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Supporting Information

Catalytic enantioselective allene-anhydride approach to β,γ-unsaturated enones bearing an α-all-carbon-quaternary center

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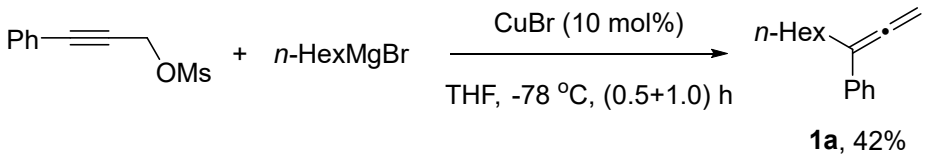
General Information. NMR spectra were taken with a Bruker Avance III spectrometer (400 MHz for ^{1}H NMR, 100 MHz for ^{13}C NMR, 376 MHz for ^{19}F NMR) in $CDCl_3$. All ^{1}H NMR experiments were measured with tetramethylsilane (0 ppm) in $CDCl_3$; ^{13}C NMR experiments were measured in relative to the signal of $CDCl_3$ (77.0 ppm); ^{19}F NMR experiments were measured in relative to the signal of $CFCl_3$ (0 ppm). The enantiomeric excess values were determined by chiral HPLC using an Agilent 1260 Infinity II instrument with the sepicific column. All reactions were carried out in oven-dried Schlenk tubes. Allenes were prepared according to the reported procedures.[1,2] Anhydrides were purchased from Macklin Co., Alfa Aesar, Bide Pharmatech Ltd. and used without purification. $Cu(OAc)_2$ was purchased from J&K Chemicals; (2*S*,5*S*)-1,2-Bis(diphenylphospholano)ethane and (2*R*,5*R*)-1,2-bis(diphenylphospholano)ethane (Ph-BPE) ligands were purchased from Laajoo Reagent and stored in a nitrogen filled glove box; $(MeO)_2MeSiH$ was purchased from TCI Chemicals. THF was dried over sodium wire with benzophenone as the indicator and distilled freshly before use. Petroleum ether (b.p. 60-90 ºC) purchased from Shanghai Titan Scientific Co., Ltd. was used for chromatography. ^{1}H NMR analysis of the crude products was conducted using dibromomethane or CH_3NO_2 as the internal standard. Column chromatography was conducted on 300-400 mesh silica gel purchased from Huanghai chemicals or Biotage Isolera One flash chromatography purification system using flash silica gel columns purchased from Santai Tech. Inc.

Experimental details and analytical data

1. Synthesis of 1,1-disubstituted allenes[1,2]

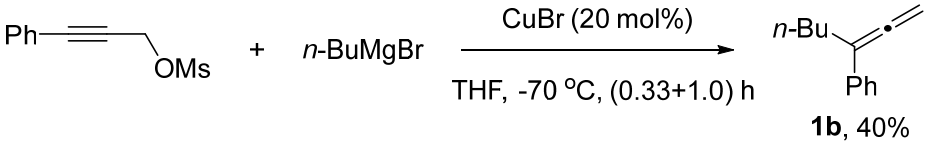
(1) Preparation of (Nona-1,2-dien-3-yl)benzene (1a) (Yy-3-080)[1]



1a, 42%

Typical Procedure I: To an oven-dried flask (100 mL) were added THF (30 mL), 3-phenylprop-2-yn-1-yl methanesulfonate (4.0788 g, 19.4 mmol) and CuBr (278.2 mg, 1.94 mmol) under argon. Then the resulting mixture was cooled to -78 °C followed by dropwise addition of freshly made *n*-hexylmagnesium bromide (1.0 M in THF, 25 mL, 25.0 mmol) over 0.5 h. The resulting mixture was stirred for 1 h at -78 °C and quenched with a saturated aqueous solution of NH_4Cl (5 mL). After extraction with ethyl ether (40 mL x 3), the organic layer was combined and dried over anhydrous Na_2SO_4. After filtration and concentration under reduced pressure, the crude product was purified by column chromatography on silica gel to afford **1a**[3] (1.6245 g, 42% yield) (eluent: Petroleum ether) as a colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.45-7.35 (d, J = 7.6 Hz, 2 H, Ar-H), 7.35-7.25 (t, J = 7.6 Hz, 2 H, Ar-H), 7.22-7.13 (t, J = 7.2 Hz, 1 H, Ar- H), 5.04 (t, J = 3.0 Hz, 2 H, =CH_2), 2.40 (tt, J_1 = 7.6 Hz, J_2 = 3.6 Hz, 2 H, CH_2), 1.62-1.48 (m, 2 H, CH_2), 1.44-1.23 (m, 6 H, CH_2 x 3), 0.89 (t, J = 6.6 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 208.6, 136.5, 128.3, 126.5, 126.0, 105.1, 78.0, 31.7, 29.5, 29.1, 27.8, 22.7, 14.1; **IR** (neat): ν = 2955, 2927, 2857, 1941, 1597, 1494, 1452, 1075 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 201 (M^++1, 1.29), 200 (M^+, 7.62), 130 (100).

(2) Preparation of (Hepta-1,2-dien-3-yl)benzene (1b) (Yy-3-157-1)[1]

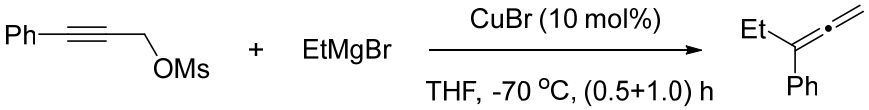


1b, 40%

Following **Typical Procedure I**: The reaction of 3-phenylprop-2-ynyl methanesulfonate (3.0000 g, 14.0 mmol), CuBr (401.5 mg, 2.8 mmol) and *n*-butylmagnesium bromide (1.0 M in THF, 15 mL, 15.0 mmol) afforded **1b**[4] (0.9756

g, 40% yield) as colorless oil (eluent: Petroleum ether); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.41 (d, *J* = 7.6 Hz, 2 H, Ar-H), 7.31 (t, *J* = 7.6 Hz, 2 H, Ar-H), 7.19 (t, *J* = 7.2 Hz, 1 H, Ar- H), 5.05 (s, 2 H, $=CH_2$), 2.48-2.37 (m, 2 H, CH_2), 1.60-1.48 (m, 2 H, CH_2), 1.48-1.35 (m, 2 H, CH_2), 0.93 (t, *J* = 7.4 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 208.6, 136.5, 128.3, 126.5, 126.0, 105.0, 78.0, 30.0, 29.2, 22.5, 14.0; **IR** (neat): *v* = 3084, 3059, 3034, 2957, 2929, 2871, 2860, 1940, 1494, 1452 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 172 (M^+, 11.06), 130 (100).

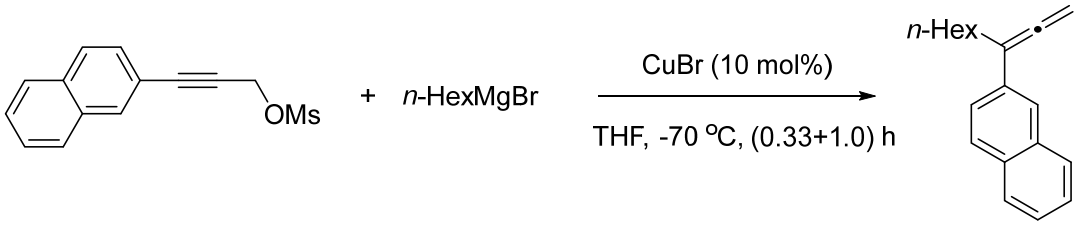
(3) Preparation of (penta-1,2-dien-3-yl)benzene (1c) (Yy-3-180)[1]



1c, 66%

Following **Typical Procedure I**: The reaction of 3-phenylprop-2-ynyl methanesulfonate (3.1530 g, 15.0 mmol), CuBr (215.1 mg, 1.50 mmol) and ethylmagnesium bromide (1.0 M in THF, 20 mL, 20.0 mmol) afforded **1c**[5] (1.4341 g, 66% yield) (eluent: Petroleum ether) as a colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.40 (d, *J* = 7.6 Hz, 2 H, Ar-H), 7.30 (t, *J* = 7.6 Hz, 2 H, Ar-H), 7.18 (t, *J* = 7.0 Hz, 1 H, Ar- H), 5.09 (t, *J* = 3.6 Hz, 2 H, $=CH_2$), 2.48-2.36 (m, 2 H, CH_2), 1.15 (t, *J* = 7.4 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 208.4, 136.5, 128.3, 126.5, 125.9, 106.7, 78.7, 22.4, 12.4; **IR** (neat): *v* = 3084, 3059, 3034, 2969, 2933, 2910, 2875, 2847, 1941, 1596, 1493, 1452, 1379, 1075, 1031 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 145 (M^++1, 5.87), 144 (M^+, 43.24), 115 (100).

(4) Preparation of 2-(Nona-1,2-dien-3-yl)naphthalene (1f) (Yy-3-119-1)[1]

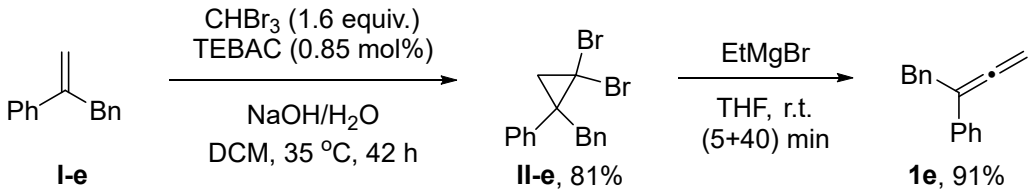


1f, 34%

Following **Typical Procedure I**: The reaction of 3-(naphthalen-2-yl)prop-2-yn-1-yl methanesulfonate (3.7366 g, 14.4 mmol), CuBr (206.5 mg, 1.44 mmol) and *n*-hexylmagnesium bromide (1.0 M in THF, 18.7 mL. 18.7 mmol afforded **1f** (1.2060

g, 34% yield) as yellow oil (eluent: Petroleum ether); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.84-7.66 (m, 4 H, Ar-H), 7.60 (d, *J* = 8.4 Hz, 1 H, Ar-H), 7.50-7.30 (m, 2 H, Ar- H), 5.11 (s, 2 H, =CH_2), 2.50 (t, *J* =7.2 Hz, 2 H, CH_2), 1.70-7.52 (m, 2 H, CH_2), 1.50-1.20 (m, 6 H, CH_2 x 3), 0.89 (t, *J* = 6.4 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 209.3, 133.9, 133.6, 132.4, 127.9, 127.7, 127.5, 126.0, 125.5, 125.3, 123.5, 105.3, 78.4, 31.8, 29.4, 29.2, 27.9, 22.7, 14.1; **IR** (neat): *v* = 3057, 2954, 2927, 2856, 1937, 1628, 1598, 1506, 1466, 1378, 1352, 1273, 1128 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 251 (M^++1, 7.69) 250 (M^+, 39.47), 180 (100); **HRMS** calcd. for $C_{19}H_{22}$ (M^+): 250.1722; Found: 250.1720.

(5) Preparation of 3,5-diphenylbuta-1,2-diene (1e) (Yy-4-034, Yy-4-047)[2]



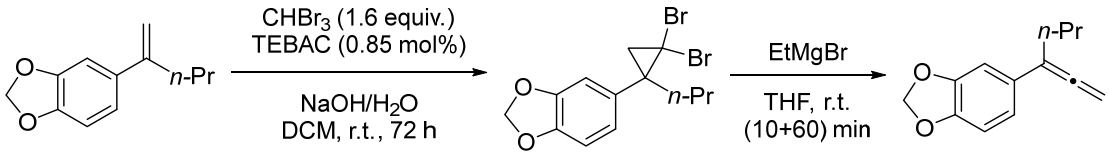
I-e **II-e**, 81% **1e**, 91%

Step 1: To a solution of alkene **I-e** (4.8112 g, 25.0 mmol), bromoform (10.1150 g, d = 2.89 g/mL, 40.0 mmol), and benzyltriethylammonium chloride (TEBAC, 44.3 mg, 0.2125 mmol) in dichloromethane (100 mL) was added dropwise an aqueous solution of 50% NaOH (72 mL) followed by stirring at 35 °C until full conversion was observed as monitored by TLC (42 h). After the addition of H_2O (50 mL) and DCM (50 mL), the aqueous phase was extracted with DCM (50 mL x 3). The combined organic phase was washed with a saturated NaCl solution (100 mL), dried over Na_2SO_4, filtrated and concentrated *in vacuo*. The crude product was purified by Biotage Isolera One flash chromatography purification system to afford **II-e** (7.3820 g, 81% yield) as a white soild: m.p. 102.1-102.8 °C (Petroleum ether/ CH_2Cl_2) (120 g silica column, eluent: Petroleum ether/ EtOAc = 100/1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.32-7.18 (m, 3 H, Ar-H), 7.17-7.00 (m, 5 H, Ar-H), 6.90-6.74 (m, 2 H, Ar-H), 3.48 (d, *J* = 13.6 Hz, 1 H, one proton of CH_2), 3.09 (d, *J* = 14.0 Hz, 1 H, one proton of CH_2), 2.12-1.98 (m, 2 H, CH_2); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 140.2, 137.9, 129.7, 129.4, 128.00, 127.99, 127.2, 126.5, 46.1, 41.1, 36.2, 32.7; **IR** (neat): *v* = 1494, 1444, 1072, 1013 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 287 [M^+(^{81}Br)-Br, 17.57], 285

[M^+(^{79}Br)-Br, 17.65], 205 (100); **Anal.** calcd. for $C_{16}H_{14}Br_2$ (M^+): C 52.49, H 3.85; Found: C 52.59, H 4.09.

Step 2: To a solution of **II-e** (3.6610 g, 10.0 mmol) in THF (20 ml) was added EtMgBr (1.0 M in THF, 15 mL, 15.0 mmol) dropwise under argon atmosphere at room temperature over 5 min. The resulting mixture was stirred at room temperature for an additional 40 minutes, quenched by saturated NH_4Cl solution (20 ml), and extracted with petroleum ether (30 mL × 3). The combined organic layer was dried over anhydrous Na_2SO_4, filtrated and concentrated *in vacuo*. The crude product was purified by Biotage Isolera One flash chromatography purification system to afford **1e** (1.8719 g, 91% yield) as a yellow oil (80 g, silica gel column, eluent: Petroleum ether); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.41 (d, *J* = 7.6 Hz, 2 H, Ar-H), 7.32-7.24 (m, 6 H, Ar-H), 7.22-7.12 (m, 2 H, Ar-H), 5.03 (t, *J* = 2.4 Hz, 2 H, =CH_2), 3.80 (t, *J* = 2.6 Hz, 2 H, CH_2); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 209.8, 139.3, 135.8, 128.7, 128.3, 128.2, 126.6, 126.2, 104.1, 78.0, 36.7; **IR** (neat): *v* = 3084, 3061, 3027, 2975, 1912, 2840, 1940, 1597, 1494, 1452, 1075, 1030, 1014 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 207 (M^++1, 8.21), 206 (M^+, 44.92), 91 (100).

(6) Preparation of 4-(hexa-1,2-dien-3-yl)benzo[*d*][1,3]dioxole (1g) (Yy-4-037, Yy-4-053)[2]



I-g **II-g**, 69% **1g**, 83%

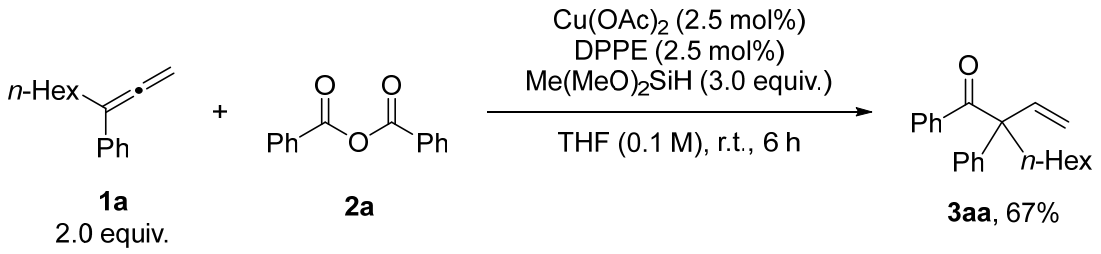
Step 1: To a solution of alkene **I-g**[6] (6.1845 g, 32.5 mmol), bromoform (13.2940 g, d = 2.89 g/mL, 52.6 mmol), and benzyltriethylammonium chloride (TEBAC, 60.6 mg, 0.272 mmol) in dichloromethane (128 mL) was added dropwise an aqueous solution of 50% NaOH (92 mL) followed by stirring at room temperature until full conversion was observed as monitored by TLC (72 h). After the addition of H_2O (60 mL) and DCM (60 mL) the aqueous phase was extracted with DCM (60 mL x 3). The combined organic phase was washed with a saturated NaCl solution (120 mL), dried over Na_2SO_4, filtrated, and concentrated *in vacuo*. The crude product was purified by

Biotage Isolera One flash chromatography purification system to afford **II-g** (8.0084 g, 69% yield) as a yellow soild: m.p. 107.3-107.9 ºC (Petroleum ether/ CH_2Cl_2) (120 g silica column, eluent: Petroleum ether/ EtOAc = 98/2 x 7 CV to 95/5 x 8 CV); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 6.80-6.75 (m, 2 H, CH_3), 6.68 (dd, J_1 = 7.8 Hz, J_2 = 1.4 Hz, 1 H, Ar-H), 5.97 (dd, J_1 = 5.0 Hz, J_2 = 1.4 Hz, 2 H, Ar-H), 2.15-1.98 (m, 2 H, CH_2), 1.71 (d, J = 7.6 Hz, 1 H, one proton of CH_2), 1.59-1.54 (m, 1 H, one proton of CH_2), 1.32-1.18 (m, 2 H, CH_2), 0.85 (t, J = 7.4 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 147.4, 146.6, 134.5, 122.5, 109.7, 107.9, 101.1, 42.5, 39.6, 36.9, 33.4, 20.5, 13.9; **IR** (neat): v = 2956, 2906, 2872, 2857, 1489, 1457, 1441, 1356, 1240, 1221, 1112, 1069, 1056, 1037, 1011 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 283 [$M(^{81}Br)^+$-Br, 53.33], 281 [$M(^{79}Br)^+$-Br, 53.76], 172 (100); **Anal.** calcd. for $C_{13}H_{14}Br_2O_2$ (M^+): C 43.13, H 3.90; Found: C 43.31, H 4.16.

Step 2: To a solution of **II-g** (3.6211 g, 10.0 mmol) in THF (20 ml) was added EtMgBr (1.0 M in THF, 15 mL, 15.0 mmol) dropwise under argon atmosphere at room temperature for 10 min. The resulting mixture was stirred at room temperature for an additional 60 minutes, quenched by saturated NH_4Cl solution (20 ml), and extracted with petroleum ether (30 mL × 3). The combined organic layer was dried over anhydrous Na_2SO_4, filtrated and concentrated *in vacuo*. The crude product was purified by Biotage Isolera One flash chromatography purification system to afford **1g** (1.6820 g, 83% yield) as a colorless oil (40 g, silica gel column, eluent: Petroleum ether/ EtOAc = 49/1 (500 mL)); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 6.92 (d, J = 1.6 Hz, 1 H, Ar-H), 6.85 (dd, J_1 = 8.2 Hz, J_2 = 1.8 Hz, 1 H, Ar-H), 6.76 (d, J = 8.0 Hz, 1 H, Ar-H), 5.92 (s, 2 H, CH_2), 5.03 (t, J = 3.2 Hz, 2 H, =CH_2), 2.38-2.29 (m, 2 H, CH_2), 1.56 (sextet, J = 7.4 Hz, 2 H, CH_2), 0.97 (s, J = 7.4 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 208.4, 147.8, 146.3, 130.6, 119.0, 108.0, 106.8, 104.6, 100.9, 78.0, 31.9, 21.1, 13.9; **IR** (neat): v = 2959, 2930, 2895, 2872, 1938, 1607, 1503, 1486, 1437, 1378, 1350, 1236, 1109, 1038 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 203 (M^++1, 14.43), 202 (M^+, 100); **HRMS** calcd. *m/z* for $C_{13}H_{14}O_2$ (M^+): 202.0988; Found: 202.0987.

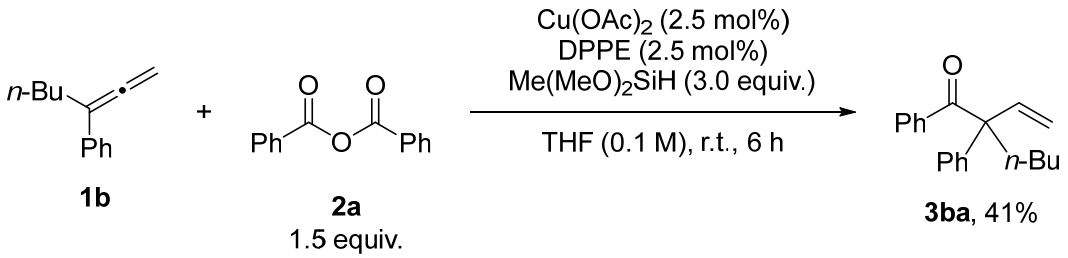
3. Preparation of racemic products

(1) Preparation of 1,2-diphenyl-2-hexylbut-3-en-1-one (3aa) (Yy-3-133, Yy-4-183)



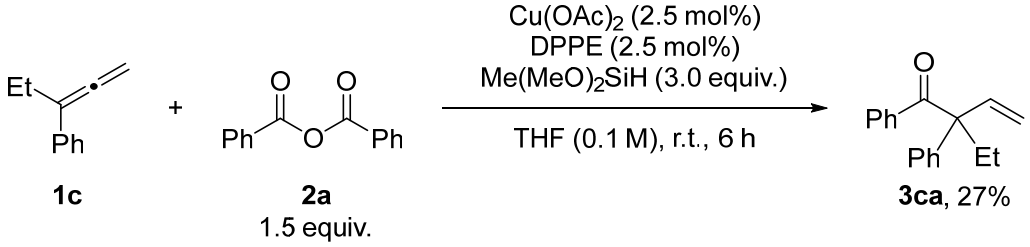
Typical Procedure II: To an oven-dried 25 mL Schlenk tube were sequentially added a stirring bar, benzoic anhydride **2a** (113.1 mg, 0.5 mmol), $Cu(OAc)_2$ (2.3 mg, 0.0127 mmol), DPPE (5.0 mg, 0.0125 mmol), allene **1a** (200.3 mg, 1.0 mmol), and THF (4 mL) under nitrogen. After beng stirred at room temperature for 5 min, dimethoxymethylsilane (163.6 mg, d = 0.861 g/mL, 0.19 mL, 1.5 mmol, diluted with 1 mL THF) was added. The resulting mixture was stirred at room temperature for 6 h and quenched with a saturated solution of NH_4F in methanol (2.5 mL). The reaction mixture was stired for 15 min at room temperature and then filtered through s short plug of celite eluted with EtOAc (10 mL x 3). The solvent was removed *in vacuo* and the crude product was purified by column chromatography on silica gel to afford **3aa** (102.6 mg, 67% yield) as a colorless oil (eluent: Petroleum ether x 200 mL to Petroleum ether/ EtOAc = 100/1 (~800 mL)); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.53 (d, J = 8.0 Hz, 2 H, Ar-H), 7.40-7.28 (m, 3 H, Ar-H), 7.28-7.15 (m, 5 H, Ar-H), 6.70 (dd, J_1 = 17.6 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.30 (d, J = 11.2 Hz, 1 H, one proton of $=CH_2$), 4.99 (d, J = 17.6 Hz, 1 H, one proton of $=CH_2$), 2.28-2.05 (m, 2 H, CH_2), 1.28-0.94 (m, 8 H, CH_2 x 4), 0.81 (t, J = 6.6 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.6, 142.6, 139.7, 136.3, 131.7, 130.0, 128.7, 127.8, 127.1, 126.8, 117.2, 61.5, 38.7, 31.5, 29.8, 23.9, 22.5, 14.0; **IR** (neat): ν = 3087, 3061, 3027, 2953, 2928, 2857, 1676, 1597, 1579, 1495, 1466, 1446, 1227, 1180 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 306 (M^+, 1.90), 105 (100); **HRMS** calcd. *m/z* for $C_{22}H_{26}O$ (M^+): 306.1978; Found: 306.1978.

(2) Preparation of 1,2-diphenyl-2-butylbut-3-en-1-one (3ba) (Yy-3-161)



Following **Typical Procedure II**, the reaction of benzoic anhydride **2a** (169.7 mg, 0.75 mmol), $Cu(OAc)_2$ (2.3 mg, 0.0127 mmol), DPPE (5.0 mg, 0.0125 mmol), allene **1b** (125.2 mg, 0.5 mmol) in THF (4 mL), and dimethoxymethylsilane (163.6 mg, d = 0.861 g/mL, 0.19 mL, 1.5 mmol, in 1 mL THF) afforded **3ba** (58.0 mg, 98% purity, 41% yield) as a colorless oil (eluent: Petroleum ether (200 mL) to Petroleum ether/ EtOAc = 100/1 (~ 500 mL)); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.53 (d, J = 7.6 Hz, 2 H, Ar-H), 7.36-7.28 (m, 3 H, Ar-H), 7.28-7.14 (m, 5 H, Ar-H), 6.70 (dd, J_1 = 17.6 Hz, J_2 = 11.2 Hz, 1 H, =CH), 5.30 (d, J = 10.8 Hz, 1 H, one proton of $=CH_2$), 5.00 (d, J = 17.6 Hz, 1 H, one proton of $=CH_2$), 2.30-2.08 (m, 2 H, CH_2), 1.30-1.15 (m, 2 H, CH_2), 1.15-0.90 (m, 2 H, CH_2), 0.78 (t, J = 7.2 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.5, 142.6, 139.6, 136.3, 131.7, 130.0, 128.7, 127.8, 127.1, 126.8, 117.2, 61.4, 38.5, 26.2, 23.2, 13.8; **IR** (neat): v = 3086, 3059, 3024, 2955, 2931, 2871, 2862, 1675, 1597, 1579, 1495, 1446, 1225, 1181, 1003 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 278 (M^+, 2.79), 105 (100); **HRMS** calcd. *m/z* for $C_{20}H_{22}O$ (M^+): 278.1665; Found: 278.1666.

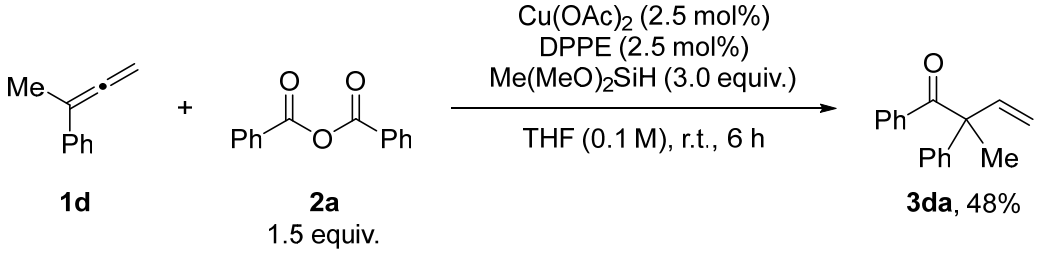
(3) Preparation of 2-ethyl-1,2-diphenylbut-3-en-1-one (3ca) (Yy-3-184)



Following **Typical Procedure II**, the reaction of benzoic anhydride **2a** (339.4 mg, 1.5 mmol), $Cu(OAc)_2$ (4.5 mg, 0.025 mmol), DPPE (10.0 mg, 0.025 mmol), allene **1c** (144.3 mg, 1.0 mmol) in THF (8 mL), and dimethoxymethylsilane (318.6 mg, d = 0.861 g/mL, 0.37 mL, 3.0 mmol, in 2 mL THF) afforded **3ca** (71.4 mg, 96% purity, 27% yield) as a colorless oil (eluent: Petroleum ether (200 mL) to Petroleum ether/

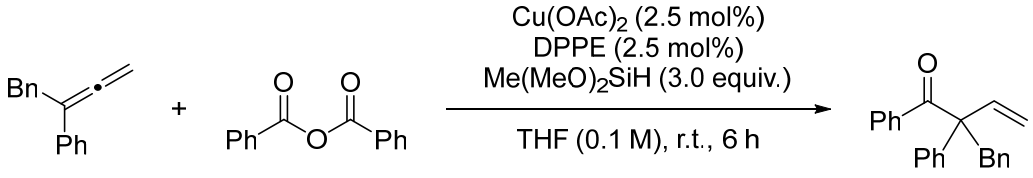
EtOAc = 100/1 (~ 800 mL)); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.58-7.48 (m, 2 H, Ar-H), 7.38-7.28 (m, 3 H, Ar-H), 7.28-7.15 (m, 5 H, Ar-H), 6.69 (dd, J_1 = 17.6 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.32(d, J = 10.8 Hz, 1 H, one proton of $=CH_2$), 5.02 (d, J = 17.6 Hz, 1 H, one proton of $=CH_2$), 2.34-2.10 (m, 2 H, CH_2), 0.71 (t, J = 7.4 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.5, 142.4, 139.1, 136.3, 131.7, 130.0, 128.7, 127.8, 127.2, 126.8, 117.5, 61.8, 31.5, 8.6; **IR** (neat): v = 3085, 3059, 3024, 2971, 2937, 2879, 1673, 1597, 1578, 1494, 1446, 1227, 1181, 1003 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 250 (M^+, 1.36), 105 (100); **HRMS** calcd. *m/z* for $C_{18}H_{18}O$ (M^+): 250.1352; Found: 250.1350.

(4) Preparation of 2-methyl-1,2-diphenylbut-3-en-1-one (3da) (Yy-4-055)



Following **Typical Procedure II**, the reaction of benzoic anhydride **2a** (169.7 mg, 0.75 mmol), $Cu(OAc)_2$ (2.3 mg, 0.0127 mmol), DPPE (5.0 mg, 0.0125 mmol), allene **1d** (65.3 mg, 0.5 mmol) in THF (4 mL), and dimethoxymethylsilane (163.6 mg, d = 0.861 g/mL, 0.19 mL, 1.5 mmol, in 1 mL THF) afforded **3da**[7] (56.7 mg, 48% yield) as a colorless oil (eluent: Petroleum ether (200 mL) to Petroleum ether/ EtOAc = 100/1 (~ 600 mL)); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.60-7.50 (m, 2 H, Ar-H), 7.40-7.30 (m, 3 H, Ar-H), 7.30-7.18 (m, 5 H, Ar-H), 6.62 (dd, J_1 = 17.2 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.29 (d, J = 10.8 Hz, 1 H, one proton of $=CH_2$), 5.16 (d, J = 17.6 Hz, 1 H, one proton of $=CH_2$), 1.67 (s, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.8, 144.4, 140.9, 136.2, 131.8, 130.0, 129.0, 127.9, 126.9, 126.4, 116.5, 58.5, 25.9; **IR** (neat): v = 3086, 3059, 3024, 2985, 2934, 1677, 1597, 1493, 1446, 1409, 1368, 1237, 1174, 1077, 1011 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 236 (M^+, 1.85), 105 (100).

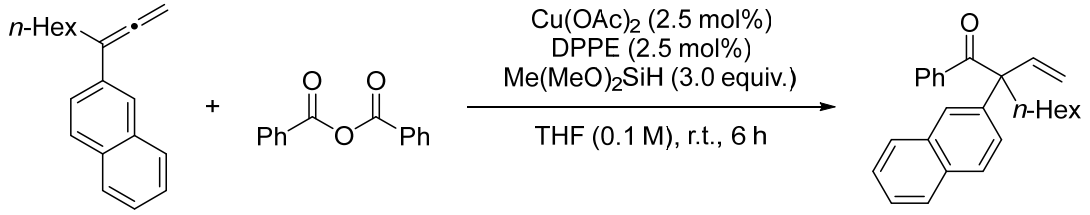
(5) Preparation of 2-benzyl-1,2-diphenylbut-3-en-1-one (3ea) (Yy-4-049)



1e **2a** 1.5 equiv. **3ea**, 63%

Following **Typical Procedure II**, the reaction of benzoic anhydride **2a** (169.7 mg, 0.75 mmol), $Cu(OAc)_2$ (2.3 mg, 0.0127 mmol), DPPE (5.1 mg, 0.0128 mmol), allene **1e** (102.9 mg, 0.5 mmol) in THF (4 mL), and dimethoxymethylsilane (163.6 mg, d = 0.861 g/mL, 0.19 mL, 1.5 mmol, in 1 mL THF) afforded **3ea** (98.1 mg, 63% yield) as a colorless oil (eluent: Petroleum ether (200 mL) to Petroleum ether/ EtOAc = 100/1 (~ 400 mL)); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.62 (d, *J* = 7.6 Hz, 2 H, Ar-H), 7.32 (t, *J* = 7.2 Hz, 1 H, Ar-H), 7.28-7.13 (m, 5 H, Ar-H), 7.13-6.90 (m, 5 H, Ar-H), 6.68-6.52 (m, 3 H, =CH and Ar-H), 5.39 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 5.14 (d, *J* = 17.6 Hz, 1 H, one proton of $=CH_2$), 3.48 (q, *J* = 13.5 Hz, 2 H, CH_2); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 199.8, 141.6, 139.3, 136.9, 135.7, 131.8, 131.2, 130.6, 128.5, 127.7, 127.5, 127.2, 126.9, 126.1, 118.5, 62.2, 47.3; **IR** (neat): *v* = 3080, 3060, 30225, 2973, 2925, 1668, 1597, 1579, 1495, 1448, 1226, 1181, 1118, 1079, 1012 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 313 (M^++1, 4.08), 312 (M^+, 16.18), 105 (100); **HRMS** calcd. *m/z* for $C_{23}H_{20}O$ (M^+): 312.1509; Found: 312.1509.

(6) Preparation of 2-(Naphth-2-yl)-1-phenyl-2-hexyl-3-buten-1-one (3fa) (Yy-3-135)

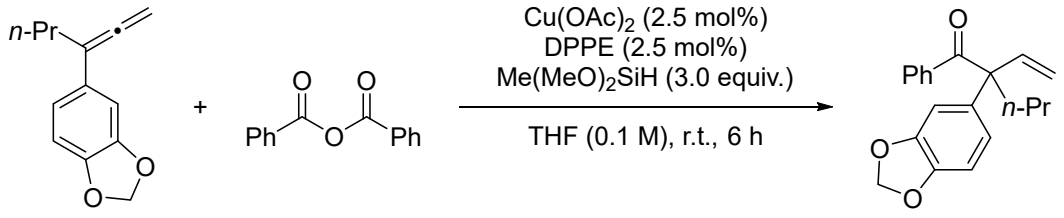


1f **2a** 1.5 equiv. **3fa**, 54%

Following **Typical Procedure II**, the reaction of benzoic anhydride **2a** (169.7 mg, 0.75 mmol), $Cu(OAc)_2$ (2.3 mg, 0.0127 mmol), DPPE (5.0 mg, 0.0125 mmol), allene **1f** (125.2 mg, 0.5 mmol) in THF (4 mL), and dimethoxymethylsilane (163.6 mg, d =

0.861 g/mL, 0.19 mL, 1.5 mmol, in 1 mL THF) afforded **3fa** (96.6 mg, 54% yield) as a colorless oil (eluent: Petroleum ether (400 mL) to Petroleum ether/ EtOAc = 100/1 (~ 200 mL)); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.88-7.70 (m, 4 H, Ar-H), 7.56 (d, *J* = 8.0 Hz, 2 H, Ar-H), 7.52-7.40 (m, 2 H, Ar-H), 7.28 (d, *J* = 8.0 Hz, 2 H, Ar-H), 7.14 (t, *J* = 7.6 Hz, 2 H, Ar-H), 6.82 (dd, J_1 = 17.6 Hz, J_2 = 11.2 Hz, 1 H, =CH), 5.34 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 5.03 (d, *J* = 17.6 Hz, 1 H, one proton of $=CH_2$), 2.40-2.18 (m, 2 H, CH_2), 1.24-0.95 (m, 8 H, CH_2 x 4), 0.78 (t, *J* = 6.6 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.6, 140.2, 139.7, 136.4, 133.5, 132.3, 131.7, 130.0, 128.5, 128.1, 127.9, 127.6, 126.2, 125.9, 125.7, 125.5, 117.4, 61.6, 38.7, 31.5, 29.8, 24.0, 22.5, 14.0; **IR** (neat): *v* = 3060, 2953, 2856, 1676, 1631, 1597, 1579, 1506, 1466, 1446, 1223, 1181 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 357 (M^++1, 2.41), 356 (M^+, 8.41), 105 (100); **HRMS** calcd. for $C_{26}H_{29}O$ ($M+H^+$): 357.2213; Found: 357.2210.

(7) Preparation of 2-(benzo[*d*][1,3]dioxol-5-yl)-1-phenyl-2-propyl-3-buten-1-one (3ga) (Yy-4-061)

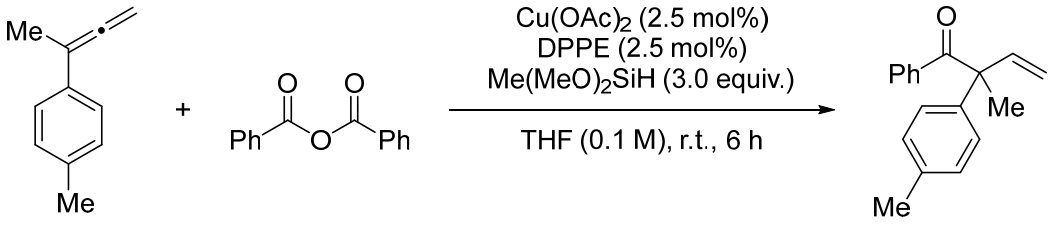


1g **2a** 1.5 equiv. **3ga**, 61%

Following **Typical Procedure II**, the reaction of benzoic anhydride **2a** (169.7 mg, 0.75 mmol), $Cu(OAc)_2$ (2.3 mg, 0.0127 mmol), DPPE (5.0 mg, 0.0125 mmol), allene **1g** (103.1 mg, 0.5 mmol) in THF (4 mL), and dimethoxymethylsilane (163.6 mg, d = 0.861 g/mL, 0.19 mL, 1.5 mmol, in 1 mL THF) afforded **3ga** (96.0 mg, 61% yield) as a colorless oil (eluent: Petroleum ether (200 mL) to Petroleum ether/ EtOAc = 100/1 (~ 200 mL) to 50/1 (~ 400 mL)); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.58 (d, *J* = 8.0 Hz, 2 H, Ar-H), 7.35 (t, *J* = 7.0 Hz, 1 H, Ar-H), 7.23 (t, *J* = 7.6 Hz, 2 H, Ar-H), 6.80-6.68 (m, 3 H, Ar-H), 6.63 (dd, J_1 = 17.6 Hz, J_2 = 10.8 Hz, 1 H, =CH), 6.00-5.88 (m, 2 H, CH_2), 5.27 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 5.00 (d, *J* = 17.6 Hz, 1 H, one proton of $=CH_2$), 2.22-2.00 (m, 2 H, CH_2), 1.20-1.00 (m, 2 H, CH_2), 0.83 (t, *J* = 7.2

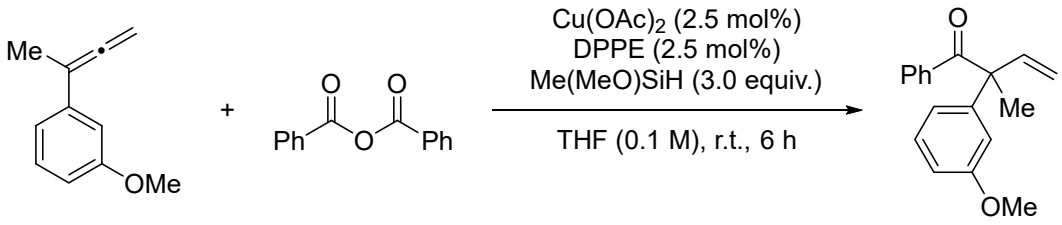
Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.3, 148.1, 146.4, 139.7, 136.4, 136.3, 131.7, 129.9, 127.8, 120.4, 117.1, 108.4, 107.6, 101.1, 61.1, 40.9, 17.4, 14.6; **IR** (neat): *v* = 3067, 3022, 2959, 2931, 2872, 1676, 1596, 1504, 1485, 1436, 1340, 1233, 1182, 1112, 1038 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 309 (M^++1, 3.93), 308 (M^+, 19.30), 203 (100); **HRMS** calcd. *m/z* for $C_{20}H_{20}O_3$ (M^+): 308.1407; Found: 308.1410.

(8) Preparation of 2-methyl-1-phenyl-2-(*p*-tolyl)but-3-en-1-one (3ha) (Yy-4-081)



Following **Typical Procedure II**, the reaction of benzoic anhydride **2a** (113.1 mg, 0.50 mmol), $Cu(OAc)_2$ (2.3 mg, 0.0127 mmol), DPPE (5.0 mg, 0.0125 mmol), allene **1h** (108.2 mg, 0.75 mmol) in THF (4 mL), and dimethoxymethylsilane (163.6 mg, d = 0.861 g/mL, 0.19 mL, 1.5 mmol, in 1 mL THF) afforded **3ha** (82.4 mg, 66% yield) as a colorless oil (eluent: Petroleum ether (200 mL) to petroleum ether/ EtOAc = 100/1 (~ 600 mL)); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.60-7.50 (m, 2 H, Ar-H), 7.35 (t, *J* = 7.4 Hz, 1 H, Ar-H), 7.22 (t, *J* = 7.8 Hz, 2 H, Ar-H), 7.18-7.10 (m, 4 H, Ar-H), 6.60 (dd, J_1 = 17.2 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.26 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 5.14 (d, *J* = 17.6 Hz, 1 H, one proton of $=CH_2$), 2.32 (s, 3 H, CH_3), 1.65 (s, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 201.0, 141.3, 141.2, 136.5, 136.3, 131.7, 130.0, 129.7, 127.9, 126.2, 116.3, 58.1, 25.9, 21.0; **IR** (neat): *v* = 3056, 3020, 2989, 2922, 1672, 1596, 1577, 1509, 1445, 1406, 1365, 1241, 1171, 1076, 1009 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 250 (M^+, 3.56), 105 (100); **HRMS** calcd. *m/z* for $C_{18}H_{18}O$ (M^+): 250.1352; Found: 250.1357.

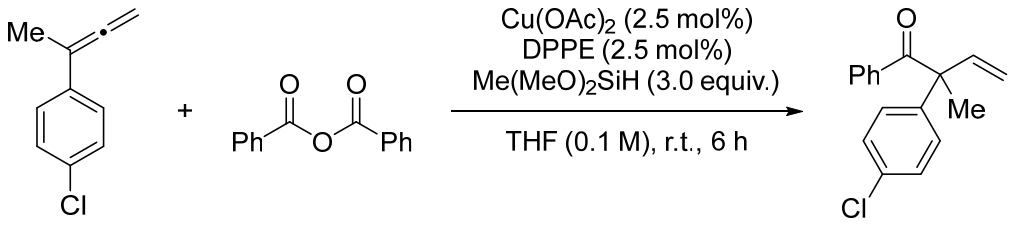
(9) Preparation of 2-(3-methoxyphenyl)-2-methyl-1-phenylbut-3-en-1-one (3ia) (Yy-4-083)



1i 1.5 equiv. **2a** **3ia**, 90%

Following **Typical Procedure II**, the reaction of benzoic anhydride **2a** (113.1 mg, 0.50 mmol), $Cu(OAc)_2$ (2.3 mg, 0.0127 mmol), DPPE (5.0 mg, 0.0125 mmol), allene **1i** (120.3 mg, 0.75 mmol) in THF (4 mL), and dimethoxymethylsilane (163.6 mg, d = 0.861 g/mL, 0.19 mL, 1.5 mmol, in 1 mL THF) afforded **3ia** (119.9 mg, 90% yield) as a colorless oil (eluent: Petroleum ether (200 mL) to Petroleum ether/ EtOAc = 100/1 (~ 200 mL) to 50/1 (~ 400 mL)); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.60-7.52 (m, 2 H, Ar-H), 7.40-7.33 (m, 1 H, Ar-H), 7.26-7.20 (m, 3 H, Ar-H), 6.88-6.82 (m, 2 H, Ar-H), 6.88-6.77 (m, 1 H, Ar-H), 6.60 (dd, J_1 = 17.2 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.28 (d, J = 10.8 Hz, 1 H, one proton of $=CH_2$), 5.16 (d, J = 17.2 Hz, 1 H, one proton of $=CH_2$), 3.75 (s, 3 H, OCH_3), 1.66 (s, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.6, 160.0, 146.0, 140.8, 136.2, 131.8, 129.93, 129.91, 127.9, 118.9, 116.5, 112.4, 111.9, 58.4, 55.1, 25.7; **IR** (neat): ν = 3058, 2987, 2936, 2835, 1677, 1596, 1580, 1485, 1433, 1409, 1317, 1290, 1239, 1169, 1073, 1046, 1013 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 267 (M^++1, 1.55), 266 (M^+, 6.90), 105 (100); **HRMS** calcd. *m/z* for $C_{18}H_{18}O_2$ (M^+): 266.1301; Found: 266.1308.

(10) Preparation of 2-(4-chlorophenyl)-2-methyl-1-phenylbut-3-en-1-one (3ja) (Yy-4-089)

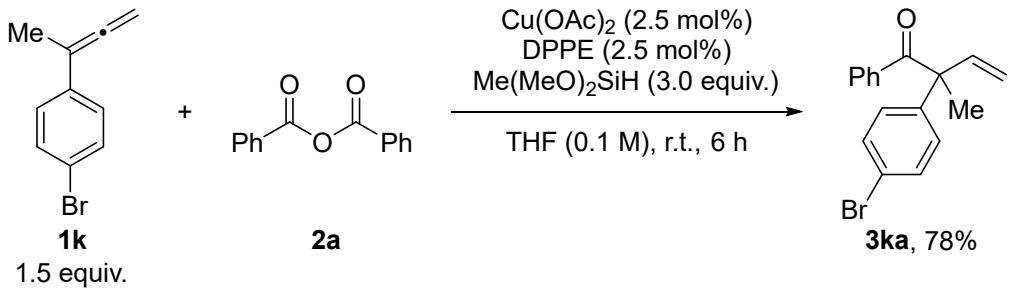


1j 1.5 equiv. **2a** **3ja**, 74%

Following **Typical Procedure III**, the reaction of benzoic anhydride **2a** (113.1 mg, 0.50 mmol), $Cu(OAc)_2$ (2.3 mg, 0.0127 mmol), DPPE (5.0 mg, 0.0125 mmol), allene

1j (124.3 mg, 0.76 mmol) in THF (4 mL), and dimethoxymethylsilane (163.6 mg, d = 0.861 g/mL, 0.19 mL, 1.5 mmol, in 1 mL THF) afforded **3ja** (100.6 mg, 74% yield) as a yellow oil (eluent: Petroleum ether (200 mL) to Petroleum ether/ EtOAc = 100/1 (~ 500 mL)); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.58-7.50 (m, 2 H, Ar-H), 7.43-7.36 (m, 1 H, Ar-H), 7.36-7.29 (m, 2 H, Ar-H), 7.29-7.18 (m, 4 H, Ar-H), 6.58 (dd, J_1 = 17.2 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.31 (d, J = 10.8 Hz, 1 H, one proton of $=CH_2$), 5.16 (d, J = 17.2 Hz, 1 H, one proton of $=CH_2$), 1.65 (s, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.3, 143.0, 140.5, 135.8, 132.9, 132.0, 130.0, 129.2, 128.1, 127.8, 117.0, 58.1, 26.0; **IR** (neat): v = 3087, 3063, 3024, 2987, 2935, 1677, 1596, 1489, 1446, 1402, 1236, 1170, 1095, 1012 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 272 [M^+(^{37}Cl), 0.30)], 270 [M^+(^{35}Cl), 1.03)], 105 (100); **HRMS** calcd. *m/z* for $C_{17}H_{15}{}^{35}ClO$ (M^+): 270.0806; Found: 270.0807.

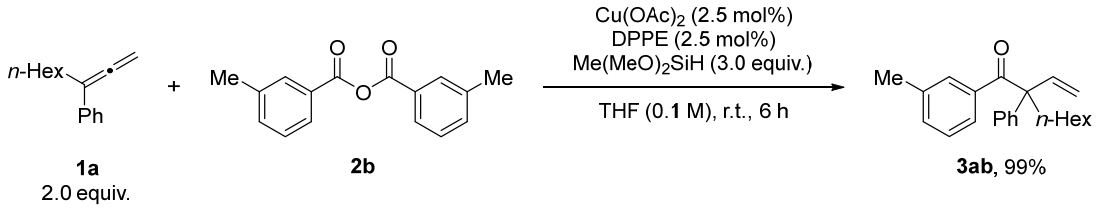
(11) Preparation of 2-(4-bromophenyl)-2-methyl-1-phenylbut-3-en-1-one (3ka) (Yy-4-091)



Following **Typical Procedure II**, the reaction of benzoic anhydride **2a** (113.1 mg, 0.50 mmol), $Cu(OAc)_2$ (2.3 mg, 0.0127 mmol), DPPE (5.0 mg, 0.0125 mmol), allene **1k** (156.6 mg, 0.75 mmol) in THF (4 mL), and dimethoxymethylsilane (163.6 mg, d = 0.861 g/mL, 0.19 mL, 1.5 mmol, in 1 mL THF) afforded **3ka** (122.9 mg, 78% yield) as a colorless oil (eluent: Petroleum ether (200 mL) to Petroleum ether/ EtOAc = 100/1 (~ 400 mL)); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.56-7.50 (m, 2 H, Ar-H), 7.50-7.43 (m, 2 H, Ar-H), 7.43-7.35 (m, 1 H, Ar-H), 7.30-7.22 (m, 2 H, Ar-H), 7.18-7.10 (m, 2 H, Ar-H), 6.57 (dd, J_1 = 17.2 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.31 (d, J = 10.8 Hz, 1 H, one proton of $=CH_2$), 5.16 (d, J = 17.2 Hz, 1 H, one proton of $=CH_2$), 1.64 (s, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.2, 143.6, 140.4, 135.8,

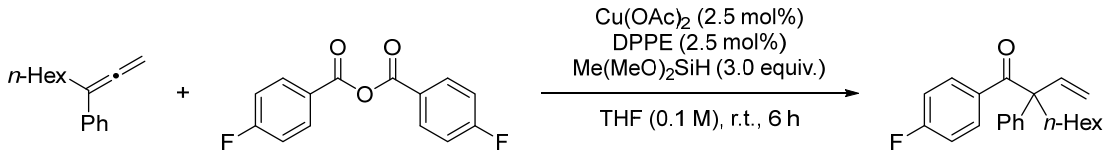
132.11, 132.06, 130.0, 128.2, 128.1, 121.0, 117.0, 58.1, 26.0; **IR** (neat): ν = 3087, 3060, 2985, 2934, 1677, 1631, 1596, 1487, 1446, 1409, 1396, 1369, 1236, 1170, 1103, 1079, 1008 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 316 [M^+(^{81}Br), 0.39], 314 [M^+(^{79}Br), 0.45], 130 (M^+-Br-Bz), 105 (100); **HRMS** calcd. *m/z* for $C_{17}H_{15}{}^{79}BrO$ (M^+): 314.0301; Found: 314.0302.

(12) Preparation of 2-phenyl-1-(*m*-tolyl)-2-hexylbuten-1-one (3ab) (Yy-4-007)



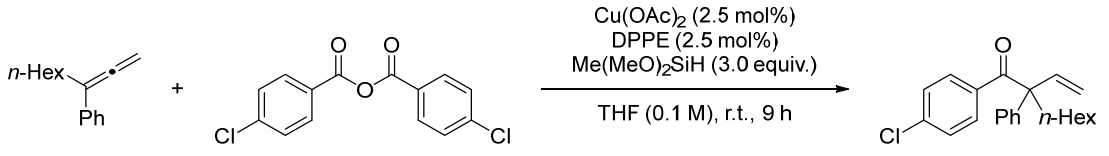
Following **Typical Procedure II**, the reaction of 3-methylbenzoic anhydride **2b** (131.3 mg, 0.5 mmol), $Cu(OAc)_2$ (2.3 mg, 0.0127 mmol), DPPE (5.0 mg, 0.0125 mmol), allene **1a** (200.3 mg, 1.0 mmol) in THF (4 mL), and dimethoxymethylsilane (163.6 mg, d = 0.861 g/mL, 0.19 mL, 1.5 mmol, in 1 mL THF) afforded **3ab** (159.1 mg, 99% yield) as a colorless oil (eluent: Petroleum ether (200 mL) to Petroleum ether/ EtOAc = 100/1 (~ 400 mL)); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.44 (s, 1 H, Ar-H), 7.35-7.28 (m, 2 H, Ar-H), 7.28-7.17 (m, 4 H, Ar-H), 7.15 (d, J = 7.6 Hz, 1 H, Ar-H), 7.04 (t, J = 7.6 Hz, 1 H, Ar-H), 6.69 (dd, J_1 = 17.6 Hz, J_2 = 11.2 Hz, 1 H, =CH), 5.29 (d, J = 10.8 Hz, 1 H, one proton of $=CH_2$), 4.99 (d, J = 17.6 Hz, 1 H, one proton of $=CH_2$), 2.27-2.06 (m, 5 H, CH_2 and CH_3), 1.24-0.95 (m, 8 H, CH_2 x 4), 0.81 (t, J = 6.8 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.8, 142.7, 139.8, 137.6, 136.4, 132.4, 130.5, 128.7, 127.5, 127.3, 127.2, 126.8, 117.1, 61.6, 38.7, 31.5, 29.8, 24.0, 22.5, 21.3, 14.0; **IR** (neat): ν = 3085, 3060, 3028, 2952, 2926, 2856, 1676, 1600, 1583, 1494, 1446, 1252, 1173, 1000 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 320 (M^+, 1.72), 119 (100); **HRMS** calcd. for $C_{23}H_{28}O$ (M^+): 320.2135; Found: 320.2139.

(13) Preparation of 1-(4-fluorophenyl)-2-phenyl-2-hexyl-3-buten-1-one (3ac) (Yy-5-049, Yy-4-018)



Following **Typical Procedure II**, the reaction of 4-fluorobenzoic anhydride **2c** (135.0 mg, 0.5 mmol), $Cu(OAc)_2$ (2.3 mg, 0.0127 mmol), DPPE (5.0 mg, 0.0125 mmol), allene **1a** (200.3 mg, 1.0 mmol) in THF (4 mL), and dimethoxymethylsilane (163.6 mg, d = 0.861 g/mL, 0.19 mL, 1.5 mmol, in 1 mL THF) afforded **3ac** (148.8 mg, 89% yield) as a colorless oil (eluent: Petroleum ether (400 mL) to Petroleum ether/ EtOAc = 100/1 (~ 800 mL)); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.62-7.52 (m, 2 H, Ar-H), 7.38-7.28 (m, 2 H, Ar-H), 7.28-7.18 (m, 3 H, Ar-H), 6.92-6.82 (m, 2 H, Ar-H), 6.69 (dd, J_1 = 17.6 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.31 (d, J = 10.8 Hz, 1 H, one proton of $=CH_2$), 4.99 (d, J = 17.6 Hz, 1 H, one proton of $=CH_2$), 2.26-2.08 (m, 2 H, CH_2), 1.28-0.92 (m, 8 H, CH_2 x 4), 0.81 (t, J = 6.8 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 199.0, 164.6 (d, J = 252.0 Hz), 142.5, 139.5, 132.7 (d, J = 9.5 Hz), 132.4 (d, J = 3.1 Hz), 128.8, 127.1, 126.9, 117.4, 114.9 (d, J = 21.3 Hz), 61.4, 39.0, 31.5, 29.8, 23.9, 22.5, 14.0; **^{19}F NMR** (376 MHz, $CDCl_3$) δ = -107.4; **IR** (neat): ν = 3084, 3061, 3025, 2954, 2928, 2857, 1678, 1597, 1504, 1466, 1447, 1407, 1378, 1297, 1231, 1156, 1098 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 324 (M^+, 2.08), 123 (100); **HRMS** calcd. *m/z* for $C_{22}H_{25}FO$ (M^+): 324.1884; Found: 324.1888.

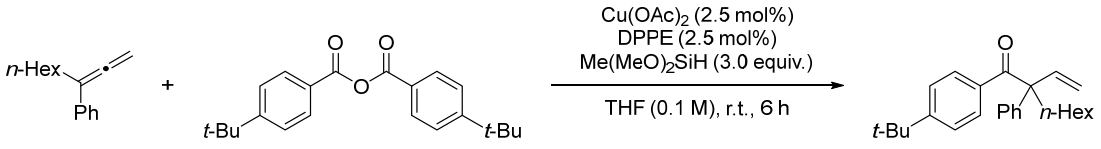
(14) Preparation of 1-(4-chlorophenyl)-2-phenyl-2-hexyl-3-buten-1-one (3ad) (Yy-5-057, Yy-4-021)



Following **Typical Procedure II**, the reaction of 4-chlorobenzoic anhydride **2d** (147.6 mg, 0.5 mmol), $Cu(OAc)_2$ (2.3 mg, 0.0127 mmol), DPPE (5.0 mg, 0.0125 mmol), allene **1a** (200.3 mg, 1.0 mmol) in THF (4 mL), and dimethoxymethylsilane (163.6

mg, d = 0.861 g/mL, 0.19 mL, 1.5 mmol, in 1 mL THF) afforded **3ad** (126.8 mg, 74% yield) as a colorless oil (eluent: Petroleum ether (400 mL) to Petroleum ether/ EtOAc = 100/1 (~ 800 mL)); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.48 (d, *J* = 8.8 Hz, 2 H, Ar-H), 7.38-7.29 (m, 2 H, Ar-H), 7.28-7.14 (m, 5 H, Ar-H), 6.68 (dd, J_1 = 17.6 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.31 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 4.99 (d, *J* = 17.6 Hz, 1 H, one proton of $=CH_2$), 2.24-2.05 (m, 2 H, CH_2), 1.26-0.94 (m, 8 H, CH_2 x 4), 0.81 (t, *J* = 6.8 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 199.3, 142.3, 139.4, 138.0, 134.5, 131.5, 128.9, 128.1, 127.1, 127.0, 117.6, 61.4, 39.0, 31.5, 29.8, 23.9, 22.5, 14.0; **IR** (neat): *v* = 3085, 3061, 3025, 2953, 2927, 2857, 1678, 1586, 1569, 1487, 1466, 1447, 1398, 1378, 1225, 1176, 1013 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 342 [M^+(^{37}Cl), 0.77)], 340 [M^+(^{35}Cl), 1.96)], 139 (100); **HRMS** calcd. *m/z* for $C_{22}H_{25}{}^{35}ClO$ (M^+): 340.1588; Found: 340.1589.

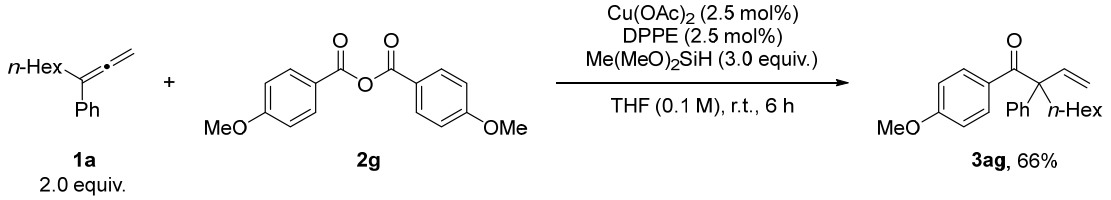
(15) Preparation of 1-(4-(*tert*-butyl)phenyl)-2-phenyl-2-hexyl-3-buten-1-one (3ae) (Yy-4-024)



Following **Typical Procedure II**, the reaction of 4-(*tert*-butyl)benzoic anhydride **2e** (169.5 mg, 0.5 mmol), $Cu(OAc)_2$ (2.3 mg, 0.0127 mmol), DPPE (5.0 mg, 0.0125 mmol), allene **1a** (200.3 mg, 1.0 mmol) in THF (4 mL), and dimethoxymethylsilane (163.6 mg, d = 0.861 g/mL, 0.19 mL, 1.5 mmol, in 1 mL THF) afforded **3ae** (173.0 mg, 95% yield) as a colorless oil (eluent: Petroleum ether (200 mL) to Petroleum ether/ EtOAc = 100/1 (~ 600 mL)); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.47 (d, *J* = 8.8 Hz, 2 H, Ar-H), 7.37-7.29 (m, 2 H, Ar-H), 7.29-7.18 (m, 5 H, Ar-H), 6.69 (dd, J_1 = 17.6 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.29 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 4.99 (d, *J* = 17.6 Hz, 1 H, one proton of $=CH_2$), 2.28-2.07 (m, 2 H, CH_2), 1.24 (s, 9 H, CH_3 x 3), 1.20-0.94 (m, 8 H, CH_2 x 4), 0.80 (t, *J* = 6.8 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.1, 155.2, 142.9, 139.9, 133.6, 130.0, 128.7, 127.2, 126.7, 124.8, 117.0, 61.5, 38.6, 34.9, 31.5, 31.0, 29.8, 23.9, 22.5, 14.0; **IR** (neat): *v* = 3085, 3059,

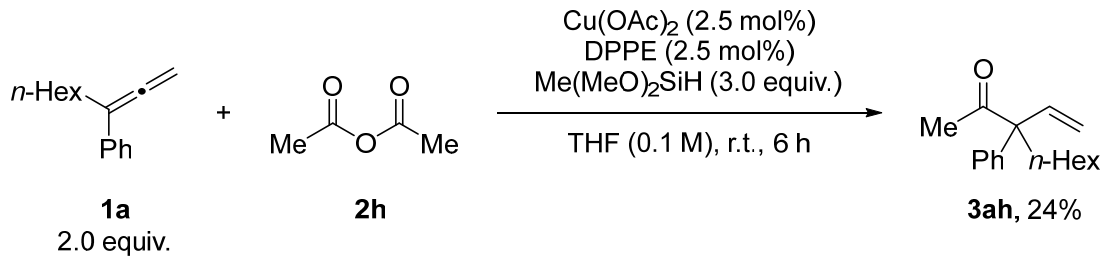
3025, 2955, 2928, 2860, 1675, 1604, 1563, 1495, 1464, 1447, 1406, 1364, 1268, 1235, 1193, 1110 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 362 (M^+, 1.13), 161 (100); **HRMS** calcd. *m/z* for $C_{26}H_{34}O$ (M^+): 362.2604; Found: 362.2607.

(16) Preparation of 1-(4-methoxyphenyl)-2-phenyl-2-hexyl-3-buten-1-one (3ag) (Yy-4-041)



Following **Typical Procedure II**, the reaction of 4-methoxybenzoic anhydride **2g** (143.3 mg, 0.5 mmol), $Cu(OAc)_2$ (2.3 mg, 0.0127 mmol), DPPE (5.0 mg, 0.0125 mmol), allene **1a** (200.3 mg, 1.0 mmol) in THF (4 mL), and dimethoxymethylsilane (163.6 mg, d = 0.861 g/mL, 0.19 mL, 1.5 mmol, in 1 mL THF) afforded **3ag** (110.5 mg, 66% yield) as a colorless oil (eluent: Petroleum ether (400 mL) to Petroleum ether/ EtOAc = 50/1 (~ 400 mL)); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.56 (d, *J* = 9.2 Hz, 2 H, Ar-H), 7.35-7.28 (m, 2 H, Ar-H), 7.28-7.19 (m, 3 H, Ar-H), 6.76-6.66 (m, 3 H, =CH and Ar-H), 5.28 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 4.98 (d, *J* = 17.6 Hz, 1 H, one proton of $=CH_2$), 3.75 (s, 3 H, CH_3), 2.25-2.05 (m, 2 H, CH_2), 1.22-0.94 (m, 8 H, CH_2 x 4), 0.81 (t, *J* = 6.8 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 199.0, 162.2, 143.2, 140.0, 132.5, 128.8, 128.7, 127.1, 126.7, 116.9, 113.0, 61.2, 55.2, 39.0, 31.5, 29.8, 24.0, 22.5, 14.0; **IR** (neat): *v* = 3083, 3059, 3024, 2953, 2928, 2856, 1669, 1598, 1575, 1508, 1495, 1458, 1446, 1417, 1307, 1259, 1238, 1169, 1115, 1030 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 336 (M^+, 1.17), 135 (100); **HRMS** calcd. *m/z* for $C_{23}H_{28}O_2$ (M^+): 336.2084; Found: 336.2085.

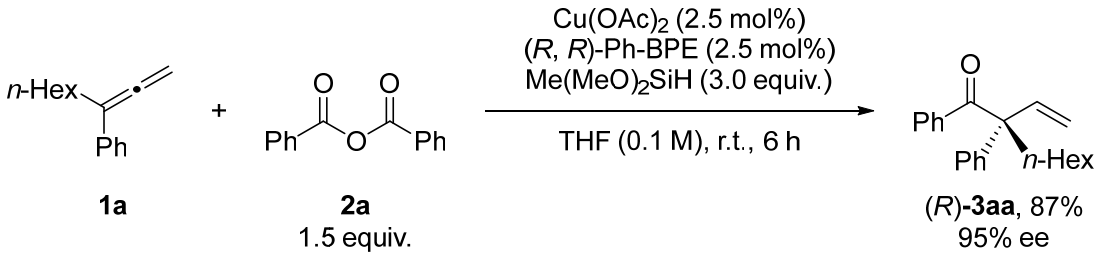
(17) Preparation of 3-phenyl-3-hexyl-3-buten-2-one (3ah) (Yy-4-039)



Following **Typical Procedure II**, the reaction of acetic anhydride **2h** (51.0 mg, 0.5 mmol), $Cu(OAc)_2$ (2.3 mg, 0.0127 mmol), DPPE (5.0 mg, 0.0125 mmol), allene **1a** (200.3 mg, 1.0 mmol) in THF (4 mL), and dimethoxymethylsilane (163.6 mg, d = 0.861 g/mL, 0.19 mL, 1.5 mmol, in 1 mL THF) afforded **3ah** (32.1 mg, 90% purity, 24% yield) as a yellow oil (eluent: Petroleum ether (300 mL) to Petroleum ether/ EtOAc = 100/1 (~ 600 mL)); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.39-7.30 (m, 2 H, Ar-H), 7.30-7.23 (m, 1 H, Ar-H), 7.23-7.14 (m, 2 H, Ar-H), 6.47 (dd, J_1 = 17.8 Hz, J_2 = 11.0 Hz, 1 H, =CH), 5.35 (d, J = 10.8 Hz, 1 H, one proton of $=CH_2$), 4.99 (d, J = 17.6 Hz, 1 H, one proton of $=CH_2$), 2.13-1.95 (m, 2 H, CH_2), 1.94 (s, 3 H, CH_3), 1.28-0.94 (m, 8 H, CH_2 x 4), 0.84 (t, J = 6.6 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 208.2, 141.5, 138.9, 128.6, 127.5, 126.9, 117.2, 63.3, 35.9, 31.6, 29.9, 26.9, 24.2, 22.6, 14.0; **IR** (neat): ν = 3085, 3059, 3024, 2927, 2857, 1709, 1632, 1599, 1494, 1447, 1352, 1174, 1119, 1004 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 244 (M^+, 1.45), 117 (100); **HRMS** calcd. *m/z* for $C_{17}H_{24}O$ (M^+): 244.1822; Found: 244.1819.

4. Preparation of optically active products

(1) Preparation of (*R*)-1,2-diphenyl-2-hexyl-3-buten-1-one [(*R*)-3aa] (Yy-3-132)

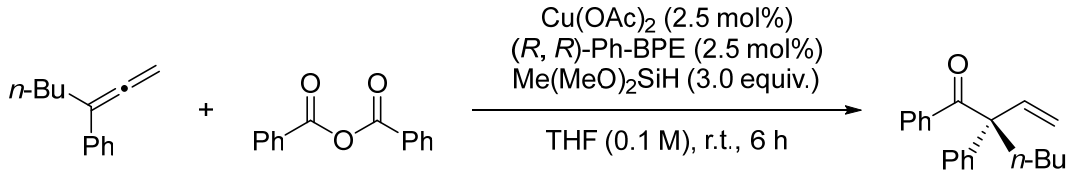


1a **2a** 1.5 equiv. (*R*)-**3aa**, 87% 95% ee

Typical Procedure III: To an oven-dried 25 mL Schlenk tube were added a stirring bar, benzoic anhydride **2a** (339.3 mg, 1.5 mmol), $Cu(OAc)_2$ (4.5 mg, 0.025 mmol), (*R*,*R*)-Ph-BPE (12.7 mg, 0.025 mmol), and allene **1a** (200.3 mg, 1.0 mmol) in THF (8 mL) under nitrogen. The resulting mixture was stirred at room temperature for 5 min followed by the addition of dimethoxymethylsilane solution (318.6 mg, d = 0.861 g/mL, 0.37 mL, 3.0 mmol, diluted with 2 mL THF). After being stirred at room temperature for 6 h, a saturated solution of NH_4F in methanol (5 mL) was added to quench the reaction. The reaction mixture was stirred for 15 min at room temperature and then filtered through s short plug of celite eluted with EtOAc (10 mL x 3). The

solvent was removed *in vacuo* and the crude product was purified by column chromatography on silica gel to afford (*R*)-**3aa** (266.7 mg, 87% yield) as a colorless oil (eluent: Petroleum ether (250 mL) to petroleum ether/ EtOAc = 100/1 (~ 500 mL)): 95% ee (HPLC conditions: AD-H column, hexane/*i*-PrOH = 95/5, 1.0 mL/min, λ = 214 nm, t_R (major) = 4.0 min, t_R (minor) = 3.8 min; $[\alpha]^{22}_D$ = +98.5 (c = 1.04, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.53 (d, *J* = 8.0 Hz, 2 H, Ar-H), 7.40-7.28 (m, 3 H, Ar-H), 7.28-7.15 (m, 5 H, Ar-H), 6.70 (dd, J_1 = 17.6 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.30 (d, *J* = 11.2 Hz, 1 H, one proton of $=CH_2$), 4.99 (d, *J* = 17.6 Hz, 1 H, one proton of $=CH_2$), 2.30-2.05 (m, 2 H, CH_2), 1.30-0.95 (m, 8 H, CH_2 x 4), 0.81 (t, *J* = 6.6 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.6, 142.6, 139.7, 136.3, 131.7, 130.0, 128.7, 127.8, 127.1, 126.8, 117.2, 61.5, 38.7, 31.5, 29.8, 23.9, 22.5, 14.0; **IR** (neat): *v* = 3088, 3062, 3026, 2953, 2927, 2857, 1676, 1597, 1579, 1466, 1446, 1227, 1180 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 306 (M^+, 2.39), 105 (100); **HRMS** calcd. *m/z* for $C_{22}H_{26}O$ (M^+): 306.1978; Found: 306.1978.

(2) Preparation of (*R*)-1,2-Diphenyl-2butyl-3-buten-1-one [(*R*)-3ba] (Yy-3-160)

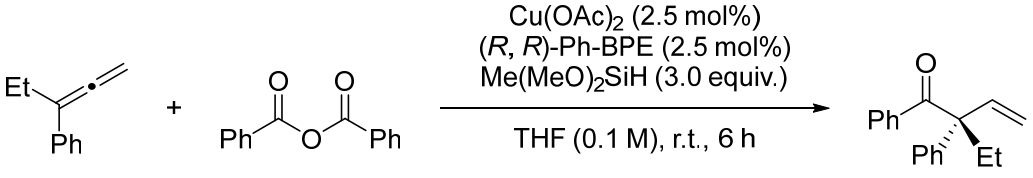


1b | **2a** 1.5 equiv. | (*R*)-**3ba**, 83% 97% ee

Following **Typical Procedure III**, the reaction of benzoic anhydride **2a** (339.3 mg, 1.5 mmol), $Cu(OAc)_2$ (4.5 mg, 0.025 mmol), (*R*,*R*)-Ph-BPE (12.7 mg, 0.025 mmol), allene **1b** (172.3 mg, 1.0 mmol) in THF (8 mL), and dimethoxymethylsilane (318.6 mg, d = 0.861 g/mL, 0.37 mL, 3.0 mmol, in 2 mL THF) afforded (*R*)-**3ba** (236.1 mg, 98% purity, 83% yield) as a colorless oil (eluent: Petroleum ether (250 mL) to Petroleum ether/ EtOAc = 100/1 (~ 500 mL)): 97% ee (HPLC conditions: AD-H column, hexane/*i*-PrOH = 95/5, 1.0 mL/min, λ = 214 nm, t_R (major) = 4.3 min, t_R (minor) = 4.0 min; $[\alpha]^{26}_D$ = +110.7 (c = 1.07, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.53 (d, *J* = 7.6 Hz, 2 H, Ar-H), 7.36-7.29 (m, 3 H, Ar-H), 7.29-7.15 (m, 5 H, Ar-H), 6.70 (dd, J_1 = 17.6 Hz, J_2 = 11.2 Hz, 1 H, =CH), 5.30 (d, *J* = 10.8 Hz, 1 H, one

proton of =CH_2), 5.00 (d, J = 17.6 Hz, 1 H, one proton of =CH_2), 2.28-2.08 (m, 2 H, CH_2), 1.30-1.15 (m, 2 H, CH_2), 1.15-0.90 (m, 2 H, CH_2), 0.78 (t, J = 7.2 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.6, 142.6, 139.7, 136.3, 131.7, 130.0, 128.7, 127.8, 127.1, 126.8, 117.2, 61.4, 38.5, 26.2, 23.2, 13.8; **IR** (neat): ν = 3086, 3058, 3024, 2955, 2931, 2871, 1675, 1597, 1578, 1495, 1446, 1225, 1181 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 278 (M^+, 1.88), 105 (100); **HRMS** calcd. *m/z* for $C_{20}H_{22}O$ (M^+): 278.1665; Found: 278.1668.

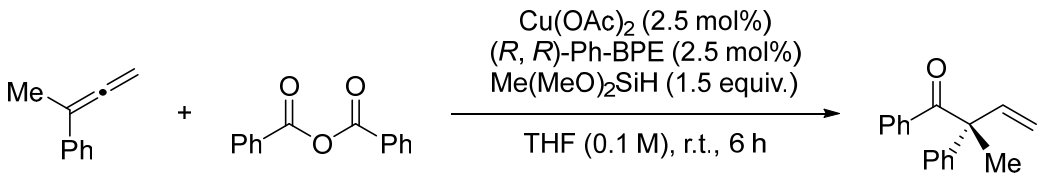
(3) Preparation of (*R*)-2-ethyl-1,2-diphenylbut-3-en-1-one [(*R*)-3ca] (Yy-3-183)



1c **2a** 1.5 equiv. (*R*)-**3ca**, 81% 95% ee

Following **Typical Procedure III**, the reaction of benzoic anhydride **2a** (339.3 mg, 1.5 mmol), $Cu(OAc)_2$ (4.5 mg, 0.025 mmol), (*R*,*R*)-Ph-BPE (12.7 mg, 0.025 mmol), allene **1c** (144.4 mg, 1.0 mmol) in THF (8 mL), and dimethoxymethylsilane (318.6 mg, d = 0.861 g/mL, 0.37 mL, 3.0 mmol, in 2 mL THF) afforded (*R*)-**3ca** (203.9 mg, 99% purity, 81% yield) as a colorless oil (eluent: Petroleum ether (200 mL) to Petroleum ether/ EtOAc = 100/1 (~ 800 mL)): 95% ee (HPLC conditions: OD-H column, hexane/*i*-PrOH = 99.5/0.5, 1.0 mL/min, λ = 214 nm, t_R (major) = 6.0 min, t_R (minor) = 5.7 min; $[\alpha]^{23}_D$ = +137.6 (c = 1.12, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.58-7.50 (m, 2 H, Ar-H), 7.37-7.29 (m, 3 H, Ar-H), 7.29-7.15 (m, 5 H, Ar-H), 6.69 (dd, J_1 = 17.6 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.32 (d, J = 11.2 Hz, 1 H, one proton of =CH_2), 5.02 (d, J = 17.6 Hz, 1 H, one proton of =CH_2), 2.35-2.10 (m, 2 H, CH_2), 0.71 (t, J = 7.4 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.5, 142.4, 139.1, 136.3, 131.7, 130.0 ,128.7, 127.8, 127.2, 126.8, 117.5, 61.8, 31.5, 8.6; **IR** (neat): ν = 3085, 3058, 3025, 2970, 2937, 2879, 1674, 1597, 1578, 1494, 1446, 1227, 1181, 1003 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 250 (M^+, 1.18), 105 (100); **HRMS** calcd. *m/z* for $C_{18}H_{18}O$ (M^+): 250.1352; Found: 250.1352.

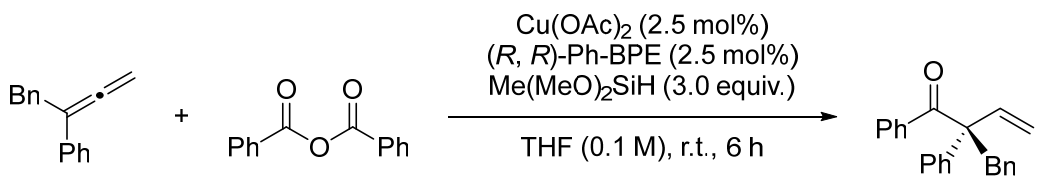
(4) Preparation of (*R*)-2-methyl-1,2-diphenylbut-3-en-1-one [(*R*)-3da] (Yy-4-066)



1d 1.5 equiv. | **2a** | (*R*)-**3da**, 86% 95% ee

Following **Typical Procedure III**, the reaction of benzoic anhydride **2a** (226.4 mg, 1.0 mmol), $Cu(OAc)_2$ (4.5 mg, 0.025 mmol), (*R*,*R*)-Ph-BPE (12.7 mg, 0.025 mmol), allene **1d** (195.5 mg, 1.5 mmol) in THF (8 mL), and dimethoxymethylsilane (163.6 mg, d = 0.861 g/mL, 0.19 mL, 1.5 mmol, in 2 mL THF) afforded (*R*)-**3da**[8] (204.2 mg, 86% yield) as a colorless oil (eluent: Petroleum ether (200 mL) to Petroleum ether/ EtOAc = 100/1 (~ 400 mL) to 50/1 (~ 400 mL)): 95% ee (HPLC conditions: AD-H column, hexane/*i*-PrOH = 99/1, 1.0 mL/min, λ = 214 nm, t_R (major) = 6.3 min, t_R (minor) = 6.9 min; $[\alpha]^{23}_D$ = +141.7 (c = 1.00, $CHCl_3$) [reported: 90% ee, $[\alpha]^{20}_D$ = +129.9 (c = 1.00, $CHCl_3$)][8]; **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.53 (d, *J* = 7.6 Hz, 2 H, Ar-H), 7.40-7.30 (m, 3 H, Ar-H), 7.30-7.18 (m, 5 H, Ar-H), 6.62 (dd, J_1 = 17.4 Hz, J_2 = 10.6 Hz, 1 H, =CH), 5.29 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 5.16 (d, *J* = 17.2 Hz, 1 H, one proton of $=CH_2$), 1.67 (s, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.8, 144.4, 141.0, 136.2, 131.8, 130.0, 129.0, 127.9, 126.9, 126.4, 116.6, 58.5, 25.9; **IR** (neat): *v* = 3085, 3058, 3024, 2979, 2930, 1674, 1595, 1579, 1493, 1446, 1407, 1364, 1236, 1165, 1078, 1007 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 236 (M^+, 2.10), 105 (100).

(5) Preparation of (*R*)-2-benzyl-1,2-diphenylbut-3-en-1-one [(*R*)-3ea] (Yy-4-048)

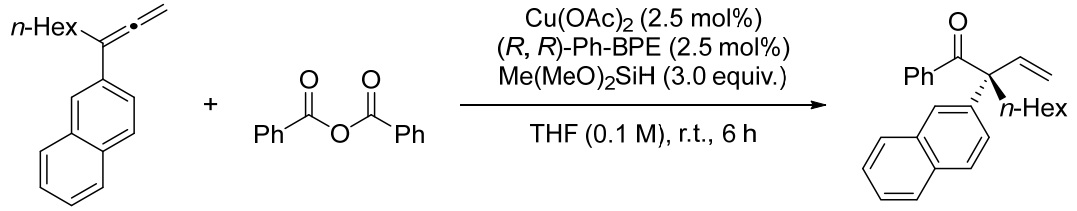


1e | **2a** 1.5 equiv. | (*R*)-**3ea**, 80% 94% ee

Following **Typical Procedure III**, the reaction of benzoic anhydride **2a** (339.9 mg, 1.5 mmol), $Cu(OAc)_2$ (4.5 mg, 0.025 mmol), (*R*,*R*)-Ph-BPE (12.7 mg, 0.025 mmol),

allene **1e** (206.6 mg, 1.0 mmol) in THF (8 mL), and dimethoxymethylsilane (318.6 mg, d = 0.861 g/mL, 0.37 mL, 3.0 mmol, in 2 mL THF) afforded (*R*)-**3ea** (249.0 mg, 80% yield) as a white soild: m.p. 111.7-112.9 ºC (Petroleum ether/ EtOAc) (eluent: Petroleum ether (200 mL) to Petroleum ether/ EtOAc = 100/1 (~ 400 mL)): 94% ee (HPLC conditions: OD-H column, hexane/*i*-PrOH = 99/1, 1.0 mL/min, λ = 214 nm, t_R (major) = 6.4 min, t_R (minor) = 5.7 min; $[\alpha]^{24}_D$ = +190.4 (c = 0.99, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.61 (d, *J* = 7.6 Hz, 2 H, Ar-H), 7.32 (t, *J* = 7.2 Hz, 1 H, Ar-H), 7.25-7.15 (m, 5 H, Ar-H), 7.15-6.90 (m, 5 H, Ar-H), 6.70-6.55 (m, 3 H, =CH and Ar-H), 5.40 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 5.14 (d, *J* = 17.6 Hz, 1 H, one proton of $=CH_2$), 3.48 (q, *J* = 13.5 Hz, 2 H, CH_2); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 199.9, 141.6, 139.3, 136.9, 135.7, 131.8, 131.2, 130.6, 128.5, 127.8, 127.5, 127.2, 126.9, 126.1, 118.5, 62.2, 47.3; **IR** (neat): *v* = 3084, 3059, 3027, 2963, 2925, 1677, 1596, 1577, 1490, 1454, 1445, 1397, ,1227, 1180, 1156, 1077 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 313 (M^++1, 4.75), 312 (M^+, 18.00), 105 (100); **HRMS** calcd. *m/z* for $C_{23}H_{20}O$ (M^+): 312.1509; Found: 312.1509.

