Sterically Controlled Reductive Oligomerisations of CO by Activated Magnesium(I) Compounds: Deltate vs. Ethenediolate Formation

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Electronic Supplementary Information (75 pages)

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1. Experimental

General considerations.

All manipulations were carried out using standard Schlenk and glove box techniques under an atmosphere of high purity dinitrogen. Pentane and diethyl ether were distilled over Na/K alloy (50:50), while hexane, cyclohexane, toluene and THF were distilled over molten potassium. $^1$H and $^{13}$C{$^1$H} NMR spectra were recorded on Bruker Avance III 400 or Bruker Avance III 600 spectrometers and were referenced to the resonances of the solvent used or external SiMe$_4$. Mass spectra were collected using an Agilent Technologies 5975D inert MSD with a solid-state probe. FTIR spectra were collected for solid samples or Nujol mulls on an Agilent Cary 630 attenuated total reflectance (ATR) spectrometer. Microanalyses were carried out at the Science Centre, London Metropolitan University. Melting points were determined in sealed glass capillaries under dinitrogen, and are uncorrected. The compounds (TCHP)NH$_2$, and [(ArNacnac)Mg]$_2$ (Ar = Xyl$^2$, Mes$^3$ or Dep$^4$), were prepared according to the literature procedures. CO gas was dried over P$_2$O$_5$ in prior to use. All other reagents were used as received.

Synthesis of TCHP$\text{NacnacH}$. 2,4,6-tricyclohexylaniline (10.0 g, 29.5 mmol), p-tolylsulfonic acid monohydrate (2.80 g, 14.7 mmol) and acetylacetone (1.50 mL, 14.7 mmol) were dissolved in toluene (150 mL) in a round bottom flask. A Dean-Stark apparatus was attached and the mixture heated at reflux for 72h. After cooling, NEt$_3$ (2.1 mL, 15.0 mmol) was added and the mixture allowed to stir for 1h. The organic phase was washed with water (2 x 30 mL), dried over MgSO$_4$ and evaporated to yield a dark red oil. Cold methanol was added to the oil to yield the title compound as an off-white solid after filtration and drying (9.16 g, 83%). Crystals suitable for X-ray crystallographic studies were obtained by slow evaporation of a solution of TCHP$\text{NacnacH}$ in diethyl ether. M.p. 103-105 °C. $^1$H NMR (400 MHz, C$_6$D$_6$, 298 K): N.B. integration of resonances for cyclohexyl groups are estimated due to complex overlapping signals, and small amounts of unknown impurities. $\delta$ 1.21-2.03 (m, 60H, Cy-CH$_2$), 1.72 (s, 6H, NCCCH$_3$), 2.52-2.59 (m, 2H, Cy-CH), 2.98-3.05 (m, 4H, Cy-CH), 4.84 (s, 1H, NCCCH), 7.18 (s, 4H, ArH), 11.63 (br, 1H, NH); $^{13}$C{$^1$H} (101 MHz, C$_6$D$_6$, 298 K): $\delta$ 21.4 (NCCCH$_3$), 26.9, 27.5, 27.6, 27.7, 34.5, 35.3, 39.3, 45.2 (Cy-C), 94.5 (NCCCH), 123.0, 139.5, 141.6, 144.6 (ArC), 161.4 (NCCCH$_3$); IR v/cm$^{-1}$ (ATR): 1654 (m), 1617 (m), 1545 (m), 1492 (m), 1117 (m), 1076 (w), 1029 (w), 949 (w), 920
(w), 861 (m), 797 (w), 777 (w), 744 (m), 699 (m); acc. mass/ESI m/z: calc. for [M+H]$^+$ 743.6238 found: 743.6231.

**Figure S1.** $^1$H NMR spectrum (400 MHz, 298 K, C$_6$D$_6$) of $^{15}$CH$_2$NacnacH.
Synthesis of [(\textsuperscript{TCHP}Nacnac)MgI(OEt\textsubscript{2})]. Mg turnings (78 mg, 3.33 mmol) were placed in a Schlenk flask and placed under vacuum. After 20 minutes, diethyl ether (5 mL) and a crystal of I\textsubscript{2} were added. After the iodine had been consumed, a reflux condenser was added and MeI (0.234 mL, 3.76 mmol) in diethyl ether (5 mL) was added. The resultant suspension was heated at reflux for 4h. The freshly prepared MeMgI solution was cooled and was subsequently added to a suspension of \textsuperscript{TCHP}NacnacH (2.00 g, 2.69 mmol) in diethyl ether (20 mL), and the mixture stirred overnight. The resultant solution was filtered, concentrated \textit{in vacuo} and stored at −30 °C to yield colourless crystals of the title compound. A second crop of crystals could be obtained from further concentration and storage of the supernatant solution at −30 °C (1.44 g, 55 %). M.p. 162-165 °C (decomp): \textsuperscript{1}H NMR (400 MHz, C\textsubscript{6}D\textsubscript{6}, 298 K) N.B. integrations for cyclohexyl groups are estimated due to complex overlapping signals: δ 1.11 (t, \textit{J}_{HH} = 7.0 Hz, 6H, OCH\textsubscript{2}CH\textsubscript{3}), 1.32-1.45 (m, 11H, Cy-H), 1.48 (s, 6H, NCCCH\textsubscript{3}), 1.51-2.00 (m, 45H, cyclohexyl CH\textsubscript{2}), 2.27-2.31 (m, 4H, Cy-CH\textsubscript{2}), 2.69-2.74 (m, 2H, Cy-CH), 2.79-2.86 (m, 4H, Cy-CH), 3.26
(q, $J_{HH} = 7.0$ Hz, 4H, CH$_3$CH$_2$O), 4.64 (s, 1H, NCCH), 7.14 (s, 4H, ArH); $^{13}$C{${}^1$H} (101 MHz, C$_6$D$_6$, 298 K): $\delta$ 15.5 (CH$_3$CH$_2$O), 25.3 (NCCH$_3$), 26.9, 27.0, 27.7, 27.9, 28.3, 34.7, 35.2, 35.9, 40.1, 44.8 (Cy-C), 66.0 (CH$_3$CH$_2$O), 95.2 (NCCH), 123.1, 141.4, 142.8, 144.0 (ArC), 170.7 (NCCH); IR $\nu$/cm$^{-1}$ (Nujol): 1618 (m), 1546 (s), 1143 (w), 1115 (w), 1086 (w), 1017 (w), 997 (w), 949 (w), 925 (w), 890 (w), 862 (m), 842 (w); EI/MS (70eV) m/z (%): 83.1 (Cy$^+$, 23), 364.3 Cy$_3$C$_6$H$_2$NCH$_3$+, 100), 659.6 (TCHP$^{+}$NacnacH–Cy$^+$, 13), 727.8 (TCHP$^{+}$NacnacH–CH$_3$+, 23), 742.8 (TCHP$^{+}$NacnacH$^+$, 13); anal. calc. for C$_{57}$H$_{87}$IMgN$_2$O: C 70.76 %, H 9.06 %, N 2.90 %; found: C 70.66 %, H 8.86 %, N 2.83 %.

Figure S3. $^1$H NMR spectrum (400 MHz, 298 K, C$_6$D$_6$) of [(TCHP$^{+}$Nacnac)MgI(OEt$_2$)].
Figure S4. $^{13}$C{$^{1}$H} NMR spectrum (101 MHz, 298 K, C$_6$D$_6$) of [($^{\text{TCHP}}$Nacnac)MgI(OEt$_2$)].

**Synthesis of [($^{\text{TCHP}}$Nacnac)Mg$_2$], 5.** [($^{\text{TCHP}}$Nacnac)MgI(OEt$_2$)] (700 mg, 0.72 mmol) was dissolved in a 4:1 mixture of toluene/diethyl ether (20 mL/5 mL) and the solution stirred over a sodium mirror (120 mg, 7.2 mmol) at room temperature. The progress of the reaction was monitored by $^1$H NMR spectroscopy until all [($^{\text{TCHP}}$Nacnac)MgI(OEt$_2$)] was consumed (ca. 96h), after which the solution was filtered, the filtrate concentrated *in vacuo* and stored at −30 °C to yield yellow crystals of [($^{\text{TCHP}}$Nacnac)Mg$_2$]. A second crop was obtained from further concentration of the supernatant solution and storage at −30 °C (405 mg, 73 %). M.p. > 260 °C. $^1$H NMR (400 MHz, C$_6$D$_6$, 298 K) N.B. integration for cyclohexyl groups are estimated due to complex overlapping signals: δ 1.21-1.41 (m, 20H, Cy-$CH_2$), 1.44 (s, 12H, NCC$_3$H), 1.46-1.60 (m, 40H, Cy-$CH_2$), 1.67-2.01 (m, 52H, Cy-$CH_2$), 2.34-2.38 (br. m, 8H, Cy-$CH_2$), 2.69-2.77 (br. m, 12H, Cy-$CH$), 4.72 (s, 2H, NCC$H$), 7.12 (s, 8H, ArH); $^{13}$C{$^{1}$H} NMR (101 MHz, C$_6$D$_6$, 298 K) δ 25.2 (NC$C$_3$H$), 26.9, 27.0, 27.7, 28.1, 28.5, 33.9, 35.1, 35.2, 39.9, 44.6 (Cy-$C$), 95.7
(NCCH), 123.0, 141.1, 143.3, 145.2 (ArC), 168.5 (NCCH₃); IR ν/cm⁻¹ (ATR): 1528 (m), 1115 (m), 1069 (m), 1028 (w), 992 (w), 920 (w), 727 (m), 695 (s); EI/MS (70eV) m/z (%): 83.1 (Cy⁺, 22), 364.3 Cy₃C₆H₂NCMe⁺, 100), 659.6 (TCHPＮacnacH–Cy⁺, 11), 727.8 (TCHPＮacnacH–CH₃⁺, 21), 742.8 (TCHPＮacnacH⁺, 13); anal. calc. for C₁₀₆H₁₅₄Mg₂N₄: C 83.05 %, H 10.13 %, N 3.65 %; found: C 82.88 %, H 9.92 %, N 3.55 %.

![Figure S5. 1H NMR spectrum (400 MHz, 298 K, C₆D₆) of [{(TCHP Nacnac)Mg}₂].](image)
Figure S6. $^{13}$C$\{^1$H$\}$ NMR spectrum (101 MHz, 298 K, C$_6$D$_6$) of [[$^{(TCHP}$Nacnac)Mg]$_2$].

**Synthesis of [(XylNacnac)(DMAP)Mg–Mg(XylNacnac)], 6.** [[$[^{(Xyl}$Nacnac)Mg]$_2$] (200 mg, 0.304 mmol) and DMAP (37 mg, 0.304 mmol) were dissolved in toluene (10 mL) at -78 °C. This resulted in an orange-red solution. The mixture was stirred for 1 h, warmed to room temperature, filtered, and the filtrate concentrated to ca. 3 mL in vacuo and layered with hexane. The filtrate was then placed at -30 °C for 2 d, after which time red-orange crystals of 6 had deposited. These were isolated and a second crop obtained from the mother liquor (129 mg, 54 %). M.p: 157-160 °C; $^1$H NMR (600 MHz, toluene-$d_8$, 298 K) δ 1.59 (s, 12H, NC$_3$H$_3$), 1.94 (s, 24H, ortho-CH$_3$), 2.19 (s, 6H, N(CH$_3$)$_2$), 4.85 (s, 2H, CH), 5.98 (d, $^3$J$_{HH}$ = 6.1 Hz, 2H, DMAP-ArH), 6.96-7.10 (m, 12H, ArH), 7.90 (d, $^3$J$_{HH}$ = 6.0 Hz, 2H, DMAP-ArH); $^{13}$C $^1$H NMR (151 MHz, toluene-$d_8$, 298 K) δ 20.1 (ortho-CH$_3$), 24.0 (NC$_3$H$_3$), 38.4 (N(CH$_3$)$_2$), 94.9 (CH), 106.5 (DMAP-ArC), 123.8, 128.7, 132.7, 149.8 (ArC), 150.5, 154.9 (DMAP-ArC), 165.4 (NC$_3$H$_3$); IR ν/cm$^{-1}$ (Nujol): 1610 (m), 1517 (m), 1266 (m), 1225 (m), 1178 (s), 1005 (m), 833 (m), 755 (s); MS (EI, 70 eV): m/z (%): 659.6 ([($^{(Xyl}$Nacnac)Mg]$_2$ $^+$), 5), 329.2 ([($^{(Xyl}$Nacnac)Mg] $^+$, 68), 146.1 (MeCNXyl $^+$, 100);
anal. calc. for C_{49}H_{60}Mg_{2}N_{6}: C 75.29 %, H 7.74 %, N 10.75 %; found: C 75.19 %, H 7.91 %, N 10.56 %.

Figure S7. Variable temperature $^1$H NMR spectra (400 MHz, toluene-$d_8$) of 6.
Figure S8. $^1$H NMR spectrum (600 MHz, 298 K, toluene-$d_8$) of 6.

Figure S9. $^{13}$C{$^{1}$H} NMR spectrum (151 MHz, 298 K, toluene-$d_8$) of 6.
Synthesis of $\left\{\left(\text{XylNacnac}\right)\text{Mg}\left(\text{DMAP}\right)\right\}_2$. \left\{\left(\text{XylNacnac}\right)\text{Mg}\right\}_2$ (150 mg, 0.228 mmol) and DMAP (56 mg, 0.456 mmol) were dissolved in toluene (8 mL) at room temperature. This resulted in an intense red solution. The mixture was stirred for 1h, filtered, and the filtrate concentrated to ca. 4 mL in vacuo. The filtrate was then placed at -30 °C for 1 d, after which time dark red crystals of the title compound had deposited. These were isolated and a second crop obtained from the mother liquor (111 mg, 54 %). M.p. 148-151 °C; $^1$H NMR (400 MHz, C$_6$D$_6$, 298 K) δ 1.69 (s, 12H, NCC$_3$H$_3$), 2.02 (s, 24H, ortho-CH$_3$), 2.16 (s, 12H, N(C$_3$H$_3$)$_2$), 4.95 (s, 2H, CH), 6.04 (d, $^3$J$_{HH}$ = 6.0 Hz, 4H, DMAP-ArH), 7.00 (d, $^3$J$_{HH}$ = 1.7 Hz, 2H, ArH), 7.05 (d, $^3$J$_{HH}$ = 6.0 Hz, 4H, ArH), 7.11 (s, 6H, ArH), 8.23 (d, $^3$J$_{HH}$ = 5.9 Hz, 4H, DMAP-ArH); $^{13}$C\{$^1$H\} NMR (101 MHz, C$_6$D$_6$, 298 K) δ 19.9 (ortho-CH$_3$), 23.9 (NCCH$_3$), 38.1 (N(CH$_3$)$_2$), 94.2 (CH), 106.4 (DMAP-ArC), 123.3, 128.1, 132.6 (ArC), 150.0 (DMAP-ArC), 150.9 (ArC), 154.3 (DMAP-ArC), 164.7 (NCCH$_3$); IR ν/cm$^{-1}$ (Nujol): 1610 (s), 1545, 1517 (w), 1268 (m), 1177 (m), 1092 (w), 1005 (m), 806 (s), 760 (m); MS (EI, 70 eV): m/z (%) = 329.2 (\{XylNacnac\}Mg$^+$, 28),
146.1 (MeCNXyl’, 100); anal. calc. for C₅₆H₇₀Mg₂N₈: C 74.42 %, H 7.81 %, N 12.40 %: found: C 74.12 %, H 7.96 %, N 12.22 %.

