Electronic Supplementary Information for One metal is enough: A nickel complex reduces nitrate anions to nitrogen gas

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1. Experimental section

1.1 General Considerations. All manipulations were carried out using standard Schlenk or glovebox techniques under a N_2 atmosphere. Unless otherwise noted, solvents were deoxygenated and dried by thoroughly sparging with Ar gas followed by passage through an activated alumina column. Non-halogenated solvents were tested with a standard purple solution of sodium benzophenoneketyl in tetrahydrofuran in order to confirm effective oxygen and moisture removal. All reagents were purchased from commercial vendors and used without further purification unless otherwise stated. Nitric oxide and nitrous oxide were purchased from Thomas Scientific (Sigma-Aldrich Co.) and Special Gas (Daejeon, South Korea). (PNP)NiCl[S1] and (PNP)Ni(OTf)[S2] were prepared according to literature procedures. Elemental analyses were carried out at KAIST Central Research Instrument Facility on Thermo Scientific FLASH 2000 series instrument. Deuterated solvents were purchased from Cambridge Isotope Laboratories, Inc. or Euriso-top, degassed, and dried over activated 4 Å molecular sieves prior to use.

X-ray Crystallography. The diffraction data of **1** was collected on a Bruker SMART 1000. The diffraction data of **2** and **3** were collected on a Bruker D8 QUEST. A suitable size and quality of crystal was coated with Paratone-N oil and mounted on a DualThickness MicroLoops LD purchased from MiTeGen. The data were collected with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å) under a stream of N_2(g) at 120 K. Cell parameters were determined and refined by SMART program [S3]. Data reduction was performed using SAINT software [S4]. An empirical absorption correction was applied using the SADABS program [S5]. The structures were solved by direct methods, and all non-hydrogen atoms were subjected to anisotropic refinement by full-matrix least squares on F^2 by using the SHELXTL/PC package [S6]. Unless otherwise noted, hydrogen atoms were placed at their geometrically calculated positions and refined riding on the corresponding carbon atoms with isotropic thermal parameters.

Spectroscopic Measurements. Bruker 400 spectrometers were used to measure ^{1}H NMR. The chemical shifts for ^{1}H NMR spectra were quoted in part per million referenced to residual solvent peaks. ^{13}C NMR spectra were recorded on Agilent 600 spectrometers. ^{13}C NMR chemical shifts are reported in parts per million (ppm) referenced to internal solvent peaks. ^{31}P NMR spectra were recorded on Bruker 400 and were decoupled by broad band proton decoupling. The chemical shifts for ^{31}P NMR spectra were quoted in part per million (ppm) referenced to external phosphoric acid as 0.0 ppm. ^{15}N NMR spectra were recorded on Agilent 600 spectrometer and were decoupled by broad band proton decoupling. The chemical shifts for ^{15}N NMR spectra were quoted in part per million (ppm) referenced to external formamide as –267.8 ppm. The following abbreviations were used to describe peak splitting patterns when appropriate: s = singlet, d = doublet, t = triplet, m = multiplet, dt = doublet of triplet. Coupling constants, *J*, were reported in hertz unit (Hz). UV-Vis spectra were measured by Agilent Cary 60 UV-Vis spectrophotometer using a 1 cm two-window quartz spectrophotometer cell sealed with a screw-cap purchased from Hellma Analytics (117.100-

QS). Infrared spectra were recorded in KBr pellet by Brucker VECTOR 33. Frequencies are given in reciprocal centimeters (cm^{-1}) and only selected absorbances were reported.

Gas Chromatography. Gas chromatography experiments were performed on an Acme 6100 GC with a thermal conductivity detector and a flame ionization detector equipped with a methanizer. The constituent gases were separated by passing through a Carboxen 1000 column using argon as the carrier gas. The reaction components were loaded into a gas-tight piece of glassware, outfitted with a rubber septum, in a glove box. The headspace was sampled using a gas-tight syringe. Gas calibration curves (N_2O, CO_2, N_2) were constructed by sampling different volumes of gas (1 atm) and plotting the area versus the moles of gas. Comparison of the area yielded the number moles of gas in the headspace. Assuming ideal gas behavior the molar concentration of gas in solution was determined. From these values the total number of moles of gas and yield were calculated.