(6) Preparation of (*R*)-2-(Naphthalen-2-yl)-1-phenyl-2-hexylbut-3-en-1-one [(*R*)-3fa] (Yy-3-134)

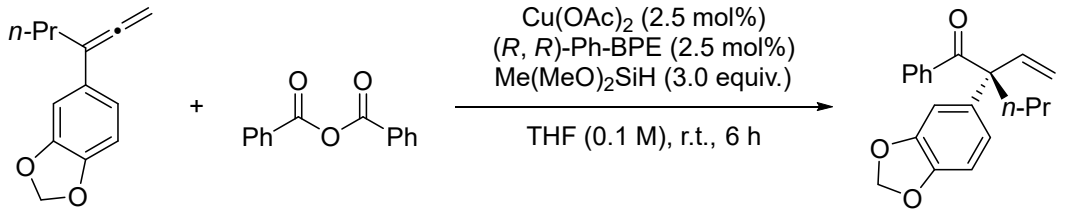


1f **2a** 1.5 equiv. (*R*)-**3fa**, 96% 99% ee

Following **Typical Procedure III**, the reaction of benzoic anhydride **2a** (339.3 mg, 1.5 mmol), $Cu(OAc)_2$ (4.5 mg, 0.025 mmol), (*R*,*R*)-Ph-BPE (12.7 mg, 0.025 mmol), allene **1f** (250.4 mg, 1.0 mmol) in THF (8 mL), and dimethoxymethylsilane (318.6 mg, d = 0.861 g/mL, 0.37 mL, 3.0 mmol, in 2 mL THF) afforded (*R*)-**3fa** (341.6 mg, 96% yield) as a colorless oil (eluent: Petroleum ether (500 mL) to Petroleum ether/ EtOAc = 100/1 (~ 400 mL)): 99% ee (HPLC conditions: AD-H column, hexane/*i*-PrOH = 99/1, 1.0 mL/min, λ = 214 nm, t_R (major) = 9.4 min, t_R (minor) = 8.6 min; $[\alpha]^{21}_D$ = +97.8 (c = 1.55, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.90-7.70 (m,

4 H, Ar-H), 7.56 (d, J = 7.6 Hz, 2 H, Ar-H), 7.50-7.40 (m, 2 H, Ar-H), 7.35-7.20 (m, 2 H, Ar-H), 7.15 (t, J = 7.6 Hz, 2 H, Ar-H), 6.82 (dd, J_1 = 17.6 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.35 (d, J = 10.8 Hz, 1 H, one proton of $=CH_2$), 5.03 (d, J = 17.6 Hz, 1 H, one proton of $=CH_2$), 2.40-2.18 (m, 2 H, CH_2), 1.24-0.95 (m, 8 H, CH_2 x 4), 0.78 (t, J = 6.2 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.6, 140.2, 139.7, 136.4, 133.5, 132.3, 131.7, 130.0, 128.5, 128.1, 127.9, 127.6, 126.2, 125.9, 125.7, 125.5, 117.4, 61.6, 38.7, 31.5, 29.8, 24.0, 22.5, 14.0; **IR** (neat): ν = 3060, 3033, 2956, 2920, 2856, 1718, 1668, 1630, 1597, 1579, 1504, 1478, 1447, 1269, 1235, 1179, 1108 cm^{-1}; **MS** (70 eV, EI) *m/z* (%):357 (M^++1, 2.64), 356 (M^+, 9.57), 105 (100); **HRMS** calcd. for $C_{26}H_{29}O$ ($M+H^+$): 357.2213; Found: 357.2212.

(7) Preparation of (*R*)-2-(benzo[*d*][1,3]dioxol-5-yl)-1-phenyl-2-propylbut-3-en-1-one [(*R*)-3ga] (Yy-4-060)

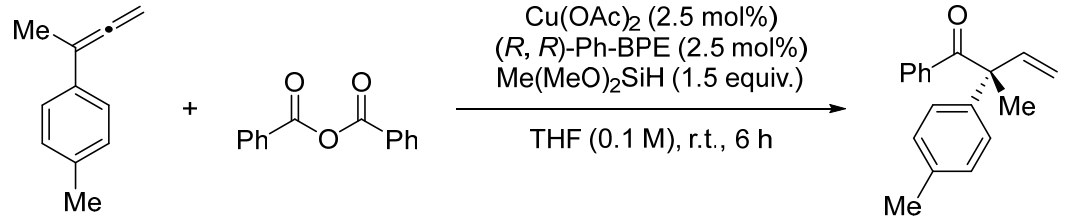


1g **2a** 1.5 equiv. (*R*)-**3ga**, 75% 92% ee

Following **Typical Procedure III**, the reaction of benzoic anhydride **2a** (339.3 mg, 1.5 mmol), $Cu(OAc)_2$ (4.5 mg, 0.025 mmol), (*R*,*R*)-Ph-BPE (12.7 mg, 0.025 mmol), allene **1g** (202.0 mg, 1.0 mmol) in THF (8 mL), and dimethoxymethylsilane (318.6 mg, d = 0.861 g/mL, 0.37 mL, 3.0 mmol, in 2 mL THF) afforded (*R*)-**3ga** (230.0 mg, 75% yield) as a colorless oil (eluent: Petroleum ether (100 mL) to Petroleum ether/ EtOAc = 50/1 (~ 400 mL)): 92% ee (HPLC conditions: AD-H column, hexane/*i*-PrOH = 98/2, 1.0 mL/min, λ = 214 nm, t_R (major) = 8.3 min, t_R (minor) = 10.1 min; $[\alpha]^{23}_D$ = +107.9 (c = 0.84, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.58 (d, J = 7.6 Hz, 2 H, Ar-H), 7.36 (t, J = 7.4 Hz, 1 H, Ar-H), 7.23 (t, J = 7.8 Hz, 2 H, Ar-H), 6.80-6.66 (m, 3 H, Ar-H), 6.62 (dd, J_1 = 17.6 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.94 (d, J = 2.0 Hz, 2 H, CH_2), 5.28 (d, J = 10.8 Hz, 1 H, one proton of $=CH_2$), 4.99 (d, J = 17.6 Hz, 1 H, one proton of $=CH_2$), 2.20-2.00 (m, 2 H, CH_2), 1.18-0.98 (m, 2 H, CH_2), 0.83

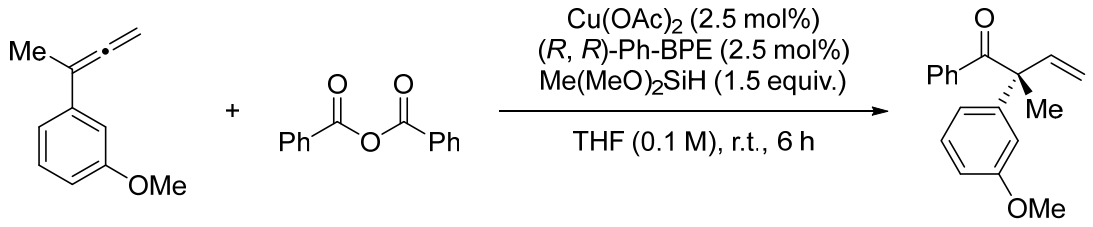
(t, J = 7.2 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.3, 148.1, 146.4, 139.7, 136.44, 136.37, 131.7, 130.0, 127.9, 120.4, 117.1, 108.4, 107.7, 101.1, 61.2, 41.0, 17.4, 14.6; **IR** (neat): v = 2969, 2953, 2935, 2898, 2873, 1672, 1596, 1503, 1484, 1447, 1433, 1232, 1185, 1111, 1039 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 309 (M^++1, 5.37), 308 (M^+, 21.71), 203 (100); **HRMS** calcd. *m/z* for $C_{20}H_{20}O_3$ (M^+): 308.1407; Found: 308.1410.

(8) Preparation of (*R*)-2-methyl-1-phenyl-2-(*p*-tolyl)but-3-en-1-one [(*R*)-3ha] (Yy-4-080)



Following **Typical Procedure III**, the reaction of benzoic anhydride **2a** (226.0 mg, 1.0 mmol), $Cu(OAc)_2$ (4.5 mg, 0.025 mmol), (*R*,*R*)-Ph-BPE (12.7 mg, 0.025 mmol), allene **1h** (216.3 mg, 1.5 mmol) in THF (8 mL), and dimethoxymethylsilane (163.6 mg, d = 0.861 g/mL, 0.19 mL, 1.5 mmol, in 2 mL THF) afforded (*R*)-**3ha**[8] (233.7 mg, 93% yield) as a yellow oil (eluent: Petroleum ether (200 mL) to Petroleum ether/ EtOAc = 100/1 (~ 600 mL)): 94% ee (HPLC conditions: AD-H column, hexane/*i*-PrOH = 99/1, 1.0 mL/min, λ = 214 nm, t_R (major) = 6.0 min, t_R (minor) = 7.1 min; $[\alpha]^{23}_D$ = +124.6 (c = 1.11, $CHCl_3$) [reported: 89% ee, $[\alpha]^{20}_D$ = +108.7 (c = 1.00, $CHCl_3$)][8]; **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.59-7.51 (m, 2 H, Ar-H), 7.40-7.32 (m, 1 H, Ar-H), 7.27-7.19 (m, 2 H, Ar-H), 7.19-7.10 (m, 4 H, Ar-H), 6.60 (dd, J_1 = 17.4 Hz, J_2 = 10.6 Hz, 1 H, =CH), 5.27 (d, J = 10.8 Hz, 1 H, one proton of $=CH_2$), 5.14 (d, J = 17.6 Hz, 1 H, one proton of $=CH_2$), 2.33 (s, 3 H, CH_3), 1.65 (s, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 201.1, 141.3, 141.2, 136.6, 136.3, 131.8, 130.0, 129.7, 127.9, 126.3, 116.3, 58.2, 25.9, 21.0; **IR** (neat): v = 3062, 3025, 2984, 2937, 1676, 1511, 1446, 1408, 1366, 1239, 1168, 1112, 1078, 1010 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 250 (M^+, 6.24), 105 (100).

(9) Preparation of (*R*)-2-(3-methoxyphenyl)-2-methyl-1-phenylbut-3-en-1-one [(*R*)-3ia] (Yy-4-082)



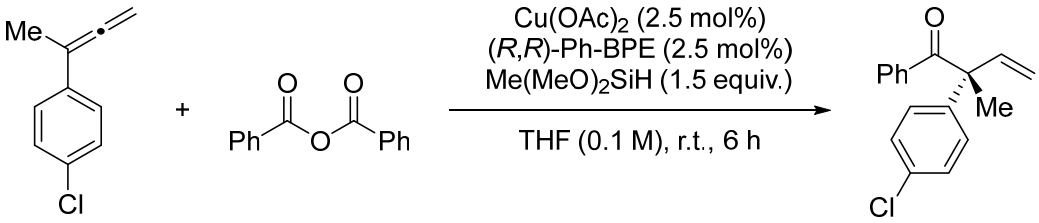
1i
1.5 equiv.

2a

(*R*)-**3ia**, 87%
95% ee

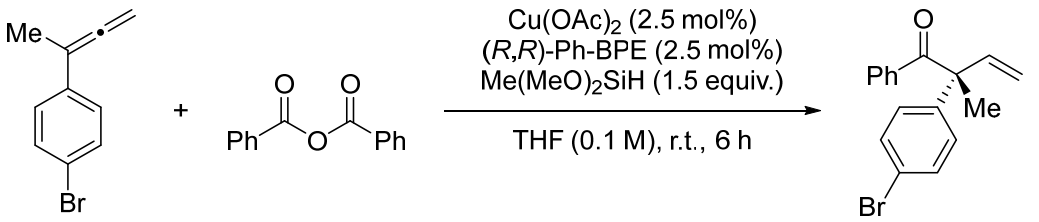
Following **Typical Procedure III**, the reaction of benzoic anhydride **2a** (226.1 mg, 1.0 mmol), $Cu(OAc)_2$ (4.5 mg, 0.025 mmol), (*R*,*R*)-Ph-BPE (12.7 mg, 0.025 mmol), allene **1i** (240.3 mg, 1.5 mmol) in THF (8 mL), and dimethoxymethylsilane (163.6 mg, d = 0.861 g/mL, 0.19 mL, 1.5 mmol, in 2 mL THF) afforded (*R*)-**3ia** (231.1 mg, 87% yield) as a colorless oil (eluent: Petroleum ether (200 mL) to Petroleum ether/ EtOAc = 100/1 (~ 200 mL) to 50/1 (~ 400 mL)): 95% ee (HPLC conditions: AD-H column, hexane/*i*-PrOH = 98/2, 1.0 mL/min, λ = 214 nm, t_R (major) = 6.7 min, t_R (minor) = 7.4 min; $[\alpha]^{24}_D$ = +125.2 (c = 1.08, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.60-7.52 (m, 2 H, Ar-H), 7.40-7.33 (m, 1 H, Ar-H), 7.26-7.19 (m, 3 H, Ar-H), 6.88-6.77 (m, 3 H, Ar-H), 6.60 (dd, J_1 = 17.2 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.28 (d, J = 10.4 Hz, 1 H, one proton of $=CH_2$), 5.16 (d, J = 17.2 Hz, 1 H, one proton of $=CH_2$), 3.75 (s, 3 H, OCH_3), 1.66 (s, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.6, 160.0, 146.0, 140.8, 136.2, 131.8, 129.94, 129.91, 127.9, 118.9, 116.5, 112.4, 111.9, 58.4, 55.1, 25.7; **IR** (neat): ν = 3061, 2986, 2936, 2835, 1677, 1596, 1580, 1485, 1447, 1432, 1409, 1290, 1239, 1129, 1045, 1013 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 266 (M^+, 7.09), 105 (100); **HRMS** calcd. *m/z* for $C_{18}H_{18}O_2$ (M^+): 266.1301; Found: 266.1305.

(10) Preparation of (*R*)-2-(4-chlorophenyl)-2-methyl-1-phenylbut-3-en-1-one [(*R*)-3ja] (Yy-4-088)



Following **Typical Procedure III**, the reaction of benzoic anhydride **2a** (226.2 mg, 1.0 mmol), $Cu(OAc)_2$ (4.5 mg, 0.025 mmol), (*R*,*R*)-Ph-BPE (12.7 mg, 0.025 mmol), allene **1j** (247.5 mg, 1.5 mmol) in THF (8 mL), and dimethoxymethylsilane (163.6 mg, d = 0.861 g/mL, 0.19 mL, 1.5 mmol, in 2 mL THF) afforded (*R*)-**3ja**[8] (204.7 mg, 76% yield) as a colorless oil (eluent: Petroleum ether (200 mL) to Petroleum ether/ EtOAc = 100/1 (~ 505 mL)): 93% ee (HPLC conditions: AD-H column, hexane/*i*-PrOH = 99/1, 1.0 mL/min, λ = 214 nm, t_R (major) = 5.9 min, t_R (minor) = 6.4 min; $[\alpha]^{24}_D$ = +117.0 (c = 1.12, $CHCl_3$) [reported: 94% ee, $[\alpha]^{20}_D$ = +110.9 (c = 1.00, $CHCl_3$)][8]; **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.58-7.50 (m, 2 H, Ar-H), 7.44-7.36 (m, 1 H, Ar-H), 7.36-7.29 (m, 2 H, Ar-H), 7.29-7.18 (m, 4 H, Ar-H), 6.58 (dd, J_1 = 17.2 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.31 (d, J = 10.8 Hz, 1 H, one proton of $=CH_2$), 5.16 (d, J = 17.2 Hz, 1 H, one proton of $=CH_2$), 1.65 (s, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.3, 143.0, 140.5, 135.8, 132.9, 132.0, 130.0, 129.2, 128.1, 127.8, 117.0, 58.1, 26.0; **IR** (neat): ν = 3067, 2987, 2937, 1723, 1675, 1629, 1598, 1581, 1490, 1457, 1446, 1407, 1367, 1240, 1168, 1127, 1094, 1007 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 272 [M^+(^{37}Cl), 0.31)], 270 [M^+(^{35}Cl), 1.03)], 105 (100).

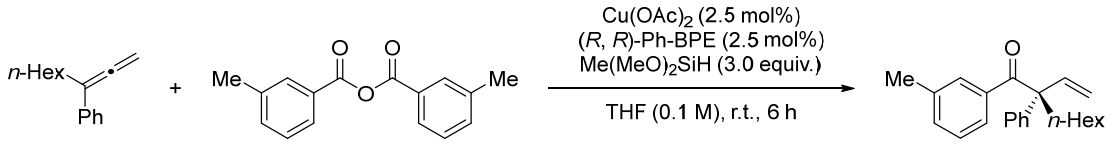
(11) Preparation of (*R*)-2-(4-bromophenyl)-2-methyl-1-phenylbut-3-en-1-one [(*R*)-3ka] (Yy-4-090)



Following **Typical Procedure III**, the reaction of benzoic anhydride **2a** (226.2 mg,

1.0 mmol), $Cu(OAc)_2$ (4.5 mg, 0.025 mmol), (*R*,*R*)-Ph-BPE (12.7 mg, 0.025 mmol), allene **1k** (313.5 mg, 1.5 mmol) in THF (8 mL), and dimethoxymethylsilane (163.6 mg, d = 0.861 g/mL, 0.19 mL, 1.5 mmol, in 2 mL THF) afforded (*R*)-**3ka** (245.7 mg, 78% yield) as a colorless oil (eluent: Petroleum ether (200 mL) to Petroleum ether/ EtOAc = 100/1 (~ 600 mL)): 96% ee (HPLC conditions: AD-H column, hexane/*i*-PrOH = 99/1, 1.0 mL/min, λ = 214 nm, t_R (major) = 7.7 min, t_R (minor) = 9.3 min; $[\alpha]^{23}_D$ = +100.8 (c = 1.14, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.56-7.50 (m, 2 H, Ar-H), 7.47 (d, *J* = 8.4 Hz, 2 H, Ar-H), 7.40 (t, *J* = 7.4 Hz, 1 H, Ar-H), 7.26 (d, *J* = 7.8 Hz, 2 H, Ar-H), 7.15 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.57 (dd, J_1 = 17.2 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.31 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 5.16 (d, *J* = 17.2 Hz, 1 H, one proton of $=CH_2$), 1.64 (s, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.2, 143.6, 140.4, 135.8, 132.12, 132.07, 130.0, 128.2, 128.1, 121.0, 117.1, 58.1, 26.0; **IR** (neat): *v* = 3063, 2985, 2937, 1675, 1629, 1597, 1581, 1489, 1446, 1408, 1398, 1365, 1241, 1170, 1105, 1081, 1007 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 316 [M^+(^{81}Br), 0.57], 314 [M^+(^{79}Br), 0.59], 130 (M^+-Br-Bz), 105 (100); **HRMS** calcd. *m/z* for $C_{17}H_{15}{}^{79}BrO$ (M^+): 314.0301; Found: 314.0303.

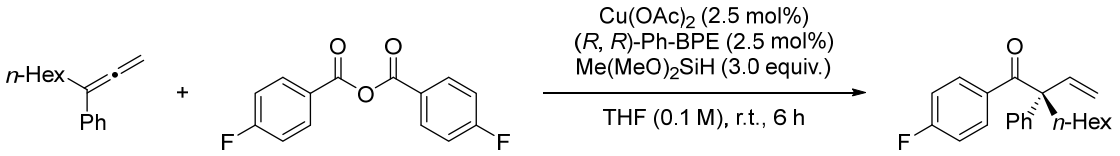
(12) Preparation of (*R*)-2-phenyl-1-(m-tolyl)-2-hexylbut-en-1-one [(*R*)-3ab] (Yy-4-006)



Following **Typical Procedure III**, the reaction of 3-methylbenzoic anhydride **2b** (262.1 mg, 1.0 mmol), $Cu(OAc)_2$ (4.5 mg, 0.025 mmol), (*R*,*R*)-Ph-BPE (12.7 mg, 0.025 mmol), allene **1a** (400.9 mg, 2.0 mmol) in THF (8 mL), and dimethoxymethylsilane (318.6 mg, d = 0.861 g/mL, 0.37 mL, 3.0 mmol, in 2 mL THF) afforded (*R*)-**3ab** (302.1 mg, 94% yield) as a colorless oil (eluent: Petroleum ether (200 mL) to Petroleum ether/ EtOAc = 100/1 (~ 400 mL)): 96% ee (HPLC conditions: AD-H column, hexane/*i*-PrOH = 99/1, 1.0 mL/min, λ = 214 nm, t_R (major)

= 5.5 min, t_R (minor) = 4.8 min; $[\alpha]^{31}_D$ = +94.5 (c = 1.18, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.44 (s, 1 H, Ar-H), 7.35-7.28 (m, 2 H, Ar-H), 7.28-7.17 (m, 4 H, Ar-H), 7.14 (d, *J* = 7.6 Hz, 1 H, Ar-H), 7.04 (t, *J* = 7.8 Hz, 1 H, Ar-H), 6.69 (dd, J_1 = 17.6 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.29 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 5.00 (d, *J* = 17.6 Hz, 1 H, one proton of $=CH_2$), 2.27-2.06 (m, 5 H, CH_2 and CH_3), 1.24-0.95 (m, 8 H, CH_2 x 4), 0.81 (t, *J* = 6.8 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.8, 142.7, 139.8, 137.6, 136.4, 132.4, 130.5, 128.7, 127.5, 127.3, 127.2, 126.7, 117.1, 61.5, 38.7, 31.5, 29.8, 23.9, 22.5, 21.3, 14.0; **IR** (neat): *v* = 3084, 3060, 3026, 2953, 2926, 2857, 1676, 1600, 1583, 1494, 1446, 1252, 1173, 1001 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 320 (M^+, 1.54), 119 (100); **HRMS** calcd. for $C_{23}H_{28}O$ (M^+): 320.2135; Found: 320.2140.

(13) Preparation of (*R*)-1-(4-fluorophenyl)-2-phenyl-2-hexylbut-3-en-1-one [(*R*)-3ac] (Yy-5-050, Yy-4-017)

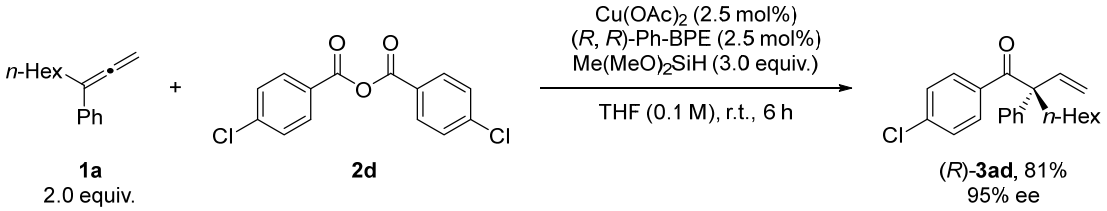


1a 2.0 equiv. **2c** (*R*)-**3ac**, 90% 96% ee

Following **Typical Procedure III**, the reaction of 4-fluorobenzoic anhydride **2c** (270.5 mg, 1.0 mmol), $Cu(OAc)_2$ (4.5 mg, 0.025 mmol), (*R*,*R*)-Ph-BPE (12.7 mg, 0.025 mmol), allene **1a** (400.2 mg, 2.0 mmol) in THF (8 mL), and dimethoxymethylsilane (318.6 mg, d = 0.861 g/mL, 0.37 mL, 3.0 mmol, in 2 mL THF) afforded (*R*)-**3ac** (302.5 mg, 90% yield) as a colorless oil (eluent: Petroleum ether (500 mL) to Petroleum ether/ EtOAc = 100/1 (~ 1000 mL)): 96% ee (HPLC conditions: AD-H column, hexane/*i*-PrOH = 99/1, 1.0 mL/min, λ = 214 nm, t_R (major) = 5.9 min, t_R (minor) = 5.3 min; $[\alpha]^{31}_D$ = +93.3 (c = 1.03, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.64-7.52 (m, 2 H, Ar-H), 7.38-7.28 (m, 2 H, Ar-H), 7.28-7.18 (m, 3 H, Ar-H), 6.92-6.82 (m, 2 H, Ar-H), 6.69 (dd, J_1 = 17.6 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.31 (d, *J* = 11.2 Hz, 1 H, one proton of $=CH_2$), 4.99 (d, *J* = 17.6 Hz, 1 H, one proton of $=CH_2$), 2.26-2.05 (m, 2 H, CH_2), 1.24-0.94 (m, 8 H, CH_2 x 4), 0.81 (t, *J* = 6.8 Hz, 3

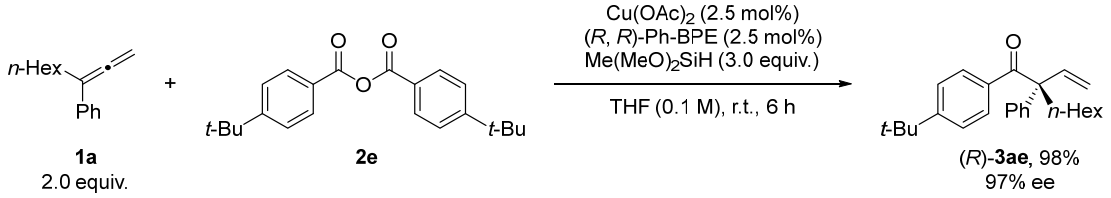
H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 199.0, 164.6 (d, *J* = 252.0 Hz), 142.5, 139.5, 132.7 (d, *J* = 8.7 Hz), 132.4 (d, *J* = 3.1 Hz), 128.8, 127.1, 126.9, 117.4, 114.9 (d, *J* = 21.3 Hz), 61.4, 39.0, 31.5, 29.8, 23.9, 22.5, 14.0; **^{19}F NMR** (376 MHz, $CDCl_3$) δ = -107.4; **IR** (neat): *v* = 3084, 3025, 2954, 2928, 2857, 1678, 1597, 1504, 1466, 1447, 1407, 1231, 1156 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 324 (M^+, 2.07), 123 (100); **HRMS** calcd. *m/z* for $C_{22}H_{25}FO$ (M^+): 324.1884; Found: 324.1888.

(14) Preparation of (*R*)-1-(4-chlorophenyl)-2-phenyl-2-vinyloctan-1-one [(*R*)-3ad] (Yy-5-053, Yy-4-020)



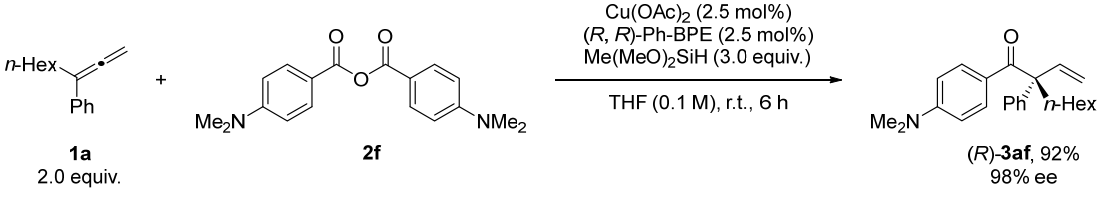
Following **Typical Procedure III**, the reaction of 4-chlorobenzoic anhydride **2d** (295.1 mg, 1.0 mmol), $Cu(OAc)_2$ (4.5 mg, 0.025 mmol), (*R*,*R*)-Ph-BPE (12.7 mg, 0.025 mmol), allene **1a** (400.6 mg, 2.0 mmol) in THF (8 mL), and dimethoxymethylsilane (318.6 mg, d = 0.861 g/mL, 0.37 mL, 3.0 mmol, in 2 mL THF) afforded (*R*)-**3ad** (276.2 mg, 81% yield) as a colorless oil (eluent: Petroleum ether (400 mL) to Petroleum ether/ EtOAc = 100/1 (~ 800 mL)): 95% ee (HPLC conditions: AD-H column, hexane/*i*-PrOH = 99/1, 1.0 mL/min, λ = 214 nm, t_R (major) = 6.3 min, t_R (minor) = 6.0 min; $[\alpha]^{30}_D$ = +96.7 (c = 1.19, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.48 (d, *J* = 8.8 Hz, 2 H, Ar-H), 7.38-7.29 (m, 2 H, Ar-H), 7.28-7.14 (m, 5 H, Ar-H), 6.68 (dd, J_1 = 17.6 Hz, J_2 = 11.2 Hz, 1 H, =CH), 5.31 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 4.99 (d, *J* = 17.6 Hz, 1 H, one proton of $=CH_2$), 2.25-2.05 (m, 2 H, CH_2), 1.25-0.92 (m, 8 H, CH_2 x 4), 0.81 (t, *J* = 6.8 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 199.3, 142.3, 139.4, 138.0, 134.5, 131.5, 128.9, 128.1, 127.1, 127.0, 117.6, 61.4, 39.0, 31.5, 29.8, 23.9, 22.5, 14.0; **IR** (neat): *v* = 3085, 3061, 3025, 2953, 2927, 2857, 1678, 1586, 1487, 1447, 1398, 1224, 1176, 1093, 1013 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 342 [M^+(^{37}Cl), 0.63)], 340 [M^+(^{35}Cl), 1.66)], 139 (100); **HRMS** calcd. *m/z* for $C_{22}H_{25}{}^{35}ClO$ (M^+): 340.1588; Found: 340.1590.

(15) Preparation of (*R*)-1-(4-(*tert*-butyl)phenyl)-2-phenyl-2-hexylbut-3-en-1-one [(*R*)-3ae] (Yy-5-054, Yy-4-023)



Following **Typical Procedure III**, the reaction of 4-(*tert*-butyl)benzoic anhydride **2e** (338.5 mg, 1.0 mmol), $Cu(OAc)_2$ (4.5 mg, 0.025 mmol), (*R*,*R*)-Ph-BPE (12.7 mg, 0.025 mmol), allene **1a** (400.6 mg, 2.0 mmol) in THF (8 mL), and dimethoxymethylsilane (318.6 mg, d = 0.861 g/mL, 0.37 mL, 3.0 mmol, in 2 mL THF) afforded (*R*)-**3ae** (353.9 mg, 98% yield) as a colorless oil (eluent: Petroleum ether (200 mL) to Petroleum ether/ EtOAc = 100/1 (~ 800 mL)): 97% ee (HPLC conditions: AD-H column, hexane/*i*-PrOH = 97/3, 1.0 mL/min, λ = 214 nm, t_R (major) = 4.9 min, t_R (minor) = 4.4 min; $[\alpha]^{30}_D$ = +95.5 (c = 1.09, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.47 (d, *J* = 8.8 Hz, 2 H, Ar-H), 7.37-7.28 (m, 2 H, Ar-H), 7.28-7.18 (m, 5 H, Ar-H), 6.70 (dd, J_1 = 17.6 Hz, J_2 = 11.2 Hz, 1 H, =CH), 5.28 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 4.99 (d, *J* = 17.6 Hz, 1 H, one proton of $=CH_2$), 2.28-2.08 (m, 2 H, CH_2), 1.24 (s, 9 H, CH_3 x 3), 1.20-0.95 (m, 8 H, CH_2 x 4), 0.80 (t, *J* = 6.8 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.1, 155.2, 142.9, 139.9, 133.6, 130.0, 128.7, 127.2, 126.7, 124.8, 117.0, 61.4, 38.5, 34.8, 31.5, 31.0, 29.8, 23.9, 22.5, 14.0; **IR** (neat): *v* = 3086, 3059, 3025, 2955, 2928, 2860, 1674, 1604, 1495, 1464, 1447, 1407, 1364, 1268, 1236, 1193, 1110 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 362 (M^+, 1.37), 161 (100); **HRMS** calcd. *m/z* for $C_{26}H_{34}O$ (M^+): 362.2604; Found: 362.2607.

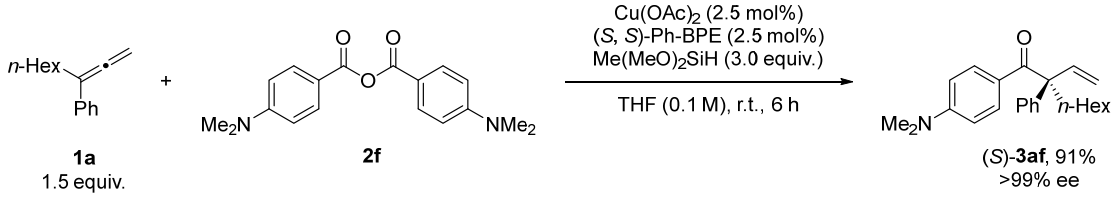
(16) Preparation of (*R*)-1-(4-(dimethylamino)phenyl)-2-phenyl-2-hexylbut-3-en-1-one [(*R*)-3af] (Yy-4-027)



Following **Typical Procedure III**, the reaction of 4-(dimethylamino)benzoic

anhydride **2f** (312.4 mg, 1.0 mmol), $Cu(OAc)_2$ (4.5 mg, 0.025 mmol), (*R*,*R*)-Ph-BPE (12.7 mg, 0.025 mmol), allene **1a** (400.6 mg, 2.0 mmol) in THF (8 mL), and dimethoxymethylsilane (318.6 mg, d = 0.861 g/mL, 0.37 mL, 3.0 mmol, in 2 mL THF) afforded (*R*)-**3af** (321.7 mg, 92% yield) as a white soild: m.p. 87.7-88.5 ºC (Petroleum ether/ CH_2Cl_2) (eluent: Petroleum ether (300 mL) to Petroleum ether/ EtOAc = 20/1 (~ 420 mL)): 98% ee (HPLC conditions: AD-H column, hexane/*i*-PrOH = 90/10, 1.0 mL/min, λ = 214 nm, t_R (major) = 8.5 min, t_R (minor) = 6.9 min; $[\alpha]^{24}_D$ = +143.3 (c = 1.12, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.52 (d, *J* = 9.2 Hz, 2 H, Ar-H), 7.35-7.27 (m, 2 H, Ar-H), 7.25-7.18 (m, 3 H, Ar-H), 6.73 (dd, J_1 = 17.4 Hz, J_2 = 11.0 Hz, 1 H, =CH), 6.42 (d, *J* = 9.2 Hz, 2 H, Ar-H), 5.25 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 4.97 (d, *J* = 17.6 Hz, 1 H, one proton of $=CH_2$), 2.95 (s, 6 H, NMe_2), 2.25-2.05 (m, 2 H, CH_2), 1.24-0.96 (m, 8 H, CH_2 x 4), 0.81 (t, *J* = 6.8 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 198.4, 152.2, 144.0, 140.6, 132.4, 128.4, 127.1, 126.3, 123.4, 116.2, 110.0, 60.9, 39.7, 39.0, 31.5, 29.9, 24.0, 22.5, 14.0; **IR** (neat): *v* = 2945, 2924, 2849, 1655, 1600, 1546, 1529, 1494, 1467, 1446, 1376, 1258, 1186, 1067, 1005 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 349 (M^+, 1.79), 148 (100); **Anal.** calcd. for $C_{24}H_{31}NO$: C 82.47, H 8.94; Found: C 82.37, H 8.86.

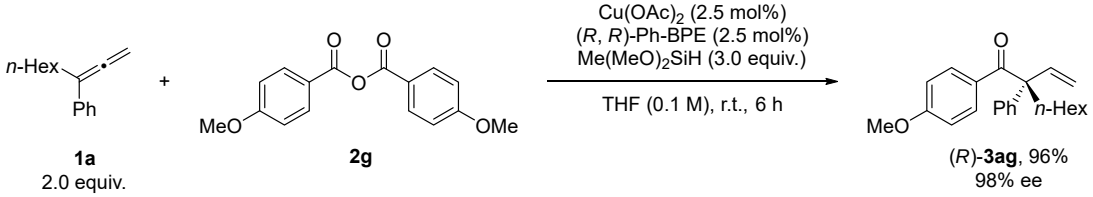
(17) Preparation of (*S*)-1-(4-(dimethylamino)phenyl)-2-phenyl-2-hexylbut-3-en-1-one [(*S*)-3af] (Yy-4-036)



Following **Typical Procedure III**, the reaction of 4-(dimethylamino)benzoic anhydride **2f** (156.3 mg, 0.5 mmol), $Cu(OAc)_2$ (2.3 mg, 0.0125 mmol), (*S*,*S*)-Ph-BPE (6.3 mg, 0.0125 mmol), allene **1a** (150.2 mg, 0.75 mmol) in THF (4 mL), and dimethoxymethylsilane (163.6 mg, d = 0.861 g/mL, 0.19 mL, 1.5 mmol, in 1 mL THF) afforded (*S*)-**3af** (158.5 mg, 91% yield) as a white soild: m.p. 88.0-88.7 ºC (Petroleum ether/ CH_2Cl_2) (eluent: Petroleum ether (300 mL) to Petroleum ether/ EtOAc = 20/1 (~ 420 mL)): >99% ee (HPLC conditions: AD-H column, hexane/*i*-PrOH = 90/10, 1.0

mL/min, λ = 214 nm, t_R (major) = 6.9 min; $[\alpha]^{24}_D$ = -141.4 (c = 1.14, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.56-7.49 (m, 2 H, Ar-H), 7.35-7.27 (m, 2 H, Ar-H), 7.25-7.18 (m, 3 H, Ar-H), 6.73 (dd, J_1 = 17.6 Hz, J_2 = 10.8 Hz, 1 H, =CH), 6.46-6.39 (m, 2 H, Ar-H), 5.25 (d, J = 11.2 Hz, 1 H, one proton of $=CH_2$), 4.97 (d, J = 17.6 Hz, 1 H, one proton of $=CH_2$), 2.95 (s, 6 H, NMe_2), 2.26-2.06 (m, 2 H, CH_2), 1.30-0.95 (m, 8 H, CH_2 x 4), 0.81 (t, J = 7.0 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 198.4, 152.2, 144.0, 140.6, 132.4, 128.4, 127.1, 126.3, 123.4, 116.2, 110.0, 60.9, 39.7, 39.0, 31.5, 29.9, 24.0, 22.5, 14.0; **IR** (neat): ν = 2944, 2925, 2856, 1655, 1597, 1546, 1528, 1494, 1467, 1446, 1375, 1256, 1172, 1067, 1005 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 349 (M^+, 1.21), 148 (100); **Anal.** calcd. for $C_{24}H_{31}NO$: C 82.47, H 8.94; Found: C 82.17, H 9.25.

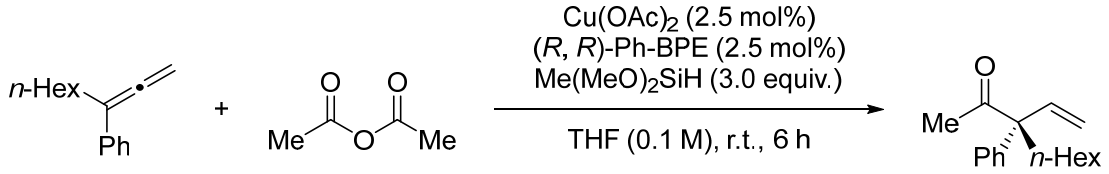
(18) Preparation of (*R*)-1-(4-methoxyphenyl)-2-phenyl-2-hexylbut-3-en-1-one [(*R*)-3ag] (Yy-4-040)



Following **Typical Procedure III**, the reaction of 4-methoxybenzoic anhydride **2g** (286.3 mg, 1.0 mmol), $Cu(OAc)_2$ (4.5 mg, 0.025 mmol), (*R*,*R*)-Ph-BPE (12.7 mg, 0.025 mmol), allene **1a** (400.6 mg, 2.0 mmol) in THF (8 mL), and dimethoxymethylsilane (318.6 mg, d = 0.861 g/mL, 0.37 mL, 3.0 mmol, in 2 mL THF) afforded (*R*)-**3ag** (321.5 mg, 96% yield) as a colorless oil (eluent: Petroleum ether (400 mL) to Petroleum ether/ EtOAc = 50/1 (~ 400 mL)): 98% ee (HPLC conditions: AD-H column, hexane/*i*-PrOH = 98/2, 1.0 mL/min, λ = 214 nm, t_R (major) = 9.1 min, t_R (minor) = 7.8 min; $[\alpha]^{24}_D$ = +108.5 (c = 0.99, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.57 (d, J = 9.2 Hz, 2 H, Ar-H), 7.33-7.25 (m, 2 H, Ar-H), 7.25-7.16 (m, 3 H, Ar-H), 6.80-6.60 (m, 3 H, =CH and Ar-H), 5.27 (d, J = 10.8 Hz, 1 H, one proton of $=CH_2$), 4.98 (d, J = 17.6 Hz, 1 H, one proton of $=CH_2$), 3.71 (s, 3 H, CH_3), 2.38-2.07 (m, 2 H, CH_2), 1.26-0.95 (m, 8 H, CH_2 x 4), 0.80 (t, J = 6.8 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 198.9, 162.1, 143.1, 140.0, 132.4, 128.7, 128.6, 127.0, 126.6,

116.8, 112.9, 61.2, 55.1, 39.0, 31.5, 29.8, 23.9, 22.5, 13.9; **IR** (neat): ν = 3083, 3060, 3024, 2928, 2856, 1669, 1598, 1575, 1508, 1459, 1446, 1417, 1307, 1258, 1238, 1169, 1117, 1030 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 336 (M^+, 1.02), 135 (100); **HRMS** calcd. *m/z* for $C_{23}H_{28}O_2$ (M^+): 336.2084; Found: 336.2086.

(19) Preparation of (*R*)-3-phenyl-3-hexylpent-4-en-2-one [(*R*)-3ah] (Yy-4-038)



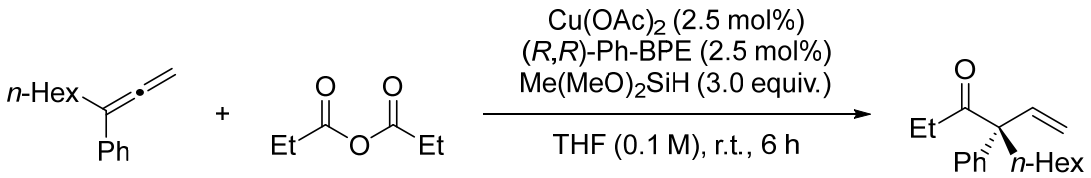
1a
2.0 equiv.

2h

(*R*)-**3ah**, 92%
91% ee

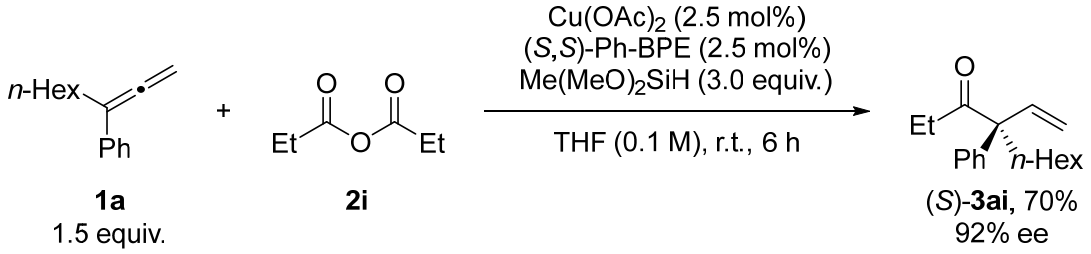
Following **Typical Procedure III**, the reaction of acetic anhydride **2h** (102.1 mg, 1.0 mmol), $Cu(OAc)_2$ (4.5 mg, 0.025 mmol), (*R*,*R*)-Ph-BPE (12.7 mg, 0.025 mmol), allene **1a** (400.6 mg, 2.0 mmol) in THF (8 mL), and dimethoxymethylsilane (318.6 mg, d = 0.861 g/mL, 0.37 mL, 3.0 mmol, in 2 mL THF) afforded (*R*)-**3ah** (225.3 mg, 92% yield) as a colorless oil (eluent: Petroleum ether (300 mL) to Petroleum ether/ EtOAc = 100/1 (~ 600 mL)): 91% ee (HPLC conditions: AS-H column, hexane/*i*-PrOH = 98/2, 1.0 mL/min, λ = 214 nm, t_R (major) = 3.9 min, t_R (minor) = 4.6 min; $[\alpha]^{24}_D$ = +10.7 (c = 1.14, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.34 (t, *J* = 7.4 Hz, 2 H, Ar-H), 7.26 (t, *J* = 7.2 Hz, 1 H, Ar-H), 7.19 (d, *J* = 7.6 Hz, 2 H, Ar-H), 6.48 (dd, J_1 = 17.6 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.35 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 4.99 (d, *J* = 17.6 Hz, 1 H, one proton of $=CH_2$), 2.14-1.97 (m, 2 H, CH_2), 1.94 (s, 3 H, CH_3), 1.35-0.94 (m, 8 H, CH_2 x 4), 0.84 (t, *J* = 6.6 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 208.1, 141.5, 138.9, 128.6, 127.4, 126.9, 117.2, 63.3, 35.9, 31.5, 29.9, 26.8, 24.1, 22.5, 14.0; **IR** (neat): ν = 3085, 3059, 3024, 2953, 2927, 2857, 1709, 1632, 1599, 1494, 1446, 1352, 1174, 1119, 1082, 1004 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 244 (M^+, 2.25), 117 (100); **HRMS** calcd. *m/z* for $C_{17}H_{24}O$ (M^+): 244.1822; Found: 244.1823.

(20) Preparation of (*R*)-4-phenyl-4-hexylhex-5-en-3-one [(*R*)-3ai] (Yy-4-096)



Following **Typical Procedure III**, the reaction of propionic anhydride **2i** (130.6 mg, 1.0 mmol), $Cu(OAc)_2$ (4.5 mg, 0.025 mmol), (*R*,*R*)-Ph-BPE (12.7 mg, 0.025 mmol), allene **1a** (400.6 mg, 2.0 mmol) in THF (8 mL), and dimethoxymethylsilane (318.6 mg, d = 0.861 g/mL, 0.37 mL, 3.0 mmol, in 2 mL THF) afforded (*R*)-**3ai** (220.1 mg, 85% yield) as a colorless oil (eluent: Petroleum ether (300 mL) to Petroleum ether/ EtOAc = 100/1 (~ 600 mL)): 93% ee (HPLC conditions: AS-H column, hexane/*i*-PrOH = 99.5/0.5, 1.0 mL/min, λ = 214 nm, t_R (major) = 3.8 min, t_R (minor) = 4.1 min; $[\alpha]^{23}_D$ = +14.2 (c = 0.95, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.33 (t, *J* = 7.6 Hz, 2 H, Ar-H), 7.25 (t, *J* = 7.2 Hz, 1 H, Ar-H), 7.18 (d, *J* = 7.6 Hz, 2 H, Ar-H), 6.50 (dd, J_1 = 17.8 Hz, J_2 = 11.0 Hz, 1 H, =CH), 5.33 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 4.97 (d, *J* = 18.0 Hz, 1 H, one proton of $=CH_2$), 2.34-1.96 (m, 4 H, CH_2 x 2), 1.32-0.97 (m, 8 H, CH_2 x 4), 0.94 (t, *J* = 7.4 Hz, 3 H, CH_3), 0.84 (t, *J* = 6.6 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 211.2, 141.7, 139.1, 128.5, 127.5, 126.8, 117.0, 63.1, 35.9, 32.2, 31.6, 29.9, 24.1, 22.6, 14.0, 8.8; **IR** (neat): *v* = 3084, 3062, 3023, 2929, 2857, 1709, 1494, 1459, 1446, 1409, 1376, 1339, 1102, 1006 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 258 (M^+, 2.70), 117 (100); **HRMS** calcd. *m/z* for $C_{18}H_{26}O$ (M^+): 258.1978; Found: 258.1984.

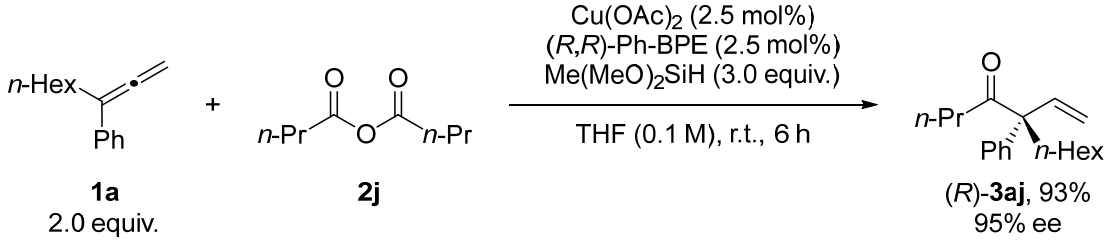
(21) Preparation of (*S*)-4-phenyl-4-hexylhex-5-en-3-one [(*S*)-3ai] (Yy-4-100)



Following **Typical Procedure III**, the reaction of propionic anhydride **2i** (64.5 mg, 0.5 mmol), $Cu(OAc)_2$ (2.3 mg, 0.0127 mmol), (*S*,*S*)-Ph-BPE (6.3 mg, 0.0124 mmol),

allene **1a** (150.1 mg, 0.75 mmol) in THF (4 mL), and dimethoxymethylsilane (163.6 mg, d = 0.861 g/mL, 0.19 mL, 1.5 mmol, in 1 mL THF) afforded (*S*)-**3ai** (89.8 mg, 70% yield) as a colorless oil (eluent: Petroleum ether (300 mL) to Petroleum ether/ EtOAc = 100/1 (~ 500 mL)): 92% ee (HPLC conditions: AS-H column, hexane/*i*-PrOH = 99.5/0.5, 1.0 mL/min, λ = 214 nm, t_R (major) = 4.1 min, t_R (minor) = 3.8 min; $[\alpha]^{23}_D$ = -13.1 (c = 0.51, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.34 (t, *J* = 7.6 Hz, 2 H, Ar-H), 7.25 (t, *J* = 7.2 Hz, 1 H, Ar-H), 7.18 (d, *J* = 8.0 Hz, 2 H, Ar-H), 6.49 (dd, J_1 = 18.0 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.33 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 4.97 (d, *J* = 18.0 Hz, 1 H, one proton of $=CH_2$), 2.34-1.98 (m, 4 H, CH_2 x 2), 1.32-0.96 (m, 8 H, CH_2 x 4), 0.94 (t, *J* = 7.4 Hz, 3 H, CH_3), 0.84 (t, *J* = 6.8 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 211.3, 141.7, 139.1, 128.5, 127.5, 126.8, 117.1, 63.1, 35.9, 32.2, 31.6, 29.9, 24.2, 22.6, 14.0, 8.8; **IR** (neat): *v* = 3084, 3062, 3023, 2928, 2857, 1709, 1494, 1459, 1446, 1408, 1376, 1339, 1103, 1006 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 258 (M^+, 3.15), 117 (100); **HRMS** calcd. *m/z* for $C_{18}H_{26}O$ (M^+): 258.1978; Found: 258.1981.

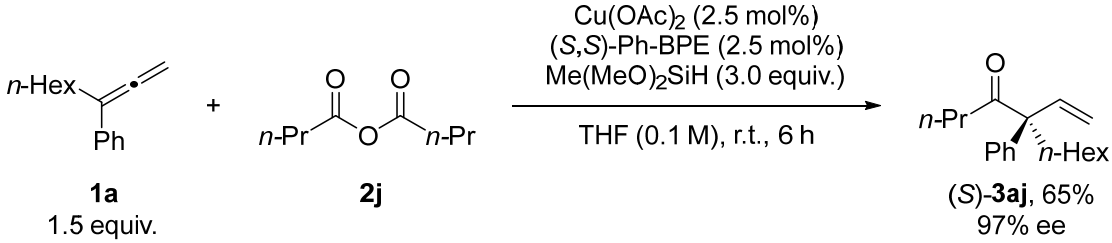
(22) Preparation of (*R*)-5-phenyl-5-hexylhept-6-en-4-one [(*R*)-3aj] (Yy-4-098)



Following **Typical Procedure III**, the reaction of butyric anhydride **2j** (158.9 mg, 1.0 mmol), $Cu(OAc)_2$ (4.5 mg, 0.025 mmol), (*R*,*R*)-Ph-BPE (12.7 mg, 0.025 mmol), allene **1a** (400.6 mg, 2.0 mmol) in THF (8 mL), and dimethoxymethylsilane (318.6 mg, d = 0.861 g/mL, 0.37 mL, 3.0 mmol, in 2 mL THF) afforded (*R*)-**3aj** (253.9 mg, 93% yield) as a colorless oil (eluent: Petroleum ether (300 mL) to Petroleum ether/ EtOAc = 100/1 (~ 600 mL)): 95% ee (HPLC conditions: AS-H column, hexane, 0.3 mL/min, λ = 214 nm, t_R (major) = 19.0 min, t_R (minor) = 21.9 min; $[\alpha]^{23}_D$ = +16.2 (c = 1.17, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.34 (t, *J* = 7.6 Hz, 2 H, Ar-H), 7.30-7.22 (m, 1 H, Ar-H), 7.22-7.15 (m, 2 H, Ar-H), 6.49 (dd, J_1 = 17.6 Hz, J_2 = 10.8

Hz, 1 H, =CH), 5.34 (d, J = 10.8 Hz, 1 H, one proton of =CH_2), 4.99 (d, J = 18.0 Hz, 1 H, one proton of =CH_2), 2.30-1.96 (m, 4 H, CH_2 x 2), 1.55-1.40 (m, 2 H, CH_2), 1.30-0.90 (m, 8 H, CH_2 x 4), 0.84 (t, J = 6.8 Hz, 3 H, CH_3), 0.76 (t, J = 7.4 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 210.3, 141.6, 139.0, 128.5, 127.6, 126.8, 117.2, 63.1, 41.0, 35.8, 31.6, 29.9, 24.1, 22.6, 17.9, 14.0, 13.7; **IR** (neat): v = 3084, 3059, 3022, 2956, 2928, 2871, 1708, 1494, 1465, 1446, 1408, 1378, 1354, 1134, 1116, 1059, 1004 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 272 (M^+, 3.00), 117 (100); **HRMS** calcd. *m/z* for $C_{19}H_{28}O$ (M^+): 272.2135; Found: 272.2139.

(23) Preparation of (*S*)-5-phenyl-5-hexylhept-6-en-4-one [(*S*)-3aj] (Yy-4-101)



1a
1.5 equiv.

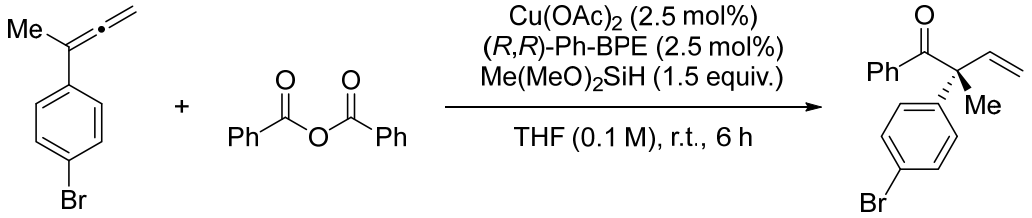
2j

(*S*)-**3aj**, 65%
97% ee

Following **Typical Procedure III**, the reaction of butyric anhydride **2j** (78.8 mg, 0.5 mmol), $Cu(OAc)_2$ (2.3 mg, 0.0127 mmol), (*S*,*S*)-Ph-BPE (6.3 mg, 0.0124 mmol), allene **1a** (150.2 mg, 0.75 mmol) in THF (4 mL), and dimethoxymethylsilane (163.6 mg, d = 0.861 g/mL, 0.19 mL, 1.5 mmol, in 1 mL THF) afforded (*S*)-**3aj** (88.2 mg, 65% yield) as a colorless oil (eluent: Petroleum ether (300 mL) to Petroleum ether/ EtOAc = 100/1 (~ 500 mL)): 97% ee (HPLC conditions: AS-H column, hexane, 1.0 mL/min, λ = 214 nm, t_R (major) = 21.0 min, t_R (minor) = 19.1 min; $[\alpha]^{23}_D$ = -15.4 (c = 0.51, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.34 (t, J = 7.4 Hz, 2 H, Ar-H), 7.30-7.21 (m, 1 H, Ar-H), 7.21-7.14 (m, 2 H, Ar-H), 6.49 (dd, J_1 = 17.6 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.34 (d, J = 10.8 Hz, 1 H, one proton of =CH_2), 4.99 (d, J = 18.0 Hz, 1 H, one proton of =CH_2), 2.30-1.97 (m, 4 H, CH_2 x 2), 1.55-1.40 (m, 2 H, CH_2), 1.30-0.90 (m, 8 H, CH_2 x 4), 0.84 (t, J = 6.8 Hz, 3 H, CH_3), 0.76 (t, J = 7.4 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 210.3, 141.6, 139.0, 128.5, 127.6, 126.8, 117.2, 63.1, 41.0, 35.8, 31.6, 29.9, 24.1, 22.6, 17.9, 14.0, 13.7; **IR** (neat): v = 3084, 3063, 3024, 2956, 2928, 2871, 1708, 1494, 1465, 1446, 1408, ,1378, 1354, 1278,

1116, 1059, 1003 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 272 (M^+, 3.32), 117 (100); **HRMS** calcd. *m/z* for $C_{19}H_{28}O$ (M^+): 272.2135; Found: 272.2135.

(24) Preparation of (*R*)-2-(4-bromophenyl)-2-methyl-1-phenylbut-3-en-1-one [(*R*)-3ka] on gram scale (Yy-4-102)



1k
15 mmol

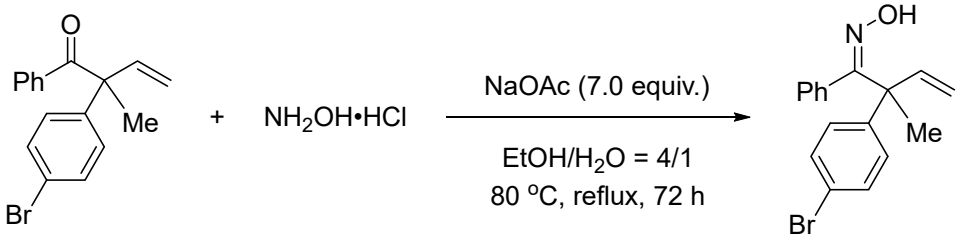
2a
10 mmol

(*R*)-3ka
79%, 96% ee
2.4974 g

Following **Typical Procedure III**, the reaction of benzoic anhydride **2a** (2.2625 g, 10.0 mmol), $Cu(OAc)_2$ (45.4 mg, 0.25 mmol), (*R*,*R*)-Ph-BPE (126.7 mg, 0.25 mmol), allene **1k** (3.1364 g, 15.0 mmol) in THF (80 mL) and dimethoxymethylsilane (1.5929 g, d = 0.861 g/mL, 1.85 mL, 15.0 mmol, in 20 mL THF) afforded (*R*)-**3ka** (2.4974 g, 79% yield) as a colorless oil (eluent: Petroleum ether (600 mL) to Petroleum ether/ EtOAc = 100/1 (~ 2000 mL)): 96% ee (HPLC conditions: AD-H column, hexane/*i*-PrOH = 99/1, 1.0 mL/min, λ = 214 nm, t_R (major) = 7.8 min, t_R (minor) = 9.5 min; **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.46 (d, *J* = 7.2 Hz, 2 H, Ar-H), 7.39 (d, *J* = 8.4 Hz, 2 H, Ar-H), 7.32 (t, *J* = 7.2 Hz, 1 H, Ar-H), 7.18 (t, *J* = 7.6 Hz, 2 H, Ar-H), 7.07 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.50 (dd, J_1 = 17.2 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.24 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 5.09 (d, *J* = 17.6 Hz, 1 H, one proton of $=CH_2$), 1.57 (s, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.2, 143.6, 140.4, 135.8, 132.10, 132.06, 130.0, 128.2, 128.1, 121.0, 117.0, 58.1, 26.0.

5. Synthetic applications:

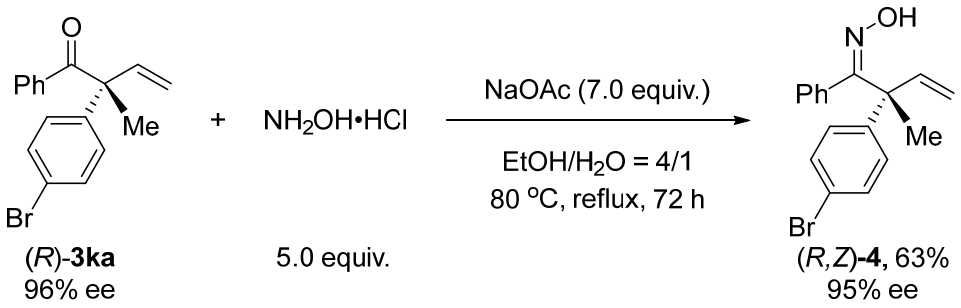
(1) Synthesis of (*Z*)-2-(4-bromophenyl)-2-methyl-1-phenylbut-3-en-1-one oxime [(*Z*)-4] (Yy-5-007)[9]



3ka 5.0 equiv. (*Z*)-**4**, 60%

To a Schlenk tube were added $NH_2OH{\cdot}HCl$ (173.7 mg, 2.5 mmol)/H_2O (1 mL), NaOAc (287.3 mg, 3.50 mmol)/EtOH (1 mL), and **3ka** (157.9 mg, 0.5 mmol)/EtOH (3 mL) sequentially under argon. The resulting mixture was allowed to reflux at 80 °C for 72 h and then cooled to room temperature and diluted with 5 mL of CH_2Cl_2 and 5 mL of H_2O. After extraction with CH_2Cl_2 (10 mL x 3), the organic layer was combined and concentrated *in vacuo*, the residue was purified by column chromatography on silica gel to afford (*Z*)-**4** (105.9 mg, 94% purity, 60% yield) as a white soild: m.p. 130.2-130.9 °C (Petroleum ether/ CH_2Cl_2) (eluent: petroleum ether/ethyl acetate = 100/1 (~ 200 mL) to 10/1 (~ 330 mL)); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 8.18 (s, 1 H, N-OH), 7.47 (d, *J* = 8.4 Hz, 2 H, Ar-H), 7.30-7.16 (m, 5 H, Ar-H), 6.81(d, *J* = 6.8 Hz, 2 H, Ar-H), 6.26 (dd, J_1 = 17.4 Hz, J_2 = 10.6 Hz, 1 H, =CH), 5.19 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 4.92 (d, *J* = 17.6 Hz, 1 H, one proton of $=CH_2$), 1.51 (s, 3 H , CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 163.1, 142.7, 142.1, 132.7, 131.4, 129.5, 128.4, 127.92, 127.91, 121.0, 114.6, 51.3, 24.1; **IR** (neat): *v* = 3271, 1636, 1489, 1443, 1410, 1395, 1371, 1267, 1080, 1007 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 331 [M(^{81}Br)$^+$, 17.98], 329 [M(^{79}Br)$^+$, 17.32], 130 (100); **Anal.** calcd. for $C_{17}H_{16}BrNO$ (M^+): C 61.83, H 4.88; Found: C 61.81, H 4.98.

(2) Synthesis of (*R,Z*)-2-(4-bromophenyl)-2-methyl-1-phenylbut-3-en-1-one oxime [(*R,Z*)-4] (Yy-5-008)[9]



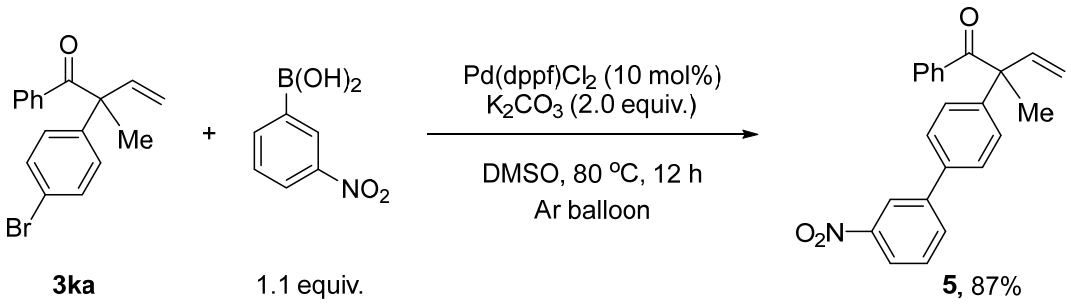
(*R*)-**3ka** 96% ee

5.0 equiv.

(*R,Z*)-**4**, 63% 95% ee

To a Schlenk tube were added $NH_2OH{\cdot}HCl$ (69.5 mg, 1.0 mmol)/H_2O (0.4 mL), NaOAc (114.8 mg, 1.4 mmol), and (*R*)-**3ka** (63.0 mg, 0.2 mmol)/EtOH (1.6 mL) sequentially under argon. The resulting mixture was allowed to reflux at 80 °C for 72 h and then cooled to room temperature and diluted with 5 mL of CH_2Cl_2 and 5 mL of H_2O. After extraction with CH_2Cl_2 (5 mL x 3), the organic layer was combined and concentrated *in vacuo*, the residue was purified by column chromatography on silica gel to afford (*R,Z*)-**4** (42.8 mg, 97% purity, 63% yield) as a white soild: m.p. 125.0-125.8 °C (Petroleum ether/ CH_2Cl_2) (eluent: petroleum ether/ethyl acetate = 100/1 (~ 200 mL) to 10/1 (~ 220 mL)): 95% ee (HPLC conditions: AD-H column, hexane/*i*-PrOH = 97/3, 1.0 mL/min, λ = 214 nm, t_R (major) = 22.1 min, t_R (minor) = 21.0 min; $[\alpha]^{25}_D$ = -14.0 (c = 1.04, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 8.05 (s, 1 H, N-OH), 7.47 (d, *J* = 8.4 Hz, 2 H, Ar-H), 7.30-7.20 (m, 5 H, Ar-H), 6.81 (m, 2 H, Ar-H), 6.27 (dd, J_1 = 17.6 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.19 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 4.93 (d, *J* = 17.6 Hz, 1 H, one proton of $=CH_2$), 1.51 (s, 3 H , CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 163.1, 142.8, 142.1, 132.7, 131.4, 129.5, 128.4, 127.93, 127.92, 121.0, 114.6, 51.3, 24.2; **IR** (neat): *v* = 3229, 1634, 1489, 1464, 1445, 1412, 1395, 1263, 1078, 1024, 1007 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 331 [M(^{81}Br)$^+$, 16.25], 329 [M(^{79}Br)$^+$, 16.21], 130 (100); **Anal.** calcd. for $C_{17}H_{16}BrNO$ (M^+): C 61.83, H 4.88; Found: C 61.98, H 5.15.

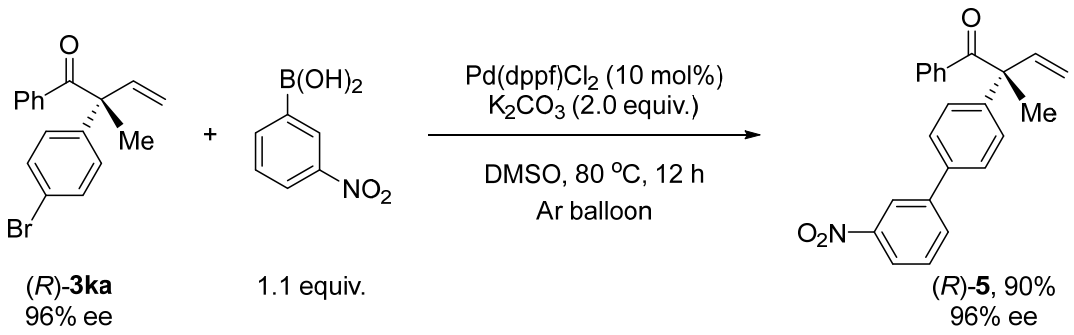
(3) Synthesis of 2-methyl-2-(3'-nitro-[1,1'-biphenyl]-4-yl)-1-phenylbut-3-en-1-one (5) (Yy-4-110)[10]



3ka 1.1 equiv. **5**, 87%

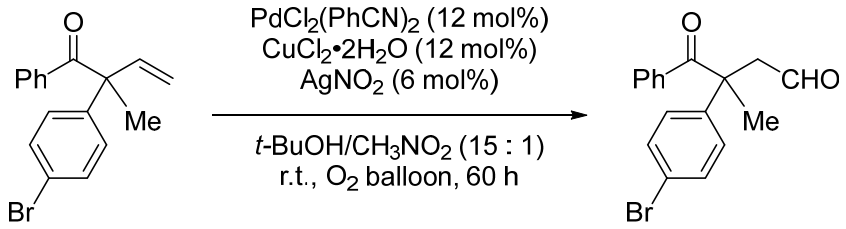
To a flame-dried Schlenk tube were added $Pd(dppf)Cl_2$ (14.6 mg, 0.02 mmol), (3-nitrophenyl)boronic acid (36.7 mg, 0.22 mmol), K_2CO_3 (55.3 mg, 0.4 mmol), and **3ka** (63.0 mg, 0.2 mmol) sequentially. After addition of all these chemicals, the tube was degassed and refilled with argon for three times. Then DMSO (2 mL) was added under argon. The resulting mixture was stirred at 80 °C with a balloon of argon for 12 h, diluted with 2 mL of ethyl acetate, cooled to room temperature, and quenched with 10 mL of H_2O. After extraction with ethyl acetate (10 mL x 3) and washing with a saturated solution of NaCl (10 mL x 3), the organic layer was dried over anhydrous Na_2SO_4. After filtration and concentration *in vacuo*, the residue was purified by column chromatography on silica gel to afford **5** (61.9 mg, 87% yield) as a yellow oil (eluent: petroleum ether/ethyl acetate = 50/1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 8.44 (s, 1 H, Ar-H), 8.18 (d, *J* = 8.0 Hz, 1 H, Ar-H), 7.91 (d, *J* = 7.6 Hz, 1 H, Ar-H), 7.70-7.53 (m, 5 H, Ar-H), 7.47-7.34 (m, 3 H, Ar-H), 7.26 (t, *J* = 7.6 Hz, 2 H, Ar-H), 6.67 (dd, J_1 = 17.4 Hz, J_2 = 10.6 Hz, 1 H, =CH), 5.35 (d, *J* = 10.58 Hz, 1 H, one proton of $=CH_2$), 5.21 (d, *J* = 17.6 Hz, 1 H, one proton of $=CH_2$), 1.72 (s, 3 H , CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.4, 148.7, 145.0, 142.0, 140.6, 137.1, 135.9, 132.8, 132.0, 130.0, 129.7, 128.0, 127.7, 127.2, 122.0, 121.7, 116.9, 58.2, 26.0; **IR** (neat): *v* = 3064, 2968, 2935, 2878, 1676, 1596, 1487, 1445, 1397, 1344, 1303, 1232, 1182, 1151, 1106, 1088, 1075, 1005 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 357 (M^+, 0.19), 252 (M^+-PhCO, 2.88), 105 (100); **HRMS** Calcd *m/z* for $C_{23}H_{19}NO_3$: 357.1359; Found: 357.1359.

(4) Synthesis of (*R*)-2-methyl-2-(3'-nitro-[1,1'-biphenyl]-4-yl)-1-phenylbut-3-en-1-one [(*R*)-5] (Yy-4-103)[10]



To a flame-dried Schlenk tube were added $Pd(dppf)Cl_2$ (14.6 mg, 0.02 mmol), (3-nitrophenyl)boronic acid (36.7 mg, 0.22 mmol), K_2CO_3 (55.4 mg, 0.4 mmol), and (*R*)-**3ka** (63.0 mg, 0.2 mmol) sequentially. After addition of all these chemicals, the tube was degassed and refilled with argon for three times. Then DMSO (2 mL) was added under argon. The resulting mixture was stirred at 80 °C with a balloon of argon for 12 h, diluted with 2 mL of ethyl acetate, cooled to room temperature, and quenched with 10 mL of H_2O. After extraction with ethyl acetate (10 mL x 3) and washing with a saturated solution of NaCl (10 mL x 3), the organic layer was dried over anhydrous Na_2SO_4. After filtration and concentration *in vacuo*, the residue was purified by column chromatography on silica gel to afford (*R*)-**5** (64.6 mg, 90% yield) as a yellow oil (eluent: petroleum ether/ethyl acetate = 50/1): 96% ee (HPLC conditions: AD-H column, hexane/*i*-PrOH = 85/15, 0.5 mL/min, λ = 214 nm, t_R (major) = 17.7 min, t_R (minor) = 16.9 min; $[\alpha]^{27}_D$ = +77.7 (c = 1.08, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 8.50 (s, 1 H, Ar-H), 8.19 (d, *J* = 8.0 Hz, 1 H, Ar-H), 7.91 (d, *J* = 7.6 Hz, 1 H, Ar-H), 7.70-7.55 (m, 5 H, Ar-H), 7.46-7.35 (m, 3 H, Ar-H), 7.26 (t, *J* = 7.6 Hz, 2 H, Ar-H), 6.66 (dd, J_1 = 17.6 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.35 (d, *J* = 10.58 Hz, 1 H, one proton of $=CH_2$), 5.21 (d, *J* = 17.6 Hz, 1 H, one proton of $=CH_2$), 1.72 (s, 3 H , CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 200.4, 148.7, 145.0, 142.1, 140.6, 137.2, 135.9, 132.8, 132.0, 130.0, 129.7, 128.0, 127.7, 127.2, 122.1, 121.8, 116.9, 58.3, 26.0; **IR** (neat): *v* = 3065, 2970, 2936, 2879, 1676, 1594, 1488, 1455, 1446, 1397, 1384, 1232, 1182, 1152, 1106, 1089, 1075, 1005 cm^{-1}; **MS** (70 eV, EI) *m/z* (%): 357 (M^+, 0.57), 252 (M^+-PhCO, 3.24), 105 (100); **HRMS** Calcd *m/z* for $C_{23}H_{19}NO_3$: 357.1359; Found: 357.1364.

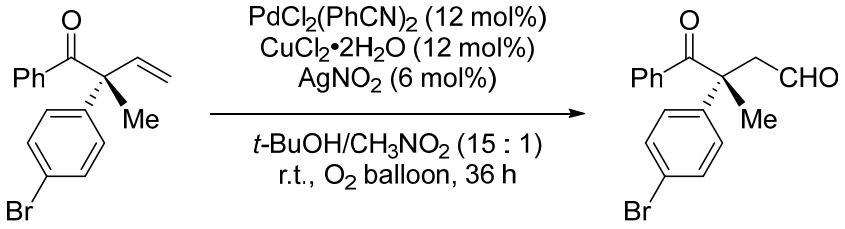
(5) Synthesis of 3-(4-bromophenyl)-3-methyl-4-oxo-4-phenylbutanal (6) (Yy-4-150)[11]



3ka **6**, 75%

To a Schlenk tube were added $Pd(PhCN)_2Cl_2$ (9.2 mg, 0.024 mmol), $CuCl_2•2H_2O$ (3.6 mg, 0.024 mmol) and $AgNO_2$ (1.8 mg, 0.012 mmol). After the addition of CH_3NO_2 and *t*-BuOH, the mixture was stirred at room temperature and sparged with O_2 (balloon) for 3 minutes. Then **3ka** (63.0 mg, 0.2 mmol) was added and the resulting mixture was allowed to stirred at room temperature and sparged with O_2 (balloon) for another 3 minutes. The mixture was then stirred at room temperature for 60 h with a balloon of O_2. After that, the reaction mixture was diluted with water (4 mL) and extracted with dichloromethane (5 mL x 3). The organic phase was dried over anhydrous Na_2SO_4, then filtered and concentrated in *vacuo*. The residue was purified by column chromatography on silica gel to afford **6** (49.6 mg, 75% yield) as a yellow oil (eluent: petroleum ether/ethyl acetate = 15/1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 9.69 (s, 1 H, CHO), 7.52 (d, *J* = 8.4 Hz, 2 H, Ar-H), 7.49-7.36 (m, 3 H, Ar-H), 7.31-7.14 (m, 4 H, Ar-H), 3.08 (d, *J* = 16.0 Hz, 1 H, one proton of CH_2), 2.79 (d, *J* = 16.0 Hz, 1 H, one proton of CH_2), 1.82 (s, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 201.6, 200.3, 141.4, 135.3, 132.5, 132.3, 129.6, 128.2, 127.8, 121.7, 54.5, 53.2, 23.4; **IR** (neat): *v* = 3061, 2987, 2941, 2838, 2739, 1718, 1672, 1596, 1578, 1488, 1446, 1397, 1258, 1236, 1182, 1147, 1083, 1008 cm^{-1}; **MS** (ESI) *m/z* (%): 331 $[M(^{79}Br)+H]^+$; **HRMS** Calcd *m/z* for $C_{17}H_{16}{}^{79}BrO_2(M+H)^+$: 331.0328; Found: 331.0313.

(6) Synthesis of (*R*)-3-(4-bromophenyl)-3-methyl-4-oxo-4-phenylbutanal [(*R*)-6] (Yy-4-146)[11]

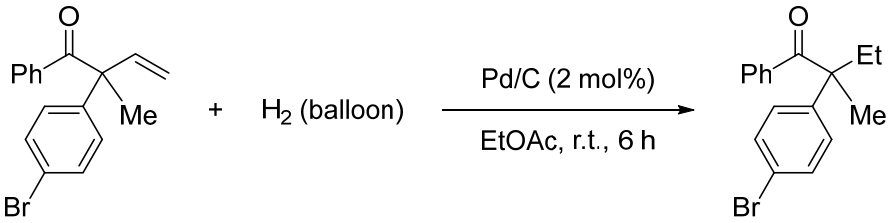


(*R*)-**3ka**
96% ee

(*R*)-**6**, 63%, 25% NMR recovery
93% ee

To a Schlenk tube were added $Pd(PhCN)_2Cl_2$ (9.2 mg, 0.024 mmol), $CuCl_2 \cdot 2H_2O$ (3.6 mg, 0.024 mmol) and $AgNO_2$ (1.8 mg, 0.012 mmol). After the addition of CH_3NO_2 and *t*-BuOH, the resulting mixture was stirred at room temperature and sparged with O_2 (balloon) for 3 minutes. Then (*R*)-**3ka** (63.0 mg, 0.2 mmol) was added and the mixture was allowed to stirred at room temperature and sparged with O_2 (balloon) for another 3 minutes. The mixture was then stirred at room temperature for 36 h with a balloon of O_2. The resulting reaction mixture was diluted with water (4 mL) and extracted with dichloromethane (5 mL x 3). The organic phase was dried over anhydrous Na_2SO_4, then filtered and concentrated in *vacuo*. The residue was purified by column chromatography on silica gel to afford (*R*)-**6** (41.8 mg, 63% yield) as a yellow oil (eluent: petroleum ether/ethyl acetate = 15/1): 93% ee (HPLC conditions: AD-H column, hexane/*i*-PrOH = 95/5, 1.0 mL/min, λ = 214 nm, t_R (major) = 12.9 min, t_R (minor) = 12.2 min; $[\alpha]^{20}_D$ = -149.7 (c = 0.76, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 9.69 (t, *J* = 1.8 Hz, 1 H, CHO), 7.53 (d, *J* = 8.8 Hz, 2 H, Ar-H), 7.48-7.38 (m, 3 H, Ar-H), 7.30-7.20 (m, 4 H, Ar-H), 3.08 (dd, J_1 = 16.2 Hz, J_2 = 1.8 Hz, 1 H, one proton of CH_2), 2.79 (dd, J_1 = 16.2 Hz, J_2 = 1.8 Hz, 1 H, one proton of CH_2), 1.82 (s, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 201.5, 200.3, 141.4, 135.3, 132.5, 132.3, 129.6, 128.2, 127.8, 121.7, 54.4, 53.2, 23.4; **IR** (neat): *v* = 3061, 2990, 2934, 2839, 2739, 1717, 1672, 1596, 1578, 1488, 1459, 1446, 1397, 1258, 1236, 1182, 1147, 1083, 1036, 1008 cm^{-1}; **MS** (ESI) *m/z* (%): 333 $[M(^{81}Br)+H]^+$, 331 $[M(^{79}Br)+H]^+$; **HRMS** Calcd *m/z* for $C_{17}H_{16}{}^{79}BrO_2(M+H)^+$: 331.0328; Found: 331.0312.

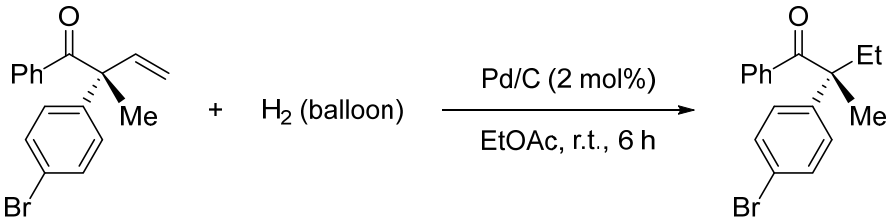
(7) Synthesis of 2-(4-bromophenyl)-2-methyl-1-phenylbutan-1-one (7) via Pd/C reduction of 3ka (Yy-4-107)



3ka **7**, 97%

To a Schlenk tube fulfilled with argon were added Pd/C (8.5 mg, 0.004 mmol) and **3ka** (63.0 mg, 0.2 mmol) sequentially. After addition of these chemicals, the tube was degassed and refilled with H_2 by a balloon of H_2. Then EtOAc (2 mL) was added and the resulting mixture was stirred at room temperature for 6 h. The H_2 balloon was removed and the resulting mixture was filtered through a short column of silica gel (2 cm), eluted with ethyl acetate (5 mL x 3), and concentrated. The residue was purified by column chromatography on silica gel to afford **7** (61.6 mg, 97% yield) as a colorless oil (eluent: petroleum ether/ethyl acetate = 100/1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.54-7.42 (m, 4 H, Ar-H), 7.40-7.34 (m, 1 H, Ar-H), 7.26-7.20 (m, 2 H, Ar-H), 7.19-7.10 (m, 2 H, Ar-H), 2.40-1.96 (m, 2 H, CH_2), 1.53 (s, 3 H, CH_3), 0.74 (t, *J* = 7.4 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 203.1, 143.5, 136.6, 132.0, 131.7, 129.3, 128.03, 127.99, 120.8, 54.6, 32.1, 23.6, 8.5; **IR** (neat): *v* = 3065, 2970, 2937, 2879, 1676, 1596, 1488, 1455, 1446, 1397, 1384, 1232, 1182, 1152, 1107, 1089, 1075, 1006 cm^{-1}; **MS** (ESI) *m/z* (%): 319 $[M(^{81}Br)+H]^+$, 317 $[M(^{79}Br)+H]^+$; **HRMS** Calcd *m/z* for $C_{17}H_{18}{}^{79}BrO(M+H)^+$: 317.0536; Found: 317.0539.