Figure S11. "H NMR spectrum (400 MHz, 298 K, C₆D₆) of [(XylNacnac)Mg(DMAP)]₂."
Figure S12. $^{13}$C{$^1$H} NMR spectrum (101 MHz, 298 K, C$_6$D$_6$) of [($^{\text{Xyl}}$Nacnac)Mg(DMAP)$_2$].
Synthesis of [(DepNacnac)(DMAP)Mg—Mg(DepNacnac)], 8. [(DepNacnac)Mg]$_2$ (150 mg, 0.195 mmol) and DMAP (24 mg, 0.195 mmol) were dissolved in toluene (8 mL) at -78 °C. This resulted in an orange-red solution. The mixture was stirred for 1h, warmed to room temperature, filtered, and the filtrate concentrated to ca. 2 mL in vacuo and layered with hexane. The filtrate was then placed at -30 °C for 3 d, after which time red-orange crystals of 8 had deposited. These were isolated and a second crop obtained from the mother liquor (71 mg, 41 %). M.p. 124-127 °C; $^1$H NMR (400 MHz, C$_6$D$_6$, 298 K) δ 1.11 (t, $^3$J$_{HH}$ = 7.5 Hz, 24H, CH$_2$C$_3$H), 1.64 (s, 12H, NCCCH$_3$), 2.19 (s, 6H, N(CH$_3$)$_2$), 2.32 – 2.38 (m, 8H, CH$_2$CH$_3$), 2.43 – 2.50 (m, 8H, CH$_2$CH$_3$), 4.94 (s, 2H, CH), 6.02 (d, $^3$J$_{HH}$ = 6.0 Hz, 2H, DMAP-ArH), 7.15 (s, 12H, ArH), 7.99 (d, $^3$J$_{HH}$ = 6.1 Hz, 2H, DMAP-ArH); $^{13}$C {$^1$H} NMR (101 MHz, C$_6$D$_6$, 298 K) δ 14.5 (CH$_2$CH$_3$), 24.1 (NCCH$_3$), 25.2 (CH$_2$CH$_3$), 38.1 (N(CH$_3$)$_2$), 95.0 (CH), 106.1 (DMAP-ArC), 123.9, 125.8, 137.6, 149.1 (ArC), 149.7, 154.5 (DMAP-ArC), 165.9 (NCCH$_3$); IR v/cm$^{-1}$ (Nujol): 1510 (s), 1520 (s), 1265 (m), 1226 (s), 1174 (s), 1003 (m), 796 (m), 755 (s); MS (EI, 70 eV): $m/z$ (%) = 557.5
(\{^{\text{DepNacnac}}Mg\}_2-4\text{CH}_2\text{CH}_3^+, 49), 385.3 (\{^{\text{DepNacnac}}Mg^+, 82\}, 174.2 (\text{MeCNDep}^+, 100); \text{anal. calc. for } C_{57}H_{76}Mg_2N_6: C \text{ 76.59 }\% , H 8.57 \%, N 9.40 \%; \text{ found: } C 76.42 \%, H 8.63 \%, N 9.48 \%.

**Figure S14.** Variable temperature $^1$H NMR spectra (400 MHz, toluene-$d_8$) of 8.
Figure S15. Excerpt of variable temperature $^1$H NMR spectra (400 MHz, toluene-$d_8$) of 8.

Figure S16. $^1$H NMR spectrum (400 MHz, 298 K, C$_6$D$_6$) of 8.
Figure S17. $^{13}$C($^1$H) NMR spectrum (101 MHz, 298 K, C$_6$D$_6$) of 8.

Figure S18. HMQC spectrum ($^1$H: 400 MHz; $^{13}$C: 101 MHz, 298 K, C$_6$D$_6$) of 8.
Synthesis of $\left[\text{[DepNacnac]Mg(DMAP)}\right]_2$. $\left[\text{[DepNacnac]Mg}\right]_2$ (200 mg, 0.259 mmol) and DMAP (63 mg, 0.518 mmol) were dissolved in toluene (8 mL) at room temperature. This resulted in an intense red solution. The mixture was stirred for 1 h, filtered, and the filtrate concentrated to ca. 4 mL in vacuo. The filtrate was then placed at -30 °C for 2 d, after which time dark red crystals of the title compound had deposited. These were isolated and a second crop obtained from the mother liquor (108 mg, 41 %). M.p. 145-148 °C; $^1$H NMR (400 MHz, C$_6$D$_6$, 298 K) δ 1.11 (t, $^3$J$_{HH} = 7.6$ Hz, 24H, CH$_2$CH$_3$), 1.68 (s, 12H, NCH$_3$), 2.20 (s, 12H, N(CH$_3$)$_2$), 2.20 – 2.38 (m, 8H, CH$_2$CH$_3$), 2.47 – 2.55 (m, 8H, CH$_2$CH$_3$), 4.98 (s, 2H, CH), 6.03 (br, 4H, DMAP-ArH), 7.14-7.18 (m, 12H, ArH), 8.19 (br, 4H, DMAP-ArH); $^{13}$C-$^1$H NMR (101 MHz, C$_6$D$_6$, 298 K) δ 14.6 (CH$_2$CH$_3$), 24.3 (NCCH$_3$), 25.2 (CH$_2$CH$_3$), 38.2 (N(CH$_3$)$_2$), 94.8 (CH), 106.3 (DMAP-ArC), 123.7, 125.7, 137.8, 149.9 (ArC), 150.1, 154.3 (DMAP-ArC), 165.5 (NCCH$_3$); IR ν/cm$^{-1}$ (Nujol): 1608 (s), 1514 (s), 1268 (m), 1225 (m), 1173 (s), 1103 (w), 1002 (s), 927 (w), 799 (m), 760 (m); MS (EI, 70 eV): m/z (%) = 557.5 ($\left[\text{[DepNacnac]Mg}\right]_2$-4CH$_2$-CH$_3^+$, 43), 385.4 ($\text{[DepNacnac]Mg}^+$, 86), 174.2 (MeCNDep$^+$, 100); anal. calc. for C$_{64}$H$_{86}$Mg$_2$N$_8$: C 75.66 %, H 8.53 %, N 11.03 %; found: C 75.49 %, H 8.71 %, N 10.90 %.

Figure S19. $^1$H NMR spectrum (400 MHz, 298 K, C$_6$D$_6$) of $\left[\text{[DepNacnac]Mg(DMAP)}\right]_2$. S18
Figure S20. $^{13}$C{$^1$H} NMR spectrum (101 MHz, 298 K, C$_6$D$_6$) of [{(DepNacnac)Mg(DMAP)}$_2$].

Figure S21. HMQC spectrum ($^1$H: 400 MHz; $^{13}$C: 101 MHz, , 298 K, C$_6$D$_6$) of [{(DepNacnac)Mg(DMAP)}$_2$].
Comments on variable temperature $^1$H NMR spectroscopic studies of DMAP adduct complexes 6 and 8.

Similar to the previous report on 4,5 variable temperature NMR spectroscopic studies of the adducts 6 and 8 revealed fluxional behavior, which is believed to arise from rapid "hopping" of the DMAP ligand between the two Mg centers. This is rapid on the NMR timescale at room temperature, as evidenced by the presence of one set of β-diketiminate signals in their spectra. Cooling $d_8$-toluene solutions of 6 and 8 leads to their $^1$H NMR spectra resolving to exhibit two sets of ligand β-diketiminate signals, typically at temperatures below -20 °C.

Synthesis of [(DepNacnac)Mg(µ-C₃O₂)Mg(DMAP)(DepNacnac)]₂, 9. [(DepNacnac)Mg]₂ (150 mg, 0.195 mmol) and DMAP (24 mg, 0.195 mmol) were dissolved in toluene (7 mL) at -78 °C. This resulted in an orange-red solution. The mixture was stirred for 1h, then warmed to room temperature. The orange-red solution was cooled to -78 °C for 30 minutes, then the reaction vessel placed under vacuum, and backfilled with excess CO gas. The solution was stirred for 1h, warmed to room temperature, and left overnight to yield a dark red brown solution. The mixture was then filtered, and the filtrate concentrated to ca. 2 mL in vacuo, and layered with hexane in a long, thin Schlenk flask. This was then placed at -30 °C for 3 d, after which time colourless crystals of 9 had deposited. These were isolated and a second crop obtained from the mother liquor (36 mg, 19 %). M.p. 213-216 °C; $^1$H NMR (400 MHz, THF-$d_8$, 298 K) δ 0.90 (t, $^3$J$_{HH}$ = 7.6 Hz, 24H, CH$_2$CH$_3$), 1.11 (t, $^3$J$_{HH}$ = 7.6 Hz, 24H, CH$_2$CH$_3$), 1.45 (s, 12H, NCCH$_3$), 1.67 (s, 12H, NCCH$_3$), 2.40 (q, $^3$J$_{HH}$ = 7.5 Hz, 8H, CH$_2$CH$_3$), 2.46 – 2.53 (m, 8H, CH$_2$CH$_3$), 2.56 (q, $^3$J$_{HH}$ = 7.5 Hz, 16H, CH$_2$CH$_3$), 2.94 (s, 12H, N(CH$_3$)$_2$), 4.56 (s, 2H, CH), 4.89 (s, 2H, CH$_2$), 6.48 (d, $^3$J$_{HH}$ = 6.8 Hz, 4H, DMAP-ArH), 6.85 (s, 12H, ArH), 7.03 – 7.09 (m, 12H, ArH), 7.94 (d, $^3$J$_{HH}$ = 5.9 Hz, 4H, DMAP-ArH); $^{13}$C{$^1$H} NMR (101 MHz, THF-$d_8$, 298 K) δ 14.7, 14.8 (CH$_2$CH$_3$), 23.7 (NCCH$_3$) 24.6, 24.7 (CH$_2$CH$_3$), 39.0 (N(CH$_3$)$_2$), 93.5, 94.9 (CH), 107.3 (DMAP-ArC), 124.1, 125.1, 125.9, 126.4, 137.5, 138.3, 147.5, 148.5 (ArC), 150.0, 155.6 (DMAP-ArC), 166.9, 169.0 (NCCH$_3$), C$_3$O$_2$ resonance not observed; IR ν/cm$^{-1}$ (Nujol): 1621 (s), 1526 (m), 1391 (m), 1267 (m), 1228 (w), 1176 (s), 1106 (w), 1011 (vs), 801 (m), 760 (m); MS (EI, 70 eV): m/z (%) = 362.3 (DepNacnacH$^+$, 31), 347.3 (DepNacnacH-CH$_3^+$, 36), 333.2 (DepNacnacH-CH$_2$CH$_3^+$, 25),
174.1 (MeCNDep⁺, 100). Due to persistent contamination with trace amounts of an unknown impurity, a satisfactory reproducible microanalysis could not be obtained.

Figure S22. ¹H NMR spectrum (400 MHz, 298 K, THF-d₈) of 9.
Figure S23. $^{13}\text{C}^{1\text{H}}$ NMR spectrum (101 MHz, 298 K, THF-$d_8$) of 9.

Figure S24. HMQC spectrum ($^1\text{H}$: 400 MHz; $^{13}\text{C}$: 101 MHz, 298 K, THF-$d_8$) of 9.
Synthesis of \[\{(\text{XylNacnac})\text{Mg}\{\mu-\text{OC(H)=C(DMAP-H)}\text{O}\}\text{Mg(\text{XylNacnac})}\}\], 10.

\[\{(\text{XylNacnac})\text{Mg}\}\] (150 mg, 0.228 mmol) and DMAP (28 mg, 0.228 mmol) were dissolved in toluene (6 mL) at -78 °C. This resulted in an orange-red solution. The mixture was stirred for 1 h, then warmed to room temperature. The orange-red solution was cooled down to -78 °C for 30 minutes, then the reaction vessel was placed under vacuum, before being backfilled with excess CO gas. The solution was then stirred for 1 h, warmed to room temperature, and stirred overnight, yielding a dark red-brown solution with a colourless solid suspended. The colourless solid was isolated and extracted with hot THF (ca. 20 mL), then placed at -30 °C for 2 days, after which time a few colourless crystals of 10 had deposited. The dark red-brown filtrate was concentrated to ca. 3 mL in vacuo, placed at room temperature for 3 d, after which time colourless 10 deposited. The two crops of the title compound were then combined (71 mg, 37 %). N.B. Once crystallised, compound 10 has negligible solubility in THF-\(d_8\), so meaningful solution state spectroscopic data could not be obtained. M.p. > 260 °C; IR ν/cm\(^{-1}\) (Nujol): 1582 (s), 1513 (m), 1279 (m), 1202 (m), 1180 (w), 1094 (w), 1056 (w), 1008 (s), 904 (m), 836 (w), 763 (s); MS (EI, 70 eV): \(m/z\) (%) = 837.6 (M/2+H\(^+\), 19), 329.1 (\{(\text{XylNacnac})\text{Mg}\}\(^+\), 16), 146.1 (MeCNXyl\(^+\), 100); anal. calc. for \(\text{C}_{102}\text{H}_{120}\text{Mg}_4\text{N}_{12}\text{O}_4\): C 73.12 %, H 7.22 %, N 10.03 %; found: C 72.77 %, H 7.36 %, N 9.61 %.

Synthesis of \[\{(\text{MesNacnac})\text{Mg}\{\mu-\text{OC(H)=C(DMAP-H)}\text{O}\}\text{Mg(\text{MesNacnac})}\}\], 11.

\[\{(\text{MesNacnac})\text{Mg}\}\] (151 mg, 0.211 mmol) and DMAP (26 mg, 0.211 mmol) were dissolved in toluene (6 mL) at -78 °C. This resulted in an orange-red solution. The mixture was stirred for 1 h, then warmed to room temperature. The orange-red solution was cooled down to -78 °C for 30 minutes, then the reaction vessel was placed under vacuum, and backfilled with excess CO gas. The solution was then stirred for 1 h, warmed to room temperature, and stirred overnight, yielding a dark purple solution. This was filtered, and the filtrate concentrated to ca. 3 mL in vacuo, then layered with hexane. After 4 d at room temperature colourless crystals of 11 deposited. These were isolated and a second crop obtained from the mother liquor (78 mg, 41 %). N.B. Compound 11 is only partially soluble in THF-\(d_8\), and when dissolved, spectra unavoidably contain signals resulting from the β-diketimine, \(\text{MesNacnac}\)-H. M.p. > 260 °C; \(^1\)H NMR (600 MHz, THF-\(d_8\), 298 K) δ 0.84 (s, 12H, NCCH\(_3\)), 0.93 (s, 12H, ArCH\(_3\)), 1.43 (s, 12H, S23
NCC\textsubscript{3}), 1.63 (s, 12H, ArCH\textsubscript{3}), 1.94 (s, 12H, ArCH\textsubscript{3}), 2.12 (s, 24H, ArCH\textsubscript{3}), 2.31 (s, 12H, ArCH\textsubscript{3}), 2.97 (s, 12H, N(CH\textsubscript{3})\textsubscript{2}), 4.08 (s, 2H, CH), 4.91 (s, 2H, CH), 6.00 (d, J = 2.6 Hz, 2H, DMAP-ArH), 6.13 (dd, J = 6.6, 2.6 Hz, 2H, DMAP-ArH), 6.27 (s, 2H, OHC=COC), 6.61 (s, 4H, ArH), 6.62 (s, 4H, ArH), 6.66 (s, 4H, ArH), 6.67 (s, 4H, ArH), 8.26 (d, J = 6.5 Hz, 2H, DMAP-ArH); $^{13}$C\textsuperscript{1}H NMR (151 MHz, THF-\textit{d}8, 298 K) δ 18.9, 19.0, 19.2, 19.4, 20.9, 21.6 (ArCH\textsubscript{3}), 22.9, 24.2 (NCH\textsubscript{3}), 39.1 (N(CH\textsubscript{3})\textsubscript{2}), 87.5 (CH), 94.5 (DMAP-ArC), 96.3 (CH), 103.4 (DMAP-ArC), 128.2, 129.4, 129.6, 130.1, 130.6, 131.1, 132.1, 133.1, 133.4, 134.0, 137.4 (ArC), 138.4 (OHC=COC), 147.4 (DMAP-ArC), 147.9 (ArC), 148.5, 154.8 (DMAP-ArC), 159.9 (OHC=COC), 168.8, 169.3 (NCH\textsubscript{3}); IR ν/cm\textsuperscript{-1} (Nujol): 1617 (w), 1576 (w), 1514 (w), 1278 (w), 1227 (m), 1193 (s), 1060 (m), 1005 (s), 904 (w), 852 (s), 798 (m), 728 (s); MS (EI, 70 eV): m/z (%) = 334.3 (\textsuperscript{14}MeCNacnacH\textsuperscript{+}, 21), 160.2 (MeCNMes\textsuperscript{+}, 41); anal. calc. for C\textsubscript{110}H\textsubscript{136}Mg\textsubscript{4}N\textsubscript{12}O\textsubscript{4}: C 73.91 %, H 7.67 %, N 9.40 %; found: C 73.46 %, H 7.98 %, N 9.61 %.