Synthesis of (PNP)Ni(ONO_2) (1). Sodium nitrate (0.183 g, 2.15 mmol) was added to a yellow solution of (PNP)Ni(OTf) (0.274 g, 0.431 mmol) in 20 mL of diethyl ether and 2 mL of THF in a 50 mL Schlenk tube. The mixture was stirred for 6 hrs at 45 °C. Volatiles were removed under vacuum and a resulting green solid was dissolved in benzene. The solution was filtered through Celite and the filtrate was evaporated under reduced pressure to afford a green powder of (PNP)Ni(ONO_2) (**1**, 0.199 g, 0.362 mmol, 84.5%). ^{1}H NMR (400 MHz, C_6D_6, ppm) δ 7.29 (d, *J* = 8.00 Hz, 2H, Ar-H), 6.75 (s, 2H, Ar-H), 6.64 (d, *J* = 8.00 Hz, 2H, Ar-H), 2.08 (s, 6H, Ar-CH_3), 2.01 (m, 4H, C*H*CH_3), 1.38 (q, *J* = 8.00 Hz, 12H, CHC*H*$_3$), 1.13 (q, *J* = 8.00 Hz, 12H, CHC*H*$_3$). ^{13}C NMR (151 MHz, C_6D_6, ppm) δ 161.33 (CN_{Ar}, t, *J* = 13.56 Hz), 132.20 (C_{Ar}), 131.41 (C_{Ar}), 125.47 (C_{Ar}), 118.62 (C_{Ar}), 116.90 (C_{Ar}, t, *J* = 6.03 Hz), 23.07 ($CH_{i\mathrm{Pr}}$, t, *J* = 10.55 Hz), 19.94 (Me_{Ar}), 17.62 ($Me_{i\mathrm{Pr}}$, t, *J* = 4.52 Hz), 16.08 ($Me_{i\mathrm{Pr}}$). ^{31}P NMR (162 MHz, C_6D_6, ppm) δ 35.79 (s). UV-Vis [THF, nm (L mol^{-1} cm^{-1})]: 388 (2700), 435 (1600), 677 (240). IR (KBr pellet, cm^{-1}): ν_{NO2} = 1482, 1280, ν_{NO} = 1000. Anal. Calcd. for $C_{26}H_{40}N_2NiO_3P_2$: C, 56.86; H, 7.34; N, 5.10. Found: C, 57.25; H, 7.49; N, 5.11. Crystals suitable for X-ray diffraction were obtained by slow diffusion of pentane into a saturated THF solution of **1**.

Synthesis of (PNP)Ni($O^{15}NO_2$) (1-$O^{15}NO_2$). (PNP)Ni($O^{15}NO_2$) (**1-$O^{15}NO_2$**) was synthesized by same procedure of (PNP)Ni(ONO_2) (**1**) except with $Na^{15}NO_3$ instead of $NaNO_3$. Spectroscopic features in the ^{1}H NMR, ^{13}C NMR and ^{31}P NMR were identical for **1**. ^{15}N NMR (61 MHz, C_6D_6, ppm) δ –12.42 (s). IR (KBr pellet, cm^{-1}): ν_{NO2} = 1442, 1257, ν_{NO} = 983.

Synthesis of (PNP)Ni(NO_2) (2). Sodium nitrite (1.389 g, 20.03 mmol) was added to a green solution of (PNP)NiCl (2.033 g, 3.973 mmol) in 50 mL of THF in a 250 mL Schlenk tube. After the solution was stirred for additional 3 hrs at 60 °C, all volatiles were removed under vacuum. After dissolved in benzene, a dark purple solution was filtered through Celite and volatiles were removed under vacuum. The resulting product (PNP)Ni(NO_2) (**2**, 1.716 g, 3.261 mmol, 82.1%) was isolated as a purple solid after washing with pentane.