(8) Synthesis of (*R*)-2-(4-bromophenyl)-2-methyl-1-phenylbutan-1-one [(*R*)-7] via Pd/C reduction of (*R*)-3ka (Yy-4-106)



(*R*)-**3ka** 96% ee (*R*)-**7**, 98% 96% ee

To a Schlenk tube fulfilled with argon were added Pd/C (8.5 mg, 0.004 mmol) and (*R*)-**3ka** (63.2 mg, 0.2 mmol) sequentially. After addition of these chemicals, the

tube was degassed and refilled with H_2 by a balloon of H_2. Then EtOAc (2 mL) was added and the resulting mixture was stirred at room temperature for 6 h. After that, the H_2 balloon was removed and the resulting mixture was filtered through a short column of silica gel (2 cm) eluted with ethyl acetate (5 mL x 3), and concentrated. The residue was purified by column chromatography on silica gel to afford (*R*)-**7** (62.2 mg, 98% yield) as a colorless oil (eluent: petroleum ether/ethyl acetate = 100/1): 96% ee (HPLC conditions: AD-H column, hexane/*i*-PrOH = 99/1, 0.7 mL/min, λ = 214 nm, t_R (major) = 15.7 min, t_R (minor) = 14.0 min; $[\alpha]^{27}_D$ = -40.0 (c = 1.10, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.56-7.42 (m, 4 H, Ar-H), 7.37 (t, *J* = 7.4 Hz, 1 H, Ar-H), 7.26-7.19 (m, 2 H, Ar-H), 7.17 (d, *J* = 8.4 Hz, 2 H, Ar-H), 2.40-1.95 (m, 2 H, CH_2), 1.53 (s, 3 H, CH_3), 0.74 (t, *J* = 7.4 Hz, 3 H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 203.1, 143.5, 136.6, 132.0, 131.7, 129.3, 128.02, 127.99, 120.7, 54.6, 32.1, 23.6, 8.5; **IR** (neat): *v* = 3065, 2970, 2936, 2879, 1676, 1596, 1488, 1455, 1446, 1397, 1384, 1232, 1152, 1107, 1089, 1075, 1006 cm^{-1}; **MS** (ESI) *m/z* (%): 319 $[M(^{81}Br)+H]^+$, 317 $[M(^{79}Br)+H]^+$; **HRMS** Calcd *m/z* for $C_{17}H_{18}{}^{79}BrO(M+H)^+$: 317.0536; Found: 317.0539.

Computational Method.

All calculations were performed with the Gaussian 09 program.[12] Geometries have been fully optimized with the density functional theory of B3LYP method.[13] The standard 6-31G(d)[14] basis set was used for carbon, hydrogen and oxygen atoms and LANL2DZ basis set[15] with effective core potential (ECP) for copper. Harmonic vibration frequency calculations were carried out for all the stationary points to confirm each structure being either a minimum (no imaginary frequency) or a transition structure (one imaginary frequency). Intrinsic reaction coordinate (IRC)[16] calculations were performed to confirm the connection of the transition structures with their corresponding reactants and products. The single point energies and solvent effects in THF (ε = 7.43) were computed with M06/SDD[17]-6-311+G(d,p) basis sets by using SMD[18] solvation model. The reported relative energies are the Gibbs free energies (ΔG_{sol}) in THF unless otherwise specified.

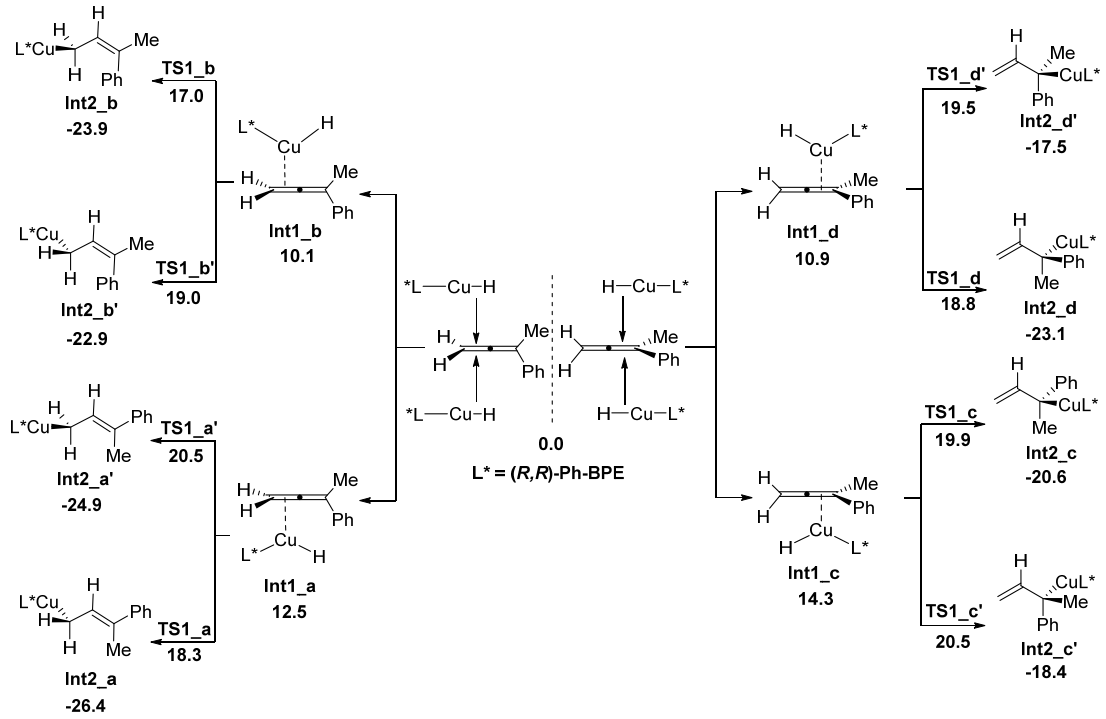


Figure S1 Eight transition structures associated with the hydrocupration step. All energies are in kcal/mol with respect of CuH and allene (**1d**).

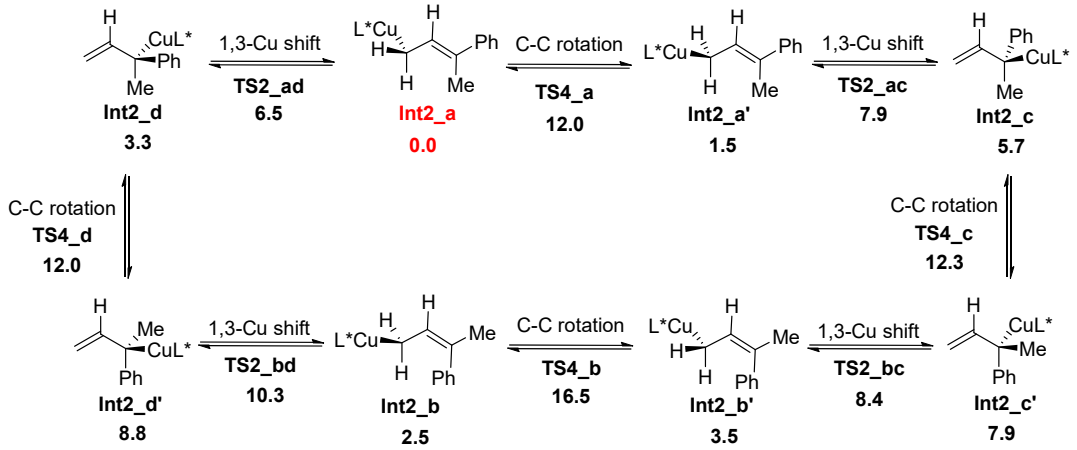


Figure S2 Facial isomerization of **Int2_a-d**. All energies are given in kcal/mol with respect of **Int2_a**.

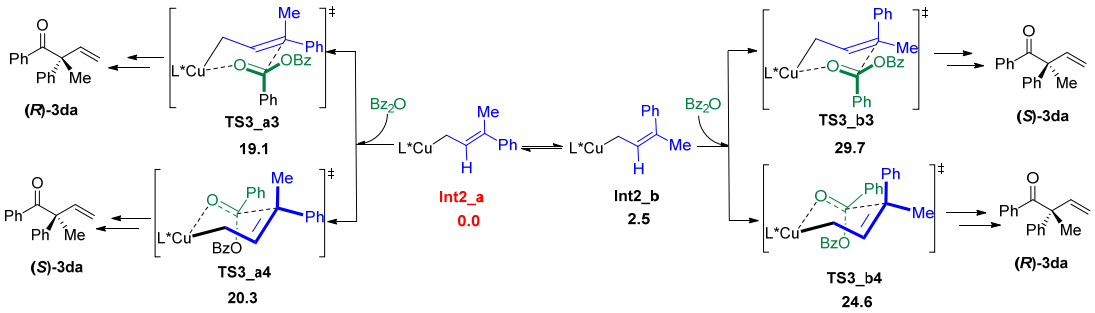


Figure S3 Less favored transition states with *Si*-face **2a** participation. All energies are given in kcal/mol with respect of **Int2_a**.

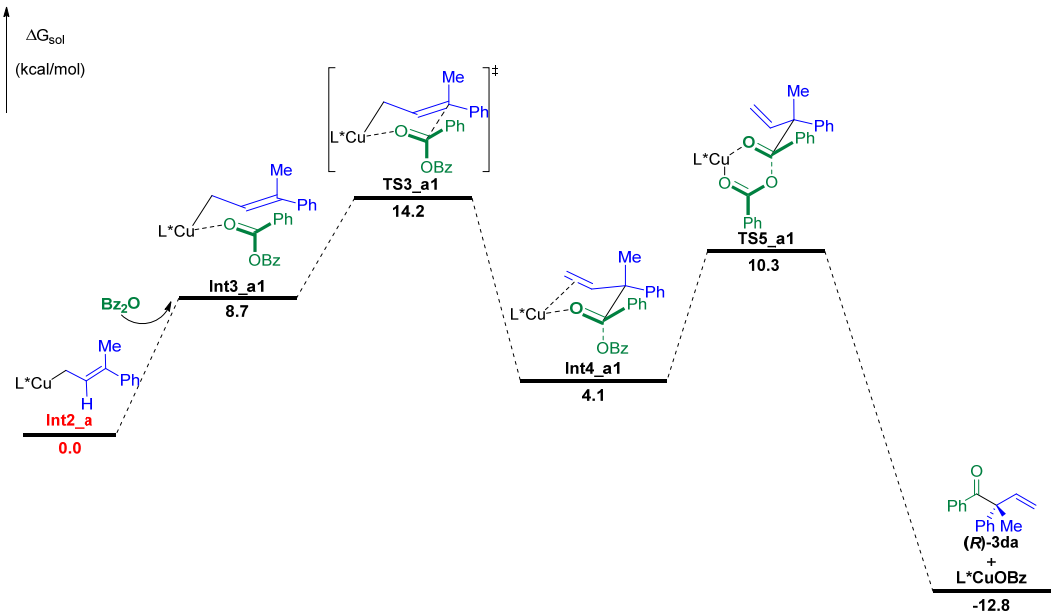
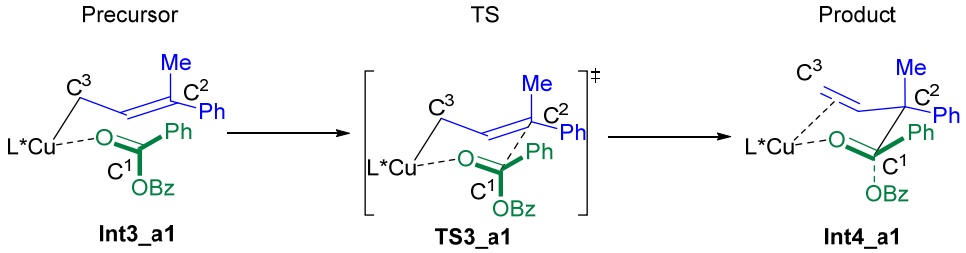


Figure S4. Energy profile for the hydroacylation process from **Int_2a**. Free energies are given in kcal/mol.

Table S1. Bond length variation from **Int3_a1** to **Int4_a1** via **TS3_a1**



	Int3_a1	δ1 [c]	TS3_a1	δ2 [d]	Int4_a1
C^1-C^2	3.589	1.324	2.265	0.635	1.630
Cu-C^3	2.031	0.208	2.239	0.183	2.422

[a] Calculated at M06/6-311+G(d,p)/SDD/SMD(THF)//B3LYP/6-31G(d)/LANL2DZ level.
[b] Bond lengths are given in angstroms.
[c] Bond length changes between precursor and TS.
[d] Bond length changes between TS and product.

We reasoned that **TS3** is a late transition state from geometry analysis of the bond length variations from **Int3** to **Int4** via **TS3**. Take the most favorable **TS3_a1** for example, the bond length variations between **TS3_a1** and **Int4_a1** are obviously smaller than that between **Int3_a1** and **TS3_a1**, indicating **TS3_a1** most resembles product **Int4_a1** and therefore should be a late transition state (Table S1).

Table S2. Comparative energetic results of TS3s

		Re-face particapation of 2a				*Si*-face particapation of 2a			
Int2_a	Int2_b	TS3_a1	TS3_a2	TS3_b1	TS3_b2	TS3_a3	TS3_a4	TS3_b3	TS3_b4
M06/6-311+G(d,p)/SDD/SMD(THF)//B3LYP/6-31G(d)/LANL-2DZ									
0.0	2.5	14.2	20.4	17.3	24.6	19.1	20.3	29.7	24.6
M06/6-311+G(d,p)/SDD/SMD(THF)//B3LYP-D3(BJ)/6-31G(d)/LANL2DZ									
0.0	1.4	15.1	21.0	17.6	26.6	16.5	19.5	31.1	23.5
M06/6-311+G(d,p)/SDD/SMD(THF)//M06/6-31G(d)/LANL2DZ									
0.0	2.8	15.0	20.0	19.3	25.7	19.5	21.1	33.8	24.6
M06/6-311+G(d,p)/SDD/SMD(THF)//wB97X-D/6-31G(d)/LANL2DZ									
0.0	0.5	13.2	20.2	15.7	25.1	15.7	18.0	30.3	20.8

Considering dispersion corrections are not involved in the geometry optimization ultizing B3LYP method, extra geometry optimizations of the eight competing TS3s with methods including dispersion corrections, such as B3LYP-D3(BJ), M06 and wB97X-D were conducted. Single point calculations on the obtained geometries have been performed including solvent effect (THF) at the same level with larger basis set. The comparisons of the energetic results are listed in Table S2. It is obvious that these results reproduce the trend observed with B3LYP optimizations. Careful examinations on the geometries didn't show significant changes from the B3LYP structures.

Energies of intermediates and transition states

Table S2. Electronic energies (E_{elec}), Gibbs free energies (G_{298}), thermal correction to Gibbs free energy ($cor\ G_{gas}$), solvation energies (Esol), solvation free energies (G_{sol}) in THF (ε = 7.43) for all stationary points of the process. Calculations were carried out at M06/6-311+G(d,p)/SDD/SMD(THF)//B3LYP/6-31G(d)/LANL-2DZ level.

species	E_{elec} (a.u.)	G_{298} (a.u.)	$cor\ G_{gas}$ (a.u.)	E_{sol} (a.u.)	G_{sol} (a.u.)
1d	-387.033394	-386.901312	0.132081	-386.820688	-386.688607
L*CuH	-2196.754939	-2196.210189	0.544751	-2197.342444	-2196.797693
Int1_a	-2583.773815	-2583.074160	0.699655	-2584.165995	-2583.466340
Int1_b	-2583.779618	-2583.079270	0.700348	-2584.170630	-2583.470282
Int1_c	-2583.769501	-2583.069137	0.700364	-2584.163879	-2583.463515
Int1_d	-2583.774133	-2583.073792	0.700342	-2584.169342	-2583.469000
TS1_a	-2583.761067	-2583.060890	0.700176	-2584.157244	-2583.457068
TS1_a'	-2583.759451	-2583.058860	0.700590	-2584.154289	-2583.453699
TS1_b	-2583.764467	-2583.064657	0.699810	-2584.159046	-2583.459236
TS1_b'	-2583.762268	-2583.062970	0.699299	-2584.155397	-2583.456098
TS1_c	-2583.758996	-2583.057299	0.701697	-2584.156250	-2583.454553
TS1_c'	-2583.758773	-2583.057786	0.700987	-2584.154640	-2583.453653
TS1_d	-2583.762960	-2583.060456	0.702504	-2584.158798	-2583.456294
TS1_d'	-2583.759582	-2583.058916	0.700666	-2584.155842	-2583.455176
Int2_a	-2583.841747	-2583.138116	0.703631	-2584.231965	-2583.528334
Int2_a'	-2583.840829	-2583.136119	0.704710	-2584.230703	-2583.525993
Int2_b	-2583.839595	-2583.134383	0.705212	-2584.229580	-2583.524368
Int2_b'	-2583.839975	-2583.133319	0.706656	-2584.229420	-2583.522764
Int2_c	-2583.830174	-2583.122548	0.707626	-2584.226816	-2583.519190
Int2_c'	-2583.828112	-2583.120604	0.707509	-2584.223194	-2583.515685
Int2_d	-2583.830233	-2583.125963	0.704270	-2584.227326	-2583.523056
Int2_d'	-2583.825285	-2583.117258	0.708028	-2584.222275	-2583.514247
TS2_ac	-2583.828388	-2583.118607	0.709781	-2584.225563	-2583.515782
TS2_ad	-2583.829223	-2583.121102	0.708120	-2584.226099	-2583.517979
TS2_bc	-2583.825319	-2583.115359	0.709961	-2584.224889	-2583.514928
TS2_bd	-2583.822733	-2583.112803	0.709930	-2584.221810	-2583.511880
TS4_a	-2583.826658	-2583.121014	0.705644	-2584.214787	-2583.509143
TS4_b	-2583.822033	-2583.116784	0.705249	-2584.207312	-2583.502063
TS4_c	-2583.818952	-2583.110732	0.708220	-2584.216964	-2583.508744
TS4_d	-2583.821496	-2583.113395	0.708102	-2584.217254	-2583.509152
2a	-765.208202	-765.045084	0.163118	-764.904973	-764.741855
Int3_a1	-3349.045610	-3348.154164	0.891446	-3349.147790	-3348.256344
Int3_a2	-3349.044361	-3348.156732	0.887629	-3349.145227	-3348.257598

Int3_a3	-3349.039747	-3348.150329	0.889418	-3349.143943	-3348.254525
Int3_a4	-3349.044494	-3348.155452	0.889042	-3349.144039	-3348.254997
Int3_b1	-3349.040258	-3348.144764	0.895493	-3349.142637	-3348.247144
Int3_b2	-3349.041053	-3348.147838	0.893215	-3349.142857	-3348.249642
Int3_b3	-3349.039085	-3348.148034	0.891052	-3349.144503	-3348.253451
Int3_b4	-3349.040896	-3348.148160	0.892736	-3349.144395	-3348.251659
TS3_a1	-3349.035358	-3348.139191	0.896168	-3349.143749	-3348.247581
TS3_a2	-3349.025491	-3348.129152	0.896338	-3349.133965	-3348.237627
TS3_a3	-3349.029722	-3348.130879	0.898843	-3349.138641	-3348.239798
TS3_a4	-3349.028859	-3348.130425	0.898433	-3349.136226	-3348.237793
TS3_b1	-3349.032264	-3348.132420	0.899844	-3349.142440	-3348.242596
TS3_b2	-3349.020914	-3348.123592	0.897322	-3349.128250	-3348.230928
TS3_b3	-3349.013470	-3348.115263	0.898207	-3349.121112	-3348.222905
TS3_b4	-3349.022878	-3348.122187	0.900691	-3349.131610	-3348.230919
Int4_a1	-3349.049053	-3348.149066	0.899987	-3349.163669	-3348.263682
Int4_a2	-3349.041514	-3348.140970	0.900544	-3349.154371	-3348.253827
Int4_b1	-3349.045127	-3348.145124	0.900004	-3349.159806	-3348.259802
Int4_b2	-3349.041341	-3348.139179	0.902162	-3349.155404	-3348.253242
TS5_a1	-3349.049428	-3348.152366	0.897061	-3349.150799	-3348.253738
(*R*)-3da	-732.637375	-732.399463	0.237913	-732.285008	-732.047095
(*S*)-3da	-732.638313	-732.400772	0.237541	-732.285309	-732.047768
L*CuOBz	-2616.444497	-2615.811065	0.633432	-2616.877001	-2616.243569

Cartesian coordinates for the optimized structures in Table S2

1d

C	1.93008400	-1.47135900	-0.00004600
C	0.57139400	-1.17613800	-0.00004100
C	0.11762000	0.15638700	0.00001400
C	1.08046400	1.17884700	0.00005900
C	2.44491000	0.88170800	0.00005200
C	2.87772300	-0.44276000	0.00000300
H	2.25311100	-2.50931900	-0.00008700
H	-0.15720200	-1.98174200	-0.00008000
H	0.76984100	2.21842300	0.00009500
H	3.16853300	1.69285400	0.00008700
H	3.93941200	-0.67422500	0.00000000
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C	-1.77886100	1.92797900	-0.00005400
H	-1.40153900	2.45622500	0.88451200
H	-1.40134300	2.45621000	-0.88454500
H	-2.86888400	1.99867500	-0.00017500
C	-2.25465500	-0.47172500	-0.00014200
C	-3.17532900	-1.39848200	0.00011400
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H	-3.58042000	-1.80618300	0.92624800

L*CuH

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H	-1.51679500	-0.23428000	-1.66977300
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P	-0.93449200	1.34935400	0.04432900
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Cu	0.00000200	0.00022600	1.84157700
C	-2.70501100	1.98953600	-0.19220600
H	-2.94680500	1.83302600	-1.25215800
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C	0.15772800	-3.08111500	-0.16561900
H	-0.05926300	-3.37124300	0.87015200
C	2.70513300	-1.98933400	-0.19183400

H	2.94698600	-1.83290300	-1.25178500
C	-2.58355500	3.51749600	0.03473000
C	-1.30286300	3.98326000	-0.66854500
H	-3.47521100	4.03320100	-0.34105700
H	-2.52141800	3.72669300	1.11058800
H	-1.08297100	5.04006000	-0.47277900
H	-1.43456900	3.87838800	-1.75273100
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C	-4.97166700	0.90620600	0.03928500
C	-3.60939600	1.08870000	2.01939200
C	-5.98921200	0.31006200	0.78756000
H	-5.11267000	1.06508300	-1.02799400
C	-4.62383800	0.49106200	2.76821300
H	-2.67648800	1.35690900	2.50826800
C	-5.81788400	0.10067800	2.15704900
H	-6.91378300	0.01144800	0.29967500
H	-4.47331500	0.32343500	3.83124800
H	-6.60586500	-0.36556400	2.74259500
C	1.15208000	3.08727800	-0.92434600
C	1.24060100	3.36375500	-2.29687800
C	2.33657000	2.76709400	-0.23749300
C	2.46983300	3.31685300	-2.96031900
H	0.35074900	3.62977000	-2.85966600
C	3.56318300	2.71154900	-0.89837000
H	2.29214800	2.55251700	0.82821300
C	3.63449700	2.98711500	-2.26667400
H	2.51349300	3.54241700	-4.02287800
H	4.45930700	2.44897000	-0.34335000
H	4.58907700	2.95077400	-2.78471700
C	2.58392200	-3.51728800	0.03521900
C	1.30333100	-3.98330200	-0.66808700
H	3.47567500	-4.03288300	-0.34049100
H	2.52175200	-3.72643200	1.11108500
H	1.43505100	-3.87835400	-1.75226600
H	1.08365900	-5.04015700	-0.47236400
C	3.77006200	-1.30597500	0.64191900
C	3.60913800	-1.08806900	2.01973600
C	4.97152500	-0.90547000	0.03971600
C	4.62338300	-0.49011700	2.76856800
H	2.67623800	-1.35638400	2.50856500
C	5.98888100	-0.30902000	0.78801100
H	5.11265500	-1.06442900	-1.02753500
C	5.81739500	-0.09953200	2.15746100
H	4.47273000	-0.32239500	3.83156900

H	6.91342700	-0.01026200	0.30016600
H	6.60522200	0.36694600	2.74302700
C	-1.15186100	-3.08784900	-0.92369200
C	-1.24063200	-3.36520900	-2.29601900
C	-2.33621500	-2.76710800	-0.23684700
C	-2.46997300	-3.31858900	-2.95929800
H	-0.35091200	-3.63171200	-2.85878200
C	-3.56292300	-2.71186000	-0.89755800
H	-2.29159300	-2.55186900	0.82872000
C	-3.63448300	-2.98827900	-2.26568600
H	-2.51382200	-3.54483000	-4.02170600
H	-4.45894000	-2.44885300	-0.34256500
H	-4.58914400	-2.95215800	-2.78359500
H	0.00082400	-0.00041500	3.41977900

Int1_a

Cu	-0.62356600	0.37133300	-0.74131000
C	-2.00200800	2.96636800	-1.96781300
C	-1.04315400	2.04509800	-1.95507100
C	0.10205500	1.48390900	-2.42933300
H	1.08266100	1.80364500	-2.08144200
H	0.08533000	0.82909900	-3.30106500
C	-3.22701200	2.97688700	-1.12150100
C	-3.73362900	4.18751000	-0.61689100
C	-3.94136400	1.79699500	-0.85536100
C	-4.90138000	4.21634000	0.14628400
H	-3.20598200	5.11760100	-0.80815900
C	-5.11482300	1.82798000	-0.10323300
H	-3.56576600	0.85432500	-1.23303900
C	-5.59965000	3.03529500	0.40426100
H	-5.26597500	5.16364800	0.53590100
H	-5.64915000	0.89999900	0.08416400
H	-6.51451600	3.05716800	0.99120500
H	-1.80255200	0.13820400	0.29010100
C	-1.85314800	4.11620600	-2.96052800
H	-1.70980500	5.07453700	-2.44488400
H	-0.99307900	3.95644700	-3.61497800
H	-2.75551300	4.21533600	-3.57672500
C	0.93286500	-2.14297200	0.91193400
C	1.84719900	-1.01248700	1.42056500
H	2.76981500	-0.97989900	0.82967300
H	2.13333600	-1.22238700	2.45845700
H	0.05717400	-2.22889800	1.56436200

H	1.46826700	-3.09993100	0.95623400
C	1.50893300	-2.72697200	-1.96281200
H	1.26329400	-2.31363600	-2.95060800
C	-0.99023400	-3.32527800	-0.93592600
H	-0.90632800	-3.85624500	0.02040100
C	2.55009800	1.80023100	1.78958200
H	3.27060900	1.16110600	2.31803700
C	0.13964200	1.00684700	2.90286300
H	-0.70533700	1.61670700	2.56446100
P	0.24122000	-1.86913600	-0.80866300
P	1.08690800	0.69307900	1.26138000
C	1.06566500	1.89502800	3.76610100
C	1.91808800	2.75539500	2.82917600
H	0.47572700	2.50395500	4.46240500
H	1.73412800	1.27731300	4.37707800
H	2.69405900	3.31176100	3.36928000
H	1.28915500	3.49758900	2.32014600
C	1.10240000	-4.21159100	-1.96923800
C	-0.42617400	-4.24991400	-2.04493900
C	2.95438300	-2.39160000	-1.67218700
C	3.47752800	-1.16506000	-2.11714800
C	3.80475800	-3.24627500	-0.95422900
C	4.79409300	-0.79749000	-1.84399700
H	2.83795800	-0.48955100	-2.68044800
C	5.12725000	-2.88417600	-0.68475000
H	3.44422400	-4.20954600	-0.60673000
C	5.62701800	-1.65817100	-1.12396500
H	5.16577500	0.16315900	-2.18871100
H	5.76700600	-3.56750600	-0.13196100
H	6.65560300	-1.37776900	-0.91347600
C	-2.44060400	-2.94225600	-1.13354600
C	-3.39630900	-3.27695000	-0.16620800
C	-2.87416300	-2.27589100	-2.28999500
C	-4.74451800	-2.95962600	-0.34402500
H	-3.08028300	-3.78984100	0.73953600
C	-4.21916000	-1.95814600	-2.47366200
H	-2.15339600	-1.99418000	-3.05419400
C	-5.16200800	-2.29988300	-1.50020100
H	-5.46744800	-3.23161800	0.42088000
H	-4.53204000	-1.44119500	-3.37717300
H	-6.21082000	-2.05466100	-1.64455500
C	3.26922500	2.49318000	0.65417100
C	2.59602000	3.36360500	-0.22000400
C	4.64524200	2.30446600	0.46545200

C	3.27843300	4.02506400	-1.24099900
H	1.52628400	3.51986800	-0.10399600
C	5.33269900	2.96480300	-0.55633600
H	5.18617300	1.63464300	1.13029300
C	4.65163400	3.82902600	-1.41414700
H	2.73617800	4.69546500	-1.90287700
H	6.40162600	2.80626200	-0.67633900
H	5.18320100	4.34656900	-2.20824500
C	-0.43498000	-0.21567500	3.59081100
C	0.29882600	-0.98830600	4.50660700
C	-1.75500000	-0.60957500	3.30969500
C	-0.26280000	-2.11169800	5.11812400
H	1.31845400	-0.71315500	4.76124900
C	-2.31687100	-1.73208700	3.91863200
H	-2.32972000	-0.04112100	2.58457700
C	-1.57395200	-2.48990100	4.82724200
H	0.32719700	-2.68730200	5.82718000
H	-3.34120900	-2.01034700	3.68379400
H	-2.01312200	-3.36074100	5.30714200
H	-0.82216600	-5.26616700	-1.93232200
H	-0.75449600	-3.89062200	-3.02828100
H	1.57061200	-4.74913600	-2.80376800
H	1.42965400	-4.70627400	-1.04607000

Int1_b

Cu	-0.19774700	0.96971700	-0.02793700
C	-2.00131100	0.63137200	1.15821000
C	-2.22368300	1.60273400	0.24207800
C	-2.93134400	2.51264200	-0.42379200
C	-4.37672800	2.71807600	-0.08349900
C	-5.12592300	3.71311100	-0.73846900
C	-5.04430700	1.93446600	0.87823300
C	-6.47548700	3.91766500	-0.44502600
H	-4.65558800	4.33997000	-1.48728900
C	-6.38991700	2.13777600	1.17074300
H	-4.49755600	1.15646500	1.40036700
C	-7.11749600	3.13246000	0.51076700
H	-7.02310800	4.69649900	-0.96987700
H	-6.87397500	1.51520700	1.91934000
H	-8.16808200	3.29031000	0.73952800
H	-2.25845700	-0.40703800	0.95642900
H	-1.73011300	0.88114100	2.18433400
H	0.43979900	2.01041500	-1.04735900

C	2.48755200	-1.16583500	0.34507800
C	1.56552700	-2.10358000	-0.45671700
P	1.58930000	0.11414800	1.37930400
P	0.21830100	-1.19852200	-1.39634000
C	3.05514900	1.17136900	1.98677200
H	3.95473300	0.60552900	1.71027000
C	1.34590500	-0.70189400	3.10116000
H	0.48578300	-0.15520500	3.50926100
C	0.96263000	-0.82962500	-3.12385100
H	0.42733900	0.08147200	-3.41612400
C	-0.82582000	-2.65588700	-2.04982100
H	-0.23264200	-3.56788800	-1.89982800
C	-2.33798100	3.36244600	-1.52558100
H	-2.87551400	3.21281400	-2.47154700
H	-2.41030800	4.42949100	-1.27713000
H	-1.28690000	3.10494600	-1.66240600
C	-0.91054200	-2.39628100	-3.57319600
C	0.48802300	-1.97909600	-4.03772500
C	2.94467100	1.13435200	3.53018300
C	2.58216800	-0.29887900	3.92895400
C	0.97429300	-2.16779700	3.06221200
C	-0.37266200	-2.53062300	2.89035700
C	1.92163500	-3.19875200	3.16410600
C	-0.76007200	-3.86757100	2.80736700
H	-1.12529000	-1.74987700	2.81636700
C	1.53682900	-4.53966300	3.08908000
H	2.97098500	-2.96364200	3.31356700
C	0.19635900	-4.88111100	2.90612700
H	-1.80805100	-4.11409800	2.66154400
H	2.29036400	-5.31819100	3.17728700
H	-0.10088500	-5.92469000	2.84767200
C	3.18389700	2.56245900	1.40656300
C	4.38262000	2.95274000	0.79358800
C	2.14996000	3.50509600	1.50331900
C	4.55026400	4.24699500	0.29645300
H	5.19579300	2.23490100	0.70749600
C	2.31422300	4.79903200	1.01178400
H	1.19976500	3.22191500	1.94761400
C	3.51541800	5.17638100	0.40690700
H	5.49028000	4.52765600	-0.17211700
H	1.49684700	5.51073600	1.09134400
H	3.64076200	6.18471200	0.02134100
C	2.44329400	-0.50412100	-3.13432500
C	2.85535000	0.81197400	-2.85750500

C	3.43459800	-1.46448600	-3.39150000
C	4.20789200	1.15150600	-2.83201400
H	2.10341500	1.56215700	-2.62602700
C	4.78982600	-1.12335900	-3.37353200
H	3.15927200	-2.48959400	-3.62121900
C	5.18349700	0.18507700	-3.09225900
H	4.49567200	2.17438600	-2.60408400
H	5.53666000	-1.88507400	-3.58391700
H	6.23771500	0.44977700	-3.07989500
C	-2.16407100	-2.84071300	-1.36783000
C	-2.49264100	-4.06744600	-0.77396600
C	-3.11985000	-1.81163300	-1.33259300
C	-3.73534800	-4.26619400	-0.16677000
H	-1.76730500	-4.87809300	-0.79085000
C	-4.36126700	-2.00486300	-0.72586800
H	-2.88628900	-0.84294100	-1.76758700
C	-4.67484300	-3.23485300	-0.14044200
H	-3.96818900	-5.22905000	0.28138600
H	-5.07944600	-1.18935300	-0.70439200
H	-5.64243900	-3.38604200	0.33065700
H	-1.63039300	-1.59206700	-3.77401700
H	-1.27367400	-3.28802700	-4.09843900
H	0.49989300	-1.67082800	-5.09066200
H	1.15590000	-2.84489300	-3.95270600
H	2.16224800	1.82879900	3.86383900
H	3.88292100	1.46825600	3.98885900
H	2.38267600	-0.39463100	5.00362100
H	3.43181500	-0.95471900	3.70204200
H	3.11487300	-0.58767500	-0.34232000
H	3.15957700	-1.75826400	0.97822500
H	2.17338300	-2.71734900	-1.13316800
H	1.04465500	-2.78729400	0.22372500

Int1_c

Cu	-1.08114000	-0.90354500	-1.09256400
C	-1.50795600	-2.03402000	-3.84574500
C	-1.01302200	-2.24565400	-2.64066100
C	-0.39927400	-3.00896600	-1.68390100
H	-1.46908000	-2.82165600	-4.60177700
H	-1.97018400	-1.09304000	-4.12178000
H	-1.93813400	0.26518500	-1.74456500
P	-1.29854500	-0.47649900	1.24846200
P	0.83208500	1.47851300	-0.75960100

C	-0.96296700	1.34609200	1.50983900
C	0.38405900	1.89670000	1.01166600
C	-0.04969600	2.76229500	-1.89758200
H	-0.55664500	2.12004400	-2.62261800
C	2.48160200	2.41299800	-0.91462700
H	2.40792300	3.31976400	-0.29710400
C	-3.07808000	-0.57373300	1.95291400
H	-3.27368100	0.43948700	2.32589600
C	-0.54978700	-1.34109100	2.78359400
H	-0.48992100	-2.39386800	2.47382700
C	-2.97892900	-1.50815300	3.18199700
C	-1.63707100	-1.23928800	3.86816400
C	2.43954000	2.85337300	-2.39426800
C	1.09056700	3.55522300	-2.60745800
C	-1.10803300	3.63488600	-1.25242200
C	-2.46878800	3.34489700	-1.45133300
C	-0.78743800	4.74405100	-0.44991800
C	-3.46696000	4.13312400	-0.87590400
H	-2.73726100	2.47795500	-2.04813700
C	-1.78382300	5.53270900	0.12876500
H	0.25347600	5.00630400	-0.27758800
C	-3.13049400	5.23202600	-0.08222000
H	-4.51140600	3.89015800	-1.05635900
H	-1.50468100	6.38601400	0.74208600
H	-3.90703300	5.84915900	0.36221700
C	3.73349300	1.67175100	-0.50714600
C	4.63185100	2.26068200	0.39544600
C	4.05931500	0.41321700	-1.03679300
C	5.82291800	1.62490300	0.75120000
H	4.39609800	3.23450600	0.81971200
C	5.24925000	-0.22443700	-0.68531700
H	3.37158100	-0.07980400	-1.71800700
C	6.13893000	0.37870400	0.20802200
H	6.50400400	2.10655600	1.44856400
H	5.47407300	-1.20072400	-1.10560700
H	7.06731700	-0.11829200	0.47775300
C	-4.17077500	-0.91315300	0.96120100
C	-4.40738800	-2.22645800	0.52847500
C	-4.99621000	0.10346000	0.46034100
C	-5.43131200	-2.51261200	-0.37534700
H	-3.79043000	-3.04023800	0.89911700
C	-6.01952700	-0.17714500	-0.44539700
H	-4.83133700	1.12972200	0.78088900
C	-6.24246500	-1.48840700	-0.86751000

H	-5.59750900	-3.53916600	-0.69210900
H	-6.64492200	0.62993300	-0.81807500
H	-7.04128300	-1.71125900	-1.56959900
C	0.84882700	-0.88665100	3.14047000
C	1.11692600	-0.03154200	4.21922600
C	1.93018900	-1.31634900	2.35183500
C	2.42144100	0.38881200	4.49395100
H	0.31094300	0.30958600	4.86151500
C	3.23018000	-0.89103300	2.61833200
H	1.74755900	-1.98101000	1.51034900
C	3.48158800	-0.03283000	3.69224600
H	2.60386400	1.04928600	5.33804400
H	4.04397600	-1.21750200	1.97821200
H	4.49414200	0.30314600	3.89701600
C	1.07782200	-3.18020400	-1.66232900
C	1.89143300	-2.62746300	-2.67257000
C	1.70178000	-3.98260800	-0.68772800
C	3.25935400	-2.88011700	-2.71268600
H	1.43142300	-2.01460900	-3.44148900
C	3.07547100	-4.22858700	-0.72520800
H	1.11078000	-4.43662800	0.10099700
C	3.86292700	-3.68481400	-1.73982400
H	3.85753700	-2.45620000	-3.51562600
H	3.52605500	-4.85871400	0.03746200
H	4.92890900	-3.89219700	-1.78030000
C	-1.25551800	-3.95702800	-0.85280200
H	-2.31369800	-3.72178200	-0.98212000
H	-1.08974400	-4.99401900	-1.17920000
H	-1.02565700	-3.90991900	0.21750500
H	-3.82924400	-1.34430200	3.85462700
H	-3.02220000	-2.55801600	2.86788300
H	-1.44524300	-1.94099900	4.68978000
H	-1.65362700	-0.23275100	4.30443600
H	2.52923800	1.97233700	-3.04384700
H	3.28235400	3.51307400	-2.63516600
H	0.86164700	3.67631600	-3.67293600
H	1.15340900	4.56561600	-2.18930300
H	-1.77969700	1.84952200	0.98009200
H	-1.07685000	1.57898300	2.57688000
H	1.20554000	1.48826200	1.61136200
H	0.38388400	2.98300000	1.16260800

Int1_d

Cu	-0.63553900	-0.23725100	-1.39298300
C	-0.63938800	-0.97514700	-4.33161700
C	-0.38954200	-1.39526100	-3.10616500
C	0.01012900	-2.31651700	-2.18001900
C	-0.95215900	-3.30033800	-1.61804400
C	-0.52340900	-4.31837300	-0.74392700
C	-2.31852600	-3.27555600	-1.97104200
C	-1.42108600	-5.25960600	-0.23457000
H	0.52313900	-4.38858800	-0.46573300
C	-3.21100500	-4.21343900	-1.45971300
H	-2.66986100	-2.50990600	-2.65596200
C	-2.77078300	-5.21162000	-0.58306300
H	-1.05752500	-6.03621000	0.43389500
H	-4.25724200	-4.17008100	-1.75237900
H	-3.46868400	-5.94479400	-0.18827300
H	-0.49175200	-1.64433500	-5.18238900
H	-0.99855100	0.02732600	-4.53507000
C	1.49586900	-2.50971000	-1.92021600
H	1.74650500	-2.50568600	-0.85446000
H	1.82629400	-3.47295900	-2.33593700
H	2.07499200	-1.71683300	-2.39357600
H	-1.41369900	0.99409400	-2.03039800
P	-0.98706800	-0.29813400	0.98856900
P	1.48641300	1.43477000	-0.65381100
C	-0.21052100	1.26032500	1.66534500
C	1.23267900	1.52847000	1.20237700
C	1.03464500	3.17731400	-1.34308500
H	0.53872200	2.92319000	-2.28575900
C	3.36180900	1.80211900	-0.76330200
H	3.62919800	2.33968600	0.15715300
C	-2.74810200	-0.17287100	1.69611200
H	-2.66231100	0.50954000	2.55325000
C	-0.51862400	-1.74042400	2.17513300
H	-0.43522800	-2.59343500	1.49262100
C	-3.00866500	-1.58629900	2.26219000
C	-1.76360200	-1.97752400	3.06411700
C	3.44353200	2.80942300	-1.92900100
C	2.37956500	3.87722600	-1.66110500
C	0.05425200	3.99560200	-0.52511700
C	-1.31687700	3.93570100	-0.82841000
C	0.45404400	4.81670800	0.54313800
C	-2.25064300	4.66842900	-0.09501200
H	-1.64903200	3.27869600	-1.62721900
C	-0.47883600	5.55311200	1.27681500

H	1.50429800	4.89642600	0.80959300
C	-1.83640400	5.48359100	0.96106900
H	-3.30426000	4.59499500	-0.35052200
H	-0.13991100	6.18440400	2.09467400
H	-2.56182000	6.05986400	1.52968400
C	4.25780800	0.58959200	-0.86906500
C	4.98444100	0.15592300	0.25033200
C	4.40729800	-0.12867100	-2.06680600
C	5.83052600	-0.95258300	0.18063700
H	4.88960000	0.69836700	1.18841100
C	5.25511700	-1.23431900	-2.14193600
H	3.85853500	0.17862800	-2.95279800
C	5.97133700	-1.65283800	-1.01813700
H	6.38741100	-1.26069700	1.06211600
H	5.35755700	-1.76889300	-3.08290500
H	6.63437100	-2.51171600	-1.07874800
C	-3.82263700	0.36851200	0.78107500
C	-4.24651800	-0.32989200	-0.35903800
C	-4.44786500	1.58563800	1.08485600
C	-5.26783700	0.17170200	-1.16425300
H	-3.76961400	-1.26814300	-0.62526800
C	-5.46898500	2.09283600	0.27837300
H	-4.13211300	2.14249100	1.96458200
C	-5.88416500	1.38518100	-0.85003400
H	-5.57921100	-0.38405000	-2.04502000
H	-5.94248500	3.03664600	0.53739200
H	-6.67967300	1.77476500	-1.47976900
C	0.80098900	-1.60411400	2.90242000
C	0.94114400	-0.86692000	4.09062100
C	1.94827400	-2.22584000	2.38289700
C	2.17847600	-0.75017000	4.72588100
H	0.07727500	-0.38095400	4.53480200
C	3.18810400	-2.10943700	3.01221400
H	1.86476500	-2.81391600	1.47232000
C	3.30938900	-1.36840600	4.18912200
H	2.25633500	-0.17621100	5.64576900
H	4.05657400	-2.59903900	2.58033200
H	4.27159900	-1.27857900	4.68604100
H	-3.91368800	-1.59032700	2.88142500
H	-3.17363700	-2.29945200	1.44492200
H	-1.71532000	-1.35699800	3.96684400
H	-1.79841800	-3.02146600	3.39838600
H	4.44959500	3.24017500	-2.00523600
H	3.23755400	2.30764800	-2.88325800

H	2.26238000	4.56271100	-2.50937900
H	2.70544500	4.48606600	-0.81024700
H	1.90642800	0.77358500	1.62647200
H	1.55322700	2.50320700	1.59012400
H	-0.86740900	2.06732200	1.32114100
H	-0.24935900	1.25499500	2.76119800

TS1_a

Cu	-0.12225500	0.38240200	-0.84028100
C	-0.29587100	3.30054800	-2.26415300
C	0.00294200	1.98879900	-2.19940300
C	0.91277000	1.06273700	-2.66770800
H	1.98020000	1.25376900	-2.57398400
H	0.61355000	0.25624500	-3.33571400
C	-1.14313100	4.05616500	-1.31960600
C	-1.82376200	5.21884700	-1.73846700
C	-1.29861600	3.67195900	0.02768100
C	-2.63754700	5.94017700	-0.86745000
H	-1.72960200	5.55776100	-2.76481200
C	-2.11416400	4.39330300	0.89979800
H	-0.76518400	2.80016900	0.38244700
C	-2.79128400	5.53082500	0.45924500
H	-3.15503100	6.82596900	-1.22792100
H	-2.21324800	4.06882700	1.93346100
H	-3.42173800	6.09615400	1.14070100
H	-1.44389600	1.27449800	-1.17029400
C	0.24610600	4.05980600	-3.47014900
H	0.76866200	4.97561600	-3.16397800
H	0.93984400	3.43473700	-4.03523100
H	-0.55862500	4.36369300	-4.15428000
C	-0.03003900	-2.44637900	0.96773700
C	1.05652700	-1.59425700	1.64855000
H	2.04098600	-1.85745400	1.24505000
H	1.07549000	-1.80970500	2.72415900
H	-0.98638500	-2.31507300	1.48687500
H	0.23477500	-3.50899000	1.03370800
C	0.77758800	-3.03869000	-1.89687900
H	0.88886300	-2.42747200	-2.80122200
C	-1.90004600	-3.02387800	-1.19182800
H	-1.95965600	-3.74899700	-0.36896300
C	2.53483900	0.89332200	2.01582200
H	3.02246300	0.02500000	2.47758500
C	-0.10135800	0.90484000	2.85785700

H	-0.51407800	1.85380800	2.49218800
P	-0.36860200	-1.95924600	-0.80875400
P	0.86854800	0.24859100	1.34862900
C	2.14830000	1.86858100	3.15561300
C	0.96797200	1.24709500	3.91121000
C	-1.50262400	-3.81105900	-2.46432600
C	-0.05528400	-4.27908000	-2.27545700
C	2.16138700	-3.25681100	-1.32469800
C	3.13950300	-2.26352100	-1.50818000
C	2.51267900	-4.39850400	-0.58791000
C	4.41806400	-2.40041200	-0.96843600
H	2.88582400	-1.36794600	-2.06969600
C	3.79508300	-4.54073600	-0.05134200
H	1.79039300	-5.19505800	-0.43522300
C	4.75241100	-3.54261400	-0.23618600
H	5.14935500	-1.61139600	-1.11998100
H	4.04432900	-5.43823900	0.50916600
H	5.74990800	-3.65611200	0.17998200
C	-3.22971500	-2.30841700	-1.28329700
C	-4.32910400	-2.79223000	-0.55925300
C	-3.41623400	-1.18975900	-2.10935200
C	-5.58296300	-2.18618000	-0.66235900
H	-4.20191000	-3.65700100	0.08900900
C	-4.66706700	-0.58166800	-2.21394800
H	-2.57363600	-0.76935500	-2.64955900
C	-5.75578500	-1.07793100	-1.49332900
H	-6.42212500	-2.58163100	-0.09545200
H	-4.78564700	0.29091400	-2.85046000
H	-6.72892900	-0.60099200	-1.57491300
C	3.48066200	1.47308200	0.98702700
C	4.80000800	1.00572700	0.90738200
C	3.08791300	2.50553700	0.12055100
C	5.70577700	1.55303900	-0.00446500
H	5.12247500	0.20558900	1.57033300
C	3.98985200	3.05482600	-0.79084400
H	2.06532000	2.87299100	0.14142200
C	5.30306900	2.58152300	-0.85716500
H	6.72529400	1.17750500	-0.04387100
H	3.66243900	3.85156600	-1.45331200
H	6.00416200	3.01058600	-1.56805400
C	-1.26719900	0.02963500	3.26587300
C	-2.43742900	0.05090200	2.48505800
C	-1.22653000	-0.82839400	4.37449700
C	-3.52315000	-0.76730800	2.79487700

H	-2.48572700	0.70217300	1.61548300
C	-2.31795800	-1.64264300	4.69115000
H	-0.34654700	-0.86072800	5.01011600
C	-3.46776600	-1.61926700	3.90193800
H	-4.40815200	-0.74132200	2.16529600
H	-2.26564300	-2.29390900	5.56012100
H	-4.31488300	-2.25367800	4.14918400
H	-2.19162500	-4.64838100	-2.62628900
H	-1.57983100	-3.15868700	-3.34422300
H	0.34698300	-4.76122000	-3.17496800
H	-0.02824400	-5.02602000	-1.47239800
H	3.00921700	2.05480700	3.80860200
H	1.85360600	2.83696100	2.73099900
H	1.31273300	0.34088000	4.42560900
H	0.56671200	1.92009400	4.67927100

TS1_a’

Cu	-0.06289600	0.45577900	-0.68359700
C	-1.70755000	2.95786000	-2.06722700
C	-0.74803600	2.04114200	-1.88638100
C	0.44105400	1.57710600	-2.44987700
C	-2.93913500	3.12655600	-1.24849900
C	-3.32096900	4.39872600	-0.78866300
C	-3.77755000	2.03871400	-0.94894000
C	-4.48152000	4.57507500	-0.03379600
H	-2.69436700	5.25971300	-1.00529500
C	-4.94342500	2.21541100	-0.20303000
H	-3.51296700	1.05279800	-1.31204600
C	-5.29941700	3.48296100	0.26245200
H	-4.74619000	5.56782800	0.32213100
H	-5.57517800	1.35589300	0.00782600
H	-6.20728600	3.62014300	0.84458400
H	-1.41498500	1.29258900	-0.36505200
C	-1.55216500	3.92700800	-3.23104300
H	-1.50119000	4.96772000	-2.88504200
H	-0.64224900	3.70968000	-3.79465000
H	-2.41415500	3.86231300	-3.90829900
C	0.72628800	-2.31425100	1.00645000
C	1.76205400	-1.30721100	1.54189700
H	2.70747400	-1.42034800	0.99975500
H	1.96423100	-1.51747100	2.59982100
H	-0.14745400	-2.32846000	1.66762600
H	1.15484400	-3.32458900	1.01099900

C	1.21205200	-2.78851600	-1.91161100
H	0.99691600	-2.28832500	-2.86533600
C	-1.31319700	-3.22560900	-0.86580900
H	-1.24557700	-3.82299300	0.05192100
C	2.84974200	1.39142800	1.83930800
H	3.53274000	0.61044500	2.19790100
C	0.33230000	0.95497800	2.90491800
H	-0.24427300	1.83565400	2.59455100
P	0.04773900	-1.89139600	-0.69145500
P	1.25642300	0.48236400	1.30215700
C	2.42655000	2.24592900	3.06183900
C	1.42525300	1.42670000	3.88121800
C	-0.85721200	-4.11887700	-2.04830800
C	0.66972400	-4.22547400	-2.00442300
C	2.68586200	-2.60510000	-1.62205700
C	3.30617600	-1.39371700	-1.97546600
C	3.46633800	-3.58881000	-0.99641700
C	4.65539800	-1.16987300	-1.70443200
H	2.71484600	-0.61551200	-2.45142400
C	4.82036800	-3.36835400	-0.72865600
H	3.02665400	-4.54289700	-0.72233600
C	5.42011400	-2.15841400	-1.07852300
H	5.10619400	-0.22015100	-1.97794600
H	5.40553000	-4.14916200	-0.24921900
H	6.47359600	-1.98897100	-0.87189600
C	-2.73234100	-2.71867700	-0.99457600
C	-3.70046800	-3.08295900	-0.04902300
C	-3.13062200	-1.91820300	-2.07668900
C	-5.02852000	-2.67014200	-0.18054300
H	-3.41124500	-3.70057600	0.79838300
C	-4.45632100	-1.50810100	-2.21517200
H	-2.39642700	-1.60529200	-2.81494400
C	-5.41246000	-1.88375100	-1.26727800
H	-5.76259800	-2.97048300	0.56290000
H	-4.74254600	-0.89008500	-3.06200500
H	-6.44592100	-1.56650000	-1.37778900
C	3.55625100	2.17773600	0.75685500
C	4.91633100	1.95745700	0.49996900
C	2.89361900	3.17111200	0.01803300
C	5.60005100	2.70628300	-0.46130100
H	5.44700500	1.19195900	1.06206900
C	3.57263200	3.92112700	-0.94214600
H	1.83430800	3.35156800	0.18416800
C	4.92958100	3.69205400	-1.18606400

H	6.65637900	2.52029500	-0.63887700
H	3.03909700	4.68349400	-1.50359700
H	5.45726300	4.27719900	-1.93445000
C	-0.65353700	-0.08321800	3.39657900
C	-1.92443400	-0.15672000	2.79816100
C	-0.35030500	-0.99482100	4.41944400
C	-2.85328600	-1.11486600	3.20358500
H	-2.17313700	0.53237100	1.99491300
C	-1.28249600	-1.95222800	4.82926400
H	0.61431500	-0.95727600	4.91652900
C	-2.53662600	-2.01870900	4.22172900
H	-3.82537200	-1.15308700	2.71967900
H	-1.02603400	-2.64205900	5.62952900
H	-3.26294800	-2.76048700	4.54392000
H	-1.34485500	-5.09957800	-1.99526900
H	-1.16753000	-3.66200800	-2.99646400
H	1.07226100	-4.74636000	-2.88232600
H	0.96407700	-4.80910800	-1.12284600
H	3.30646800	2.53718100	3.64798800
H	1.95305400	3.17367200	2.71590100
H	1.94591400	0.57020400	4.32874500
H	0.99448100	2.00694300	4.70689800
H	1.38789200	2.06304400	-2.22582100
H	0.41360600	0.94441800	-3.33652300

TS1_b

Cu	-0.13700800	0.70491700	0.32484600
C	-1.83015200	0.96409700	1.75365700
C	-1.89634800	1.80376600	0.66634200
C	-2.74633500	2.44632400	-0.15946300
C	-4.10995000	2.81188800	0.31514800
C	-5.12734000	3.11146000	-0.61396400
C	-4.44434400	2.89531500	1.68295400
C	-6.41198800	3.46742100	-0.19890700
H	-4.91872000	3.05502500	-1.67743800
C	-5.72244800	3.25834800	2.09572100
H	-3.68325900	2.67911800	2.42483900
C	-6.72018900	3.54538900	1.15829500
H	-7.17270800	3.68420400	-0.94520800
H	-5.94103800	3.32289500	3.15913400
H	-7.71871100	3.82575300	1.48313600
H	-2.52757700	0.13211900	1.83579600
H	-1.26729800	1.22931200	2.64744100

H	-0.20857700	2.30687600	-0.01061200
C	2.45648000	-1.37431700	-0.05785300
C	1.38001600	-2.05587700	-0.92515800
P	1.76972400	-0.24837900	1.27317100
P	-0.00235500	-0.90515200	-1.45634800
C	3.35294800	0.58129400	1.92254900
H	4.18155000	-0.02625400	1.53371200
C	1.55324000	-1.30799800	2.85097600
H	0.74088400	-0.78735600	3.37313500
C	0.49794300	-0.22050200	-3.16860000
H	-0.05650200	0.72531000	-3.21393600
C	-1.25342900	-2.13448400	-2.19814200
H	-0.71941900	-3.09025200	-2.28532100
C	-2.36154000	2.84236300	-1.56475400
H	-2.73691600	2.13582000	-2.32013600
H	-2.75815000	3.83116800	-1.82490600
H	-1.26934900	2.85847500	-1.64443800
C	3.29403900	0.34663900	3.45183700
C	2.84215600	-1.10192800	3.67097800
C	-0.13184500	-1.18103500	-4.19565400
C	-1.49334600	-1.60793000	-3.63483800
C	1.96970600	0.10860400	-3.30087200
C	2.45258600	1.30221700	-2.73442900
C	2.88758600	-0.73866300	-3.93922000
C	3.80651800	1.63098800	-2.79389800
H	1.75780800	1.96616800	-2.22517900
C	4.24364500	-0.40634400	-4.00728400
H	2.55060700	-1.66143600	-4.40192800
C	4.70957900	0.77625900	-3.43271000
H	4.15382500	2.55327100	-2.33658300
H	4.93408800	-1.07561700	-4.51456200
H	5.76424400	1.03312000	-3.48656200
C	-2.51319000	-2.36698500	-1.39165200
C	-2.92603900	-3.67491000	-1.10062900
C	-3.31507000	-1.30312600	-0.94858700
C	-4.10608300	-3.91792900	-0.39322900
H	-2.31790000	-4.51319300	-1.43445100
C	-4.49428800	-1.54141800	-0.24208800
H	-3.00783900	-0.27714900	-1.13083700
C	-4.89496800	-2.85057300	0.03827600
H	-4.40811300	-4.94112600	-0.18357400
H	-5.09443700	-0.69954400	0.09242800
H	-5.81314500	-3.03544900	0.58948400
C	3.59393900	2.01820300	1.51405100

C	2.61732100	3.01223000	1.67728100
C	4.84310200	2.39112600	0.99690900
C	2.88711200	4.33887100	1.34124200
H	1.62883200	2.74518700	2.03782600
C	5.11685500	3.71852200	0.66054100
H	5.61205400	1.63319300	0.86110500
C	4.13777800	4.69841200	0.83376600
H	2.11201700	5.09009500	1.46648000
H	6.09420200	3.98493100	0.26593200
H	4.34529300	5.73247900	0.57148600
C	1.09017900	-2.72575200	2.59532500
C	-0.28031200	-2.96790600	2.39580900
C	1.96990500	-3.81629000	2.52015300
C	-0.75490700	-4.25063800	2.12355500
H	-0.97659700	-2.13411700	2.44149100
C	1.49618000	-5.10375700	2.25397900
H	3.03435800	-3.67325700	2.68048300
C	0.13378600	-5.32667600	2.05207600
H	-1.81828900	-4.40502500	1.96409000
H	2.19722200	-5.93337500	2.20864800
H	-0.23295500	-6.32890500	1.84700300
H	-1.97414000	-2.37757700	-4.25027500
H	-2.17629700	-0.74890200	-3.60479700
H	-0.21882500	-0.70428300	-5.17989700
H	0.49061900	-2.07532900	-4.32554000
H	4.26998800	0.55076000	3.90775300
H	2.57653700	1.04241900	3.90660000
H	2.67128000	-1.32798600	4.73064300
H	3.63687700	-1.77408000	3.32481200
H	3.07949900	-0.72461200	-0.68363000
H	3.11370100	-2.13373400	0.38328700
H	0.88948300	-2.85032800	-0.35089600
H	1.85356200	-2.52662600	-1.79584600

TS1_b’

Cu	0.44273600	-0.27839500	-0.42516900
C	2.58229700	-0.19611800	0.09886200
C	2.27909400	-1.33401000	-0.62177200
C	2.68918000	-2.59390800	-0.86267100
C	4.10614000	-2.97600300	-0.59010500
C	4.45660900	-4.33289400	-0.44183200
C	5.14719500	-2.02994200	-0.49806900
C	5.77521400	-4.72390000	-0.20222500

H	3.68870800	-5.09708300	-0.50128100
C	6.46297600	-2.42046200	-0.26832700
H	4.91336200	-0.97764700	-0.61540100
C	6.78927900	-3.77155800	-0.11470000
H	6.00574400	-5.78013500	-0.08459200
H	7.24205000	-1.66357600	-0.21294900
H	7.81708800	-4.07384900	0.06845200
H	2.84932400	0.74030100	-0.38536000
H	2.83582900	-0.28927200	1.15465000
H	0.77390200	-1.25857400	-1.68955400
C	-2.39592100	0.90581000	0.97910100
C	-1.80796800	2.13943700	0.26835300
P	-1.14367300	-0.43832500	1.35023200
P	-0.61348300	1.72329600	-1.11638900
C	-2.28350200	-1.81846500	1.99637800
H	-3.23511000	-1.32650300	2.24059600
C	-0.43532700	-0.07811200	3.09390000
H	0.57027300	-0.51099100	3.03041400
C	-1.69435300	1.62805400	-2.68527100
H	-1.05333400	1.07719800	-3.38587200
C	0.04367700	3.46523400	-1.55669400
H	-0.51495400	4.15377500	-0.91009400
C	1.78860600	-3.66492700	-1.42808300
H	2.30503700	-4.25284300	-2.19716400
H	1.45091700	-4.37178200	-0.65648000
H	0.89871300	-3.20008300	-1.86298900
C	-1.63247500	-2.23612800	3.33685800
C	-1.25563800	-0.94514300	4.07216400
C	-1.80146500	3.07916000	-3.18614800
C	-0.41582000	3.70894500	-3.01649500
C	-2.97341100	0.83698400	-2.51518600
C	-2.90740200	-0.56775700	-2.49228600
C	-4.22835700	1.44383600	-2.35933400
C	-4.05412000	-1.33802600	-2.30442000
H	-1.94083500	-1.05420300	-2.59984000
C	-5.38036200	0.67224100	-2.17963100
H	-4.32154600	2.52529800	-2.38893800
C	-5.29802700	-0.71971400	-2.14736000
H	-3.97354000	-2.42072800	-2.27409500
H	-6.34300500	1.16516600	-2.06815100
H	-6.19380100	-1.31865400	-2.00604000
C	1.52015400	3.69289200	-1.31965000
C	1.94482100	4.66375700	-0.40212100
C	2.49901300	2.97280400	-2.02305100

C	3.30317300	4.91329600	-0.19210200
H	1.20224400	5.23357500	0.15218900
C	3.85638800	3.22035600	-1.81781100
H	2.20053000	2.20389600	-2.73168700
C	4.26478900	4.19262400	-0.90077300
H	3.60734600	5.67519100	0.52123800
H	4.59596400	2.64992000	-2.37338300
H	5.32233200	4.38503800	-0.74191900
C	-2.58019800	-2.96817400	1.05868800
C	-1.56691000	-3.63837900	0.35722400
C	-3.89957800	-3.42213700	0.91653300
C	-1.86616600	-4.73084400	-0.45735900
H	-0.54120900	-3.28925900	0.42802300
C	-4.20228900	-4.51682000	0.10452700
H	-4.69929200	-2.91263400	1.45030600
C	-3.18412500	-5.17631100	-0.58642000
H	-1.06618700	-5.22998500	-0.99738700
H	-5.23223300	-4.85244900	0.01282200
H	-3.41459000	-6.02801300	-1.22097500
C	-0.27524800	1.39102500	3.42026000
C	0.90105600	2.05365000	3.02871900
C	-1.26456400	2.14086900	4.07596700
C	1.08101000	3.41433700	3.27688600
H	1.67613600	1.49359500	2.51236500
C	-1.08502800	3.50299300	4.32974100
H	-2.18348500	1.66463100	4.40511800
C	0.08672900	4.14697400	3.93005100
H	2.00011000	3.89869600	2.95850800
H	-1.86385200	4.05878000	4.84579900
H	0.22650600	5.20568900	4.13172500
H	-0.41552900	4.78204400	-3.24186000
H	0.29116400	3.23822900	-3.71094200
H	-2.14655200	3.11493200	-4.22700600
H	-2.52773500	3.64408100	-2.58774400
H	-2.32063900	-2.85965200	3.91993000
H	-0.73696200	-2.84176500	3.14352600
H	-0.68642500	-1.14029300	4.98926400
H	-2.17626000	-0.42986600	4.37182500
H	-2.62343800	2.77477600	-0.10085700
H	-1.22849000	2.73648100	0.98214200
H	-3.14086500	0.42608300	0.33387100
H	-2.91027800	1.21808800	1.89617100

TS1_c

Cu	-0.27899200	-0.15959800	-1.26821000
C	1.27030100	0.01388800	-3.95852500
C	0.75143800	-0.82178200	-3.05870000
C	0.91696200	-2.06764200	-2.48070500
H	2.03162000	-0.34297500	-4.65151900
H	0.94289300	1.04409600	-4.05522000
H	-0.89311300	-0.13395700	-2.78624800
P	-1.16366400	-0.95942500	0.75904400
P	0.31693200	1.91364400	-0.07410700
C	-1.32319500	0.54296200	1.85929000
C	-0.18933300	1.57327300	1.70118100
C	-0.81366100	3.34928700	-0.63769400
H	-0.75904400	3.28185600	-1.73190200
C	1.80627100	3.08036500	0.22198300
C	-2.78549500	-1.87015400	1.12940400
C	-0.09928800	-2.25903500	1.68009800
H	0.44724200	-2.74925700	0.86674300
C	-1.10101900	-3.28399800	2.26244800
C	-2.32534500	-3.33216000	1.34044600
H	-3.10909600	-1.49112200	2.10898500
C	-0.08603300	4.63697100	-0.20963600
C	1.40646400	4.41210100	-0.46131000
H	1.81865100	3.25345900	1.30576400
C	-2.26847300	3.20082700	-0.24308200
C	-3.09675500	2.34857200	-0.99470700
C	-2.82775500	3.86313800	0.86001400
C	-4.43274500	2.15323200	-0.64650800
H	-2.67762400	1.81585200	-1.84522400
C	-4.16941900	3.67539900	1.20500600
H	-2.22450900	4.54161800	1.45553100
C	-4.97562300	2.81741400	0.45697900
H	-5.04600000	1.47535400	-1.23295800
H	-4.58159200	4.20554100	2.06007200
H	-6.01760500	2.66871900	0.72735500
C	3.17203500	2.57332700	-0.18454200
C	4.19635800	2.47657700	0.76785000
C	3.47240700	2.25218300	-1.51747500
C	5.48616300	2.08463000	0.40281100
H	3.98301500	2.71970600	1.80652600
C	4.76040600	1.86523700	-1.88709900
H	2.69089000	2.28797000	-2.27208200
C	5.77460800	1.78305100	-0.92877400
H	6.26515400	2.02267600	1.15842000

H	4.97043500	1.62164100	-2.92510800
H	6.77886900	1.48619100	-1.21909700
C	0.92946800	-1.67996600	2.62860200
C	0.64175500	-1.36993000	3.96773500
C	2.22292300	-1.40929500	2.15072300
C	1.61109200	-0.80402000	4.79900100
H	-0.34311700	-1.57526900	4.37785400
C	3.19093500	-0.83983100	2.97890200
H	2.47621000	-1.64839600	1.12151300
C	2.88937000	-0.53314800	4.30792000
H	1.36483300	-0.57833300	5.83357600
H	4.18170900	-0.64177700	2.57935000
H	3.64366600	-0.09537600	4.95653100
C	-3.93572600	-1.69550600	0.16176600
C	-3.78117600	-1.85768500	-1.22299400
C	-5.21660500	-1.41260500	0.65900600
C	-4.87585800	-1.74557100	-2.08090900
H	-2.79642200	-2.04782400	-1.63644100
C	-6.31465300	-1.30327900	-0.19598100
H	-5.35595900	-1.28081900	1.73012800
C	-6.14772200	-1.47093900	-1.57196300
H	-4.73116900	-1.86876000	-3.15104000
H	-7.29817900	-1.08759500	0.21376300
H	-6.99951500	-1.38729000	-2.24181000
C	2.15296800	-2.48051500	-1.79949300
C	3.25649500	-1.60985900	-1.62344800
C	2.30596200	-3.80129300	-1.31359500
C	4.42222200	-2.02899000	-0.99473600
H	3.18491700	-0.59050300	-1.98622500
C	3.48230700	-4.21855200	-0.68636800
H	1.50532200	-4.52179500	-1.44450400
C	4.55169800	-3.34083700	-0.51753300
H	5.23987700	-1.32151700	-0.87801300
H	3.55864400	-5.24473500	-0.33340000
H	5.46769900	-3.66772300	-0.03308200
C	-0.18845400	-3.08146600	-2.69566300
H	-1.08911000	-2.57612900	-3.05674400
H	0.09296400	-3.82807400	-3.45352400
H	-0.44870600	-3.63582700	-1.78329400
H	-3.13835500	-3.93282600	1.76524200
H	-2.06403900	-3.78378500	0.37405900
H	-1.42815100	-2.98003000	3.26384900
H	-0.62387700	-4.26559700	2.36812000
H	2.02249800	5.23489600	-0.07920100

H	1.59740800	4.34638800	-1.53996300
H	-0.24076500	4.83521100	0.85840600
H	-0.47206600	5.50670900	-0.75571000
H	-2.28210100	0.99431300	1.58016200
H	-1.39835900	0.23932200	2.91024600
H	0.71760000	1.19816500	2.18940100
H	-0.46956200	2.50640400	2.20637000

TS1_c'

Cu	0.23897700	1.01233500	0.53326800
C	1.36164500	3.38051500	2.30256300
C	0.33164100	2.67185200	1.84973500
C	-0.95049700	2.27103400	2.21659400
H	1.24698500	3.97787800	3.20785200
H	2.32176600	3.40013400	1.79959500
H	0.89154200	2.44937200	0.13836700
P	1.48384500	-1.02039100	0.96214300
P	-0.63781900	-0.00705600	-1.42516700
C	1.45130500	-1.85428700	-0.71515000
C	0.12527100	-1.71446000	-1.48247700
C	-0.00141500	1.01274600	-2.91996700
H	0.09863100	2.00868400	-2.47748300
C	-2.30745200	-0.34331700	-2.26341400
C	3.31251800	-1.29594500	1.43659600
C	0.86624700	-2.30500200	2.24586300
H	0.44104600	-1.66628300	3.02991200
C	2.13355900	-2.97090000	2.82211800
C	3.24229800	-1.91401300	2.85082900
H	3.66176500	-2.08541800	0.75736100
C	-1.16346900	1.05185000	-3.94138000
C	-2.48469100	0.89022800	-3.17732900
H	-2.11929900	-1.20272800	-2.92293700
C	1.36233700	0.60531900	-3.43572000
C	2.50726100	1.22131700	-2.90065800
C	1.54435300	-0.39160300	-4.40793000
C	3.78622000	0.85252300	-3.31897800
H	2.38559500	1.98567400	-2.13721900
C	2.82370100	-0.75752200	-4.83280600
H	0.68458700	-0.88704000	-4.85058400
C	3.95062400	-0.13894400	-4.28938100
H	4.65283200	1.34182500	-2.88258800
H	2.93684000	-1.52673100	-5.59273400
H	4.94547200	-0.42264400	-4.62265400

C	-3.48897000	-0.68802700	-1.38762600
C	-4.23167200	-1.84662400	-1.66087200
C	-3.90611900	0.13912300	-0.33428200
C	-5.36492700	-2.17092200	-0.91288900
H	-3.92185600	-2.49889700	-2.47487300
C	-5.03666300	-0.18495100	0.41667200
H	-3.35046800	1.04031900	-0.09328500
C	-5.77197600	-1.33852100	0.13114800
H	-5.92843000	-3.07033300	-1.14861900
H	-5.34136100	0.47579800	1.22268100
H	-6.65610200	-1.58307100	0.71443400
C	-0.23763400	-3.21589900	1.75584100
C	0.01019700	-4.46491300	1.16485700
C	-1.57310700	-2.79234700	1.86368400
C	-1.03972200	-5.25880800	0.69687700
H	1.02699900	-4.83496500	1.07228000
C	-2.62309100	-3.57776300	1.38928500
H	-1.78894200	-1.82957600	2.32078700
C	-2.35938400	-4.81797200	0.80303300
H	-0.82168600	-6.22548900	0.24981300
H	-3.64337300	-3.21523500	1.46984300
H	-3.17492800	-5.43474900	0.43536900
C	4.24748400	-0.11782400	1.28751400
C	4.15243900	1.01630100	2.10798400
C	5.27046900	-0.15800100	0.32899200
C	5.05876700	2.06875800	1.97983600
H	3.35575400	1.08836800	2.84253300
C	6.17583100	0.89653000	0.19367900
H	5.36256400	-1.02922800	-0.31609200
C	6.07494300	2.01419000	1.02272200
H	4.96770800	2.93624300	2.62823100
H	6.96364000	0.83848700	-0.55316100
H	6.77998900	2.83532800	0.92534300
C	-2.12452100	2.90659700	1.60979400
C	-2.00386000	3.76446700	0.48741400
C	-3.42249200	2.72897800	2.14356000
C	-3.11695500	4.38612700	-0.07115100
H	-1.01965500	3.94033500	0.06613000
C	-4.53003900	3.37180300	1.59008100
H	-3.56445000	2.09279900	3.01158600
C	-4.39206700	4.19969100	0.47408300
H	-2.98540400	5.03897600	-0.93157100
H	-5.50989200	3.22614300	2.04010300
H	-5.25654700	4.69866000	0.04489600

C	-1.11875200	1.40961500	3.45897600
H	-0.15928600	0.97326300	3.75159000
H	-1.48378900	2.00376800	4.31235100
H	-1.83478400	0.58913200	3.31573100
H	4.21264500	-2.34062500	3.13136800
H	3.00741400	-1.13929700	3.59222400
H	2.45786200	-3.80291200	2.18555400
H	1.93310000	-3.38989500	3.81578200
H	-3.33523100	0.74864400	-3.85466900
H	-2.69756000	1.78040500	-2.57099200
H	-1.07465700	0.23113000	-4.66281500
H	-1.13048000	1.98381300	-4.51814000
H	2.25716900	-1.36949600	-1.27944900
H	1.71215600	-2.91576200	-0.62130800
H	-0.63249900	-2.37100900	-1.03873800
H	0.26807000	-2.03580600	-2.52112300

TS1_d

Cu	-0.05517300	-0.25233600	-1.16768500
C	0.83416400	-0.95158000	-4.09744900
C	0.42421900	-1.38429200	-2.90671600
C	0.54607900	-2.45813600	-2.03348100
C	-0.60694400	-3.30385600	-1.71321400
C	-0.50223200	-4.39260800	-0.81404500
C	-1.87452200	-3.08295800	-2.30786500
C	-1.60047300	-5.19778000	-0.51510200
H	0.45419600	-4.62106100	-0.35405100
C	-2.96893200	-3.88731800	-1.99920000
H	-1.98123900	-2.27862100	-3.02760400
C	-2.84632300	-4.95014200	-1.09804900
H	-1.47863900	-6.03070200	0.17401200
H	-3.92577700	-3.69061700	-2.47772400
H	-3.69964700	-5.58285000	-0.86941100
H	1.32045400	-1.64147300	-4.78717900
H	0.67943600	0.06886900	-4.43262000
C	1.93379600	-2.88765400	-1.58616100
H	2.00771500	-3.05500800	-0.50357000
H	2.22398000	-3.83440500	-2.06867400
H	2.67562300	-2.13344900	-1.85294200
H	-0.90104300	-0.15290900	-2.54931300
P	-0.97901700	-0.32347500	0.99918500
P	1.38433700	1.57250300	-0.39207800
C	-0.43941300	1.26704200	1.81799500

C	0.98100500	1.72527300	1.43551500
C	0.90848100	3.25734500	-1.15978000
H	0.78622200	3.00832400	-2.22158300
C	3.24717900	2.00750900	-0.36348500
C	-2.78378100	-0.46302800	1.55694100
C	-0.42662100	-1.79961700	2.09269400
H	-0.11250900	-2.53755700	1.34741400
C	-1.71695400	-2.33515800	2.76374300
C	-2.91657000	-1.96885700	1.88035300
H	-2.83135400	0.07838400	2.51271800
C	2.16298300	4.14084500	-1.02650500
C	3.37464700	3.24231400	-1.28835300
H	3.44666000	2.34253300	0.66272700
C	-0.40816200	3.82308500	-0.67026300
C	-1.60813400	3.31348500	-1.19768600
C	-0.48824400	4.82536300	0.30792200
C	-2.84438000	3.78102700	-0.75383800
H	-1.56736000	2.52455600	-1.94515400
C	-1.72688400	5.30167300	0.74728200
H	0.41623300	5.25498400	0.72782900
C	-2.90876600	4.77980800	0.22182900
H	-3.75603800	3.35731600	-1.16443600
H	-1.76273000	6.08508300	1.50032500
H	-3.87159200	5.14837800	0.56556100
C	4.21024700	0.88713900	-0.68592400
C	5.16694800	0.48956600	0.25892700
C	4.21103700	0.25294100	-1.93835000
C	6.10347700	-0.50383600	-0.03588300
H	5.18293200	0.96949800	1.23520600
C	5.14951700	-0.73465800	-2.23836900
H	3.46240800	0.51828700	-2.68058600
C	6.10076700	-1.11715900	-1.28893600
H	6.83791700	-0.79164300	0.71215100
H	5.13221300	-1.21136900	-3.21487800
H	6.83022100	-1.88730300	-1.52457400
C	0.75157600	-1.52221700	3.00081400
C	0.61388200	-0.92815000	4.26650800
C	2.04918800	-1.84046100	2.56618800
C	1.72872800	-0.66275300	5.06412800
H	-0.37272600	-0.67343800	4.64340000
C	3.16648400	-1.57264200	3.35806300
H	2.18319700	-2.30525500	1.59272500
C	3.01115700	-0.98142200	4.61357400
H	1.59207500	-0.20747200	6.04176400

H	4.15654000	-1.83040100	2.99146000
H	3.87789600	-0.77648700	5.23617400
C	-3.85124700	0.10588300	0.64937800
C	-3.98437700	-0.29561900	-0.68875400
C	-4.77422700	1.02863200	1.16330800
C	-5.01443000	0.20956900	-1.48263200
H	-3.27416500	-0.99593800	-1.11521100
C	-5.80857800	1.53189800	0.37195900
H	-4.68590300	1.35170400	2.19864900
C	-5.93261500	1.12258800	-0.95684000
H	-5.09771700	-0.11184700	-2.51766600
H	-6.51591200	2.24093200	0.79491000
H	-6.73720800	1.50953400	-1.57688700
H	-3.86977400	-2.16998200	2.38370300
H	-2.90724800	-2.55702600	0.95461900
H	-1.63906900	-3.41761700	2.91790300
H	-1.85298400	-1.88160300	3.75253500
H	3.38352400	2.92275700	-2.33816900
H	4.32411200	3.75948600	-1.10499400
H	2.24147100	4.55440500	-0.01322900
H	2.11974900	4.99186600	-1.71753700
H	-0.51703900	1.18510600	2.90827200
H	-1.17424200	2.01258800	1.49213200
H	1.71943500	1.09350300	1.94365100
H	1.14141700	2.75376600	1.78296600

TS1_d’

Cu	-0.21301000	-0.08587700	-1.26953200
C	-1.34180900	-1.74420900	-3.78565500
C	-0.34490400	-1.33155100	-3.00938100
C	0.93699900	-1.67861300	-2.59102100
C	1.18556300	-2.90143000	-1.81062100
C	2.49853700	-3.26986900	-1.42910600
C	0.14897200	-3.79648100	-1.44317700
C	2.75142400	-4.43910500	-0.71060000
H	3.33501600	-2.63469400	-1.70176400
C	0.40713300	-4.95953600	-0.72412900
H	-0.86779200	-3.57408000	-1.75109000
C	1.71186300	-5.29507100	-0.34320300
H	3.77675200	-4.68298700	-0.44075800
H	-0.41907000	-5.62132300	-0.47146200
H	1.91204500	-6.20793800	0.21070400
H	-1.19388500	-2.61269400	-4.42867800

H	-2.30627200	-1.24872000	-3.81488700
C	2.10528300	-0.93788500	-3.22226700
H	2.88988000	-0.67611900	-2.50612800
H	2.57113900	-1.54297100	-4.01666500
H	1.75436800	-0.00833600	-3.68155200
H	-1.02280100	0.29579100	-2.63080400
P	-0.99214800	-0.72519700	0.90515500
P	0.63249900	1.94366900	-0.30510300
C	-0.94775200	0.88294000	1.85878100
C	0.25932600	1.77789200	1.52530800
C	-0.39101100	3.44235100	-0.91307300
H	-0.49836200	3.22962300	-1.98350800
C	2.24955200	2.97097000	-0.22212400
C	-2.66675500	-1.43796500	1.45551600
C	0.00456800	-2.01741800	1.91006000
H	0.41578000	-2.65976100	1.12524800
C	-1.04532000	-2.84403700	2.68749500
C	-2.32363900	-2.89507100	1.84416900
H	-2.92079100	-0.90616900	2.38302300
C	0.53050900	4.66858100	-0.76172200
C	1.95464800	4.21384100	-1.09131700
H	2.30145200	3.30957400	0.82111900
C	-1.78426000	3.54350200	-0.32685600
C	-2.82392200	2.79223000	-0.90268700
C	-2.08545900	4.34379200	0.78611100
C	-4.11550600	2.83109900	-0.37804300
H	-2.60337500	2.15381500	-1.75440700
C	-3.38084500	4.38954900	1.30847400
H	-1.31369300	4.94992900	1.25107400
C	-4.40027400	3.63202400	0.73115600
H	-4.89668800	2.22930200	-0.83348000
H	-3.59022100	5.02324200	2.16673800
H	-5.40755900	3.66864000	1.13768900
C	3.54350200	2.25434600	-0.53481900
C	4.44685600	1.96384700	0.49847600
C	3.90222600	1.89816700	-1.84383000
C	5.66929100	1.34217400	0.23688300
H	4.19043800	2.23122300	1.52103700
C	5.12406100	1.27935000	-2.10998900
H	3.22099100	2.09858100	-2.66592800
C	6.01432700	0.99884800	-1.07086600
H	6.35419700	1.13489500	1.05524700
H	5.37964700	1.01506100	-3.13270800
H	6.96700900	0.51987800	-1.27992600