**Figure S25.** $^{1}$H NMR spectrum (600 MHz, 298 K, THF-\textit{d}8) of 11 (FL denotes signal arising from co-crystallised \textsuperscript{14}MeCNacnacH).
Figure S26. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (151 MHz, 298 K, THF-$d_8$) of 11 (FL denotes signal arising from co-crystallised $\text{Me}^\text{NacnacH}$).
Figure S27. HMQC spectrum ($^1$H: 600 MHz; $^{13}$C: 151 MHz, 298 K, THF-$d_8$) of 11.

2. X-Ray Crystallographic Studies

Crystals suitable for X-ray structural determination were mounted in silicone oil. Crystallographic measurements were made using either an Rigaku Xtalab Synergy Dualflex diffractometer with a graphite monochromator with Mo Kα radiation ($\lambda = 0.71073$ Å) or Cu Kα radiation ($\lambda = 1.54180$ Å); or the MX2 beamline of the Australian Synchrotron ($\lambda = 0.71090$ Å). The software package Blu-Ice$^6$ was used for synchrotron data acquisition, while the program XDS$^7$ was employed for synchrotron data reduction. All structures were solved by direct methods and refined on $F^2$ by full matrix least squares (SHELX-16$^8$) using all unique data. Hydrogen atoms are typically included in calculated positions (riding model). Compound 5 co-crystallised with 1.7 % of the bridging iodide compound, $\{[(^{\text{TCHP}}\text{Nacnac})\text{Mg}(\mu-\text{I})]\}_2$, and 6.5 % of the bridging hydroxide compound, $\{[(^{\text{TCHP}}\text{Nacnac})\text{Mg}(\mu-\text{OH})]\}_2$. Repeated re-crystallisations could not remove these contaminants, as has been found previously in the synthesis of magnesium(I) compounds.$^3$ Compound 10 crystallised with 4 molecules of heavily disordered THF in the asymmetric unit (8 THFs/molecule of 10). All attempts to model this disorder were
unsatisfactory. As a result, the SQUEEZE program\textsuperscript{9} was used to remove their contribution to the structure factors. The final refinement of the structure included the contribution of the THF molecules to the empirical formula and F(000). The relatively high R1 and wR2 values for the crystal structures of 9 and 10 are due to weak diffraction data above \( \theta \) angles of 23°. Despite this, the molecular connectivities of the compounds are unambiguous, and their presented metrical parameters are reliable within the calculated esd values. Crystal data, details of data collections and refinements for all structures can be found in their CIF files and are summarized in Table S1.
Table S1. Crystal data for 5, 6, 8-11, TCHPNaClH 1S, [(TCHPNaClH)MgI(OEt)] 2S, [(Xy1NaClH)Mg(DMAP)] 3S and [(DepNaClH)Mg(DMAP)] 4S.

|                      | 5·(toluene)_{4.5} | 6 | 8 | 9·(cyclohexyl)_{4}·(toluene) | 10·(THF)_{4} | 11·(toluene) |
|----------------------|-------------------|---|---|-----------------------------|--------------|------------|
| **empirical formula** | C_{137.50}H_{189.63}Mg_{2}N_{4}O_{0.13} | C_{45}H_{60}Mg_{2}N_{6} | C_{57}H_{60}Mg_{2}N_{6} | C_{151}H_{208}Mg_{2}N_{12}O_{6} | C_{134}H_{184}Mg_{4}N_{12}O_{12} | C_{117}H_{144}Mg_{4}N_{12}O_{4} |
| **formula weight**   | 1953.69           | 781.65                     | 893.85                      | 2384.52                    | 2252.16                | 1879.67            |
| **crystal system**   | monoclinic        | monoclinic                 | monoclinic                  | triclinic                  | monoclinic             | triclinic            |
| **space group**      | P_{2}/n           | P_{2}/c                     | P_{2}/c                      | P-1                        | P_{2}/c                 | P-1                  |
| **a (Å)**            | 18.2067(10)       | 12.4858(2)                 | 18.7194(2)                  | 17.9190(6)                 | 15.480(3)               | 15.1058(2)          |
| **b (Å)**            | 26.32970(10)      | 12.0704(2)                 | 11.31290(10)                | 19.6004(9)                 | 15.114(3)               | 19.0783(2)          |
| **c (Å)**            | 25.8355(2)        | 31.1338(2)                 | 26.0645(3)                  | 20.9467(7)                 | 27.505(6)               | 20.0582(2)          |
| **α (°)**            | 90                | 90                         | 90                          | 79.292(3)                  | 90                      | 85.7620(10)         |
| **β (°)**            | 105.8060(10)      | 92.7620(10)                | 103.7910(10)                | 75.685(3)                  | 103.08(3)               | 88.9090(10)         |
| **γ (°)**            | 90                | 90                         | 90                          | 86.860(3)                  | 90                      | 66.9980(10)         |
| **V (Å³)**           | 11916.66(13)      | 4686.68(13)                | 5360.57(10)                 | 7004.0(5)                  | 6268(2)                 | 5306.17(11)         |
| **Z**                | 4                 | 4                          | 4                           | 2                          | 2                       | 2                    |
| **T (K)**            | 123(2)            | 123(2)                     | 123(2)                      | 123(2)                     | 100(2)                  | 123(2)               |
| **ρ_{calc} (g·cm⁻³)**| 1.089             | 1.108                      | 1.108                       | 1.131                      | 1.193                   | 1.176                |
| **μ (mm⁻¹)**         | 0.623             | 0.743                      | 0.704                       | 0.687                      | 0.094                   | 0.767                |
| **F(000)**           | 4278              | 1680                       | 1936                        | 2588                       | 2432                    | 2020                 |
| **reflms collected** | 121487            | 45801                      | 51963                       | 137379                     | 71723                   | 100505               |
|                         | 1S·(Et₂O) | 2S | 3S·(toluene)₂ | 4S·(toluene)₂ |
|-------------------------|-----------|----|---------------|---------------|
| empirical formula       | C₅₇H₈₈N₂O | C₅₇H₆₇Mg₂N₂O | C₇₀H₆₈Mg₂N₈ | C₇₁H₈₄Mg₂N₈ |
| formula weight          | 817.29    | 967.49 | 1154.54       | 1108.16       |
| crystal system          | monoclinic | triclinic | monoclinic   | monoclinic   |
| space group             | P2₁/n     | P-1     | C2/c          | P2₁/c         |
| a (Å)                   | 16.2198(7) | 10.4370(2) | 18.7699(3)   | 12.8246(2)    |
| b (Å)                   | 10.7700(6) | 14.8235(4) | 15.7829(2)   | 21.5786(3)    |
| c (Å)                   | 28.9971(15)| 18.7188(5) | 22.8274(4)   | 24.2161(3)    |
| α (°)                   | 90         | 84.547(2)  | 90            | 90            |
| β (°)                   | 96.100(4)  | 75.886(2)  | 109.172(2)    | 103.4930(10)  |
| γ (°)                   | 90         | 71.426(2)  | 90            | 90            |
| V (Å³)                  | 5036.7(4)  | 2661.85(12)| 6387.40(19)  | 6516.52(16)   |
| Z                       | 4          | 2          | 4             | 4             |
| Parameter                          | Value 1 | Value 2 | Value 3 | Value 4 |
|-----------------------------------|---------|---------|---------|---------|
| T (K)                             | 123(2)  | 123(2)  | 123(2)  | 123(2)  |
| $\rho_{\text{calc}}$ (g·cm$^{-3}$) | 1.078   | 1.207   | 1.131   | 1.130   |
| $\mu$ (mm$^{-1}$)                 | 0.463   | 0.652   | 0.084   | 0.084   |
| F(000)                            | 1808    | 1032    | 2344    | 2400    |
| reflns collected                  | 41363   | 35036   | 33068   | 64489   |
| unique reflns                     | 9509    | 9893    | 6275    | 11777   |
| $R_{\text{int}}$                  | 0.1874  | 0.0522  | 0.0154  | 0.0216  |
| $R1$ [I > 2$\sigma$(I)]          | 0.0785  | 0.0375  | 0.0400  | 0.0518  |
| wR2 (all data)                    | 0.1626  | 0.0951  | 0.1086  | 0.1362  |
| largest peak and hole (e·Å$^{-3}$)| 0.331, -0.257 | 0.525, -0.755 | 0.351, -0.243 | 0.994, -0.409 |
| CCDC no.                          | 1983483 | 1983484 | 1983485 | 1983487 |
Figure S28. Molecular structure of 6 (25% thermal ellipsoids are shown; hydrogen atoms omitted; aryl substituents shown as wireframe for clarity). Selected bond lengths (Å) and angles (°): Mg(1)-N(3) 2.167(2), Mg(1)-Mg(2) 2.8925(9), N(2)-Mg(1)-N(1) 89.12(7), N(3)-Mg(1)-Mg(2) 115.31(5), N(6)-Mg(2)-N(5) 89.17(8).

Figure S29. Molecular structure of 10 (25% thermal ellipsoids are shown; hydrogen atoms, except alkenic protons, omitted; aryl substituents shown as wireframe for clarity). Selected bond lengths (Å) and angles (°): Mg(1)-O(1)’ 2.016(5), Mg(1)-O(1) 2.020(4), Mg(1)-O(2) 2.110(4), O(1)-C(22) 1.318(7), Mg(2)-O(2) 1.976(4), Mg(2)-N(3) 2.118(5), O(2)-C(23) 1.375(7), C(22)-C(23) 1.364(8), O(1)’-Mg(1)-O(1) 75.24(18), O(1)’-Mg(1)-O(2) 152.0(2), N(5)-Mg(2)-N(6) 91.3(2), O(2)-Mg(2)-N(3) 80.61(19).
**Figure S30.** Molecular structure of $\text{TCHP}_2\text{NacnacH}$ 1S (25% thermal ellipsoids are shown; hydrogen atoms, except amine proton, omitted; aryl substituents shown as wireframe for clarity). Selected bond lengths (Å): N(1)-C(28) 1.346(4), N(2)-C(25) 1.314(4), C(25)-C(27) 1.425(4), C(27)-C(28) 1.375(4).

**Figure S31.** Molecular structure of $[(\text{TCHP}_2\text{Nacnac})\text{MgI(OEt}_2)]$ 2S (25% thermal ellipsoids are shown; hydrogen atoms omitted; aryl substituents shown as wireframe for clarity). Selected bond lengths (Å) and angles (°): I(1)-Mg(1) 2.6700(8), Mg(1)-O(1) 2.0431(19), Mg(1)-N(2) 2.048(2), Mg(1)-N(1) 2.054(2), N(2)-Mg(1)-N(1) 96.98(8), O(1)-Mg(1)-I(1) 101.90(6).
**Figure S32.** Molecular structure of \([\{(\text{XylNacnac})\text{Mg(DMAP)}\}_2\] 3S (25% thermal ellipsoids are shown; hydrogen atoms omitted; aryl substituents shown as wireframe for clarity). Selected bond lengths (Å) and angles (°): Mg(1)-N(3) 2.2071(11), Mg(1)-Mg(1)' 2.9464(7), N(1)-Mg(1)-N(2) 88.31(4), N(3)-Mg(1)-Mg(1)' 111.28(3).

**Figure S33.** Molecular structure of \([\{(\text{DepNacnac})\text{Mg(DMAP)}\}_2\] 4S (25% thermal ellipsoids are shown; hydrogen atoms omitted; aryl substituents shown as wireframe for clarity). Selected bond lengths (Å) and angles (°): Mg(1)-N(3) 2.2229(14), Mg(1)-Mg(2) 3.0368(7), Mg(2)-N(7) 2.2226(18), N(1)-Mg(1)-N(2) 87.04(5), N(3)-Mg(1)-Mg(2) 109.69(4), N(6)-Mg(2)-N(5) 87.01(6), N(7)-Mg(2)-Mg(1) 113.76(4).
3. Computational Studies

Geometry optimizations were performed using Gaussian09 suite of programs\textsuperscript{10} using the Becke’s 3-parameter hybrid functional,\textsuperscript{11} combined with the non-local correlation functional provided by Perdew/Wang.\textsuperscript{12} The 6-311+G(d) all-electron basis set was used for the magnesium atoms and the 6-31G(d,p) for the remaining atoms.\textsuperscript{13} All stationary points have been identified for minimum (Nimag=0) or transition states (Nimag=1). Intrinsic Reaction Paths (IRPs)\textsuperscript{14} were traced from the various transition structures to obtain the connected intermediates.