^{1}H NMR (400 MHz, C_6D_6, ppm) δ 7.45 (d, *J* = 8.00 Hz, 2H, Ar-H), 6.79 (s, 2H, Ar-H), 6.71 (d, *J* = 8.00 Hz, 2H, Ar-H), 2.15 (m, 4H, C*H*CH_3), 2.10 (s, 6H, Ar-CH_3), 1.37 (q, *J* = 8.00 Hz, 12H, CHC*H*$_3$), 1.13 (q, *J* = 8.00 Hz, 12H, CHC*H*$_3$). ^{13}C NMR (151 MHz, C_6D_6, ppm) δ 160.79 (CN_{Ar}, t, *J* = 12.49 Hz), 131.82 (C_{Ar}), 131.09 (C_{Ar}), 124.61 (C_{Ar}, t, *J* = 3.02 Hz), 117.30 (C_{Ar}, t, *J* = 9.06 Hz), 115.60 (C_{Ar}, t, *J* = 5.29 Hz), 22.46 ($CH_{i\text{Pr}}$, t, *J* = 3.02 Hz), 19.40 (Me_{Ar}), 17.11 ($Me_{i\text{Pr}}$, t, *J* = 1.51 Hz), 16.11 ($Me_{i\text{Pr}}$). ^{31}P NMR (162 MHz, C_6D_6, ppm) δ 42.29 (s). UV-Vis [THF, nm (L mol^{-1} cm^{-1})]: 387 (2700), 435 (1100), 560 (400). IR (KBr pellet, cm^{-1}): $\nu_{NO2\ sym}$ = 1334, $\nu_{NO2\ asym}$ = 1361. Anal. Calcd. for $C_{26}H_{40}N_2NiO_2P_2$: C, 58.56; H, 7.56; N, 5.25. Found: C, 58.20; H, 7.51; N, 5.00. Crystals suitable for X-ray diffraction were obtained by slow diffusion of pentane into a saturated THF solution of **2**.

Synthesis of (PNP)Ni($^{15}NO_2$) (2-$^{15}NO_2$). (PNP)Ni($^{15}NO_2$) (**2-$^{15}NO_2$**) was synthesized by same procedure of (PNP)Ni(NO_2) (**2**) except with $Na^{15}NO_2$ instead of $NaNO_2$. Spectroscopic features in the ^{1}H NMR and ^{13}C NMR were identical for **2**. ^{15}N NMR (61 MHz, C_6D_6, ppm) δ 89.89 (t, *J* = 7.93 Hz). ^{31}P NMR (162 MHz, C_6D_6, ppm) δ 42.29 (d, *J* = 8.10 Hz). IR (KBr pellet, cm^{-1}): $\nu_{NO2\ sym}$ = 1309, $\nu_{NO2\ asym}$ = 1342.