C	1.16498600	-1.46416600	2.70794800
C	1.01838100	-0.94298500	4.00433000
C	2.44790700	-1.45154600	2.13502500
C	2.11161600	-0.42218600	4.69963800
H	0.04559900	-0.94830900	4.48808900
C	3.54160900	-0.92985600	2.82731400
H	2.58697200	-1.86669100	1.13987100
C	3.37863600	-0.41037300	4.11362100
H	1.97127500	-0.02995200	5.70381200
H	4.52168500	-0.93364200	2.35832100
H	4.23023300	-0.00992300	4.65740000
C	-3.83182100	-1.29037400	0.50293600
C	-3.77990700	-1.76949200	-0.81508200
C	-5.02446700	-0.70265000	0.94858700
C	-4.88882600	-1.66949800	-1.65493100
H	-2.86135100	-2.20398100	-1.19685000
C	-6.13696500	-0.60144800	0.11041500
H	-5.08414300	-0.32357100	1.96672000
C	-6.07316900	-1.08688800	-1.19652600
H	-4.82450500	-2.04532800	-2.67278400
H	-7.05200300	-0.14632600	0.48117900
H	-6.93658100	-1.01192600	-1.85231800
H	-3.15939000	-3.35410000	2.38575000
H	-2.15519300	-3.49329800	0.93991100
H	-0.65452500	-3.84543400	2.90354200
H	-1.27428000	-2.37475900	3.65187500
H	2.02681100	3.96054100	-2.15641800
H	2.69608300	4.99855000	-0.89880400
H	0.51134700	5.04715700	0.26756800
H	0.19641600	5.48842300	-1.40930300
H	-0.97378200	0.69298100	2.93828200
H	-1.87903300	1.39694500	1.59486300
H	1.16778300	1.34871500	1.96413100
H	0.11741700	2.76873700	1.97537000

Int2_a

C	-1.11799000	-1.03618800	1.80041700
C	-2.17646500	0.03488700	1.46607400
Cu	-0.23069500	0.15307100	-1.37514000
C	-3.74765900	-0.78346300	-0.99433400
H	-3.53100200	-0.86495900	-2.06729200
C	-3.50110700	1.90358200	-0.35487000
H	-3.84326400	2.00995900	0.68286400

C	1.41099500	-2.43650500	1.29881700
H	0.97093600	-2.77390400	2.24728900
C	1.64490000	0.28907100	1.74064800
H	2.18467100	0.78681300	0.92737200
P	-2.36754200	0.37806100	-0.36907300
P	0.45643000	-0.87768800	0.79391100
C	0.98070600	0.60567000	-2.93326700
H	0.68203600	1.58006900	-3.33215900
H	0.80575000	-0.17322500	-3.68526700
C	2.33266800	0.54568600	-2.37894200
C	3.12633300	1.53444500	-1.86790800
H	2.72655700	-0.46923300	-2.29831800
C	2.67484500	2.97845500	-1.87846900
H	3.50513400	3.65907400	-2.10660300
H	1.89567100	3.14140300	-2.62835200
H	2.25665800	3.30838500	-0.91312700
C	4.41495800	1.22124300	-1.21718900
C	4.98084900	2.09902700	-0.26489200
C	5.15023400	0.04499200	-1.49905000
C	6.18158200	1.80857000	0.38357200
H	4.46442900	3.02140400	-0.01621900
C	6.34518400	-0.24753500	-0.84798700
H	4.79388100	-0.63500300	-2.26735900
C	6.87392500	0.62985300	0.10439100
H	6.57619500	2.51193900	1.11380200
H	6.88019300	-1.16030300	-1.10158800
H	7.81174400	0.40441800	0.60516100
C	2.65032900	-0.63633500	2.46434000
C	2.82859200	-1.89686400	1.60980600
H	3.60010600	-0.11245600	2.62111800
H	2.27187300	-0.92776700	3.45192700
H	3.42450700	-2.66093300	2.12307100
H	3.35442600	-1.65079000	0.67872000
C	-4.72296700	1.47872300	-1.20695800
C	-5.05153900	0.02584700	-0.84661600
C	0.95872700	1.35704700	2.56431000
C	0.57797700	1.16407500	3.90175700
C	0.65053300	2.59113000	1.96612500
C	-0.08588900	2.16658300	4.61313000
H	0.80715700	0.22912500	4.40450500
C	-0.01819000	3.59202500	2.67084300
H	0.93943800	2.76540000	0.93282800
C	-0.39005100	3.38374700	4.00121700
H	-0.36283800	1.99389600	5.65015200

H	-0.24602800	4.53231100	2.17656800
H	-0.90503700	4.16296900	4.55680400
C	1.36179500	-3.58830900	0.31804100
C	1.01402100	-4.87160300	0.76317700
C	1.69060500	-3.42211800	-1.03707400
C	0.99848400	-5.95994100	-0.11253700
H	0.75707100	-5.02152000	1.80971800
C	1.67431500	-4.50568800	-1.91479100
H	1.94812500	-2.43476500	-1.40927900
C	1.32801700	-5.78029400	-1.45688200
H	0.73130800	-6.94645400	0.25808700
H	1.93266100	-4.35365100	-2.95957700
H	1.31844500	-6.62404600	-2.14173900
C	-3.69949800	-2.17962200	-0.41164800
C	-2.80665700	-3.11522200	-0.96210200
C	-4.48486600	-2.58046500	0.67916800
C	-2.68958400	-4.40048400	-0.43550000
H	-2.18944600	-2.82628800	-1.81038400
C	-4.37650900	-3.87118800	1.20441500
H	-5.19774400	-1.89212300	1.12323800
C	-3.47718100	-4.78454800	0.65327400
H	-1.97987900	-5.09662700	-0.87239500
H	-5.00058100	-4.16057000	2.04614400
H	-3.39308100	-5.78695200	1.06423900
C	-2.85643500	3.20675100	-0.77620900
C	-2.20506000	3.34118300	-2.01258100
C	-2.92920200	4.32778900	0.06242000
C	-1.65048900	4.56161000	-2.39843500
H	-2.11148900	2.48144300	-2.67059400
C	-2.37402900	5.55108800	-0.32072400
H	-3.42874800	4.24227200	1.02513900
C	-1.73287400	5.67186200	-1.55445800
H	-1.14686500	4.64230000	-3.35797100
H	-2.44666600	6.40821000	0.34397000
H	-1.29841200	6.62111200	-1.85582000
H	-5.56799900	2.15320600	-1.02542300
H	-4.47559600	1.55559900	-2.27368900
H	-5.41457600	-0.00903700	0.18810900
H	-5.84446600	-0.39045200	-1.47998900
H	-1.88044200	0.99511300	1.90535400
H	-3.14095300	-0.24065100	1.91041100
H	-0.90675200	-1.01815700	2.87641800
H	-1.50826800	-2.03262300	1.56148000

Int2_a'

C	1.11238800	1.35815100	1.77089700
C	2.43750700	0.84159800	1.17604800
Cu	0.18708200	-0.43652600	-1.07124100
C	2.88493700	2.11070700	-1.54820300
H	2.40889000	2.01605100	-2.53263100
C	4.03359400	-0.34701400	-0.97188900
H	4.61689700	-0.20001900	-0.05326000
C	-1.80040100	1.52257700	1.87720600
H	-1.31570800	2.17754000	2.61395200
C	-0.73216100	-0.98105700	2.37949600
H	-1.27403300	-1.70402400	1.75731800
P	2.35818600	0.49844300	-0.66681200
P	-0.40884600	0.44799200	1.15344100
C	-0.77206100	-1.75191200	-2.27449600
H	-0.08680300	-2.60828900	-2.28716700
H	-0.83186600	-1.32581500	-3.28101600
C	-2.06328400	-2.09722500	-1.67923700
C	-3.30945300	-1.62324700	-1.97475200
H	-2.00313600	-2.83997200	-0.88079700
C	-3.50240900	-0.65533400	-3.12558900
H	-4.38746700	-0.02446600	-2.98171100
H	-2.63622700	0.00933600	-3.22372300
H	-3.62588900	-1.16228500	-4.09517500
C	-4.50162900	-2.07850200	-1.23312900
C	-5.78518000	-2.05244100	-1.82270900
C	-4.43288500	-2.55539900	0.09713600
C	-6.91901100	-2.48722800	-1.13677700
H	-5.89353100	-1.70661200	-2.84643100
C	-5.56305700	-2.99612800	0.78020700
H	-3.47366000	-2.56519300	0.60792800
C	-6.82086700	-2.96568400	0.17062600
H	-7.88654300	-2.45671700	-1.63330700
H	-5.46349600	-3.35345500	1.80314800
H	-7.70456400	-3.30167300	0.70655800
C	-1.73153500	-0.42139000	3.41265900
C	-2.68130600	0.51754300	2.65956300
H	-2.26656000	-1.23557000	3.91658500
H	-1.20864300	0.14904300	4.19074000
H	-3.35859100	1.05165400	3.33636200
H	-3.30773800	-0.05442500	1.96328800
C	4.69241300	0.50815600	-2.08243600
C	4.40736300	1.97828000	-1.75757300

C	0.51746600	-1.66509400	2.88891000
C	1.14060600	-1.31582100	4.09666000
C	1.10913900	-2.67436000	2.10926800
C	2.31568300	-1.95019100	4.50846600
H	0.70566900	-0.55115700	4.73325400
C	2.28561900	-3.30437700	2.51401900
H	0.64044900	-2.96530900	1.17159100
C	2.89542700	-2.94370300	3.71861000
H	2.77472400	-1.66685700	5.45226400
H	2.72405300	-4.07422400	1.88549600
H	3.80828700	-3.43725400	4.04113200
C	-2.54418100	2.39643900	0.89055400
C	-2.65439300	3.77362500	1.12903900
C	-3.16531100	1.86296300	-0.25033200
C	-3.36683400	4.60153200	0.25842500
H	-2.18005200	4.20215600	2.00958200
C	-3.87566000	2.68931400	-1.12164500
H	-3.09468100	0.79900100	-0.46469900
C	-3.97980200	4.06038700	-0.87233600
H	-3.44542600	5.66550200	0.46806800
H	-4.34822800	2.25734900	-1.99903200
H	-4.53669400	4.69925700	-1.55269900
C	2.36188500	3.37869900	-0.90958400
C	1.06252200	3.81458900	-1.22085200
C	3.10784400	4.13387700	0.00806300
C	0.52139600	4.95611300	-0.63056200
H	0.46616900	3.24659900	-1.93168300
C	2.57120300	5.28213700	0.59640700
H	4.12105600	3.83885700	0.26376700
C	1.27633000	5.69638900	0.28308100
H	-0.49046800	5.26025000	-0.88117000
H	3.17187100	5.85416900	1.29898900
H	0.86079500	6.58966800	0.74147900
C	3.97992900	-1.83163200	-1.26265900
C	3.21818200	-2.34971100	-2.32218900
C	4.73063200	-2.72459900	-0.48556900
C	3.21312600	-3.71725600	-2.59644700
H	2.60744700	-1.68376600	-2.92555900
C	4.72800800	-4.09486700	-0.75745500
H	5.32733100	-2.34218800	0.33994400
C	3.96853600	-4.59591500	-1.81546100
H	2.61238300	-4.09678100	-3.41850200
H	5.32278500	-4.76738100	-0.14445200
H	3.96297100	-5.66111800	-2.03007500

H	5.76637300	0.29620700	-2.14203100
H	4.26010900	0.24722000	-3.05705000
H	4.94964100	2.25166800	-0.84406100
H	4.75222200	2.65374700	-2.55006300
H	2.69955700	-0.11976900	1.63369900
H	3.24826300	1.54339400	1.40784300
H	1.16835400	1.33847800	2.86633100
H	0.95633000	2.40197200	1.47279400

Int2_b

C	1.02910600	2.34638900	0.19288700
C	2.11167600	1.65572600	-0.66096500
H	0.28312800	2.81298800	-0.46174400
H	1.48473100	3.14666000	0.78841700
H	2.48388100	2.35085300	-1.42344100
H	2.96365400	1.38122300	-0.02720800
Cu	0.11356800	-1.01249700	0.15545700
C	0.84367200	0.47629500	-3.16399500
H	0.14324900	-0.34729300	-3.35234000
C	3.17765200	-0.62929500	-2.15057200
H	3.89470400	0.20087800	-2.10033700
C	-1.32083900	2.30168800	1.93126400
H	-0.97089100	3.32848800	1.75683500
C	0.93614800	1.07542200	2.96794200
H	0.68515800	0.06425400	3.31059800
P	1.54952600	0.04527400	-1.44155600
P	0.04870700	1.16808100	1.27361000
C	-0.49515800	-2.86013200	0.72033100
H	0.42028700	-3.28809300	1.14961200
H	-0.76891200	-3.43111200	-0.17179800
C	-1.54006300	-2.75909800	1.74136300
C	-2.90912600	-2.79966900	1.70919700
H	-1.13126300	-2.61930600	2.74698100
C	-3.64984600	-2.73400700	3.03488700
H	-4.43298300	-1.96181000	3.04161800
H	-4.14653500	-3.68214000	3.29061300
H	-2.95731400	-2.51108000	3.85375100
C	-3.73715700	-2.92967300	0.49587600
C	-3.25911000	-2.63329200	-0.80363400
C	-5.09549700	-3.31955400	0.58700600
C	-4.07585100	-2.74118400	-1.92794700
H	-2.24292600	-2.28217800	-0.92759900
C	-5.90895800	-3.43205800	-0.53952900

H	-5.52217300	-3.55014900	1.55736300
C	-5.40651900	-3.14877000	-1.81112000
H	-3.66693300	-2.49898800	-2.90713500
H	-6.94375100	-3.74602400	-0.42028400
H	-6.03916900	-3.23879700	-2.69038000
C	-1.28644500	2.06188800	3.45970400
C	0.18848600	2.07194200	3.88069300
C	2.85980200	-0.87872700	-3.64547200
C	2.02706900	0.30947300	-4.13996800
C	3.77238400	-1.81210800	-1.41647900
C	5.09737200	-1.75843300	-0.96173500
C	3.04034100	-2.98991400	-1.19633700
C	5.68070400	-2.84792000	-0.31052200
H	5.68064700	-0.85406600	-1.12245300
C	3.61981200	-4.07950000	-0.54626600
H	2.00338300	-3.05055200	-1.51512400
C	4.94263500	-4.01358200	-0.10100900
H	6.71184400	-2.78501000	0.02806100
H	3.03290500	-4.97918600	-0.38250900
H	5.39215800	-4.86336900	0.40560600
C	0.05164300	1.76491400	-3.21060300
C	-1.30100100	1.74756100	-2.82870200
C	0.61522900	2.99360400	-3.58642600
C	-2.06149400	2.91617300	-2.80708600
H	-1.76167500	0.80585900	-2.53822000
C	-0.14674800	4.16494400	-3.57513700
H	1.65296100	3.04609000	-3.90233600
C	-1.48493200	4.13279400	-3.18159000
H	-3.09977300	2.87330100	-2.49172400
H	0.31025000	5.10368000	-3.87792700
H	-2.07503400	5.04516000	-3.17157500
C	2.44423400	1.16806600	2.89503000
C	3.14128600	2.38243700	2.99324200
C	3.19030700	-0.00419700	2.68223300
C	4.53308500	2.42287500	2.87851000
H	2.60292900	3.30902200	3.17014800
C	4.57925100	0.03360900	2.56048000
H	2.67133100	-0.95741500	2.60752600
C	5.25807000	1.25095700	2.65842200
H	5.05010600	3.37517700	2.96544000
H	5.12684200	-0.88854700	2.38764200
H	6.34069300	1.28460100	2.57091200
C	-2.68141000	2.15091100	1.28316700
C	-3.29501500	0.89885700	1.11908900

C	-3.37261100	3.29491500	0.85871600
C	-4.56373300	0.79781000	0.54526700
H	-2.78243700	-0.00981600	1.42634300
C	-4.64439600	3.19746900	0.28993600
H	-2.91027200	4.27304300	0.97712700
C	-5.24299000	1.94644100	0.13016600
H	-5.01195700	-0.18303000	0.41729500
H	-5.16424000	4.09835800	-0.02701300
H	-6.23084000	1.86500600	-0.31567900
H	-1.74514600	1.09246900	3.69430700
H	-1.87134500	2.82887500	3.98092200
H	0.32170000	1.80506900	4.93619700
H	0.58473800	3.08699100	3.75491400
H	3.78635900	-1.00299000	-4.21820100
H	2.28962900	-1.81053600	-3.75379400
H	1.66764500	0.16579400	-5.16626200
H	2.65727400	1.20744500	-4.14409500

Int2_b’

C	-1.58025500	0.78412200	1.71273300
C	-0.86691600	2.06411300	1.23605700
H	-2.61641600	0.77886500	1.35319600
H	-1.61550900	0.76882900	2.80829500
H	-1.45673900	2.94619100	1.51383800
H	0.10516000	2.15175400	1.73598500
Cu	-0.03370700	-0.22334400	-1.21496000
C	-1.94646200	2.93990400	-1.45939700
H	-1.90316500	2.53738900	-2.47959000
C	0.65482500	3.58242600	-0.74813200
H	0.58525900	4.10558000	0.21480900
C	-2.05450400	-2.10244200	1.64156300
H	-2.63644200	-1.62635700	2.44271300
C	0.54138200	-1.34518900	2.26516600
H	1.26282300	-1.84844700	1.61127000
P	-0.48063000	2.06664800	-0.59882300
P	-0.82130100	-0.79212800	1.03708100
C	0.72448800	-1.27289500	-2.77862300
H	1.68987900	-0.82296900	-3.02739700
H	0.03191200	-1.10825500	-3.61285300
C	0.76303300	-2.69025800	-2.41401600
C	1.67069400	-3.49615600	-1.77431500
H	-0.14970100	-3.21713500	-2.70683600
C	1.32029200	-4.96904700	-1.63686100

H	1.98947000	-5.61944300	-2.22005900
H	1.37730000	-5.32322000	-0.59648900
H	0.30312200	-5.16065100	-1.99459500
C	2.96696500	-3.07496100	-1.21640300
C	3.35337000	-1.71961800	-1.06023700
C	3.90414800	-4.03947500	-0.76809700
C	4.58831500	-1.36390300	-0.51646800
H	2.67717600	-0.93044700	-1.35644400
C	5.13682300	-3.68159500	-0.22671400
H	3.66935700	-5.09463800	-0.85390000
C	5.49601500	-2.33852600	-0.09733900
H	4.84050000	-0.30869600	-0.43049300
H	5.82339600	-4.46226800	0.09401800
H	6.46037800	-2.05881100	0.31891400
C	-1.14848400	-3.17079200	2.29830600
C	-0.12035300	-2.42264200	3.15412500
C	-0.03741500	4.47239100	-1.81045000
C	-1.54435000	4.42707400	-1.53301300
C	2.11403800	3.28262800	-1.01921900
C	3.10504400	3.83018800	-0.19263000
C	2.51570500	2.48629300	-2.10357500
C	4.45960300	3.59717300	-0.44120300
H	2.81252700	4.44817600	0.65365300
C	3.86767500	2.25058800	-2.35416500
H	1.76726000	2.02782100	-2.74439600
C	4.84556600	2.80649400	-1.52446600
H	5.21094800	4.03580300	0.21055600
H	4.15673600	1.62457800	-3.19373500
H	5.89817500	2.62230900	-1.72148300
C	-3.30312200	2.58968200	-0.88842000
C	-3.93359100	1.40527500	-1.30741500
C	-3.95349400	3.37730100	0.07340500
C	-5.16146900	1.01228200	-0.77635900
H	-3.45007300	0.78211700	-2.05679400
C	-5.18852200	2.99094600	0.60101900
H	-3.50586800	4.30685300	0.41197100
C	-5.79563600	1.80651000	0.18284200
H	-5.61710800	0.08438600	-1.10967400
H	-5.67598300	3.62207700	1.33973600
H	-6.75554300	1.50759600	0.59514900
C	1.26797700	-0.21904700	2.96795600
C	0.79710500	0.36810700	4.15375700
C	2.45235100	0.28689800	2.40611400
C	1.48023300	1.42996600	4.75061400

H	-0.10555900	-0.00603700	4.62860900
C	3.13303600	1.35166900	2.99770800
H	2.84731800	-0.16885700	1.50131900
C	2.64847200	1.93028100	4.17318600
H	1.09830800	1.86328400	5.67161600
H	4.04430200	1.72416900	2.53793600
H	3.18015700	2.75548300	4.63952000
C	-3.02081000	-2.62401000	0.60163300
C	-2.57044900	-3.23826100	-0.57782700
C	-4.40263000	-2.52611600	0.81561200
C	-3.47771100	-3.74068700	-1.51040400
H	-1.50461800	-3.31281600	-0.77487900
C	-5.31347900	-3.02946100	-0.11650000
H	-4.77004400	-2.05488600	1.72488200
C	-4.85322700	-3.63895700	-1.28444900
H	-3.10784600	-4.21206000	-2.41726600
H	-6.38074700	-2.94897800	0.07450500
H	-5.55817000	-4.03312500	-2.01158400
H	-0.64034100	-3.75794400	1.52272600
H	-1.74917300	-3.87110900	2.89078000
H	0.63997300	-3.09527000	3.56867000
H	-0.63580800	-1.96022700	4.00481600
H	0.36166700	5.49282000	-1.77353600
H	0.17238700	4.08285900	-2.81511100
H	-2.12424600	4.95099500	-2.30281800
H	-1.74557600	4.93224500	-0.58015800

Int2_c

Cu	0.07070400	-0.32003200	-1.06696500
C	1.43149300	-0.62293400	-4.56510000
C	1.24007400	-1.33266200	-3.43067700
C	-0.01314900	-1.59986400	-2.69518000
H	0.62516300	-0.13420700	-5.10480300
H	2.42600800	-0.51896400	-4.99120800
H	2.13413200	-1.78767000	-3.00414600
P	-1.03089500	-0.48952000	1.15305500
P	0.99198700	1.72515900	-0.29751700
C	-0.70428100	1.17623000	1.95592300
C	0.62271300	1.83832100	1.53516800
C	0.23011700	3.27339600	-1.12212200
H	0.03857200	2.93081000	-2.14638000
C	2.76063700	2.41323600	-0.37956900
C	-2.80229100	-0.84109900	1.75679900

C	-0.26494700	-1.81964300	2.29667100
H	-0.04620400	-2.63491500	1.59679800
C	-1.41475700	-2.28499000	3.21503500
C	-2.70406500	-2.25064700	2.38817300
H	-2.98358000	-0.12686300	2.57122600
C	1.37567400	4.30601400	-1.18605800
C	2.67387700	3.53343900	-1.44388600
H	2.93314200	2.89514900	0.59222800
C	-1.09164500	3.72078100	-0.53690300
C	-2.28149500	3.15073400	-1.02067700
C	-1.18726200	4.66841600	0.49396300
C	-3.52147500	3.50397700	-0.48907300
H	-2.23244000	2.41833500	-1.82349800
C	-2.42826800	5.02924100	1.02453800
H	-0.29225800	5.14216800	0.88624900
C	-3.59971900	4.44733200	0.53856000
H	-4.42260300	3.03795300	-0.87645000
H	-2.47623100	5.77100100	1.81772800
H	-4.56419100	4.73022600	0.95155200
C	3.86105100	1.39937300	-0.60532400
C	4.91216400	1.29376600	0.31613000
C	3.88018600	0.57224400	-1.73974700
C	5.95976400	0.39226800	0.11334600
H	4.91213000	1.92673200	1.20111700
C	4.92542900	-0.32932400	-1.94278900
H	3.07083600	0.61281900	-2.46443500
C	5.96966000	-0.42337900	-1.01882100
H	6.76763700	0.33219400	0.83836700
H	4.92141000	-0.96096900	-2.82721400
H	6.78304700	-1.12551300	-1.18136100
C	1.03665700	-1.41785700	2.95508000
C	1.09671300	-0.78244200	4.20564500
C	2.24591200	-1.66188900	2.28180300
C	2.32083900	-0.39746700	4.75803000
H	0.18636400	-0.59101000	4.76631600
C	3.46906700	-1.27169600	2.82697500
H	2.21988500	-2.16780700	1.32004100
C	3.51159500	-0.63515500	4.07001000
H	2.34087000	0.08639000	5.73137600
H	4.38618500	-1.46376000	2.27752400
H	4.46292100	-0.33513000	4.50123600
C	-3.90119300	-0.67322200	0.73153100
C	-3.94072300	-1.45173100	-0.43594600
C	-4.93097400	0.25225700	0.94979300

C	-4.98150600	-1.30779600	-1.35326800
H	-3.14898100	-2.16959100	-0.63338800
C	-5.97508800	0.39784000	0.03281400
H	-4.91814700	0.86216200	1.85065700
C	-6.00331600	-0.38229000	-1.12363600
H	-4.99340900	-1.91985800	-2.25131800
H	-6.76730000	1.11666900	0.22706500
H	-6.81430600	-0.27362600	-1.83879200
C	-0.04444000	-2.89415100	-1.94716500
C	1.07757100	-3.38262600	-1.22340700
C	-1.20733300	-3.70034800	-1.88146900
C	1.02533200	-4.55266500	-0.47109700
H	2.00743700	-2.81924600	-1.23768000
C	-1.26266800	-4.86687600	-1.11421000
H	-2.08456300	-3.41859100	-2.45417400
C	-0.15253000	-5.30632300	-0.39264500
H	1.91598500	-4.88095900	0.06158000
H	-2.18292000	-5.44824000	-1.10202500
H	-0.19222500	-6.21955800	0.19469800
C	-1.27202500	-1.26836400	-3.49819200
H	-1.21131400	-0.25546600	-3.91167500
H	-1.41668700	-1.95199400	-4.35442100
H	-2.18099700	-1.30264500	-2.88863700
H	-2.66439400	-3.01369500	1.60078100
H	-3.59275700	-2.45845500	2.99604200
H	-1.52512200	-1.61236100	4.07457800
H	-1.20663400	-3.28503000	3.61428200
H	3.55811400	4.17935400	-1.39026500
H	2.65875300	3.09223100	-2.44862200
H	1.17760300	5.05547600	-1.96188500
H	1.46593800	4.84568600	-0.23539000
H	0.63688800	2.88300500	1.87002000
H	1.46189200	1.32996400	2.02479900
H	-1.54615900	1.80729300	1.64697900
H	-0.74250700	1.09831300	3.04928800

Int2_c’

Cu	-0.00200500	-0.35783000	-1.08355900
C	2.11817400	-2.13245000	-3.82616900
C	0.98853200	-1.45145000	-3.54017800
C	-0.14017700	-1.73567400	-2.61743600
H	2.37123900	-3.08217900	-3.36537100
H	2.81774400	-1.74898100	-4.56486400

H	0.83594800	-0.52748500	-4.10678600
P	-1.02999800	-0.40200100	1.17349100
P	0.94164600	1.72957400	-0.44319200
C	-0.73889500	1.32412000	1.85180700
C	0.57112000	1.98145100	1.37534000
C	0.18636300	3.20554200	-1.39518100
H	-0.02329600	2.77284500	-2.38113700
C	2.70789800	2.40629400	-0.57190700
C	-2.77226000	-0.76994200	1.85265900
C	-0.19004100	-1.62661600	2.38312800
H	0.04380500	-2.47662000	1.73119100
C	-1.30087900	-2.07395700	3.35655600
C	-2.60985500	-2.13401300	2.56329000
H	-2.94886900	-0.01393300	2.62975900
C	1.34080300	4.21581000	-1.57029300
C	2.63158000	3.40796300	-1.74979000
H	2.86504500	2.99331000	0.34337100
C	-1.12359200	3.71459800	-0.83428100
C	-2.32320500	3.10682400	-1.24233700
C	-1.19832600	4.75059600	0.10944600
C	-3.55238900	3.50995200	-0.72118100
H	-2.28955000	2.30354900	-1.97508500
C	-2.42854700	5.16137200	0.62872000
H	-0.29486200	5.25380600	0.44097800
C	-3.60984800	4.54163500	0.21926200
H	-4.46138300	3.01333100	-1.04785900
H	-2.46044200	5.97101800	1.35334700
H	-4.56582900	4.86296000	0.62380300
C	3.82258100	1.38579000	-0.67183300
C	4.96336700	1.52973500	0.13105200
C	3.77403500	0.31420600	-1.57624600
C	6.03075200	0.63452400	0.03242200
H	5.01757800	2.35383600	0.83968000
C	4.83682900	-0.58450800	-1.67299200
H	2.89950300	0.15273000	-2.20021700
C	5.97041600	-0.42794600	-0.87134900
H	6.90705400	0.76879700	0.66177000
H	4.76444700	-1.40908900	-2.37678800
H	6.79804400	-1.12810000	-0.94938500
C	1.10985600	-1.13882800	2.98503600
C	1.17321700	-0.42938700	4.19483000
C	2.31227300	-1.37939000	2.29845100
C	2.39449100	0.02873300	4.69555100
H	0.26847700	-0.23579100	4.76376900

C	3.53206100	-0.91607400	2.79112600
H	2.28412000	-1.93837100	1.36665100
C	3.57795800	-0.20792900	3.99474800
H	2.41791200	0.56959400	5.63835100
H	4.44326900	-1.10605800	2.23140000
H	4.52693700	0.14980600	4.38515600
C	-3.90714100	-0.68822300	0.85676400
C	-4.01357700	-1.58680000	-0.21676300
C	-4.90375600	0.28603100	1.00890000
C	-5.08674400	-1.51241600	-1.10486400
H	-3.24979300	-2.34518000	-0.36694700
C	-5.97862500	0.36366100	0.11997400
H	-4.84029800	0.98903300	1.83680800
C	-6.07416100	-0.53714600	-0.94127400
H	-5.14992000	-2.21792100	-1.92913800
H	-6.74352700	1.12282800	0.26360800
H	-6.91023300	-0.48309100	-1.63334200
C	-0.08791600	-2.99589400	-1.81756600
C	1.07253300	-3.36508700	-1.08715900
C	-1.20101000	-3.85781400	-1.68114300
C	1.10565200	-4.49101800	-0.26890200
H	1.95713500	-2.73837300	-1.16212700
C	-1.17097600	-4.98240300	-0.85087100
H	-2.10684700	-3.65160600	-2.24155800
C	-0.02183100	-5.31112400	-0.13206800
H	2.02086300	-4.73303800	0.26822500
H	-2.05391800	-5.61526600	-0.78211100
H	0.00503600	-6.19123500	0.50483200
C	-1.47543700	-1.48559600	-3.34187000
H	-1.44102000	-0.53255300	-3.88433900
H	-1.69958300	-2.26704800	-4.09112300
H	-2.32980400	-1.43490700	-2.65794200
H	-2.56070200	-2.94278900	1.82382500
H	-3.47557000	-2.33483500	3.20567400
H	-1.41473800	-1.35496700	4.17726400
H	-1.04757600	-3.04011000	3.80947400
H	3.52197900	4.04737200	-1.76631000
H	2.61117600	2.86086400	-2.70148700
H	1.14537800	4.88325700	-2.41827200
H	1.44044800	4.84904500	-0.68012900
H	0.56447700	3.04899400	1.62775600
H	1.42164000	1.52840700	1.89816400
H	-1.59763800	1.91217200	1.50555700
H	-0.76824400	1.32251400	2.94815700

Int2_d

Cu	0.05400300	-0.29203000	-0.96803700
C	-1.58076300	0.14165800	-4.06377500
C	-1.41675000	-0.75739400	-3.06113200
C	-0.19607500	-1.46606000	-2.64751600
H	-0.78726600	0.39964300	-4.75983800
H	-2.53536700	0.63941500	-4.21235400
H	-2.29822500	-0.94930100	-2.44657100
P	1.18514600	1.66219900	-0.24161700
P	-0.96135400	-0.40123900	1.25812300
C	0.87723800	1.79562200	1.60435100
C	-0.47335800	1.21943700	2.07205300
C	-0.23594600	-1.79019700	2.34950700
H	-0.21545100	-2.64453400	1.66093900
C	-2.72004800	-0.62245100	1.97078700
C	3.00141000	2.22455300	-0.34085400
C	0.53009100	3.27175700	-1.02571800
C	1.71204400	4.25900900	-0.96740700
H	1.56228700	5.08922000	-1.66841900
C	2.97673500	3.45424300	-1.28466500
H	3.24750900	2.58643900	0.66599600
H	2.95357500	3.11719000	-2.32897500
H	3.89084000	4.04661100	-1.16046400
C	-1.31151600	-2.07305200	3.41588200
C	-2.66906800	-1.98025000	2.71350000
H	-2.82084600	0.16603500	2.72806700
C	1.18042600	-1.54592300	2.82086500
C	2.24857000	-1.89490600	1.97652200
C	1.48252400	-0.96027900	4.05998100
C	3.57068400	-1.65202900	2.34733100
H	2.03283800	-2.36601000	1.02055900
C	2.80707700	-0.72257900	4.43719800
H	0.68555500	-0.69447900	4.74819600
C	3.85586200	-1.06194400	3.58157400
H	4.37657300	-1.92202000	1.67111000
H	3.01623900	-0.27473700	5.40550400
H	4.88537900	-0.87729600	3.87651700
C	-3.86659300	-0.48061700	0.99420400
C	-4.81861500	0.53244700	1.17278200
C	-4.03349100	-1.36958600	-0.07938300
C	-5.90914600	0.65718000	0.30858300
H	-4.70689900	1.22964200	2.00046100

C	-5.12145600	-1.24731100	-0.94352500
H	-3.30552100	-2.15805600	-0.25219500
C	-6.06481800	-0.23396100	-0.75357400
H	-6.63824200	1.44706800	0.47108900
H	-5.23075200	-1.94501000	-1.76964300
H	-6.91262600	-0.14202700	-1.42708700
C	-0.81206900	3.72974100	-0.49883000
C	-0.94148200	4.65085400	0.55183700
C	-1.98388000	3.19623500	-1.06352600
C	-2.20155000	5.02172300	1.02857200
H	-0.05866100	5.09695700	1.00060300
C	-3.24176400	3.56060600	-0.58355400
H	-1.90660700	2.48734800	-1.88592400
C	-3.35599000	4.47557700	0.46649200
H	-2.27737000	5.74319600	1.83824100
H	-4.13171100	3.12630000	-1.02967700
H	-4.33553600	4.76598100	0.83688200
C	4.01462900	1.16667600	-0.72162900
C	3.87836200	0.40419400	-1.89192600
C	5.14754700	0.96137000	0.07755000
C	4.84720000	-0.53237300	-2.25169700
H	3.00206100	0.53182100	-2.52092200
C	6.12129000	0.02599700	-0.28060500
H	5.27035300	1.54225100	0.98915800
C	5.97391700	-0.72487500	-1.44770400
H	4.71897900	-1.11366400	-3.16084400
H	6.99444500	-0.11249000	0.35197600
H	6.72904900	-1.45368800	-1.72958900
C	-0.37385500	-2.82510300	-2.05159000
C	0.72004900	-3.51426000	-1.46703300
C	-1.61519000	-3.50355900	-2.01507400
C	0.57265900	-4.75013400	-0.84411000
H	1.70343300	-3.04927500	-1.48515700
C	-1.76803700	-4.73621900	-1.37414000
H	-2.47228000	-3.06820400	-2.51935400
C	-0.68112800	-5.37052500	-0.77215200
H	1.44379100	-5.23417600	-0.40653900
H	-2.74524600	-5.21589000	-1.37273300
H	-0.79738200	-6.33461200	-0.28440500
C	0.96264700	-1.35063000	-3.64080800
H	0.72059100	-1.83808800	-4.60219200
H	1.19321500	-0.30225800	-3.86812800
H	1.88155900	-1.81009600	-3.26501500
H	1.80595200	4.69709200	0.03424400

H	0.39146200	2.98678700	-2.07629800
H	-3.50780600	-2.06041900	3.41519000
H	-2.77139900	-2.80234900	1.99464200
H	-1.15179800	-3.05419300	3.87967600
H	-1.26993500	-1.32650900	4.21911800
H	0.97017400	2.83716200	1.93714500
H	1.69734700	1.23488500	2.06802900
H	-1.27986200	1.91614300	1.81388700
H	-0.46964200	1.12070100	3.16471800

Int2_d’

Cu	-0.06205600	-0.37495800	-0.98859600
C	-1.62247200	-3.09789400	-3.35627300
C	-0.97169900	-1.91960100	-3.25686900
C	0.33010200	-1.53537000	-2.65356300
H	-1.23638700	-4.03184000	-2.96170900
H	-2.57204000	-3.15403100	-3.88337600
H	-1.46397200	-1.07154100	-3.74259400
P	0.72092800	1.84820200	-0.21709100
P	-1.10860500	-0.57631700	1.15341900
C	0.24377200	1.91446000	1.60110000
C	-1.01172700	1.10416000	1.97346400
C	-0.21571800	-1.82459500	2.29040500
H	0.09579000	-2.60283300	1.58416600
C	-2.83552800	-1.14961300	1.69559900
C	2.36968400	2.82418500	-0.14754900
C	-0.21563400	3.30654400	-1.01259700
C	0.65857800	4.54221300	-0.73603900
H	0.37007000	5.38408100	-1.37791700
C	2.11077500	4.11388000	-0.96669700
H	2.47751900	3.11262400	0.90543600
H	2.26951000	3.91611200	-2.03373300
H	2.82493500	4.89488800	-0.68001800
C	-1.31880100	-2.42582400	3.18762600
C	-2.58485300	-2.53960100	2.33122600
H	-3.12402200	-0.46921600	2.50845900
C	1.03379200	-1.30006800	2.96316100
C	2.27220800	-1.45344600	2.31593200
C	1.01153300	-0.64299100	4.20376700
C	3.44510100	-0.95380900	2.88295800
H	2.31763200	-1.97757600	1.36406800
C	2.18602300	-0.14709600	4.77478600
H	0.07485600	-0.52188500	4.74075800

C	3.40737000	-0.29626500	4.11512900
H	4.38791000	-1.08383300	2.35915700
H	2.14444600	0.35180500	5.73979800
H	4.32122500	0.08614500	4.56222900
C	-3.93171900	-1.12252800	0.65115900
C	-5.18603400	-0.58953300	0.98332900
C	-3.75416200	-1.66025100	-0.63245000
C	-6.23785600	-0.59541400	0.06510800
H	-5.34134100	-0.16729000	1.97418800
C	-4.80270100	-1.66375400	-1.55312000
H	-2.79273100	-2.06319300	-0.93868200
C	-6.04889200	-1.13334800	-1.20952300
H	-7.20229000	-0.17992600	0.34651600
H	-4.63360700	-2.08280200	-2.54110100
H	-6.86458200	-1.13995600	-1.92783800
C	-1.68420800	3.37141300	-0.65151900
C	-2.20557000	4.30946100	0.25040300
C	-2.56883600	2.44144700	-1.22599700
C	-3.56619700	4.31233400	0.57372900
H	-1.55733000	5.05513600	0.70038800
C	-3.92361700	2.43621600	-0.89938800
H	-2.18412100	1.70526800	-1.92911600
C	-4.42830500	3.37494300	0.00557100
H	-3.94876600	5.05387400	1.27061200
H	-4.58147000	1.69573600	-1.34444800
H	-5.48445000	3.37494600	0.26061100
C	3.61142400	2.05912200	-0.54991700
C	3.82204000	1.63927400	-1.87210600
C	4.60113100	1.77326400	0.40069400
C	4.98423300	0.95795500	-2.23244100
H	3.06744100	1.83801200	-2.62825300
C	5.76685600	1.09152400	0.04422600
H	4.45720800	2.08782000	1.43192200
C	5.96345100	0.68222300	-1.27496300
H	5.12374200	0.64152700	-3.26264700
H	6.52281600	0.88615600	0.79792400
H	6.86987000	0.15299100	-1.55585300
C	1.13636300	-2.58294700	-1.95682700
C	2.54801200	-2.63933300	-2.05406600
C	0.54307500	-3.54664500	-1.09682200
C	3.30538800	-3.57031100	-1.33977000
H	3.06895100	-1.93844800	-2.69641100
C	1.29822200	-4.48190000	-0.39453300
H	-0.53519900	-3.54559700	-0.97450200

C	2.69390200	-4.50419100	-0.50321400
H	4.38790900	-3.56800600	-1.45163600
H	0.79170300	-5.20497900	0.24243000
H	3.28323900	-5.23647100	0.04202600
C	1.12219600	-0.67970700	-3.65886000
H	1.52638400	-1.28143700	-4.49318700
H	0.47091100	0.08351700	-4.10315200
H	1.96583200	-0.15537500	-3.19843500
H	0.54070100	4.87589400	0.30293500
H	-0.14707200	3.08744900	-2.08715000
H	-3.45735400	-2.85370000	2.91621800
H	-2.44240000	-3.28709800	1.54007800
H	-1.00105700	-3.39555200	3.58960300
H	-1.52392800	-1.77475400	4.04674200
H	0.12208500	2.95532700	1.92757300
H	1.11155200	1.50847200	2.13423700
H	-1.91100600	1.63383300	1.63812800
H	-1.07853900	1.00973700	3.06432300

TS2_ac

C	0.19759500	-2.26930400	0.85833500
C	1.41679100	-1.53909100	1.45105800
Cu	-0.04895600	0.82065500	-0.53454600
C	3.09059600	0.76262300	2.01930200
C	0.51024500	0.86730700	3.02141000
C	-1.99468300	-2.55091200	-1.05262500
P	1.33325600	0.33723900	1.38456700
P	-0.44017200	-1.51623900	-0.73153200
C	1.27679200	1.79286000	-3.07905600
H	2.09979100	2.34703000	-2.63834500
H	1.51569400	1.15799900	-3.92782700
C	-0.01167900	1.89617200	-2.63317900
C	-0.53199800	2.62182100	-1.47550900
H	-0.74906900	1.30576300	-3.18126200
C	0.38110800	3.72661000	-0.93814100
H	0.44834600	4.57205100	-1.64610900
H	1.40016100	3.36273200	-0.77514000
H	0.02651700	4.13045800	0.01541300
C	-1.98487900	2.95779100	-1.46316200
C	-2.60255700	3.45641200	-0.29036600
C	-2.81928800	2.84480100	-2.59846400
C	-3.94993800	3.79941300	-0.24848100
H	-2.00616200	3.56196700	0.61300600

C	-4.17722500	3.17153800	-2.55487200
H	-2.39487700	2.52664500	-3.54593800
C	-4.75920600	3.65356400	-1.38188800
H	-4.37618000	4.17859100	0.67818300
H	-4.77592400	3.07241800	-3.45828900
H	-5.81115800	3.92549600	-1.35262300
C	0.51194100	-2.29633900	-2.19964100
C	-1.88006600	-2.90081700	-2.55498200
C	-0.43789000	-3.36130100	-2.79669300
C	2.85356200	1.58383100	3.30944700
C	1.65856800	0.96517100	4.04285800
H	-2.61071900	-3.67204600	-2.82582600
H	-2.10925500	-2.01471200	-3.16183200
H	-0.28883600	-4.33022500	-2.30540900
H	-0.22318000	-3.51001600	-3.86176500
H	1.35813900	1.55610900	4.91690600
H	1.93990800	-0.02992600	4.41009300
H	2.63063400	2.62791000	3.05692700
H	3.76026000	1.59262400	3.92596200
H	0.17330400	1.88942600	2.80410300
H	3.51593800	-0.20408000	2.31807600
C	-0.71040100	0.05060400	3.38852600
C	-1.92636200	0.30955500	2.73136300
C	-0.67687400	-0.98328300	4.33537000
C	-3.06447700	-0.45079500	2.99578400
H	-1.97759300	1.10953700	1.99573600
C	-1.82018900	-1.73930800	4.61113700
H	0.23974400	-1.20151600	4.87502300
C	-3.01505600	-1.48084100	3.93942500
H	-3.98495500	-0.24329800	2.45847200
H	-1.77201800	-2.53080200	5.35489300
H	-3.90174900	-2.07281000	4.14908000
C	4.03284300	1.39098000	1.01641900
C	3.85391200	2.70238300	0.54937800
C	5.13648800	0.66640800	0.54429800
C	4.74662400	3.26794000	-0.36113500
H	3.00709300	3.28952800	0.89299300
C	6.03351100	1.22940800	-0.36608300
H	5.29647300	-0.35073300	0.89492900
C	5.84134100	2.53351800	-0.82328300
H	4.58499100	4.28429000	-0.70996200
H	6.88579200	0.64959900	-0.71155300
H	6.53754900	2.97532100	-1.53086100
C	1.93108000	-2.73008100	-1.90099100

C	2.24448200	-3.98783400	-1.36026800
C	2.98764200	-1.83870800	-2.15370100
C	3.56637300	-4.34142300	-1.08119000
H	1.45636100	-4.70843900	-1.16074400
C	4.30890100	-2.18936500	-1.87378600
H	2.76562800	-0.85749200	-2.56687800
C	4.60494700	-3.44394000	-1.33577400
H	3.78321700	-5.32359700	-0.66882100
H	5.10454300	-1.47857700	-2.07868400
H	5.63378600	-3.72254100	-1.12364300
C	-3.32225500	-1.95753900	-0.63370700
C	-3.70947900	-0.65901100	-0.99766800
C	-4.22378300	-2.74117000	0.10179400
C	-4.96298400	-0.16120300	-0.63836100
H	-3.02759300	-0.01819200	-1.54937600
C	-5.47993900	-2.24879300	0.45975900
H	-3.93951800	-3.75028600	0.39347500
C	-5.85330100	-0.95524300	0.08976000
H	-5.23156800	0.85140000	-0.92426300
H	-6.16406600	-2.87588900	1.02612100
H	-6.83033900	-0.56744900	0.36653700
H	-1.84743000	-3.48434600	-0.49151100
H	0.56930200	-1.46097200	-2.90615600
H	2.31267300	-1.79696600	0.87375300
H	1.58572600	-1.87855200	2.48079400
H	-0.64740300	-2.21335200	1.55479500
H	0.43649300	-3.33053100	0.71934600

TS2_ad

C	-0.75634900	1.11636200	1.94147000
C	0.53703800	1.83633500	1.51546500
Cu	0.04427400	-0.23052400	-1.05356900
C	0.02266200	3.37687600	-1.06970400
H	-0.17432500	3.06197600	-2.10110100
C	2.59903800	2.62248400	-0.38148300
H	2.73342400	3.08020700	0.60794000
C	-0.20576900	-1.84749600	2.20134800
H	-0.04532100	-2.68254400	1.50780200
P	0.86839900	1.82708000	-0.32901200
P	-1.03958200	-0.53399500	1.09203800
C	-1.21532000	-0.01928400	-3.56906700
H	-0.46250300	0.50932500	-4.14704600
H	-2.23675900	0.33834300	-3.65209600

C	-0.94133900	-1.15310200	-2.84078300
C	0.34053900	-1.75555100	-2.52114900
H	-1.81174600	-1.60146000	-2.36398100
C	1.50683500	-1.41777600	-3.44375400
H	1.47071100	-2.01339000	-4.37298400
H	1.49193500	-0.36400000	-3.74260700
H	2.48153900	-1.59841900	-2.98251500
C	0.36739400	-3.08525800	-1.86937400
C	1.58116500	-3.63882700	-1.38567700
C	-0.78568000	-3.88864100	-1.67696000
C	1.62837400	-4.85827900	-0.71516500
H	2.50590600	-3.08391200	-1.51691600
C	-0.73926700	-5.10567900	-0.99532500
H	-1.73544300	-3.57366200	-2.09743000
C	0.46531400	-5.60407300	-0.49559200
H	2.58663000	-5.22938600	-0.35688800
H	-1.65507700	-5.68303000	-0.88083900
H	0.50282400	-6.55628900	0.02631300
C	-2.78990900	-0.96598200	1.72632200
H	-3.01132300	-0.21057100	2.49158000
C	-1.28905300	-2.27637200	3.20974200
C	-2.61610800	-2.32497000	2.44679800
C	1.11311800	4.46813000	-1.11019900
C	2.44782400	3.77503400	-1.40264300
H	3.29748400	4.46408100	-1.32882000
H	2.45075700	3.37246200	-2.42397900
H	0.86880700	5.23015900	-1.86016400
H	1.18485300	4.98307800	-0.14451500
C	1.14452700	-1.43751900	2.74702900
C	2.28687200	-1.62603700	1.94961600
C	1.30944700	-0.84822100	4.01004100
C	3.54726200	-1.22587400	2.39270000
H	2.17985400	-2.09784900	0.97569500
C	2.57272700	-0.45327100	4.45849300
H	0.45314100	-0.70214800	4.66176700
C	3.69568600	-0.63520400	3.65057400
H	4.41239300	-1.37438100	1.75304500
H	2.67597500	-0.00630400	5.44419800
H	4.67790300	-0.32839200	4.00026900
C	-1.30680900	3.74166900	-0.44607900
C	-2.48385200	3.17706100	-0.96670300
C	-1.42090200	4.61007700	0.65124900
C	-3.72916100	3.46291600	-0.40698000
H	-2.41685700	2.50034600	-1.81541400

C	-2.66743200	4.90111600	1.21042300
H	-0.53632900	5.07748000	1.07415400
C	-3.82674800	4.32774900	0.68578300
H	-4.62131900	3.00719600	-0.82680000
H	-2.72995000	5.58227500	2.05531200
H	-4.79630700	4.55848200	1.11910900
C	3.77214500	1.70210000	-0.63272000
C	3.85154000	0.90609200	-1.78512800
C	4.83955600	1.66453600	0.27517800
C	4.96682800	0.10374200	-2.02485500
H	3.03059500	0.90198900	-2.49552400
C	5.95865400	0.86292700	0.03863100
H	4.79561100	2.27266400	1.17613200
C	6.02645900	0.07936300	-1.11417600
H	5.00613000	-0.50479200	-2.92432600
H	6.77673400	0.85467000	0.75443500
H	6.89577800	-0.54483700	-1.30266700
C	-3.89530700	-0.92462900	0.69465100
C	-4.91406600	0.03285900	0.79355900
C	-3.95028000	-1.84437600	-0.36486800
C	-5.95774400	0.07463300	-0.13408700
H	-4.89160500	0.75355300	1.60792100
C	-4.99088700	-1.80573700	-1.29280400
H	-3.17036600	-2.59383300	-0.46905200
C	-5.99991600	-0.84534800	-1.18200400
H	-6.74035000	0.82235700	-0.03164200
H	-5.01319700	-2.52745900	-2.10512800
H	-6.81108400	-0.81781100	-1.90450200
H	-3.46980300	-2.51659600	3.10783800
H	-2.58865800	-3.13938500	1.71291100
H	-1.37331000	-1.54963600	4.02780000
H	-1.03774400	-3.24314300	3.66272300
H	-1.62434600	1.72915700	1.67047900
H	-0.76769400	1.00214400	3.03282500
H	0.52710700	2.86654200	1.89204800
H	1.40450600	1.33632600	1.96201400

TS2_bc

C	1.36556500	1.90841900	1.07664800
C	-0.02891100	1.70964300	1.69915000
Cu	0.01157300	-0.62314200	-0.76060700
C	-0.25553700	-1.12547900	2.81867300
H	-0.24757100	-2.11176800	2.34122700

C	-2.52958600	0.26549000	2.06430300
H	-2.46533700	1.15416800	2.70757500
C	1.09219900	2.79381000	-1.77672300
H	0.91804500	2.34296000	-2.76323900
P	-0.77678500	0.02338500	1.37931200
P	1.52832800	1.28806500	-0.69175900
C	1.46303800	-3.42650100	-0.75055500
H	0.86044300	-4.04665100	-0.09813900
H	2.54015600	-3.54360400	-0.67044500
C	0.95904000	-2.60246700	-1.71554500
C	-0.39275100	-2.17584700	-2.11305100
H	1.72798300	-2.11667100	-2.31987400
C	3.41043700	1.52528500	-0.95465500
H	3.76955100	1.96513200	-0.01595300
C	2.39221900	3.61223600	-1.86511600
C	3.53193600	2.60742700	-2.05789700
C	-1.43663400	-1.10326400	3.81323900
C	-2.72529000	-0.95601300	2.99457300
H	-3.60577900	-0.81248200	3.63184800
H	-2.90403600	-1.85582900	2.39208100
H	-1.43714300	-2.01021900	4.42993900
H	-1.35314300	-0.25111500	4.49893400
C	-0.17833400	3.50703500	-1.36879200
C	-1.41797600	2.91794400	-1.67391600
C	-0.17798800	4.72691200	-0.67749300
C	-2.61591600	3.51689700	-1.28878300
H	-1.43977200	1.97134200	-2.20975000
C	-1.37854000	5.33459600	-0.29748700
H	0.75919300	5.22084600	-0.43955500
C	-2.59990100	4.73153100	-0.59671800
H	-3.55867600	3.03115600	-1.52139300
H	-1.35359900	6.28408300	0.23139800
H	-3.53219300	5.20272200	-0.29771100
C	1.13517900	-0.87255000	3.35831400
C	2.22877300	-1.51993400	2.75668300
C	1.39119400	0.00673100	4.42225900
C	3.53204600	-1.28973100	3.19815300
H	2.05465000	-2.20251700	1.92729500
C	2.69538300	0.23366800	4.86872500
H	0.57080100	0.51497400	4.92071100
C	3.77192700	-0.41111600	4.25774800
H	4.35810800	-1.80273800	2.71318400
H	2.86696100	0.91309700	5.69977800
H	4.78554500	-0.23737600	4.60919200

C	-3.64337200	0.49527700	1.06513800
C	-3.84562000	-0.35299500	-0.03411200
C	-4.53853300	1.55675000	1.26421600
C	-4.91452000	-0.14213900	-0.90630700
H	-3.16938600	-1.18183800	-0.21742600
C	-5.61152900	1.76649200	0.39558400
H	-4.39617100	2.22399400	2.11209100
C	-5.80193700	0.91660800	-0.69582200
H	-5.04826800	-0.81636700	-1.74726400
H	-6.29642500	2.59199900	0.57327400
H	-6.63659200	1.07504900	-1.37392600
C	4.20700100	0.26416600	-1.21001600
C	5.14271900	-0.17776200	-0.26437400
C	4.05579400	-0.48070800	-2.38976600
C	5.90434500	-1.32727100	-0.48591700
H	5.27703000	0.38634800	0.65603800
C	4.81507900	-1.62849300	-2.61595500
H	3.33258000	-0.16789700	-3.13889700
C	5.74318400	-2.05750800	-1.66372100
H	6.62668600	-1.64761800	0.26062200
H	4.67787200	-2.19123100	-3.53527800
H	6.33411500	-2.95195500	-1.84028700
C	-1.59244000	-2.93009600	-1.67160700
C	-1.72021000	-3.49885000	-0.37735700
C	-2.70713800	-3.11265900	-2.52742800
C	-2.85907000	-4.19503200	0.02233500
H	-0.92095100	-3.36223900	0.34091500
C	-3.85024900	-3.80509300	-2.12422300
H	-2.67939400	-2.71226100	-3.53461400
C	-3.94183100	-4.35844000	-0.84646000
H	-2.89996800	-4.61410100	1.02621300
H	-4.67346700	-3.92146900	-2.82669400
H	-4.82915800	-4.90312400	-0.53576100
C	-0.43984400	-1.65682100	-3.55425800
H	0.46459300	-1.08042000	-3.78298400
H	-0.50037800	-2.46910900	-4.30141800
H	-1.29488100	-0.99450300	-3.73470300
H	3.44795800	2.14262200	-3.04783700
H	4.51847100	3.08377400	-2.01448700
H	2.34530100	4.34405100	-2.68123700
H	2.55988700	4.17547100	-0.93823500
H	0.01659800	1.91501500	2.77554100
H	-0.73845300	2.42206800	1.26242100
H	2.10644900	1.33693800	1.64878800

H	1.65257900	2.96575200	1.14225300

TS2_bd

C	0.51522400	1.77370800	1.58590700
C	-0.78141100	1.01007600	1.91181800
Cu	0.36598600	-0.25543500	-1.05851600
C	-2.84091200	-0.95140100	1.41605500
C	-0.33869600	-2.00691400	1.92374600
C	2.60000300	2.80533200	-0.15749000
P	-1.05174600	-0.55328400	0.91153400
P	0.91979700	1.89972100	-0.24131700
C	-1.12229100	-1.10793700	-3.78017800
H	-1.83350400	-1.87305000	-3.49590800
H	-1.46155200	-0.39545200	-4.52719600
C	0.16826500	-1.04538600	-3.34148700
C	0.98004400	-1.78329700	-2.35808400
H	0.74871100	-0.24452900	-3.80915600
C	0.00891200	3.44744500	-0.90409000
C	2.40581000	4.05432700	-1.04689900
C	1.00999900	4.61095500	-0.75181600
C	-2.77692500	-2.42735100	1.88161800
C	-1.51783200	-2.56917600	2.74542700
C	0.55800500	-3.08992600	-1.79664300
C	-0.79603200	-3.45923100	-1.58440300
C	1.51681600	-4.06026700	-1.40405100
C	-1.15690100	-4.68703100	-1.03216900
H	-1.58353000	-2.76082700	-1.82934400
C	1.15437200	-5.28379100	-0.83998300
H	2.57205500	-3.85847700	-1.54763100
C	-0.18687700	-5.61723800	-0.64782700
H	-2.21302100	-4.91900100	-0.90593500
H	1.93526100	-5.98778200	-0.55917000
H	-0.46983800	-6.57537500	-0.22046300
C	2.48007900	-1.66316300	-2.65115000
H	2.71196600	-0.67655800	-3.06430700
H	2.82423900	-2.41330700	-3.38596700
H	3.10528500	-1.77851400	-1.75890200
H	0.74460000	5.44077800	-1.41811500
H	0.99471800	5.00543000	0.27138900
H	2.48062800	3.78242400	-2.10721700
H	3.19548500	4.78899500	-0.85003900
H	-1.65583300	-2.00512000	3.67674300
H	-1.32596000	-3.61177700	3.02551400

H	-3.68876900	-2.69479000	2.42918800
H	-2.71129200	-3.09062800	1.01077600
H	-3.01872000	-0.34385700	2.31443400
H	-0.10568200	-2.74030200	1.14384500
C	0.94772300	-1.68298100	2.64985400
C	2.16851200	-1.84398300	1.97135400
C	0.98250900	-1.19364300	3.96506400
C	3.37956800	-1.51434500	2.58023700
H	2.16094200	-2.23983300	0.95851900
C	2.19496700	-0.86843400	4.57861600
H	0.06092900	-1.07364200	4.52754400
C	3.39806700	-1.02247300	3.88794500
H	4.30804300	-1.64407700	2.03116700
H	2.19658500	-0.49828700	5.60086100
H	4.34071200	-0.77221100	4.36761100
C	-3.95491300	-0.64730800	0.43293700
C	-5.20803700	-0.26174300	0.93520100
C	-3.81003500	-0.77467400	-0.95539100
C	-6.28640600	-0.02271500	0.08267100
H	-5.33942800	-0.14942700	2.00973200
C	-4.88576200	-0.53279000	-1.81252400
H	-2.84624300	-1.03655700	-1.37901800
C	-6.12920200	-0.15902500	-1.29875500
H	-7.24703600	0.27252400	0.49721400
H	-4.74433900	-0.63443900	-2.88539400
H	-6.96612400	0.02636700	-1.96688600
H	-0.08436300	3.23032100	-1.97576000
H	2.67253900	3.15376100	0.88121200
C	-1.38700000	3.64917100	-0.35518400
C	-2.46467100	2.97631500	-0.95576700
C	-1.65470800	4.46370200	0.75586200
C	-3.76167500	3.09985500	-0.45813200
H	-2.28185600	2.33954700	-1.81817900
C	-2.95425700	4.59686700	1.25131400
H	-0.85096000	5.00950800	1.24071600
C	-4.01168400	3.91343200	0.64978500
H	-4.57238000	2.55416500	-0.93171100
H	-3.13699600	5.23927500	2.10903800
H	-5.02157500	4.01493400	1.03757300
C	3.83199600	1.97893500	-0.45138800
C	4.16254500	1.57016900	-1.75220600
C	4.69813800	1.62386400	0.59310300
C	5.32280400	0.83712600	-2.00039100
H	3.50693200	1.81928000	-2.58213900

C	5.85825400	0.88628900	0.34965000
H	4.46296600	1.93247100	1.60931800
C	6.17665100	0.49189500	-0.95047300
H	5.55693700	0.53068100	-3.01620900
H	6.51587800	0.62831500	1.17582600
H	7.08071100	-0.07850600	-1.14524500
H	-1.64760600	1.64228300	1.68591200
H	-0.81347600	0.79075000	2.98610000
H	0.47743400	2.77369600	2.03620900
H	1.37394000	1.25243600	2.02706900

TS4_a

C	1.25440900	1.52710000	1.66889100
C	2.52759600	0.84791800	1.12461900
Cu	0.30503200	-0.57017300	-1.12452700
C	2.96079200	1.79238200	-1.74119700
H	2.42574000	1.61726200	-2.68271400
C	4.06520200	-0.60770000	-0.89790300
H	4.68684600	-0.32805300	-0.03665100
C	-1.61750000	2.00565700	1.74500300
H	-1.07468100	2.66790000	2.43302200
C	-0.81643800	-0.55891300	2.40832500
H	-1.44305200	-1.25958100	1.84204200
P	2.41907900	0.30697900	-0.66574800
P	-0.35287100	0.74600600	1.08650200
C	-1.05788400	-1.69996100	-2.02287000
H	-0.66188900	-2.72771600	-2.07084400
H	-1.12038000	-1.38229500	-3.07823800
C	-2.44261500	-1.71449900	-1.41435600
C	-3.52362100	-2.41831500	-1.82315500
H	-2.59613500	-1.10381200	-0.52114600
C	-3.45938200	-3.36627000	-3.00122700
H	-4.33622800	-3.25764000	-3.65206100
H	-2.55999400	-3.18407800	-3.59409100
H	-3.42968500	-4.41806000	-2.68115400
C	-4.82370600	-2.31620800	-1.10610600
C	-5.68835600	-3.42308400	-1.00548400
C	-5.25131500	-1.11026400	-0.51498700
C	-6.90129000	-3.33999900	-0.32075300
H	-5.40161000	-4.36836200	-1.45708200
C	-6.46156400	-1.02524900	0.17146300
H	-4.63894800	-0.22016100	-0.62511300
C	-7.29492800	-2.14162400	0.27670900

H	-7.54080100	-4.21719500	-0.25451700
H	-6.76430000	-0.07641000	0.60854500
H	-8.24257200	-2.07423000	0.80483100
C	-1.73129600	0.17326400	3.41062900
C	-2.58823400	1.15142900	2.59923200
H	-2.34088700	-0.54015900	3.97881000
H	-1.13779000	0.74164700	4.13823300
H	-3.20529200	1.79381300	3.23894400
H	-3.27342500	0.59861700	1.94322600
C	4.68513700	0.05937300	-2.15000700
C	4.46351500	1.56993600	-2.01480800
C	0.36238600	-1.34040800	2.94543700
C	1.00714700	-1.02371600	4.15033500
C	0.86468600	-2.41556500	2.19065400
C	2.11905000	-1.75239700	4.58279700
H	0.63854700	-0.21122000	4.76932900
C	1.97897800	-3.13848000	2.61491300
H	0.37772000	-2.67984800	1.25424200
C	2.61261600	-2.80845500	3.81640200
H	2.59635000	-1.49219100	5.52433000
H	2.35236800	-3.95576100	2.00449100
H	3.47754100	-3.37329800	4.15386400
C	-2.29502000	2.86769600	0.69801700
C	-2.52079000	4.22675700	0.96043300
C	-2.74683900	2.34393600	-0.52408400
C	-3.18315500	5.04019700	0.03837800
H	-2.17440800	4.65251100	1.90005200
C	-3.40842100	3.15421300	-1.44813300
H	-2.56314200	1.30072200	-0.76654900
C	-3.63009200	4.50566000	-1.17139900
H	-3.34865500	6.09022500	0.26644700
H	-3.74786000	2.72654600	-2.38787400
H	-4.14539900	5.13512100	-1.89200900
C	2.52738500	3.14443200	-1.21749000
C	1.24293000	3.61854700	-1.53448000
C	3.33983000	3.94156600	-0.39685300
C	0.77876300	4.83739200	-1.04098100
H	0.59550100	3.01777000	-2.16933400
C	2.88140600	5.16753300	0.09255400
H	4.34316900	3.61637500	-0.13823500
C	1.59949600	5.61891000	-0.22357000
H	-0.22418700	5.17070000	-1.29109400
H	3.53214200	5.76999100	0.72130200
H	1.24406800	6.57166200	0.15941500

C	3.98927900	-2.11880100	-0.95132400
C	3.14751900	-2.78812600	-1.85387300
C	4.80251100	-2.88679700	-0.10620700
C	3.12354400	-4.18181700	-1.90733700
H	2.48839200	-2.21835500	-2.50306900
C	4.78227700	-4.28235600	-0.15864500
H	5.46175800	-2.38597600	0.59980900
C	3.94101500	-4.93525600	-1.06074700
H	2.45924900	-4.67921300	-2.60891800
H	5.42475100	-4.85638700	0.50425200
H	3.92066200	-6.02089900	-1.10419900
H	5.74733900	-0.19851100	-2.23473900
H	4.19063900	-0.31691400	-3.05502700
H	5.06948100	1.94275900	-1.18006300
H	4.78014400	2.11834000	-2.91031400
H	2.72290400	-0.07631100	1.68135500
H	3.39308800	1.50558200	1.27372100
H	1.30445400	1.56578700	2.76414400
H	1.20927200	2.56172100	1.30971200

TS4_b

C	-2.33639300	-1.41009900	0.86454000
C	-2.98648800	-0.25097500	0.08283100
H	-2.30222600	-2.30748400	0.23554300
H	-2.95170500	-1.65226500	1.73995500
H	-3.94264000	-0.57777200	-0.34445600
H	-3.20297700	0.57992200	0.76467500
Cu	0.35648200	0.43206800	-0.56215800
C	-2.27483100	-0.45205200	-2.86200800
H	-1.35105700	-0.32875100	-3.44109500
C	-2.86469800	2.02233300	-1.76019500
H	-3.85612800	1.91280100	-1.30059700
C	-0.03996700	-2.80377400	2.00309800
H	-0.96102800	-3.39901000	2.05681000
C	-0.62965800	-0.33659500	3.11659100
H	0.32066000	0.20808000	3.18932600
P	-1.88312300	0.48137600	-1.24382100
P	-0.55115200	-1.08629600	1.35618700
C	2.29592900	0.84570100	-0.73699300
H	2.43621500	1.82633800	-1.21788200
H	2.69438000	0.11778600	-1.46399900
C	3.09269000	0.78057600	0.54549100
C	4.41077400	0.96273200	0.83021700

H	2.50373200	0.54667100	1.43794800
C	4.82966400	0.81886700	2.28601200
H	5.59367900	0.04136000	2.42343100
H	5.25003300	1.74957100	2.69125700
H	3.97031100	0.55078700	2.90808100
C	5.50117000	1.29484800	-0.12671800
C	5.31284700	1.41029000	-1.52262300
C	6.81603700	1.50873800	0.34593900
C	6.36727300	1.71816200	-2.38031400
H	4.32915000	1.25664500	-1.93938300
C	7.87043300	1.81898200	-0.51200400
H	7.02793500	1.43474000	1.40617300
C	7.65577100	1.92669500	-1.88568300
H	6.17565400	1.79534000	-3.44829200
H	8.86461300	1.97623400	-0.09994300
H	8.47566200	2.16777400	-2.55755100
C	0.42979300	-2.54202800	3.45575800
C	-0.54716500	-1.53848200	4.07819500
C	-3.04485800	1.85770500	-3.29023200
C	-3.37046200	0.38298400	-3.55446200
C	-2.28792100	3.35327600	-1.32460700
C	-3.10164000	4.28088700	-0.65900800
C	-0.95742900	3.70954700	-1.59736100
C	-2.60740800	5.53076100	-0.27871300
H	-4.13525300	4.02259500	-0.43814700
C	-0.46042400	4.95619800	-1.21676800
H	-0.29606800	2.99968600	-2.08654700
C	-1.28314500	5.87252300	-0.55692300
H	-3.25856000	6.23565200	0.23214800
H	0.57480100	5.20764200	-1.43096300
H	-0.89370200	6.84283300	-0.26074600
C	-2.50586300	-1.93708800	-2.68424700
C	-1.39336300	-2.79113500	-2.58731600
C	-3.78428300	-2.50432900	-2.57581600
C	-1.54957100	-4.16028300	-2.37520800
H	-0.39271600	-2.37253600	-2.67149300
C	-3.94431700	-3.87784000	-2.37273000
H	-4.66885100	-1.88004200	-2.65977200
C	-2.82983400	-4.71031600	-2.26687600
H	-0.67043300	-4.79252500	-2.29033600
H	-4.94542900	-4.29509900	-2.29950500
H	-2.95661500	-5.77780600	-2.10800000
C	-1.74326200	0.66732500	3.31666500
C	-2.98510700	0.32935800	3.87568800

C	-1.54982000	1.99445000	2.89414500
C	-3.99941900	1.28253200	4.00166900
H	-3.16802300	-0.68110500	4.22883700
C	-2.56256500	2.94578100	3.01113400
H	-0.59297000	2.28127200	2.46307000
C	-3.79534900	2.59238700	3.56680300
H	-4.95016700	0.99709100	4.44487200
H	-2.38695500	3.96029700	2.66488900
H	-4.58519300	3.33219800	3.66556800
C	0.95713400	-3.55129900	1.14172400
C	2.16436500	-2.96513700	0.72823500
C	0.69872300	-4.87745500	0.76670300
C	3.08326400	-3.68762200	-0.03302100
H	2.38857700	-1.93282100	0.98424400
C	1.61758200	-5.60348200	0.00506100
H	-0.23182700	-5.34791000	1.07796700
C	2.81450600	-5.00941600	-0.39789000
H	4.00880600	-3.21096000	-0.34447400
H	1.39783200	-6.63240400	-0.26915700
H	3.53180000	-5.56992600	-0.99153000
H	1.44488900	-2.12411200	3.44631700
H	0.47657400	-3.48144600	4.01943200
H	-0.23383500	-1.21952300	5.08019400
H	-1.52819200	-2.01835200	4.18631100
H	-3.82985000	2.52926300	-3.65727400
H	-2.11656400	2.13780300	-3.80472000
H	-3.41957400	0.15323400	-4.62588000
H	-4.35689700	0.15668800	-3.13090500

TS4_c

Cu	0.44953900	-0.19157000	-1.29858500
C	2.55542300	-1.47954300	-3.65327700
C	1.21679100	-1.46924200	-3.77718700
C	0.12003700	-1.57281300	-2.75737000
H	3.06195100	-1.51634200	-2.69345000
H	3.19328900	-1.44840400	-4.53375000
H	0.84786200	-1.37718200	-4.80637100
P	-1.23674700	-0.49004300	1.00934600
P	1.06740400	1.73214000	-0.17967200
C	-0.85552500	1.11615200	1.91037000
C	0.51014500	1.75885600	1.60570700
C	0.33210100	3.28054800	-1.01514700
H	0.34677100	3.01183600	-2.07928200

C	2.79675600	2.50680200	-0.01529100
C	-2.99489200	-0.80156500	1.69752100
C	-0.48341700	-1.89855100	2.07732600
H	-0.30490600	-2.68548200	1.33565200
C	-1.61745900	-2.38660100	3.00455300
C	-2.93327400	-2.25093500	2.23363700
H	-3.10607800	-0.13614400	2.56454800
C	1.38252000	4.38894900	-0.80726200
C	2.75942800	3.73436500	-0.95952700
H	2.83168900	2.88794300	1.01381800
C	-1.10395900	3.57535900	-0.63794800
C	-2.13323900	2.84400100	-1.25558500
C	-1.45812000	4.53340400	0.32263900
C	-3.46918200	3.05085300	-0.91692900
H	-1.87930700	2.09445200	-2.00195900
C	-2.79799800	4.74967900	0.65795100
H	-0.69243700	5.12830400	0.81123800
C	-3.80705400	4.00805100	0.04387000
H	-4.24436500	2.46057400	-1.39627200
H	-3.04897600	5.50298400	1.40044900
H	-4.84788800	4.17329600	0.30792300
C	3.98695200	1.59494600	-0.21426000
C	4.93947900	1.46093200	0.80550800
C	4.19962600	0.90874500	-1.41954500
C	6.07782200	0.67142900	0.62894900
H	4.78974600	1.98329800	1.74793500
C	5.33627200	0.12012600	-1.59907100
H	3.46828400	0.97292000	-2.22085200
C	6.28111100	-0.00084000	-0.57675600
H	6.80489900	0.58632100	1.43250100
H	5.47978400	-0.40363500	-2.54004600
H	7.16631000	-0.61463200	-0.71997800
C	0.84321100	-1.57295300	2.72685500
C	0.94534800	-0.97495400	3.99360100
C	2.03386900	-1.85185700	2.03335300
C	2.19036300	-0.65650800	4.54151000
H	0.04994900	-0.75968700	4.56950600
C	3.27828900	-1.52816700	2.57505300
H	1.97701600	-2.33817500	1.06228100
C	3.36236600	-0.92582800	3.83288600
H	2.24147300	-0.20051600	5.52725500
H	4.18208400	-1.74741300	2.01350500
H	4.33071500	-0.67870600	4.25988400
C	-4.14005000	-0.52648200	0.74883800

C	-4.24260500	-1.17840100	-0.49029100
C	-5.15535300	0.37012700	1.11021500
C	-5.32374000	-0.93997400	-1.33841000
H	-3.46551700	-1.87433500	-0.79268300
C	-6.24208300	0.60943100	0.26563600
H	-5.09638300	0.88442900	2.06710700
C	-6.32985800	-0.04422400	-0.96426600
H	-5.38117700	-1.45594000	-2.29333500
H	-7.02005800	1.30448600	0.57175000
H	-7.17432900	0.13770000	-1.62369400
C	0.04948600	-2.86686600	-1.99373900
C	1.19829000	-3.53921700	-1.50711800
C	-1.18877600	-3.48876200	-1.70137200
C	1.11263200	-4.71444100	-0.76369900
H	2.17914800	-3.13445300	-1.72598600
C	-1.27585100	-4.66252400	-0.94794200
H	-2.10634100	-3.06266500	-2.09047900
C	-0.12746300	-5.28614000	-0.45994700
H	2.02864200	-5.19077800	-0.41955200
H	-2.25479900	-5.10078200	-0.76140800
H	-0.19252100	-6.20115500	0.12263100
C	-1.21688800	-1.18339300	-3.42018400
H	-1.09650600	-0.26129000	-4.00096900
H	-1.58575700	-1.95869800	-4.11776400
H	-2.01564000	-0.99499900	-2.69447700
H	-2.95249100	-2.96091800	1.39719400
H	-3.80682000	-2.46597400	2.86128600
H	-1.67261900	-1.77370900	3.91287500
H	-1.43181900	-3.41862000	3.32661100
H	3.57688100	4.42324000	-0.71687900
H	2.91052700	3.41072800	-1.99729700
H	1.23061000	5.20863800	-1.51990000
H	1.30144500	4.81894500	0.19891700
H	0.51784200	2.79447400	1.97046900
H	1.30017200	1.22456700	2.14667400
H	-1.65728900	1.79589900	1.59889200
H	-0.94875500	0.98780800	2.99621400

TS4_d

Cu	0.23392400	-0.32862600	-1.15421000
C	-1.87398900	-0.58853000	-3.57913600
C	-0.75209600	-1.31352300	-3.70342500
C	0.21858800	-1.74511900	-2.63939800

H	-2.20930800	-0.20672300	-2.61588800
H	-2.50907600	-0.37319400	-4.43622000
H	-0.50296600	-1.64632000	-4.72129600
P	1.12943200	1.69816000	-0.33929100
P	-0.98357000	-0.43434600	1.08985300
C	0.78942700	1.80562800	1.49902800
C	-0.54739200	1.18081100	1.94137200
C	-0.20810700	-1.84859000	2.12444900
H	-0.03725400	-2.62567000	1.37078600
C	-2.72310500	-0.73692100	1.80822500
C	2.89852400	2.38807800	-0.43061900
C	0.36574500	3.25067600	-1.15616300
C	1.51450200	4.27852100	-1.23970000
H	1.31135500	5.02173800	-2.02018600
C	2.80847700	3.50101400	-1.50195600
H	3.06927400	2.87864200	0.53713300
H	2.78479700	3.05378100	-2.50422700
H	3.69510200	4.14455400	-1.45953800
C	-1.32925200	-2.35005800	3.06149100
C	-2.65864200	-2.19662800	2.31542800
H	-2.79428100	-0.08711800	2.69148000
C	1.12730300	-1.51766900	2.75341300
C	2.30646200	-1.77675500	2.03375100
C	1.24842400	-0.92935900	4.02269000
C	3.55858400	-1.44707900	2.55313400
H	2.23492300	-2.24804400	1.05654500
C	2.50104500	-0.60457500	4.54889300
H	0.36230200	-0.72757000	4.61755100
C	3.66131500	-0.85681300	3.81525000
H	4.45191300	-1.64979800	1.96934600
H	2.56736500	-0.15596400	5.53701600
H	4.63531000	-0.60383500	4.22559400
C	-3.89185400	-0.42058500	0.90221500
C	-4.86574000	0.50114000	1.31152800
C	-4.05652700	-1.05511500	-0.33919800
C	-5.97576300	0.78136800	0.51105900
H	-4.75693700	1.00207000	2.27118100
C	-5.16180400	-0.77452900	-1.14247500
H	-3.31434200	-1.77098600	-0.68040900
C	-6.12717700	0.14446000	-0.72141500
H	-6.72152400	1.49447200	0.85368000
H	-5.26690800	-1.27512200	-2.10135600
H	-6.98957200	0.35828200	-1.34731100
C	-0.94460800	3.71074100	-0.55532900

C	-1.01731800	4.64924700	0.48563400
C	-2.14611400	3.16336300	-1.03602600
C	-2.24860300	5.02292300	1.02976400
H	-0.11217600	5.10498300	0.87621500
C	-3.37620400	3.52840300	-0.48980200
H	-2.11305300	2.43929000	-1.84704200
C	-3.43204500	4.46241800	0.54766700
H	-2.27940500	5.75709400	1.83087900
H	-4.28777800	3.07865200	-0.87172800
H	-4.38893700	4.75329500	0.97247600
C	4.00680500	1.38192600	-0.64824600
C	4.03094100	0.54334200	-1.77324800
C	5.06418500	1.29547500	0.26799300
C	5.08279400	-0.34974600	-1.97623800
H	3.21354500	0.57370300	-2.48779900
C	6.12009000	0.40338500	0.06719800
H	5.06215500	1.93615600	1.14726800
C	6.13313400	-0.42280900	-1.05736000
H	5.07848800	-0.99158000	-2.85302500
H	6.93194900	0.35798300	0.78869500
H	6.95308000	-1.11770100	-1.21765600
C	-0.17696800	-3.00116600	-1.91276500
C	0.77810200	-3.77912000	-1.21017200
C	-1.50892600	-3.47676400	-1.86071700
C	0.42219300	-4.91359100	-0.48039900
H	1.82400600	-3.48677400	-1.23072500
C	-1.86485200	-4.61271700	-1.13294400
H	-2.27253900	-2.94532400	-2.41926700
C	-0.90694800	-5.34184900	-0.42296800
H	1.19660600	-5.47293600	0.04136200
H	-2.90345700	-4.93911200	-1.13523100
H	-1.18379700	-6.22925800	0.13985500
C	1.61697000	-1.85391400	-3.28668900
H	1.68245100	-2.70343400	-3.99194600
H	1.84235100	-0.94337300	-3.85555000
H	2.42548200	-1.97403200	-2.55957900
H	1.61486500	4.82665800	-0.29504500
H	0.15716900	2.90589800	-2.17635100
H	-3.52095600	-2.41641300	2.95649000
H	-2.69634700	-2.89253000	1.46813300
H	-1.14105900	-3.38873000	3.35852600
H	-1.36608800	-1.75472900	3.98238500
H	0.84389100	2.84716000	1.83991800
H	1.62234600	1.26809000	1.96791200

H	-1.37195900	1.85713700	1.68608200
H	-0.55017000	1.06322000	3.03175100

2a

C	-4.78352900	-0.00138200	-0.34374800
C	-3.59750600	-0.69465600	-0.56520600
C	-2.37850700	-0.16293300	-0.11819500
C	-2.35821800	1.06784800	0.55357100
C	-3.54899200	1.75781600	0.77345000
C	-4.76027600	1.22592200	0.32524500
H	-5.72594700	-0.41546500	-0.69077100
H	-3.59132300	-1.64963200	-1.08019000
H	-1.41555700	1.47459700	0.90167900
H	-3.53237100	2.71023400	1.29575800
H	-5.68675500	1.76697900	0.49832900
C	-1.14912500	-0.95361200	-0.37986800
O	-1.11124800	-2.03479300	-0.90732400
O	0.00002300	-0.26041800	-0.00025500
C	1.14905700	-0.95356700	0.37971700
O	1.11108000	-2.03466300	0.90734600
C	2.37849600	-0.16294600	0.11814500
C	2.35834000	1.06774000	-0.55379600
C	3.59740500	-0.69462700	0.56544800
C	3.54916400	1.75765700	-0.77356400
H	1.41574600	1.47445400	-0.90212800
C	4.78347900	-0.00140300	0.34409900
H	3.59111300	-1.64953000	1.08056500
C	4.76036100	1.22580600	-0.32507100
H	3.53265000	2.71000000	-1.29601100
H	5.72582800	-0.41545300	0.69134600
H	5.68687900	1.76682500	-0.49806900

Int3_a1

C	-3.43575000	-1.35761900	0.79724700
C	-3.93503700	0.01215000	0.29711200
H	-3.61743300	-2.12000900	0.03132700
H	-4.01276600	-1.64936500	1.68457100
H	-3.93662900	0.72782800	1.12717900
H	-4.97707700	-0.09301700	-0.03287700
P	-2.89242200	0.82753700	-1.04050300
P	-1.60746700	-1.48644800	1.17544400
C	0.65427100	-0.54823700	-2.31832100