**Figure S34.** HOMO (left) and NBO charges (right) of 7.
Figure S35. HOMO of TS1.
Figure S36. Fully labelled computed (B3PW91) enthalpy profile at 298 K for the formation of ethenediolate complex 11, or deltate complex 12, from magnesium(I)-adduct complex 7, and two or three molecules of CO, respectively.
Table S2. *Cartesian coordinates* of the optimized structures.

| Complex 7 | X | Y | Z       |
|-----------|---|---|---------|
| C         | -0.050083 | 0.740164 | -3.274967 |
| C         | 1.090230 | 1.067130 | -2.511932 |
| C         | 2.242975 | 0.262290 | -2.599533 |
| C         | 2.234747 | -0.845757 | -3.451907 |
| C         | 1.119043 | -1.188863 | -4.215889 |
| C         | -0.011686 | -0.376364 | -4.112603 |
| N         | 1.035925 | 2.184443 | -1.626603 |
| C         | 1.359530 | 3.383383 | -2.099716 |
| C         | 1.919077 | 3.509728 | -3.504413 |
| C         | 3.478907 | 0.575186 | -1.798247 |
| C         | 1.125002 | -2.406344 | -5.104350 |
| C         | -1.300114 | 1.571661 | -3.177963 |
| Mg        | 0.366457 | 1.853085 | 0.375688 |
| N         | 2.399918 | 1.880401 | 1.322421 |
| C         | 2.842970 | 0.939620 | 2.173360 |
| C         | 4.122950 | 0.910211 | 2.696522 |
| C         | 5.047990 | 1.919598 | 2.344258 |
| C         | 4.573573 | 2.910001 | 1.452295 |
| C         | 3.275225 | 2.844943 | 0.983525 |
| N         | 6.321945 | 1.938586 | 2.835257 |
| C         | 6.781367 | 0.865912 | 3.695069 |
| N         | -0.086691 | 3.932670 | 0.561136 |
| C         | 0.437790 | 4.863652 | -0.231422 |
| C         | 0.210108 | 6.307068 | 0.083893 |
| C         | -1.017119 | 4.341951 | 1.561256 |
| C         | -2.373904 | 4.511464 | 1.213268 |
| C         | -3.289243 | 4.880056 | 2.201508 |
| C         | -2.909358 | 5.075747 | 3.530841 |
| C         | -1.563588 | 4.895968 | 3.852369 |
| C         | -0.611350 | 4.529195 | 2.896972 |
| C         | -2.836422 | 4.288280 | -0.201587 |
| C         | -3.922043 | 5.442628 | 4.850009 |
| C         | 0.827396 | 4.353455 | 3.302949 |
| C         | 7.251747 | 2.961291 | 2.398814 |
| C         | 1.191443 | 4.597749 | -1.395520 |
| Mg        | -1.352620 | -0.329890 | 1.379975 |
| N         | -3.266835 | -1.122348 | 0.950389 |
| C         | -3.961498 | -0.526405 | -0.143141 |
| C         | -3.825177 | -1.057108 | -1.440332 |
| C         | -4.516780 | -0.452147 | -2.493069 |
| C         | -5.322149 | 0.672309 | -2.303597 |
| C         | -5.423269 | 1.191466 | -1.010914 |
| C         | -4.754798 | 0.617563 | 0.072942 |
| C         | -2.948050 | -2.254785 | -1.693690 |
| C         | -6.035134 | 1.324610 | -3.460292 |
| C         | -4.884326 | 1.206800 | 1.452219 |
| C         | -3.880384 | -2.096590 | 1.620275 |
| C         | -5.275034 | -2.526811 | 1.208679 |
| C         | -3.325337 | -2.781506 | 2.718114 |
| C         | -2.078539 | -2.613207 | 3.349956 |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | -1.796296 | -3.534890 | 4.515122  |
| N       | -1.162415 | -1.714842 | 2.976577  |
| C       | 0.050810  | -1.662202 | 3.717766  |
| C       | 0.161463  | -0.799001 | 4.828618  |
| C       | 1.357519  | -0.770779 | 5.547837  |
| C       | 2.452907  | -1.565930 | 5.198510  |
| C       | 2.335649  | -2.377096 | 4.068321  |
| C       | 1.157703  | -2.434985 | 3.315516  |
| C       | -0.994168 | 0.076791  | 5.232646  |
| C       | 1.075087  | -3.308334 | 2.092009  |
| C       | 3.707512  | -1.563411 | 6.034788  |
| H       | -3.956255 | -3.551868 | 3.147235  |
| H       | -0.902383 | -4.142012 | 4.331802  |
| H       | -2.637757 | -4.206708 | 4.700734  |
| H       | -1.600813 | -2.963352 | 5.429537  |
| H       | -4.420977 | -0.875515 | -3.492279 |
| H       | -5.977071 | -1.687308 | 1.267573  |
| H       | -5.644778 | -3.332900 | 1.846981  |
| H       | -5.291870 | -2.871011 | 0.168677  |
| H       | 1.431590  | -0.112695 | 6.412936  |
| H       | -1.252136 | 0.785115  | 4.434296  |
| H       | -0.751116 | 0.655643  | 6.129688  |
| H       | -1.900565 | -0.504977 | 5.437577  |
| H       | -6.045477 | 2.068603  | -0.836572 |
| H       | -3.914129 | 1.557411  | 1.828757  |
| H       | -5.257696 | 0.476318  | 2.180081  |
| H       | -5.567368 | 2.062161  | 1.448609  |
| H       | 3.180333  | -2.994838 | 3.764686  |
| H       | -1.892887 | -2.019802 | -1.502223 |
| H       | -3.030213 | -2.583984 | -2.734647 |
| H       | -3.203935 | -3.102435 | -1.047435 |
| H       | 2.014447  | -3.847586 | 1.931249  |
| H       | 0.870336  | -2.709848 | 1.193974  |
| H       | 0.267453  | -4.404659 | 2.163649  |
| H       | 4.000315  | -0.546364 | 6.322757  |
| H       | 4.547516  | -2.021765 | 5.501005  |
| H       | 3.568041  | -2.130104 | 6.965045  |
| H       | -6.999502 | 1.744548  | -3.152698 |
| H       | -6.221920 | 0.611107  | -4.270336 |
| H       | -5.443297 | 2.148435  | -3.881625 |
| H       | 2.907899  | 3.598742  | 0.290583  |
| H       | 5.207508  | 3.722802  | 1.117981  |
| H       | 1.563159  | 5.477952  | -1.909327 |
| H       | 4.384352  | 0.104955  | 3.371283  |
| H       | 0.979593  | 4.671861  | 4.339869  |
| H       | 1.140896  | 3.306466  | 3.222518  |
| H       | 1.508170  | 4.930343  | 2.666256  |
| H       | 3.134724  | -1.456185 | -3.521335 |
| H       | -4.332910 | 5.017114  | 1.920717  |
| H       | -1.236865 | 5.050638  | 4.880305  |
| H       | -0.895480 | -0.615958 | -4.702713 |
| H       | -2.044307 | 1.243922  | -3.910182 |
| H       | -1.753410 | 1.479123  | -2.182510 |
| H       | -1.104573 | 2.637955  | -3.338778 |
| H       | 3.330792  | 0.358635  | -0.734166 |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | 4.327441  | -0.023598 | -2.146665 |
| H    | 3.758082  | 1.632517  | -1.863457 |
| H    | -2.658222 | 3.252996  | -0.516257 |
| H    | -3.908419 | 4.488953  | -0.296662 |
| H    | -2.308312 | 4.926887  | -0.919544 |
| H    | 1.150960  | 3.257496  | -3.704274 |
| H    | 2.262887  | 4.527723  | -3.04274  |
| H    | 2.749557  | 2.815838  | -3.671467 |
| H    | 6.883124  | 3.966776  | 2.639763  |
| H    | 8.204008  | 2.823528  | 2.913494  |
| H    | 7.439111  | 2.912682  | 1.316670  |
| H    | 0.441260  | 6.551795  | 1.131540  |
| H    | 0.821788  | 6.972443  | -0.555488 |
| H    | -0.840959 | 6.603847  | -0.066228 |
| H    | -4.733815 | 6.049337  | 4.168160  |
| H    | -4.380984 | 4.548430  | 5.028304  |
| H    | -3.463503 | 6.010298  | 5.40328   |
| H    | 6.762121  | -0.107411 | 3.184461  |
| H    | 7.808888  | 1.067509  | 4.002056  |
| H    | 6.168284  | 0.789669  | 4.602087  |
| H    | 2.137488  | -2.650428 | 5.444616  |
| H    | 0.737995  | -3.289088 | -4.577270 |
| H    | 0.498083  | -2.259284 | -5.991052 |
| H    | 2.125510  | 0.167984  | 2.443845  |

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| 131  | C 1.157703 | -2.434985 | 3.315516  |
|      | C 0.050810 | -1.662202 | 3.717766  |
|      | C 0.161463 | -0.799001 | 4.828618  |
|      | C 1.357519 | -0.770779 | 5.547837  |
|      | C 2.452907 | -1.565930 | 5.198510  |
|      | C 2.335649 | -2.377096 | 4.068321  |
| N    | -1.162415 | -1.714842 | 2.976577  |
|      | C -2.078539 | -2.613207 | 3.343956  |
|      | C -1.796296 | -3.534890 | 4.515122  |
|      | C -0.994168 | 0.076791  | 5.232646  |
|      | C 3.707512  | -1.563411 | 6.034788  |
|      | C 1.075087  | -3.308334 | 2.092009  |
|      | C -3.325337 | -2.781506 | 2.718114  |
|      | C -3.880384 | -2.096590 | 1.620275  |
|      | C -5.275034 | -2.526811 | 1.208678  |
| N    | -3.266835  | -1.122348 | 0.950389  |
|      | C -3.961497 | -0.526405 | -0.143141 |
|      | C -3.825176 | -1.057108 | -1.440332 |
|      | C -4.516779 | -0.452147 | -2.493070 |
|      | C -5.322148 | 0.672309  | -2.303598 |
|      | C -5.423268 | 1.191466  | -1.010915 |
|      | C -4.754797 | 0.617563  | 0.072941  |
|      | C -2.948049 | -2.254785 | -1.693690 |
|      | C -6.055133 | 1.324610  | -3.460293 |
|      | C -4.884326 | 1.206800  | 1.452218  |
| Mg   | -1.352620  | -0.329890 | 1.379975  |
| Mg   | 0.366458   | 1.853085  | 0.375688  |
|  | X       | Y       | Z       |
|---|---------|---------|---------|
| N | -0.339357 | 3.533596 | -0.738813 |
| C | -1.720953 | 3.876573 | -0.655099 |
| C | -2.613087 | 3.389777 | -1.633882 |
| C | -3.971013 | 3.699597 | -1.531420 |
| C | -4.481321 | 4.467256 | -0.482602 |
| C | -3.581058 | 4.931787 | 0.476843  |
| C | -2.213501 | 4.648944 | 0.414801  |
| C | -2.114586 | 2.538109 | -2.770265 |
| C | -5.955745 | 4.761195 | -0.377363 |
| C | -1.289913 | 5.181059 | 1.477595  |
| N | 2.052716  | 1.704756 | -0.928799 |
| C | 2.456273  | 2.695934 | -1.716656 |
| C | 1.766550  | 3.918054 | -1.888512 |
| C | 0.444330  | 4.260798 | -1.530626 |
| C | -0.090095 | 5.544412 | -2.139247 |
| C | 2.748637  | 0.460971 | -0.990753 |
| C | 2.331709  | -0.512990| -1.921888 |
| C | 2.986515  | -1.745765| -1.957072 |
| C | 4.039709  | -2.052281| -1.093242 |
| C | 4.434664  | -1.073422| -0.181085 |
| C | 3.809162  | 0.174744 | -0.108923 |
| C | 1.185145  | -0.237405| -2.856137 |
| C | 4.281040  | 1.185877 | 0.902231  |
| C | 4.710323  | -3.401558| -1.130467 |
| C | 3.722787  | 2.534611 | -2.536502 |
| N | 1.418886  | 2.970087 | 2.011755  |
| C | 1.371704  | 2.620344 | 3.308256  |
| C | 2.082703  | 3.258429 | 4.308376  |
| C | 2.914513  | 4.355468 | 3.987051  |
| C | 2.955525  | 4.721957 | 2.621192  |
| C | 2.208225  | 4.014338 | 1.698964  |
| N | 3.634380  | 5.021866 | 4.936844  |
| C | 4.518539  | 6.103299 | 4.549928  |
| C | 3.609844  | 4.567937 | 6.313187  |
| H | -3.956255 | -3.551868| 3.147235  |
| H | -0.902383 | -4.142012| 4.331802  |
| H | -2.637757 | -4.206708| 4.700734  |
| H | -1.600813 | -2.963352| 5.429537  |
| H | -4.420975 | -0.875515| -3.492279 |
| H | -5.977071 | -1.687308| 1.267572  |
| H | -5.644778 | -3.332900| 1.846980  |
| H | -5.291870 | -2.871011| 0.168676  |
| H | 1.431590  | -0.112695| 6.412936  |
| H | -1.252136 | 0.785115 | 4.434296  |
| H | -0.751116 | 0.655643 | 6.129688  |
| H | -1.900565 | -0.504977| 5.437577  |
| H | -6.045476 | 2.068603 | -0.836573 |
| H | -3.914129 | 1.557411 | 1.828756  |
| H | -5.257696 | 0.476318 | 2.180080  |
| H | -5.567368 | 2.062161 | 1.448608  |
| H | 3.180333  | -2.994838| 3.764686  |
| H | -1.892886 | -2.019802| -1.502223 |
| H | -3.030212 | -2.583984| -2.734647 |
| H | -3.203934 | -3.102435| -1.047435 |
| H | 2.014447  | -3.847586| 1.931249  |
H  0.870336 -2.709848  1.193974
H  0.267453 -4.046459  2.163649
H  4.000315 -0.546364  6.965045
H  4.547516 -2.021765  5.501005
H  3.568041 -2.130104  6.322757
H  4.000315  1.744548 -3.152699
H  6.221918  0.611107 -4.270337
H  5.443296  2.148435 -3.881626
H  2.242833  4.286091  0.646223
H  3.567151  5.546018  2.273167
H  5.261234 -1.281822  0.497703
H  4.650216  3.326534 -2.297172
H  3.949802  5.540742  1.301783
H  5.261234 -1.281822  0.497703
H  4.650216  3.326534 -2.297172
H  3.949802  5.540742  1.301783
H  5.261234 -1.281822  0.497703
H  4.650216  3.326534 -2.297172
C  0.172941  0.698343 -3.411410
H  3.554768  1.308441  1.713777
H  5.231269  0.872392  1.348032
H  4.422635  2.178320  0.460475
H  5.231269  0.872392  1.348032
H  4.422635  2.178320  0.460475
C  0.172941  0.698343 -3.411410
O  0.089624 -2.300485 -6.181046
131
INT1
C  -0.561176 -1.424080  4.049770
C  -0.463993 -2.520993  3.168996
C   0.720873 -3.280048  3.114699
C  1.776195 -2.950630  3.971143
C  1.698734 -1.880595  4.864193
C  0.521265 -1.128542  0.485628
N  -1.535459 -2.820949  2.281213
C  -2.444491 -3.727590  2.638187
C  -3.501910 -1.880595  4.864193
C  -0.521265 -1.128542  0.485628
C  -4.995970 -4.554508 -0.123916
C  -0.853559 -4.203046  2.140259
C  -2.512121 -1.530039  5.770423
C  -1.809757 -0.583395  4.093270
C  -4.995970 -4.554508 -0.123916
C  -0.853559 -4.203046  2.140259
C  -2.512121 -1.530039  5.770423
C  -1.809757 -0.583395  4.093270
Mg  -1.619155 -1.763288  0.505101
C  -0.729313  0.109515  0.010507
C  -3.576689 -2.704771 -1.594567
C  -2.997819 -3.455373 -2.636047
C  -3.404540 -3.214491 -3.950740
C  -4.361266 -2.246413 -4.264336
C  -4.896073 -1.494437 -3.215619
C  -4.519357 -1.699094 -1.885673
C  -1.952161 -4.497656 -2.339276
C  -5.105285 -0.851892 -0.787001
C  -4.822160 -2.038366 -5.684446
O  -1.911495  0.260076  0.485335
Mg  0.594469  1.770374 -0.661234
N  0.391890  3.797256 -0.154356
C  0.033253  4.106081  1.94093
C  -1.312870  3.976344  1.601186
C  -1.643697  4.233343  2.93016
C  -0.688194  4.609810  3.879854
C  0.633591  4.731072  3.453904
C  1.014172  4.483798  2.130906
C  -2.382158  3.549541  0.630969
C  -1.078943  4.874236  5.311423
C  2.461851  4.619141  1.737177
C  -2.360177 -4.361219  4.012206
N  2.510216  1.035004  0.074860
C  2.541203 -0.141336  0.731251
C  3.691946 -0.696483  1.258035
C  4.927069 -0.021707  1.120061
C  4.886597  1.211720  0.426038
C  3.682109  1.680009 -0.062161
N  6.088690 -0.527915  1.623222
C  7.335257  0.187231  1.432492
N  0.881660  2.211998 -2.690038
C  0.986020  1.098877 -3.577042
C  2.239175  0.647555 -4.034534
C  2.294459 -0.486614 -4.851037
C  1.151542 -1.196479 -5.216632
C  -0.080581 -0.728859 -4.753123
C  -0.186211  0.403979 -3.944956
C  3.518992  1.348001 -3.657367
C  1.240092 -2.436112 -6.069222
C  -1.537238  0.882427 -3.484434
C  6.089213 -1.819175  2.283696
C  0.797240  3.439962  -3.197840
C  0.618588  4.613028  -2.436201
C  0.386736  4.779913  -1.054978
C  0.072093  6.194205  -0.607200
C  0.860609  3.627816  -4.700961
H  -4.158824  -4.897094  2.267366
H  -1.430548  -4.930462  4.127108
H  -3.200502  -5.036233  4.189776
H  -2.354337  -5.562825  1.971838
H  -0.438323  -0.283400  5.562825
H  -1.971838  -0.058086  3.144140
H  -1.742171  0.170393  4.884136
H  -2.705543  -1.189899  4.275203
H  -5.631956  -0.722122  3.463139
H  -4.331323  -0.250061  0.295418
H  -5.576210  -1.459521  2.297369
H  -5.862320  -0.168950  1.186108
H  2.681260  -3.557517  3.942543
H  -1.068582  -4.050795  -1.864656
H  -1.624305  -4.994165  -3.258356
H  -2.319057  -5.267884  -1.650220
H  1.837197  -4.894742  2.223380
H  0.729385  -4.072243  1.105961
H  0.092723  -5.193983  2.297369
H  3.603828  -2.326067  5.786849
H  2.516964  -1.367697  6.802034
H  3.349505  -0.606413  5.446903
H  -5.691805  -2.667729  -5.917657
H  -4.036475  -2.931444  -6.404180
H  -5.118282  -0.998851  -5.863156
H  3.644037  2.624907  -0.597647
H  5.780365  1.802151  0.263486
H  0.581284  5.528832  -3.015628
H  3.612600  -1.642325  1.779336
H  3.028598  5.138417  2.517529
H  2.925494  3.636321  1.591009
H  2.589176  5.171550  0.799811
H  3.266743  -0.822977  -5.210371
H  -2.685578  4.137058  3.236909
H  1.398119  5.032133  4.169395
H  -0.991652  -1.260667  -5.022482
H  -2.332347  0.243584  -3.879348
H  -1.618700  0.870597  -2.390297
H  -1.734451  1.914141  -3.801593
H  3.863794  1.033755  -2.664589
H  4.315209  1.108440  -4.370767
H  3.406747  2.436079  -3.623983
H  -2.345916  2.463170  0.463036
H  -3.375704  3.785454  1.028336
H  -2.279228  4.041971  -0.341875
H  0.041783  3.086002  -5.188829