Synthesis of (PNP)Ni(NO) (3). In a 250 mL Schlenk tube, (PNP)Ni(NO_2) (**2**, 0.982 g, 1.842 mmol) was dissolved in 50 mL of benzene. The solution was degassed by three freeze-pump-thaw cycles on the Schlenk line and CO gas was added at ambient pressure. The reaction mixture was vigorously stirred for additional 3 hrs at 40 °C, all volatiles were removed under vacuum. After dissolved in pentane, a brown solution was filtered through Celite and the volatiles were removed *in vacuo*. The resulting product (PNP)Ni(NO) (**3**, 0.832 g, 1.610 mmol, 87.4%) was isolated as a brown solid after washing with cold pentane (–35 °C) and drying under vacuum. ^{1}H NMR (400 MHz, C_6D_6, ppm) δ 7.71 (d, *J* = 8.00 Hz, 2H, Ar-H), 6.97 (s, 2H, Ar-H), 6.95 (s, 2H, Ar-H), 2.22 (s, 6H, Ar-CH_3), 2.13 (m, 4H, C*H*CH_3), 1.04 – 0.95 (m, 24H, CHC*H*$_3$). ^{13}C NMR (151 MHz, C_6D_6, ppm) δ 159.17 (CN_{Ar}, t, *J* = 11.34 Hz), 131.34 (C_{Ar}), 130.84 (C_{Ar}), 122.95 (C_{Ar}, t, *J* = 3.02 Hz), 120.22 (C_{Ar}, dt, *J* = 42.28 Hz, 21.14 Hz), 116.67 (C_{Ar}, t, *J* = 3.02 Hz), 23.62 ($CH_{i\text{Pr}}$, t, *J* = 6.04 Hz), 19.74 (Me_{Ar}), 17.96 ($Me_{i\text{Pr}}$, t, *J* = 3.02 Hz), 17.51 ($Me_{i\text{Pr}}$). ^{31}P NMR (162 MHz, C_6D_6, ppm) δ 52.57 (s, 1P). UV-Vis [THF, nm (L mol^{-1} cm^{-1})]: 403 (3400), 479 (1000). IR (KBr pellet, cm^{-1}): ν_{NO} = 1646. Solution IR (KBr window, THF, cm^{-1}): ν_{NO} = 1673. Anal. Calcd. for $C_{26}H_{40}N_2NiOP_2$: C, 60.37; H, 7.79; N, 5.42. Found: C, 59.87; H, 7.79; N, 5.26. Crystals suitable for X-ray diffraction were obtained by slow evaporation of a saturated pentane solution of **3**.

Synthesis of (PNP)Ni(^{15}NO) (3-^{15}NO). (PNP)Ni(^{15}NO) (**3-^{15}NO**) was synthesized by same procedure of (PNP)Ni(NO) (**3**) except with **2-$^{15}NO_2$** instead of **2**. Spectroscopic features in the ^{1}H NMR and ^{13}C NMR were identical for **3**. ^{15}N NMR (61 MHz, C_6D_6, ppm) δ 241.44 (t, *J* = 14.64 Hz). ^{31}P NMR (162 MHz, C_6D_6, ppm) δ 52.57 (d, *J* = 14.58 Hz). IR (KBr pellet, cm^{-1}): ν_{NO} = 1616.

Reaction of (PNP)Ni(ONO_2) (1) with CO. In a 250 mL Schlenk tube (PNP)Ni(ONO_2) (**1**, 0.215 g, 0.391 mmol) was dissolved in 50 mL of benzene. The solution was degassed by three freeze-pump-thaw cycles on the Schlenk line and CO gas was added at ambient pressure. The reaction mixture was vigorously stirred for additional 1 hr at room temperature, and all volatiles were removed under vacuum. After dissolved in pentane, a brown solution was filtered through Celite and volatiles were removed *in vacuo*. The resulting product (PNP)Ni(NO) (**3**, 0.176 g, 0.340 mmol, 87.0%) was isolated as a brown solid after washing with cold pentane (–35°C) and drying under vacuum. Spectroscopic features in the ^{1}H NMR and ^{31}P NMR were identical to that reported above for **3**.

Reaction of (PNP)Ni(ONO_2) (1) with 1 equivalent of CO. A solution of **1** (0.013 g, 0.024 mmol) in benzene (5.0 mL) was placed into a gas-tight piece of glassware (11.5 mL) capped with a rubber septum. CO(g) (0.60 mL, 1.0 atm, 0.024 mmol) was slowly injected to the solution of **1** at room temperature and stirred for 2 hrs. Volatiles were removed under vacuum and a resulting purple solid was dissolved in benzene. The solution was filtered through Celite and the filtrate was evaporated under reduced pressure. Spectroscopic features in the ^{1}H NMR and ^{31}P NMR were identical to that reported above for **2** (0.011 g, 0.022 mmol, 90.5%).