C	2.05243700	-0.14694600	-2.26614400
H	0.55235400	-1.59720800	-2.62195400
C	2.13967300	1.14845800	1.07949500
C	2.62758400	1.07825700	-2.47533400
Cu	-0.29634400	-0.56430800	-0.52386200
O	0.97737000	0.81381400	0.96136400
C	-3.86367300	2.47320400	-1.20936000
H	-4.74602700	2.38125500	-0.56324700
C	-3.62449400	0.14282300	-2.67976600
H	-2.81442800	0.32536000	-3.39836200
C	-1.38262100	-0.88679800	2.97212400
H	-0.32813100	-0.59054400	2.98749800
C	-1.47171700	-3.32475000	1.65468900
H	-2.50702800	-3.68049800	1.74229700
C	1.78666600	2.29720100	-2.78573700
H	1.63956100	2.94321100	-1.90601300
H	2.24795800	2.91902900	-3.56387000
H	0.79117700	2.00869800	-3.13624200
C	4.09176800	1.25763000	-2.42450900
C	4.66715600	2.52192800	-2.16401600
C	4.99510400	0.19705700	-2.67701300
C	6.04959000	2.70808900	-2.12766700
H	4.02004900	3.37192100	-1.97229900
C	6.37500500	0.38238200	-2.63599500
H	4.60310900	-0.77839800	-2.94947700
C	6.91868700	1.64084100	-2.35666500
H	6.44795100	3.69840900	-1.91724400
H	7.03280500	-0.45655300	-2.85559300
H	7.99543000	1.78729800	-2.33734100
C	2.62770000	2.54011400	1.09699300
C	3.97159600	2.86102200	1.34975100
C	1.69337800	3.56934300	0.88447200
C	4.36923700	4.19523300	1.40350200
H	4.69426700	2.06847100	1.50206800
C	2.09898500	4.89948000	0.93808800
H	0.65935100	3.31332000	0.67991800
C	3.43598100	5.21516200	1.20108400
H	5.40933600	4.43852200	1.60059800
H	1.36950200	5.68799000	0.77802600
H	3.74997900	6.25468800	1.24584900
H	2.73279800	-0.95320600	-1.98524300
H	0.02145400	0.08808600	-2.94731200
O	3.17229400	0.22842300	1.22044500
C	2.98545000	-1.00687000	1.80972200

O	2.06844400	-1.25324000	2.56164700
C	4.07958600	-1.94659100	1.46176100
C	4.11472900	-3.18301000	2.12693800
C	5.05730000	-1.63819000	0.50345000
C	5.11865500	-4.10200500	1.83623800
H	3.35209800	-3.40340300	2.86632800
C	6.05845000	-2.56485000	0.21597500
H	5.02712400	-0.69121800	-0.02273400
C	6.09210400	-3.79327000	0.88027800
H	5.14448400	-5.05728900	2.35277500
H	6.80923700	-2.32318000	-0.53066600
H	6.87546900	-4.51172400	0.65351000
C	-4.78911300	1.08210600	-3.04650200
C	-4.35347900	2.50146100	-2.67873600
H	-5.05116600	0.98989000	-4.10833200
H	-5.68901300	0.82766600	-2.47293100
H	-5.16298400	3.23146500	-2.80173600
H	-3.53468700	2.82231500	-3.33576200
C	-0.85998600	-3.30141700	3.07737800
C	-1.52512100	-2.15266100	3.84115600
H	-1.07220600	-1.99619700	4.82785500
H	-2.58150800	-2.39918500	4.00718900
H	-1.00882200	-4.26957500	3.57079900
H	0.21957700	-3.12489900	3.01607700
C	-3.10464500	3.71649800	-0.79865600
C	-3.63673100	4.58586400	0.16406500
C	-1.88228400	4.06191600	-1.39742000
C	-2.97968000	5.76845100	0.51256900
H	-4.58058900	4.33464200	0.64290600
C	-1.22555100	5.24500000	-1.05803900
H	-1.43587200	3.39879100	-2.13409800
C	-1.77275200	6.10557000	-0.10150000
H	-3.41684800	6.42880600	1.25737000
H	-0.28543800	5.49371800	-1.54339800
H	-1.26600800	7.03168100	0.15766500
C	-3.90487500	-1.34481000	-2.68747000
C	-5.17959300	-1.88161300	-2.44857100
C	-2.84745200	-2.24033900	-2.92579700
C	-5.38823800	-3.26363100	-2.44006500
H	-6.02656400	-1.22436300	-2.27712500
C	-3.05139300	-3.61952600	-2.91116000
H	-1.85176400	-1.84756300	-3.11373600
C	-4.32578600	-4.13869100	-2.66696200
H	-6.38715500	-3.65312900	-2.25945600

H	-2.21265800	-4.28746700	-3.08484300
H	-4.48907000	-5.21315300	-2.66136400
C	-2.21615900	0.31865400	3.35122800
C	-3.44697800	0.21770500	4.01786000
C	-1.75334600	1.60225100	3.01170500
C	-4.19257800	1.35815900	4.32876100
H	-3.83187700	-0.75417300	4.31151900
C	-2.49860600	2.74107200	3.31523700
H	-0.80277100	1.69792700	2.49409900
C	-3.72444900	2.62428900	3.97639700
H	-5.13978100	1.25256400	4.85200500
H	-2.12239000	3.72012300	3.03203200
H	-4.30402500	3.51087800	4.22002700
C	-0.74934000	-4.21748600	0.67052600
C	-1.41430200	-5.30146000	0.08187100
C	0.60106100	-4.01088000	0.34639400
C	-0.75444600	-6.15794900	-0.80301000
H	-2.46099400	-5.47821800	0.31980000
C	1.26365700	-4.86444000	-0.53517000
H	1.13609700	-3.17508400	0.78661500
C	0.58837700	-5.94202600	-1.11486600
H	-1.29024600	-6.99528100	-1.24326900
H	2.31033100	-4.68682400	-0.76754000
H	1.10582700	-6.60702600	-1.80129600

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C	-3.59196400	0.68028700	1.42568400
C	-3.12727900	-0.73957400	1.80357300
H	-3.01221500	1.41940500	1.99053100
H	-4.64343600	0.80676600	1.71451000
H	-3.83769000	-1.47723400	1.41328800
H	-3.12249700	-0.84466400	2.89605400
P	-1.46058500	-1.23842100	1.10241200
P	-3.33086000	1.13241100	-0.38070300
C	0.44391900	0.67993800	-2.96830800
Cu	-1.30059600	-0.40142200	-1.07816300
C	-1.39169500	-3.07159600	1.61681600
H	-2.32436700	-3.24722400	2.16777000
C	-0.18127100	-0.70912400	2.40128300
H	0.76663700	-0.75899100	1.85427200
C	-4.94918900	0.59136000	-1.24100700
H	-4.66849000	0.58235400	-2.30320300
C	-3.86582400	2.97157700	-0.34357500

H	-4.17150300	3.17055900	0.69134400
C	1.79649900	0.55447200	-2.81040200
C	-0.16122800	-1.85721000	3.42721700
C	-0.21220600	-3.16165000	2.62355500
H	0.74232200	-1.79605400	4.04465200
H	-1.02798900	-1.80369100	4.09945700
H	-0.33624800	-4.04033300	3.26792000
H	0.72803800	-3.28516100	2.07812600
C	-5.13096600	3.04621300	-1.23723700
C	-5.93192200	1.75746500	-1.03330700
H	-6.78443100	1.68611800	-1.72077300
H	-6.33922800	1.74487500	-0.01419900
H	-5.71538200	3.94285500	-0.99817800
H	-4.83331000	3.13352400	-2.28987500
C	-1.32021900	-4.07253600	0.48338700
C	-0.28436000	-4.03593100	-0.46476400
C	-2.28229500	-5.08594900	0.37798400
C	-0.21981400	-4.98412600	-1.48582700
H	0.47474400	-3.26145900	-0.40513300
C	-2.21706600	-6.03972400	-0.64138900
H	-3.09139100	-5.12984800	1.10397500
C	-1.18519700	-5.99054600	-1.57914900
H	0.58461800	-4.93204100	-2.21515900
H	-2.97154000	-6.82050600	-0.69879100
H	-1.13251100	-6.72825200	-2.37549800
C	-0.36491500	0.70510600	2.90450100
C	-1.00047100	1.00668500	4.11820400
C	0.09512800	1.77453500	2.11633300
C	-1.17953700	2.33203300	4.52507700
H	-1.35166500	0.20691400	4.76317900
C	-0.08705800	3.09762100	2.51638200
H	0.60238200	1.56409500	1.17751200
C	-0.72891700	3.38260400	3.72503200
H	-1.66932300	2.53966200	5.47332700
H	0.27323300	3.90319500	1.88328500
H	-0.86758700	4.41259700	4.04324300
C	-5.41697500	-0.80342200	-0.88556800
C	-6.47052600	-1.04822100	0.00740700
C	-4.76479700	-1.90992800	-1.45809600
C	-6.85556300	-2.35484300	0.32236900
H	-7.01014100	-0.21988100	0.45609800
C	-5.14317500	-3.21375400	-1.14171100
H	-3.94441600	-1.74305100	-2.15301600
C	-6.19297200	-3.44208100	-0.24710800

H	-7.68001700	-2.51844600	1.01186700
H	-4.61387900	-4.04916600	-1.59038200
H	-6.49504100	-4.45717000	-0.00332100
C	-2.79453400	3.97261200	-0.72024700
C	-2.45021800	5.00403400	0.16407500
C	-2.15273200	3.92755200	-1.96821500
C	-1.50039900	5.96712800	-0.18526100
H	-2.93344600	5.05445600	1.13736400
C	-1.20582500	4.88837900	-2.32261900
H	-2.38664500	3.12760800	-2.66668600
C	-0.87608100	5.91388600	-1.43171800
H	-1.25360600	6.76001300	0.51634100
H	-0.71962700	4.83245800	-3.29274100
H	-0.13923900	6.66280100	-1.70919000
C	-0.57806200	-0.36571000	-2.96509000
H	-1.43064600	-0.11056900	-3.60520100
H	-0.21265300	-1.36518000	-3.21552200
C	2.68741600	1.72539700	-2.85330100
C	4.04348100	1.60263000	-3.23810800
C	2.24629600	3.02936900	-2.52073200
C	4.89055500	2.70907800	-3.31562300
H	4.43203800	0.62720500	-3.51606500
C	3.08826600	4.13346700	-2.60827900
H	1.23032200	3.17153700	-2.16532300
C	4.42185100	3.98866300	-3.00935400
H	5.92182500	2.56936700	-3.63358200
H	2.70411800	5.11674900	-2.34370100
H	5.07782100	4.85262900	-3.08126900
C	2.40928600	-0.82198100	-2.65769500
H	1.75437000	-1.46879700	-2.06214600
H	2.57099700	-1.33093700	-3.62110800
H	3.37971400	-0.78371700	-2.14999600
C	3.74630900	-2.04814100	0.63021300
O	2.57042700	-2.26246400	0.81443200
H	0.05948000	1.69017600	-3.11763900
O	4.35454800	-0.86538900	1.01120100
C	4.68214100	-2.96321000	-0.06610300
C	4.16753200	-4.17125700	-0.56274700
C	6.04308100	-2.66313800	-0.22854400
C	5.00681900	-5.06872900	-1.21596300
H	3.11373000	-4.38959700	-0.42472800
C	6.87827100	-3.56539800	-0.88492300
H	6.43693300	-1.72968000	0.15688600
C	6.36232300	-4.76624100	-1.37858900

H	4.60702300	-6.00322800	-1.59902800
H	7.93155100	-3.33189600	-1.01135300
H	7.01651300	-5.46723800	-1.89007900
C	3.89819200	-0.16402500	2.13317000
O	3.39959900	-0.72480800	3.07743500
C	4.17493400	1.28527100	2.02680300
C	4.00450800	2.06207900	3.18479100
C	4.56697700	1.89318400	0.82429600
C	4.23856400	3.43238200	3.14193600
H	3.68827900	1.57385600	4.10051300
C	4.78673600	3.26957600	0.78456700
H	4.67808400	1.30298500	-0.07802700
C	4.62924700	4.03604800	1.94166700
H	4.11193600	4.03180000	4.03908600
H	5.06258500	3.73632000	-0.15558100
H	4.80476100	5.10826600	1.90786000

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C	3.42984200	-1.28054200	1.20109200
C	2.58257600	-2.47551100	0.72516100
H	4.25042300	-1.10098000	0.49671900
H	3.88054600	-1.51137100	2.17299900
H	1.88028600	-2.76304600	1.51695200
H	3.23584000	-3.33965500	0.54799300
P	1.52288000	-2.11130800	-0.78720300
P	2.49100000	0.33850500	1.27365600
C	0.59816600	1.48719600	-2.30944400
C	-0.85568100	1.52909500	-2.47083800
H	1.00601400	2.49171300	-2.14489300
C	-2.13748600	1.87932100	1.22215900
C	-1.68484600	0.72456400	-3.19913100
Cu	1.13356900	0.38083400	-0.69006600
O	-1.22209700	1.09558900	1.31510200
C	0.52204000	-3.74475100	-0.92460900
H	0.93044300	-4.38372900	-0.12884300
C	2.64784200	-2.57735300	-2.26017400
H	2.16482400	-2.06729200	-3.10404700
C	1.70622400	0.50958600	3.01552700
H	0.78237400	1.05519500	2.79949800
C	3.88832800	1.56070200	1.67180900
H	4.69631800	0.95686800	2.10779100
C	-1.13737300	-0.44884900	-3.98219800
H	-1.27543500	-1.40296100	-3.44958400

H	-1.62617800	-0.55324600	-4.95978000
H	-0.06445100	-0.33389400	-4.16255400
C	-3.14375300	0.93982400	-3.22817800
C	-4.02562000	-0.08906400	-3.63225000
C	-3.74220100	2.18254500	-2.90468500
C	-5.40482100	0.10622200	-3.70709600
H	-3.62365500	-1.06544000	-3.88261700
C	-5.11930300	2.37498900	-2.96847600
H	-3.11094600	3.02458500	-2.63780600
C	-5.96928600	1.33953400	-3.37613700
H	-6.04177300	-0.71486300	-4.02998700
H	-5.53183900	3.35244800	-2.72643900
H	-7.04162800	1.50104200	-3.45493700
H	-1.33883600	2.30722300	-1.87827000
H	1.12727600	1.02431000	-3.15176600
C	2.44439400	-4.09009100	-2.45695000
C	0.94708200	-4.35416600	-2.27608800
H	2.80443800	-4.41234900	-3.44205100
H	3.00594100	-4.66090000	-1.70645400
H	0.70685000	-5.42361600	-2.31702200
H	0.40247700	-3.86921300	-3.09555700
C	3.29724600	2.41940300	2.81501500
C	2.64703900	1.45057600	3.80624200
H	2.08775900	1.97356800	4.59145200
H	3.43332200	0.87344400	4.30755100
H	4.07994200	3.02852900	3.28283200
H	2.54886300	3.11406300	2.41056100
C	-0.96982300	-3.60032200	-0.67893200
C	-1.42144400	-3.16155400	0.57637500
C	-1.93100100	-3.91759100	-1.64836400
C	-2.78100800	-3.02988800	0.84928700
H	-0.70210200	-2.91485400	1.35366100
C	-3.29647900	-3.78948200	-1.37624600
H	-1.62547300	-4.27609600	-2.62599300
C	-3.72853700	-3.34222600	-0.12921100
H	-3.09855200	-2.67172500	1.82432100
H	-4.02055900	-4.03990800	-2.14734400
H	-4.78870700	-3.23228400	0.08019100
C	4.06674400	-2.06022300	-2.16664000
C	5.14324400	-2.86212800	-1.75900900
C	4.32676000	-0.71484600	-2.48217800
C	6.43440400	-2.33499700	-1.66262200
H	4.98552700	-3.91028400	-1.52373500
C	5.61211400	-0.18488700	-2.38012800

H	3.50608900	-0.07568500	-2.79908000
C	6.67388000	-0.99522800	-1.96799200
H	7.25340500	-2.97850800	-1.35088700
H	5.78146900	0.86157400	-2.61606800
H	7.67767900	-0.58604700	-1.89120500
C	1.31592100	-0.77571100	3.71515400
C	2.24509400	-1.57521100	4.40217400
C	-0.02780300	-1.18723300	3.69999800
C	1.84896600	-2.75071000	5.04313600
H	3.28896900	-1.27732200	4.45354800
C	-0.42464800	-2.35987100	4.34602600
H	-0.77039400	-0.57998500	3.19009100
C	0.51146400	-3.14986000	5.01666000
H	2.58731600	-3.35007200	5.56992700
H	-1.47309400	-2.64549300	4.33093600
H	0.20154200	-4.06105100	5.52142900
C	4.47293000	2.35883300	0.52576100
C	5.86565900	2.45736700	0.39267000
C	3.66865900	3.05831600	-0.38729400
C	6.44206700	3.23363300	-0.61474800
H	6.50675900	1.92179900	1.08979100
C	4.24076200	3.83051500	-1.39901500
H	2.58787800	2.97534900	-0.32645400
C	5.62998100	3.92404800	-1.51615100
H	7.52440800	3.29709000	-0.69411900
H	3.59772600	4.35475400	-2.10115500
H	6.07381500	4.52812600	-2.30307000
O	-3.46743500	1.49644400	1.30197000
C	-3.86749600	0.38946700	2.04428200
O	-3.25010800	-0.01491300	3.00008100
C	-5.16067900	-0.14817600	1.56086900
C	-5.69608100	0.19738800	0.31126900
C	-5.84022900	-1.05322200	2.39267400
C	-6.90307900	-0.36708300	-0.10027300
H	-5.16859900	0.88382900	-0.34179600
C	-7.04929900	-1.60443200	1.97953600
H	-5.40732300	-1.30717600	3.35486900
C	-7.58056700	-1.26215800	0.73073100
H	-7.30062200	-0.10846400	-1.07643000
H	-7.57802300	-2.29913200	2.62621700
H	-8.52291300	-1.69623300	0.40658600
C	-2.00034700	3.33288600	0.96117100
C	-3.08997000	4.21411300	1.02890900
C	-0.72145100	3.82348400	0.65350300

C	-2.89578600	5.57514200	0.79965400
H	-4.07732100	3.83119500	1.26001900
C	-0.53485000	5.18299300	0.42004900
H	0.10234200	3.12085500	0.57945600
C	-1.62104800	6.06027400	0.49619400
H	-3.73931800	6.25727600	0.85544800
H	0.45408400	5.55937500	0.17415900
H	-1.47440000	7.12166000	0.31470500

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C	-3.99337700	-0.34180600	0.42652300
C	-3.27082000	-1.56402400	1.02710100
H	-4.02612200	0.46312000	1.16843800
H	-5.03380000	-0.62093000	0.21341800
H	-3.38420300	-2.42869800	0.36341800
H	-3.74691400	-1.82809500	1.98049900
P	-1.42507800	-1.39413000	1.29541900
P	-3.18364600	0.42609500	-1.08886400
C	3.21435700	-0.18274900	2.04435700
C	1.75717700	0.10015100	-2.52063100
Cu	-0.36350700	-0.69466200	-0.64823700
C	-1.00532100	-3.10794900	2.01371400
H	-1.97380400	-3.59480400	2.18861200
C	-1.21733400	-0.51262500	2.97653100
H	-0.21162100	-0.08610300	2.89947400
C	-3.99701900	-0.51689800	-2.54966300
H	-3.31350400	-0.31187300	-3.38475600
C	-4.34048200	1.93711900	-1.32114500
H	-5.11327700	1.86812700	-0.54478300
C	3.02127100	-0.41067200	-2.58964600
C	-1.16651700	-1.65070900	4.01696700
C	-0.37349000	-2.80164900	3.39434400
H	-0.71318500	-1.29614300	4.95064700
H	-2.17598200	-2.00403200	4.26302400
H	-0.38446200	-3.70046600	4.02282600
H	0.67245900	-2.50054700	3.27132000
C	-5.02408000	1.71901400	-2.69562100
C	-5.31560400	0.22316800	-2.83871200
H	-5.70478400	-0.02998800	-3.83340100
H	-6.08745100	-0.06008400	-2.11166100
H	-5.93072000	2.33095700	-2.77792500
H	-4.34893700	2.04390200	-3.49799000
C	-0.17692100	-4.01312500	1.12926200

C	1.13962400	-3.68343500	0.76977700
C	-0.70439100	-5.22970300	0.67531600
C	1.90552800	-4.54931300	-0.01052100
H	1.56953500	-2.74278300	1.10220100
C	0.05798300	-6.09699800	-0.11095000
H	-1.72301200	-5.50234800	0.94288100
C	1.36754900	-5.76005500	-0.45507100
H	2.92280900	-4.27354600	-0.27332500
H	-0.37105600	-7.03759100	-0.44745900
H	1.96503000	-6.43352000	-1.06377800
C	-2.19084800	0.61753200	3.24137200
C	-3.37170700	0.44745200	3.98088900
C	-1.91465700	1.89599500	2.72580200
C	-4.24903800	1.51442200	4.19243200
H	-3.61501600	-0.52049900	4.40803500
C	-2.79126400	2.96088600	2.93169600
H	-1.00356600	2.04556500	2.15355100
C	-3.96515500	2.77515900	3.66687700
H	-5.15391000	1.35662000	4.77411900
H	-2.55724900	3.93631500	2.51451900
H	-4.64636000	3.60544200	3.83396500
C	-4.05539300	-2.01898500	-2.37294100
C	-5.22611800	-2.69895200	-2.00527500
C	-2.88478600	-2.77521400	-2.56316300
C	-5.22582700	-4.08545400	-1.82555600
H	-6.15435700	-2.15334400	-1.86636900
C	-2.88083600	-4.15718000	-2.37940000
H	-1.96535500	-2.26797100	-2.84504000
C	-4.05429500	-4.82008600	-2.00769100
H	-6.14817200	-4.58918600	-1.54688800
H	-1.95922300	-4.71433300	-2.52190800
H	-4.05565100	-5.89813400	-1.86990100
C	-3.65791900	3.28290300	-1.19238600
C	-4.17480300	4.26225600	-0.33258000
C	-2.52446300	3.60618000	-1.95616300
C	-3.58916900	5.52737800	-0.24223100
H	-5.04935400	4.03128900	0.27151400
C	-1.93800400	4.86925800	-1.87309100
H	-2.09275000	2.85990500	-2.61871700
C	-2.46978900	5.83750200	-1.01589100
H	-4.01347100	6.27146600	0.42727800
H	-1.06610300	5.09733000	-2.48088100
H	-2.02013800	6.82555200	-0.95799000
O	2.33806500	-0.51598600	2.80801400

C	0.46862800	-0.59592400	-2.47877200
H	-0.29303100	-0.03322500	-3.03460400
H	0.50732100	-1.61973800	-2.86560400
O	3.24254000	1.06829800	1.43585300
C	4.20794100	0.46339800	-2.65886600
C	5.43688200	-0.01998200	-3.16655400
C	4.20242200	1.80975600	-2.22057500
C	6.57238000	0.78752200	-3.24634600
H	5.49857500	-1.04240800	-3.52559300
C	5.33468800	2.61594400	-2.30166100
H	3.29727100	2.22837100	-1.79204800
C	6.53534400	2.11451000	-2.81526000
H	7.49146800	0.37445600	-3.65731500
H	5.28037600	3.64280100	-1.94620400
H	7.41990000	2.74318400	-2.87394500
C	3.24822500	-1.90628700	-2.66916200
H	2.38141000	-2.45632300	-2.29443900
H	3.43295800	-2.25347500	-3.69798800
H	4.11551000	-2.21456200	-2.07066300
C	4.40809000	-0.98584300	1.69588800
C	5.28680200	-0.61159600	0.66785900
C	4.63458600	-2.16902900	2.41931200
C	6.38126300	-1.42151600	0.36654600
H	5.10541100	0.28960600	0.09441400
C	5.73445400	-2.96662400	2.11976800
H	3.94223500	-2.44325700	3.20840200
C	6.60800300	-2.59322900	1.09222100
H	7.04526400	-1.13532100	-0.44316300
H	5.91128900	-3.87901500	2.68222500
H	7.46397900	-3.22004000	0.85606700
C	2.08329400	1.76900900	1.15108700
O	1.00270900	1.23802100	1.03193800
C	2.34616900	3.21676500	0.96839300
C	1.28881900	4.02041400	0.51215400
C	3.59401600	3.79509900	1.24860400
C	1.47739100	5.38927500	0.34499500
H	0.33240100	3.56067900	0.28627500
C	3.77499000	5.16692700	1.08164900
H	4.41055500	3.17178600	1.59405100
C	2.71919600	5.96422800	0.63147000
H	0.65472900	6.00391000	-0.00836000
H	4.74005900	5.61401100	1.30233500
H	2.86535400	7.03330000	0.50181500
H	1.67083800	1.18807000	-2.51283900

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C	0.79871500	-3.27799000	1.14689900
C	-0.71344800	-3.38683400	0.87140200
H	1.35943100	-3.73882100	0.32547600
H	1.04683000	-3.83505000	2.05938900
H	-1.27081000	-3.12753400	1.77903200
H	-0.96161100	-4.42842100	0.62857100
P	-1.37039900	-2.21585000	-0.44565000
P	1.45604200	-1.52898700	1.26010700
C	0.65170000	0.53814800	-2.35108900
C	0.38335000	1.97210700	-2.40320300
H	1.69771600	0.32027800	-2.59791900
C	-0.17328300	2.76975900	1.05250700
C	-0.72755900	2.71747000	-2.69629800
Cu	0.48934100	-0.27374100	-0.48474800
O	-0.18158500	1.55828200	1.06027800
C	-3.23668700	-2.64147300	-0.33753100
H	-3.30511400	-3.52386200	0.31232000
C	-1.16833600	-3.17888100	-2.09538300
H	-1.15634200	-2.37223000	-2.83918500
C	1.23542900	-0.97277400	3.07620200
H	1.17000000	0.11590100	2.97868400
C	3.31996900	-1.85133500	1.47153000
H	3.40990200	-2.92129000	1.70262900
C	-1.35288700	3.64026800	1.23280000
C	-1.24127100	5.03394400	1.37125500
C	-2.61708600	3.03149200	1.29789300
C	-2.38236200	5.80522700	1.58257300
H	-0.26548200	5.50291900	1.32149700
C	-3.75191400	3.80877100	1.50931100
H	-2.69682800	1.95697400	1.17394100
C	-3.63723200	5.19487900	1.65407000
H	-2.29238500	6.88215200	1.69300500
H	-4.72484700	3.32980700	1.56129000
H	-4.52510900	5.79900700	1.82075600
H	1.24373400	2.57240900	-2.09309300
H	-0.00597400	-0.08499100	-2.95705200
O	0.98826600	3.51224900	0.85021200
C	2.23668600	3.03766600	1.20591600
O	2.40624700	2.17222400	2.03428700
C	3.31970400	3.77205900	0.50439300
C	4.64524500	3.48392100	0.86658400

C	3.06006200	4.72716000	-0.49058100
C	5.69879900	4.14025200	0.23644300
H	4.82926800	2.74565000	1.63966800
C	4.11919300	5.38004300	-1.11902800
H	2.03668100	4.94762300	-0.77024000
C	5.43679200	5.08834500	-0.75745900
H	6.72310000	3.91390000	0.51830300
H	3.91573900	6.11446300	-1.89291700
H	6.25984100	5.59924000	-1.24987800
C	-2.47904300	-3.96691100	-2.28719400
C	-3.61733800	-3.08548800	-1.76993200
H	-2.61524000	-4.24862400	-3.33903300
H	-2.46284300	-4.89782700	-1.70679100
H	-4.58051800	-3.61056000	-1.76476900
H	-3.73555100	-2.20608300	-2.41565400
C	3.69184100	-1.06353700	2.75129000
C	2.57395400	-1.30139700	3.77115500
H	2.70036600	-0.68672900	4.67083600
H	2.60197300	-2.34996600	4.09269400
H	4.67050300	-1.38694800	3.12668900
H	3.76183200	0.00584200	2.52317400
C	-4.13950700	-1.57042400	0.23219500
C	-4.89668900	-1.83002600	1.38413800
C	-4.29712400	-0.32625900	-0.39933400
C	-5.79541000	-0.88660500	1.88724100
H	-4.78644600	-2.78758000	1.88854200
C	-5.20227000	0.61386600	0.09448800
H	-3.72090000	-0.08610800	-1.28879600
C	-5.95638600	0.33874300	1.23901000
H	-6.37713500	-1.11599500	2.77671600
H	-5.31676800	1.55882600	-0.42859700
H	-6.66865200	1.06834200	1.61654500
C	0.12668800	-3.94957900	-2.23931400
C	0.24065200	-5.31257100	-1.92270500
C	1.27802600	-3.28079600	-2.69111800
C	1.46141800	-5.98110800	-2.04757100
H	-0.62729900	-5.86975500	-1.58357700
C	2.49874400	-3.94420600	-2.81122600
H	1.21482400	-2.22499400	-2.94031000
C	2.59639800	-5.30039900	-2.48899200
H	1.52022100	-7.03868100	-1.80193800
H	3.37375800	-3.39791500	-3.15125100
H	3.54514800	-5.82147300	-2.58709100
C	-0.03064800	-1.46306500	3.74517700

C	-0.08914100	-2.65234800	4.48931800
C	-1.21323900	-0.71559200	3.60652000
C	-1.28547300	-3.08165200	5.06917400
H	0.80420200	-3.25337600	4.63098700
C	-2.41003200	-1.14445400	4.18051000
H	-1.19054100	0.20566600	3.03075300
C	-2.45217600	-2.33191500	4.91575600
H	-1.30115500	-4.00389200	5.64478500
H	-3.31087800	-0.55213100	4.04734600
H	-3.38231000	-2.66553900	5.36833200
C	4.19225300	-1.55403200	0.27237800
C	4.99183100	-2.56217500	-0.28325500
C	4.25857300	-0.26884400	-0.28939600
C	5.83578800	-2.29988100	-1.36531000
H	4.95520700	-3.56455700	0.13800400
C	5.10031100	-0.00274300	-1.36897100
H	3.64257600	0.52639100	0.11856000
C	5.89283600	-1.01759700	-1.91267700
H	6.44991700	-3.09761500	-1.77584100
H	5.13652200	1.00051700	-1.78525300
H	6.54843400	-0.80910300	-2.75409700
C	-2.02461900	2.17651300	-3.15890100
C	-2.12858300	1.06020900	-4.01917000
C	-3.23632400	2.81412600	-2.80796200
C	-3.36239200	0.59351000	-4.47104800
H	-1.22217700	0.58447100	-4.37461700
C	-4.47178000	2.34927000	-3.26069700
H	-3.21043600	3.68751400	-2.16343700
C	-4.54840500	1.22868800	-4.09011900
H	-3.39562600	-0.25818700	-5.14758600
H	-5.38021200	2.87243500	-2.96860800
H	-5.50957200	0.86794500	-4.44681300
C	-0.65698200	4.22773100	-2.54285000
H	0.38217400	4.55093700	-2.41252200
H	-1.05377400	4.74505800	-3.42775200
H	-1.22228400	4.61292600	-1.68018300

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C	-3.66326500	-1.39563500	0.57457700
C	-2.56956000	-2.29483100	1.18603300
H	-3.94549700	-0.62295200	1.29774500
H	-4.55792000	-2.00797000	0.39872700
H	-2.41170300	-3.17398300	0.55132700

H	-2.91639300	-2.66477200	2.16021900
P	-0.86864800	-1.53926800	1.39814000
P	-3.18277200	-0.45130700	-0.97994700
C	1.07263400	1.25418400	-2.54490600
Cu	-0.09927700	-0.52189900	-0.55061800
C	0.07785900	-3.00732600	2.16335200
H	-0.68456600	-3.77481100	2.35076900
C	-0.92846700	-0.57727100	3.04561300
H	-0.09079600	0.12101600	2.94104800
C	-3.62863000	-1.67006200	-2.39756100
H	-3.05781200	-1.27447400	-3.24846800
C	-4.79657900	0.55309500	-1.23552800
H	-5.49508000	0.23794800	-0.44960000
C	2.34703800	1.72687900	-2.72374900
C	-0.54548600	-1.61276400	4.12222600
C	0.56813700	-2.48207100	3.53537200
H	-0.23157000	-1.10985900	5.04502600
H	-1.40120100	-2.25070500	4.37797600
H	0.82865000	-3.32243800	4.19016000
H	1.47158600	-1.87616100	3.40681500
C	-5.36145600	0.07305800	-2.59624300
C	-5.12145800	-1.43517100	-2.69260200
H	-5.40102200	-1.83824600	-3.67456300
H	-5.74878000	-1.94199200	-1.94842100
H	-6.42316400	0.33339500	-2.68773700
H	-4.83833100	0.58509700	-3.41427900
C	1.15889000	-3.62084100	1.30151800
C	2.34246000	-2.92691600	1.00473700
C	1.01241600	-4.92369700	0.80601500
C	3.35097000	-3.52291800	0.24799500
H	2.48227700	-1.91502800	1.37384900
C	2.01706000	-5.52134400	0.04125400
H	0.10241400	-5.47812500	1.02459700
C	3.19244100	-4.82327900	-0.23843100
H	4.26055600	-2.96666700	0.04018900
H	1.88282800	-6.53539800	-0.32707100
H	3.97909200	-5.28781500	-0.82702400
C	-2.18793400	0.22955800	3.28388500
C	-3.25742700	-0.24093500	4.06149400
C	-2.30501000	1.50541300	2.70500900
C	-4.40671700	0.53201700	4.24742500
H	-3.20002400	-1.21412200	4.53893300
C	-3.45260700	2.27659200	2.88569200
H	-1.48414300	1.88525200	2.10371200

C	-4.51159200	1.79220800	3.65840900
H	-5.21831800	0.14645500	4.85960500
H	-3.52080100	3.25502400	2.41865400
H	-5.40449600	2.39411900	3.80583900
C	-3.17509400	-3.09695000	-2.17585600
C	-4.04179700	-4.11161800	-1.74194900
C	-1.82613000	-3.43083100	-2.39351400
C	-3.57693400	-5.41219200	-1.52671500
H	-5.09362600	-3.89854600	-1.57839300
C	-1.35911900	-4.72626800	-2.17525500
H	-1.13438000	-2.66109700	-2.72696900
C	-2.23444200	-5.72539800	-1.73948600
H	-4.27131000	-6.18125600	-1.19730100
H	-0.30998600	-4.95273700	-2.34259900
H	-1.87456400	-6.73786200	-1.57619300
C	-4.62689800	2.05510300	-1.14610600
C	-5.42159400	2.80918300	-0.27145500
C	-3.70719900	2.73915600	-1.95790500
C	-5.31219400	4.20069200	-0.21180300
H	-6.13671100	2.29927400	0.37016100
C	-3.59691200	4.12883300	-1.90558100
H	-3.06808300	2.17902400	-2.63626700
C	-4.40088000	4.86727300	-1.03183700
H	-5.94481500	4.76237000	0.47102700
H	-2.88404600	4.63496800	-2.55170400
H	-4.32108400	5.95070400	-0.99568700
C	0.48439000	-0.08033900	-2.43695500
H	-0.50323500	-0.08503600	-2.91766600
H	1.08840000	-0.89286300	-2.84824700
C	3.18643900	1.02187000	1.96592200
O	2.44327900	0.60273600	2.82429500
H	0.32109500	2.04629200	-2.48442800
C	3.56055900	0.89921800	-2.84775300
C	4.73527200	1.42846400	-3.43624200
C	3.64052600	-0.43704500	-2.38583400
C	5.89090500	0.66490300	-3.59628600
H	4.73963500	2.45173000	-3.79610600
C	4.79519300	-1.19954700	-2.55202000
H	2.79822400	-0.87371200	-1.86532300
C	5.92978300	-0.66296500	-3.16553000
H	6.76252900	1.11028800	-4.07157000
H	4.80515900	-2.22674900	-2.19521100
H	6.82482500	-1.26483100	-3.30140200
C	2.52303400	3.22453000	-2.91038000

H	3.30488500	3.64451500	-2.26082600
H	2.80220500	3.48809500	-3.94197100
H	1.59247000	3.75502200	-2.68716600
C	4.58962500	0.59011200	1.76288400
C	5.32602600	0.93623100	0.61979200
C	5.17367700	-0.20916700	2.75977300
C	6.63644600	0.48109600	0.47885400
H	4.86963700	1.52937300	-0.16351800
C	6.48580700	-0.64931600	2.61824900
H	4.58651200	-0.46885300	3.63446900
C	7.21750400	-0.30460100	1.47667400
H	7.19204100	0.72919100	-0.41979700
H	6.93855100	-1.26193600	3.39276900
H	8.24027600	-0.65459500	1.36368800
O	2.83166300	2.03576300	1.08865600
C	1.50115300	2.34335000	0.83353200
O	0.62086500	1.51108500	0.87407000
C	1.31012800	3.77209800	0.50577700
C	0.03247200	4.18711000	0.09420400
C	2.34513300	4.71312600	0.62274000
C	-0.20513300	5.52774100	-0.19228400
H	-0.75794200	3.45036600	-0.00337400
C	2.09985700	6.05463600	0.33500200
H	3.33040900	4.39112600	0.93974600
C	0.82747800	6.46358400	-0.07158900
H	-1.19627400	5.84029700	-0.50778800
H	2.90219200	6.78106300	0.42762400
H	0.64031600	7.51053000	-0.29506700

Int3_b3

C	3.40627800	-1.34123500	1.09306800
C	2.60556200	-2.56997700	0.62368000
H	4.18397500	-1.10063200	0.35848900
H	3.91312500	-1.57020200	2.03846600
H	1.98199800	-2.93737700	1.44727000
H	3.30021000	-3.37739300	0.35930600
P	1.39891100	-2.23669400	-0.77558200
P	2.39225500	0.22490300	1.25656500
C	0.52822200	1.34352000	-2.34278500
C	-0.39309000	2.45745500	-2.13142300
H	1.52687100	1.73648400	-2.57836700
C	-2.01434600	1.98807600	1.22157000
C	-1.72156100	2.66121100	-2.40442200

Cu	0.98643500	0.31985800	-0.64226600
O	-1.05147400	1.25679700	1.26425400
C	0.55124500	-3.94573400	-0.88207400
H	1.16356800	-4.62239000	-0.27122300
C	2.38207100	-2.52370300	-2.39616400
H	1.82249600	-1.91736100	-3.11976300
C	1.66153100	0.25601000	3.02051700
H	0.76105000	0.86414600	2.88560200
C	3.74843500	1.49068700	1.67621300
H	4.63158300	0.89878200	1.95158200
H	0.09478700	3.32688500	-1.68061700
H	0.22354200	0.63715800	-3.12067400
C	2.16385200	-4.00560800	-2.76276200
C	0.73115100	-4.36661500	-2.36046000
H	2.35171000	-4.17528200	-3.83026900
H	2.85837100	-4.64973300	-2.20938800
H	0.52135100	-5.43603000	-2.48329500
H	0.01352500	-3.82578500	-2.99112300
C	3.23508300	2.17243200	2.96819500
C	2.66340000	1.06996900	3.86635900
H	2.17224100	1.47625000	4.75906100
H	3.48614500	0.43451200	4.21672700
H	4.04417100	2.72982500	3.45527200
H	2.45126200	2.89971800	2.71829300
C	-0.87274300	-4.01392400	-0.37765500
C	-1.23771500	-4.98072600	0.56903800
C	-1.86849500	-3.15461600	-0.86684000
C	-2.55864400	-5.09428800	1.00922000
H	-0.47958600	-5.65384200	0.96386900
C	-3.18860000	-3.26478200	-0.43264400
H	-1.60602700	-2.38126600	-1.58329400
C	-3.53894200	-4.23748900	0.50783800
H	-2.81868200	-5.85364700	1.74259100
H	-3.94005200	-2.58511700	-0.82343500
H	-4.56731000	-4.31811100	0.84887200
C	3.80471900	-2.00771900	-2.37889200
C	4.90444000	-2.81307900	-2.04397600
C	4.04621900	-0.65713800	-2.68592700
C	6.19811500	-2.28562900	-2.01122500
H	4.76226600	-3.86510600	-1.81558600
C	5.33529100	-0.12634200	-2.64677000
H	3.20905100	-0.01594200	-2.94951500
C	6.41937700	-0.94033100	-2.30813300
H	7.03380100	-2.93250400	-1.75584100

H	5.48989300	0.92377500	-2.87792600
H	7.42602000	-0.53157400	-2.28280700
C	1.22491600	-1.08982500	3.55885400
C	2.09316000	-1.94910600	4.25137500
C	-0.09719100	-1.51433500	3.34169300
C	1.65844500	-3.19848500	4.70036500
H	3.11680300	-1.64660000	4.45422700
C	-0.52953300	-2.76502700	3.78357500
H	-0.79535100	-0.85782200	2.82996000
C	0.34719800	-3.61447000	4.46282900
H	2.34742100	-3.84466200	5.23886400
H	-1.55477100	-3.06904600	3.59338700
H	0.01017300	-4.58712400	4.81187500
C	4.15277300	2.44502200	0.57311500
C	5.50548500	2.58374800	0.23170600
C	3.21329400	3.23630600	-0.10663300
C	5.91281200	3.48639900	-0.75336600
H	6.24943200	1.97870400	0.74573000
C	3.61540200	4.13784500	-1.09209700
H	2.15558700	3.12794800	0.11549900
C	4.96762400	4.26775900	-1.41937600
H	6.96813400	3.57788600	-0.99770100
H	2.86914100	4.73371800	-1.61093200
H	5.27950300	4.96996000	-2.18789000
O	-3.29482800	1.51057500	0.96496500
C	-3.75382500	0.35843500	1.58994300
O	-3.24564800	-0.08873900	2.58972300
C	-4.97208500	-0.16973000	0.92995300
C	-5.37393500	0.24080800	-0.34960000
C	-5.72214300	-1.12816600	1.63023500
C	-6.52062000	-0.31133500	-0.92132400
H	-4.78539300	0.96413700	-0.90248000
C	-6.87256000	-1.66410600	1.05922500
H	-5.38779000	-1.43497800	2.61581600
C	-7.27143500	-1.25666000	-0.21869400
H	-6.81449500	-0.00630900	-1.92067600
H	-7.45843400	-2.39804100	1.60577200
H	-8.16660100	-1.67989600	-0.66701700
C	-1.98808500	3.45704200	1.40521400
C	-3.16159500	4.22282600	1.47615600
C	-0.73960300	4.08441300	1.54000300
C	-3.08237000	5.59959100	1.68134400
H	-4.12511800	3.73796300	1.36989100
C	-0.66482300	5.45908200	1.73979000

H	0.15723800	3.47765200	1.48099100
C	-1.83742800	6.21885300	1.81187600
H	-3.99286100	6.18938200	1.73685400
H	0.30394100	5.94058700	1.83927300
H	-1.77915900	7.29252200	1.96919000
C	-2.63278200	1.66728200	-2.99589500
C	-3.82194400	2.07302200	-3.64922600
C	-2.40172800	0.27193900	-2.92717200
C	-4.69445500	1.15458000	-4.23268400
H	-4.05805000	3.12946300	-3.72184400
C	-3.27612500	-0.64446100	-3.50877900
H	-1.54056700	-0.09081400	-2.37958600
C	-4.42655100	-0.21490900	-4.17643600
H	-5.58515500	1.51556200	-4.74303800
H	-3.06072100	-1.70850900	-3.43549300
H	-5.09972000	-0.93245500	-4.63845600
C	-2.28916600	4.05043000	-2.17078000
H	-1.58782600	4.66468400	-1.59729500
H	-2.48759200	4.58675900	-3.11174300
H	-3.23953000	4.03183500	-1.61843800

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C	-3.34541200	-1.92609000	0.45044800
C	-2.15148800	-2.53491800	1.21219400
H	-3.85962300	-1.20728300	1.09738600
H	-4.06331300	-2.72711300	0.23004900
H	-1.75513700	-3.39493300	0.66003000
H	-2.50183900	-2.91100600	2.18217600
P	-0.66819500	-1.42785500	1.50006100
P	-2.92046700	-0.96063600	-1.10636300
C	2.59042400	1.97288600	2.24533500
C	1.42662100	1.39448000	-2.34854700
Cu	0.05110200	-0.43300500	-0.47482900
C	0.46284100	-2.59455900	2.48623600
H	-0.18904000	-3.41531300	2.81447700
C	-1.06011100	-0.34010800	3.02252100
H	-0.45453300	0.55220500	2.83731900
C	-2.96643700	-2.28826600	-2.49316100
H	-2.40293100	-1.81099600	-3.30640900
C	-4.66724100	-0.31610700	-1.56131700
H	-5.36551800	-0.74253600	-0.82969200
C	2.73517300	1.72269400	-2.58334600
C	-0.44261200	-1.08534100	4.22642100

C	0.83691200	-1.77173900	3.74200700
H	-0.24713900	-0.38255100	5.04462700
H	-1.13013500	-1.84812700	4.61244600
H	1.27188400	-2.42574200	4.50741000
H	1.59029400	-1.01514800	3.49456800
C	-4.98245900	-0.94408300	-2.94258300
C	-4.43775200	-2.37471400	-2.93889000
H	-4.52761400	-2.85557200	-3.92151700
H	-5.02355600	-2.97759200	-2.23317700
H	-6.05959600	-0.90775700	-3.14693500
H	-4.49026100	-0.36209000	-3.73277700
C	1.63234800	-3.19663500	1.74155500
C	2.69011000	-2.40666900	1.26550600
C	1.70129200	-4.58353300	1.54824900
C	3.78636200	-2.98695600	0.62759200
H	2.66249400	-1.32859800	1.39393100
C	2.79414300	-5.16861500	0.90499100
H	0.89151400	-5.21320900	1.91055900
C	3.84290000	-4.37138700	0.44450400
H	4.59134900	-2.35226900	0.26963400
H	2.82732600	-6.24709600	0.77190500
H	4.69874500	-4.82359600	-0.04987500
C	-2.50436300	0.09661900	3.15683700
C	-3.45717700	-0.63372100	3.88479000
C	-2.92345000	1.27818800	2.52135500
C	-4.78314800	-0.20204300	3.97013300
H	-3.17084900	-1.54597200	4.39956900
C	-4.24798300	1.70839300	2.60127800
H	-2.19676300	1.85603400	1.95766100
C	-5.18570300	0.96892300	3.32670200
H	-5.50008700	-0.78278700	4.54530700
H	-4.54720000	2.62060500	2.09289000
H	-6.21687900	1.30554100	3.39562800
C	-2.25543100	-3.57867600	-2.14894400
C	-2.93116300	-4.73122200	-1.72051700
C	-0.85214500	-3.62899800	-2.23104500
C	-2.22904400	-5.89019600	-1.37650000
H	-4.01524100	-4.73843200	-1.66097200
C	-0.14917400	-4.78098800	-1.88105700
H	-0.30777100	-2.74752900	-2.56145900
C	-0.83646400	-5.91947600	-1.45028000
H	-2.77714700	-6.77208300	-1.05393700
H	0.93542400	-4.78737300	-1.94068600
H	-0.29117600	-6.82042600	-1.18215100

C	-4.81250100	1.19129100	-1.53369900
C	-5.85221900	1.79036700	-0.80904200
C	-3.94694900	2.02607100	-2.25930600
C	-6.03064800	3.17606300	-0.81099400
H	-6.53147800	1.16233500	-0.23689100
C	-4.12239900	3.40995700	-2.26691400
H	-3.12404800	1.59009000	-2.82059900
C	-5.16661000	3.99209700	-1.54213800
H	-6.84823700	3.61527300	-0.24479700
H	-3.44336500	4.03327900	-2.84349500
H	-5.30698400	5.06988300	-1.55110200
O	1.90522200	1.72208700	3.20827100
C	0.68641600	0.13023400	-2.30358400
H	-0.30016100	0.27403700	-2.76645000
H	1.18897700	-0.70844300	-2.79459600
O	2.19085500	2.87676900	1.26176700
C	3.95003600	1.44913400	1.98819300
C	4.52480900	1.48277200	0.70895200
C	4.64785100	0.86923500	3.06090600
C	5.79055600	0.93314500	0.50477700
H	3.96829800	1.89806600	-0.12315000
C	5.91871700	0.34223900	2.85529300
H	4.18189800	0.84609000	4.04081900
C	6.48908700	0.37303400	1.57733400
H	6.21855800	0.93514500	-0.49296400
H	6.46407500	-0.09755400	3.68553600
H	7.47837200	-0.04770800	1.41731600
C	0.85721900	3.01364100	0.91822000
O	0.06015500	2.10967300	1.03286000
C	0.55643400	4.35111400	0.35734700
C	-0.72523800	4.56696000	-0.17459700
C	1.49739200	5.39234700	0.35960100
C	-1.06046100	5.81315000	-0.69567100
H	-1.44185100	3.75237100	-0.17790800
C	1.15418200	6.63832400	-0.16210800
H	2.48704800	5.22045100	0.76691100
C	-0.12239900	6.85007700	-0.68924800
H	-2.05315900	5.97505100	-1.10569200
H	1.88308100	7.44364900	-0.15901600
H	-0.38567200	7.82270800	-1.09631900
H	0.77942800	2.26216300	-2.19376000
C	3.82834800	0.76286200	-2.83202300
C	5.00735000	1.16946700	-3.50113500
C	3.78698900	-0.58180200	-2.39409600

C	6.05665000	0.28530200	-3.75077700
H	5.10013800	2.19332700	-3.84800300
C	4.83507600	-1.46533100	-2.64858500
H	2.94011500	-0.92686400	-1.81447400
C	5.97766200	-1.04508400	-3.33395200
H	6.93835100	0.63947700	-4.28068400
H	4.75708400	-2.49207000	-2.29828100
H	6.79106300	-1.73787400	-3.53417300
C	3.08982100	3.19795600	-2.68302400
H	3.96947600	3.46438500	-2.07811600
H	3.32190200	3.50546300	-3.71402100
H	2.25626900	3.82170100	-2.34585400

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C	3.21670700	1.40709700	0.81365200
C	3.76416500	0.05029700	0.33488800
H	3.37970700	2.16532500	0.03777200
H	3.76680200	1.73193200	1.70536900
H	3.75410800	-0.66880400	1.16235900
H	4.80760700	0.16647700	0.01919500
P	2.74149200	-0.75209300	-1.00985800
P	1.36948600	1.43220200	1.14502900
C	-0.38657300	0.93685700	-2.44496600
C	-1.72536200	0.81400400	-2.12823600
H	0.08560100	1.90844700	-2.31647800
C	-2.15939900	-1.29843700	-0.35547200
C	-2.58117400	-0.31204700	-2.35037800
Cu	0.46678300	0.06288800	-0.56901100
O	-0.90933800	-1.42261100	-0.34457900
C	3.56023200	-2.45600900	-1.12325600
H	4.57689100	-2.32179600	-0.72645400
C	3.44581300	-0.19621800	-2.70839400
C	1.16088600	0.94789800	2.97762400
H	0.12146700	0.60288800	3.02114900
C	1.11395300	3.29193000	1.49728000
C	-2.00662300	-1.39521300	-3.24443900
H	-2.57688000	-2.32523500	-3.20018000
H	-1.96787900	-1.07664600	-4.29684300
H	-0.98725700	-1.63781800	-2.92824500
C	-4.04817800	-0.06920900	-2.41637100
C	-4.91771500	-0.99864500	-3.02869200
C	-4.66217200	1.09060400	-1.88565500
C	-6.29619500	-0.79234800	-3.09667400

H	-4.51620900	-1.90347900	-3.46894800
C	-6.03796300	1.29589900	-1.94865300
H	-4.05599000	1.86304700	-1.42586100
C	-6.87385200	0.35450800	-2.55525000
H	-6.91935900	-1.54008700	-3.58183600
H	-6.45909200	2.20769700	-1.53026400
H	-7.94675200	0.51780700	-2.61019400
C	-3.05204700	-2.48662000	-0.43205500
C	-4.41176700	-2.43428700	-0.08588300
C	-2.51150800	-3.71071900	-0.86454700
C	-5.20242100	-3.58178800	-0.15280800
H	-4.84837700	-1.49657500	0.23631700
C	-3.30693200	-4.85172200	-0.93887700
H	-1.46238100	-3.75342000	-1.13351100
C	-4.65655400	-4.79365400	-0.57867600
H	-6.25153000	-3.52387200	0.12500200
H	-2.87109000	-5.79047300	-1.27176000
H	-5.27591500	-5.68532000	-0.63063100
H	-2.14266300	1.65619000	-1.58351900
H	0.08513100	0.26498800	-3.15791800
C	-2.50845800	-0.24494900	1.78938200
O	-2.74405400	-0.23686800	0.45536600
O	-1.79933000	-1.04438100	2.37033200
C	-3.22756200	0.86324900	2.49637300
C	-4.14061200	1.70792100	1.84857900
C	-2.98650700	1.02601900	3.86902300
C	-4.79119500	2.71210600	2.56688700
H	-4.34951200	1.56057200	0.79570000
C	-3.63401700	2.03362800	4.58097700
H	-2.29863900	0.34456600	4.35895000
C	-4.53614100	2.88031200	3.92984500
H	-5.50240400	3.36063100	2.06249100
H	-3.44236100	2.15501800	5.64368300
H	-5.04407600	3.66425600	4.48545700
C	1.25737900	2.27364700	3.75733500
H	0.82743000	2.16715200	4.76090900
H	2.30418100	2.57602600	3.88810200
C	0.52877000	3.33820100	2.92934900
H	-0.54504500	3.11688700	2.91045900
H	0.64083500	4.34314900	3.35370300
H	2.12646800	3.71360100	1.54225800
C	2.03673100	-0.20592000	3.41703800
C	1.61200400	-1.51889500	3.14475200
C	3.27156900	-0.02428300	4.05791300

C	2.40895800	-2.61208100	3.48451900
H	0.64946300	-1.67722200	2.66431400
C	4.06465500	-1.12053300	4.40808200
H	3.62180600	0.97498100	4.29991400
C	3.64002700	-2.41740100	4.11704500
H	2.06745200	-3.61588700	3.24910500
H	5.01455500	-0.95641400	4.91106900
H	4.25879200	-3.26971100	4.38509900
C	3.70330300	-2.67632200	-2.64747800
H	4.33703100	-3.54678600	-2.85453600
H	2.71889900	-2.88363400	-3.08854800
C	4.29546000	-1.38363800	-3.22203700
H	2.54489800	-0.14004400	-3.33026900
H	5.33260500	-1.29054700	-2.87837200
H	4.32339100	-1.38915200	-4.31834200
C	2.91764900	-3.60214900	-0.36666700
C	3.74681100	-4.59413700	0.18048600
C	1.52982500	-3.73474100	-0.21594500
C	3.21028200	-5.69448200	0.84950700
H	4.82675900	-4.50185800	0.08077900
C	0.99127800	-4.83215200	0.46081100
H	0.86008500	-2.96732700	-0.59152900
C	1.82629700	-5.81743500	0.99166800
H	3.87275800	-6.45051900	1.26357400
H	-0.08616700	-4.90450300	0.58066800
H	1.40306500	-6.66957300	1.51720100
C	4.09338700	1.17124000	-2.72755400
C	3.32893000	2.29238700	-3.09179000
C	5.43520200	1.38183000	-2.36884000
C	3.87658600	3.57577800	-3.08693700
H	2.29146700	2.15417400	-3.38531200
C	5.98779800	2.66409900	-2.36730900
H	6.06489600	0.54017100	-2.09460100
C	5.21089000	3.76811400	-2.72244200
H	3.25916700	4.42261300	-3.37446000
H	7.03036400	2.79800700	-2.09030900
H	5.64294600	4.76516400	-2.72315600
C	0.34152500	4.05487800	0.44417000
C	-1.03985800	3.87955500	0.26355100
C	1.00480300	4.97597600	-0.37967500
C	-1.73231100	4.60840100	-0.70371900
H	-1.58260300	3.16852100	0.88024800
C	0.31514800	5.70218600	-1.35321000
H	2.07456800	5.12941000	-0.25416800

C	-1.05840700	5.52205900	-1.51816300
H	-2.80308800	4.46279200	-0.82084500
H	0.85137200	6.41393900	-1.97587300
H	-1.60002500	6.08788800	-2.27118500

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C	-3.84743700	0.02617200	0.95792100
C	-3.34151100	-1.40266200	1.23980700
H	-4.94025600	0.01704000	0.85140200
H	-3.61471300	0.67225700	1.81232700
H	-3.67308700	-1.70767000	2.24034400
H	-3.78932400	-2.10267900	0.52569900
P	-1.48916100	-1.61672600	1.05315400
P	-3.07386400	0.88729400	-0.51835200
C	-0.06193100	0.40637900	-2.74694000
C	1.15976600	1.02314900	-2.57396500
H	-0.88658600	0.98911100	-3.15107400
C	2.18696000	0.64803800	-0.01126200
C	2.39233900	0.40443700	-2.17700800
Cu	-0.79737100	0.17762500	-0.61472700
O	1.04286100	0.19863500	0.26625900
C	-0.73769700	-1.16888600	2.74698800
C	-1.31393900	-3.49396900	1.35986100
H	-2.30601900	-3.84017800	1.67886000
C	-3.94562500	2.58945900	-0.40550900
H	-4.60510100	2.50688300	0.46736800
C	-4.13621900	0.33846400	-2.00636200
C	2.37565800	-1.11413600	-2.23205900
H	3.25772900	-1.55611000	-1.76702100
H	2.31546200	-1.47719700	-3.26895500
H	1.50458900	-1.49851500	-1.69433500
C	3.65648100	1.07948300	-2.59982800
C	4.80554500	0.33320600	-2.93838900
C	3.77183700	2.48398700	-2.69787100
C	5.99116400	0.94724200	-3.34579000
H	4.77286200	-0.75002800	-2.90840700
C	4.95250000	3.09755700	-3.10970600
H	2.93228500	3.11694000	-2.43108000
C	6.07618400	2.33594200	-3.43770400
H	6.84865800	0.32959600	-3.60358500
H	4.99403500	4.18272400	-3.16677700
H	6.99685300	2.81583800	-3.75890200
H	1.16635900	2.10612600	-2.68537600

H	-0.12935100	-0.67007100	-2.89374900
C	-0.36157200	-3.59851200	2.57814000
C	-0.73346700	-2.48061100	3.55599100
H	0.30045500	-0.93401900	2.48728800
C	-1.33171000	0.05559200	3.40733900
C	-2.41616100	-0.00428600	4.29717000
C	-0.78799200	1.31786600	3.11092100
C	-2.94998700	1.15856500	4.85944900
H	-2.84781000	-0.96378800	4.56768300
C	-1.32379700	2.47994600	3.66616800
H	0.06632300	1.37620300	2.44275100
C	-2.41066100	2.40632400	4.54203500
H	-3.78536100	1.08556600	5.55176800
H	-0.88492000	3.44234400	3.41706600
H	-2.82328400	3.30982100	4.98382300
C	-0.88393400	-4.31791000	0.16687700
C	-1.65268100	-5.41184600	-0.25272400
C	0.30617500	-4.03805300	-0.52340600
C	-1.24888300	-6.20653100	-1.32861500
H	-2.57730300	-5.64546100	0.27079000
C	0.71188300	-4.82748400	-1.59901200
H	0.91691600	-3.19211300	-0.21913700
C	-0.06466400	-5.91592700	-2.00723400
H	-1.85893300	-7.05373300	-1.63237500
H	1.63637900	-4.59097200	-2.11904500
H	0.25370900	-6.53239300	-2.84374200
C	-4.83827600	2.67649100	-1.67123500
C	-5.35921200	1.27423600	-1.98863600
H	-3.51991100	0.62075000	-2.87103200
C	-4.40144200	-1.14925800	-2.10368300
C	-5.59866200	-1.73558500	-1.66647800
C	-3.41564900	-1.98920000	-2.64879600
C	-5.79793700	-3.11572400	-1.76134700
H	-6.39282300	-1.11918700	-1.25658300
C	-3.60726900	-3.36705500	-2.73618200
H	-2.48461900	-1.55438800	-3.00366200
C	-4.80277200	-3.93719700	-2.29095600
H	-6.73709100	-3.54539300	-1.42203800
H	-2.82135800	-3.99502700	-3.14508100
H	-4.95735200	-5.01029600	-2.36202300
C	-3.06412200	3.80363300	-0.21137200
C	-3.20871500	4.60126100	0.93216900
C	-2.13888300	4.20556100	-1.18799200
C	-2.47008400	5.77583700	1.08991900

H	-3.91403300	4.30293500	1.70431200
C	-1.40228300	5.37999700	-1.03688300
H	-1.99487200	3.59887000	-2.07882600
C	-1.57025100	6.17451300	0.10089600
H	-2.60593700	6.38226000	1.98155100
H	-0.69557500	5.67490900	-1.80777600
H	-1.00307000	7.09456800	0.21374800
C	2.55297700	2.07189200	0.26769200
C	3.87819500	2.47743300	0.48997900
C	1.53324900	3.03523800	0.33777500
C	4.17281300	3.80732200	0.79187400
H	4.67774600	1.74898300	0.43023300
C	1.83156700	4.36492300	0.63150300
H	0.50420100	2.73351300	0.17256800
C	3.15312000	4.75660600	0.86384900
H	5.20492000	4.09946800	0.96751200
H	1.02606700	5.09103700	0.68977100
H	3.38392400	5.79222800	1.10068400
O	3.31626600	-0.22812400	0.27623200
C	3.41813300	-0.85057900	1.47360200
O	2.62891000	-0.75241900	2.39360700
C	4.65601900	-1.69110400	1.55067700
C	5.62044000	-1.71250500	0.53262000
C	4.84780300	-2.46417100	2.70457900
C	6.75990900	-2.50543600	0.67068100
H	5.47928400	-1.10234600	-0.35253200
C	5.98472800	-3.25781700	2.83643300
H	4.09519600	-2.42439300	3.48513700
C	6.94283200	-3.27999200	1.81873400
H	7.50716100	-2.51669500	-0.11823600
H	6.12669500	-3.85699200	3.73187300
H	7.83138000	-3.89754700	1.92206800
H	-0.43176000	-4.59480600	3.03149300
H	0.67641900	-3.46494200	2.24942300
H	-1.72189400	-2.68907200	3.98676600
H	-0.02493600	-2.41299600	4.39039400
H	-5.64958400	3.39677000	-1.51295700
H	-4.24571400	3.04899300	-2.51586900
H	-6.07047600	0.96894100	-1.21115100
H	-5.89484100	1.23809600	-2.94534400

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C	3.87309800	-0.33011700	0.59266200

C	3.49573900	-1.63710500	-0.12690800
H	4.33444000	0.36328400	-0.12120600
H	4.61863700	-0.53818300	1.37025800
H	3.19427600	-2.39454800	0.60597500
H	4.37259700	-2.02757700	-0.65652000
P	2.02982600	-1.47931400	-1.27863200
P	2.42553100	0.61269000	1.32616100
C	0.27027600	1.93224900	-1.70961100
C	-0.95672500	2.35946100	-1.24515100
H	1.14766600	2.53765000	-1.49607600
C	-2.30486900	0.40635700	0.23664500
C	-2.23890000	1.77414200	-1.51302800
Cu	0.66567100	0.28772000	-0.24820600
O	-1.26059600	-0.28999600	0.11216200
C	1.74864300	-3.28587100	-1.76466900
H	2.72061600	-3.78242700	-1.62974000
C	2.68526300	-1.01468500	-3.02320500
C	2.25704900	-0.02261100	3.11654400
H	1.23070300	0.25824900	3.38637200
C	3.30836500	2.21759700	1.86565500
H	4.37430600	2.02563900	1.68818700
C	-2.23943600	0.70309000	-2.59052200
H	-3.18393900	0.15895600	-2.63558800
H	-2.04200900	1.12906900	-3.58581500
H	-1.46230600	-0.03715100	-2.37824300
C	-3.42637500	2.67268200	-1.44574000
C	-4.55189400	2.45942600	-2.27189200
C	-3.49505300	3.78428100	-0.57492500
C	-5.67006500	3.29282300	-2.22801300
H	-4.54899000	1.64147500	-2.98319600
C	-4.60856400	4.62030900	-0.53460600
H	-2.67132100	3.99891900	0.09699600
C	-5.71023400	4.38328100	-1.35919300
H	-6.50992200	3.09093200	-2.88911800
H	-4.61459100	5.46226400	0.15382600
H	-6.57813500	5.03650300	-1.32701400
H	-0.92967400	3.19584200	-0.54989700
H	0.33702200	1.27779300	-2.57532200
O	-3.54274900	-0.21199800	-0.20177500
C	-2.53958000	1.29837700	1.41220500
C	-3.81832300	1.76408000	1.75755200
C	-1.45177500	1.67291400	2.21808400
C	-4.00067300	2.57540400	2.87840300
H	-4.67133100	1.48793000	1.14980500

C	-1.63458500	2.48958900	3.33219400
H	-0.46582500	1.29886300	1.96653900
C	-2.91273600	2.94565900	3.66910500
H	-5.00003000	2.92065200	3.12969900
H	-0.78187100	2.75807200	3.95239400
H	-3.05725600	3.57669100	4.54212600
C	-3.97964900	-1.31549400	0.45560600
C	-5.28441700	-1.80793400	-0.08602300
C	-5.81371000	-2.98591900	0.46035300
C	-5.99091600	-1.12959600	-1.08938000
C	-7.02814200	-3.48865100	0.00006100
H	-5.25957900	-3.48715300	1.24705400
C	-7.20902800	-1.63432800	-1.54473100
H	-5.59219800	-0.20696600	-1.49524700
C	-7.72709000	-2.81405500	-1.00520100
H	-7.43218300	-4.40349100	0.42522100
H	-7.75557100	-1.10447900	-2.32023600
H	-8.67583500	-3.20515700	-1.36371000
O	-3.39621800	-1.84534900	1.38077200
C	1.50548500	-3.19982800	-3.28937900
H	1.50449600	-4.20076700	-3.73682500
H	0.51911600	-2.75892800	-3.48705700
C	2.62299400	-2.31705700	-3.85930700
H	3.57141600	-2.86254600	-3.78974900
H	2.46929900	-2.08291600	-4.91951600
H	1.90609600	-0.34286000	-3.40097500
C	3.09888500	2.28343600	3.39865900
C	3.21434100	0.85534700	3.94422600
H	2.97399700	0.80019100	5.01308500
H	4.25085100	0.51385900	3.83019000
H	3.82962200	2.96223600	3.85401900
H	2.10491100	2.68826000	3.62664000
C	0.71794100	-4.07892200	-0.98583300
C	0.96347700	-5.44159900	-0.75156200
C	-0.48104800	-3.52456200	-0.51469600
C	0.03595700	-6.23594200	-0.07772100
H	1.89364700	-5.88472300	-1.10310800
C	-1.40652900	-4.31607700	0.17174700
H	-0.69488000	-2.46767500	-0.64621200
C	-1.15460100	-5.67268900	0.38749100
H	0.24689200	-7.28944900	0.08911800
H	-2.31110100	-3.85390700	0.55442900
H	-1.87727500	-6.28495600	0.92110200
C	3.98849800	-0.24567900	-3.04540000

C	3.96064500	1.15855300	-3.09002000
C	5.24367700	-0.87452600	-2.99749500
C	5.13785600	1.90759200	-3.07827300
H	3.00204600	1.66922900	-3.13791900
C	6.42379300	-0.12822400	-2.99019200
H	5.30949100	-1.95863900	-2.97451100
C	6.37749300	1.26646500	-3.02760700
H	5.08272500	2.99233900	-3.11562100
H	7.38177500	-0.64093000	-2.95889500
H	7.29670000	1.84595900	-3.02540300
C	2.92867000	3.46790400	1.10292600
C	3.87017600	4.09211500	0.27186400
C	1.65243900	4.04432000	1.20800900
C	3.55330800	5.25617700	-0.43219500
H	4.86535700	3.66258600	0.17792000
C	1.33459100	5.20953100	0.50996400
H	0.89196300	3.57928800	1.82930400
C	2.28309900	5.82072300	-0.31424300
H	4.30213900	5.72329200	-1.06679400
H	0.34147700	5.63977200	0.60864500
H	2.03230200	6.72727000	-0.85803000
C	2.36635300	-1.52752900	3.24321100
C	3.53123100	-2.17012300	3.68695600
C	1.26809600	-2.32236300	2.86888500
C	3.59958600	-3.56498200	3.74907500
H	4.39308000	-1.58829700	3.99999100
C	1.33869800	-3.71391300	2.92095700
H	0.35355900	-1.84711200	2.52040200
C	2.50733500	-4.34135700	3.36207100
H	4.51056100	-4.04116100	4.10313600
H	0.48244700	-4.30401600	2.60865800
H	2.56243200	-5.42570700	3.40585300

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C	2.96168000	-2.30743000	0.35294900
C	3.62539300	-1.06425200	0.97494200
H	3.73731500	-3.00773200	0.01772600
H	2.36556000	-2.82771800	1.11233600
H	4.11796200	-1.34958200	1.91254100
H	4.40424400	-0.68641000	0.30276800
P	2.47165600	0.38701800	1.24686900
P	1.75551600	-1.96755100	-1.03944200
C	0.33911700	1.36045200	-2.27442700

C	-1.02832000	1.54035800	-2.20300900
H	0.72464100	0.65520000	-3.00774000
C	-1.97457300	1.30455000	0.43130800
C	-1.74552100	2.52436500	-1.45048800
Cu	0.65963200	0.07444000	-0.47506500
O	-0.82109600	0.86765000	0.67678900
C	1.73293800	0.16171800	2.99284800
C	3.71802800	1.71119300	1.83298500
H	4.66380100	1.17768200	1.99570600
C	1.19355200	-3.74661900	-1.44269500
H	1.91672500	-4.39118300	-0.92558300
C	2.79970500	-1.83463200	-2.64279600
C	-0.89013600	3.64456800	-0.88662800
H	-1.42146900	4.25387400	-0.15338400
H	-0.52411800	4.31307200	-1.68034600
H	-0.01894300	3.22564900	-0.37500600
C	-3.11152900	2.88603600	-1.92507000
C	-3.67959200	4.14359800	-1.62683900
C	-3.90985800	2.01733100	-2.70581600
C	-4.95411900	4.50509900	-2.06693200
H	-3.11740800	4.86485500	-1.04637600
C	-5.18136800	2.37596900	-3.14528300
H	-3.53320600	1.03953600	-2.98499200
C	-5.72076600	3.62602600	-2.82899700
H	-5.34348900	5.48775900	-1.81079400
H	-5.75296400	1.67371700	-3.74840700
H	-6.71142500	3.90704600	-3.17596500
C	-2.60822100	2.31477500	1.32905000
C	-3.97723500	2.62223300	1.27442400
C	-1.80502600	2.97942400	2.27085100
C	-4.52551400	3.56215700	2.14751500
H	-4.61255800	2.12299000	0.55261000
C	-2.35421400	3.92169200	3.13697600
H	-0.74988900	2.73314600	2.31862000
C	-3.71936200	4.21693000	3.08016400
H	-5.58832200	3.78335900	2.09480900
H	-1.71879400	4.42013100	3.86499200
H	-4.15034100	4.94804600	3.75924200
H	-1.62059400	0.80108000	-2.73753300
H	1.03266700	2.13560200	-1.95679200
C	-3.41412500	-0.57265000	0.77752200
O	-2.95299300	0.36293400	-0.09641500
O	-2.95510200	-0.76278900	1.88625200
C	-4.58113900	-1.34040100	0.24242400

C	-5.18043200	-1.05048000	-0.99045300
C	-5.09683300	-2.37321100	1.03861300
C	-6.27514700	-1.79881000	-1.42635300
H	-4.79958000	-0.23253400	-1.58912800
C	-6.19030400	-3.11706400	0.60152700
H	-4.62544600	-2.57313600	1.99487600
C	-6.77912300	-2.83392000	-0.63502200
H	-6.73967600	-1.56800400	-2.38134300
H	-6.58748800	-3.91433400	1.22427700
H	-7.63322100	-3.41315600	-0.97648600
C	3.18400800	2.15260400	3.21825700
C	2.69368400	0.89824200	3.94744700
H	0.80449200	0.74117800	2.92637200
C	1.35020300	-1.26105300	3.33942300
C	2.23028500	-2.15362100	3.97183300
C	0.06782000	-1.72054900	2.99283300
C	1.84512500	-3.46990000	4.24025100
H	3.22209800	-1.82645300	4.27139000
C	-0.31372400	-3.03637200	3.25581900
H	-0.63880100	-1.04542200	2.51753100
C	0.57345400	-3.91819000	3.87871700
H	2.54052900	-4.14174700	4.73768700
H	-1.31011500	-3.36296400	2.97286100
H	0.27368600	-4.94149600	4.09011800
C	3.98008100	2.85196400	0.87454100
C	5.28656100	3.13330300	0.45248200
C	2.94365800	3.68153600	0.41776500
C	5.55416700	4.20854900	-0.39872600
H	6.10475000	2.50456600	0.79700300
C	3.20509400	4.75355300	-0.43492600
H	1.92116100	3.48631200	0.72903700
C	4.51324400	5.02213500	-0.84750300
H	6.57715700	4.41067200	-0.70636500
H	2.38489300	5.37881000	-0.77739900
H	4.71732600	5.85921300	-1.50971700
C	1.45139800	-3.89200100	-2.96031900
C	2.80927100	-3.25215000	-3.25443600
H	2.17320400	-1.20390500	-3.28595100
C	4.14156200	-1.14691700	-2.50549800
C	5.31824100	-1.83998300	-2.17806000
C	4.22952300	0.24109500	-2.70242900
C	6.53563100	-1.16818900	-2.04647000
H	5.29661900	-2.91548200	-2.02944200
C	5.44251200	0.91614000	-2.56692300

H	3.33427800	0.79901600	-2.96519700
C	6.60318600	0.21270800	-2.23714400
H	7.43297200	-1.72928800	-1.79812800
H	5.47702100	1.99148000	-2.71415100
H	7.55107700	0.73436400	-2.13622900
C	-0.19223500	-4.15597500	-1.00125700
C	-0.34887700	-5.19644500	-0.07534700
C	-1.34580000	-3.56567200	-1.54057500
C	-1.61803900	-5.64427500	0.29679600
H	0.53359600	-5.66541800	0.35443500
C	-2.61459300	-4.01392400	-1.17623800
H	-1.25290700	-2.74636700	-2.24952800
C	-2.75527800	-5.05673200	-0.25654300
H	-1.71438300	-6.45514100	1.01433500
H	-3.49571900	-3.54537700	-1.60349400
H	-3.74608600	-5.39906200	0.02768000
H	3.96443800	2.68303900	3.77715000
H	2.35238300	2.85669700	3.08640300
H	3.55688400	0.26803500	4.19604300
H	2.19248000	1.13967300	4.89295500
H	3.59609700	-3.86499600	-2.79876000
H	3.02425100	-3.20620700	-4.32900700
H	1.41835100	-4.94842100	-3.25184900
H	0.66222600	-3.38070900	-3.52626300

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C	3.36537900	0.45615200	0.73712000
C	3.24302500	-1.07083100	0.88284700
H	3.82752300	0.69982800	-0.22763900
H	4.02588700	0.84919800	1.51994800
H	2.93629300	-1.32334600	1.90436400
H	4.22111000	-1.53582300	0.71234800
P	1.93674700	-1.84057700	-0.21359100
P	1.73039600	1.37821500	0.74211600
C	-0.15196900	0.30758600	-2.64590600
C	-1.42343800	0.82594600	-2.46963200
H	0.65838200	1.01764200	-2.79968500
C	-2.67506700	-0.01361700	-0.14232200
C	-2.71338800	0.20752300	-2.41508900
Cu	0.28039300	-0.06370600	-0.48405100
O	-1.60767300	-0.62224600	0.10557500
C	1.90423300	-3.61536500	0.44773300
H	2.88341700	-3.77015500	0.92361100

C	2.77381100	-2.36778300	-1.85820300
C	1.34977100	1.78767100	2.56776500
H	0.26254400	1.92336400	2.56319800
C	2.34428400	3.14441100	0.36275800
C	-3.86338000	1.17033600	-2.67418800
C	-4.00808200	-0.63139200	0.08373800
C	-5.17292100	0.13283000	0.26706700
C	-4.10692800	-2.03318500	0.12697900
C	-6.40118200	-0.48958100	0.49147100
H	-5.11428400	1.21510000	0.24502500
C	-5.33628700	-2.64969100	0.34522900
H	-3.21344000	-2.62806400	-0.01603700
C	-6.48947600	-1.88197400	0.53029900
H	-7.29021400	0.11807900	0.63983100
H	-5.39390000	-3.73474600	0.37209600
H	-7.44727000	-2.36527400	0.70445100
H	-1.44810600	1.89759600	-2.26893500
H	-0.00206800	-0.68457600	-3.06328000
C	-2.47055600	1.86204200	1.36884600
O	-2.69627300	1.42779600	0.10706200
O	-2.24387100	1.14706000	2.32575200
C	-2.53436700	3.35633300	1.46794600
C	-2.81410000	4.17914700	0.36707100
C	-2.31762800	3.93563800	2.72698600
C	-2.86410100	5.56457200	0.52504500
H	-2.99496300	3.72953300	-0.60256500
C	-2.36707000	5.31963300	2.88102900
H	-2.12036100	3.28156500	3.57005300
C	-2.63860200	6.13647500	1.77946500
H	-3.08191000	6.19788900	-0.33058200
H	-2.19925700	5.76199000	3.85922400
H	-2.67833100	7.21588500	1.89942900
H	-3.65574400	2.14656100	-2.22623400
H	-4.02667900	1.33690900	-3.74968300
H	-4.80862400	0.80736200	-2.25663900
C	-2.91839000	-1.18926700	-2.88427800
C	-4.06497800	-1.54275400	-3.62855000
C	-2.01350800	-2.23553900	-2.59267300
C	-4.28209200	-2.84578400	-4.07510000
H	-4.80160800	-0.78637600	-3.87500100
C	-2.23497600	-3.54014100	-3.03260700
H	-1.15236500	-2.03281800	-1.97041800
C	-3.36617400	-3.85755300	-3.78613600
H	-5.17589500	-3.06825600	-4.65353500

H	-1.51724300	-4.31749600	-2.77731100
H	-3.53335400	-4.87336200	-4.13480500
C	1.89733900	-4.46930200	-0.84204800
H	2.06974600	-5.52614500	-0.60644800
H	0.91344200	-4.40469300	-1.32615300
C	2.98981000	-3.89646800	-1.75318000
H	3.96768300	-4.11824900	-1.30940800
H	2.98257900	-4.35332600	-2.75008300
H	1.98050100	-2.19627300	-2.59482300
C	0.83752800	-3.97875000	1.46220100
C	1.15236200	-4.91342800	2.46134000
C	-0.46166300	-3.45289000	1.42641800
C	0.19764600	-5.32341800	3.39230600
H	2.15899800	-5.32484400	2.50915400
C	-1.41723800	-3.85731500	2.36199800
H	-0.73140600	-2.69862900	0.69440800
C	-1.09474600	-4.79559600	3.34459400
H	0.46497800	-6.04995800	4.15561400
H	-2.41318200	-3.42471300	2.32166300
H	-1.84133500	-5.10805300	4.07016600
C	3.96346200	-1.52911100	-2.27322300
C	5.27056600	-1.78841700	-1.82940300
C	3.76410200	-0.42107100	-3.11421300
C	6.33589400	-0.96905700	-2.20863600
H	5.46914400	-2.64164000	-1.18704800
C	4.82552500	0.40205000	-3.49147800
H	2.76227700	-0.20348400	-3.47547600
C	6.11890100	0.13160500	-3.03913300
H	7.33854300	-1.19591200	-1.85530000
H	4.63889200	1.25161100	-4.14289600
H	6.94920900	0.76669000	-3.33597300
C	1.99882800	3.16353100	2.81972000
H	1.54842500	3.64959400	3.69378400
H	3.07064500	3.05852000	3.02937700
C	1.81926700	3.99472400	1.54390100
H	0.75764700	4.23042800	1.40240400
H	2.35529200	4.95017600	1.59278000
H	3.43696900	3.09212700	0.45710400
C	1.65938600	0.66611700	3.53575000
C	2.88129800	0.56421000	4.21840100
C	0.69728600	-0.33995100	3.73641200
C	3.13971600	-0.51523300	5.06734400
H	3.64082900	1.33189200	4.10065300
C	0.95998900	-1.42348700	4.57473200

H	-0.26191100	-0.26788000	3.22947200
C	2.18363400	-1.51641600	5.24328800
H	4.09091500	-0.56991100	5.59120800
H	0.20794800	-2.19721200	4.69906000
H	2.38682700	-2.35880000	5.89920600
C	2.02451400	3.66551400	-1.02030900
C	3.05344900	3.84466000	-1.95621100
C	0.71436800	3.99025300	-1.40636000
C	2.78777500	4.33115700	-3.23831000
H	4.07663000	3.60362800	-1.67570200
C	0.44645000	4.47994400	-2.68472200
H	-0.10528000	3.85992600	-0.70544400
C	1.48121400	4.65149600	-3.60786500
H	3.60389300	4.46579000	-3.94373400
H	-0.57510200	4.72768700	-2.96122400
H	1.26961000	5.03234200	-4.60324600

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C	-3.02904000	-1.76901400	1.05840700
C	-1.84568900	-2.64316200	1.51598600
H	-3.93873800	-2.38457700	1.02717300
H	-3.20828400	-0.97930100	1.79672300
H	-2.05388100	-2.97595400	2.54150800
H	-1.79339200	-3.54435700	0.89482900
P	-0.12493400	-1.88467400	1.39535900
P	-2.89269100	-0.84860300	-0.56412400
C	-0.53996900	0.83276700	-3.08523600
C	0.06825100	2.05548400	-2.85793500
H	-1.56118500	0.83589800	-3.46263300
C	1.18899800	2.31248700	-0.31603500
C	1.42487000	2.38936200	-2.54496800
Cu	-1.01254900	0.37691800	-0.96033800
O	0.48195200	1.29696800	-0.06797700
C	0.07874900	-0.86136300	3.01227100
C	0.86894800	-3.35529500	2.11884900
H	0.13438400	-4.06232500	2.52734900
C	-4.61195600	-0.02002400	-0.61606100
H	-5.10887900	-0.36318000	0.29950100
C	-3.34022000	-2.10499500	-1.91887400
C	1.77760700	3.83984100	-2.85151300
H	-0.60908700	2.91208100	-2.83061900
H	0.04826500	-0.04827300	-3.33292800
C	1.64531200	-2.75010800	3.31295400