S43
|  | X        | Y        | Z        |
|---|----------|----------|----------|
| H | 0.787538 | 4.683276 | -4.973390|
| H | 1.789398 | 3.223507 | -5.117735|
| H | 7.295481 | 1.189661 | 1.878558 |
| H | 8.142411 | -0.362734| 1.918604 |
| H | 7.58643  | 0.292046 | 0.368278 |
| H | 0.732264 | 6.514762 | 0.205646 |
| H | 0.165216 | 6.902497 | -1.433766|
| H | 0.950565 | -0.362734| 1.918604 |
| H | 7.588643 | 0.292046 | 0.368278 |
| H | 0.732264 | 6.514762 | 0.205646 |
| H | 0.165216 | 6.902497 | -1.433766|
| H | 0.950565 | -0.362734| 1.918604 |
| H | 7.588643 | 0.292046 | 0.368278 |
| H | 0.732264 | 6.514762 | 0.205646 |
| H | 0.165216 | 6.902497 | -1.433766|
| H | 0.950565 | -0.362734| 1.918604 |

| Adduct 1 |
|----------|
| C | 0.704807 | -3.112908 | 3.315895 |
| C | -0.458327 | -2.318810 | 3.290636 |
| C | -0.535479 | -1.152275 | 4.077483 |
| C | 0.544894  | -0.818729 | 4.897048 |
| C | 1.701498  | -1.599840 | 4.956744 |
| C | 1.758913  | -2.742482 | 4.156483 |
| C | -1.526366 | -2.659697 | 2.412629 |
| C | -2.466313 | -3.510114 | 2.827367 |
| C | -2.425893 | -4.021262 | 4.252924 |
| C | -1.761152 | -0.278467 | 4.036801 |
| C | 2.857742  | -1.202597 | 5.838567 |
| C | 0.816172  | -4.336768 | 2.445296 |
| C | -3.518125 | -3.985890 | 2.023420 |
| C | -3.786428 | -3.769612 | 0.655679 |
| C | -4.965027 | -4.532240 | 0.084702 |
| C | -3.083835 | -2.964753 | -0.141590|
| C | -3.444274 | -2.889792 | -1.521779|
| C | -2.853968 | -3.774375 | -2.445142|
| C | -3.197094 | -3.670799 | -3.794414|
| C | -4.102306 | -2.713290 | -4.256890|
| C | -4.653117 | -1.833074 | -3.324120|
| C | -4.339203 | -1.897417 | -1.963790|
| C | -1.857552 | -4.808119 | -1.990772|
| C | -4.490015 | -2.649847 | -5.712089|
| C | -4.943780 | -0.914178 | -0.996008|
| Mg| -1.578430 | -1.743910 | 0.567592 |
| O | -1.844411 | 0.268199  | 0.273926 |
| C | -0.598685 | 0.112887  | 0.095373 |
| C | -0.015190 | -1.452704 | -1.419943|
| O | 1.097255  | -1.759642 | -1.575365|
| Mg| 0.747684  | 1.695106  | -0.768086|
| N | 2.643255  | 0.978358  | 0.013279 |
| C | 2.655062  | -0.113603 | 0.802766 |
| Element | X           | Y           | Z           |
|---------|-------------|-------------|-------------|
| C       | 3.803385    | -0.645738   | 1.356588    |
| C       | 5.055661    | -0.042012   | 1.097560    |
| C       | 5.033173    | 1.108616    | 0.272174    |
| C       | 3.829883    | 1.564279    | -0.228576   |
| N       | 6.217337    | -0.536142   | 1.612080    |
| C       | 7.480675    | 0.102142    | 1.298329    |
| N       | 1.016685    | 2.298901    | -2.751996   |
| C       | 1.137971    | 3.576957    | -3.111353   |
| C       | 1.091603    | 4.673207    | -2.225861   |
| C       | 0.726728    | 4.728263    | -0.864350   |
| C       | 0.509312    | 6.118691    | -0.299318   |
| C       | 0.907294    | 1.312602    | -3.780725   |
| N       | 0.520686    | 3.665843    | -0.087739   |
| C       | 0.019716    | 3.877792    | 1.233010    |
| C       | -1.372721   | 3.854628    | 1.458375    |
| C       | -1.850292   | 4.029229    | 2.759300    |
| C       | -0.995915   | 4.222087    | 3.846635    |
| N       | 0.520686    | 3.665843    | -0.087739   |
| H       | -2.337649   | 3.625388    | 0.325273    |
| C       | -1.541712   | 4.447141    | 5.233522    |
| C       | 2.394974    | 4.070276    | 2.111151    |
| N       | 6.195410    | -1.737637   | 2.424337    |
| H       | -4.208556   | -4.655932   | 2.523123    |
| H       | -1.506206   | -4.586088   | 4.443039    |
| H       | -3.278603   | -4.669945   | 4.465916    |
| H       | -2.432536   | -3.189628   | 4.966588    |
| H       | -2.739863   | -4.359086   | -4.504253   |
| H       | -5.690170   | -3.850295   | -0.372929   |
| H       | -5.471948   | -5.113777   | 0.858064    |
| H       | -4.641908   | -5.217129   | -0.707582   |
| H       | 0.477226    | 0.080984    | 5.507101    |
| H       | -1.909881   | 0.158994    | 3.042151    |
| H       | -1.672295   | 0.546662    | 4.749875    |
| H       | -2.672947   | -0.839464   | 4.274866    |
| H       | -5.351651   | -1.068346   | -3.661575   |
| H       | -4.176391   | -0.261647   | -0.562457   |
| H       | -5.445476   | -1.414102   | -0.158761   |
| H       | -5.680503   | -0.279499   | -1.499430   |
| H       | 2.647076    | -3.373487   | 4.190059    |
| H       | -0.963864   | -4.337558   | -1.561938   |
| H       | -1.534302   | -5.432162   | -2.830242   |
| H       | -2.265988   | -5.467921   | -1.216008   |
| H       | 1.783358    | -4.830765   | 2.586194    |
| H       | 0.719750    | -4.079370   | 1.382682    |
| H       | 0.030178    | -5.071437   | 2.656831    |
| Atom | X    | Y    | Z    | X    | Y    | Z    |
|------|------|------|------|------|------|------|
| H    | 3.527938 | -2.048607 | 6.026948 | H    | 2.513065 | -0.827729 | 6.809140 |
| H    | 3.454462 | -0.402235 | 5.380098 | H    | -3.649082 | -2.910951 | -6.364288 |
| H    | -4.835693 | -1.648782 | -5.992074 | H    | -5.305058 | -3.350367 | -5.939804 |
| H    | 3.803194 | 2.448218 | -0.860774 | H    | 5.940202 | 1.644487 | 0.019712 |
| H    | 1.237642 | 5.640013 | -2.694734 | H    | 3.710267 | -1.521799 | 1.986434 |
| H    | 2.910910 | 4.318593 | 3.044734 | H    | 2.759514 | 3.093620 | 1.775172 |
| H    | 2.704165 | 3.093620 | 1.775172 | H    | 2.778831 | -0.794465 | -5.680169 |
| H    | -2.927029 | 4.013654 | 2.92428 |
| H    | 1.066899 | 4.374738 | 4.430588 | H    | -1.477514 | -0.326292 | -5.565482 |
| H    | -2.506063 | 1.225915 | -4.184028 | H    | -1.717538 | 1.390542 | -2.610948 |
| H    | -1.584118 | 2.691403 | -3.791959 | H    | 3.587749 | 0.620349 | -2.786048 |
| H    | 4.194179 | 0.571267 | -4.446133 | H    | 3.603196 | 2.092516 | -3.753142 |
| H    | -2.332848 | 2.570291 | 0.019954 | H    | -3.359117 | 3.873339 | 0.633696 |
| H    | -2.092129 | 4.227186 | -0.556307 | H    | 0.389255 | 3.643606 | -5.134644 |
| H    | 1.462823 | 4.993614 | -4.718555 | H    | 2.119606 | 3.372160 | -5.038563 |
| H    | 7.503302 | 1.144355 | 1.643723 | H    | 8.287569 | -0.433906 | 1.800135 |
| H    | 7.685876 | 0.091150 | 0.218985 | H    | 1.056511 | 6.266403 | 0.637224 |
| H    | 0.817011 | 6.887874 | -1.011600 | H    | -0.551247 | 6.272117 | -0.065748 |
| H    | -1.835499 | 5.495051 | 5.383182 | H    | -2.431035 | 3.834417 | 5.420216 |
| H    | -0.798740 | 4.205553 | 6.001467 | H    | 5.802439 | -2.597844 | 1.865572 |
| H    | 7.212277 | -1.975162 | 2.740459 | H    | 5.583269 | -1.602990 | 3.325374 |
| H    | 1.407768 | -1.909089 | -7.363323 | H    | 0.246633 | -2.737310 | -6.319690 |
| H    | -0.321953 | -1.547951 | -7.494300 | H    | 1.683889 | -0.569105 | 0.990842 |

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TS second inserion

| Atom | X    | Y    | Z    |
|------|------|------|------|
| C    | 0.584416 | -2.725533 | 3.078801 |
| C    | -0.624519 | -2.008782 | 3.192555 |
| C    | -0.706899 | -0.884308 | 4.032949 |
| C    | 0.418305 | -0.509152 | 4.772924 |
| C    | 1.620210 | -1.213174 | 4.698744 |
| C    | 1.678258 | -2.318880 | 3.845926 |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | -2.265893 | 3.321063  | 0.170824  |
| C       | -2.120609 | 4.126111  | 5.147741  |
| C       | 2.185861  | 3.593666  | 2.586176  |
| C       | 7.102848  | -1.244650 | 2.171788  |
| H       | -4.254323 | -4.596358 | 2.711549  |
| H       | -1.389966 | -4.395374 | 4.327794  |
| H       | -3.141473 | -4.578562 | 4.548808  |
| H       | -2.318726 | 3.070400  | 5.008450  |
| H       | -3.365108 | -4.040695 | -4.417438 |
| H       | -0.643436 | -3.610999 | -0.051142 |
| H       | -5.647898 | -5.113015 | 1.148660  |
| H       | -4.930856 | -5.150072 | -0.475633 |
| H       | 0.348120  | 0.360856  | 5.423586  |
| H       | -2.173497 | 0.469935  | 3.202444  |
| H       | -1.919676 | 0.648141  | 4.936022  |
| H       | -2.854782 | -0.724304 | 4.309089  |
| H       | -6.117265 | -0.949808 | -3.307943 |
| H       | -4.764593 | -0.125083 | -0.315082 |
| H       | -5.911142 | -1.362387 | 0.203607  |
| H       | -6.345777 | -0.240833 | -1.098728 |
| H       | 2.604844  | -2.888136 | 3.773962  |
| H       | -1.357730 | -3.955692 | -1.702885 |
| H       | -2.030162 | -5.123163 | -2.844073 |
| H       | -2.537439 | -5.138360 | -1.145782 |
| H       | 1.625701  | -4.458490 | 2.337900  |
| H       | 0.776912  | -3.541413 | 1.088042  |
| H       | -0.136167 | -4.574911 | 2.188047  |
| H       | 3.354947  | -1.643251 | 5.920937  |
| H       | 2.550764  | -0.114628 | 6.312896  |
| H       | 3.546799  | -0.243625 | 4.859252  |
| H       | -4.498630 | -2.674215 | -6.164236 |
| H       | -5.650281 | -1.409767 | -5.702206 |
| H       | -6.127469 | -3.108965 | -5.638677 |
| H       | 3.728141  | 2.668560  | -0.537583 |
| H       | 6.024095  | 2.253199  | 0.197692  |
| H       | 1.631950  | 5.380288  | -2.297547 |
| H       | 4.620276  | -1.531975 | 1.793561  |
| H       | 2.582843  | 3.865993  | 3.569977  |
| H       | 2.550945  | 2.589126  | 2.344226  |
| H       | 2.622299  | 4.273001  | 1.845051  |
| H       | 3.154963  | -0.971098 | -5.480487 |
| H       | -3.195465 | 3.736141  | 2.671425  |
| H       | 0.568643  | 3.945546  | 4.706858  |
| H       | -1.089851 | -0.402242 | -5.575111 |
| H       | -2.137712 | 1.217609  | -4.276408 |
| H       | -1.538023 | 1.071837  | -2.619225 |
| H       | -1.192202 | 2.532381  | -3.553192 |
| H       | 3.826772  | 0.379447  | -2.486651 |
| H       | 4.528811  | 0.289439  | -4.107669 |
| H       | 3.952382  | 1.837637  | -3.464847 |
| H       | -2.164848 | 2.285133  | -0.183727 |
| H       | -3.328149 | 3.516652  | 0.354363  |
| H       | -1.934820 | 3.977705  | -0.641794 |
| H       | 0.805366  | 3.611341  | -4.858210 |
| H       | 1.997427  | 4.816869  | -4.338396 |
| Atom | X Coord  | Y Coord  | Z Coord  |
|------|----------|----------|----------|
| H    | 2.497413 | 3.157925 | -4.748848|
| H    | 7.728960 | 1.922597 | 1.712759 |
| H    | 8.838781 | 0.545230 | 1.671234 |
| H    | 8.072280 | 1.096554 | 0.172456 |
| H    | 1.106918 | 5.875739 | 1.018735 |
| H    | 1.072066 | 6.564463 | -0.620905|
| H    | -0.408527| 5.950853 | 0.136976 |
| H    | -2.430944| 5.175989 | 5.237539 |
| H    | -3.027395| 3.517772 | 5.229932 |
| H    | -1.483471| 3.901083 | 6.010002 |
| H    | 6.877229 | -2.101328| 1.522407 |
| H    | 8.160185 | -1.290539| 2.436498 |
| H    | 6.518643 | -1.347548| 3.095682 |
| H    | 1.813809 | -1.926465| -7.337463|
| H    | 0.729171 | -2.856332| -6.298693|
| H    | 0.063931 | -1.655183| -7.409665|
| H    | 2.394928 | -0.931146| 0.979853 |