Monitoring the formation of CO_2 by gas chromatography upon reaction of (PNP)Ni(NO_2) (2) with CO. A solution of **2** (0.013 g, 0.024 mmol) in benzene (5.0 mL) was placed into a gas-tight piece of glassware (11.5 mL) capped with a rubber septum. CO(g) (0.60 mL, 1.0 atm, 0.024 mmol) was slowly injected to the solution of **2** at room temperature and stirred for 2 hrs. A 1000 µL sample of the headspace was sampled using a gas-tight syringe and a gas chromatogram was recorded revealing the presence of CO_2. The amount of CO_2 was determined to be 0.0143 mmol, 60% yield (see Figure S16).

Monitoring the formation of CO_2 by gas chromatography upon reaction of (PNP)Ni(ONO_2) (1) with CO. A solution of **1** (0.013 g, 0.024 mmol) in benzene (5.0 mL) was placed into a gas-tight piece of glassware (11.5 mL) capped with a rubber septum. CO(g) (1.20 mL, 1.0 atm, 0.049 mmol) was slowly injected to the solution of **1** at room temperature and stirred for 2 hrs. A 1000 µL sample of the headspace was sampled using a gas-tight syringe and a gas chromatogram was recorded revealing the presence of CO_2. The amount of CO_2 was determined to be 0.0287mmol, 119% yield (see Figure S17).

Reaction of (PNP)Ni(NO) (3) with 2 equivalent of NO(g). A solution of **3** (0.017 g, 0.033 mmol) in benzene (5.0 mL) was placed into a gas-tight piece of glassware (11.5 mL) capped with a rubber septum. NO(g) (1.66 mL, 1.0 atm, 0.066 mmol) was slowly injected to the solution of **3** at room temperature and stirred for 2 hrs. A 1000 µL sample of the headspace was sampled using a gas-tight syringe and a gas chromatogram was recorded revealing the presence of N_2O. The amount of N_2O was determined to be

0.0178 mmol, 54% yield (see Figure S18). Spectroscopic features of remained product in the ^{1}H NMR and ^{31}P NMR were identical to that reported above for **2** (0.015 g, 0.029 mmol, 87.8%).

Reaction of (PNP)Ni(NO) (3) with tritylthionitrite. A solution of **3** (0.030 g, 0.059 mmol) in benzene (5.0 mL) was placed into a gas-tight piece of glassware (11.5 mL) capped with a rubber septum. Tritylthionitrite (0.036 mg, 0.118 mmol) was added to the solution of **3** at room temperature and stirred for 4 hrs. A 1000 µL sample of the headspace was sampled using a gas-tight syringe and a gas chromatogram was recorded revealing the presence of N_2O. The amount of N_2O was determined to be 0.0330 mmol, 56% yield (see Supplementary Fig. 19). Spectroscopic features of remained product after purification in the ^{1}H NMR and ^{31}P NMR were identical to that reported above for **2** (0.029 g, 0.053 mmol, 91.0%).

Monitoring the catalytic CO and NO conversion to CO_2 and N_2O. A solution of **3** (0.006 g, 0.010 mmol) in benzene (1.0 mL) was placed into a gas-tight piece of glassware (11.5 mL) capped with a rubber septum. CO(g) (2.50 mL, 1.0 atm, 0.099 mmol) and NO(g) (5.0 mL, 1.0 atm, 0.2 mmol) were slowly injected to the solution of **3** at room temperature and stirred for 140 mins. A 1000 µL sample of the headspace was sampled using a gas-tight syringe and a gas chromatogram was recorded revealing the presence of CO_2 and N_2O (see Figure S20).

Reaction of (PNP)Ni(NO) (3) with N_2O(g). In a 250 mL Schlenk tube (PNP)Ni(NO) (**3**, 0.154 g, 0.297 mmol) was dissolved in 50 mL of benzene. The solution was degassed by three freeze-pump-thaw cycles on the Schlenk line and N_2O gas was added at ambient pressure. The reaction mixture was vigorously stirred for additional 36 hrs at 60°C, and all volatiles were removed under vacuum. The major product, **2** (0.074 g, 0.135 mmol, 45.5%) was obtained as a purple solid after washing with pentane and drying under vacuum.