C	0.68041600	-1.82408800	4.05571400
H	0.85586900	-0.14003000	2.73574400
C	-1.13370400	-0.06520800	3.44324300
C	-2.12164800	-0.57928700	4.29951300
C	-1.29199300	1.24823400	2.96620600
C	-3.23692100	0.18476600	4.65388300
H	-2.02422300	-1.58185600	4.70620700
C	-2.40695800	2.01046300	3.31607500
H	-0.52509100	1.66882100	2.32284200
C	-3.38802300	1.48161400	4.15960800
H	-3.98376500	-0.23443400	5.32413100
H	-2.50026200	3.02328300	2.93310400
H	-4.25151700	2.07872400	4.44224100
C	1.74312100	-4.10583500	1.13833800
C	2.74813400	-3.45938400	0.39999400
C	1.59730800	-5.49132500	0.98070300
C	3.58203500	-4.17846500	-0.45658500
H	2.87899700	-2.38418800	0.49318000
C	2.42606900	-6.21436900	0.11923800
H	0.82607400	-6.01135500	1.54495200
C	3.42407900	-5.55988500	-0.60335300
H	4.36203800	-3.65811300	-1.00624700
H	2.29461500	-7.28911100	0.01967500
H	4.07635600	-6.11824000	-1.26962400
C	-5.33943900	-0.66648900	-1.82399600
C	-4.87956800	-2.12276500	-1.93769400
H	-3.00635800	-1.60501900	-2.83876100
C	-2.61730000	-3.43375700	-1.82896700
C	-3.26265300	-4.61968500	-1.45307000
C	-1.24527700	-3.49096200	-2.13020400
C	-2.55700800	-5.82419000	-1.37248800
H	-4.32499200	-4.61774200	-1.22971100
C	-0.53763100	-4.68777500	-2.04088200
H	-0.72553100	-2.58130000	-2.42205900
C	-1.19347100	-5.86221400	-1.66037100
H	-3.08009400	-6.73253400	-1.08433800
H	0.52643600	-4.70338000	-2.25741000
H	-0.64224000	-6.79549600	-1.59030000
C	-4.63254400	1.49346800	-0.61379400
C	-5.16849400	2.18571500	0.48103500
C	-4.16583100	2.24174900	-1.70695300
C	-5.25304700	3.57956500	0.48142400
H	-5.52633900	1.62670200	1.34229200
C	-4.24917600	3.63402200	-1.71117300

H	-3.73897200	1.73490800	-2.56854500
C	-4.79954600	4.30914400	-0.61824000
H	-5.68050900	4.09261600	1.33885300
H	-3.88748900	4.19209200	-2.57058700
H	-4.87547400	5.39309800	-0.62713900
C	0.71105400	3.69229400	0.00234400
C	1.59701300	4.74847700	0.27046200
C	-0.66981800	3.94340200	0.05729000
C	1.11448100	6.01914500	0.58304400
H	2.66592800	4.57011900	0.24018200
C	-1.14926600	5.21559400	0.36510800
H	-1.36775300	3.13473500	-0.13263300
C	-0.25968100	6.26032600	0.62987600
H	1.81666100	6.82159400	0.79424400
H	-2.22176000	5.38489300	0.40363500
H	-0.63429500	7.25083400	0.87469200
O	2.60364300	2.16099200	-0.06948700
C	3.00000900	1.79647700	1.17799400
O	2.26487000	1.73425800	2.14470500
C	4.46365400	1.50573200	1.23548300
C	5.26573800	1.44677800	0.08675200
C	5.03349400	1.28139500	2.49745100
C	6.62697700	1.16648700	0.20768900
H	4.82327400	1.61209000	-0.88867500
C	6.39377600	1.00669300	2.61235900
H	4.39282800	1.33012200	3.37190000
C	7.19271200	0.94892800	1.46621100
H	7.24472900	1.11517000	-0.68469400
H	6.83237000	0.83758900	3.59217500
H	8.25442100	0.73275700	1.55494700
C	2.50847500	1.39507100	-2.81449800
C	3.67410600	1.76678200	-3.51674600
C	2.43079700	0.05214500	-2.38569500
C	4.68523400	0.84759600	-3.80423900
H	3.79448400	2.78760000	-3.86170400
C	3.43987800	-0.86595500	-2.67162000
H	1.59261800	-0.26616900	-1.77850900
C	4.57320200	-0.47980100	-3.39082400
H	5.56040400	1.17466300	-4.36130300
H	3.33554200	-1.89087100	-2.32484800
H	5.35547700	-1.19885900	-3.62032500
H	2.67206000	4.16686400	-2.31040900
H	1.96908000	3.99534500	-3.92337100
H	0.95987800	4.50907400	-2.57129600

H	2.04306100	-3.54468700	3.95657900
H	2.50542200	-2.17587400	2.94513900
H	-0.10104900	-2.43193600	4.52954200
H	1.17809400	-1.26333700	4.85688400
H	-6.42539800	-0.58148900	-1.70099800
H	-5.08216300	-0.12810800	-2.74419200
H	-5.25750700	-2.60431200	-2.84792200
H	-5.27027900	-2.69406000	-1.08601600

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C	3.51683200	1.18311300	-1.01637100
C	2.70985000	2.42334800	-0.59421500
H	4.25579600	0.94329900	-0.24316400
H	4.07241800	1.40342700	-1.93656300
H	2.11565600	2.78627700	-1.44124000
H	3.39951400	3.22875400	-0.31373400
P	1.45708200	2.12073900	0.76458800
P	2.50447200	-0.38067100	-1.22828500
C	0.44938000	-1.24648200	2.24195900
C	-0.33822600	-2.26888400	1.74192600
H	1.51733400	-1.43622800	2.33881800
C	-1.99069700	-1.53108200	-0.44628500
C	-1.75979500	-2.42943400	1.68599500
Cu	0.66969600	-0.14270000	0.35641500
O	-1.11796200	-0.62478300	-0.52040100
C	0.66868000	3.85026400	0.89234700
H	1.38195600	4.53038200	0.40695900
C	2.37320800	2.31122000	2.44069300
C	1.98227600	-0.41741300	-3.06240400
H	1.12129100	-1.09719400	-3.05715000
C	3.90739300	-1.64951200	-1.49349600
C	-2.18002300	-3.89358600	1.58966800
H	0.21391000	-3.08332800	1.26876600
H	0.02990800	-0.49371600	2.90520900
O	-3.31072300	-0.91921700	-0.44926900
C	-1.84850900	-2.77052400	-1.28211100
C	-0.54164200	-3.13339100	-1.65730500
C	-2.90993200	-3.56514600	-1.74218500
C	-0.29997100	-4.25406000	-2.44800200
H	0.27866100	-2.51376800	-1.31493500
C	-2.66559500	-4.68365800	-2.54219300
H	-3.92819300	-3.33498400	-1.46499400
C	-1.36501000	-5.03907800	-2.89787700

H	0.72064600	-4.51454200	-2.72013200
H	-3.50588900	-5.28081000	-2.88706800
H	-1.18201900	-5.91253200	-3.51805900
C	-4.50777600	-1.37988400	-0.03852400
C	-5.58214900	-0.35997300	-0.25978900
C	-5.37393700	0.80659200	-1.00856200
C	-6.84944100	-0.62190000	0.27847100
C	-6.42626200	1.69931700	-1.21402300
H	-4.39303200	1.00272900	-1.42616200
C	-7.89515400	0.27703700	0.07989600
H	-6.99086800	-1.53339500	0.84935800
C	-7.68600200	1.43863700	-0.66858900
H	-6.26396300	2.59748200	-1.80443900
H	-8.87373500	0.07196400	0.50561100
H	-8.50324600	2.13731700	-0.82863900
O	-4.73708700	-2.47733700	0.43241700
H	-3.21402200	-3.99772200	1.25811600
H	-1.54141400	-4.43134400	0.88185700
H	-2.07904400	-4.40462800	2.55976500
C	-2.61563400	-1.54686800	2.53343600
C	-3.58461000	-2.08436500	3.40549900
C	-2.49801100	-0.14150000	2.50536500
C	-4.37051100	-1.26930300	4.21901000
H	-3.73040600	-3.15778800	3.44831700
C	-3.28993000	0.67582600	3.31243000
H	-1.80388100	0.30912800	1.80600500
C	-4.22789600	0.11896000	4.18334600
H	-5.10150900	-1.72479900	4.88324900
H	-3.17783500	1.75689200	3.25492400
H	-4.84222800	0.75523100	4.81524200
C	0.70319500	4.15601700	2.40755000
H	0.48605000	5.21529000	2.58887200
H	-0.07342400	3.57709300	2.92418600
C	2.09146400	3.75586500	2.91428200
H	2.83430400	4.44833900	2.50049100
H	2.16991200	3.82218100	4.00613700
H	1.81201700	1.63278700	3.09413500
C	-0.67985000	4.04606900	0.23862300
C	-0.85372200	5.05914000	-0.71493200
C	-1.79300700	3.27298900	0.59835300
C	-2.10447100	5.30191300	-1.28682400
H	-0.00158300	5.66892600	-1.00793000
C	-3.04466400	3.51300500	0.03321700
H	-1.68055400	2.46881600	1.31879500

C	-3.20529300	4.53036900	-0.91153100
H	-2.21701800	6.09666900	-2.01998600
H	-3.89088400	2.89971000	0.32716800
H	-4.18193400	4.72001800	-1.34925200
C	3.81957800	1.86570100	2.46251500
C	4.13802800	0.56549500	2.88763300
C	4.87552800	2.70228700	2.06376800
C	5.45715400	0.11099100	2.90372800
H	3.34057900	-0.09740900	3.21386400
C	6.19712500	2.25233000	2.08176300
H	4.67337700	3.71977500	1.74180200
C	6.49451800	0.95369600	2.49904900
H	5.66972500	-0.90209600	3.23274900
H	6.99570600	2.92220200	1.77323100
H	7.52390100	0.60592500	2.51662500
C	3.13462400	-1.12721900	-3.79796800
H	2.80662200	-1.49639500	-4.77743900
H	3.96775500	-0.43591300	-3.97801800
C	3.61788800	-2.26116800	-2.88642700
H	4.51421800	-2.75612600	-3.27868900
H	2.83976600	-3.03043300	-2.80423800
H	4.82095000	-1.04784700	-1.58476200
C	1.50400600	0.91956400	-3.58699600
C	2.31006800	1.76797600	-4.35985200
C	0.20530200	1.34924300	-3.25800300
C	1.83693900	3.01249800	-4.78634200
H	3.31134900	1.46091300	-4.64740200
C	-0.26270300	2.59479000	-3.67498700
H	-0.43346400	0.70588600	-2.65666200
C	0.55241000	3.43287200	-4.44175700
H	2.47650500	3.65030600	-5.39146400
H	-1.26313300	2.91211400	-3.39526500
H	0.18611300	4.40150000	-4.77142700
C	4.12190300	-2.65152000	-0.37986700
C	5.34439100	-2.68349200	0.30578400
C	3.13614500	-3.58393600	-0.01800800
C	5.58022200	-3.61585900	1.31891500
H	6.12206900	-1.97032400	0.04162500
C	3.36759400	-4.51632100	0.99324300
H	2.17575500	-3.58416600	-0.52556300
C	4.59156300	-4.53640400	1.66711100
H	6.53951200	-3.62457200	1.83036700
H	2.58934800	-5.22826100	1.25485800
H	4.77128900	-5.26400500	2.45381400

TS3_b4

C	1.72853000	-2.92222400	0.74562700
C	2.70382700	-1.88697400	1.33210000
H	2.25109500	-3.87545900	0.59835300
H	0.91281000	-3.10474900	1.45663500
H	2.95209300	-2.16751500	2.36250900
H	3.63801100	-1.89372100	0.75925900
P	2.11052400	-0.11437100	1.25599400
P	0.85180000	-2.41370500	-0.82835500
C	0.57338100	1.09855900	-2.49314500
C	-0.73007700	1.56095000	-2.53553800
H	0.82267600	0.24487600	-3.12126500
C	-1.93648700	1.79095100	-0.05169900
C	-1.33785200	2.74763500	-2.01192600
Cu	0.42007300	-0.06064300	-0.59179200
O	-0.92684600	1.17167800	0.37126100
C	1.14693300	0.25725900	2.86543100
C	3.67114100	0.78746100	1.86600700
H	4.25149800	0.03053200	2.41205300
C	-0.13367800	-4.00395900	-1.19339500
H	0.43460800	-4.79460200	-0.68392000
C	2.04524200	-2.72350900	-2.30502900
C	-2.65834500	3.09615200	-2.68667800
C	-2.46661500	2.98543100	0.66780300
C	-3.77216400	3.46911800	0.47801600
C	-1.63222200	3.64878700	1.58203200
C	-4.22384200	4.58818200	1.17711700
H	-4.44168100	2.96008200	-0.20598800
C	-2.08426400	4.76881500	2.27499500
H	-0.63014100	3.27107600	1.74318600
C	-3.38185800	5.24604200	2.07527600
H	-5.23976900	4.94225800	1.02168700
H	-1.42256600	5.26839600	2.97795300
H	-3.73497400	6.11843400	2.61886100
H	-1.44701400	0.87141500	-2.98557100
H	1.40067100	1.76219600	-2.25582500
C	-3.79083800	0.27826900	0.19893500
O	-3.00533000	0.99342200	-0.64652400
O	-3.58144600	0.13796500	1.38693800
C	-4.99154600	-0.29108300	-0.49101300
C	-5.18706100	-0.20029000	-1.87575100
C	-5.95869500	-0.92048100	0.30509700

C	-6.33471400	-0.74161900	-2.45648900
H	-4.44004800	0.28867400	-2.49003100
C	-7.10793200	-1.45237400	-0.27537700
H	-5.78811100	-0.97881000	1.37478700
C	-7.29682700	-1.36644100	-1.65833100
H	-6.48114000	-0.67063800	-3.53093300
H	-7.85759300	-1.93272700	0.34773600
H	-8.19308500	-1.78156800	-2.11201400
C	3.11899900	1.77818900	2.91880000
C	2.13972800	0.99007300	3.79613900
H	0.40123100	0.97924800	2.51670200
C	0.39346500	-0.92053500	3.44719200
C	0.98537700	-1.84637500	4.32216600
C	-0.94913900	-1.11608600	3.08054200
C	0.26122300	-2.93699900	4.80951300
H	2.01650800	-1.71780200	4.64072900
C	-1.67087000	-2.20821200	3.56371200
H	-1.43635100	-0.40884300	2.41525600
C	-1.06901000	-3.12495700	4.42907600
H	0.73851600	-3.63673900	5.49142200
H	-2.70580600	-2.33148300	3.25816100
H	-1.63228200	-3.97239300	4.81172900
C	4.58086800	1.40581600	0.82695800
C	5.96714000	1.21063600	0.91347100
C	4.09214900	2.22493900	-0.20167800
C	6.83992000	1.81891800	0.00869800
H	6.36819300	0.57838000	1.70289700
C	4.95937100	2.83473600	-1.10874900
H	3.02380500	2.38211700	-0.30130300
C	6.33873900	2.63490300	-1.00721500
H	7.91083600	1.65580400	0.10039500
H	4.55303700	3.46901400	-1.89215500
H	7.01493800	3.11305800	-1.71096800
C	0.07526200	-4.20878400	-2.70709900
C	1.57584700	-4.04265000	-2.96599500
H	1.79407600	-1.90200900	-2.98518600
C	3.52528600	-2.62344900	-2.00378000
C	4.26149300	-3.69339600	-1.46866900
C	4.20251000	-1.41798200	-2.24928700
C	5.62202000	-3.55973700	-1.18505600
H	3.77673000	-4.64532000	-1.27103500
C	5.56051200	-1.27827500	-1.96173000
H	3.65640600	-0.57534600	-2.66608000
C	6.27704900	-2.35098100	-1.42747200

H	6.16965900	-4.40455300	-0.77500000
H	6.05313200	-0.32886900	-2.14871100
H	7.33553400	-2.24692600	-1.20508100
C	-1.55605000	-4.08032500	-0.69068000
C	-1.83148200	-4.79182300	0.48685500
C	-2.63159000	-3.50457800	-1.38324900
C	-3.13745300	-4.93179100	0.95756100
H	-1.01236900	-5.24986500	1.03713000
C	-3.93985400	-3.65301700	-0.92266900
H	-2.45315600	-2.94282700	-2.29604100
C	-4.19828000	-4.36694900	0.24938900
H	-3.32350500	-5.49058800	1.87109500
H	-4.75850600	-3.20661400	-1.47822900
H	-5.21868500	-4.47779400	0.60544900
C	-0.49823000	3.91444000	-1.61485000
C	0.65376200	3.77984100	-0.81045200
C	-0.83838400	5.22545800	-2.00945400
C	1.42908700	4.88082100	-0.44704700
H	0.90920800	2.80047900	-0.42562200
C	-0.06187100	6.32720800	-1.65034300
H	-1.71948200	5.39471300	-2.61776000
C	1.08347700	6.16488400	-0.87125900
H	2.30897900	4.73309300	0.17534100
H	-0.35760900	7.31880900	-1.98521100
H	1.69075300	7.02224300	-0.59281400
H	-3.26166800	3.77763200	-2.07818600
H	-2.50386400	3.58297700	-3.66120700
H	-3.25048800	2.19555200	-2.86632000
H	3.93826700	2.21643500	3.50142700
H	2.60261500	2.60705900	2.41640200
H	2.70671200	0.27189000	4.40083000
H	1.59946800	1.63797900	4.49686200
H	-0.28924200	-5.19536600	-3.01688400
H	-0.49117500	-3.46329100	-3.27975600
H	2.10500800	-4.89755700	-2.52998900
H	1.81458000	-4.03686400	-4.03620900

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C	3.18905600	1.22984200	1.22862700
C	3.69518700	-0.16703600	0.82348600
H	3.58625000	1.98356300	0.53950100
H	3.56826100	1.47442400	2.22863400
H	3.43517700	-0.89410400	1.60149000

H	4.78967600	-0.15711500	0.74470900
P	2.93408300	-0.84901200	-0.74797200
P	1.32194700	1.41011500	1.16998200
C	-0.04327800	0.50830100	-2.77958500
C	-1.17927200	0.37837300	-2.06009400
H	0.46136300	1.46957400	-2.83218700
C	-2.07491800	-1.19469500	-0.35143300
C	-2.07406600	-0.84749500	-1.94360500
Cu	0.65314600	-0.14648600	-0.55410600
O	-0.85425200	-1.29872200	0.10108500
C	3.70378500	-2.59978500	-0.77088500
H	4.43112800	-2.59729600	0.05090600
C	4.05594100	-0.23280900	-2.17217500
H	3.40244600	-0.31553700	-3.05049300
C	0.73811800	0.98266800	2.92530500
H	-0.33371600	0.79146500	2.79585900
C	1.13474200	3.29126600	1.44423200
H	2.15717400	3.67271300	1.55938900
C	-1.43662400	-2.05571400	-2.65915300
H	-2.00035500	-2.97150800	-2.47094500
H	-1.40067000	-1.89499700	-3.74237800
H	-0.42492500	-2.22255600	-2.28350500
C	-3.45941700	-0.54112000	-2.54939200
C	-4.31209500	-1.58249900	-2.95705200
C	-3.92285300	0.77156000	-2.75043100
C	-5.56315500	-1.32827400	-3.52130600
H	-4.00896000	-2.61426500	-2.82701200
C	-5.17229200	1.03127600	-3.31664500
H	-3.30270100	1.61684100	-2.47589200
C	-6.00430500	-0.01840600	-3.70521300
H	-6.19215000	-2.16382800	-3.81826600
H	-5.48940100	2.06157700	-3.45962900
H	-6.97635400	0.18115900	-4.14846000
C	-2.97071300	-2.37784000	0.03901400
C	-4.36552100	-2.29180100	0.14706100
C	-2.35354000	-3.60950500	0.29477900
C	-5.12266400	-3.41026200	0.50114700
H	-4.86101500	-1.34470600	-0.03297700
C	-3.11037700	-4.72993800	0.64012300
H	-1.27250200	-3.66808100	0.23677500
C	-4.49951500	-4.63543700	0.74472700
H	-6.20264000	-3.32039100	0.59005100
H	-2.61109400	-5.67561000	0.83897100
H	-5.09038000	-5.50545300	1.02095600

H	-1.51626300	1.24676200	-1.50181100
H	0.34497000	-0.28370100	-3.41326100
O	-2.83684000	0.09111100	0.18412300
C	4.49796700	-2.66514100	-2.09756800
C	5.15846500	-1.30206000	-2.31454700
H	5.23003700	-3.48049900	-2.06253800
H	3.81830800	-2.88468300	-2.93055600
H	5.64693000	-1.22835400	-3.29402600
H	5.93884300	-1.15705900	-1.55744800
C	2.75624100	-3.75817400	-0.54871900
C	2.88035000	-4.55509400	0.59754200
C	1.76591200	-4.09272100	-1.48443700
C	2.04678600	-5.65636200	0.80320800
H	3.63816200	-4.31040100	1.33815400
C	0.93114100	-5.19142800	-1.28363000
H	1.63926800	-3.48740400	-2.37817100
C	1.06963000	-5.98000600	-0.13856400
H	2.16510600	-6.26183000	1.69807700
H	0.16798900	-5.42869200	-2.01960900
H	0.42050200	-6.83739700	0.01673900
C	4.50769500	1.20882500	-2.07985800
C	5.69633000	1.59242300	-1.43771900
C	3.71544900	2.21895900	-2.64960900
C	6.07086600	2.93561100	-1.35968600
H	6.34680100	0.84210900	-0.99878500
C	4.08390600	3.56175500	-2.57084400
H	2.79848100	1.94572500	-3.16555800
C	5.26579100	3.92726000	-1.92239800
H	6.99870700	3.20463700	-0.86149000
H	3.44710300	4.31938300	-3.01877700
H	5.56080600	4.97145700	-1.86472200
C	0.41494200	3.42442200	2.81209000
C	0.90365200	2.29054800	3.72055400
H	0.60143400	4.41516600	3.24370400
H	-0.66899900	3.33615200	2.67344900
H	1.95585900	2.46278100	3.98299000
H	0.34119400	2.25022800	4.66159300
C	0.47868400	4.03934300	0.30415200
C	-0.86813200	3.82703000	-0.03265500
C	1.20565300	4.98052700	-0.43797200
C	-1.46690200	4.53736100	-1.07286400
H	-1.45982600	3.10494300	0.52324400
C	0.61025100	5.69010100	-1.48416800
H	2.24963400	5.16162700	-0.19205400

C	-0.72980100	5.47177900	-1.80565000
H	-2.51524500	4.36487400	-1.30205800
H	1.19298000	6.42030300	-2.04045200
H	-1.19779200	6.02711300	-2.61406600
C	1.35021600	-0.28399200	3.48516900
C	2.41577500	-0.27530100	4.39740500
C	0.83653400	-1.52359900	3.05989600
C	2.96205700	-1.47161800	4.87198500
H	2.81886400	0.66605700	4.75994700
C	1.38753600	-2.71491400	3.53221900
H	0.00469200	-1.54633500	2.35809100
C	2.45232300	-2.69586600	4.43881000
H	3.78126800	-1.44201500	5.58649700
H	0.97746500	-3.66114500	3.19058100
H	2.87258000	-3.62625100	4.81294600
C	-2.90173800	0.34652800	1.48734000
O	-2.38917100	-0.30463000	2.38542600
C	-3.70306700	1.59130900	1.78446300
C	-3.72215000	2.06318300	3.10462000
C	-4.43781100	2.26875200	0.80070500
C	-4.44861800	3.20623200	3.43449500
H	-3.16986500	1.50905200	3.85679300
C	-5.17143100	3.40828400	1.13519200
H	-4.44263400	1.88817200	-0.21459600
C	-5.17406900	3.88224300	2.44932200
H	-4.45632400	3.56664100	4.45993600
H	-5.74646800	3.92394300	0.37019600
H	-5.74469800	4.77102200	2.70653000

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C	-2.82247000	2.43776100	0.49712600
C	-3.58430100	1.21584900	1.04436400
H	-2.18506100	2.85537700	1.28508900
H	-3.53815000	3.22008400	0.21279800
H	-4.39095000	0.94205200	0.35509000
H	-4.05183900	1.48356200	2.00015300
P	-2.54212600	-0.33137600	1.22989700
P	-1.65234500	2.09419000	-0.92567500
C	1.85018400	-1.48457400	0.23625800
C	0.85043800	-1.13453400	-2.02238300
C	1.52000500	-2.21295500	-1.18675600
Cu	-0.65568100	0.01252500	-0.36407700
C	-3.88391500	-1.58650100	1.77170000

H	-4.80312200	-0.99799300	1.88632000
C	-1.78496600	-0.23221400	2.97377900
H	-0.94344600	-0.93085100	2.89693100
C	-2.73312300	2.18291900	-2.50540900
H	-2.13861200	1.62797900	-3.24299400
C	-0.94169800	3.84688000	-1.20165400
H	-1.54031700	4.49383900	-0.54752700
C	0.52425300	-3.35331900	-0.89544000
H	0.26770800	-3.89263100	-1.81363100
H	0.93437800	-4.07268100	-0.18461500
H	-0.38966800	-2.94738000	-0.45725300
C	2.75061400	-2.76008300	-1.94038100
C	3.24757900	-4.04707200	-1.66963300
C	3.40879400	-2.02588600	-2.94373700
C	4.34817200	-4.56776300	-2.35262300
H	2.78056700	-4.65960400	-0.90824000
C	4.50670000	-2.54342700	-3.63288500
H	3.06348800	-1.03320800	-3.20811700
C	4.98698600	-3.82007400	-3.34074500
H	4.70198000	-5.56625800	-2.10804400
H	4.98206200	-1.94413700	-4.40576000
H	5.84034800	-4.22611300	-3.87739600
C	-3.44059800	-2.05261700	3.18190700
C	-2.84074800	-0.84790700	3.91183700
H	-4.28971300	-2.48887800	3.72185200
H	-2.68384300	-2.84185800	3.09012200
H	-2.39138300	-1.13056000	4.87190600
H	-3.63687200	-0.12539000	4.13312600
C	-4.16627700	-2.71472500	0.80430900
C	-5.44447100	-2.86829500	0.24997600
C	-3.18036800	-3.65431800	0.46271600
C	-5.73363300	-3.92528400	-0.61686100
H	-6.22346300	-2.15245200	0.50270400
C	-3.46350400	-4.70969700	-0.40376800
H	-2.18045500	-3.56145300	0.87785600
C	-4.74299100	-4.85027200	-0.94823500
H	-6.73539400	-4.02743000	-1.02685400
H	-2.68327100	-5.42425700	-0.65240100
H	-4.96459300	-5.67505700	-1.62015500
C	-1.20891500	1.11730600	3.34966100
C	-1.94674900	2.09219700	4.03976900
C	0.11668200	1.41092000	2.98377500
C	-1.37948100	3.33189500	4.34804100
H	-2.96648800	1.88918800	4.35563900

C	0.68006000	2.64981200	3.29190100
H	0.71101600	0.66978500	2.45336900
C	-0.06520600	3.61668600	3.97225200
H	-1.96533700	4.07033600	4.89050900
H	1.70743800	2.84306000	2.99815700
H	0.37655900	4.57909600	4.21876300
C	-1.30931100	4.19691800	-2.66383400
C	-2.71879400	3.66574700	-2.92686400
H	-1.23517600	5.27891400	-2.82396600
H	-0.59621300	3.72481000	-3.35160000
H	-3.43387100	4.24441400	-2.32958000
H	-3.01737600	3.77428700	-3.97684800
C	0.51537500	4.06835600	-0.86639600
C	1.54213000	3.42031400	-1.57021200
C	0.87025000	4.99292200	0.12467300
C	2.88073500	3.69809600	-1.29947700
H	1.29414500	2.69114900	-2.33840400
C	2.21024500	5.27178800	0.40138200
H	0.08860100	5.50282500	0.68340100
C	3.21987700	4.62760800	-0.31269300
H	3.66245000	3.18160200	-1.84787100
H	2.46158800	5.99426500	1.17362600
H	4.26430800	4.83321000	-0.09905600
C	-4.08757400	1.51108500	-2.41916600
C	-5.25734400	2.20438600	-2.07001400
C	-4.19537200	0.13746600	-2.69286500
C	-6.48678100	1.54570000	-1.98941300
H	-5.22215600	3.27005100	-1.86605500
C	-5.41945300	-0.52467000	-2.60830400
H	-3.30520500	-0.41970000	-2.97365800
C	-6.57344800	0.17858100	-2.25443900
H	-7.37840900	2.10745800	-1.72287200
H	-5.46907500	-1.58967900	-2.81426400
H	-7.53059600	-0.33228300	-2.19410000
O	0.78594300	-0.86488100	0.69978300
C	-0.36346300	-1.18723900	-2.60444000
H	-1.01011900	-2.05708800	-2.54120200
H	-0.70651300	-0.37454300	-3.23948900
H	1.44008100	-0.23051900	-2.15579400
C	2.48249400	-2.44190200	1.26281100
C	3.83149600	-2.82128700	1.23079200
C	1.66682400	-2.97485600	2.26880700
C	4.34811400	-3.70514300	2.18048400
H	4.48712700	-2.41362200	0.46981800

C	2.17749400	-3.86491800	3.21402200
H	0.62781900	-2.66683900	2.30466800
C	3.52326800	-4.23451700	3.17404100
H	5.40034500	-3.97639500	2.14306100
H	1.52603500	-4.26241000	3.98897900
H	3.92632800	-4.92204200	3.91353300
O	2.97890000	-0.51919000	-0.19294800
C	3.52303600	0.30716500	0.71190000
O	3.12224300	0.49589400	1.84661700
C	4.75912400	0.99067100	0.18871500
C	5.30175000	0.71442900	-1.07359500
C	5.39746300	1.91667300	1.02481800
C	6.45963900	1.36953900	-1.49714500
H	4.82296800	-0.02165700	-1.70887100
C	6.55441500	2.56835400	0.60165000
H	4.96934800	2.10467500	2.00374500
C	7.08607400	2.29923900	-0.66338200
H	6.87802100	1.14769800	-2.47567700
H	7.04571800	3.28224600	1.25801800
H	7.98947700	2.80571200	-0.99397100

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C	3.14202100	-0.14170100	1.42655000
C	2.69454700	-1.60689700	1.57684600
H	3.90056500	-0.06461800	0.63924800
H	3.61172300	0.19467000	2.35883300
H	2.03541100	-1.70353800	2.44781900
H	3.56664600	-2.24559000	1.76439200
P	1.70656300	-2.25955200	0.12058800
P	1.76331600	1.02578400	0.91979600
C	0.24630400	-0.32529900	-2.84895000
C	-0.72096400	0.52250100	-2.43892700
H	1.25167100	0.04607300	-3.03089500
C	-2.47800100	0.41769000	-0.65675700
C	-2.20833500	0.25551900	-2.24905400
Cu	0.31452000	-0.37374200	-0.40943600
O	-1.64088600	-0.25814500	0.06947800
C	1.26147600	-4.01456400	0.74604500
H	1.83521800	-4.11866800	1.67913100
C	3.01348100	-2.92597800	-1.11127000
H	2.46676100	-2.93719200	-2.06294800
C	1.04868900	1.71927900	2.54250400
H	0.06571000	2.09185900	2.23580100

C	2.76604500	2.61132000	0.55870400
H	3.79598600	2.37148300	0.85288300
C	-3.95144100	0.24242500	-0.26782900
C	-4.93785600	1.21120200	-0.50094200
C	-4.33348800	-0.96555500	0.32873500
C	-6.26939800	0.97493900	-0.15391500
H	-4.66287700	2.16837500	-0.92967800
C	-5.66454400	-1.20574000	0.67053400
H	-3.57256500	-1.70996600	0.52844300
C	-6.64053700	-0.23742500	0.42896100
H	-7.01540700	1.74531900	-0.33406800
H	-5.93859800	-2.15238500	1.13065100
H	-7.67760800	-0.42221500	0.69814800
H	-0.44031500	1.55786000	-2.25684300
H	0.03764800	-1.35728600	-3.11460900
O	-2.21540100	2.03331100	-0.51787000
C	1.89166700	-4.96997600	-0.28909500
C	3.24719700	-4.39157900	-0.69600100
H	1.99498200	-5.98117300	0.12144900
H	1.24176500	-5.04412800	-1.17103000
H	3.70874500	-4.95758500	-1.51438500
H	3.93304300	-4.44875700	0.15806500
C	-0.20138300	-4.26780500	1.07629400
C	-0.83886800	-5.46065900	0.70047100
C	-0.93169500	-3.34249200	1.83735200
C	-2.16042800	-5.72013100	1.07327800
H	-0.30491000	-6.20604200	0.11980500
C	-2.25044500	-3.59972700	2.21098700
H	-0.47733300	-2.40452400	2.14167500
C	-2.87226900	-4.79083700	1.83077300
H	-2.62931300	-6.65270500	0.76986100
H	-2.79387300	-2.85865000	2.79014100
H	-3.90065400	-4.98994500	2.11957500
C	4.24904700	-2.07392200	-1.30847100
C	5.40759500	-2.22763500	-0.52946500
C	4.25987000	-1.09128000	-2.31171400
C	6.52895100	-1.42257900	-0.74039000
H	5.44776000	-2.98746200	0.24481600
C	5.37698800	-0.28379200	-2.52443100
H	3.38028700	-0.96208700	-2.93707600
C	6.51906900	-0.44539900	-1.73697700
H	7.41463400	-1.56669400	-0.12699100
H	5.35201200	0.46872400	-3.30722500
H	7.39465700	0.17593000	-1.90442000

C	2.22161100	3.65958000	1.56140800
C	1.93201000	2.93737000	2.88079400
H	2.94260300	4.47691100	1.68307200
H	1.29627300	4.10436600	1.17674000
H	2.87847900	2.62322700	3.33991600
H	1.42653900	3.59013700	3.60274600
C	2.78350600	3.05981300	-0.88592400
C	1.61803700	3.50109500	-1.53352200
C	3.98482700	3.06617300	-1.60816800
C	1.65729100	3.93453500	-2.85880900
H	0.67161600	3.51090600	-0.99968600
C	4.02689300	3.49852100	-2.93613100
H	4.89897600	2.72958000	-1.12445400
C	2.86174400	3.93430800	-3.56759800
H	0.74391800	4.27756700	-3.33782200
H	4.97269000	3.50144300	-3.47243000
H	2.89048400	4.27503300	-4.59906800
C	0.80996200	0.70478700	3.64043300
C	1.78303100	0.37795600	4.59807500
C	-0.44350600	0.07003800	3.71582100
C	1.51891400	-0.56062100	5.59891200
H	2.75275500	0.86762200	4.58193700
C	-0.70537700	-0.86379000	4.71994100
H	-1.21235600	0.32604200	2.98992500
C	0.27348800	-1.18680500	5.66330700
H	2.28588100	-0.79292700	6.33374200
H	-1.68425800	-1.33345900	4.77034700
H	0.06414700	-1.91103900	6.44617400
C	-2.21232800	2.60382000	0.67520100
O	-2.35605700	2.04898600	1.75716300
C	-2.00075600	4.10103300	0.60407800
C	-1.90614800	4.81066000	1.80968500
C	-1.91981600	4.79987600	-0.60844700
C	-1.71887400	6.19209000	1.80402900
H	-1.99437600	4.25610700	2.73832700
C	-1.73571200	6.18351800	-0.61399600
H	-2.01063900	4.25504000	-1.54175500
C	-1.63198800	6.88182500	0.59123500
H	-1.64685500	6.73302900	2.74411200
H	-1.67673900	6.71748800	-1.55895200
H	-1.48900900	7.95937600	0.58568200
C	-2.60923100	-1.16711500	-2.70257500
C	-2.19561000	-2.31323800	-1.99692500
C	-3.38225400	-1.37703800	-3.85706100

C	-2.53743800	-3.59695100	-2.42426400
H	-1.62752200	-2.19221100	-1.08371700
C	-3.72319800	-2.66096500	-4.28981700
H	-3.73826800	-0.53686900	-4.44047400
C	-3.30153000	-3.78130800	-3.57716300
H	-2.21270800	-4.45212100	-1.83729000
H	-4.32642600	-2.77743100	-5.18702500
H	-3.57002100	-4.78098400	-3.90978700
C	-2.93744900	1.32744300	-3.09471500
H	-2.65119300	1.24993400	-4.14908700
H	-4.02263400	1.21647700	-3.02548400
H	-2.67397200	2.32642700	-2.74847000

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C	1.78339900	-2.71589800	0.92997400
C	2.91620800	-1.69078900	1.10359000
H	1.19862900	-2.79036800	1.85473800
H	2.21105400	-3.70579600	0.73408100
H	3.61073100	-1.76659700	0.25735000
H	3.48675400	-1.92168200	2.01180600
P	2.37382900	0.10622800	1.11651600
P	0.51947100	-2.26845200	-0.37011100
C	-1.99474200	1.91575100	-0.30349800
C	-0.30195600	1.49321400	-2.08977900
C	-1.07069400	2.63128300	-1.42473100
Cu	0.34003400	0.12545600	-0.21810600
C	4.09661800	0.94196500	1.10601800
H	4.79125200	0.12122100	1.32971300
C	2.05886800	0.56298900	2.94211400
H	1.38108100	1.42202600	2.85792300
C	1.11028100	-2.89209900	-2.08966600
H	0.89316100	-2.04150800	-2.74448300
C	-0.71507300	-3.68344100	-0.18790800
H	-0.11425300	-4.55474800	0.11256500
C	4.07610400	1.86729600	2.34303700
C	3.40594700	1.08521900	3.47864000
H	5.09465100	2.18078900	2.60156100
H	3.50314500	2.77748700	2.12960300
H	3.25754800	1.70074100	4.37436000
H	4.05918600	0.25272800	3.76780900
C	4.54345800	1.57119300	-0.19490200
C	5.49282200	0.91474800	-0.99308400
C	4.05581500	2.81254500	-0.63308800

C	5.94081000	1.47414000	-2.19145800
H	5.89196700	-0.04397400	-0.66912000
C	4.50386400	3.37483500	-1.82932800
H	3.31685000	3.34793300	-0.04512100
C	5.44726600	2.70885700	-2.61522400
H	6.68363400	0.94889200	-2.78681000
H	4.10805100	4.33660800	-2.14379200
H	5.79685500	3.15021100	-3.54469900
C	1.33857000	-0.51060700	3.73034000
C	1.99809400	-1.36838000	4.62272600
C	-0.04568400	-0.67792600	3.54283300
C	1.29730700	-2.36443900	5.30876400
H	3.06337000	-1.25949100	4.80288200
C	-0.74300200	-1.67694800	4.22179300
H	-0.57760000	-0.03120900	2.84677300
C	-0.07358100	-2.52443000	5.10906400
H	1.82833800	-3.01259400	6.00159100
H	-1.80739900	-1.79782500	4.04703500
H	-0.61846900	-3.30083900	5.63919700
C	-1.14895700	-3.92612500	-1.65095600
C	0.14400700	-4.05084900	-2.46939300
H	-1.76506900	-4.82959000	-1.72684400
H	-1.76542500	-3.08852100	-2.00303300
H	0.61224400	-5.01493100	-2.24104700
H	-0.04720600	-4.04378100	-3.54879600
C	-1.83916000	-3.53525900	0.81488500
C	-2.56824300	-2.34868800	0.97005800
C	-2.20106700	-4.65007400	1.58826200
C	-3.64424300	-2.28564300	1.85948800
H	-2.28719600	-1.45367300	0.42373000
C	-3.27103000	-4.58933500	2.48112100
H	-1.64039200	-5.57739700	1.48438000
C	-4.00011400	-3.40542100	2.61472700
H	-4.19437500	-1.35394100	1.93981700
H	-3.53447700	-5.46558500	3.06848800
H	-4.83842400	-3.35505400	3.30514900
C	2.58808300	-3.19442700	-2.21770200
C	3.16049500	-4.38504300	-1.73782000
C	3.44135300	-2.25759500	-2.82300600
C	4.52999300	-4.62635100	-1.85696200
H	2.53343600	-5.13997800	-1.27142400
C	4.81157500	-2.49407300	-2.94283200
H	3.02516500	-1.33098400	-3.21107800
C	5.36341800	-3.68160200	-2.45919900

H	4.94495600	-5.55785000	-1.48072100
H	5.44329400	-1.74977900	-3.41999300
H	6.42875500	-3.87233700	-2.55557800
O	-1.29975100	1.09966700	0.46180900
C	1.03485200	1.35175000	-2.20552900
H	1.73576700	2.07084700	-1.79702100
H	1.45645700	0.54926100	-2.80628900
H	-0.94800600	0.76634700	-2.57909200
C	-2.90178700	2.88932300	0.47321500
C	-3.92916400	3.62749000	-0.13210000
C	-2.70036500	3.04894000	1.84875400
C	-4.70358200	4.52190000	0.60800900
H	-4.15890300	3.48051300	-1.18089000
C	-3.47149900	3.94211500	2.59247900
H	-1.94712200	2.44000200	2.33421600
C	-4.47256400	4.69175400	1.97368400
H	-5.49743700	5.07821000	0.11529800
H	-3.29464700	4.04489700	3.66062000
H	-5.07544100	5.38862000	2.55060800
O	-2.95275300	1.09139300	-1.25969500
C	-3.98222300	0.40326900	-0.76877300
O	-4.36601700	0.41237900	0.38927100
C	-4.67316100	-0.42268400	-1.82435200
C	-4.22014400	-0.49685100	-3.14901500
C	-5.81623600	-1.14137500	-1.44944400
C	-4.90025100	-1.28091400	-4.08190000
H	-3.33990200	0.06415700	-3.44312100
C	-6.49658900	-1.92172700	-2.38202900
H	-6.15153200	-1.07192200	-0.42024200
C	-6.03931300	-1.99417700	-3.70071200
H	-4.54362400	-1.33229200	-5.10757600
H	-7.38308000	-2.47439100	-2.08197300
H	-6.56944500	-2.60292000	-4.42886200
C	-0.12413100	3.67431200	-0.78464300
C	0.30568100	3.59299300	0.55190700
C	0.35222600	4.76144300	-1.53865500
C	1.12664200	4.57261100	1.11560600
H	-0.02810700	2.75847200	1.15281900
C	1.19192200	5.73156900	-0.98574500
H	0.06367500	4.87162700	-2.57742600
C	1.57697800	5.65074100	0.35209900
H	1.40487900	4.49503000	2.16449300
H	1.52829200	6.56108500	-1.60308300
H	2.21209600	6.41514500	0.79234100

C	-1.89038000	3.29675000	-2.56619400
H	-1.24939600	3.52517100	-3.42392800
H	-2.67531200	2.62378500	-2.91221200
H	-2.34770000	4.23040800	-2.23013300

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C	-2.92422100	2.29035400	0.21328700
C	-3.74765200	1.03761300	0.57200100
H	-2.56213900	2.76754500	1.13158500
H	-3.58546500	3.01479200	-0.28098200
H	-4.32709000	0.72203100	-0.30316900
H	-4.47357300	1.32682400	1.34381200
P	-2.83189300	-0.52373400	1.09448400
P	-1.38019100	2.11271500	-0.82113800
C	3.09255300	-1.03949600	4.03379500
C	3.14742200	-1.02218800	2.70158200
H	3.42519300	-0.18312000	4.61501300
C	1.96473500	-1.46945300	0.55485100
C	2.74903100	-2.15267500	1.75478600
Cu	0.18155500	0.63875900	-0.20736300
O	1.07815800	-0.64522500	0.98313900
C	-4.36944700	-1.61439400	1.45018600
H	-5.24530800	-0.95446100	1.39360800
C	-2.48276500	-0.28382300	2.96998300
H	-1.65699900	-0.98578700	3.14380900
C	-1.88398800	1.93743000	-2.65457600
H	-1.04148900	1.37756500	-3.07808100
C	-0.87385800	3.93341600	-1.01328200
H	-1.76770500	4.51088600	-0.74101600
C	1.70870000	-3.07456700	2.43925000
H	1.27349800	-3.78822600	1.73451500
H	2.17307400	-3.64487000	3.24953300
H	0.89725000	-2.46980300	2.84912200
C	3.99643900	-2.96426300	1.34409100
C	3.90660600	-4.31740900	0.97905300
C	5.27811300	-2.38772800	1.35654600
C	5.03954500	-5.05781200	0.63299300
H	2.94211300	-4.81173300	0.95458500
C	6.41278300	-3.12236100	1.01175400
H	5.39564200	-1.35210800	1.65316100
C	6.30091200	-4.46484800	0.64544000
H	4.92941500	-6.10328600	0.35551700
H	7.38884900	-2.64379800	1.03921700

H	7.18426400	-5.04025600	0.38082400
C	1.56932900	-2.35994100	-0.62228700
C	2.48239500	-2.91231300	-1.53298300
C	0.20601600	-2.64981000	-0.77960800
C	2.03856100	-3.72373600	-2.57795700
H	3.53721900	-2.68737900	-1.43864900
C	-0.23700200	-3.46796900	-1.82205600
H	-0.50898200	-2.21830900	-0.08639900
C	0.67887400	-4.00760800	-2.72617300
H	2.76036500	-4.13234500	-3.28065600
H	-1.29864600	-3.67994100	-1.92115100
H	0.33782000	-4.64122700	-3.54122700
H	3.52512700	-0.13141300	2.20661900
H	2.72288000	-1.88802700	4.60285800
O	3.31922000	-0.56198200	-0.18026700
C	-4.21014200	-2.05051100	2.92702400
C	-3.71973600	-0.82963200	3.70923600
H	-5.15623500	-2.44476800	3.31813100
H	-3.47417000	-2.86209100	2.99868900
H	-3.48002900	-1.07267300	4.75233600
H	-4.52232500	-0.08173800	3.73316200
C	-4.58346600	-2.75990400	0.48472800
C	-5.79506500	-2.88275000	-0.20965800
C	-3.60271400	-3.74391200	0.27814400
C	-6.02607000	-3.95029600	-1.08073000
H	-6.56935100	-2.13269100	-0.06369600
C	-3.82867600	-4.81276500	-0.58917600
H	-2.64920500	-3.67062400	0.79532500
C	-5.04256700	-4.92076400	-1.27448800
H	-6.97657900	-4.02383500	-1.60336900
H	-3.05463100	-5.56295300	-0.72931000
H	-5.21881600	-5.75489800	-1.94840700
C	-1.98751400	1.09216500	3.35994700
C	-2.83790800	2.09217200	3.85639300
C	-0.62338200	1.39956000	3.20079800
C	-2.34680300	3.36196600	4.17393300
H	-3.89344700	1.88694900	4.00806200
C	-0.13561600	2.66956100	3.50978500
H	0.05907500	0.63937400	2.82688100
C	-0.99524600	3.65838700	3.99642800
H	-3.02544000	4.11688900	4.56391900
H	0.91884500	2.88829900	3.36628100
H	-0.61227900	4.64632200	4.23661300
C	-0.66766200	4.09655900	-2.53864100

C	-1.82360900	3.36811300	-3.23247000
H	-0.62843100	5.15924100	-2.80551700
H	0.29178000	3.65381500	-2.83451000
H	-2.75544900	3.90989100	-3.02982600
H	-1.70188700	3.33754800	-4.32184300
C	0.27507200	4.42007600	-0.15681900
C	1.55204600	3.84236100	-0.23715800
C	0.08623600	5.50148500	0.71464700
C	2.60612400	4.33581800	0.53256900
H	1.72502800	2.99373200	-0.89259800
C	1.13990600	5.99721000	1.48578300
H	-0.89619300	5.96316000	0.78878800
C	2.40515600	5.41524100	1.39712900
H	3.58689300	3.87473500	0.45118300
H	0.97047000	6.83941500	2.15192500
H	3.22824600	5.79952700	1.99373600
C	-3.14116700	1.13126900	-2.90266500
C	-4.41006700	1.71868200	-3.01699900
C	-3.04861300	-0.26801600	-2.99590300
C	-5.54929800	0.93342600	-3.21191100
H	-4.52131200	2.79740900	-2.95992600
C	-4.18517300	-1.05451400	-3.18027800
H	-2.07497000	-0.74525200	-2.91002700
C	-5.44267900	-0.45545600	-3.28939600
H	-6.52088600	1.41242300	-3.30377900
H	-4.09079900	-2.13531200	-3.23140900
H	-6.32865700	-1.06715900	-3.43468700
C	3.08083600	0.32043400	-1.09444300
O	1.95256800	0.69103000	-1.49154300
C	4.31201400	0.92968500	-1.71503000
C	4.17322600	1.94284000	-2.67388300
C	5.59525600	0.48940200	-1.36065100
C	5.29977400	2.51777200	-3.25999200
H	3.17537800	2.26241300	-2.95436900
C	6.72107700	1.06392300	-1.94973800
H	5.69676900	-0.30851100	-0.63362500
C	6.57647100	2.08069200	-2.89719000
H	5.18315000	3.30417500	-4.00116200
H	7.71274100	0.71636400	-1.67194300
H	7.45536500	2.52776500	-3.35476400

(*R*)-3da

C	2.26937700	3.18272200	0.41529500

C	1.64664600	2.22172800	-0.26561600
H	2.90905400	3.89586400	-0.09738600
C	-0.59079800	1.15623600	-0.50247900
C	0.74903300	1.12380200	0.30058600
O	-0.73051300	1.96669200	-1.40591900
C	0.42698500	1.37293700	1.78840800
H	-0.17239400	0.56883400	2.21948000
H	1.34385300	1.46714300	2.37702800
H	-0.13179200	2.30788300	1.89674600
C	1.47952600	-0.21204700	0.04187500
C	2.12224100	-0.92861400	1.06054200
C	1.55862200	-0.71073900	-1.26886200
C	2.81400200	-2.10909500	0.77977900
H	2.08877000	-0.57242000	2.08484200
C	2.24783100	-1.88939200	-1.55039800
H	1.07203500	-0.17292000	-2.07866800
C	2.87953200	-2.59582300	-0.52549400
H	3.30378900	-2.64669700	1.58769000
H	2.28928200	-2.25573600	-2.57278000
H	3.41691300	-3.51499600	-0.74224700
C	-1.73885800	0.24429700	-0.15566900
C	-1.62098600	-0.95299000	0.56888800
C	-3.00835600	0.63037800	-0.62003600
C	-2.74609800	-1.73689500	0.82508000
H	-0.65127200	-1.29449700	0.91072200
C	-4.13139600	-0.14639500	-0.35289700
H	-3.08854500	1.54911000	-1.19124300
C	-4.00303300	-1.33457500	0.37138400
H	-2.63743600	-2.66634500	1.37737900
H	-5.10682500	0.17147000	-0.71123400
H	-4.87804800	-1.94542600	0.57752500
H	1.78536900	2.16926700	-1.34211000
H	2.17572500	3.31272000	1.48929200

(*S*)-3da

C	2.87112200	-2.38234700	-0.10461200
C	1.56296700	-2.36617800	0.14557300
H	3.39051300	-3.32186900	-0.27350800
C	-0.61248300	-1.25082600	-0.34566300
C	0.71048600	-1.14399600	0.47955500
O	-0.74050300	-2.15569100	-1.15700200
C	-1.76063600	-0.29923600	-0.12841600
C	-1.66052100	0.94886600	0.50749300

C	-3.01224800	-0.70518900	-0.62402400
C	-2.78491000	1.76263700	0.64738800
H	-0.70379700	1.30447800	0.86977800
C	-4.13483700	0.10281800	-0.47447000
H	-3.07829100	-1.66452400	-1.12596500
C	-4.02398800	1.34156000	0.16291200
H	-2.68931800	2.73031500	1.13238400
H	-5.09610500	-0.23022200	-0.85650700
H	-4.89841000	1.97683300	0.27749200
H	1.01506300	-3.30538100	0.17249400
H	3.47001200	-1.47810400	-0.15886600
C	1.44231600	0.15620500	0.12004200
C	1.99971600	1.00642700	1.08399400
C	1.59657100	0.49863900	-1.23365000
C	2.67818700	2.16969100	0.70899000
H	1.90803100	0.76996200	2.13908300
C	2.26947300	1.65946100	-1.60957800
H	1.19036200	-0.15843100	-1.99795500
C	2.81269400	2.50313200	-0.63788900
H	3.10187700	2.81302000	1.47590200
H	2.37060900	1.90426600	-2.66363700
H	3.33762800	3.40890200	-0.92913000
C	0.34934900	-1.26303700	1.98631500
H	-0.21436400	-2.18630400	2.15874000
H	1.26040700	-1.32064500	2.58900100
H	-0.25972600	-0.42852100	2.34296100

L*CuOBz

C	0.41180700	-2.62314500	0.38867800
C	1.49743500	-1.85278200	1.17215000
H	-0.45577300	-2.79585400	1.03675900
H	0.79813600	-3.60662000	0.09341400
H	2.44606200	-1.89200500	0.62425100
H	1.66078200	-2.33896800	2.14173500
P	1.13332300	-0.02521400	1.38306800
P	-0.28651300	-1.71777900	-1.10080100
Cu	-0.29656500	0.48739900	-0.43222200
C	2.78400800	0.64554400	2.02748700
H	3.38878300	-0.23252700	2.29236200
C	0.25045900	0.20313600	3.05173900
H	-0.29894000	1.14002300	2.89508300
C	0.79727900	-2.18092100	-2.60044500
H	0.64969400	-1.32866900	-3.27579900

C	-1.70195700	-2.87197200	-1.61726100
H	-1.55127600	-3.80071900	-1.05092400
C	2.40662700	1.36033400	3.35227800
C	1.37184800	0.48328300	4.06961700
H	3.30150000	1.53363800	3.96162100
H	1.97520700	2.34447200	3.12745800
H	0.97469700	0.96544700	4.97142600
H	1.85340000	-0.45034400	4.38795200
C	3.58510400	1.49657800	1.05957800
C	4.98476400	1.39742300	1.06264600
C	2.98343400	2.41239500	0.18149900
C	5.76677800	2.19026800	0.22067100
H	5.46748500	0.68919300	1.73341300
C	3.76460900	3.20309700	-0.66373400
H	1.90138100	2.49427100	0.12125600
C	5.15714800	3.09801100	-0.64782100
H	6.84970100	2.09635400	0.24274800
H	3.27562500	3.89747500	-1.34157700
H	5.76122900	3.71466800	-1.30822400
C	-0.76964800	-0.87197300	3.35384600
C	-0.49794300	-1.97458700	4.17656900
C	-2.03785600	-0.78362200	2.75107700
C	-1.46340200	-2.96297100	4.38932700
H	0.46599900	-2.06561800	4.66920500
C	-2.99771400	-1.77443600	2.95626900
H	-2.26478900	0.06724500	2.11164000
C	-2.71400000	-2.86950300	3.77789700
H	-1.23470000	-3.80508100	5.03786500
H	-3.96586000	-1.68957700	2.47073700
H	-3.46328300	-3.63898600	3.94452200
C	-1.40702000	-3.18276500	-3.10617200
C	0.10523500	-3.40216800	-3.23890300
H	-1.98372800	-4.05489800	-3.43589200
H	-1.72202800	-2.33620000	-3.73017700
H	0.37814400	-4.32491500	-2.71167700
H	0.41611900	-3.52598800	-4.28350000
C	-3.10090400	-2.36722200	-1.33366400
C	-3.53059600	-1.10004100	-1.75746200
C	-4.01270200	-3.18632000	-0.65314300
C	-4.83318300	-0.66856800	-1.50931600
H	-2.83699500	-0.43446500	-2.26404900
C	-5.31871400	-2.75831200	-0.40504000
H	-3.69644800	-4.17072800	-0.31423800
C	-5.73294500	-1.49603400	-0.83275000

H	-5.14044500	0.32102500	-1.83573900
H	-6.00959900	-3.41155600	0.12198000
H	-6.74685000	-1.15700700	-0.63782800
C	2.27659500	-2.26693300	-2.29358200
C	2.93019700	-3.47645800	-2.01525400
C	3.03080500	-1.08125400	-2.24777500
C	4.29094700	-3.49889100	-1.69694600
H	2.38471300	-4.41467700	-2.05398300
C	4.38653900	-1.09953600	-1.92196700
H	2.54434500	-0.13150400	-2.45896400
C	5.02325000	-2.31244200	-1.64465400
H	4.77714600	-4.44940400	-1.49213100
H	4.94015000	-0.16602200	-1.87998800
H	6.08073300	-2.33189200	-1.39526100
O	-0.33110800	2.42716300	-1.31944500
C	-1.36159100	2.71075900	-0.62435400
O	-1.88152000	1.87182000	0.17442900
C	-1.97192300	4.07706100	-0.75513400
C	-3.09654400	4.42282700	0.00591800
C	-1.42283400	5.01632600	-1.63825900
C	-3.66404200	5.69095300	-0.11431200
H	-3.51008400	3.68385900	0.68421100
C	-1.99106900	6.28410000	-1.75889400
H	-0.55250500	4.73300000	-2.22070100
C	-3.11256600	6.62377300	-0.99708700
H	-4.53635800	5.95340400	0.47922000
H	-1.56089100	7.00823000	-2.44639100
H	-3.55550500	7.61232300	-1.09115200

Table S3. Electronic energies (E_{elec}), Gibbs free energies (G_{298}), thermal correction to Gibbs free energy ($cor\ G_{gas}$), solvation energies (Esol), solvation free energies (G_{sol}) in THF (ε = 7.43) for all stationary points of the process. Calculations were carried out at M06/6-311+G(d,p)/SDD/SMD(THF)//B3LYP-D3(BJ)/6-31G(d)/LANL2DZ level.

species	E_{elec} (a.u.)	G_{298} (a.u.)	$cor\ G_{gas}$ (a.u.)	E_{sol} (a.u.)	G_{sol} (a.u.)
Int2_a	-2584.127187	-2583.410408	0.716779	-2584.240175	-2583.523396
Int2_b	-2584.125186	-2583.408679	0.716507	-2584.237671	-2583.521164
2a	-765.263319	-765.099996	0.163323	-764.905268	-764.741945
TS3_a1	-3349.415896	-3348.505222	0.910674	-3349.151948	-3348.241274
TS3_a2	-3349.405920	-3348.498114	0.907806	-3349.139733	-3348.231927
TS3_a3	-3349.408636	-3348.500960	0.907676	-3349.146704	-3348.239028
TS3_a4	-3349.407251	-3348.499824	0.907426	-3349.141667	-3348.234241
TS3_b1	-3349.415803	-3348.504335	0.911468	-3349.148831	-3348.237363
TS3_b2	-3349.406466	-3348.494698	0.911768	-3349.134708	-3348.222940
TS3_b3	-3349.396229	-3348.485750	0.910478	-3349.126236	-3348.215758
TS3_b4	-3349.402603	-3348.491282	0.911322	-3349.139242	-3348.227920

Cartesian coordinates for the optimized structures in Table S3

Int2_a

C	−0.99171300	1.03866100	1.94087500
C	0.27032000	1.88864900	1.71424600
Cu	−0.07087600	0.31520100	−1.32372900
C	−0.18911500	3.62428000	−0.66291900
H	−0.16965800	3.54114700	−1.75679500
C	2.38675700	3.00545500	0.08632900
H	2.51823300	3.18739500	1.16009600
C	−2.85358900	−1.07702200	1.22449400
H	−3.13409300	−0.57954900	2.16175900
C	−0.20982500	−1.80392500	1.41145100
H	−0.00753500	−2.42385000	0.53451400
P	0.74724900	2.09096000	−0.07859300
P	−1.19024200	−0.35082000	0.71169500
C	−0.07940300	−0.69381200	−3.08562100
H	0.76231100	−0.40829900	−3.71986100
H	−1.03691700	−0.50410600	−3.57886300
C	0.00391700	−1.99223000	−2.43819300
C	1.10701600	−2.73564500	−2.10723300
H	−0.95062800	−2.36065000	−2.06123300

C	2.48341600	-2.30223300	-2.55477200
H	3.14507700	-3.16267100	-2.70752000
H	2.42429300	-1.75637300	-3.50213800
H	2.98790800	-1.63270100	-1.84035600
C	0.98806000	-3.87648700	-1.18994100
C	2.07617900	-4.26801900	-0.37878900
C	-0.22252100	-4.58826500	-1.00782500
C	1.94823700	-5.26269400	0.58904700
H	3.02576200	-3.75302700	-0.47799700
C	-0.34977000	-5.57884600	-0.03956000
H	-1.07096200	-4.36866800	-1.64873700
C	0.73244800	-5.92078600	0.77870600
H	2.80569400	-5.51544900	1.20790900
H	-1.29798100	-6.10070200	0.06700400
H	0.63288600	-6.69597400	1.53309400
C	-1.19256700	-2.58177600	2.29758800
C	-2.53284500	-2.55685600	1.55326400
H	-0.83277900	-3.60316000	2.46121900
H	-1.31106700	-2.10415600	3.27891600
H	-3.34801800	-3.00559500	2.13212000
H	-2.44011800	-3.12917400	0.62209800
C	2.14067600	4.37491400	-0.59755100
C	0.70572200	4.80729300	-0.26802100
C	1.11147300	-1.34949800	1.96727800
C	1.32288500	-1.07294900	3.32254900
C	2.15503600	-1.09823100	1.06236400
C	2.53880300	-0.53642300	3.75745100
H	0.53784200	-1.26915700	4.04647600
C	3.36825800	-0.56755800	1.49100700
H	1.99852500	-1.31774300	0.01237200
C	3.56098100	-0.27403400	2.84405100
H	2.68401100	-0.32396400	4.81342500
H	4.15782300	-0.38016300	0.77175400
H	4.50398800	0.14690200	3.18135900
C	-3.96488200	-0.87370100	0.22462800
C	-5.23735000	-0.48804000	0.66248200
C	-3.75988500	-1.06409200	-1.14918800
C	-6.28046000	-0.29170500	-0.24383700
H	-5.40769300	-0.32976400	1.72477100
C	-4.79813200	-0.86805600	-2.05849800
H	-2.77252600	-1.33115400	-1.51214800
C	-6.06316000	-0.47874100	-1.60996400
H	-7.25925900	0.01294900	0.11653000
H	-4.61574300	-1.01184800	-3.11987500

H	-6.87040700	-0.32077900	-2.31943500
C	-1.62581700	3.57213900	-0.21160100
C	-2.50116500	2.69588500	-0.87501800
C	-2.09999500	4.26890100	0.90515400
C	-3.80342600	2.49993500	-0.42354100
H	-2.14316200	2.14058400	-1.73944700
C	-3.40786800	4.07592900	1.36098100
H	-1.45029800	4.96129900	1.43128700
C	-4.25906100	3.18586300	0.70570500
H	-4.45533700	1.80693900	-0.94330100
H	-3.75712400	4.62261500	2.23280800
H	-5.27127300	3.02645200	1.06562800
C	3.59882200	2.25734200	-0.41689800
C	3.55688400	1.46694700	-1.57318000
C	4.80630700	2.35295600	0.28568000
C	4.69133300	0.77978400	-2.00542600
H	2.62317600	1.35272100	-2.11653700
C	5.94463700	1.67205800	-0.14669100
H	4.84848700	2.95492600	1.19045300
C	5.88901000	0.87776200	-1.29341300
H	4.63294000	0.15677400	-2.89296900
H	6.86973400	1.75328500	0.41735200
H	6.76932400	0.33624100	-1.62747700
H	2.88720100	5.10642200	-0.26894800
H	2.25477200	4.26248600	-1.68317800
H	0.62747500	5.01203100	0.80718300
H	0.41558600	5.72358100	-0.79546100
H	1.13424300	1.40381800	2.17983000
H	0.15140300	2.87132600	2.18625200
H	-0.99689300	0.65081600	2.96607700
H	-1.88669100	1.65626100	1.81567500

Int2_b

C	0.39762200	-1.75011000	-1.68953500
C	1.73529800	-1.89582500	-0.94565600
H	-0.29614100	-2.52901000	-1.35601300
H	0.56212100	-1.90096500	-2.76313300
H	1.99518400	-2.95630200	-0.84121800
H	2.53472900	-1.41725800	-1.52039000
Cu	0.65560900	0.90041800	0.70927300
C	1.10574100	-2.29291500	1.95600400
H	0.82899000	-1.66923700	2.81543700
C	3.59464000	-1.36614000	1.21332200

H	4.01283400	-2.02215700	0.43972600
C	-2.04235800	-0.50216800	-2.49995100
H	-1.79307800	-1.40338600	-3.07476200
C	0.19998400	1.08644300	-2.63360800
H	-0.05222000	2.05511800	-2.18750200
P	1.80428700	-1.06010000	0.71007200
P	-0.53722900	-0.15425500	-1.38726900
C	0.15325900	2.76440500	1.24506300
H	1.07175500	3.35852800	1.16894000
H	-0.16844300	2.72557900	2.29031900
C	-0.86383600	3.24673500	0.31134900
C	-2.22928500	3.22903300	0.34415800
H	-0.44588900	3.70899900	-0.58783100
C	-2.99312900	3.89576400	-0.78357600
H	-3.78467200	3.24853800	-1.18782600
H	-3.48439200	4.82876900	-0.47068400
H	-2.31737400	4.15456800	-1.60595800
C	-3.03204500	2.62834200	1.42409200
C	-2.55978700	1.55171200	2.20663700
C	-4.35450600	3.05684400	1.66987200
C	-3.35516700	0.94711400	3.17536900
H	-1.56901700	1.16006600	2.01393000
C	-5.14409100	2.46622700	2.65594300
H	-4.77000900	3.86986200	1.08400400
C	-4.65270700	1.40457700	3.41792300
H	-2.96027700	0.10591400	3.74083000
H	-6.15284800	2.83559800	2.82436900
H	-5.27030800	0.93899500	4.18081900
C	-2.06965000	0.68758200	-3.48365700
C	-0.62380400	0.93626500	-3.92143000
C	3.48992700	-2.18604200	2.52356500
C	2.30912700	-3.15251100	2.37042800
C	4.45869100	-0.13215500	1.30498200
C	5.73158900	-0.13026500	0.72315400
C	4.02205200	1.02447800	1.96577100
C	6.54996400	0.99814900	0.78926500
H	6.07825300	-1.01888500	0.20113900
C	4.83374900	2.15637400	2.02901000
H	3.02827300	1.05498800	2.40327600
C	6.10053700	2.14865600	1.43929600
H	7.53291700	0.98073400	0.32664400
H	4.47115900	3.04806100	2.53244300
H	6.73019500	3.03254900	1.48543000
C	-0.14315900	-2.95377400	1.43292400

C	-1.34315200	-2.22447200	1.44844800
C	-0.14121200	-4.22569300	0.85011500
C	-2.50569100	-2.74065600	0.88388300
H	-1.35822900	-1.22973200	1.88537100
C	-1.30773000	-4.74875000	0.28370000
H	0.76956500	-4.81604300	0.83221700
C	-2.48868400	-4.00704200	0.29294100
H	-3.41605600	-2.15220700	0.89194400
H	-1.28788300	-5.73788700	-0.16602100
H	-3.39302000	-4.40412000	-0.15735700
C	1.70005400	0.98033300	-2.71362800
C	2.35660700	0.17660900	-3.65454800
C	2.47726600	1.63354600	-1.74252300
C	3.74254700	0.00321900	-3.60335900
H	1.78858200	-0.32810300	-4.42940900
C	3.85751900	1.45608400	-1.68168100
H	1.98676600	2.27486900	-1.01474800
C	4.49590900	0.62981100	-2.60960800
H	4.23083300	-0.62801500	-4.34116800
H	4.43080400	1.95427000	-0.90748100
H	5.57099200	0.48457800	-2.55907900
C	-3.33410000	-0.74562600	-1.76558600
C	-3.78398100	0.15432500	-0.79269400
C	-4.10850700	-1.87688100	-2.04584000
C	-4.97537300	-0.07179800	-0.10574600
H	-3.17960300	1.01987400	-0.54864900
C	-5.30564900	-2.10762300	-1.36551100
H	-3.76483900	-2.58721100	-2.79433600
C	-5.73985600	-1.20708000	-0.39075100
H	-5.28966900	0.63118900	0.65809900
H	-5.89457300	-2.99242000	-1.59310300
H	-6.66643600	-1.38954800	0.14663800
H	-2.46691600	1.57537300	-2.97597200
H	-2.73396900	0.47196900	-4.32835600
H	-0.52510600	1.82374200	-4.55786500
H	-0.27703700	0.07730800	-4.50897700
H	4.43409800	-2.70271800	2.72753500
H	3.30644800	-1.50466900	3.36390500
H	2.10300500	-3.70883800	3.29206900
H	2.54419700	-3.88870100	1.59183800

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C	-4.77263700	0.00799100	-0.33294600

C	-3.59330400	-0.69512400	-0.55480700
C	-2.37014800	-0.16740200	-0.11823300
C	-2.33599500	1.06783600	0.54259300
C	-3.52001600	1.76772000	0.76264200
C	-4.73675400	1.24028500	0.32534600
H	-5.71967000	-0.40180200	-0.67113600
H	-3.59450600	-1.65410400	-1.06152200
H	-1.38768200	1.46842600	0.88103600
H	-3.49441200	2.72414800	1.27636900
H	-5.65819100	1.78905600	0.49863300
C	-1.14777100	-0.96413400	-0.37798000
O	-1.11288700	-2.04746400	-0.90083500
O	-0.00000100	-0.27192700	-0.00011600
C	1.14771800	-0.96415000	0.37783300
O	1.11278000	-2.04748600	0.90068100
C	2.37014200	-0.16744700	0.11817700
C	2.33610800	1.06766000	-0.54290100
C	3.59321400	-0.69504800	0.55513100
C	3.52016000	1.76753300	-0.76282200
H	1.38786100	1.46816500	-0.88163200
C	4.77257900	0.00804800	0.33338700
H	3.59432400	-1.65392300	1.06204400
C	4.73681500	1.24021100	-0.32515600
H	3.49464600	2.72386000	-1.27673800
H	5.71954700	-0.40165800	0.67186800
H	5.65827700	1.78897000	-0.49835100

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C	-3.17048200	-1.62929900	0.60536800
C	-3.77207200	-0.26358400	0.24453900
H	-3.26558700	-2.31173300	-0.24690900
H	-3.72235200	-2.07194300	1.44277600
H	-3.84268500	0.36762100	1.13524500
H	-4.78740500	-0.39495600	-0.14421600
P	-2.72065700	0.70205300	-0.94931300
P	-1.34085100	-1.57111100	0.99135100
C	0.42523400	-0.81034500	-2.36820800
C	1.74243700	-0.61124900	-1.99783500
H	0.00827300	-1.80553700	-2.24546200
C	2.00545100	1.44204300	-0.10419600
C	2.53431600	0.55117700	-2.20330800
Cu	-0.49384200	-0.02947900	-0.51203700
O	0.75677800	1.51370700	-0.14089400

C	-3.62432100	2.35361200	-0.97791400
H	-4.62434500	2.15861000	-0.56749800
C	-3.30593000	0.22745700	-2.69873600
C	-1.26068400	-1.22130100	2.84055800
H	-0.23143000	-0.88497600	2.99883000
C	-0.96566900	-3.41611800	1.19594000
C	1.90527700	1.63677300	-3.04475800
H	2.45637200	2.57740200	-3.00922100
H	1.82518100	1.33764900	-4.10033200
H	0.89243500	1.84439700	-2.68012400
C	4.00269100	0.43241900	-2.14753300
C	4.84469400	1.52341500	-2.45276800
C	4.65345300	-0.76457200	-1.76218300
C	6.23217600	1.43646400	-2.35046700
H	4.41307200	2.46860200	-2.75809300
C	6.03723600	-0.84741800	-1.64718600
H	4.07084000	-1.65810400	-1.57185800
C	6.84543400	0.25585400	-1.93618800
H	6.83415200	2.30999700	-2.58777000
H	6.48997200	-1.79028700	-1.34803300
H	7.92646000	0.18903000	-1.85343700
C	2.86339700	2.63513900	-0.14623400
C	4.20069000	2.61012500	0.27558500
C	2.32466800	3.83581300	-0.64243500
C	4.97531900	3.76793000	0.22075200
H	4.63015100	1.68389300	0.63642500
C	3.10628700	4.98381100	-0.70794500
H	1.29354000	3.84857700	-0.97388600
C	4.43585200	4.95579600	-0.27189700
H	6.00961900	3.73349200	0.55070300
H	2.67800800	5.90519800	-1.09317600
H	5.04430500	5.85462700	-0.31889000
H	2.17643400	-1.41435500	-1.41247300
H	-0.05020700	-0.17303200	-3.11010200
C	2.26693400	0.09792100	1.87507600
O	2.61653900	0.34545400	0.59315100
O	1.48386400	0.75828000	2.52930400
C	2.96164400	-1.11372500	2.39601600
C	3.99128100	-1.74109500	1.68174200
C	2.55388400	-1.62857300	3.63323700
C	4.58577100	-2.89292100	2.19398800
H	4.31201900	-1.32714400	0.73371400
C	3.14087700	-2.78882100	4.13368700
H	1.77846600	-1.10789300	4.18481000

C	4.15355100	-3.42572700	3.41110800
H	5.38477900	-3.37783800	1.64039600
H	2.81333400	-3.19452400	5.08644600
H	4.61057100	-4.33100800	3.80056400
C	-1.44004900	-2.59502700	3.50218300
H	-1.13855700	-2.57142800	4.55633300
H	-2.49190900	-2.90539900	3.47535500
C	-0.59378200	-3.58371000	2.68730500
H	0.46430400	-3.35112700	2.84012700
H	-0.74427600	-4.62129400	3.00589400
H	-1.91634900	-3.93234900	1.01661100
C	-2.18198900	-0.08459300	3.20069300
C	-1.78963400	1.22067000	2.85585500
C	-3.44997200	-0.28238400	3.75953500
C	-2.65638900	2.29434200	3.04511100
H	-0.80570000	1.38359000	2.42570800
C	-4.31884500	0.79603400	3.94963800
H	-3.77154300	-1.27965600	4.04372800
C	-3.92881000	2.08468000	3.58426600
H	-2.34130000	3.29221500	2.76240600
H	-5.30121600	0.62402700	4.38186000
H	-4.60587500	2.92317400	3.72127700
C	-3.80028500	2.64334600	-2.48483500
H	-4.50171400	3.47084900	-2.63969900
H	-2.83786000	2.95017400	-2.91531600
C	-4.28433300	1.33906500	-3.12762000
H	-2.39717100	0.32772900	-3.30297400
H	-5.29592200	1.12245400	-2.76474000
H	-4.34198500	1.40558300	-4.22015800
C	-3.00000600	3.47592200	-0.18249500
C	-3.83583400	4.40092000	0.45711700
C	-1.61284500	3.63423500	-0.07112000
C	-3.30387600	5.46275700	1.18858100
H	-4.91472900	4.28043200	0.38770300
C	-1.07769100	4.68902000	0.66970300
H	-0.94036400	2.90934800	-0.51486000
C	-1.91930300	5.60867000	1.29890600
H	-3.96901700	6.16733000	1.68061100
H	0.00027800	4.77574900	0.76752100
H	-1.50025600	6.42551300	1.87985800
C	-3.77129400	-1.20214500	-2.79659900
C	-2.84979300	-2.20127700	-3.14425700
C	-5.08054100	-1.59355200	-2.48015000
C	-3.21710800	-3.54618300	-3.16141700

H	-1.83387800	-1.91877800	-3.39808400
C	-5.44974100	-2.93914600	-2.49013300
H	-5.82308700	-0.84546900	-2.22097700
C	-4.51870200	-3.92355300	-2.82577800
H	-2.48456700	-4.29726900	-3.44284100
H	-6.46937500	-3.21726700	-2.23811400
H	-4.80760900	-4.97053400	-2.83657700
C	0.03627300	-3.89180500	0.17306800
C	1.41350100	-3.70409600	0.34169700
C	-0.41629000	-4.46189400	-1.02435400
C	2.31138700	-4.06985700	-0.66039400
H	1.79624000	-3.25955000	1.25148100
C	0.47866500	-4.82061100	-2.03250400
H	-1.48277800	-4.60978400	-1.17141400
C	1.84945000	-4.62336200	-1.85571800
H	3.37468600	-3.91335700	-0.50217500
H	0.10572100	-5.25595100	-2.95599500
H	2.54906000	-4.89829100	-2.63948600

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C	-3.81066100	-1.26249200	0.48179500
C	-2.87162000	-2.40126600	0.92491100
H	-4.75232300	-1.67959500	0.10358200
H	-4.05693700	-0.62945000	1.33996700
H	-3.20246600	-2.78294400	1.89816200
H	-2.93137800	-3.22938000	0.21258300
P	-1.06518700	-1.92824900	0.97518200
P	-3.09737400	-0.09053500	-0.77515200
C	-0.12973900	0.87537200	-2.61714400
C	0.85774000	1.74466300	-2.22435500
H	-1.06714800	1.26608800	-3.00277000
C	1.79639400	1.33309500	0.36213500
C	2.17411400	1.38826800	-1.77635400
Cu	-0.83873400	0.09807800	-0.50606900
O	0.80949900	0.56154600	0.51020100
C	-0.83670100	-1.19198200	2.70408200
C	-0.27172700	-3.58104800	1.46011200
H	-1.08337700	-4.31658500	1.51957600
C	-4.49773000	1.16337800	-0.95238600
H	-5.29378700	0.82364300	-0.27915800
C	-3.45398200	-0.91399800	-2.43725500
C	2.52569500	-0.07225500	-1.97067300
H	3.46721700	-0.34046600	-1.49254900

H	2.59789400	-0.33379900	-3.03619300
H	1.75168100	-0.70517700	-1.52660000
C	3.25709900	2.38960700	-1.95511400
C	4.58901700	1.98942500	-2.18463500
C	3.02027600	3.77879200	-1.88260300
C	5.62411500	2.91536600	-2.30890100
H	4.82295800	0.93663200	-2.28610800
C	4.05166900	4.70411000	-2.01255300
H	2.02039200	4.15061200	-1.69075500
C	5.36583400	4.28303300	-2.22131800
H	6.63672100	2.56122900	-2.48647000
H	3.82385600	5.76406400	-1.93574400
H	6.17043000	5.00645700	-2.31843300
H	0.58619000	2.79709700	-2.17570200
H	0.10329000	-0.14930300	-2.89447900
C	0.29618400	-3.34820700	2.88514500
C	-0.65437000	-2.40407600	3.62635000
H	0.12555000	-0.67585200	2.62277900
C	-1.90453500	-0.18093700	3.02610900
C	-3.06973300	-0.49331900	3.73725000
C	-1.76699300	1.11886800	2.51054200
C	-4.08868800	0.45299700	3.88737700
H	-3.19501800	-1.48115100	4.16973200
C	-2.78416600	2.05932200	2.64694900
H	-0.85028800	1.37334600	1.99152500
C	-3.95857700	1.72474000	3.32751500
H	-4.98726200	0.19034300	4.43985500
H	-2.66238700	3.04970300	2.21950700
H	-4.75577100	2.45524500	3.43140100
C	0.76281200	-4.06771200	0.47671700
C	0.77447300	-5.39887700	0.04665900
C	1.74969800	-3.19665000	-0.00628100
C	1.74318500	-5.85134400	-0.85216700
H	0.01185500	-6.08306900	0.41158700
C	2.72188700	-3.64439900	-0.89838500
H	1.74408400	-2.16153100	0.31661000
C	2.71877900	-4.97407600	-1.32923800
H	1.73405900	-6.88758400	-1.17977600
H	3.48151000	-2.95420800	-1.25270100
H	3.47355700	-5.32356100	-2.02810400
C	-4.98989900	0.99658400	-2.41349200
C	-4.88902200	-0.48837800	-2.78025000
H	-2.77806200	-0.41011700	-3.13903700
C	-3.09965700	-2.37980300	-2.40849500

C	-4.05550400	-3.38970800	-2.25101300
C	-1.74411600	-2.74541500	-2.44295600
C	-3.66424600	-4.72423500	-2.10600500
H	-5.11196400	-3.14188500	-2.23219100
C	-1.34906900	-4.07173800	-2.29630200
H	-0.98801700	-1.97519600	-2.55310100
C	-2.31231600	-5.06830200	-2.11749000
H	-4.42158400	-5.49332900	-1.98047700
H	-0.29454300	-4.32433000	-2.30558900
H	-2.00727400	-6.10329600	-1.99351100
C	-4.12370900	2.57728100	-0.58398000
C	-4.94070400	3.32413700	0.27150400
C	-2.96726000	3.17875600	-1.09931700
C	-4.61405000	4.63855500	0.60886900
H	-5.83477000	2.86575800	0.68645800
C	-2.63996900	4.49289500	-0.77135200
H	-2.30418600	2.60861500	-1.74240300
C	-3.46121200	5.22782100	0.08789000
H	-5.25836400	5.19976300	1.27988100
H	-1.73433700	4.93628000	-1.17369900
H	-3.20357200	6.25059200	0.34794300
C	1.72021900	2.76657700	0.74399700
C	2.85026100	3.49391100	1.13803300
C	0.47673300	3.41652700	0.68677400
C	2.73728300	4.83995800	1.48509500
H	3.81501600	3.00319100	1.16373600
C	0.36835400	4.76066900	1.03227000
H	-0.40084200	2.86375400	0.37108800
C	1.49900600	5.47856700	1.43447200
H	3.62393200	5.39052600	1.78654600
H	-0.60352600	5.24341600	1.00165100
H	1.41169200	6.52674400	1.70708500
O	3.09917900	0.78482600	0.67162000
C	3.24384500	-0.27188400	1.50323800
O	2.44238900	-0.62293400	2.34859700
C	4.52845900	-0.98664200	1.24917900
C	5.52362000	-0.45567000	0.41676400
C	4.71364500	-2.23989400	1.84623100
C	6.69014200	-1.18079600	0.18112800
H	5.37558100	0.51582100	-0.03933300
C	5.87522800	-2.96619800	1.59818500
H	3.93154200	-2.63355700	2.48539300
C	6.86482200	-2.43794100	0.76523300
H	7.46158500	-0.76618000	-0.46154600