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| Atom | X Coord  | Y Coord  | Z Coord  |
|------|----------|----------|----------|
| INT2 | 0.084094 | -1.023204| 4.790467 |
| C    | -0.439459| -1.992658| 3.914182 |
| C    | 0.282164 | -3.173034| 3.647627 |
| C    | 1.501010 | -3.379353| 4.297580 |
| C    | 2.029377 | -2.448111| 5.194640 |
| C    | 1.307855 | -1.274067| 5.416874 |
| N    | -1.670973| -1.747026| 3.235723 |
| C    | -2.795738| -2.264167| 3.733228 |
| C    | -2.746329| -3.011779| 5.049955 |
| C    | -0.237488| -4.189995| 2.665138 |
| C    | 3.325784 | -2.714032| 5.916030 |
| C    | -0.649101| 0.268741 | 5.036588 |
| Mg   | -1.689251| -0.463187| 1.636370 |
| N    | -3.615010| -0.924461| 1.084259 |
| C    | -4.443263| -1.575072| 1.902447 |
| C    | -5.904439| -1.705024| 1.524239 |
| O    | -0.081149| 0.149012 | 0.607541 |
| C    | -0.698686| 1.306142 | 1.191234 |
| C    | -0.340904| 2.539075 | 1.356687 |
| O    | -0.232347| 3.718901 | 1.554000 |
| Mg   | 1.293165 | 0.498194 | -0.713605|
| N    | 0.435622 | 1.897853 | -2.111784|
| C    | -0.802849| 2.417831 | -1.999970|
| C    | -1.339090| 3.313721 | -2.904423|
| C    | -0.577477| 3.734560 | -4.019172|
| C    | 0.719481 | 3.177396 | -4.131299|
| C    | 1.164587 | 2.287091 | -3.174850|
| N    | -1.060828| 4.625231 | -4.931075|
| C    | -2.375473| 5.209596 | -4.745520|
| N    | 3.185653 | 1.260022 | -0.298377|
| C    | 4.204032 | 1.003279 | -1.113783|
| C    | 5.535900 | 1.689823 | -0.885555|
| C    | 3.429593 | 2.065542 | 0.860326 |
| C    | 3.236188 | 3.459297 | 0.827353 |
| C    | 3.463041 | 4.198436 | 1.990597 |
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C -2.478164 -2.429102 5.235496
C 0.678618 -3.225517 3.594011
C 2.838002 -0.265005 7.061047
C -1.388448 1.253933 4.765442
Mg -1.387263 -0.529399 1.422828
N -3.284587 -1.122550 0.944426
C -4.028721 -1.866815 1.763165
C -5.405939 -2.309375 1.316144
O 0.188317 0.189869 0.257653
C -0.447822 1.060562 0.243430
O -0.328199 2.140849 0.986343
O -0.527587 3.248183 1.379900
Mg 1.571809 -0.132300 -1.206967
N 0.392437 1.287585 -2.196249
C -0.860404 1.447311 -1.581746
C -1.594208 2.664304 -1.796262
C -0.999019 3.284587 -2.386881
C 0.335624 3.608850 -2.886324
C 0.936550 4.963629 -2.768388
N -1.668887 4.963629 -2.544584
C -2.903111 5.161918 -1.814526
N 3.491641 0.415361 -0.611247
C -4.582787 -0.157539 -1.109718
C 5.948725 0.293988 -0.626750
C 3.643899 1.360584 0.452519
C 3.842203 2.730795 0.205003
C 3.932119 3.606321 1.292824
C 3.821325 3.171895 2.611668
C 3.637215 1.804380 2.832513
C 3.549376 0.893281 1.780466
C 3.955238 3.290429 -1.189324
C 3.365888 -0.573844 2.060944
C 3.874002 4.144100 3.761367
C 4.582912 -1.196538 -2.064510
C 3.520418 -1.965659 -2.572951
N 2.227683 -1.776926 -2.287580
C 1.289142 -2.714661 -2.813221
C 0.977656 -3.875389 -2.076644
C 0.067018 -4.792677 -2.606431
C -0.552684 -4.590563 -3.841842
C -0.255235 -3.415123 -4.534473
C 0.650730 -2.469793 -4.045051
C 1.623967 -4.129568 -0.740221
C -1.490742 -5.619745 -4.419071
C 0.945239 -1.219298 -4.830551
C 3.915946 -3.102616 -3.495222
C -3.855840 -0.682773 -0.288996
C -4.582787 0.522858 -0.328342
C -5.111322 0.948170 -1.549453
C -4.924846 0.226892 -2.730920
C -4.188516 -0.957399 -2.663694
C -3.644419 -1.425390 -1.464607
C -4.775681 1.347240 0.917261
C -5.467370 0.730930 -4.042809
C -2.840334 -2.696722 -1.434997
| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| C    | -0.961023 | 6.130536 | -3.026609 |
| C    | -3.635653 | -2.268073 | 3.054628 |
| H    | -4.366558 | -2.867404 | 3.584960 |
| H    | -6.059408 | -1.445681 | 1.149383 |
| H    | -5.873644 | -2.957928 | 2.061026 |
| H    | -5.354779 | -2.847706 | 0.363440 |
| H    | 0.751859  | 1.367342 | 6.404828 |
| H    | -1.611104 | -3.062078 | 5.450706 |
| H    | -3.385542 | -2.991212 | 5.466196 |
| H    | -2.415578 | -1.575733 | 5.920697 |
| H    | -4.025907 | -1.537266 | 3.570964 |
| H    | -1.789087 | -2.502844 | -1.186182 |
| H    | -2.848690 | -3.188130 | -2.411095 |
| H    | -3.215120 | -3.407215 | -0.688720 |
| H    | 2.489300  | -2.427311 | 5.433410 |
| H    | 0.708610  | -3.017637 | 2.517170 |
| H    | -0.216905 | -3.833929 | 3.767643 |
| H    | 1.552980  | -3.836585 | 3.839126 |
| H    | -5.683530 | 1.874640  | -1.576888 |
| H    | -1.301814 | 1.747967  | 3.788332 |
| H    | -1.304810 | 2.035670  | 5.527125 |
| H    | -2.396913 | 0.829251  | 4.822234 |
| H    | -5.406133 | 2.218890  | 0.714302 |
| H    | -3.814789 | 1.713103  | 1.301843 |
| H    | -5.241755 | 0.775992  | 1.728811 |
| H    | -4.729092 | 1.359518  | -4.558137 |
| H    | -6.368525 | 1.337077  | -3.899164 |
| H    | -5.719554 | -0.094339 | -4.717613 |
| H    | 2.573966  | -0.685526 | 8.040784 |
| H    | 3.021355  | 0.804925  | 7.206475 |
| H    | 3.780764  | -0.730422 | 6.753231 |
| H    | 1.933810  | 2.235656  | -3.182239 |
| H    | 0.865617  | 4.411183  | -3.382925 |
| H    | 5.566087  | -1.501816 | -2.404200 |
| H    | -2.617125 | 2.690469  | -1.442656 |
| H    | 0.390864  | -1.214377 | -5.774782 |
| H    | 0.666273  | -0.320793 | -4.266619 |
| H    | 2.012648  | -1.126409 | 5.066137 |
| H    | 4.090505  | 4.665757  | 1.093926 |
| H    | -0.159778 | -5.693086 | -2.036662 |
| H    | -0.736198 | -3.226132 | -5.493426 |
| H    | 3.554570  | 1.432726  | 3.852459 |
| H    | 3.350903  | -0.763650 | 3.137567 |
| H    | 2.416949  | -0.936501 | 1.648139 |
| H    | 4.161662  | -1.182217 | 1.613555 |
| H    | 2.992172  | 3.696961  | -1.521771 |
| H    | 4.684451  | 4.108245  | -1.220710 |
| H    | 4.258216  | 2.533173  | -1.917602 |
| H    | 1.437832  | -3.304884 | -0.041280 |
| H    | 1.239815  | -5.050657 | -0.289893 |
| H    | 2.714098  | -4.222318 | -0.818441 |
| H    | 6.048116  | 0.130172  | 0.452570 |
| H    | 6.748931  | -0.249590 | -1.134122 |
| H    | 6.094465  | 1.366920  | -0.791159 |
| H    | -0.512845 | 5.939466  | -4.008238 |
| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| C    | 0.341807 | 0.116641 | 4.959951 |
| C    | 0.358548 | -1.071085 | 4.204248 |
| C    | 0.683432 | -2.009149 | 4.332029 |
| C    | 1.706921 | -1.758955 | 5.249047 |
| C    | 1.736087 | -0.601421 | 6.030188 |
| C    | 0.707146 | 0.326622 | 5.858951 |
| N    | -1.427800 | -1.312692 | 3.283218 |
| C    | -2.487492 | -2.001749 | 3.727631 |
| C    | -2.489882 | -2.511257 | 5.15942 |
| C    | 0.700316 | -3.262604 | 3.497462 |
| C    | 2.827819 | -0.374355 | 7.043910 |
| C    | 1.429859 | 1.148763 | 4.812117 |
| Mg   | -1.360623 | -0.602979 | 1.371908 |
| N    | -3.277049 | -1.094334 | 0.890463 |
| C    | -4.031253 | -1.846013 | 1.694848 |
| C    | -5.413519 | -2.260275 | 1.238059 |
| O    | 0.195561 | -0.152623 | 0.276263 |
| C    | -0.386934 | 1.125851 | 0.159081 |
| O    | -0.249979 | 2.112946 | 1.037808 |
| O    | -0.325014 | 3.095105 | 1.686745 |
| Mg   | 1.603601 | -0.133649 | -1.215192 |
| N    | 0.397333 | 1.268238 | -2.125629 |
| C    | -0.807542 | 1.468525 | -1.342737 |
| C    | -1.519250 | 2.764002 | -1.541815 |
| C    | -1.026547 | 3.743654 | -2.351012 |
| C    | 0.217809 | 3.507257 | -3.054318 |
| C    | 0.824532 | 2.292807 | -2.898200 |
| N    | -1.715489 | 4.940574 | -2.608172 |
| C    | -3.024599 | 5.091082 | -2.016851 |
| N    | 3.516392 | 0.387562 | -0.591707 |
| C    | 4.611008 | -0.196457 | -1.071799 |
| C    | 5.973215 | 0.281893 | -0.612329 |
| C    | 3.659617 | 1.390545 | 0.416908 |
| C    | 3.805001 | 2.750225 | 0.083973 |
| C    | 3.888280 | 3.689523 | 1.117306 |
| C    | 3.819865 | 3.328995 | 2.461972 |
| C    | 3.681677 | 1.972344 | 2.766032 |
| El | X      | Y      | Z      |
|----|--------|--------|--------|
| C  | 3.600675 | 0.998542 | 1.770108 |
| C  | 3.862997 | 3.221790 | -1.345350 |
| C  | 3.458504 | -0.454217 | 2.136076 |
| C  | 3.86915  | 4.368737 | 3.551415 |
| C  | 4.608482 | -1.265923 | -1.992934 |
| C  | 3.542861 | -2.035170 | -2.493502 |
| N  | 0.989899 | -3.918761 | -1.992932 |
| C  | 0.99740  | -3.936561 | -3.744732 |
| C  | -0.554444 | 1.276956 | 4.759263 |
| C  | -3.844809 | -1.265777 | -1.551359 |
| H  | 4.380433 | -2.888416 | -3.490255 |
| H  | 6.056728 | -1.385240 | 1.091322 |
| H  | -0.009279 | 1.387316 | -3.635724 |
| H  | -1.786922 | 2.438699 | -1.314299 |
| H  | -2.895118 | -3.104757 | -2.503070 |
| H  | -3.208661 | -3.265050 | -0.771324 |
| H  | 2.505361 | -2.492325 | 5.353316 |
| H  | 0.739386 | -3.030760 | 2.425731 |
| H  | -0.194434 | 3.877907 | 3.650108 |
| H  | 1.574964 | -3.876271 | 3.734402 |
| H  | 5.638684 | 1.989337 | -1.561371 |
| H  | -1.355020 | 1.683387 | 3.856014 |
| H  | -1.359228 | 1.901387 | 5.603759 |
| H  | 2.430561 | 0.704559 | 4.853382 |
| H  | 5.370214 | 2.273343 | 0.734279 |
| H  | -3.803232 | 1.719762 | 1.341048 |
| H  | 5.255146 | 0.799118 | 1.708774 |
| H  | -4.661793 | 1.549176 | -4.543039 |
| H  | -6.309206 | 1.525069 | -3.904336 |
| H  | -5.665903 | 0.111545 | -4.758187 |
| H  | 2.561298 | -0.806123 | 8.018004 |
H  3.012669  0.693415  7.202613
H  3.770003 -0.837534  6.731520
H  1.737066  2.084542 -3.459471
H  0.593293  4.205891 -3.791916
H  5.591422  1.584258 -2.321159
H -2.458791  2.878843  1.013163
H  0.413684 -1.285021  5.712148
H  0.651523 -0.378605 -4.205936
H  2.022877 -1.172949  4.977274
H  4.007037  4.740055  0.854453
H  2.861099  3.473328 -1.716745
H  4.479494  4.123883 -1.429765
H  4.273257  2.462020 -2.016937
H  1.505092 -3.322433  0.021683
H  1.229910 -5.064915  0.184071
H  2.728564 -4.310163 -0.750725
H  6.081549  0.157141  0.471276
H  6.775407 -0.271398 -1.105929
H  6.106801  1.349904 -0.815528
H  0.019562  6.043779 -3.055527
H -1.494483  6.961689  3.100166
H -0.761590  6.519662 -1.536315
H  3.415835 -3.124674  3.611426
H  5.009648 -3.199931 -3.579657
H  3.648125 -4.151193 -2.957041
H -0.964041 -6.419678  4.898643
H -2.040608 -6.194946 -3.517947
H -2.243131 -5.205959  4.974281
H -2.998301  5.190561 -0.915554
H -3.498253  5.989581  2.427462
H -3.647354  4.227385 -2.269119
H  4.384639  5.275067  3.219012
H  2.855188  4.665451  3.858713
H  4.381235  3.994403  4.443908
H -1.496067  0.619797 -1.529177