Monitoring the formation of N_2 by gas chromatography upon reaction of (PNP)Ni(NO) (3) with N_2O. A solution of **3** (0.011 g, 0.021 mmol) in benzene (5.0 mL) was placed into a gas-tight piece of glassware (11.5 mL) capped with a rubber septum under an Ar atmosphere. N_2O(g) (0.50 mL, 1.0 atm, 0.020 mmol) was slowly injected to the solution of **3** at 60°C and stirred for 72 hrs. A 1000 µL sample of the headspace was sampled using a gas-tight syringe and a gas chromatogram was recorded revealing the presence of N_2. The amount of N_2 was determined to be 0.0086mmol, 41% yield (see Figure S21).

Kinetic Experiment of 1 with CO. A solution of **1** (10 mL, 2.80 mM in THF) was added to a Schlenk tube, and an initial UV−Vis spectrum (350 nm < λ < 800 nm) was measured at 273 K. After CO(g) was bubbled through a solution with a needle connected to the Schlenk line, spectra were collected with 0.2 min intervals over the course of 5 min. The time-stacked UV−Vis spectra show the consumption of **1** (λ_{max} 677 nm) and

an increase in absorbance of **2** (λ_{max} 560 nm) indicating the formation of **2**. Isosbestic points were shown at λ 500 and 620 nm.

Kinetic Experiment of 2 with CO. A solution of **2** (10 mL, 1.13 mM in THF) was added to a Schlenk tube, and an initial UV−Vis spectrum (350 nm < λ < 800 nm) was measured at room temperature. After CO(g) was bubbled through a solution with a needle connected to the Schlenk line, spectra were collected with 0.2 min intervals over the course of 50 min. The time-stacked UV−Vis spectra show the consumption of **2** (λ_{max} 560 nm) and an increase in absorbance of **3** (λ_{max} 480 nm) indicating the formation of **3**.

Figure S1. ^{1}H NMR spectrum (C_6D_6, 400 MHz) of (PNP)Ni(ONO_2) (**1**) at room temperature.

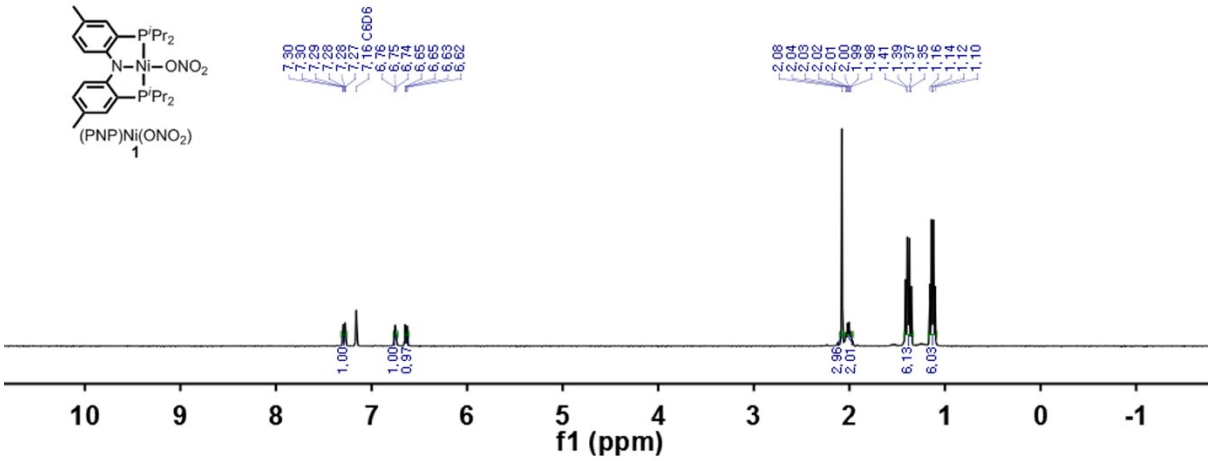


Figure S2. ^{13}C NMR spectrum (C_6D_6, 151 MHz) of (PNP)Ni(ONO_2) (**1**) at room temperature.