H	6.00820900	-3.94496100	2.04979000
H	7.77113700	-3.00529600	0.57196600
H	0.43290400	-4.30522100	3.40186600
H	1.27712000	-2.86828300	2.80387400
H	-1.61074900	-2.91163000	3.81010500
H	-0.25307000	-2.10099800	4.60071800
H	-6.00708600	1.38859200	-2.52215900
H	-4.34598200	1.58518900	-3.07884800
H	-5.61346700	-1.05713800	-2.18444200
H	-5.12104100	-0.67183900	-3.83587700

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C	-3.56660700	1.28135800	0.96847700
C	-2.86745600	2.49251000	0.33736400
H	-4.37924300	0.93431800	0.32280400
H	-4.00885800	1.56796900	1.92948800
H	-2.26250400	3.00533300	1.09067800
H	-3.61692500	3.20789000	-0.02155800
P	-1.66541300	2.07739200	-1.02550800
P	-2.46461100	-0.20332500	1.19768700
C	-0.66589900	-1.64474600	-2.19579400
C	0.43995400	-2.32141000	-1.74313400
H	-1.64272800	-2.10876500	-2.09228000
C	1.93646900	-0.94827900	0.09604600
C	1.81622900	-1.90506800	-1.81290400
Cu	-0.86419000	-0.09030000	-0.49188400
O	1.06243200	-0.03710800	0.05959600
C	-0.92524700	3.78834300	-1.32178200
H	-1.49882900	4.47179700	-0.68315000
C	-2.70333300	2.11892000	-2.60842500
C	-1.64690600	0.03325700	2.88739500
H	-0.76558400	-0.61507700	2.84628800
C	-3.71801500	-1.46206600	1.83704800
H	-4.65063100	-0.90457700	1.98821400
C	2.07398000	-0.69793000	-2.69251600
H	3.04619500	-0.24498100	-2.49288400
H	2.02550600	-0.95861100	-3.75925100
H	1.32167500	0.06932100	-2.49891500
C	2.86760700	-2.95539800	-1.77934000
C	4.14143400	-2.72126900	-2.33687000
C	2.67299100	-4.20697800	-1.15862700
C	5.16070500	-3.66924900	-2.26589100
H	4.33992300	-1.78552200	-2.84525100

C	3.68810100	-5.15764900	-1.09313700
H	1.72311200	-4.44328600	-0.69342600
C	4.94427500	-4.89808200	-1.64186500
H	6.12768300	-3.44559400	-2.70985400
H	3.49426800	-6.10488000	-0.59656700
H	5.73655400	-5.63930600	-1.58765500
H	0.23639000	-3.23537900	-1.19021900
H	-0.58489000	-0.83856800	-2.92089800
O	3.29807700	-0.48847800	-0.07694700
C	1.86548500	-2.09080500	1.05055900
C	3.00497100	-2.78497400	1.47560000
C	0.60908100	-2.52561500	1.49691400
C	2.88741300	-3.87515500	2.33849000
H	3.98090300	-2.47949700	1.11934400
C	0.48894000	-3.62577700	2.34003200
H	-0.26930000	-1.99185800	1.15826900
C	1.63320300	-4.30514200	2.77002400
H	3.78297400	-4.40023000	2.65825400
H	-0.49584900	-3.95498300	2.66219800
H	1.54476700	-5.16161100	3.43245500
C	3.77750000	0.38911500	0.84027900
C	5.14835500	0.85153000	0.47893100
C	5.67925000	1.93838400	1.18520600
C	5.89716400	0.24004000	-0.53501400
C	6.94553800	2.42288800	0.86835000
H	5.07869200	2.38732400	1.96887900
C	7.16905000	0.72248500	-0.84116200
H	5.48490400	-0.61209700	-1.06284900
C	7.69137600	1.81547300	-0.14627700
H	7.35410500	3.27005900	1.41192800
H	7.75294300	0.24543300	-1.62317200
H	8.68032400	2.19246500	-0.39221300
O	3.17801000	0.75882400	1.82795600
C	-1.28554500	4.11236500	-2.79297000
H	-1.19241200	5.18738700	-2.98313100
H	-0.57731400	3.60434600	-3.46017400
C	-2.70737400	3.59084500	-3.04459100
H	-3.41376600	4.17124500	-2.43804100
H	-3.01257900	3.69921900	-4.09205600
H	-2.10476900	1.55413500	-3.33483200
C	-3.17853300	-1.85597300	3.23384500
C	-2.63565600	-0.57915600	3.89092000
H	-2.14791400	-0.78355100	4.85090600
H	-3.46846300	0.10738900	4.08846300

H	-3.96480000	-2.33489900	3.82804400
H	-2.36763300	-2.58612100	3.12124300
C	0.53843600	3.93899400	-0.98088000
C	0.99869200	5.13446000	-0.41410800
C	1.46184700	2.91846900	-1.23181100
C	2.34852100	5.30684000	-0.10466800
H	0.28922800	5.93115600	-0.20140000
C	2.81151300	3.08930300	-0.93189200
H	1.12305200	1.96272000	-1.61104300
C	3.26136300	4.28195600	-0.36388900
H	2.68464000	6.23776600	0.34414000
H	3.50836600	2.28253600	-1.12922400
H	4.31213900	4.40140800	-0.11625600
C	-4.00104400	1.38479300	-2.39292300
C	-3.96994400	-0.01907800	-2.37389000
C	-5.20594500	2.02660100	-2.08450900
C	-5.09177000	-0.76333300	-2.02071500
H	-3.04211600	-0.52624200	-2.61251400
C	-6.33833000	1.28339400	-1.73749500
H	-5.26651700	3.11025000	-2.10288400
C	-6.28273000	-0.11030800	-1.69117800
H	-5.03285300	-1.84624400	-1.98936300
H	-7.26420600	1.79945200	-1.49804700
H	-7.15958300	-0.68551200	-1.40807500
C	-4.00134600	-2.60771600	0.89776000
C	-5.32389200	-2.98643500	0.63877300
C	-2.96953100	-3.31153900	0.26033100
C	-5.61428300	-4.03276000	-0.23849700
H	-6.13461100	-2.44518100	1.12059100
C	-3.25413300	-4.35330500	-0.62108400
H	-1.93685700	-3.03104400	0.43393400
C	-4.57897500	-4.71626000	-0.87770000
H	-6.64843200	-4.30718200	-0.42794800
H	-2.43912500	-4.87878500	-1.11114800
H	-4.80053200	-5.52499900	-1.56802500
C	-1.16877100	1.45325400	3.05594000
C	-1.93302900	2.44800100	3.67853200
C	0.04839400	1.81176000	2.45398000
C	-1.50743900	3.77961900	3.66558500
H	-2.86863800	2.19348200	4.16809600
C	0.46950700	3.13938500	2.43541500
H	0.66342500	1.05700000	1.97615200
C	-0.31427200	4.13143900	3.03079400
H	-2.11339700	4.54126700	4.14958300

H	1.40669400	3.38917100	1.94961200
H	0.00908000	5.16859900	3.00951500

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C	-3.07635700	2.31288700	0.39906400
C	-3.59626400	1.05626500	1.12651200
H	-3.91991200	2.90388200	0.02258300
H	-2.52233600	2.94394300	1.09943300
H	-3.94118300	1.33096400	2.13029400
H	-4.45087600	0.63831400	0.58580400
P	-2.33776100	-0.31128000	1.20098900
P	-1.87439100	1.96628700	-0.98560100
C	-0.16808600	-0.83036400	-2.62277300
C	1.19536500	-1.00465700	-2.43929300
H	-0.49600200	0.03044600	-3.19993400
C	1.73062700	-1.54874900	0.28824000
C	1.85564600	-2.15183200	-1.92870700
Cu	-0.75738500	-0.07416000	-0.62738700
O	0.51878800	-1.28188700	0.46332600
C	-1.29316500	0.07521900	2.73135300
C	-3.27721200	-1.71606200	2.03803100
H	-4.26503700	-1.33051300	2.32019600
C	-1.37763500	3.71353300	-1.49705100
H	-1.96128700	4.39790800	-0.86882200
C	-2.98340400	1.71257900	-2.49886300
C	1.01339700	-3.40506700	-1.83380900
H	1.48488200	-4.18443500	-1.23388800
H	0.79523500	-3.82319800	-2.82726200
H	0.05884800	-3.17206800	-1.35399900
C	3.30897500	-2.29001300	-2.15707600
C	3.93464800	-3.55273900	-2.14813000
C	4.15328300	-1.17348400	-2.35192600
C	5.31366500	-3.69271500	-2.30640000
H	3.33948100	-4.44673500	-2.01018100
C	5.52803200	-1.31143300	-2.50734400
H	3.73233200	-0.17530900	-2.36054300
C	6.12637600	-2.57541000	-2.48104900
H	5.75065700	-4.68782700	-2.28717300
H	6.13922000	-0.42345700	-2.65290400
H	7.20054400	-2.68196900	-2.60188200
C	2.35634000	-2.75601300	0.86315400
C	3.74732000	-2.93649000	0.88701700
C	1.52745300	-3.75980000	1.39137100

C	4.29439500	-4.09709200	1.43055700
H	4.39640300	-2.17385800	0.47540200
C	2.07850000	-4.91893800	1.92729200
H	0.45382500	-3.61330900	1.37880500
C	3.46593700	-5.09268000	1.94917200
H	5.37304700	-4.22459900	1.43820700
H	1.42623200	-5.68613900	2.33571400
H	3.89610700	-5.99745500	2.36966700
H	1.81099900	-0.13688300	-2.66436900
H	-0.83412900	-1.68949100	-2.64993200
C	2.86638900	0.22500700	1.36414900
O	2.63735200	-0.43024600	0.19161200
O	2.31843200	-0.04290300	2.41297600
C	3.84762000	1.33127900	1.20421900
C	4.82553000	1.31468100	0.20276000
C	3.78673600	2.39623900	2.11118900
C	5.73704800	2.36554400	0.10956100
H	4.87494100	0.47618700	-0.48116400
C	4.68512100	3.45409900	1.99985300
H	3.02444800	2.38231800	2.88229400
C	5.66326700	3.43841500	1.00162400
H	6.50563100	2.34664300	-0.65800600
H	4.62680000	4.28852100	2.69262400
H	6.37126100	4.25907900	0.92278700
C	-2.47124800	-1.99106000	3.33272600
C	-2.01096300	-0.63823000	3.88646400
H	-0.34910100	-0.44365400	2.53314500
C	-0.99777200	1.54839100	2.85191200
C	-1.72663800	2.41320400	3.67684300
C	0.00511500	2.09791200	2.03679700
C	-1.47052300	3.78818400	3.67366400
H	-2.50158500	2.02032500	4.32742300
C	0.27256300	3.46386700	2.03742800
H	0.56877600	1.43846500	1.39099400
C	-0.47454200	4.31888800	2.85310200
H	-2.05088600	4.44248400	4.31896200
H	1.05724800	3.85708800	1.40112700
H	-0.27519800	5.38695200	2.85229800
C	-3.45592600	-2.92018900	1.14586100
C	-4.68887200	-3.57707400	1.07688400
C	-2.39117800	-3.40412000	0.37003200
C	-4.86372700	-4.68784700	0.24840800
H	-5.52301200	-3.20675100	1.66837900
C	-2.56249900	-4.51130300	-0.45878900

H	-1.43419400	-2.89085300	0.39522900
C	-3.80134000	-5.15578900	-0.52630900
H	-5.83066300	-5.18177600	0.20399900
H	-1.72751400	-4.86713300	-1.05591600
H	-3.93568600	-6.01564300	-1.17647600
C	-1.88488900	3.85404000	-2.95440900
C	-3.23014800	3.12477700	-3.04842300
H	-2.34292000	1.18536000	-3.21598700
C	-4.15684200	0.82205900	-2.17675000
C	-5.42848500	1.31968600	-1.86973300
C	-3.94191700	-0.56228900	-2.07836700
C	-6.44716100	0.45989600	-1.44818900
H	-5.63074200	2.38308300	-1.94915100
C	-4.95177100	-1.42233100	-1.65548200
H	-2.96148300	-0.96454400	-2.31040000
C	-6.21003900	-0.90990300	-1.32828600
H	-7.42651700	0.86646400	-1.21045600
H	-4.75279200	-2.48515600	-1.57079600
H	-6.99838600	-1.57614000	-0.98993400
C	0.08858900	4.02871600	-1.31644700
C	0.47660600	5.30809300	-0.90124800
C	1.08531700	3.07322400	-1.55836400
C	1.82335600	5.62429200	-0.71632500
H	-0.28704800	6.05681500	-0.70318200
C	2.43094700	3.38375200	-1.37123500
H	0.80632800	2.06706400	-1.85694400
C	2.80576800	4.65947600	-0.94490500
H	2.10283600	6.61988200	-0.38224900
H	3.18714000	2.62402400	-1.53456800
H	3.85338900	4.88902500	-0.78119900
H	-3.07601200	-2.55801000	4.04951200
H	-1.59556200	-2.60460500	3.08792900
H	-2.88945300	-0.06835800	4.21552900
H	-1.34971000	-0.74957200	4.75368800
H	-3.97028700	3.65608900	-2.43724300
H	-3.61769800	3.09270400	-4.07358100
H	-1.95665900	4.91038300	-3.23629800
H	-1.16083600	3.38765500	-3.63481200

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C	2.72742800	-1.90699100	0.88403900
C	1.59437800	-2.94180300	0.88437000
H	3.36096800	-2.04503700	0.00198100

H	3.35865300	-2.04515200	1.76932600
H	1.10745400	-2.96613500	1.86412000
H	2.00313600	-3.94052500	0.69578100
P	0.21936500	-2.55885400	-0.31394200
P	2.13984200	-0.13993500	0.78685400
C	0.23826900	0.49569800	-2.61558400
C	-0.46827600	1.66749800	-2.40642000
H	1.31532900	0.58736500	-2.72253300
C	-1.98048100	1.72498300	-0.07156800
C	-1.86174700	1.95732600	-2.36501300
Cu	0.22004800	-0.16725900	-0.50130500
O	-1.58840600	0.55538600	0.13631700
C	-0.99085100	-3.93803900	0.10268800
H	-0.40513600	-4.69685400	0.63911300
C	0.71264900	-3.34350000	-1.97605900
C	1.87795000	0.41233700	2.57274400
H	1.17331900	1.24293300	2.49358000
C	3.78257200	0.76678700	0.60263300
C	-2.19657800	3.42284900	-2.57189900
C	-3.38084100	2.14579100	0.10268500
C	-3.73428800	3.47804900	0.36735000
C	-4.39694900	1.18458600	-0.02741000
C	-5.07329600	3.83537600	0.51611700
H	-2.95838800	4.22896600	0.45977700
C	-5.73192600	1.54814000	0.11353400
H	-4.12964600	0.16399000	-0.26372800
C	-6.07714900	2.87331400	0.39059500
H	-5.33162900	4.86861600	0.73100300
H	-6.50478500	0.79386300	-0.00344600
H	-7.12039900	3.15501000	0.50299200
H	0.15498500	2.52743400	-2.16174900
H	-0.22066300	-0.36313400	-3.09661500
C	-0.58880100	2.92456200	1.45460200
O	-1.02651800	2.78958400	0.18055600
O	-1.03439100	2.31433700	2.40601300
C	0.53469600	3.89858900	1.55746700
C	1.04344800	4.57695800	0.44316100
C	1.10859400	4.10174100	2.81996400
C	2.13653300	5.42984600	0.58701600
H	0.58628300	4.42325000	-0.52723800
C	2.19726500	4.95766100	2.96148100
H	0.69024500	3.57162400	3.66880800
C	2.71664900	5.61727300	1.84333400
H	2.54019700	5.94064900	-0.28187900

H	2.64485500	5.10829300	3.93947100
H	3.57225800	6.27767900	1.95187900
H	-1.41263900	4.05502200	-2.14303600
H	-2.27758100	3.67881300	-3.63863500
H	-3.14095700	3.70627500	-2.09692900
C	-2.88948300	0.97110600	-2.74536000
C	-4.12447500	1.39082400	-3.28344800
C	-2.75059600	-0.41384600	-2.49345300
C	-5.15304200	0.49130500	-3.55432800
H	-4.29060800	2.44251900	-3.48424300
C	-3.78549200	-1.30964200	-2.74933900
H	-1.85089900	-0.78477700	-2.02697200
C	-4.99548900	-0.86879600	-3.28764500
H	-6.08808100	0.86090000	-3.96766200
H	-3.64900500	-2.36163200	-2.51013800
H	-5.79959500	-1.57047800	-3.49099500
C	-1.33798100	-4.53594100	-1.27861600
H	-1.87692300	-5.48331700	-1.16602800
H	-1.99857000	-3.84989400	-1.82445200
C	-0.00858000	-4.70341600	-2.02522300
H	0.58349800	-5.47364900	-1.51697600
H	-0.14808500	-5.03434600	-3.06070000
H	0.24331600	-2.68599400	-2.71644200
C	-2.16764200	-3.56130800	0.97091900
C	-2.63532400	-4.48898400	1.91174200
C	-2.80913100	-2.32004400	0.87426100
C	-3.72171500	-4.19277500	2.73434700
H	-2.13435900	-5.45020800	2.00465000
C	-3.89196000	-2.01851200	1.70182100
H	-2.43905200	-1.56173100	0.19502300
C	-4.35442900	-2.95225600	2.63104800
H	-4.06602600	-4.92445500	3.46032400
H	-4.35740100	-1.04054500	1.63283800
H	-5.19287500	-2.71025600	3.27821100
C	2.20313400	-3.29789200	-2.19077400
C	3.06530100	-4.31201700	-1.75177300
C	2.77075100	-2.14303000	-2.75096700
C	4.45035800	-4.16327200	-1.84598400
H	2.65974100	-5.22346700	-1.32370000
C	4.15252800	-1.98826200	-2.84335500
H	2.11745700	-1.35219500	-3.10127500
C	5.00051600	-2.99785800	-2.38232700
H	5.09988800	-4.96115400	-1.49625100
H	4.56053900	-1.07469500	-3.26348600

H	6.07867600	-2.88203700	-2.44878700
C	3.23496000	0.97774800	3.01943200
H	3.11904800	1.63283900	3.89070600
H	3.92031500	0.17110800	3.30768200
C	3.81658100	1.72944600	1.81379200
H	3.20500900	2.61127900	1.59743000
H	4.83824100	2.08227000	1.99463300
H	4.56674700	0.01260100	0.74296300
C	1.20828200	-0.68127800	3.36480900
C	1.91872600	-1.58813000	4.16013600
C	-0.17465500	-0.86923000	3.19538100
C	1.26936500	-2.67349200	4.75482000
H	2.98559000	-1.45831300	4.31550300
C	-0.82107500	-1.95310500	3.78630000
H	-0.73808100	-0.16939800	2.58523600
C	-0.09921400	-2.86481100	4.56140600
H	1.83766700	-3.36965600	5.36621100
H	-1.88566900	-2.08951600	3.63334100
H	-0.60437900	-3.71394600	5.01305400
C	3.97284500	1.41775600	-0.74335900
C	5.11585600	1.15800800	-1.50665100
C	3.00651900	2.29063200	-1.26208800
C	5.29280800	1.75324500	-2.75810200
H	5.86972100	0.47631300	-1.12034700
C	3.17868600	2.88779100	-2.50850600
H	2.10485300	2.48459400	-0.69297100
C	4.32283700	2.61873900	-3.26447200
H	6.18750700	1.53829600	-3.33632900
H	2.41226400	3.55298300	-2.89695300
H	4.45460500	3.07849300	-4.23969100

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C	2.72886400	2.64833100	0.67190900
C	1.37289200	3.06160700	1.27409700
H	3.28299700	3.53803300	0.34781700
H	3.33384700	2.14666200	1.43266200
H	1.53646200	3.43913100	2.29070400
H	0.94717500	3.88300000	0.68960600
P	0.04368200	1.73987300	1.27097900
P	2.64382900	1.42918800	-0.72470500
C	0.64571100	-0.75130700	-2.75750500
C	0.31098600	-2.06349300	-2.46997200
H	1.64922800	-0.55163700	-3.12528700

C	-0.77341700	-2.41547800	0.11245400
C	-0.95046600	-2.64925400	-2.17703700
Cu	0.91945300	-0.01895500	-0.61583200
O	-0.28811200	-1.27525900	0.30711700
C	0.41500300	0.73266100	2.84224200
C	-1.34268300	2.72816000	2.13380700
H	-0.92383300	3.71890600	2.34846600
C	4.46934600	1.09684600	-1.06287100
H	5.02386800	1.73044900	-0.36012900
C	2.41218300	2.47659500	-2.27477200
C	-1.01750700	-4.15286300	-2.36926000
H	1.15129500	-2.75466300	-2.37961600
H	-0.11495900	-0.04477800	-3.07969400
C	-1.58396700	1.99528300	3.47601500
C	-0.23067600	1.51377600	3.99463300
H	-0.16428000	-0.18265200	2.68150100
C	1.86690300	0.35946100	2.97957600
C	2.79098100	1.12786200	3.69982000
C	2.33456100	-0.78107400	2.30748600
C	4.14739800	0.78928500	3.71134400
H	2.46003300	2.00292000	4.25012200
C	3.68601700	-1.11556300	2.30660500
H	1.61678300	-1.39824400	1.78140500
C	4.60267600	-0.32292800	3.00240200
H	4.84766900	1.40041900	4.27518300
H	4.02463100	-1.98940700	1.75880300
H	5.65783400	-0.57966400	2.99921200
C	-2.60045400	2.89935700	1.32312500
C	-3.32264600	1.78081300	0.88691300
C	-3.10010900	4.17366200	1.03056100
C	-4.52561600	1.92825900	0.19943500
H	-2.94091800	0.78828300	1.09551100
C	-4.29227600	4.32890500	0.32034500
H	-2.54622800	5.04987100	1.35865800
C	-5.01152800	3.20583400	-0.09301400
H	-5.07377000	1.04475700	-0.11017900
H	-4.66310100	5.32637400	0.09897700
H	-5.94581100	3.32408700	-0.63494800
C	4.70461800	1.64357900	-2.49522300
C	3.83417900	2.89484800	-2.67444300
H	2.04977300	1.76611200	-3.02750200
C	1.34603300	3.52180200	-2.05907500
C	1.63940200	4.86439100	-1.79783600
C	0.00388400	3.10835300	-2.01093900

C	0.62013800	5.76471700	-1.47212300
H	2.66568100	5.21565600	-1.83962100
C	-1.01225000	3.99901600	-1.67760800
H	-0.23928600	2.06795800	-2.20310900
C	-0.70446700	5.33369600	-1.39919600
H	0.86739400	6.80336400	-1.26978600
H	-2.03803700	3.65171200	-1.61392700
H	-1.49513500	6.02761200	-1.13008400
C	4.90275000	-0.33504500	-0.85926200
C	6.06508100	-0.62124500	-0.13498500
C	4.16901100	-1.40464800	-1.39066500
C	6.48339500	-1.93815400	0.06222900
H	6.64014800	0.19668200	0.29161100
C	4.58136900	-2.72203300	-1.19715600
H	3.25317000	-1.20930400	-1.93752300
C	5.74041300	-2.99492600	-0.46596800
H	7.38585900	-2.13745700	0.63341900
H	3.98941400	-3.53455800	-1.60802700
H	6.06102500	-4.02124700	-0.31140700
C	-0.01649900	-3.65191700	0.40517200
C	-0.65149600	-4.84387400	0.77997800
C	1.38498600	-3.62864100	0.30462000
C	0.10020800	-5.98767700	1.04714100
H	-1.73172500	-4.86515000	0.86336300
C	2.13080500	-4.77140900	0.57337800
H	1.88359300	-2.71119300	0.01517400
C	1.49166500	-5.95853600	0.94479400
H	-0.40455500	-6.90408900	1.34029300
H	3.21400900	-4.73074200	0.50260400
H	2.07458500	-6.85038700	1.15662400
O	-2.18099600	-2.55040200	0.33040700
C	-2.74070100	-1.87894400	1.37508600
O	-2.12369900	-1.48196700	2.34513500
C	-4.20399700	-1.68350300	1.19871100
C	-4.85272800	-1.97278900	-0.00746000
C	-4.92493400	-1.13195100	2.26768700
C	-6.21449600	-1.70633100	-0.14115100
H	-4.29004700	-2.37955000	-0.83619200
C	-6.28449800	-0.87199900	2.13098000
H	-4.39816900	-0.90475100	3.18800300
C	-6.93112100	-1.15755900	0.92413600
H	-6.70717300	-1.91612200	-1.08560200
H	-6.83988700	-0.43999200	2.95827200
H	-7.99145500	-0.94639600	0.81459700

C	-2.18867500	-1.89199200	-2.48303700
C	-3.24930500	-2.49597800	-3.18867400
C	-2.36271700	-0.54400500	-2.10280500
C	-4.39694800	-1.78279300	-3.53761800
H	-3.17267200	-3.53498800	-3.48776600
C	-3.50408600	0.16927700	-2.45712300
H	-1.61589100	-0.06309700	-1.48450200
C	-4.52855900	-0.44006100	-3.18429800
H	-5.18635000	-2.28148800	-4.09485100
H	-3.59882100	1.20417400	-2.14615500
H	-5.41662700	0.12097800	-3.46184200
H	-1.83396000	-4.60034300	-1.79168200
H	-1.17398800	-4.42392300	-3.42336900
H	-0.08714400	-4.62850200	-2.04893000
H	-2.09938100	2.65607800	4.18292900
H	-2.23037100	1.12765400	3.30476900
H	0.38128800	2.37996400	4.27776000
H	-0.33087900	0.88276100	4.88583500
H	5.76919900	1.84436400	-2.65769400
H	4.40605500	0.88055100	-3.22504300
H	3.86677600	3.27761700	-3.70118300
H	4.20448000	3.69255800	-2.01813700

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C	-3.37378900	1.46054400	1.02677000
C	-2.51285900	2.66017400	0.60700100
H	-4.19938800	1.32609300	0.32218800
H	-3.81111500	1.64481100	2.01429300
H	-1.91757100	3.01105400	1.45613100
H	-3.15719400	3.48890700	0.29160400
P	-1.25731200	2.28329500	-0.71559800
P	-2.46088400	-0.16281600	1.02714400
C	-0.15975900	-0.84816600	-2.42559700
C	0.39023700	-2.02883100	-1.95159600
H	-1.18815400	-0.88861800	-2.77771700
C	1.67020700	-1.75594300	0.57420600
C	1.73601600	-2.39065900	-1.64965600
Cu	-0.61878800	0.02645400	-0.47897300
O	0.92933900	-0.73824900	0.60289300
C	-0.44129400	3.97570500	-0.89376500
H	-1.11607400	4.69061900	-0.40541800
C	-2.17926800	2.42415100	-2.37363600
C	-1.71848300	-0.31540300	2.76089300

H	-0.88402600	-1.01107500	2.62012500
C	-3.87795400	-1.34902900	1.38895800
C	1.96125200	-3.89770000	-1.65692500
H	-0.33151600	-2.81742800	-1.73180500
H	0.46621800	-0.08364600	-2.87831700
O	3.02438600	-1.36163700	0.83364200
C	1.19915800	-3.04652400	1.14952800
C	-0.18032700	-3.30619000	1.07927700
C	2.02900100	-4.00450200	1.74496400
C	-0.71235400	-4.50317300	1.54419300
H	-0.82305200	-2.55804500	0.63689300
C	1.48975900	-5.19665700	2.23253800
H	3.09438900	-3.83735800	1.80357100
C	0.12461900	-5.45950400	2.12744500
H	-1.77823600	-4.69084300	1.44545600
H	2.14997700	-5.92789700	2.69074900
H	-0.28485100	-6.39632800	2.49458500
C	4.19678700	-1.91884700	0.45225300
C	5.28948600	-0.90793300	0.47492300
C	5.10168200	0.38399400	0.98131900
C	6.53150800	-1.27727900	-0.05327400
C	6.15627600	1.29401200	0.96638900
H	4.13092900	0.66383300	1.37212400
C	7.57894500	-0.35999600	-0.08068900
H	6.64763600	-2.28014000	-0.44798700
C	7.39387900	0.92586400	0.43188700
H	6.01277900	2.29273000	1.36979700
H	8.53854000	-0.64573700	-0.50190400
H	8.21209200	1.64075200	0.41460700
O	4.37000000	-3.08371200	0.15393100
H	2.86580800	-4.17711200	-1.11738800
H	1.11821800	-4.41084900	-1.18502600
H	2.03932000	-4.28347200	-2.68458400
C	2.84437300	-1.53922900	-2.14862700
C	3.96191800	-2.10125300	-2.79681000
C	2.84500400	-0.14049300	-1.97219300
C	5.00770300	-1.30925900	-3.26488400
H	4.01995800	-3.17563100	-2.92449800
C	3.88837400	0.65264500	-2.44542700
H	2.04390400	0.31035400	-1.40188400
C	4.97684100	0.07625800	-3.09993000
H	5.85406600	-1.78015800	-3.75854000
H	3.85585800	1.72798400	-2.29530900
H	5.79445900	0.69418700	-3.45969100

C	-0.50328200	4.24397600	-2.41318100
H	-0.26583100	5.29130000	-2.63041400
H	0.24496400	3.62852300	-2.92930600
C	-1.91582100	3.85850900	-2.86930000
H	-2.63033300	4.55982500	-2.42273800
H	-2.03627500	3.92493900	-3.95657200
H	-1.63477700	1.73521700	-3.02911600
C	0.91900000	4.09696500	-0.25932700
C	1.19134800	5.14513000	0.62731800
C	1.93563800	3.17598400	-0.53999400
C	2.44887300	5.27463200	1.21923300
H	0.40758800	5.86134900	0.86186500
C	3.19287300	3.29886600	0.04796500
H	1.73478400	2.34936900	-1.21258500
C	3.45335600	4.34939900	0.93191900
H	2.64020600	6.09420000	1.90651900
H	3.96295600	2.57054700	-0.17896600
H	4.43301200	4.44506700	1.39218300
C	-3.60559500	1.94276200	-2.26632800
C	-3.87136700	0.56762300	-2.36490500
C	-4.67252300	2.79931700	-1.96384600
C	-5.14960500	0.05738200	-2.14756900
H	-3.05940800	-0.11473600	-2.58983100
C	-5.95596500	2.29385100	-1.74441900
H	-4.50757200	3.86914700	-1.88731700
C	-6.19865600	0.92190300	-1.82722500
H	-5.32033000	-1.01142300	-2.21918600
H	-6.76657600	2.97717200	-1.50604300
H	-7.19586300	0.52929500	-1.65045900
C	-2.80127700	-1.01395000	3.59961000
H	-2.37224600	-1.45658800	4.50587400
H	-3.56954400	-0.29902900	3.91902400
C	-3.44802800	-2.06856600	2.69215800
H	-4.30921800	-2.55566800	3.16365900
H	-2.71873200	-2.85061700	2.45845300
H	-4.74027500	-0.71583100	1.63548500
C	-1.16077800	1.00853900	3.22529100
C	-1.89666500	1.91113700	4.00340500
C	0.10579700	1.40253900	2.76017500
C	-1.39565300	3.18606800	4.28222600
H	-2.87053000	1.63051000	4.39249400
C	0.60224800	2.67543500	3.03135900
H	0.68655100	0.71096800	2.15831000
C	-0.15157500	3.57782700	3.78631000

H	-1.98402600	3.87306800	4.88490200
H	1.57205900	2.96589300	2.64115400
H	0.23219200	4.57366700	3.98939500
C	-4.28839400	-2.26724200	0.25909300
C	-5.61823100	-2.70378100	0.18926300
C	-3.39457800	-2.70457400	-0.72659000
C	-6.04520300	-3.55076400	-0.83327200
H	-6.32799500	-2.36472600	0.94044300
C	-3.81542000	-3.55267200	-1.75118500
H	-2.37255700	-2.34585400	-0.71802400
C	-5.14349800	-3.97855900	-1.81050400
H	-7.08279300	-3.87106900	-0.87109200
H	-3.10416700	-3.87092500	-2.50846100
H	-5.47398400	-4.63323400	-2.61168100

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C	1.50299100	-3.10477300	0.79559100
C	2.60941100	-2.15443500	1.27186700
H	1.92754500	-4.09440400	0.58845000
H	0.75346100	-3.22871600	1.58447100
H	2.88003100	-2.39843100	2.30498200
H	3.50660900	-2.28439700	0.65942200
P	2.19146900	-0.34611700	1.12388700
P	0.52998000	-2.51989400	-0.68391200
C	0.67748000	0.89335600	-2.46897400
C	-0.55544000	1.52443800	-2.49242900
H	0.79588000	0.01290900	-3.09777400
C	-1.69311400	1.86840800	0.01999200
C	-1.00126400	2.77209000	-1.96712400
Cu	0.41487000	-0.19382700	-0.55539700
O	-0.72936500	1.17972400	0.43011400
C	1.29139500	0.12381500	2.73005500
C	3.82889200	0.40734800	1.69374100
H	4.37648100	-0.40571400	2.18877500
C	-0.63291000	-4.00444300	-0.89318100
H	-0.20360900	-4.77933900	-0.24574300
C	1.57757600	-3.00553500	-2.19560600
C	-2.27682200	3.28881300	-2.60543300
C	-2.08141100	3.13050000	0.68335000
C	-3.33047800	3.73816400	0.48289100
C	-1.14546500	3.76074800	1.51820900
C	-3.62486200	4.95872900	1.08788900
H	-4.07254200	3.25225000	-0.13989400

C	-1.43732900	4.98539100	2.10782800
H	-0.18877700	3.28301700	1.68027300
C	-2.67750000	5.59189900	1.89382300
H	-4.59780100	5.41519800	0.92789100
H	-0.69466200	5.46841400	2.73638000
H	-2.90585900	6.54815700	2.35620000
H	-1.35953300	0.93394700	-2.93488100
H	1.59064500	1.44149300	-2.25567000
C	-3.68213900	0.57547600	0.26709800
O	-2.80986400	1.17883400	-0.58126500
O	-3.48057400	0.40169800	1.45107800
C	-4.94354700	0.18701500	-0.42243200
C	-5.12881700	0.36198500	-1.79899000
C	-5.96469700	-0.37192800	0.35487900
C	-6.32415300	-0.03770600	-2.39502300
H	-4.33340800	0.79641000	-2.39182900
C	-7.16020500	-0.76309700	-0.24087500
H	-5.79186700	-0.50005800	1.41754700
C	-7.33922800	-0.60215200	-1.61810900
H	-6.46515200	0.09188300	-3.46415900
H	-7.95151300	-1.19690900	0.36373400
H	-8.27009100	-0.91250100	-2.08452600
C	3.40019700	1.40673700	2.79203300
C	2.37445700	0.68077700	3.66992600
H	0.64442600	0.94780700	2.41445200
C	0.40503300	-0.99401700	3.21917200
C	0.85888500	-2.01047900	4.07071200
C	-0.90348600	-1.07472900	2.71755300
C	0.03669500	-3.09539000	4.38597100
H	1.85990500	-1.96725600	4.48963800
C	-1.72432000	-2.15589000	3.03019600
H	-1.27983800	-0.28751600	2.07551700
C	-1.25327300	-3.17843200	3.85759200
H	0.40745700	-3.87556400	5.04586500
H	-2.72760900	-2.19032900	2.61932100
H	-1.88970600	-4.02550900	4.09973500
C	4.71759400	0.99165200	0.62577800
C	6.10106700	0.78102500	0.67373000
C	4.20137800	1.78417300	-0.40564100
C	6.94699100	1.35313600	-0.27781900
H	6.51758400	0.15880900	1.46237900
C	5.04027500	2.36770100	-1.35326100
H	3.13280200	1.93020500	-0.47907800
C	6.41956200	2.15267200	-1.29412000

H	8.01756500	1.17463900	-0.22477300
H	4.61116300	2.98591400	-2.13668000
H	7.07628900	2.60130000	-2.03400300
C	-0.41227600	-4.45446000	-2.35238000
C	1.09463200	-4.40688900	-2.60745800
H	1.25418400	-2.29810000	-2.96834900
C	3.05577500	-2.80909900	-1.97133000
C	3.88811100	-3.83289300	-1.49911900
C	3.61474100	-1.53641800	-2.16511800
C	5.23180900	-3.58601700	-1.20882800
H	3.49255000	-4.83147000	-1.34554100
C	4.95540500	-1.28745200	-1.88069500
H	2.98612200	-0.72837100	-2.52540500
C	5.76866500	-2.31154600	-1.39155100
H	5.85681100	-4.39421000	-0.83838900
H	5.36117200	-0.29386600	-2.03037700
H	6.81061500	-2.11318200	-1.15855500
C	-2.07015500	-3.81639400	-0.48999600
C	-2.55793800	-4.46654200	0.64943800
C	-2.96083400	-3.05369400	-1.25804500
C	-3.90257500	-4.37258200	1.00985900
H	-1.87429400	-5.04940600	1.26107900
C	-4.30869200	-2.97660300	-0.91490700
H	-2.60099700	-2.52382100	-2.13610200
C	-4.78401200	-3.63368900	0.22215000
H	-4.25933200	-4.88326000	1.90029900
H	-4.98963500	-2.40191000	-1.53168400
H	-5.83381500	-3.56133700	0.48888500
C	-0.06331500	3.79739700	-1.46321100
C	1.07707700	3.46312200	-0.70395600
C	-0.32322900	5.17129700	-1.64065400
C	1.91780400	4.43919200	-0.17400600
H	1.25051300	2.42445300	-0.46360500
C	0.51476100	6.14891300	-1.10861000
H	-1.19634100	5.48602600	-2.19976400
C	1.64749900	5.79296300	-0.37629900
H	2.78783100	4.13792300	0.40396200
H	0.27769900	7.19768100	-1.26899200
H	2.30342600	6.55550200	0.03442700
H	-2.82014500	3.97131800	-1.94480600
H	-2.07147400	3.83601200	-3.53726900
H	-2.94543100	2.46111500	-2.85487900
H	4.27163500	1.75274000	3.35956400
H	2.94368600	2.29062900	2.32683900

H	2.88042100	-0.13025900	4.20753200
H	1.93153700	1.34041000	4.42492400
H	-0.83364600	-5.45334100	-2.51122200
H	-0.92955100	-3.77386500	-3.03965700
H	1.57845700	-5.17702900	-1.99625700
H	1.35154300	-4.61686300	-3.65207000

Table S4. Electronic energies (E_{elec}), Gibbs free energies (G_{298}), thermal correction to Gibbs free energy ($cor\ G_{gas}$), solvation energies (Esol), solvation free energies (G_{sol}) in THF (ε = 7.43) for all stationary points of the process. Calculations were carried out at M06/6-311+G(d,p)/SDD/SMD(THF)//M06/6-31G(d)/LANL2DZ level.

species	E_{elec} (a.u.)	G_{298} (a.u.)	$cor\ G_{gas}$ (a.u.)	E_{sol} (a.u.)	G_{sol} (a.u.)
Int2_a	-2582.495081	-2581.782036	0.713045	-2584.244562	-2583.531517
Int2_b	-2582.493309	-2581.778662	0.714647	-2584.241721	-2583.527074
2a	-764.702311	-764.539513	0.162799	-764.906101	-764.743302
TS3_a1	-3347.200210	-3346.294148	0.906062	-3349.156950	-3348.250888
TS3_a2	-3347.189160	-3346.286667	0.902493	-3349.145431	-3348.242938
TS3_a3	-3347.191161	-3346.285254	0.905907	-3349.149588	-3348.243681
TS3_a4	-3347.190593	-3346.284473	0.906120	-3349.147309	-3348.241189
TS3_b1	-3347.196031	-3346.288140	0.907892	-3349.151987	-3348.244095
TS3_b2	-3347.189356	-3346.280506	0.908850	-3349.142682	-3348.233832
TS3_b3	-3347.177027	-3346.266104	0.910923	-3349.131876	-3348.220953
TS3_b4	-3347.186488	-3346.278681	0.907808	-3349.143373	-3348.235565

Cartesian coordinates for the optimized structures in Table S4

Int2_a

C	-1.02555000	1.02585400	1.91473700
C	0.23069700	1.87148000	1.70785300
Cu	-0.06367100	0.31193400	-1.32748800
C	-0.18941800	3.62390200	-0.65278800
H	-0.14815500	3.54609600	-1.75247900
C	2.36465300	2.98572100	0.11607300
H	2.48483200	3.15681200	1.19947600
C	-2.86682500	-1.09202400	1.25212200
H	-3.14892500	-0.54213800	2.16662800
C	-0.23905100	-1.82395600	1.50771600
H	-0.04859900	-2.50477100	0.66111200
P	0.72582100	2.08305100	-0.07356500
P	-1.19480400	-0.39794300	0.72034600

C	-0.08602600	-0.62992300	-3.10037900
H	0.74872800	-0.31264100	-3.73494600
H	-1.05523300	-0.44624800	-3.57872500
C	0.02510500	-1.92756800	-2.46878600
C	1.13439800	-2.65717600	-2.13641900
H	-0.93060400	-2.31745900	-2.10119000
C	2.49941400	-2.19519400	-2.55900800
H	3.15644300	-3.04014900	-2.81043200
H	2.43412800	-1.55496400	-3.44838800
H	3.02689000	-1.60357900	-1.78620900
C	1.02930500	-3.81591000	-1.24677500
C	2.13943000	-4.24192200	-0.49200400
C	-0.17778700	-4.51823600	-1.03403000
C	2.03725800	-5.25452400	0.45503400
H	3.09763900	-3.73942000	-0.62111300
C	-0.27799800	-5.52973900	-0.08956900
H	-1.05528400	-4.27501700	-1.63412300
C	0.82653000	-5.90213900	0.67617900
H	2.91824400	-5.53363400	1.03275400
H	-1.23120200	-6.04304500	0.04140200
H	0.74619300	-6.69490400	1.41811100
C	-1.23826000	-2.52061000	2.42526100
C	-2.55290900	-2.54255300	1.65589700
H	-0.88885800	-3.52994000	2.68644700
H	-1.37558300	-1.96303000	3.36698200
H	-3.38399600	-2.97272100	2.23203000
H	-2.43204600	-3.16131500	0.75031500
C	2.12914100	4.35083500	-0.55710500
C	0.70500300	4.78682000	-0.23384300
C	1.08506500	-1.36992000	2.04192300
C	1.31645000	-1.08792700	3.38929800
C	2.12409800	-1.15158600	1.12748100
C	2.54505000	-0.57641900	3.80613100
H	0.53334300	-1.26571300	4.12682900
C	3.34886300	-0.64480100	1.53900900
H	1.95207100	-1.38775500	0.07511800
C	3.56049100	-0.34351100	2.88381500
H	2.70740100	-0.36150600	4.86175700
H	4.14041900	-0.48367600	0.80652500
H	4.51922100	0.05875800	3.20957100
C	-3.96795500	-0.93668300	0.24274800
C	-5.21298900	-0.44259900	0.63522100
C	-3.78272200	-1.28447000	-1.09917100
C	-6.24760800	-0.29332000	-0.28415500

H	-5.36856000	-0.16218600	1.67843300
C	-4.81048800	-1.13241600	-2.02231600
H	-2.81227200	-1.66229600	-1.42706800
C	-6.04732600	-0.63356700	-1.61827100
H	-7.21106800	0.09492800	0.04378600
H	-4.64231400	-1.40162000	-3.06405500
H	-6.85094800	-0.51234800	-2.34276600
C	-1.62843200	3.58588800	-0.22973800
C	-2.49702900	2.70413000	-0.88850200
C	-2.12264800	4.32330400	0.84742500
C	-3.80989300	2.54269400	-0.46608800
H	-2.12638900	2.11745100	-1.73448900
C	-3.44109700	4.16421700	1.27242500
H	-1.47622500	5.02889200	1.36896300
C	-4.28467300	3.26804200	0.62532800
H	-4.46460200	1.84397300	-0.98565000
H	-3.80651700	4.74694500	2.11693000
H	-5.31281600	3.13747900	0.96087000
C	3.57768100	2.25490400	-0.38997200
C	3.56591100	1.56045300	-1.60296300
C	4.76368500	2.29494200	0.34587000
C	4.71159100	0.91976100	-2.06305000
H	2.64162200	1.49818500	-2.18275300
C	5.91205800	1.65692900	-0.11219100
H	4.78035200	2.82842600	1.29800300
C	5.88817100	0.96466000	-1.31931600
H	4.68151500	0.37539900	-3.00587200
H	6.82618700	1.69614900	0.47856300
H	6.78271900	0.45934200	-1.67936300
H	2.88529400	5.07724100	-0.22827700
H	2.24618800	4.23963300	-1.64764300
H	0.62127200	4.97398900	0.84910000
H	0.42275000	5.71902300	-0.74378800
H	1.09722400	1.38007800	2.17761500
H	0.11839600	2.85396400	2.19281200
H	-1.07201300	0.66280300	2.95322000
H	-1.92587200	1.63875300	1.74477100

Int2_b

C	0.39558500	-1.77224200	-1.69024200
C	1.72048300	-1.92805600	-0.94463300
H	-0.31854100	-2.53492800	-1.33781600
H	0.55105200	-1.95809800	-2.76466900

H	1.97698700	-2.99374300	-0.83569000
H	2.53568000	-1.46192000	-1.51917100
Cu	0.69291200	0.89247000	0.70662000
C	1.13407200	-2.32087300	1.95074400
H	0.89992900	-1.69726200	2.83063900
C	3.59377300	-1.37269100	1.18747600
H	4.02286200	-1.99541400	0.38426200
C	-2.03026000	-0.56136000	-2.52153400
H	-1.78673000	-1.50502800	-3.03886300
C	0.19838500	1.01753400	-2.73518600
H	-0.09641500	2.00864400	-2.34799300
P	1.79986100	-1.08390100	0.70142200
P	-0.52798800	-0.16220400	-1.43042300
C	0.18445600	2.73214100	1.24101100
H	1.10926800	3.32291800	1.15908500
H	-0.12914600	2.69417500	2.29250700
C	-0.83460800	3.21823200	0.31880400
C	-2.19739300	3.22127000	0.36426600
H	-0.41892200	3.68135200	-0.58752700
C	-2.95813600	3.91672600	-0.73642300
H	-3.79842000	3.31108600	-1.11561500
H	-3.39296100	4.87687700	-0.41354300
H	-2.29785900	4.14018700	-1.58560900
C	-2.99700300	2.63105500	1.44786100
C	-2.53585200	1.55047800	2.22402700
C	-4.30602900	3.07897500	1.70633700
C	-3.32878400	0.96127900	3.19983700
H	-1.54436400	1.14496100	2.02399600
C	-5.09312800	2.50321600	2.69784400
H	-4.71351300	3.90457800	1.12443600
C	-4.61282100	1.43789100	3.45362100
H	-2.94015000	0.11480700	3.76771500
H	-6.09539800	2.89200500	2.87773400
H	-5.23072000	0.98292300	4.22620100
C	-2.04149400	0.55389000	-3.57561600
C	-0.59950100	0.76219600	-4.01164800
C	3.51150700	-2.22881900	2.46463600
C	2.33930700	-3.18859500	2.30387200
C	4.42368000	-0.12639200	1.32181500
C	5.66774000	-0.04089600	0.69531000
C	3.98161100	0.96301600	2.07963500
C	6.45140400	1.10364800	0.81088500
H	6.02092900	-0.88415500	0.09919000
C	4.75726200	2.11065700	2.19230000

H	3.00482200	0.92426500	2.56650500
C	5.99522500	2.18587600	1.55686900
H	7.41860200	1.15109200	0.31219300
H	4.39048100	2.95272000	2.77715600
H	6.60101300	3.08621500	1.64397800
C	-0.13655700	-2.96222800	1.47748500
C	-1.32032900	-2.21383500	1.51903800
C	-0.17996100	-4.24799400	0.93681000
C	-2.50965300	-2.72149100	1.01326400
H	-1.29895500	-1.20524500	1.94037600
C	-1.37447900	-4.76547700	0.43755800
H	0.72195600	-4.85957700	0.90697200
C	-2.53735100	-4.00409800	0.46656200
H	-3.41306900	-2.11069400	1.03737100
H	-1.39208500	-5.77288700	0.02374400
H	-3.46825400	-4.40819600	0.07205500
C	1.69591900	0.95312100	-2.78923300
C	2.38782100	0.18098100	-3.72589200
C	2.44091200	1.62937800	-1.81242000
C	3.77547900	0.06046200	-3.66735100
H	1.84444900	-0.33688200	-4.51576500
C	3.82216600	1.49839900	-1.74069900
H	1.91964600	2.25712500	-1.08468200
C	4.49578000	0.70422100	-2.66699900
H	4.29337400	-0.54404500	-4.41099200
H	4.37491200	2.01043000	-0.95265200
H	5.57893200	0.60166800	-2.61116400
C	-3.32781400	-0.74079700	-1.79006200
C	-3.77104800	0.20945400	-0.86686500
C	-4.12957300	-1.85551300	-2.04109700
C	-4.98747700	0.05193300	-0.21226900
H	-3.14174200	1.07268300	-0.63723600
C	-5.35000000	-2.01709900	-1.39100100
H	-3.78774500	-2.60811600	-2.75419300
C	-5.78106200	-1.06371600	-0.47346800
H	-5.30541400	0.80322800	0.51120000
H	-5.96399500	-2.89211600	-1.60219500
H	-6.73415900	-1.18869500	0.03839400
H	-2.43745200	1.48077100	-3.12845600
H	-2.70746900	0.29187400	-4.40984400
H	-0.48528600	1.58769700	-4.72911200
H	-0.24679400	-0.15180000	-4.51593700
H	4.46512600	-2.74325400	2.64529100
H	3.33556200	-1.57163700	3.33163500

H	2.15410600	-3.78578600	3.20798400
H	2.55980900	-3.89802200	1.48975000

2a

C	-4.75446300	0.00870800	-0.32911000
C	-3.57883100	-0.69496600	-0.54212300
C	-2.35935800	-0.16720200	-0.10972200
C	-2.32520400	1.06969500	0.53876900
C	-3.50499700	1.77043400	0.75088400
C	-4.71741600	1.24236600	0.31685700
H	-5.70329500	-0.40259500	-0.66779400
H	-3.57943400	-1.66057400	-1.04340300
H	-1.37505200	1.47457200	0.87799300
H	-3.47922800	2.73293100	1.25809400
H	-5.64059400	1.79460200	0.48464600
C	-1.14385400	-0.96728600	-0.36776000
O	-1.11657400	-2.04794400	-0.88591800
O	0.00011200	-0.28052500	-0.00085300
C	1.14364100	-0.96724300	0.36711800
O	1.11605300	-2.04769700	0.88574800
C	2.35933200	-0.16733400	0.10952800
C	2.32563100	1.06914200	-0.53977500
C	3.57846400	-0.69477900	0.54323200
C	3.50556400	1.76979300	-0.75141000
H	1.37572100	1.47375000	-0.88002600
C	4.75424400	0.00878300	0.33065100
H	3.57870200	-1.66006200	1.04513400
C	4.71766400	1.24203200	-0.31612600
H	3.48015800	2.73195200	-1.25928100
H	5.70282700	-0.40228800	0.67031700
H	5.64096200	1.79416900	-0.48357500

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C	-3.24103500	-1.38056900	0.67711400
C	-3.74075300	0.00409400	0.27435500
H	-3.38594000	-2.09246400	-0.15505200
H	-3.81735000	-1.76542100	1.53274200
H	-3.75629500	0.67872900	1.14585900
H	-4.77228300	-0.05781200	-0.10434500
P	-2.63697500	0.85344900	-0.95637300
P	-1.41270100	-1.46101700	1.03647200
C	0.38120600	-0.86927100	-2.33822700

C	1.71923800	-0.68544500	-2.03517300
H	-0.02185900	-1.87997700	-2.22803800
C	2.08972600	1.25851600	-0.07562000
C	2.50627100	0.47747300	-2.21971200
Cu	-0.46478600	-0.06275000	-0.52946200
O	0.85966700	1.43661600	-0.09219200
C	-3.42991700	2.55451900	-1.02097200
H	-4.45579500	2.42442300	-0.63206500
C	-3.28217200	0.38202400	-2.68298700
C	-1.23409900	-1.07588000	2.86656400
H	-0.17180200	-0.80036300	2.96159400
C	-1.21141700	-3.31935300	1.28474000
C	1.84969700	1.59721900	-2.98050500
H	2.37284500	2.55433100	-2.87056900
H	1.78065700	1.38194400	-4.05944700
H	0.82594200	1.75783700	-2.60844000
C	3.97406800	0.35118200	-2.26687800
C	4.78762300	1.41056300	-2.70918300
C	4.65498000	-0.80887300	-1.84256500
C	6.17565600	1.33446000	-2.68722400
H	4.33247200	2.33215900	-3.06619400
C	6.03991600	-0.88273200	-1.80798400
H	4.08919500	-1.68977400	-1.54404700
C	6.82003100	0.19383800	-2.22482600
H	6.75733100	2.19037900	-3.02928000
H	6.51477700	-1.80239500	-1.46443000
H	7.90685700	0.13527500	-2.20305400
C	3.06063200	2.36305700	-0.07242000
C	4.39517400	2.18501400	0.30670900
C	2.63338700	3.63063600	-0.48840800
C	5.27667400	3.25932900	0.28784500
H	4.75067800	1.19619600	0.59399700
C	3.51958400	4.69796900	-0.51468900
H	1.59693500	3.75681300	-0.79835000
C	4.84497900	4.51631900	-0.12126200
H	6.31453800	3.10363400	0.57825900
H	3.17456600	5.67845900	-0.84034000
H	5.53956000	5.35476400	-0.13905200
H	2.18155500	-1.52416100	-1.50908700
H	-0.11624700	-0.23000300	-3.07300700
C	2.36584700	-0.07664200	1.87581700
O	2.59336000	0.08160100	0.55765100
O	1.75297100	0.69863700	2.57464000
C	2.95175400	-1.35011500	2.37165400

C	3.83641800	-2.10789100	1.59993600
C	2.58556700	-1.79026800	3.64592700
C	4.32562100	-3.31284500	2.09063800
H	4.13663800	-1.74221100	0.61900600
C	3.06727100	-3.00115400	4.12763400
H	1.92108100	-1.16717000	4.24374700
C	3.93072400	-3.76628800	3.34661100
H	5.01372300	-3.90352100	1.48781300
H	2.77073500	-3.34978800	5.11542000
H	4.30557900	-4.71652900	3.72376700
C	-1.45083200	-2.41395400	3.56705900
H	-1.09087400	-2.38526500	4.60627100
H	-2.52340500	-2.66601100	3.60606400
C	-0.71837400	-3.46056600	2.73128300
H	0.36548100	-3.27088900	2.78397700
H	-0.87974900	-4.48291800	3.09960800
H	-2.22954500	-3.73873600	1.22817100
C	-2.05490500	0.12277000	3.23859800
C	-1.60084400	1.38436900	2.82836800
C	-3.28406900	0.03017500	3.89334000
C	-2.37094100	2.51873800	3.05048500
H	-0.63674200	1.46954900	2.31943700
C	-4.05492600	1.17000400	4.11727900
H	-3.64930300	-0.93833100	4.23588300
C	-3.60610000	2.41442500	3.68796100
H	-2.00892200	3.48868400	2.70928600
H	-5.01209400	1.07980200	4.62979400
H	-4.21012900	3.30590300	3.85368600
C	-3.54531200	2.82074900	-2.52619000
H	-4.14656600	3.72004500	-2.72118400
H	-2.54026800	3.00731200	-2.94342800
C	-4.14908500	1.56225100	-3.13381900
H	-2.36601900	0.38257500	-3.29606800
H	-5.17774400	1.45221600	-2.75620600
H	-4.21502400	1.60575500	-4.22973100
C	-2.75981700	3.64421200	-0.23160600
C	-3.55218000	4.60069400	0.40887200
C	-1.36959800	3.74903400	-0.13297000
C	-2.97640800	5.63986900	1.13213300
H	-4.63889200	4.52206400	0.34166800
C	-0.79186900	4.77837400	0.60420200
H	-0.72750000	2.99661300	-0.59477200
C	-1.59097500	5.72832300	1.23557600
H	-3.61120300	6.37534600	1.62453600

H	0.29285800	4.82579400	0.70052900
H	-1.13408900	6.53050700	1.81301700
C	-3.87691100	-0.99405100	-2.73919100
C	-3.05648700	-2.08386000	-3.05400700
C	-5.21724300	-1.24875000	-2.42723000
C	-3.55322400	-3.38226400	-3.04562100
H	-2.01050000	-1.90651300	-3.30964800
C	-5.71493600	-2.54793100	-2.41272900
H	-5.88895100	-0.42289700	-2.19227500
C	-4.88445200	-3.62195400	-2.71717200
H	-2.89351900	-4.21000300	-3.30252700
H	-6.76189700	-2.72022100	-2.16709600
H	-5.27613600	-4.63775100	-2.71141000
C	-0.37791400	-3.93187900	0.19839700
C	1.00770200	-3.75235000	0.15283200
C	-0.99319500	-4.62914100	-0.84350900
C	1.75582700	-4.26619600	-0.89940300
H	1.51166300	-3.19251500	0.94317300
C	-0.24631500	-5.13942100	-1.90213200
H	-2.07674900	-4.76782500	-0.82394300
C	1.13241400	-4.95992300	-1.93408800
H	2.83707100	-4.12458800	-0.91245200
H	-0.74309600	-5.68777400	-2.70213900
H	1.71962300	-5.35865000	-2.75928200

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C	-3.87490400	-0.23996700	0.99669900
C	-3.27174100	-1.62409600	1.24293700
H	-4.96430100	-0.31689000	0.85327400
H	-3.71412400	0.39819700	1.87973500
H	-3.53026900	-1.96721800	2.25673700
H	-3.69905500	-2.35474400	0.53955600
P	-1.43238900	-1.70049700	0.96391300
P	-3.12131400	0.71593500	-0.41229500
C	-0.16485200	0.38861000	-2.69527700
C	1.02114300	1.08666900	-2.52173300
H	-1.02065100	0.93302300	-3.10318400
C	2.05680900	0.65614200	0.03589000
C	2.28814500	0.54034400	-2.20276000
Cu	-0.88730200	0.07864300	-0.67214500
O	0.94440000	0.14569600	0.25390100
C	-0.69639900	-1.18642900	2.62459600
C	-1.09970500	-3.53610000	1.27281400

H	-2.06987600	-3.99049200	1.53624200
C	-4.07786000	2.33811200	-0.25919800
H	-4.68610800	2.24008200	0.65515000
C	-4.12826600	0.14352900	-1.90363300
C	2.37256300	-0.96023500	-2.31657700
H	3.27843400	-1.37693700	-1.86385600
H	2.33679800	-1.28914700	-3.36883200
H	1.52130600	-1.42260000	-1.79967400
C	3.50508100	1.33074600	-2.48742700
C	4.75041600	0.70475200	-2.67376500
C	3.50186500	2.73722500	-2.54870800
C	5.91722700	1.43276700	-2.87915300
H	4.81439400	-0.38162100	-2.67348200
C	4.66364100	3.46519000	-2.76312200
H	2.57650400	3.28993600	-2.38851400
C	5.88719600	2.82188300	-2.92379400
H	6.85930400	0.90218100	-3.01701300
H	4.60916000	4.55337500	-2.78717300
H	6.79960200	3.39314500	-3.08670100
H	0.93884300	2.17773400	-2.55704900
H	-0.13026300	-0.67435100	-2.95253800
C	-0.19460700	-3.55857000	2.51780900
C	-0.67607700	-2.46352900	3.45816400
H	0.34461700	-0.93090900	2.36857300
C	-1.35484700	0.04300800	3.17535000
C	-2.40275700	0.00900400	4.09816600
C	-0.94954300	1.28861500	2.67636800
C	-3.06158700	1.18081700	4.46926800
H	-2.72068500	-0.93949400	4.53166500
C	-1.61609500	2.45480900	3.02823300
H	-0.09672500	1.31891700	1.99775500
C	-2.68665800	2.40385300	3.92094400
H	-3.87688700	1.13328400	5.19042600
H	-1.28893300	3.40832900	2.60938500
H	-3.20944000	3.31657500	4.20514500
C	-0.52902300	-4.25306800	0.08497800
C	-1.10497800	-5.43533200	-0.38033900
C	0.60029600	-3.75438700	-0.57372500
C	-0.57552500	-6.10481400	-1.48086700
H	-1.98796000	-5.83090600	0.12492600
C	1.12862500	-4.41617300	-1.67542100
H	1.06565200	-2.82938800	-0.22029200
C	0.54091900	-5.59384200	-2.13487400
H	-1.03941400	-7.02699300	-1.82928500

H	2.00617900	-4.01002700	-2.17750000
H	0.95631900	-6.11132700	-2.99811700
C	-5.01306600	2.37108100	-1.48438900
C	-5.42363400	0.94415100	-1.81552400
H	-3.55689300	0.51961100	-2.77069000
C	-4.20154300	-1.35331800	-1.99662600
C	-5.33949100	-2.08015500	-1.64224000
C	-3.05854500	-2.06020600	-2.39196700
C	-5.32334100	-3.47425200	-1.65112800
H	-6.25213400	-1.55961700	-1.35296100
C	-3.03399900	-3.44776300	-2.39015000
H	-2.16375400	-1.50420100	-2.67679800
C	-4.16939000	-4.16191800	-2.01060900
H	-6.22148200	-4.02337000	-1.37134400
H	-2.12327200	-3.97423300	-2.67459200
H	-4.15084900	-5.25100300	-2.00517800
C	-3.22568100	3.56871900	-0.14392200
C	-3.50397200	4.53206600	0.82616500
C	-2.17500300	3.80181100	-1.03689800
C	-2.75766000	5.70472100	0.90223500
H	-4.31692100	4.35589000	1.53220500
C	-1.42874300	4.97122800	-0.96682100
H	-1.93279800	3.04881500	-1.79160500
C	-1.71999600	5.92854800	0.00363100
H	-2.98870600	6.44617800	1.66557800
H	-0.60601600	5.13005500	-1.66363100
H	-1.13458100	6.84556700	0.05795200
C	2.36160300	2.07679000	0.31174900
C	3.66878300	2.53308700	0.50811200
C	1.30405900	2.99081600	0.38856100
C	3.91000100	3.87257200	0.79121000
H	4.50227100	1.83661100	0.42439900
C	1.54927900	4.32730900	0.67187000
H	0.28254100	2.64109900	0.22857400
C	2.85434100	4.77306200	0.87533100
H	4.93410900	4.21324600	0.93585900
H	0.71134200	5.02078900	0.74224100
H	3.04555900	5.82134100	1.10072800
O	3.19676700	-0.17873900	0.24971500
C	3.36459700	-0.71478200	1.47626800
O	2.60950600	-0.56229200	2.41022700
C	4.61307100	-1.51594800	1.55043300
C	5.56796500	-1.50538500	0.53142700
C	4.83031100	-2.27452900	2.70264800

C	6.72942800	-2.25672400	0.66573400
H	5.39894300	-0.89188700	-0.35156200
C	5.98764800	-3.02976500	2.82966800
H	4.07644800	-2.25163300	3.48726700
C	6.93766200	-3.02110300	1.81069900
H	7.47733400	-2.24334100	-0.12516000
H	6.15460700	-3.62420100	3.72621900
H	7.84785600	-3.61054600	1.91120300
H	-0.19546400	-4.55615000	2.97882800
H	0.84376500	-3.34315200	2.21586100
H	-1.68170600	-2.71944600	3.83136900
H	-0.02354500	-2.35107900	4.33574800
H	-5.87140300	3.03067900	-1.29689000
H	-4.46422700	2.80200300	-2.33716900
H	-6.06700700	0.55338700	-1.01088100
H	-6.00363200	0.87945100	-2.74761600

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C	-3.82015200	0.39756100	0.76980200
C	-3.45336100	1.69934600	0.06356500
H	-4.35772300	-0.26991600	0.07456700
H	-4.49683800	0.59327900	1.61610100
H	-3.08206200	2.43900000	0.79227600
H	-4.34273600	2.13471900	-0.41711200
P	-2.06083000	1.52145200	-1.15541300
P	-2.35636600	-0.61258000	1.32734000
C	-0.44636500	-1.82496800	-1.81080300
C	0.77310400	-2.30067700	-1.35782500
H	-1.33628600	-2.42789000	-1.60984300
C	2.16752000	-0.36803200	0.16586600
C	2.05990100	-1.77531200	-1.63543700
Cu	-0.77131000	-0.30734400	-0.33274900
O	1.13942200	0.31903200	0.02965300
C	-1.78215700	3.30957400	-1.63785300
H	-2.73216500	3.83224200	-1.42510800
C	-2.82613000	1.08490900	-2.84054300
C	-1.99754500	-0.05100600	3.08522700
H	-0.97752600	-0.42527700	3.27921400
C	-3.22404500	-2.19198500	1.88745600
H	-4.30193100	-1.99657200	1.76256900
C	2.10333400	-0.69749400	-2.68776800
H	3.06629300	-0.17817400	-2.72440500
H	1.89561400	-1.09800300	-3.69401300

H	1.34514300	0.07060100	-2.47176800
C	3.23277700	-2.65422000	-1.47480700
C	4.42826600	-2.41163700	-2.17802800
C	3.24378000	-3.75571300	-0.59612300
C	5.56417500	-3.19098800	-1.99055600
H	4.47042100	-1.60232800	-2.90458000
C	4.37369900	-4.54184300	-0.41750400
H	2.35702100	-3.99509100	-0.00804700
C	5.55112100	-4.26353300	-1.10488700
H	6.46681800	-2.95959400	-2.55649700
H	4.33324000	-5.37560000	0.28351400
H	6.43919400	-4.87608300	-0.95894500
H	0.70862000	-3.13704900	-0.65641600
H	-0.49151700	-1.19393000	-2.70214800
O	3.38618500	0.20226900	-0.29711700
C	2.39521900	-1.31947000	1.27276200
C	3.66671000	-1.80951000	1.58830000
C	1.30367100	-1.73772100	2.04163500
C	3.83829600	-2.68684000	2.65446400
H	4.52739200	-1.51527600	0.98822100
C	1.47545100	-2.62006400	3.09825100
H	0.31525900	-1.35485700	1.78812900
C	2.74790100	-3.09812700	3.41133100
H	4.83537900	-3.06102900	2.88154900
H	0.61526600	-2.92605100	3.69642400
H	2.88503400	-3.78688900	4.24336000
C	3.86940000	1.25072300	0.40369100
C	5.18493900	1.69520400	-0.12098600
C	5.69787200	2.90533300	0.35135300
C	5.91885000	0.93416400	-1.03436400
C	6.92600500	3.36473500	-0.10328600
H	5.11662800	3.46758000	1.08046700
C	7.15455900	1.39175200	-1.47610000
H	5.52639000	-0.02161300	-1.37971600
C	7.65462500	2.60757800	-1.01778000
H	7.32086200	4.31225300	0.25939900
H	7.73133200	0.79519900	-2.18089700
H	8.62031000	2.96586400	-1.37175200
O	3.30437100	1.76059400	1.34380200
C	-1.64723600	3.22381500	-3.16236300
H	-1.62327900	4.22699600	-3.61045200
H	-0.69314400	2.73209300	-3.41985700
C	-2.82899200	2.39190100	-3.64320700
H	-3.75238000	2.96088200	-3.45391400

H	-2.79718000	2.18817600	-4.72229900
H	-2.07018200	0.41746900	-3.28501900
C	-2.93445100	-2.28179000	3.39354400
C	-2.96187600	-0.86035200	3.94802400
H	-2.68480900	-0.81945600	5.01113800
H	-3.98604900	-0.46040100	3.86823200
H	-3.65716900	-2.94357100	3.88966100
H	-1.93791300	-2.71994000	3.56405000
C	-0.67307600	4.03499200	-0.93084600
C	-0.88868200	5.35034600	-0.51054800
C	0.57866000	3.45232500	-0.70685300
C	0.12103500	6.07936900	0.10807400
H	-1.86713100	5.80691800	-0.67117600
C	1.58891100	4.18007400	-0.08467400
H	0.76195000	2.41083800	-0.98028600
C	1.36545100	5.49413000	0.31998500
H	-0.06702200	7.10350100	0.42826800
H	2.54956300	3.70630400	0.10861800
H	2.15900800	6.05581300	0.81071900
C	-4.11074300	0.31836000	-2.73079000
C	-4.07806500	-1.08100200	-2.69588100
C	-5.35262200	0.94955100	-2.60076400
C	-5.24349800	-1.82277500	-2.53661200
H	-3.11996900	-1.59387400	-2.80016600
C	-6.51910600	0.20968600	-2.43529300
H	-5.41667000	2.03751500	-2.63035300
C	-6.47100400	-1.18043700	-2.40090900
H	-5.18785100	-2.91066400	-2.52695300
H	-7.47384800	0.72466900	-2.33822700
H	-7.38549100	-1.75863800	-2.28016900
C	-2.84831100	-3.36548900	1.03016600
C	-3.75147400	-3.84234100	0.07820500
C	-1.57939500	-3.95058300	1.09311900
C	-3.40262900	-4.87529700	-0.78759400
H	-4.74249900	-3.38799400	0.01322800
C	-1.23001500	-4.98641800	0.23472700
H	-0.83809300	-3.58072800	1.80387200
C	-2.13946700	-5.45227500	-0.71184100
H	-4.12468400	-5.23640000	-1.51962500
H	-0.23505600	-5.42673800	0.30209700
H	-1.86264300	-6.26058400	-1.38607700
C	-1.96802300	1.44558000	3.17364100
C	-3.01838500	2.19126700	3.71104200
C	-0.87081800	2.12377800	2.62266100

C	-2.98394800	3.58439100	3.68524300
H	-3.87333500	1.68598600	4.16068300
C	-0.83947700	3.51203000	2.59378500
H	-0.03800800	1.55915800	2.19120500
C	-1.90045200	4.24749300	3.11984100
H	-3.81102000	4.15044600	4.11212300
H	0.01602600	4.01892300	2.14785600
H	-1.87484300	5.33610800	3.09078100

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C	-3.04071300	2.35745600	0.33592300
C	-3.70109100	1.11750600	0.93248300
H	-3.80480300	3.03759100	-0.07272300
H	-2.50550500	2.91603500	1.11895100
H	-4.18823400	1.37094100	1.88648200
H	-4.49034400	0.75049700	0.25937900
P	-2.55434600	-0.33161000	1.14757700
P	-1.74538500	2.02098700	-0.95509200
C	-0.28044400	-1.12550800	-2.31999600
C	1.07884300	-1.35021600	-2.18698900
H	-0.58955500	-0.34107100	-3.01521800
C	1.83608100	-1.30593000	0.46944500
C	1.71416500	-2.42570600	-1.52157300
Cu	-0.73777400	-0.05020100	-0.49224800
O	0.66240200	-0.96218000	0.70219500
C	-1.82448500	-0.09160900	2.87454300
C	-3.78749800	-1.63686500	1.73863100
H	-4.76517300	-1.13035300	1.80985400
C	-1.20701800	3.79281200	-1.32117400
H	-1.90236300	4.43401600	-0.75363100
C	-2.73375400	1.88169200	-2.56844700
C	0.80297200	-3.54749100	-1.10097900
H	1.25482100	-4.22269900	-0.36585200
H	0.48288800	-4.15663300	-1.96296000
H	-0.10067800	-3.13350300	-0.63472400
C	3.10822700	-2.76227500	-1.87588300
C	3.69017000	-3.97652600	-1.46879400
C	3.93995200	-1.89876100	-2.61636700
C	5.01691400	-4.28877900	-1.74630600
H	3.10383600	-4.69503700	-0.89957600
C	5.26706200	-2.20191600	-2.88344300
H	3.54595600	-0.95969000	-3.00172000
C	5.82442600	-3.40158600	-2.44597100

H	5.42068800	-5.23931400	-1.39803800
H	5.87008700	-1.49423600	-3.45385500
H	6.86434800	-3.64245100	-2.66004100
C	2.50289800	-2.37096900	1.24483500
C	3.88728100	-2.56893700	1.21479000
C	1.71262000	-3.22009300	2.02970600
C	4.46511400	-3.59639400	1.95175600
H	4.51538200	-1.92304400	0.60199800
C	2.29154100	-4.25172400	2.75405800
H	0.63690200	-3.05064800	2.06067400
C	3.67199100	-4.44418100	2.71678200
H	5.54392400	-3.74003800	1.91319500
H	1.66529800	-4.90429300	3.36086300
H	4.12714000	-5.25226500	3.28750900
H	1.71996300	-0.55045200	-2.56624200
H	-0.98986700	-1.94906300	-2.19737400
C	3.23088200	0.54528100	0.91789100
O	2.75562200	-0.31791800	-0.01148200
O	2.77247300	0.66711300	2.03022500
C	4.40962700	1.30473900	0.43205400
C	5.04848600	0.99072900	-0.76795800
C	4.89360400	2.34308500	1.23044000
C	6.15701500	1.72373500	-1.17566900
H	4.67514000	0.16317200	-1.36547700
C	5.99829900	3.07634400	0.81866800
H	4.38239900	2.56068700	2.16675800
C	6.62772000	2.77058900	-0.38723700
H	6.65804600	1.47251800	-2.10950200
H	6.37343800	3.88875900	1.43922500
H	7.49528000	3.34583600	-0.70745900
C	-3.32147100	-1.98902900	3.16252900
C	-2.85090300	-0.70166500	3.82427600
H	-0.93356900	-0.74167100	2.86023100
C	-1.36461200	1.32215600	3.08261000
C	-2.13760500	2.29719500	3.71690100
C	-0.13115900	1.69550600	2.53466000
C	-1.70233300	3.62152500	3.76741300
H	-3.08846700	2.02977700	4.17930000
C	0.29910600	3.01489500	2.57620600
H	0.50239700	0.93175600	2.08389200
C	-0.49346900	3.98800900	3.18316900
H	-2.31584300	4.36988700	4.26806800
H	1.26031400	3.27698000	2.13094300
H	-0.15963300	5.02493000	3.21222000

C	-3.92176200	-2.82454200	0.83029100
C	-5.17866600	-3.34779800	0.52416500
C	-2.79114500	-3.44523500	0.29173900
C	-5.30672500	-4.45751000	-0.30723100
H	-6.06916400	-2.86944200	0.93633100
C	-2.91287600	-4.54635400	-0.54687800
H	-1.80159500	-3.04424300	0.52575100
C	-4.17398500	-5.05551200	-0.85132200
H	-6.29603000	-4.85223900	-0.53514700
H	-2.01793100	-5.00646100	-0.96491000
H	-4.27127600	-5.91742100	-1.50928900
C	-1.51193700	3.97851800	-2.81447600
C	-2.85528800	3.31505600	-3.08039000
H	-2.05007800	1.34303800	-3.24611800
C	-3.97793100	1.05629400	-2.40890800
C	-5.24497900	1.61523300	-2.22528300
C	-3.85911900	-0.33887400	-2.36586200
C	-6.35079400	0.80526800	-1.97123000
H	-5.37920400	2.69560900	-2.27416800
C	-4.95706100	-1.14867800	-2.10976000
H	-2.87947000	-0.79479700	-2.51173400
C	-6.20990200	-0.57676500	-1.89921100
H	-7.32883400	1.26291900	-1.82767900
H	-4.83016400	-2.22985900	-2.06323500
H	-7.07181500	-1.20926500	-1.69015200
C	0.19414400	4.13874900	-0.91641600
C	0.42920600	5.25539200	-0.11355200
C	1.28774700	3.38420000	-1.35335800
C	1.72380600	5.62012400	0.24409600
H	-0.41930700	5.84700700	0.23421600
C	2.58248000	3.75055700	-1.00674200
H	1.11952200	2.50019900	-1.97408400
C	2.80398500	4.86897200	-0.20418100
H	1.88681600	6.49517800	0.87206300
H	3.42805600	3.15983300	-1.35742800
H	3.82112900	5.14761600	0.06728600
H	-4.12462600	-2.49230100	3.71911300
H	-2.48233600	-2.70163400	3.10013300
H	-3.71323200	-0.02875500	3.95825000
H	-2.42125100	-0.87249800	4.82179700
H	-3.63621600	3.86208700	-2.52810800
H	-3.13911100	3.33789600	-4.14224900
H	-1.50030100	5.04416900	-3.08193200
H	-0.72619100	3.49035900	-3.41430400

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C	2.70351900	-1.94828900	0.86408000
C	1.56966200	-2.97963400	0.84393500
H	3.34165100	-2.07587700	-0.01864800
H	3.33365400	-2.10403700	1.74779900
H	1.08578100	-3.02889000	1.82648400
H	1.97827100	-3.97457800	0.63317500
P	0.19768700	-2.57113600	-0.33813000
P	2.13214300	-0.18186800	0.79059400
C	0.18550500	0.53501800	-2.58078900
C	-0.51208400	1.72542800	-2.39802800
H	1.25914500	0.64003400	-2.72501400
C	-1.96528900	1.75026900	0.00653800
C	-1.88539800	2.03950100	-2.37238700
Cu	0.22060000	-0.18121800	-0.52882700
O	-1.59201700	0.58128500	0.15415000
C	-1.01740100	-3.93537900	0.07047600
H	-0.43705700	-4.69439000	0.61333500
C	0.67009100	-3.33678500	-1.99938000
C	1.87691300	0.35028700	2.57215100
H	1.17475100	1.18632700	2.50903100
C	3.77725000	0.69847000	0.61846900
C	-2.20912700	3.51192500	-2.52804000
C	-3.36534400	2.18865400	0.16145700
C	-3.69898100	3.51666300	0.44569300
C	-4.38621200	1.24329000	0.01419500
C	-5.03147800	3.88651700	0.59606000
H	-2.91595800	4.25998500	0.54765200
C	-5.71489800	1.61811900	0.15720500
H	-4.12982400	0.22231100	-0.24036000
C	-6.04230400	2.93969600	0.45367400
H	-5.27821100	4.91932500	0.82347700
H	-6.49560800	0.87505000	0.02581600
H	-7.08213600	3.23126300	0.56932000
H	0.12715700	2.57974400	-2.16300700
H	-0.27751000	-0.29752500	-3.10781900
C	-0.55433700	2.90820700	1.50280500
O	-1.00527800	2.78193500	0.23884300
O	-1.01851900	2.32274500	2.45350000
C	0.60309100	3.84319500	1.59394600
C	1.14801500	4.46633600	0.47000600
C	1.16884700	4.05526300	2.85421000

C	2.27063000	5.27678900	0.60283600
H	0.69672800	4.30461000	-0.50296300
C	2.28485000	4.87227200	2.98512100
H	0.72480000	3.56401400	3.71407700
C	2.84032300	5.47727500	1.85798100
H	2.70607200	5.74267100	-0.27534400
H	2.72776900	5.03224100	3.96328300
H	3.72014500	6.10584400	1.95829500
H	-1.41357400	4.12546300	-2.09118100
H	-2.30620500	3.80454500	-3.58346300
H	-3.14386700	3.78992200	-2.02793100
C	-2.93547900	1.07362500	-2.74594300
C	-4.16374400	1.51749000	-3.27090400
C	-2.82323400	-0.31153100	-2.50363300
C	-5.20896500	0.64082200	-3.53829400
H	-4.31471700	2.57329600	-3.46660100
C	-3.87376600	-1.18587300	-2.75800500
H	-1.92743300	-0.70500800	-2.04336900
C	-5.07607700	-0.72057100	-3.28268100
H	-6.13875000	1.03094900	-3.94387400
H	-3.75317100	-2.24192200	-2.52805800
H	-5.89361500	-1.40604700	-3.48620600
C	-1.36075200	-4.54102500	-1.30505400
H	-1.89135100	-5.49189300	-1.18693300
H	-2.02508900	-3.86272800	-1.85697200
C	-0.03144000	-4.70338000	-2.04744700
H	0.56413300	-5.46873100	-1.53489500
H	-0.16786400	-5.03709600	-3.08158400
H	0.17613100	-2.68487000	-2.73018700
C	-2.20118700	-3.56113600	0.93141500
C	-2.67418000	-4.48899100	1.86465400
C	-2.84487400	-2.32537000	0.83061400
C	-3.76458800	-4.19668300	2.67795400
H	-2.17443500	-5.45056200	1.96128100
C	-3.93039200	-2.02709400	1.65055000
H	-2.47658300	-1.56668300	0.14713600
C	-4.39614400	-2.95981000	2.57354400
H	-4.11326600	-4.93040300	3.39914300
H	-4.39981700	-1.05089900	1.58119700
H	-5.23863800	-2.71913800	3.21528900
C	2.15613600	-3.26212600	-2.24667500
C	3.04634900	-4.26228200	-1.84478000
C	2.68570300	-2.09156700	-2.80273800
C	4.42263900	-4.08211300	-1.96634700

H	2.67202700	-5.18974800	-1.42116300
C	4.05818500	-1.90379700	-2.91900500
H	2.00831700	-1.31193500	-3.13426300
C	4.93491500	-2.89869500	-2.49158200
H	5.09691900	-4.87061100	-1.64433500
H	4.43827700	-0.97569900	-3.33501200
H	6.00816000	-2.75768400	-2.57910300
C	3.23208800	0.90915700	3.02591000
H	3.11527100	1.56134700	3.89852000
H	3.91845200	0.10135500	3.31018300
C	3.81664900	1.66035600	1.82531800
H	3.21002300	2.54681600	1.60662500
H	4.83964200	2.00679100	2.00780200
H	4.55030100	-0.06597800	0.77232600
C	1.20183600	-0.74512600	3.36013400
C	1.90558600	-1.64758600	4.16010100
C	-0.17725300	-0.93233900	3.18827300
C	1.25490300	-2.72824300	4.75415800
H	2.97208100	-1.51974200	4.32186400
C	-0.82544300	-2.01211300	3.77756400
H	-0.74195500	-0.23488800	2.57374700
C	-0.10902600	-2.92022100	4.55571900
H	1.82080500	-3.42138100	5.37047300
H	-1.89045300	-2.14930200	3.61889000
H	-0.61543200	-3.76793500	5.00793100
C	4.01194500	1.35205000	-0.72058700
C	5.21391600	1.15647300	-1.40257700
C	3.04432300	2.17813100	-1.29907900
C	5.44602000	1.77035000	-2.63204000
H	5.97433000	0.50957400	-0.97103000
C	3.26932800	2.79146300	-2.52581400
H	2.09358000	2.31724700	-0.79352700
C	4.47305100	2.58850100	-3.19873400
H	6.38814400	1.60581500	-3.14733800
H	2.49646600	3.41721100	-2.96398800
H	4.64799500	3.06210000	-4.16009400