Product TS2

C  16.680621  37.327027  25.239969
C  15.797790  36.232132  25.388961
C  15.024040  36.126461  26.564144
C  15.183509  36.048786  27.572540
C  16.069982  38.150804  27.458147
C  16.806490  38.251594  26.273987
N  15.636825  35.317750  24.311302
C  15.925899  34.025607  24.474351
C  15.465395  33.000882  23.613260
C  14.371430  33.031410  22.713616
C  13.788984  31.693485  22.308542

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| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| C       | 13.998399 | 35.041295 | 26.773331 |
| C       | 16.212774  | 39.178780  | 28.550321 |
| C       | 17.476711  | 37.507261  | 23.978680 |
| N       | 13.836468  | 34.154399  | 22.238651 |
| Mg      | 15.081782  | 37.948417  | 22.376084 |
| O       | 16.496122  | 36.001852  | 20.899616 |
| Mg      | 18.14856   | 35.210867  | 20.149465 |
| N       | 20.028085  | 34.913345  | 21.06474 |
| C       | 20.382195  | 35.459332  | 23.39227 |
| C       | 20.287928  | 34.642747  | 24.84985 |
| C       | 20.624999  | 35.179549  | 24.729166 |
| C       | 21.051754  | 36.501584  | 24.875539 |
| C       | 21.14035   | 37.286173  | 23.72532 |
| C       | 20.80175   | 36.795463  | 22.95242 |
| C       | 19.838291  | 33.209653  | 23.37247 |
| C       | 21.373615  | 37.06487   | 26.234527 |
| C       | 20.919355  | 37.689075  | 21.252604 |
| C       | 12.560729  | 34.117209  | 21.602990 |
| C       | 11.392717  | 34.047191  | 22.39133 |
| C       | 10.016989  | 34.133640  | 20.37667 |
| C       | 11.85689   | 34.231329  | 19.618719 |
| C       | 12.45407   | 34.235054  | 20.204747 |
| C       | 11.473044  | 34.021043  | 23.394222 |
| C       | 13.678434  | 34.373899  | 19.343377 |
| C       | 8.65974    | 34.164586  | 19.719818 |
| O       | 14.47543   | 37.590650  | 21.841517 |
| C       | 15.038180  | 38.118614  | 20.822582 |
| C       | 16.144989  | 37.198132  | 20.297231 |
| C       | 17.099480  | 37.780244  | 19.355756 |
| N       | 18.140921  | 36.972099  | 18.995518 |
| C       | 18.975143  | 37.416013  | 18.029219 |
| C       | 18.865747  | 38.632077  | 17.406361 |
| C       | 17.818547  | 39.516878  | 17.809443 |
| C       | 16.953685  | 39.076326  | 18.813936 |
| N       | 17.684993  | 40.755221  | 17.243336 |
| C       | 18.700804  | 41.260907  | 16.342378 |
| N       | 18.332848  | 33.496245  | 18.973889 |
| C       | 17.208803  | 32.824179  | 18.399443 |
| C       | 16.645431  | 33.278017  | 17.191284 |
| C       | 15.554951  | 32.589412  | 16.652368 |
| C       | 14.999764  | 31.471044  | 17.275137 |
| C       | 15.571451  | 31.045899  | 18.476460 |
| C       | 16.661187  | 31.702516  | 19.054121 |
| C       | 17.216768  | 34.467715  | 16.466898 |
| C       | 13.806007  | 30.762820  | 16.689213 |
| C       | 17.239342  | 31.207402  | 20.354022 |
| C       | 16.653704  | 41.652098  | 17.728547 |
| C       | 19.547414  | 33.046043  | 18.650079 |
| C       | 20.753618  | 33.484888  | 19.234233 |
| C       | 20.974440  | 34.250685  | 20.396723 |
| C       | 22.400162  | 34.261848  | 20.912295 |
| C       | 19.686323  | 31.949898  | 17.611891 |
| C       | 16.775330  | 33.575494  | 25.645120 |
| H       | 15.855437  | 32.011595  | 23.829846 |
| Atoms | X       | Y       | Z       |
|-------|---------|---------|---------|
| C     | 0.91603 | 4.20359 | -3.30690 |
| C     | 2.19946 | 3.60785 | -3.41790 |
| C     | 2.42499 | 2.39080 | -2.81101 |
| C     | -0.78649 | 1.45477 | -1.28110 |
| C     | -1.81150 | 2.46381 | -3.41790 |
| O     | -2.14614 | 2.03385 | 0.57309 |
| N     | 0.64064 | 5.42248 | -3.85275 |
| N     | 0.64064 | 5.42248 | -3.85275 |
| C     | 1.04302 | 2.15628 | 2.53490 |
| C     | 0.23558 | -1.46297 | 4.75019 |
| C     | 5.72545 | -1.27790 | -0.48233 |
| H     | -0.78189 | -3.27591 | 3.26382 |
| H     | -3.86240 | -3.70208 | 2.37956 |
| H     | -2.29991 | 4.52994 | 2.28884 |
| H     | -3.12739 | -3.98434 | 0.80734 |
| H     | -1.98786 | 2.38002 | 6.96593 |
| H     | 0.97203 | -0.67201 | 4.92111 |
| H     | 0.75682 | -2.41860 | 4.64548 |
| H     | -0.38519 | -1.53642 | 5.65712 |
| H     | -5.11249 | -2.00367 | 2.55634 |
| H     | -1.83868 | -1.34887 | 1.34129 |
| H     | -2.77398 | -2.17270 | -2.60175 |
| H     | -2.20872 | -3.05603 | -1.18354 |
| H     | 1.03952 | 4.04711 | 4.43907 |
| H     | 0.42839 | 2.33561 | 1.64277 |
| H     | 1.54950 | 1.19525 | 2.40364 |
| H     | 1.80836 | 2.93810 | 2.55783 |
| H     | -7.20630 | -0.85955 | 1.00213 |
| H     | -2.85304 | -0.37750 | 4.67714 |
| H     | -3.45281 | 0.69171 | 5.95644 |
| H     | -2.21813 | -0.50936 | 6.32148 |
| H     | -6.10558 | -0.46711 | 3.00353 |
| H     | -4.46555 | 0.18445 | 2.83245 |
| H     | -4.69525 | -1.49197 | 3.31476 |
| H     | -8.30694 | -0.69831 | -1.27836 |
| H     | -8.14321 | -2.44472 | -1.47865 |
| H     | -7.47052 | -1.35396 | -2.69511 |
| H     | 0.69938 | 4.50054 | 7.27387 |
| H     | -1.05804 | 4.48938 | 7.56391 |
| H     | -0.37256 | 5.46687 | 6.25276 |
| H     | 3.40280 | 1.91974 | -2.87925 |
|     |     |     |
|-----|-----|-----|
| H   | 3.006107 | 4.080866 | -3.964944 |
| H   | 5.082255 | -1.974995 | -2.837978 |
| H   | -1.069110 | 3.840040 | -2.438770 |
| H   | 0.028171 | -0.082072 | -5.910053 |
| H   | 0.113281 | 0.467357 | -4.233484 |
| H   | 1.545121 | -0.203083 | -4.997650 |
| H   | 4.969585 | 2.260627 | 2.907935 |
| H   | -1.042589 | -5.248857 | -3.388758 |
| H   | -1.444470 | -1.877957 | -6.001404 |
| H   | 3.659346 | -1.621517 | 4.153691 |
| H   | 3.018784 | -3.248469 | 2.599317 |
| H   | 1.545121 | -0.203083 | -4.997650 |
| H   | 4.969585 | 2.260627 | 2.907935 |
| H   | 5.725464 | 0.337307 | 1.552500 |
| H   | 3.470107 | 2.343945 | -0.166120 |
| H   | 4.899091 | 2.932702 | 0.697613 |
| H   | 5.052984 | 1.674408 | -0.539433 |
| H   | 0.823108 | -3.682950 | -0.899235 |
| H   | 0.465725 | -5.261479 | -1.623500 |
| H   | 1.998134 | -4.439741 | -1.961589 |
| H   | 5.725464 | 0.337307 | -1.961589 |
| H   | 6.431232 | -1.621755 | -1.241785 |
| H   | 6.091398 | -0.337324 | -0.059590 |
| H   | 1.990967 | 5.589269 | -5.479719 |
| H   | 1.260734 | 7.100359 | -4.914262 |
| H   | 2.543227 | 6.339852 | -3.962259 |
| H   | 2.656026 | -2.393077 | -5.169908 |
| H   | 4.262455 | -2.873476 | -4.576213 |
| H   | 2.826585 | -3.86375 | -4.186476 |
| H   | -2.217066 | -5.407443 | -5.730984 |
| H   | -3.410459 | -4.367648 | -4.951865 |
| H   | -2.690978 | -3.879066 | -6.490670 |
| H   | -0.987859 | 6.097068 | -2.683755 |
| H   | -0.714914 | 6.963043 | -4.206735 |
| H   | -1.443883 | 5.345715 | -4.228040 |
| H   | 5.573535 | 1.346267 | 5.196552 |
| H   | 3.857234 | 1.260582 | 5.604418 |
| H   | 4.864293 | -0.185866 | 5.734373 |
| H   | -1.460513 | 1.003722 | -2.035514 |

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Product TS3

|     |     |     |
|-----|-----|-----|
| C   | 16.639209 | 37.501777 | 25.160072 |
| C   | 15.785605 | 36.391962 | 25.356502 |
| C   | 15.029571 | 36.306684 | 26.545059 |
| C   | 15.181192 | 37.298405 | 27.521302 |
| C   | 16.046757 | 38.376722 | 27.363600 |
| C   | 16.760723 | 38.459299 | 26.164735 |
| N   | 15.630573 | 35.439891 | 24.310880 |
| C   | 15.976763 | 34.167161 | 24.505819 |
| C   | 15.554494 | 33.098791 | 23.678224 |
| C   | 14.451537 | 33.056070 | 22.791126 |
| C   | 13.935308 | 31.681839 | 22.417206 |
| C   | 14.028905 | 35.207443 | 26.796177 |
| C   | 16.212759 | 39.417501 | 28.440225 |
| C   | 17.399614 | 37.668441 | 23.874916 |
N  13.854584  34.140623  22.302039
Mg 15.004164  35.862301  22.377290
O  16.479829  36.038217  20.899410
Mg 18.119213  35.180979  20.140788
N  19.963138  36.038217  20.899410
C  20.318916  35.364631  22.341656
C  20.219994  34.508756  23.457391
C  20.558191  34.999503  24.720449
C  20.988207  36.313822  24.915471
C  21.084335  37.137789  23.793817
C  20.752563  36.693373  22.510814
C  19.760833  33.083256  23.296089
C  21.308566  36.831421  26.294002
C  20.865560  37.633816  21.340492
C  12.575714  34.023182  21.684002
C  11.422083  33.891913  22.485564
C  10.171641  33.815734  21.869070
C  10.021139  33.883277  20.483009
C  11.173205  34.053355  19.714992
C  12.445525  34.131952  20.286969
C  11.518081  33.892444  23.987902
C  13.649777  34.346933  19.414305
C  8.663541  33.766611  19.839702
O  14.335339  37.555227  21.708552
C  15.061843  38.068279  20.744343
C  16.150137  37.227443  20.299003
C  17.156507  37.793233  19.349505
N  18.173387  36.967663  19.011425
C  19.085681  37.423472  18.131963
C  19.034780  38.685966  17.547826
C  17.972902  39.549709  17.890782
C  17.043974  39.082095  18.838034
N  17.867392  40.793574  17.341421
C  18.885221  41.278569  16.431620
N  18.262436  33.505390  18.919356
C  17.137880  32.845538  18.332079
C  16.552778  33.344058  17.152459
C  15.460321  32.667942  16.601762
C  14.922259  31.521727  17.187657
C  15.514209  31.053762  18.363071
C  16.607987  31.694837  18.949943
C  17.095067  34.574661  16.475212
C  13.723998  30.828671  16.593006
C  17.205698  31.156871  20.223746
C  16.795363  41.676964  17.760438
C  19.478450  33.078982  18.570622
C  20.685143  33.506817  19.162993
C  20.908143  34.228689  20.353674
C  22.334753  34.221143  20.866407
C  19.618709  32.025963  17.489116
C  16.854016  33.787575  25.680966
H  15.989876  32.134119  23.918385
H  12.961351  31.490302  22.881713
H  14.624988  30.899275  22.743330
H  13.789564  31.603439  21.334391
H  12.795740  31.154027  17.081006
H  13.624750  31.045344  15.524061
H  16.875262  41.939071  18.827844
H  16.838753  42.596993  17.178806
H  15.814411  41.215296  17.599587
H  20.401524  37.208303  26.789677
H  21.723151  36.045300  26.932993
H  22.026608  37.655465  26.257827
H  15.057350  37.415016  19.548396

TS4

C   0.069990  1.981665  3.914637
C  -0.823440  0.895684  4.062254
C  -1.624228  0.814214  5.221220
C  -1.484752  1.789965  6.215339
C  -0.587347  2.847716  6.3827
C   0.176242  2.923999  4.935422
N   -0.970589 -0.033001  2.995207
C  -0.662608 -1.317758  3.171171
C  -1.088604 -2.354841  2.305894
C  -2.163867 -2.347395  1.384985
C  -2.691066 -3.697986  0.946173
C  -2.656335 -0.265904  5.422915
C  -0.437190  3.872405  7.198100
C   0.900388  2.131926  2.671613
N   -2.723824 -1.234956  0.911992
Mg  -1.518540  0.437170  1.051934
C  -0.062252  0.796229  -0.377355
Mg  1.546562 -0.139200  -1.184319
N   3.392843 -0.490262  -0.279071
C   3.760522  0.022750  1.002965
C   3.660907 -0.814804  2.132643
C   4.016137 -0.308781  3.385009
C   4.465026  1.002841  3.555255
C   4.557394  1.809583  2.420685
C   4.207556  1.349826  1.147792
C   3.185019 -2.237371  1.996227
C   4.806166  1.535152  4.922736
C   4.321851  2.265363  0.04792
C  -3.987767 -1.301541  0.258515
C  -5.163242 -1.467274  1.022740
C  -6.398258 -1.493755  0.372749
C  -6.513507 -1.342703 -1.010519
C  -5.341457 -1.137946 -1.738037
C  -4.082200 -1.106192 -1.132191
C  -5.108575 -1.552068  2.525100
C  -2.855643 -0.854107 -1.963474
C  -7.856185 -1.410500 -1.691049
O  -2.186148  2.192300  0.509262
C  -1.431438  2.639431 -0.446994
C  -0.345629  1.946572 -0.940476
C   0.511359  2.437315 -1.991449
N   1.555078  1.619919 -2.325925
C   2.403293  2.019444 -3.291693

133
H  0.012977 -0.603169 -5.807856
H  0.374900  0.130688 -4.238311
H  1.589827 -0.852870 -5.630451
H  4.912468  2.834113  2.524568
H  3.254668 -2.761630  2.954656
H  2.140051 -2.281295  1.664946
H  3.768332 -0.963238  4.252688
H  3.254668 -1.509650 -5.147480
H  1.574294 -0.852870 -5.038596
H  4.912468  2.834113  2.524568
H  0.456528 -3.467343 -0.245406
H  0.120151 -5.112777 -0.802737
H  1.673706 -4.340875 -1.167248
H  5.826873 -1.742961  0.470678
H  6.428910 -1.619191 -0.838369
H  6.114599 -0.158351 -0.226420
H  2.112224  4.969431 -5.630451
H  1.707186  6.642312 -5.741744
H  3.020686  5.829257 -4.874029
H  2.465038 -3.054305 -4.730893
H  4.051268 -3.523363 -4.077092
H  2.564700 -4.287668 -3.481102
H  2.848291 -5.562691 -4.572492
H  3.822315 -4.134110 -4.216384
H  2.994505 -4.267017 -5.772221
H  0.060522  6.497116 -2.923341
H  -0.021623  7.024116 -4.615622
H  -1.009527  5.600440 -4.072822
H  3.906812  1.890362  5.442950
H  5.261310  0.763079  5.553257
H  5.504293  2.377057  4.863380
H  -1.690169  3.618810 -0.861904

Adduct TS5
C  -4.746595  1.255665 -0.210687
C  -4.156105 -0.014642 -0.353818
C  -3.953168 -0.560337 -1.638220
C  -4.367509  0.165242 -2.755964
C  -4.977834  1.417080 -2.641111
C  -5.147807  1.944980 -1.360734
N  -3.734224 -0.746609  0.796606
C  -4.617255 -1.577162  1.366357
C  -5.999804 -1.713572  0.759647
C  -3.321185 -1.916712 -1.799532
C  -5.459954  2.153457 -3.864892
C  -4.968915  1.860145  1.151213
Mg  -1.818984 -0.515875  1.530247
O  -1.520395  2.045101  2.120391
C  -0.449443  2.491117  2.415674
O  -0.046474 -0.407232  0.702166
C  0.750708  0.411407  1.508619
C  1.563418  0.148844  2.508238

S66
| H   | -4.304514 | -3.875408 | 4.549428 |
|-----|-----------|-----------|----------|
| H   | -3.223849 | -2.815680 | 5.479198 |
| H   | -4.219751 | -0.267442 | -3.744736 |
| H   | -2.294973 | -1.941694 | -1.413917 |
| H   | -3.284522 | -2.854645 | 4.658278 |
| H   | -2.294973 | -1.941694 | -1.413917 |
| H   | 1.785187  | -3.615749 | 4.651525 |
| H   | 0.058736  | -3.108275 | 1.762253 |
| H   | -1.015234 | -4.232829 | 2.587543 |
| H   | 0.740554  | -4.420726 | 2.730350 |
| H   | -5.624946 | 2.917629  | -1.244541 |
| H   | -2.186466 | 0.726189  | -2.854645 |
| H   | -1.896534 | 0.589325  | 6.397957 |
| H   | -3.094701 | -0.445010 | 5.603390 |
| H   | -5.499931 | 2.814234  | 1.069618 |
| H   | -4.022032 | 2.043930  | 1.670799 |
| H   | -5.558618 | 1.201974  | 1.800185 |
| H   | -5.796985 | 3.165944  | 1.355724 |
| H   | -6.305691 | 1.635233  | -3.617205 |
| H   | -4.673163 | 2.233353  | -4.625159 |
| H   | 2.647008  | -3.142740 | 6.948868 |
| H   | 1.957234  | -1.817034 | 7.902923 |
| H   | 3.044808  | -1.466136 | 6.554237 |
| H   | 1.802389  | 1.306126  | -3.358303 |
| H   | 0.878407  | 2.934128  | -4.929223 |
| H   | 4.778967  | -0.039208 | -3.468044 |
| H   | -2.287344 | 3.637257  | -2.043463 |
| H   | -0.873742 | -2.164441 | -4.224866 |
| H   | -0.433141 | -0.874593 | -3.091689 |
| H   | 0.739422  | -1.437053 | -4.272424 |
| H   | 3.546558  | 5.371416  | 1.355724 |
| H   | 1.589696  | -5.516904 | -0.108615 |
| H   | -1.053202 | -4.251685 | -3.232603 |
| H   | 5.745084  | 2.142750  | 3.109451 |
| H   | 5.780637  | 0.033273  | 2.179027 |
| H   | 4.250893  | -0.444511 | 1.433663 |
| H   | 5.636093  | -0.066431 | 0.414699 |
| H   | 1.466023  | 3.728925  | -0.576752 |
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| H   | 3.298648  | -4.150953 | 0.685946 |
| H   | 3.970226  | -2.953519 | -0.436760 |
| H   | 6.179276  | 1.666176  | -1.157464 |
| H   | 5.885841  | 1.718959  | -2.904096 |
| H   | 5.190381  | 2.953636  | -1.824606 |
| H   | -0.580867 | 3.874266  | -6.367340 |
| H   | -1.290011 | 5.488667  | -6.257353 |
| H   | 0.307559  | 5.183463  | 5.549178 |
| H   | 2.682533  | -2.636599 | -4.130747 |
| H   | 4.322311  | -1.963371 | -4.279256 |
| H   | 3.933575  | -3.129305 | 3.003371 |
| H   | -0.337339 | -6.948909 | 2.559559 |
| H   | -0.140377 | -7.003558 | -0.802843 |
| H   | -1.590156 | -6.278617 | -1.513198 |
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H  -3.345395  4.567778 -3.786501
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H   4.505497  4.640721  4.376216
H   6.171385  4.565721  3.796327
H  -1.214401  1.971660  -0.621940
135
TS5
C   0.410608 -2.809313 -2.621748
C   1.497593 -2.548079 -1.762921
C   1.917403 -3.529195 -0.845661
C   1.254462 -4.760048  -0.816414
C   0.185240  5.047886  -1.664421
C  -0.220721 -4.053365  -2.558238
N   2.157353 -1.283245  -1.792076
C   3.188061 -1.141166  -2.628112
C   4.029047 -0.011739  -2.684768
C   4.195468  1.027725  -1.739993
C   5.429801  1.890109  -1.925545
C   3.062005  3.260540   0.094530
C  -0.505026 -6.387420  -1.631125
C  -0.063187  1.841495  -2.703588
N   3.378452  1.251433  -0.717316
Mg  1.494211  0.289564  -0.559913
O  -0.046474 -0.407232  0.702166
Mg  2.118984 -0.515875  1.530247
N  -2.125906 -1.717649  3.167839
C  -1.067652 -1.852188  4.121074
C  -1.025013 -1.005335  5.244893
C   0.041747 -1.129169  6.137508
C   1.065982 -2.057356  5.945559
C   0.996109 -2.885079  4.824117
C  -0.047024 -2.795801  3.900306
C  -2.105514  0.016102  5.489128
C   2.236428 -2.128536  6.890371
C  -0.069757  3.686128  2.686198
C   3.826390  2.152627  0.301905
C   4.674559  1.664394  1.317705
C   5.096121  2.531381  2.325957
C   4.701622  3.869724  2.367442
C   3.865367  4.329623  1.351502
C   3.413900  3.497239  0.323039
C   5.112481  0.224279  1.333443
C   2.500584  4.056797  -0.734387
C   5.139871  4.774331  3.489807
N   0.343979  1.550812  -1.910942
C  -0.782020  2.211552  -1.587725
C  -1.380886  3.160063  -2.393584
C  -0.810313  3.475319  -3.649094
C   0.363606  2.763301  -3.991362
C   0.887549  1.839436  -3.108436
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S69
|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| C | 0.750708  | 0.411407  | 1.508619  |
| C | 1.563418  | 0.418844  | 2.508239  |
| O | 2.337711  | 0.214538  | 3.404544  |
| O | -1.579952 | 1.534283  | 2.002680  |
| C | -0.509000 | 1.980299  | 2.297963  |
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| C | -3.953168 | -0.560337 | -1.638220 |
| C | -4.367509 | 0.165242  | 2.755964  |
| C | -4.977834 | 1.417080  | 3.404544  |
| C | -5.147807 | 1.944980  | 2.397963  |
| C | -4.746595 | 1.255665  | -0.210687 |
| C | -3.321185 | -1.916712 | -1.799532 |
| C | -5.459954 | 2.153457  | -3.864892 |
| C | -4.968915 | 1.860145  | 1.151213  |
| C | -4.617255 | -1.577162 | 1.366357  |
| C | -4.375265 | -2.352315 | 2.512553  |
| C | -3.242841 | -2.416831 | 3.352059  |
| C | -3.342879 | -3.357582 | 4.534742  |
| C | -5.999804 | -1.713572 | 0.759647  |
| C | 3.549884  | -2.272855 | -3.571142 |
| H | -5.200080 | -2.987234 | 2.815043  |
| H | -6.529011 | -0.753929 | 0.771924  |
| H | -6.599350 | -2.443604 | 1.307656  |
| H | -5.946169 | -2.024397 | -0.289521 |
| H | 0.076792  | -0.469675 | 7.003398  |
| H | -2.542505 | -4.105259 | 4.504523  |
| H | -4.304515 | -3.875408 | 4.594282  |
| H | -3.223850 | -2.815680 | 5.479198  |
| H | -4.219751 | -0.267442 | -3.744736 |
| H | -2.94973  | -1.941694 | -1.413917 |
| H | -3.284522 | -2.204400 | -2.854645 |
| H | -3.872877 | -2.693630 | -1.257201 |
| H | 1.785187  | -3.615748 | 4.651525  |
| H | 0.058736  | -3.108275 | 1.762253  |
| H | -1.015234 | -4.232829 | 2.587543  |
| H | 0.740554  | -4.420726 | 2.730350  |
| H | -5.624946 | 2.917629  | -1.244541 |
| H | -2.186467 | 0.726189  | 4.658278  |
| H | -1.896535 | 0.589325  | 6.397957  |
| H | -3.094702 | -0.445010 | 5.603390  |
| H | -5.499931 | 2.814234  | 1.069618  |
| H | -4.022032 | 2.043930  | 1.670799  |
| H | -5.558618 | 1.201974  | 1.800185  |
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| H | -6.305691 | 1.635233  | -4.335370 |
| H | -4.673163 | 2.233353  | -4.625159 |
| H | 2.647008  | -3.142739 | 6.948869  |
| H | 1.957234  | -1.817033 | 7.902923  |
| H | 3.044807  | -1.466135 | 6.554237  |
| H | 1.802389  | 1.306126  | -3.358303 |
| H | 0.878407  | 2.934128  | -4.929223 |
| H | 4.778967  | -0.039208 | -3.468044 |
| H | -2.287344 | 3.637257  | -2.043463 |
| H | -0.873742 | -2.164441 | -4.224865 |
Product TS5

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C 0.418811  -4.759565  -1.896150
C -0.469542  -4.785489  -2.973835
C -0.551221  -3.645636  -3.773647
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C 3.128000  -1.290835  -2.624698
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C 4.127973  0.591717  -1.209465
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N -1.507945  -1.465011  3.630871
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| C       | 2.013174   | -1.599687  | 6.004426   |
| C       | 1.813837   | -2.500860  | 4.956964   |
| C       | 0.657725   | -2.478358  | 4.172605   |
| C       | -1.208207  | 0.441786   | 5.803470   |
| C       | 3.249551   | -1.665333  | 6.864241   |
| C       | 0.478507   | -3.468410  | 3.052418   |
| C       | 3.253631   | 1.742754   | 0.678875   |
| C       | 3.459554   | 1.116741   | 1.924664   |
| C       | 3.584390   | 1.906251   | 3.068643   |
| C       | 3.509182   | 3.299828   | 3.014718   |
| C       | 3.312974   | 3.893309   | 1.768564   |
| C       | 3.174819   | 3.144945   | 0.595624   |
| C       | 3.534905   | -0.383234  | 2.028975   |
| C       | 2.904611   | 3.856836   | -0.703441  |
| C       | 3.603346   | 4.132835   | 4.266692   |
| N       | 0.362398   | 1.616917   | -2.427266  |
| C       | -0.881425  | 2.133069   | -2.411265  |
| C       | -1.333022  | 3.079296   | -3.307506  |
| C       | -0.465114  | 3.571967   | -4.308848  |
| C       | 0.836489   | 3.013934   | -4.331033  |
| C       | 1.189296   | 2.068373   | -3.390890  |
| N       | -0.857893  | 4.525947   | -5.197871  |
| C       | 0.085261   | 5.046059   | -6.169085  |
| C       | -2.171989  | 5.129898   | -5.074599  |
| C       | -0.374313  | 1.571172   | 0.828851   |
| C       | -0.499513  | 3.007406   | 0.738716   |
| O       | -0.304875  | 4.062336   | 0.154054   |
| O       | -1.839794  | 1.870899   | 2.806088   |
| C       | -1.087361  | 2.209700   | 1.806509   |
| N       | -3.426796  | -0.778808  | 1.374684   |
| C       | -3.935482  | -0.222798  | 0.163882   |
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| C       | -4.108344  | -0.283817  | -2.247194  |
| C       | -4.836666  | 0.909745   | -2.255893  |
| C       | -5.092471  | 1.526802   | -1.031134  |
| C       | -4.657563  | 0.986126   | 0.184498   |
| C       | -2.867031  | -2.144723  | -1.087975  |
| C       | -5.344552  | 1.494629   | -3.549376  |
| C       | -4.972514  | 1.682512   | 1.482370   |
| C       | -4.158309  | -1.672049  | 2.039243   |
| C       | -3.755814  | -2.313862  | 3.227986   |
| C       | -2.550851  | -2.234194  | 3.953754   |
| C       | -2.472059  | -3.095841  | 5.198139   |
| C       | -5.528178  | -2.044785  | 1.510533   |
| C       | 3.566359   | -2.339791  | -3.628568  |
| H       | -4.490881  | -2.992022  | 3.646001   |
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| H       | -6.016108  | -2.779562  | 2.154745   |
| H       | -5.459202  | -2.460448  | 0.499169   |
| H       | 1.152012   | 0.065204   | 7.056384   |
| H       | -1.642086  | -3.808242  | 5.138642   |
| H       | -3.397658  | -3.655125  | 5.350922   |

S72
H  -2.287488 -2.478781  6.084758
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H   3.560593 -0.669274  7.198447
H  -2.297479   5.876922   -5.859649
H  -2.967437   4.382711   -5.190516
H   4.034802   5.118819   4.061788
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H   4.220321   3.644847   5.029443
H  -1.546772   1.765743   -1.636730

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