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C	2.06210600	2.88132500	0.84297700
C	0.64208700	3.07184700	1.37816900
H	2.53258600	3.86068500	0.65631600
H	2.68080900	2.37239600	1.60004200
H	0.70580300	3.43123500	2.41807700

H	0.12872400	3.85969000	0.80547200
P	-0.50043600	1.58746200	1.26501200
P	2.28064200	1.82699800	-0.66312800
C	0.94695500	-0.78241100	-2.93817400
C	0.74283900	-2.13260000	-2.67087200
H	1.91442000	-0.50152800	-3.36434100
C	-0.21631700	-2.61170400	-0.07084800
C	-0.43560900	-2.84825800	-2.35702000
Cu	1.16703500	-0.09835000	-0.92540300
O	0.09919800	-1.41820300	0.09645100
C	-0.06173600	0.61237900	2.84675100
C	-2.02534100	2.36815900	2.09384100
H	-1.71998400	3.36667100	2.45060200
C	4.14875100	1.89004800	-0.88558400
H	4.51345800	2.61198500	-0.13545300
C	1.94350300	2.94366200	-2.14018500
C	-0.34944200	-4.34223800	-2.55778100
H	1.65749800	-2.73919900	-2.61731300
H	0.11121700	-0.15985000	-3.26936600
C	-2.28631600	1.48663200	3.32306100
C	-0.93540900	1.19979500	3.95223900
H	-0.43506400	-0.39734300	2.61916000
C	1.41057500	0.50412800	3.10810300
C	2.10835700	1.38907100	3.93513600
C	2.13531500	-0.50925600	2.46558800
C	3.49112700	1.28977300	4.08331900
H	1.57343800	2.17131900	4.47383700
C	3.51427300	-0.60328000	2.60113700
H	1.58715600	-1.22811300	1.85549600
C	4.20174600	0.30437400	3.40618500
H	4.01345600	1.98858600	4.73604200
H	4.05332200	-1.39939900	2.08478800
H	5.28293300	0.22817400	3.51918000
C	-3.21940500	2.52575500	1.19882400
C	-3.81780400	1.42250900	0.58051600
C	-3.78308400	3.78686400	0.99160300
C	-4.95416500	1.57864500	-0.20638300
H	-3.39405600	0.42271200	0.71406400
C	-4.91271900	3.94910700	0.19487100
H	-3.32292700	4.65609400	1.46537000
C	-5.50525300	2.84269800	-0.40564200
H	-5.40495700	0.69930900	-0.66861000
H	-5.33459500	4.94324400	0.04897100
H	-6.39397100	2.96259200	-1.02330500

C	4.33966600	2.51433600	-2.27839300
C	3.28796500	3.60535700	-2.43386900
H	1.73550200	2.23129000	-2.95675700
C	0.72589800	3.79993400	-1.94496400
C	0.79735500	5.16528300	-1.66606600
C	-0.53718000	3.19373600	-1.99254700
C	-0.36168900	5.90333700	-1.43045700
H	1.76406700	5.66757100	-1.63456600
C	-1.69236900	3.92326700	-1.74591500
H	-0.60848200	2.12382600	-2.20449800
C	-1.60637600	5.28557200	-1.46271400
H	-0.28579500	6.96934800	-1.22024900
H	-2.66390600	3.42896700	-1.76071600
H	-2.51086400	5.86155900	-1.27227000
C	4.85079000	0.57890200	-0.67069900
C	5.88764200	0.47801100	0.25754500
C	4.48878200	-0.56729500	-1.38648200
C	6.54188400	-0.73171200	0.47434800
H	6.17838700	1.36153400	0.82797200
C	5.13637800	-1.77832000	-1.17256200
H	3.67279300	-0.51802800	-2.10992100
C	6.16627200	-1.86591200	-0.23764100
H	7.34505700	-0.78756800	1.20805300
H	4.83104800	-2.65796400	-1.73977500
H	6.67395200	-2.81467700	-0.06930100
C	0.71609200	-3.72377400	0.18987000
C	0.27008500	-5.01026200	0.50507100
C	2.09349800	-3.47602500	0.13246300
C	1.18311700	-6.03304900	0.73325800
H	-0.79837300	-5.20440900	0.57058800
C	3.00171800	-4.49999200	0.36016800
H	2.44877300	-2.46784900	-0.08894000
C	2.54990500	-5.78525000	0.65576200
H	0.82288600	-7.03087800	0.97854100
H	4.07046700	-4.28829100	0.31991000
H	3.26354600	-6.58775200	0.83522100
O	-1.57991500	-2.92671200	0.16268800
C	-2.07546600	-2.53353500	1.36479600
O	-1.38942300	-2.37797700	2.34986500
C	-3.53949700	-2.31593700	1.33235300
C	-4.28026500	-2.42054500	0.15325900
C	-4.16678500	-1.93247100	2.52259100
C	-5.64060700	-2.13343400	0.16773600
H	-3.78598200	-2.71579400	-0.77001700

C	-5.52294400	-1.64017800	2.52962400
H	-3.56542600	-1.86422800	3.42799700
C	-6.25994900	-1.73833200	1.35035400
H	-6.21299800	-2.20860800	-0.75624400
H	-6.00914600	-1.33300400	3.45377400
H	-7.32326400	-1.50273000	1.35505800
C	-1.75875900	-2.22941700	-2.59823700
C	-2.79489000	-2.95958400	-3.20630200
C	-2.05396000	-0.90049200	-2.23572100
C	-4.03071300	-2.38412800	-3.48788600
H	-2.63101700	-3.99762400	-3.48846000
C	-3.28377900	-0.32451500	-2.52192000
H	-1.32624700	-0.31844400	-1.67258600
C	-4.28160400	-1.05570400	-3.16134700
H	-4.79925300	-2.98229300	-3.97729700
H	-3.46773800	0.70733400	-2.22239400
H	-5.24346300	-0.59725500	-3.39063600
H	-1.09577900	-4.88105000	-1.95521000
H	-0.51504500	-4.62904200	-3.60884900
H	0.63975100	-4.72401600	-2.27287300
H	-2.98929000	1.97608600	4.01242300
H	-2.75673700	0.54052200	3.00392700
H	-0.51327600	2.14514600	4.33132600
H	-1.00233400	0.51163700	4.80749100
H	5.36488600	2.89061700	-2.39667500
H	4.19218900	1.74187300	-3.05122700
H	3.30048000	4.06709500	-3.43139500
H	3.49389100	4.40685900	-1.70588500

TS3_b3

C	-3.39280200	1.41165500	0.97461100
C	-2.53010500	2.60962000	0.59313400
H	-4.19534500	1.27230400	0.23390100
H	-3.87907800	1.58599800	1.94683900
H	-1.93650200	2.94492400	1.45962500
H	-3.16913600	3.45469900	0.29190200
P	-1.26337700	2.25976700	-0.72244100
P	-2.49435000	-0.21684000	1.01183100
C	-0.10789100	-0.85484100	-2.38206200
C	0.49443700	-2.02162900	-1.93507500
H	-1.12796200	-0.95388700	-2.76409100
C	1.75841200	-1.68013200	0.58224400
C	1.84198500	-2.34472400	-1.62075500

Cu	-0.63623200	-0.02878200	-0.48423400
O	1.02311900	-0.66959000	0.57768600
C	-0.45470500	3.95820100	-0.84734500
H	-1.13611000	4.65213300	-0.32616900
C	-2.17601400	2.46360300	-2.37821500
C	-1.86499800	-0.36680500	2.79113900
H	-1.03347900	-1.08670200	2.70997500
C	-3.96414500	-1.35984500	1.32316700
C	2.10379400	-3.84029400	-1.62923100
H	-0.20523700	-2.84550000	-1.74368000
H	0.48687600	-0.05390700	-2.83005000
O	3.10954600	-1.30165900	0.81856700
C	1.28378500	-2.96612400	1.16347100
C	-0.09148900	-3.22046100	1.07926100
C	2.09514100	-3.91788200	1.78390800
C	-0.63574500	-4.41037300	1.53783000
H	-0.72187400	-2.46031600	0.61940000
C	1.54539200	-5.10419300	2.26364400
H	3.16303400	-3.75188300	1.86888800
C	0.18710800	-5.36565800	2.13265400
H	-1.70462100	-4.59683800	1.42210100
H	2.19703200	-5.83557300	2.73932200
H	-0.23075100	-6.30345400	2.49522800
C	4.28016200	-1.87643800	0.47771100
C	5.37222700	-0.87045900	0.45578400
C	5.16561300	0.46558400	0.80314300
C	6.63845500	-1.29691800	0.05219800
C	6.22405400	1.36420700	0.74819300
H	4.17073500	0.78957300	1.10461200
C	7.69205400	-0.39480400	-0.00875600
H	6.77087800	-2.34278700	-0.21789600
C	7.48473400	0.93766500	0.33873300
H	6.06458500	2.40624200	1.02544300
H	8.67669800	-0.72935500	-0.33086800
H	8.30993700	1.64701200	0.29171200
O	4.45764700	-3.05254800	0.25294800
H	3.01899200	-4.10772300	-1.09090000
H	1.27485500	-4.38163500	-1.15257300
H	2.18832900	-4.22946500	-2.65770500
C	2.93089300	-1.47367200	-2.12049400
C	4.07483400	-2.02040000	-2.72693000
C	2.88883300	-0.07201100	-1.99948400
C	5.10213800	-1.21769700	-3.20785400
H	4.16852000	-3.10053400	-2.81792700

C	3.91083500	0.73124200	-2.49187800
H	2.06409300	0.38446800	-1.45411500
C	5.02560700	0.16752100	-3.10423100
H	5.97150400	-1.68348800	-3.67159800
H	3.83619700	1.81559700	-2.39058500
H	5.82730900	0.79843900	-3.48497900
C	-0.52823900	4.27851100	-2.34487000
H	-0.28030300	5.33245200	-2.53151700
H	0.21071500	3.67234000	-2.89495500
C	-1.93698700	3.91579400	-2.79433100
H	-2.65009200	4.58801200	-2.29127400
H	-2.08421600	4.04666700	-3.87544000
H	-1.60190500	1.81534500	-3.06048400
C	0.90146900	4.06015500	-0.21831000
C	1.13882800	4.99695100	0.78893400
C	1.95343000	3.23401100	-0.62349700
C	2.39590100	5.11610200	1.37461700
H	0.32051800	5.63685800	1.12389500
C	3.21057800	3.35061300	-0.04379100
H	1.78571700	2.48526700	-1.40161600
C	3.43648400	4.29229600	0.95836300
H	2.56032100	5.85500400	2.15805600
H	4.01647300	2.69688100	-0.37705300
H	4.42294500	4.38466100	1.41149500
C	-3.58608300	1.95291800	-2.31912200
C	-3.82260300	0.58722300	-2.51795600
C	-4.67279100	2.76531600	-1.98276700
C	-5.08733100	0.03931400	-2.34608900
H	-2.98987600	-0.05606200	-2.80340600
C	-5.94420100	2.22185000	-1.81410800
H	-4.53186900	3.83673800	-1.84138300
C	-6.15433100	0.85603400	-1.97913200
H	-5.23823300	-1.02966600	-2.49334400
H	-6.77544000	2.87340700	-1.54781900
H	-7.14554100	0.42755700	-1.83564000
C	-3.00267700	-1.03955300	3.55921200
H	-2.64266300	-1.46968900	4.50429000
H	-3.78784800	-0.31019700	3.81603800
C	-3.59882100	-2.08574800	2.62739500
H	-4.48313500	-2.58224600	3.05185800
H	-2.85480500	-2.87241600	2.42128200
H	-4.80737000	-0.68473500	1.55097800
C	-1.31614500	0.93904100	3.29201100
C	-2.05392000	1.82205700	4.08407100

C	-0.03527700	1.32709400	2.87525000
C	-1.53759600	3.07057300	4.42756000
H	-3.04367700	1.54272900	4.44471700
C	0.47640800	2.57381600	3.21109000
H	0.55211400	0.64468700	2.25806600
C	-0.27745200	3.45605300	3.98325200
H	-2.12901900	3.74331100	5.04758300
H	1.46871800	2.85941300	2.86221000
H	0.12298600	4.43517100	4.24479000
C	-4.38544800	-2.26340100	0.19856400
C	-5.74636400	-2.46990500	-0.04205200
C	-3.46189400	-2.94050900	-0.60196400
C	-6.17529700	-3.32274900	-1.05420100
H	-6.47964800	-1.94342000	0.57170900
C	-3.88415400	-3.79006700	-1.61873600
H	-2.39532500	-2.78639900	-0.44051200
C	-5.24376000	-3.98329500	-1.85028000
H	-7.24122300	-3.46769800	-1.22474300
H	-3.14439600	-4.30102800	-2.23380600
H	-5.57524700	-4.64673700	-2.64724200

TS3_b4

C	1.62871800	-3.07322400	0.71299700
C	2.67302700	-2.09733800	1.24292100
H	2.10112900	-4.03534800	0.45905200
H	0.87139000	-3.27773000	1.48857800
H	2.96158000	-2.37389200	2.26876700
H	3.58739900	-2.14043900	0.62898900
P	2.17291900	-0.31001000	1.17159500
P	0.62998700	-2.47132000	-0.73703400
C	0.72377800	1.00508600	-2.38730200
C	-0.53747500	1.57922100	-2.45038400
H	0.90304700	0.15788800	-3.05554600
C	-1.73349100	1.81791500	0.02819900
C	-1.06422400	2.79120900	-1.93585400
Cu	0.47740200	-0.13608600	-0.57715400
O	-0.74678800	1.18329100	0.43824000
C	1.24129000	0.04669900	2.78230000
C	3.77082700	0.47136700	1.80527200
H	4.33492400	-0.34742100	2.28550000
C	-0.46177200	-3.99203700	-0.98528300
H	0.04457900	-4.78955900	-0.41524400
C	1.67621800	-2.86867100	-2.27281900

C	-2.34007200	3.23767900	-2.61011600
C	-2.19598900	3.05716400	0.68457200
C	-3.45778900	3.61341500	0.44669200
C	-1.32297900	3.70739400	1.56469600
C	-3.82353800	4.80994400	1.05139700
H	-4.15889100	3.10132300	-0.21143900
C	-1.68777100	4.90620800	2.15906600
H	-0.35320300	3.25653900	1.76633500
C	-2.93663400	5.46561200	1.89984000
H	-4.80969000	5.23052000	0.86055400
H	-0.99378900	5.40628400	2.83297400
H	-3.22262200	6.40639100	2.36776700
H	-1.29893100	0.94623100	-2.92354100
H	1.60611800	1.61082200	-2.16330200
C	-3.65224700	0.45662100	0.23305700
O	-2.79819700	1.09184200	-0.59963400
O	-3.43898400	0.25425200	1.40566000
C	-4.91684700	0.07868800	-0.44809900
C	-5.11646000	0.25272800	-1.81855700
C	-5.92872100	-0.47533200	0.33946600
C	-6.31721200	-0.14213200	-2.39833400
H	-4.32256500	0.68285800	-2.42546800
C	-7.12939400	-0.86065200	-0.23972500
H	-5.74053200	-0.60527300	1.40364200
C	-7.32232400	-0.69855700	-1.61085700
H	-6.47066500	-0.01330100	-3.46832100
H	-7.91768000	-1.29142200	0.37538100
H	-8.26209900	-1.00531200	-2.06762300
C	3.27657900	1.40190200	2.92196100
C	2.29182200	0.58772700	3.75133500
H	0.57313300	0.87327600	2.49234900
C	0.38619600	-1.11610100	3.19664300
C	0.84267200	-2.14212200	4.02906700
C	-0.89726500	-1.22583400	2.64622500
C	0.05135500	-3.26309800	4.27442800
H	1.82668600	-2.07495700	4.49449000
C	-1.68207900	-2.34749000	2.87959500
H	-1.29091800	-0.41678300	2.03175200
C	-1.20535100	-3.37853500	3.68720400
H	0.42398600	-4.05113100	4.92812500
H	-2.66908100	-2.41004300	2.41990800
H	-1.81864700	-4.26122800	3.86849500
C	4.65178900	1.11377600	0.77497500
C	6.02329800	0.85462400	0.75170400

C	4.13080500	2.00753200	-0.16213100
C	6.85087900	1.47533700	-0.18061500
H	6.44594900	0.15133100	1.47125500
C	4.94904500	2.63276900	-1.09430300
H	3.06056000	2.20318900	-0.17031000
C	6.31728200	2.36701400	-1.10698700
H	7.91865900	1.25953800	-0.18297800
H	4.50881700	3.32946300	-1.80767400
H	6.96448000	2.85333900	-1.83505600
C	-0.28643300	-4.32275000	-2.47129200
C	1.20578000	-4.24302700	-2.75168300
H	1.33017500	-2.12353800	-3.00766600
C	3.14753300	-2.65880200	-2.05716800
C	4.00626000	-3.68410500	-1.65070500
C	3.67980200	-1.37241800	-2.20743900
C	5.35033000	-3.42689800	-1.38968300
H	3.63086200	-4.70049100	-1.53405300
C	5.01900600	-1.11219100	-1.94738800
H	3.02389100	-0.55910900	-2.52267900
C	5.86031700	-2.14080800	-1.52995600
H	6.00094200	-4.24206400	-1.07543600
H	5.40600300	-0.09957300	-2.06067000
H	6.90931100	-1.93600500	-1.31932800
C	-1.87682700	-3.91035500	-0.50364600
C	-2.30167600	-4.74428500	0.53305600
C	-2.81210400	-3.06233300	-1.10385000
C	-3.62781500	-4.74889500	0.95427200
H	-1.57524700	-5.39619700	1.02185100
C	-4.14367800	-3.08962100	-0.70802300
H	-2.49874300	-2.38011700	-1.89873700
C	-4.55617700	-3.92691400	0.32581800
H	-3.93474700	-5.40345300	1.76943000
H	-4.86882500	-2.45625400	-1.21398100
H	-5.60077400	-3.92985800	0.63483300
C	-0.19596000	3.86996600	-1.42412100
C	0.94813400	3.61174200	-0.64650800
C	-0.52949200	5.22176400	-1.61876800
C	1.72181000	4.63842600	-0.11853700
H	1.17568900	2.57935000	-0.38758200
C	0.24352600	6.24938800	-1.09232000
H	-1.41538100	5.48218600	-2.19449000
C	1.38104500	5.96844800	-0.34323800
H	2.59906400	4.39360600	0.48339700
H	-0.04940700	7.28339300	-1.27250900

H	1.98939300	6.77350100	0.06612300
H	-2.94962500	3.88902500	-1.96836400
H	-2.13768000	3.80247900	-3.53484600
H	-2.95734700	2.37519600	-2.88926200
H	4.11976000	1.78771900	3.51198100
H	2.76598000	2.27458200	2.47634800
H	2.83827900	-0.23545000	4.23917300
H	1.82311400	1.17725300	4.55150300
H	-0.71202200	-5.30942800	-2.70058000
H	-0.82859600	-3.58769100	-3.08866100
H	1.71043300	-5.04584100	-2.19221100
H	1.44991600	-4.39407200	-3.81246300

Table S5. Electronic energies (E_{elec}), Gibbs free energies (G_{298}), thermal correction to Gibbs free energy ($cor\ G_{gas}$), solvation energies (Esol), solvation free energies (G_{sol}) in THF (ε = 7.43) for all stationary points of the process. Calculations were carried out at M06/6-311+G(d,p)/SDD/SMD(THF)//wB97X-D/6-31G(d)/LANL2DZ level.

species	E_{elec} (a.u.)	G_{298} (a.u.)	$cor\ G_{gas}$ (a.u.)	E_{sol} (a.u.)	G_{sol} (a.u.)
Int2_a	-2583.326481	-2582.600810	0.725670	-2584.240506	-2583.514836
Int2_b	-2583.323425	-2582.598003	0.725422	-2584.239526	-2583.514104
2a	-764.952140	-764.785723	0.166417	-764.906043	-764.739626
TS3_a1	-3348.296327	-3347.375347	0.920980	-3349.154447	-3348.233467
TS3_a2	-3348.287638	-3347.367148	0.920490	-3349.142702	-3348.222212
TS3_a3	-3348.290710	-3347.371942	0.918767	-3349.148259	-3348.229492
TS3_a4	-3348.288116	-3347.368064	0.920051	-3349.145852	-3348.225801
TS3_b1	-3348.297015	-3347.374428	0.922588	-3349.151989	-3348.229401
TS3_b2	-3348.286553	-3347.364032	0.922520	-3349.137043	-3348.214523
TS3_b3	-3348.277209	-3347.354194	0.923016	-3349.129133	-3348.206117
TS3_b4	-3348.283399	-3347.362618	0.920781	-3349.142055	-3348.221274

Cartesian coordinates for the optimized structures in Table S5

Int2_a

C	-1.01175500	0.99886700	1.93464200
C	0.21264000	1.89769700	1.69823300
Cu	-0.06603800	0.31551300	-1.32627100
C	-0.31411100	3.64918700	-0.64388100
H	-0.31328400	3.57966800	-1.73921400
C	2.27038000	3.08014700	0.06491700
H	2.40349700	3.26412900	1.13894600

C	-2.80179600	-1.15673600	1.18365300
H	-3.10227400	-0.68511800	2.12868200
C	-0.15581100	-1.80820100	1.38768700
H	0.06978100	-2.41459100	0.50480300
P	0.65750400	2.14107800	-0.09112700
P	-1.16560400	-0.38329500	0.70294500
C	0.00340800	-0.74250200	-3.04250800
H	0.83948200	-0.45775700	-3.68719700
H	-0.95106300	-0.60562200	-3.56234800
C	0.11651200	-2.04502100	-2.39682500
C	1.22673300	-2.76745400	-2.08017800
H	-0.82920500	-2.43437400	-2.01253500
C	2.59634300	-2.30873600	-2.51771900
H	3.29950700	-3.14603100	-2.58893600
H	2.54448100	-1.83503400	-3.50421400
H	3.04398400	-1.56552700	-1.83818000
C	1.11702700	-3.91443200	-1.15828500
C	2.15161000	-4.21318200	-0.25397500
C	-0.04902300	-4.70091600	-1.07259600
C	2.00732700	-5.19790000	0.71852900
H	3.06943400	-3.63298900	-0.28073700
C	-0.19572300	-5.68093300	-0.09861400
H	-0.84750100	-4.54798300	-1.79327100
C	0.82855700	-5.93217800	0.81396700
H	2.81999800	-5.38129000	1.41637800
H	-1.11242500	-6.26426900	-0.06229300
H	0.71544200	-6.69964000	1.57412600
C	-1.11998500	-2.62692900	2.25307000
C	-2.44745400	-2.63072200	1.49006600
H	-0.72989000	-3.63843200	2.40703600
H	-1.26858600	-2.16537500	3.23856500
H	-3.25722600	-3.11110300	2.04978700
H	-2.32434600	-3.18535400	0.55064400
C	1.99582200	4.44523500	-0.60873400
C	0.56026900	4.84747700	-0.25620300
C	1.15484000	-1.33093700	1.95307200
C	1.36464900	-1.08399200	3.31030000
C	2.18632400	-1.03211900	1.05393900
C	2.56678500	-0.53084500	3.75307100
H	0.58973100	-1.31805600	4.03461000
C	3.38528400	-0.48360100	1.48975000
H	2.03213400	-1.22994900	-0.00333800
C	3.57603100	-0.22106700	2.84587500
H	2.71214800	-0.34331000	4.81331100

H	4.16636300	-0.25834900	0.76989000
H	4.50946800	0.21353100	3.19139300
C	-3.91673900	-0.96680800	0.18289600
C	-5.20349400	-0.65507200	0.62790700
C	-3.70273700	-1.10482700	-1.19224800
C	-6.25108000	-0.47978800	-0.27275700
H	-5.38463900	-0.53728600	1.69382200
C	-4.74581000	-0.92976600	-2.09571600
H	-2.70460800	-1.31838400	-1.56514100
C	-6.02480300	-0.61460500	-1.63986700
H	-7.24338600	-0.23427300	0.09484300
H	-4.55623700	-1.03540900	-3.15988900
H	-6.83734200	-0.47450600	-2.34660100
C	-1.74463300	3.56802900	-0.17313100
C	-2.61621600	2.69628800	-0.83991200
C	-2.21258600	4.23884500	0.95772500
C	-3.90684800	2.47634100	-0.37567400
H	-2.26765600	2.16416700	-1.72350000
C	-3.50898100	4.02292900	1.42527900
H	-1.56619700	4.93008700	1.49049500
C	-4.35528700	3.13524100	0.76804900
H	-4.55769300	1.78519200	-0.90203100
H	-3.85393500	4.55028000	2.31012800
H	-5.36069200	2.95873900	1.13827900
C	3.50408400	2.36671900	-0.44017800
C	3.48415700	1.54892300	-1.57386000
C	4.71320500	2.53394600	0.24023400
C	4.64095300	0.90512500	-2.00422300
H	2.55215200	1.37872700	-2.10707800
C	5.87281000	1.89588000	-0.19029500
H	4.74252600	3.16127100	1.12852900
C	5.83903500	1.07360000	-1.31384400
H	4.59920700	0.25943800	-2.87648300
H	6.80126200	2.03485300	0.35602400
H	6.73876500	0.56580600	-1.64795400
H	2.73178700	5.18762700	-0.28257100
H	2.09946200	4.34211600	-1.69648300
H	0.49747700	5.04511000	0.82172700
H	0.24367300	5.75898500	-0.77481600
H	1.10138200	1.43930500	2.14764500
H	0.06502300	2.86929700	2.18565000
H	-0.98891600	0.60574900	2.95812100
H	-1.93396200	1.58206200	1.82613300

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C	0.54804200	-2.03805600	-1.39983300
C	1.85321800	-2.00783100	-0.59020100
H	-0.14559900	-2.76548100	-0.95939000
H	0.75993000	-2.37149900	-2.42314700
H	2.14353600	-3.02772000	-0.30848100
H	2.66235500	-1.59539800	-1.20533600
Cu	0.44622700	0.88877500	0.49364500
C	1.15672400	-1.97047600	2.30864600
H	0.82358400	-1.24178200	3.05913000
C	3.58851400	-1.00974400	1.48666300
H	4.07477700	-1.74680600	0.83446900
C	-1.91180100	-0.99293400	-2.41662700
H	-1.66502900	-1.99176300	-2.80059700
C	0.29373800	0.56870100	-2.84313100
H	-0.00684900	1.59426400	-2.59282800
P	1.80920100	-0.91312000	0.90564700
P	-0.41398700	-0.44326100	-1.41602900
C	0.00354700	2.81776700	0.82515100
H	0.93594300	3.37598800	0.67132100
H	-0.32069200	2.94768700	1.86315600
C	-0.99640400	3.19977300	-0.17476400
C	-2.35571900	3.23496100	-0.15577900
H	-0.55604700	3.50260500	-1.13061300
C	-3.09764200	3.70979400	-1.38865500
H	-3.89766900	3.01341100	-1.67807000
H	-3.56894900	4.69318700	-1.25108300
H	-2.41234200	3.80418800	-2.23823900
C	-3.18662800	2.83908800	1.00124000
C	-2.76730600	1.87159200	1.93286100
C	-4.48213800	3.36086200	1.17146900
C	-3.58778400	1.45775800	2.97563200
H	-1.79494400	1.40830600	1.80910600
C	-5.29959400	2.95883700	2.22335700
H	-4.85919700	4.09893900	0.47047600
C	-4.85915900	2.00306800	3.13565300
H	-3.23225300	0.69570500	3.66499200
H	-6.28936900	3.39564000	2.32802600
H	-5.49891000	1.68486400	3.95369200
C	-1.94469500	-0.03059300	-3.62179100
C	-0.49930500	0.15075100	-4.08764400
C	3.50232600	-1.62590800	2.90217600
C	2.39210300	-2.68052600	2.87440900

C	4.37240900	0.27875600	1.40612400
C	5.68264000	0.26040300	0.92272200
C	3.82811600	1.50013900	1.81486000
C	6.43196300	1.43095800	0.83891900
H	6.11759000	-0.68094300	0.59456200
C	4.57157000	2.67295500	1.72751100
H	2.80269300	1.54686300	2.17273200
C	5.87596900	2.64361900	1.23769700
H	7.44713200	1.39546900	0.45402300
H	4.12450700	3.61312100	2.03639300
H	6.45285900	3.56079700	1.16580000
C	-0.04459800	-2.77127700	1.87356900
C	-1.27254400	-2.11068100	1.73514800
C	0.03187100	-4.11629500	1.50972400
C	-2.38691900	-2.76474300	1.22682900
H	-1.35125300	-1.05926700	2.00505600
C	-1.08589100	-4.77756600	1.00014200
H	0.96660800	-4.65909100	1.61542500
C	-2.29330300	-4.10362300	0.84875800
H	-3.32285200	-2.22680500	1.11362000
H	-1.00611000	-5.82425000	0.72023100
H	-3.16142500	-4.61129000	0.43966700
C	1.79998900	0.52025000	-2.87031400
C	2.51793400	-0.39218400	-3.64710300
C	2.51337400	1.35682800	-2.00151600
C	3.90409300	-0.49115600	-3.53018700
H	1.99918200	-1.04463600	-4.34322600
C	3.89344100	1.25527000	-1.87569800
H	1.97301500	2.08363800	-1.39776300
C	4.59487500	0.32029100	-2.63471800
H	4.44306900	-1.21052000	-4.14044500
H	4.41956600	1.90141900	-1.17978900
H	5.67221700	0.23314800	-2.53032300
C	-3.20835900	-1.08414100	-1.65296300
C	-3.63475100	-0.03489600	-0.83648000
C	-4.01211800	-2.22060000	-1.76243600
C	-4.83454500	-0.11908000	-0.13750400
H	-3.01167300	0.84899400	-0.72677700
C	-5.21575900	-2.31011600	-1.06739000
H	-3.68830100	-3.04774600	-2.39052800
C	-5.62802800	-1.25995800	-0.25047800
H	-5.13797300	0.70350500	0.50292700
H	-5.82782700	-3.20300000	-1.16066300
H	-6.56339900	-1.32946600	0.29711500

H	-2.36362700	0.93483300	-3.30907200
H	-2.59450700	-0.42686000	-4.40936200
H	-0.40718300	0.89765800	-4.88381200
H	-0.13062200	-0.80206700	-4.48904600
H	4.47041700	-2.04438400	3.19651400
H	3.25402100	-0.84175200	3.62880000
H	2.19350600	-3.10308500	3.86529800
H	2.70051100	-3.50758200	2.22179800

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C	-4.76516500	-0.01311000	-0.36692200
C	-3.57312200	-0.68645100	-0.59639900
C	-2.36962400	-0.15492300	-0.12567600
C	-2.36379700	1.05224900	0.57719000
C	-3.56038400	1.72201700	0.80584200
C	-4.75871100	1.19133100	0.33432000
H	-5.69951500	-0.42662800	-0.73323000
H	-3.55400400	-1.62765600	-1.13561300
H	-1.42816700	1.45882400	0.94422600
H	-3.55815000	2.65933900	1.35341000
H	-5.69179300	1.71680900	0.51497400
C	-1.13020600	-0.92638500	-0.39406000
O	-1.07825900	-1.99359700	-0.93733000
O	0.00002000	-0.23493800	-0.00027900
C	1.13011100	-0.92630400	0.39392000
O	1.07805300	-1.99341100	0.93739800
C	2.36960700	-0.15491400	0.12564600
C	2.36393800	1.05216600	-0.57738200
C	3.57300900	-0.68642200	0.59662400
C	3.56058800	1.72185100	-0.80594500
H	1.42838200	1.45873300	-0.94461800
C	4.76511900	-0.01316600	0.36723200
H	3.55377900	-1.62755500	1.13595900
C	4.75882500	1.19117700	-0.33417800
H	3.55847200	2.65910200	-1.35363800
H	5.69939500	-0.42668100	0.73372900
H	5.69195600	1.71658900	-0.51477000

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C	-3.29095500	-1.19677900	0.66801200
C	-3.71866700	0.22146300	0.27331800
H	-3.54728200	-1.90276700	-0.13154200

H	-3.83211800	-1.51251900	1.56814400
H	-3.67729900	0.88321100	1.14629200
H	-4.75661000	0.21219000	-0.07829900
P	-2.60799300	1.02008200	-0.98234700
P	-1.45918200	-1.38888400	0.92133500
C	0.43234000	-0.84198300	-2.46484100
C	1.78595400	-0.80450200	-2.13591300
H	-0.04465600	-1.81913100	-2.40764600
C	2.17245100	1.18223200	-0.11771200
C	2.69612000	0.24683400	-2.31593200
Cu	-0.47318900	-0.01811400	-0.68287100
O	0.96368100	1.40181000	-0.23790600
C	-3.31383900	2.75549700	-0.99620800
H	-4.29871900	2.67485500	-0.51511500
C	-3.32791200	0.59473600	-2.67644900
C	-1.15639100	-0.96981500	2.72711500
H	-0.09869800	-0.69463000	2.76440200
C	-1.33796900	-3.23988300	1.19388300
C	2.20365800	1.42439500	-3.11943400
H	2.83295900	2.31047600	-3.00928700
H	2.13488100	1.19324300	-4.19202100
H	1.19973500	1.70634600	-2.77668800
C	4.14456500	-0.00157700	-2.18829500
C	5.09169500	0.91789700	-2.67368200
C	4.66774700	-1.13684000	-1.53416700
C	6.45932900	0.73288500	-2.49412300
H	4.76100100	1.80922600	-3.19412200
C	6.02990100	-1.31966400	-1.34571000
H	3.99575300	-1.90425500	-1.16618000
C	6.94520700	-0.38091200	-1.82032800
H	7.14881700	1.47844000	-2.88148100
H	6.38071100	-2.20898900	-0.82793100
H	8.01171100	-0.52358600	-1.67466900
C	3.20261200	2.23126100	-0.17944400
C	4.52131000	2.00162300	0.22144000
C	2.83936500	3.49442600	-0.66282800
C	5.45681400	3.02843600	0.15748700
H	4.82038200	1.01514300	0.55825200
C	3.77870700	4.51376800	-0.73145100
H	1.81799500	3.65812400	-0.98910300
C	5.09058700	4.28456700	-0.31552000
H	6.48075800	2.83603500	0.46212900
H	3.48764800	5.48996600	-1.10836500
H	5.82560600	5.08244500	-0.36722000

H	2.14557500	-1.68924400	-1.61818900
H	0.04175900	-0.16779900	-3.22675100
C	2.31768800	0.02184700	1.91591500
O	2.56641600	0.01362500	0.58900800
O	1.87136200	0.97193800	2.51569500
C	2.62416600	-1.28721900	2.55873900
C	3.21873300	-2.33997800	1.86190800
C	2.26860800	-1.44909200	3.90063700
C	3.42774500	-3.56025600	2.49598000
H	3.51584800	-2.19251600	0.83030300
C	2.47906500	-2.66868700	4.53157800
H	1.82024600	-0.61152300	4.42558600
C	3.05239200	-3.72708300	3.82702800
H	3.87934900	-4.38212000	1.94946400
H	2.19662300	-2.79669800	5.57200700
H	3.20991500	-4.68280900	4.31794700
C	-1.31843300	-2.29589700	3.48166500
H	-0.83656100	-2.24916000	4.46453600
H	-2.37833800	-2.52880200	3.64590200
C	-0.69928200	-3.37813000	2.59224900
H	0.38428000	-3.22540200	2.52290300
H	-0.85823900	-4.38586300	2.99057200
H	-2.36975000	-3.60897900	1.25839900
C	-1.95266700	0.24133300	3.14327000
C	-1.48087100	1.50583000	2.76439500
C	-3.18571800	0.15315500	3.79303100
C	-2.23645300	2.64727900	3.00706800
H	-0.51882400	1.59259400	2.26443900
C	-3.94313500	1.29799100	4.03724800
H	-3.57168000	-0.81194700	4.10849400
C	-3.47591500	2.54616500	3.63652200
H	-1.85810200	3.61547200	2.69473900
H	-4.90242400	1.20899900	4.53951100
H	-4.06750600	3.43862200	3.81853300
C	-3.57000200	3.03778300	-2.48996600
H	-4.19567500	3.92842600	-2.61296300
H	-2.61731300	3.23681100	-2.99856700
C	-4.22878500	1.77922300	-3.06079900
H	-2.45368000	0.61224900	-3.33877300
H	-5.22466600	1.67252400	-2.61338100
H	-4.36529200	1.83312000	-4.14617400
C	-2.53570200	3.82545900	-0.26487000
C	-3.24060900	4.87285300	0.33660100
C	-1.14228100	3.81525800	-0.16655200

C	-2.57634900	5.88734000	1.01874700
H	-4.32691600	4.88817500	0.27556900
C	-0.47559400	4.82202900	0.52826600
H	-0.56686100	2.99687400	-0.58813500
C	-1.18709100	5.86237100	1.12024700
H	-3.14380500	6.69029300	1.48066000
H	0.60517200	4.77604600	0.62555300
H	-0.66384100	6.64266600	1.66509000
C	-3.89971500	-0.80093700	-2.70551900
C	-3.03575700	-1.87532900	-2.94819100
C	-5.23306900	-1.08446100	-2.39602700
C	-3.47465200	-3.19089800	-2.84959900
H	-2.00003000	-1.67362900	-3.20105000
C	-5.67927700	-2.40112300	-2.30288100
H	-5.93727100	-0.27756800	-2.21537600
C	-4.80075400	-3.45954100	-2.51780600
H	-2.77349300	-4.00130500	-3.02416700
H	-6.71962100	-2.59778200	-2.06005900
H	-5.15014000	-4.48479800	-2.43751300
C	-0.63204800	-3.98050500	0.08657900
C	0.68390400	-3.66278600	-0.26232600
C	-1.28028200	-4.99709200	-0.61572300
C	1.33809000	-4.35039100	-1.27720400
H	1.18875200	-2.84961500	0.25166900
C	-0.63057900	-5.68512200	-1.63917800
H	-2.30858100	-5.24784500	-0.36529200
C	0.68182300	-5.36522200	-1.97175700
H	2.35980200	-4.08678300	-1.53752200
H	-1.15187800	-6.47413000	-2.17426400
H	1.19009600	-5.89741700	-2.77015300

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C	-3.91906800	-0.80543800	0.60709400
C	-3.12089000	-2.06842500	0.97921700
H	-4.93576600	-1.08410900	0.30276800
H	-4.01207300	-0.15307400	1.48214800
H	-3.46350400	-2.43906400	1.95326800
H	-3.31311700	-2.86005600	0.24697800
P	-1.27702400	-1.82771300	0.97814000
P	-3.12863500	0.25619500	-0.69373700
C	0.00389900	0.58456900	-2.54449000
C	1.04813100	1.43934900	-2.22882700
H	-0.88462900	1.01485100	-3.00341900

C	1.92359000	1.09137000	0.44349200
C	2.34403900	1.06330900	-1.80339900
Cu	-0.80196400	0.01382400	-0.56913500
O	0.88573400	0.41989300	0.55471300
C	-0.90750600	-1.20144900	2.71079000
C	-0.67337000	-3.57161800	1.35497700
H	-1.56504800	-4.21022300	1.39616700
C	-4.31635700	1.71317400	-0.76266900
H	-5.06655600	1.53520200	0.01767500
C	-3.75616000	-0.48183300	-2.30693100
C	2.63884100	-0.41483000	-1.90645400
H	3.56954200	-0.69623900	-1.41105600
H	2.69783000	-0.75065800	-2.95192700
H	1.83532600	-0.98468800	-1.42615600
C	3.46312200	2.01977200	-1.98099300
C	4.77946000	1.56570900	-2.17859300
C	3.28384500	3.41564000	-1.94336600
C	5.85073200	2.44557900	-2.30328200
H	4.97615300	0.50231800	-2.25881500
C	4.35061100	4.29502900	-2.07368400
H	2.29692500	3.83505000	-1.77575100
C	5.64787700	3.82026600	-2.24848700
H	6.85039700	2.04642200	-2.45604300
H	4.16350300	5.36416900	-2.02101300
H	6.48150600	4.50961800	-2.34504700
H	0.81730100	2.50421400	-2.25123900
H	0.22076600	-0.44297300	-2.83486500
C	-0.05465100	-3.48550500	2.77274900
C	-0.85321600	-2.46242000	3.57933200
H	0.11008000	-0.80290400	2.62252300
C	-1.83265300	-0.08113100	3.11303400
C	-2.98301100	-0.27804100	3.88068300
C	-1.57732400	1.20504100	2.61917600
C	-3.87909600	0.76803100	4.10251700
H	-3.19786200	-1.25519800	4.30318400
C	-2.47308600	2.24628700	2.82712000
H	-0.66415300	1.37337100	2.05749000
C	-3.63935900	2.02741100	3.55993100
H	-4.77203200	0.59198200	4.69607200
H	-2.26161100	3.22715700	2.41077300
H	-4.34502000	2.83742500	3.72160700
C	0.28235900	-4.12961400	0.32933000
C	0.07978000	-5.38883300	-0.23605100
C	1.41553400	-3.40162300	-0.04708200

C	0.98341700	-5.90821300	-1.16212200
H	-0.79880200	-5.96573000	0.04459100
C	2.32262500	-3.91670800	-0.96527100
H	1.57907000	-2.41852200	0.38496400
C	2.10686000	-5.17306000	-1.53009200
H	0.80864900	-6.88916400	-1.59537200
H	3.19781800	-3.33351200	-1.23748000
H	2.81255700	-5.57604700	-2.25059700
C	-5.00915100	1.61080500	-2.14469000
C	-5.14724800	0.13129600	-2.50060400
H	-3.09405400	-0.06628400	-3.07851100
C	-3.61512900	-1.98413100	-2.32816600
C	-4.68184800	-2.84832100	-2.07285800
C	-2.34398000	-2.53892800	-2.52218500
C	-4.47544300	-4.22406200	-1.97661500
H	-5.68432900	-2.45516800	-1.93453100
C	-2.13203200	-3.90783300	-2.42084400
H	-1.50479400	-1.88256000	-2.73357500
C	-3.20006600	-4.75721700	-2.13563600
H	-5.31756200	-4.87865500	-1.77054500
H	-1.13202800	-4.30919900	-2.55074800
H	-3.03789600	-5.82742500	-2.04791100
C	-3.68161200	3.06159700	-0.52736800
C	-4.25952900	3.97064400	0.35978400
C	-2.53667100	3.45020000	-1.23067900
C	-3.71569800	5.24087600	0.53747100
H	-5.14374800	3.67867300	0.92131200
C	-1.99361100	4.71821900	-1.06156900
H	-2.05437800	2.74937900	-1.90842700
C	-2.58387500	5.62029400	-0.17751100
H	-4.17899500	5.93413100	1.23347600
H	-1.09688400	4.99689000	-1.60728200
H	-2.15828800	6.61079200	-0.04461300
C	1.97517500	2.54421600	0.74386500
C	3.16209400	3.17880400	1.11519000
C	0.79529100	3.29161600	0.66077100
C	3.16723200	4.53708200	1.41629100
H	4.08363500	2.61045100	1.15589100
C	0.80465500	4.64695800	0.96437200
H	-0.12785300	2.80806800	0.35384500
C	1.99052100	5.27439000	1.34489900
H	4.09859600	5.01903500	1.69775900
H	-0.12127200	5.21035400	0.91167500
H	1.99409700	6.33438900	1.58242300

O	3.16742300	0.46775700	0.72789800
C	3.25783800	-0.64038600	1.48682800
O	2.42881400	-1.01524400	2.28499600
C	4.53614500	-1.36617500	1.23078200
C	5.57451000	-0.79474800	0.48997000
C	4.67219100	-2.65708200	1.74565400
C	6.74150700	-1.51635500	0.26631400
H	5.46022600	0.20587100	0.08676800
C	5.83620800	-3.37897600	1.50962500
H	3.85426200	-3.08433800	2.31597300
C	6.87212300	-2.80827100	0.77251600
H	7.54953900	-1.06973400	-0.30520100
H	5.93673100	-4.38637100	1.90177900
H	7.78334000	-3.37110600	0.59161800
H	-0.03912600	-4.47461200	3.24310400
H	0.98172400	-3.13873000	2.69108500
H	-1.85923200	-2.85632100	3.77650300
H	-0.38730300	-2.25332800	4.54858700
H	-5.97281900	2.13046100	-2.12912900
H	-4.38673900	2.11205800	-2.89657100
H	-5.87534800	-0.33435800	-1.82466000
H	-5.51212900	-0.01722000	-3.52304100

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C	-3.57545900	1.20489800	0.98397300
C	-2.91084300	2.44284100	0.36954300
H	-4.37650200	0.84131500	0.32918200
H	-4.03282100	1.46709600	1.94525200
H	-2.31850800	2.96272800	1.13084500
H	-3.67999400	3.14457500	0.02405600
P	-1.71088500	2.07042800	-1.00036800
P	-2.43421300	-0.24249100	1.19106100
C	-0.55087800	-1.53082500	-2.17468500
C	0.54870100	-2.26507900	-1.75153400
H	-1.51850200	-2.02958600	-2.15349500
C	1.95980900	-0.87236200	0.25241000
C	1.91075500	-1.89269000	-1.81022600
Cu	-0.86924100	-0.10573000	-0.54664900
O	1.04856700	-0.03530200	0.17219300
C	-0.98113400	3.78024800	-1.27162800
H	-1.52018800	4.44730300	-0.58680200
C	-2.75341200	2.13399100	-2.56458800
C	-1.60570700	-0.02622200	2.86701000

H	-0.67271500	-0.59381100	2.77726300
C	-3.62931000	-1.54880200	1.80363800
H	-4.56042800	-1.01973700	2.04641300
C	2.21346900	-0.64960800	-2.61258000
H	3.20637900	-0.24605300	-2.40255400
H	2.13504700	-0.82902100	-3.69438400
H	1.49381500	0.13080800	-2.35011700
C	2.95599900	-2.93852400	-1.72020400
C	4.23040600	-2.73661200	-2.28101100
C	2.75268600	-4.16650400	-1.06228000
C	5.24039900	-3.68801200	-2.17604500
H	4.43756500	-1.82527700	-2.83151300
C	3.75742500	-5.11995000	-0.96265600
H	1.80031200	-4.38161300	-0.58834200
C	5.01479400	-4.89060900	-1.51456200
H	6.20832600	-3.48832800	-2.62871000
H	3.55404900	-6.04860300	-0.43612800
H	5.79996100	-5.63652500	-1.43489700
H	0.31580800	-3.20321800	-1.24873700
H	-0.43255400	-0.76567700	-2.94197100
O	3.28037600	-0.40572200	0.03614700
C	1.91743100	-2.06577600	1.13491500
C	3.07926900	-2.69546900	1.58351600
C	0.67533400	-2.59369500	1.50358400
C	2.99818200	-3.82122800	2.39882700
H	4.04775400	-2.31719300	1.27747000
C	0.59468000	-3.73074000	2.29467600
H	-0.22262600	-2.10778300	1.13847800
C	1.76056300	-4.34672200	2.75212500
H	3.91121100	-4.29971000	2.73950500
H	-0.37712600	-4.14322900	2.55305300
H	1.70049800	-5.23379000	3.37577200
C	3.75277500	0.56341000	0.85099700
C	5.11625300	0.99602200	0.42834700
C	5.67179300	2.11445200	1.05289800
C	5.83124200	0.31741400	-0.56153700
C	6.93123200	2.56504100	0.67563500
H	5.09781300	2.61878300	1.82348600
C	7.09448300	0.76832300	-0.93079200
H	5.40177700	-0.56459500	-1.02488600
C	7.64195000	1.89329100	-0.31850900
H	7.36155600	3.43825400	1.15675000
H	7.65227900	0.23935900	-1.69767000
H	8.62636000	2.24601800	-0.61255900

O	3.16193300	1.01164200	1.80295700
C	-1.39054800	4.15795100	-2.71449200
H	-1.32591900	5.24152000	-2.85942100
H	-0.69160100	3.69610300	-3.42387500
C	-2.80370700	3.61681500	-2.94977400
H	-3.50603300	4.16363600	-2.30762100
H	-3.13492500	3.75220900	-3.98530300
H	-2.14455800	1.61422500	-3.31618100
C	-3.01185800	-2.02131800	3.13713400
C	-2.50911700	-0.76866300	3.86183600
H	-1.96479300	-1.01144800	4.78054500
H	-3.37267700	-0.15406400	4.14672100
H	-3.74603200	-2.58152000	3.72594900
H	-2.17109700	-2.69775800	2.93748300
C	0.49794500	3.90787100	-0.99545800
C	0.99214900	5.02605300	-0.32110000
C	1.40247700	2.93874700	-1.43290000
C	2.35761700	5.17140100	-0.08756300
H	0.29894700	5.78526800	0.03449100
C	2.76517300	3.07774800	-1.20227000
H	1.03390700	2.05098800	-1.93631200
C	3.24848700	4.19558400	-0.52660800
H	2.72423400	6.04649900	0.44158000
H	3.44938700	2.30473600	-1.53950100
H	4.31328000	4.29790600	-0.34011800
C	-4.03302900	1.35780300	-2.38241700
C	-3.96826600	-0.04086600	-2.42507600
C	-5.25352100	1.95462200	-2.06141800
C	-5.07095100	-0.82409300	-2.11078100
H	-3.02801700	-0.51808700	-2.68307500
C	-6.36742600	1.17208300	-1.75584700
H	-5.34448900	3.03656800	-2.03553300
C	-6.27696500	-0.21682200	-1.76438900
H	-4.98390800	-1.90638300	-2.12645600
H	-7.30774300	1.65502200	-1.50549200
H	-7.14021800	-0.82511100	-1.51080600
C	-3.95749100	-2.63916400	0.81270300
C	-5.28783200	-3.01251200	0.60935600
C	-2.96398900	-3.29871800	0.08163600
C	-5.62321300	-4.01058400	-0.30216400
H	-6.07409000	-2.50604800	1.16448300
C	-3.29372900	-4.29156000	-0.83502500
H	-1.92190100	-3.02016500	0.20744300
C	-4.62600700	-4.65026400	-1.03304500

H	-6.66533100	-4.28036100	-0.44739300
H	-2.50568100	-4.78221500	-1.39916300
H	-4.88340000	-5.42221900	-1.75190100
C	-1.23560600	1.41480000	3.11827200
C	-2.07236100	2.30692900	3.79367500
C	-0.04695100	1.90028900	2.55784400
C	-1.74591000	3.65953200	3.87777000
H	-2.99223000	1.95633700	4.25351400
C	0.27768600	3.24968700	2.63903300
H	0.62625500	1.22493400	2.03713400
C	-0.57703100	4.13765200	3.29039200
H	-2.40913400	4.33949900	4.40531800
H	1.20067400	3.59739900	2.18607000
H	-0.32746300	5.19316700	3.35321400

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C	-3.00183900	2.42853900	0.43141700
C	-3.68599300	1.17594500	1.00689100
H	-3.76219300	3.12462300	0.05701200
H	-2.44921500	2.94756900	1.22147600
H	-4.15212100	1.42095100	1.96840200
H	-4.48359300	0.84154500	0.33360000
P	-2.55620400	-0.28732000	1.17947300
P	-1.75341000	2.05548300	-0.89299300
C	-0.36946200	-1.12410200	-2.32089400
C	1.00587200	-1.30234300	-2.23482000
H	-0.72553500	-0.37554500	-3.02821200
C	1.81472300	-1.24639000	0.50881300
C	1.69459000	-2.35183700	-1.59525200
Cu	-0.81708200	-0.03966200	-0.49265600
O	0.64753300	-0.87848200	0.69354800
C	-1.74858700	-0.09902400	2.86977400
C	-3.74617000	-1.61870000	1.75359800
H	-4.70471100	-1.12601700	1.96342000
C	-0.98133200	3.73356900	-1.21846800
H	-1.36989600	4.41439700	-0.45137700
C	-2.78583200	2.08741000	-2.46239000
C	0.83778500	-3.51346800	-1.15162300
H	1.36764800	-4.22003300	-0.51089100
H	0.42791900	-4.06947200	-2.00759600
H	-0.00718800	-3.13654300	-0.56507100
C	3.10954200	-2.59950200	-1.94502400
C	3.70684100	-3.85590300	-1.73893800

C	3.94539900	-1.59750400	-2.47868800
C	5.04854900	-4.09183900	-2.02581400
H	3.11950400	-4.67545800	-1.34231100
C	5.28228300	-1.83192600	-2.76917500
H	3.54961900	-0.60336300	-2.65781200
C	5.85355500	-3.08281700	-2.53965800
H	5.46334900	-5.07956500	-1.84304500
H	5.88565800	-1.02517600	-3.17947900
H	6.90037800	-3.26432900	-2.76353900
C	2.40125500	-2.39437900	1.23786400
C	3.76432400	-2.69774000	1.17748100
C	1.55137700	-3.19890400	2.00513700
C	4.26577300	-3.79326100	1.87241400
H	4.42932900	-2.08697200	0.57701400
C	2.05538600	-4.29315600	2.69417900
H	0.49586600	-2.95030500	2.04859000
C	3.41589800	-4.59434800	2.62881100
H	5.32516100	-4.02305200	1.81153200
H	1.38916900	-4.91123200	3.28905000
H	3.81062200	-5.45082400	3.16760100
H	1.60244200	-0.50206000	-2.66899900
H	-1.04163900	-1.96768600	-2.16417800
C	3.21792500	0.52990000	1.10297900
O	2.78602700	-0.28652700	0.10972900
O	2.67597100	0.62368300	2.17890700
C	4.45200000	1.28168700	0.74610600
C	5.24523500	0.93103600	-0.34565300
C	4.82557500	2.34433500	1.57136000
C	6.40237300	1.65315800	-0.61985300
H	4.96230200	0.08886300	-0.96564700
C	5.97825700	3.06764300	1.29166500
H	4.19950000	2.58979700	2.42274900
C	6.76714400	2.72404000	0.19376800
H	7.02365400	1.37336300	-1.46558400
H	6.26586700	3.89712600	1.93068700
H	7.67171100	3.28563100	-0.02172600
C	-3.15459700	-2.09607500	3.09851600
C	-2.66646700	-0.85091800	3.84254200
H	-0.81176600	-0.66011400	2.77016300
C	-1.39472300	1.34126900	3.14787900
C	-2.22932300	2.21109800	3.85387800
C	-0.22283600	1.85439500	2.57812600
C	-1.91909500	3.56661300	3.95636900
H	-3.13625300	1.84158100	4.32385900

C	0.08636900	3.20612300	2.67591400
H	0.45328000	1.18265500	2.05884100
C	-0.76829800	4.07215400	3.35704400
H	-2.58147400	4.22780200	4.50812200
H	0.99806900	3.57599400	2.21604300
H	-0.53187100	5.12954600	3.43638900
C	-3.98006900	-2.72016600	0.74816600
C	-5.26676600	-3.21205600	0.52297000
C	-2.91763700	-3.28061600	0.03300400
C	-5.49055500	-4.22967800	-0.40205400
H	-6.10558500	-2.78419000	1.06716200
C	-3.13497700	-4.29139000	-0.89618500
H	-1.91167100	-2.90064000	0.18888900
C	-4.42586900	-4.76887200	-1.11949100
H	-6.49951500	-4.59717200	-0.56648600
H	-2.29292100	-4.70235300	-1.44587200
H	-4.59944600	-5.55540300	-1.84782600
C	-1.52034200	4.17545300	-2.60509400
C	-2.91385100	3.57746300	-2.79923200
H	-2.14764600	1.62328700	-3.22662900
C	-4.03978300	1.25856500	-2.32529100
C	-5.29632900	1.82100900	-2.09284700
C	-3.93006700	-0.13793800	-2.34160200
C	-6.40451200	1.00946200	-1.84866500
H	-5.42282800	2.89939700	-2.09123400
C	-5.02958100	-0.94936100	-2.09448300
H	-2.96278200	-0.59547400	-2.52302600
C	-6.27335500	-0.37554600	-1.83595000
H	-7.37241500	1.46745200	-1.66561600
H	-4.91028000	-2.02844700	-2.09253900
H	-7.13301300	-1.00738800	-1.63302700
C	0.52788800	3.72933700	-1.15214000
C	1.21113300	4.72423100	-0.45266300
C	1.27207500	2.75879800	-1.83229200
C	2.60455300	4.75758600	-0.43817300
H	0.64589500	5.48017000	0.08806100
C	2.66038100	2.79045300	-1.82096300
H	0.76038500	1.95773500	-2.36207300
C	3.33266000	3.79469000	-1.12807900
H	3.12096400	5.53674300	0.11525200
H	3.22324100	2.02059100	-2.34040400
H	4.41792300	3.80744100	-1.10740200
H	-3.89885000	-2.66261300	3.66854800
H	-2.31076700	-2.77199500	2.90672100

H	-3.53662000	-0.23981100	4.11499200
H	-2.14034500	-1.09989300	4.77052400
H	-3.61754000	4.06982100	-2.11627000
H	-3.29056000	3.72860200	-3.81719500
H	-1.51820800	5.26719200	-2.68843600
H	-0.84853100	3.79441700	-3.38409500

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C	2.70346800	-1.94829900	0.86417400
C	1.56959000	-2.97962000	0.84406000
H	3.34159400	-2.07593300	-0.01855300
H	3.33360100	-2.10403000	1.74789600
H	1.08569100	-3.02882600	1.82660600
H	1.97818100	-3.97458400	0.63336500
P	0.19764100	-2.57114300	-0.33804600
P	2.13214000	-0.18186200	0.79063500
C	0.18555500	0.53499600	-2.58076800
C	-0.51202600	1.72542700	-2.39805200
H	1.25919800	0.63998200	-2.72500000
C	-1.96526200	1.75029200	0.00654400
C	-1.88533300	2.03950800	-2.37245600
Cu	0.22063900	-0.18121300	-0.52882400
O	-1.59198900	0.58131400	0.15415700
C	-1.01747100	-3.93535600	0.07060600
H	-0.43714700	-4.69433300	0.61353300
C	0.67003200	-3.33685700	-1.99927000
C	1.87697400	0.35035300	2.57218600
H	1.17484000	1.18641700	2.50906900
C	3.77727200	0.69842000	0.61845100
C	-2.20905600	3.51193100	-2.52813700
C	-3.36531600	2.18868700	0.16141600
C	-3.69894200	3.51670200	0.44564100
C	-4.38619400	1.24333600	0.01412800
C	-5.03143800	3.88657600	0.59597600
H	-2.91591100	4.26001400	0.54762000
C	-5.71487900	1.61818700	0.15710300
H	-4.12981900	0.22235100	-0.24041500
C	-6.04227200	2.93976900	0.45356400
H	-5.27816100	4.91938700	0.82338800
H	-6.49559600	0.87513000	0.02569300
H	-7.08210400	3.23134900	0.56918500
H	0.12721900	2.57974100	-2.16303000
H	-0.27747700	-0.29753400	-3.10780500

C	-0.55430000	2.90822200	1.50279400
O	-1.00525000	2.78195500	0.23883300
O	-1.01848800	2.32277100	2.45349300
C	0.60314200	3.84319200	1.59392400
C	1.14809000	4.46628200	0.46996700
C	1.16888500	4.05529600	2.85418800
C	2.27071900	5.27671900	0.60278100
H	0.69680600	4.30453400	-0.50300000
C	2.28490100	4.87229100	2.98508100
H	0.72481900	3.56408600	3.71406700
C	2.84040000	5.47724000	1.85792500
H	2.70618400	5.74255500	-0.27541300
H	2.72781300	5.03228700	3.96324200
H	3.72022800	6.10580300	1.95822800
H	-1.41347500	4.12547600	-2.09133800
H	-2.30618100	3.80451800	-3.58356500
H	-3.14376900	3.78995700	-2.02799200
C	-2.93541600	1.07363100	-2.74600300
C	-4.16368200	1.51749900	-3.27096600
C	-2.82318000	-0.31152600	-2.50368700
C	-5.20890300	0.64083200	-3.53836100
H	-4.31465700	2.57330500	-3.46666000
C	-3.87370900	-1.18586600	-2.75807400
H	-1.92738600	-0.70501000	-2.04341400
C	-5.07601500	-0.72056200	-3.28275700
H	-6.13868700	1.03096100	-3.94394200
H	-3.75311100	-2.24191900	-2.52814500
H	-5.89355100	-1.40603800	-3.48629200
C	-1.36079000	-4.54109100	-1.30489200
H	-1.89137100	-5.49196200	-1.18671700
H	-2.02514100	-3.86284100	-1.85685300
C	-0.03147200	-4.70346800	-2.04726400
H	0.56411400	-5.46877500	-1.53466000
H	-0.16788100	-5.03724800	-3.08138200
H	0.17604200	-2.68498400	-2.73009500
C	-2.20129700	-3.56108100	0.93147900
C	-2.67445100	-4.48898900	1.86458500
C	-2.84487900	-2.32525800	0.83073200
C	-3.76490700	-4.19667000	2.67781500
H	-2.17479500	-5.45061200	1.96116200
C	-3.93044500	-2.02697000	1.65060100
H	-2.47648300	-1.56654300	0.14734200
C	-4.39635200	-2.95973300	2.57346800
H	-4.11371200	-4.93043000	3.39890200

H	-4.39979000	-1.05073400	1.58128700
H	-5.23888700	-2.71905600	3.21515800
C	2.15607000	-3.26219100	-2.24661200
C	3.04629900	-4.26233800	-1.84472900
C	2.68561600	-2.09164900	-2.80273000
C	4.42258300	-4.08217900	-1.96636000
H	2.67199200	-5.18979000	-1.42106700
C	4.05809300	-1.90389200	-2.91906800
H	2.00822100	-1.31202300	-3.13425100
C	4.93484000	-2.89878000	-2.49165600
H	5.09687500	-4.87067000	-1.64435400
H	4.43816900	-0.97580800	-3.33512200
H	6.00808200	-2.75777400	-2.57923000
C	3.23217900	0.90920200	3.02588600
H	3.11541200	1.56140900	3.89848900
H	3.91854100	0.10139400	3.31014400
C	3.81669400	1.66036500	1.82525000
H	3.21003900	2.54680400	1.60653900
H	4.83968500	2.00683200	2.00768400
H	4.55030300	-0.06603800	0.77235900
C	1.20188000	-0.74501400	3.36021400
C	1.90561400	-1.64748800	4.16017800
C	-0.17722500	-0.93215900	3.18840800
C	1.25489400	-2.72809800	4.75428300
H	2.97212200	-1.51969300	4.32190000
C	-0.82545400	-2.01187600	3.77775900
H	-0.74191400	-0.23468700	2.57389700
C	-0.10905500	-2.92000400	4.55590800
H	1.82078100	-3.42125100	5.37059400
H	-1.89048600	-2.14897300	3.61915900
H	-0.61548900	-3.76767400	5.00817200
C	4.01196800	1.35191900	-0.72064200
C	5.21388000	1.15619700	-1.40269300
C	3.04439300	2.17807500	-1.29910800
C	5.44597700	1.77001900	-2.63218700
H	5.97425200	0.50923300	-0.97117200
C	3.26939100	2.79134900	-2.52587200
H	2.09369100	2.31729600	-0.79351000
C	4.47306100	2.58825300	-3.19885000
H	6.38805600	1.60537600	-3.14753300
H	2.49656700	3.41716100	-2.96402200
H	4.64800000	3.06181200	-4.16023000

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C	3.05857600	2.34605700	0.71396600
C	1.74990800	2.92506600	1.27743800
H	3.73889400	3.16088300	0.43578100
H	3.56281500	1.74979400	1.48218600
H	1.92868900	3.28873400	2.29706800
H	1.43958200	3.79044700	0.68093300
P	0.28889900	1.76547500	1.24974800
P	2.83920900	1.18520600	-0.71072300
C	0.37079400	-0.56243000	-2.68941200
C	0.02570500	-1.88553900	-2.44587200
H	1.36637000	-0.38721300	-3.09585600
C	-1.01635900	-2.27775400	0.14654300
C	-1.22223200	-2.48937300	-2.17234100
Cu	0.77197400	0.13125500	-0.62479000
O	-0.43513400	-1.19995700	0.33894300
C	0.48776000	0.78420700	2.84516700
C	-1.02054900	2.90527700	2.00121500
H	-0.53061300	3.87896800	2.12759000
C	4.59722000	0.58593200	-0.98929000
H	5.21347600	1.08708800	-0.23225300
C	2.84923300	2.30266000	-2.22210800
C	-1.27196800	-3.98970400	-2.39663200
H	0.86968700	-2.57822700	-2.38415500
H	-0.38826300	0.14348100	-3.02242400
C	-1.31941800	2.32211400	3.40435700
C	-0.03401400	1.70926400	3.94897900
H	-0.22616400	-0.04085000	2.72364600
C	1.86788400	0.19940900	3.01259500
C	2.87156000	0.81103200	3.76795400
C	2.17946300	-0.98295200	2.33056600
C	4.16093800	0.27887500	3.80239300
H	2.66069800	1.71726800	4.32810000
C	3.46437000	-1.50887100	2.35112300
H	1.39210800	-1.48089600	1.77535700
C	4.46683400	-0.87139800	3.08103600
H	4.92814400	0.77129700	4.39380100
H	3.68365400	-2.41613300	1.79440100
H	5.47293000	-1.28038100	3.09722000
C	-2.27319300	3.10229800	1.18500300
C	-3.10062300	2.01756900	0.87967400
C	-2.67352000	4.37915900	0.78737800
C	-4.31527200	2.20629400	0.23090000
H	-2.79533800	1.01644100	1.16956700

C	-3.87687100	4.57139300	0.11152900
H	-2.03864600	5.23267700	1.01474200
C	-4.70562600	3.48637100	-0.16034800
H	-4.95020300	1.34941100	0.02597200
H	-4.17270700	5.57300800	-0.18843800
H	-5.65305600	3.63576400	-0.67000300
C	4.99314100	1.14178800	-2.37911700
C	4.33369400	2.51271100	-2.54045100
H	2.41862000	1.68802500	-3.02324100
C	1.95469600	3.50114900	-2.02138700
C	2.44324600	4.76322000	-1.67868500
C	0.56675800	3.31939100	-2.08369400
C	1.56795800	5.80545900	-1.37330000
H	3.51323400	4.94338000	-1.63636000
C	-0.30835000	4.35179900	-1.77111800
H	0.16882000	2.34372600	-2.35093700
C	0.19212100	5.60059800	-1.40490600
H	1.96841500	6.77901600	-1.10531000
H	-1.37947700	4.17797200	-1.79968800
H	-0.48930700	6.40866200	-1.15541800
C	4.79080700	-0.90509400	-0.85411900
C	5.87275100	-1.41059400	-0.13167400
C	3.91802200	-1.80935800	-1.46661200
C	6.07796000	-2.78292500	-0.01553700
H	6.55646500	-0.72073400	0.35708700
C	4.12003700	-3.18086200	-1.35736400
H	3.05713700	-1.43976900	-2.01805900
C	5.20037600	-3.67364100	-0.62745500
H	6.92332400	-3.15570400	0.55550400
H	3.42230700	-3.86571300	-1.83094500
H	5.35711800	-4.74468700	-0.53822100
C	-0.36825300	-3.58802000	0.40465800
C	-1.10431300	-4.71575800	0.77302700
C	1.02266300	-3.68738000	0.28695200
C	-0.45910600	-5.92427000	1.01822900
H	-2.18182500	-4.64254900	0.86761300
C	1.66302100	-4.89397900	0.53406600
H	1.59824800	-2.81427500	-0.00541700
C	0.92394800	-6.01901100	0.89917300
H	-1.04162200	-6.79465500	1.30584000
H	2.74400000	-4.95353700	0.44564300
H	1.42528900	-6.96283600	1.09204000
O	-2.41835200	-2.30376000	0.35651600
C	-2.92532300	-1.61861100	1.40628600

O	-2.28082100	-1.26356400	2.36786800
C	-4.38166700	-1.34976200	1.25105000
C	-5.07012800	-1.65112400	0.07515600
C	-5.04374600	-0.72065300	2.30961900
C	-6.41544100	-1.31636900	-0.04058300
H	-4.55121600	-2.12459800	-0.74953400
C	-6.38774500	-0.39293000	2.19160600
H	-4.48690800	-0.48603200	3.21072000
C	-7.07405600	-0.68839200	1.01367200
H	-6.93956800	-1.53632700	-0.96535300
H	-6.89923600	0.09950900	3.01294100
H	-8.12372100	-0.42552300	0.91729900
C	-2.47151700	-1.74559600	-2.47401200
C	-3.53130000	-2.36362300	-3.16132400
C	-2.65428200	-0.39897200	-2.10783900
C	-4.68360700	-1.66474800	-3.51166000
H	-3.45379400	-3.40691000	-3.44698400
C	-3.79470400	0.30448100	-2.47620600
H	-1.90600300	0.09818400	-1.49985800
C	-4.81723900	-0.31886700	-3.18661300
H	-5.47423000	-2.17729100	-4.05396000
H	-3.88666100	1.34810600	-2.19325300
H	-5.70723200	0.23417800	-3.47303400
H	-2.08201400	-4.46138600	-1.82755200
H	-1.42468100	-4.23914300	-3.45610000
H	-0.33711600	-4.46502800	-2.08575700
H	-1.72837000	3.09924700	4.05921300
H	-2.07728800	1.53534600	3.31616600
H	0.68696400	2.50632300	4.17293800
H	-0.20428300	1.15491200	4.87859300
H	6.08272700	1.18633900	-2.47882300
H	4.62607400	0.46124200	-3.15809900
H	4.47485700	2.92654000	-3.54507200
H	4.78837300	3.21600300	-1.83085900

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C	-3.37513500	1.44546300	1.02927300
C	-2.53230300	2.65432500	0.60301600
H	-4.19892500	1.29650700	0.32217900
H	-3.82009000	1.62969000	2.01415600
H	-1.93965700	3.01989300	1.45027200
H	-3.19101000	3.47215500	0.28755800
P	-1.28191100	2.28719600	-0.71787000

P	-2.44705900	-0.16080100	1.03648000
C	-0.15800400	-0.88553100	-2.38826500
C	0.42235300	-2.06713500	-1.93980900
H	-1.17981000	-0.96900000	-2.75825000
C	1.68325700	-1.74119800	0.61770100
C	1.76305000	-2.42043600	-1.66023100
Cu	-0.64285400	0.02229500	-0.49777500
O	0.92007000	-0.75778400	0.61613700
C	-0.46877900	3.96704100	-0.89497400
H	-1.14166200	4.68385300	-0.40538300
C	-2.19628000	2.42543400	-2.36672300
C	-1.70917300	-0.31450500	2.75910400
H	-0.86276500	-0.99773700	2.61855300
C	-3.84105400	-1.36082400	1.38233300
C	2.00474000	-3.92337400	-1.64427000
H	-0.29030000	-2.86677300	-1.72130700
H	0.45202200	-0.12580700	-2.87475300
O	3.01702600	-1.32720100	0.84367700
C	1.23258500	-3.04995600	1.17907200
C	-0.13558400	-3.33515300	1.08710500
C	2.06887700	-3.98148800	1.79534300
C	-0.65127200	-4.53670500	1.54959300
H	-0.78777000	-2.60283700	0.62754900
C	1.54633500	-5.17876400	2.28107100
H	3.12979200	-3.79369300	1.88034800
C	0.19284600	-5.46893300	2.15213000
H	-1.71136100	-4.74580000	1.43181200
H	2.21257700	-5.89260600	2.75642200
H	-0.20425100	-6.41065600	2.51938800
C	4.19159400	-1.87577000	0.47216800
C	5.27387300	-0.85158400	0.47799300
C	5.09375400	0.41988800	1.02583900
C	6.49285200	-1.19341100	-0.10781000
C	6.13526500	1.33978000	0.99151500
H	4.13865800	0.68146800	1.46749300
C	7.52582100	-0.26464900	-0.15648700
H	6.60603200	-2.18288300	-0.53694100
C	7.34902100	1.00169500	0.39541500
H	5.99839800	2.32465900	1.42936200
H	8.46850500	-0.52732200	-0.62680000
H	8.15665100	1.72731500	0.36159500
O	4.37586400	-3.03654800	0.19311500
H	2.91187500	-4.18708600	-1.09809000
H	1.16812600	-4.43922800	-1.16144800

H	2.08693900	-4.32990300	-2.66316600
C	2.86522700	-1.56186000	-2.16392000
C	3.98140300	-2.11319700	-2.81631000
C	2.86016100	-0.16737500	-1.98522300
C	5.01741600	-1.31460200	-3.28694300
H	4.04901000	-3.18745300	-2.94855800
C	3.89254200	0.63355300	-2.46223300
H	2.05495600	0.28018500	-1.41415800
C	4.97881600	0.06736900	-3.12089000
H	5.86434300	-1.77890000	-3.78544400
H	3.85091000	1.70922000	-2.31141700
H	5.78962600	0.69122800	-3.48494900
C	-0.53099100	4.24431100	-2.40999300
H	-0.29971800	5.29407200	-2.61919600
H	0.21768200	3.63511600	-2.93328900
C	-1.94115400	3.85835800	-2.86311000
H	-2.65538900	4.56036000	-2.41591800
H	-2.06315800	3.92347900	-3.94949500
H	-1.64596400	1.74131800	-3.02395000
C	0.89448400	4.09418800	-0.26508300
C	1.17004600	5.15051500	0.60536700
C	1.90903000	3.17446400	-0.54111500
C	2.42823600	5.28825600	1.18668400
H	0.38886400	5.87065700	0.83722700
C	3.16625200	3.30504900	0.03744400
H	1.70849700	2.34094500	-1.20822000
C	3.42983000	4.36314800	0.90575700
H	2.62295700	6.11565700	1.86306200
H	3.93642500	2.57418200	-0.18708700
H	4.41165200	4.46694700	1.35886500
C	-3.62190100	1.93487500	-2.27412700
C	-3.87893000	0.56466100	-2.40497900
C	-4.69326800	2.77661600	-1.96112700
C	-5.15183500	0.04321000	-2.20260900
H	-3.06307900	-0.10891900	-2.64778300
C	-5.97168500	2.25993200	-1.75901300
H	-4.53774600	3.84621100	-1.85788100
C	-6.20488100	0.89200000	-1.86946200
H	-5.31611000	-1.02578100	-2.29923000
H	-6.78688200	2.93342200	-1.51003800
H	-7.19975100	0.48909200	-1.70529500
C	-2.77806300	-1.03729400	3.59134400
H	-2.34145900	-1.48134100	4.49219300
H	-3.56119500	-0.34047300	3.91597500

C	-3.40353100	-2.09055700	2.67261700
H	-4.25773200	-2.59560500	3.13684500
H	-2.66004800	-2.85833800	2.43205200
H	-4.71008100	-0.74078300	1.64180700
C	-1.16845200	1.01226200	3.23957700
C	-1.90822500	1.88645800	4.03958500
C	0.08508000	1.43380400	2.77392600
C	-1.42502600	3.16020800	4.33813300
H	-2.87488300	1.58648400	4.43363800
C	0.56413000	2.70567500	3.06450600
H	0.67492900	0.76383700	2.15437500
C	-0.19473100	3.57985700	3.84101000
H	-2.01865300	3.82539500	4.95911900
H	1.52734800	3.01684900	2.67106600
H	0.17630700	4.57687700	4.06034000
C	-4.25353500	-2.27437200	0.24880600
C	-5.57907500	-2.71529200	0.18910800
C	-3.36737400	-2.71150800	-0.73910900
C	-6.00862000	-3.56707200	-0.82379400
H	-6.28656400	-2.37781400	0.94338600
C	-3.79068400	-3.56533200	-1.75389800
H	-2.34450800	-2.35000700	-0.74353500
C	-5.11369000	-3.99672500	-1.80143500
H	-7.04468600	-3.89215600	-0.85258000
H	-3.08227200	-3.88535600	-2.51259900
H	-5.44585700	-4.65979800	-2.59451600

TS3_b4

C	1.53358800	-3.09915400	0.81154100
C	2.61676400	-2.12315000	1.28561500
H	1.98107800	-4.08189200	0.61757600
H	0.78148100	-3.23364700	1.59923900
H	2.88954000	-2.35535900	2.32133100
H	3.52186700	-2.23795200	0.67825900
P	2.16268800	-0.33266500	1.12504000
P	0.56067400	-2.54796800	-0.67330600
C	0.62501000	0.89942600	-2.46500100
C	-0.60249200	1.55652500	-2.49360600
H	0.71901700	0.04111300	-3.13123900
C	-1.73285800	1.82493500	0.05545800
C	-1.03384800	2.80225100	-1.98842500
Cu	0.45487200	-0.20415000	-0.60694800
O	-0.77441200	1.12676700	0.41184600

C	1.25921500	0.14026700	2.71395200
C	3.77092900	0.46511700	1.67091100
H	4.33024400	-0.32064700	2.19756900
C	-0.59708400	-4.02327400	-0.84926200
H	-0.18408200	-4.78187700	-0.17144600
C	1.60451000	-3.06137400	-2.16361800
C	-2.32270100	3.32146200	-2.59283800
C	-2.07403300	3.10115200	0.72349600
C	-3.30504100	3.73911300	0.54012200
C	-1.11641800	3.69180300	1.55396300
C	-3.55968200	4.95905300	1.15761100
H	-4.06558700	3.28183700	-0.08413200
C	-1.36828700	4.91544600	2.15768200
H	-0.16991000	3.18798000	1.70465900
C	-2.58990600	5.55508600	1.95893700
H	-4.51987900	5.44453900	1.01032500
H	-0.60788000	5.37172600	2.78401400
H	-2.78706000	6.51264000	2.43196100
H	-1.41163700	0.97013900	-2.93548500
H	1.54633100	1.45852500	-2.30921800
C	-3.71459400	0.56363700	0.26617500
O	-2.84679600	1.18817000	-0.55976100
O	-3.51525500	0.36714600	1.44120400
C	-4.97128900	0.18303700	-0.43800600
C	-5.14639400	0.37919200	-1.80875600
C	-5.98941600	-0.39545600	0.32123500
C	-6.33204400	-0.01763200	-2.41891800
H	-4.34961300	0.82722800	-2.39091800
C	-7.17473200	-0.78585300	-0.28902100
H	-5.82562400	-0.54298000	1.38330200
C	-7.34495500	-0.60222800	-1.66074500
H	-6.46690200	0.13008800	-3.48595700
H	-7.96632400	-1.23663100	0.30205100
H	-8.26974200	-0.91165500	-2.13885600
C	3.31987400	1.48701800	2.73416300
C	2.32085300	0.75893700	3.63624300
H	0.58266800	0.93610600	2.38484000
C	0.40703800	-0.99009700	3.23867900
C	0.89082700	-1.96035900	4.12153400
C	-0.89711300	-1.12584500	2.74776000
C	0.10401500	-3.05460500	4.47704000
H	1.89126600	-1.87505800	4.53713200
C	-1.68304300	-2.21701500	3.10026400
H	-1.30148500	-0.37146600	2.08042300

C	-1.18115700	-3.19358800	3.95829500
H	0.49849500	-3.79902000	5.16333900
H	-2.68658800	-2.29533100	2.69458600
H	-1.79219000	-4.04904500	4.23345900
C	4.66576800	1.03411400	0.59812100
C	6.04856400	0.85306200	0.67949600
C	4.15806900	1.78766300	-0.46143700
C	6.90150700	1.41702600	-0.26587800
H	6.46286600	0.26120600	1.49253700
C	5.00398700	2.36525500	-1.40235000
H	3.08743000	1.91181500	-0.56376500
C	6.38208600	2.18083700	-1.30863200
H	7.97359500	1.26237100	-0.18417600
H	4.57930100	2.95565900	-2.20898400
H	7.04595600	2.62567000	-2.04395100
C	-0.36294200	-4.52886300	-2.28605200
C	1.14318000	-4.47993600	-2.52874100
H	1.26988000	-2.38556900	-2.96058400
C	3.08286200	-2.83585600	-1.95630900
C	3.93915800	-3.84093900	-1.49754100
C	3.61464900	-1.55673500	-2.16084300
C	5.28000300	-3.57129500	-1.23086400
H	3.56645400	-4.84741700	-1.33527300
C	4.95269400	-1.28571900	-1.89963100
H	2.96533500	-0.75787100	-2.51021200
C	5.79044100	-2.29174100	-1.42431600
H	5.92531800	-4.36766700	-0.87084400
H	5.34028000	-0.28484900	-2.05765800
H	6.83313600	-2.07568700	-1.21224400
C	-2.04389500	-3.82400300	-0.47957000
C	-2.56468200	-4.47006300	0.64304400
C	-2.90792600	-3.06072700	-1.27117700
C	-3.91641100	-4.37338400	0.96350900
H	-1.90278200	-5.05617800	1.27615100
C	-4.26189100	-2.98129400	-0.96800500
H	-2.52252600	-2.53053000	-2.13885100
C	-4.77054400	-3.63513400	0.15220400
H	-4.30003500	-4.88170200	1.84365600
H	-4.92448800	-2.40245200	-1.60314000
H	-5.82777000	-3.55948500	0.38718700
C	-0.09568800	3.82456300	-1.47857000
C	1.04071800	3.48700200	-0.72252100
C	-0.34965500	5.19674000	-1.65132200
C	1.88873400	4.45566500	-0.19748600

H	1.21073300	2.44488500	-0.48403600
C	0.49373200	6.16755200	-1.12287900
H	-1.22282700	5.51888000	-2.20788000
C	1.62592500	5.80710500	-0.39808100
H	2.76098100	4.14946500	0.37558800
H	0.26282900	7.21743400	-1.28282900
H	2.28917800	6.56591100	0.00690700
H	-2.85426200	3.99960800	-1.91625500
H	-2.14269100	3.87336300	-3.52666100
H	-2.99846200	2.49580200	-2.83234600
H	4.18252400	1.87392800	3.28740100
H	2.83593000	2.34312600	2.24390000
H	2.85558400	-0.01631600	4.19896100
H	1.85661500	1.42807700	4.36847000
H	-0.77552100	-5.53603400	-2.40726300
H	-0.87854900	-3.88068100	-3.00551600
H	1.62403800	-5.22455400	-1.88351200
H	1.41060700	-4.72471700	-3.56233200

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