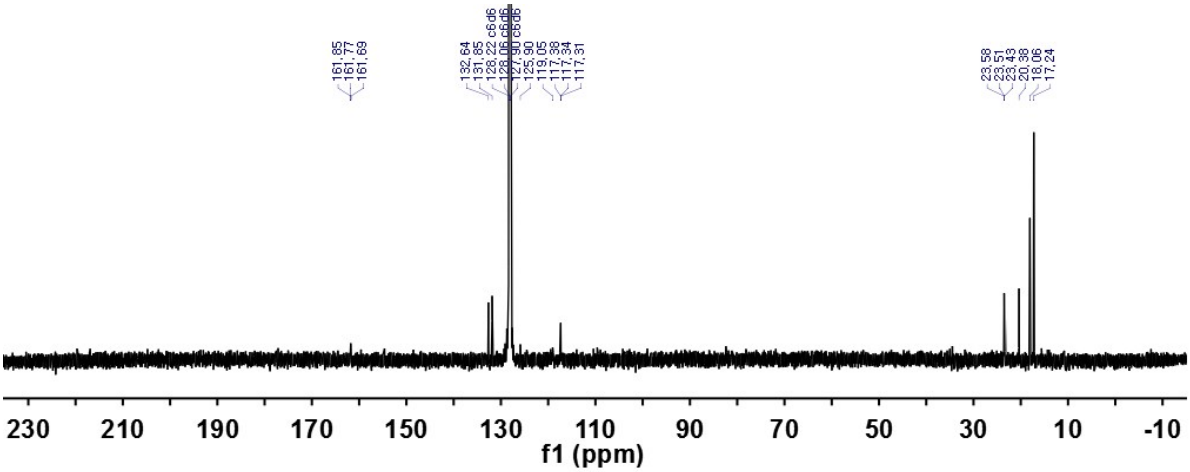


Figure S3. ^{31}P NMR spectrum (C_6D_6, 162 MHz) of (PNP)Ni(ONO_2) (**1**) at room temperature.

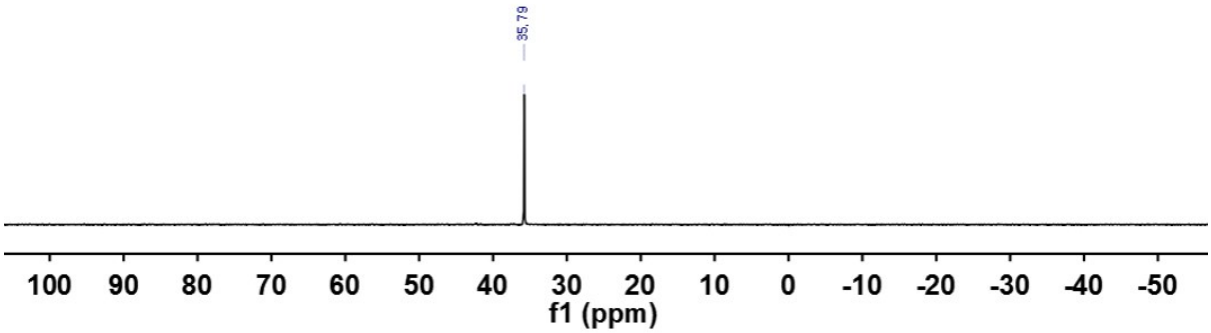


Figure S4. ^{15}N NMR spectrum (C_6D_6, 61 MHz) of (PNP)Ni($O^{15}NO_2$) (**1-$O^{15}NO_2$**) at room temperature.

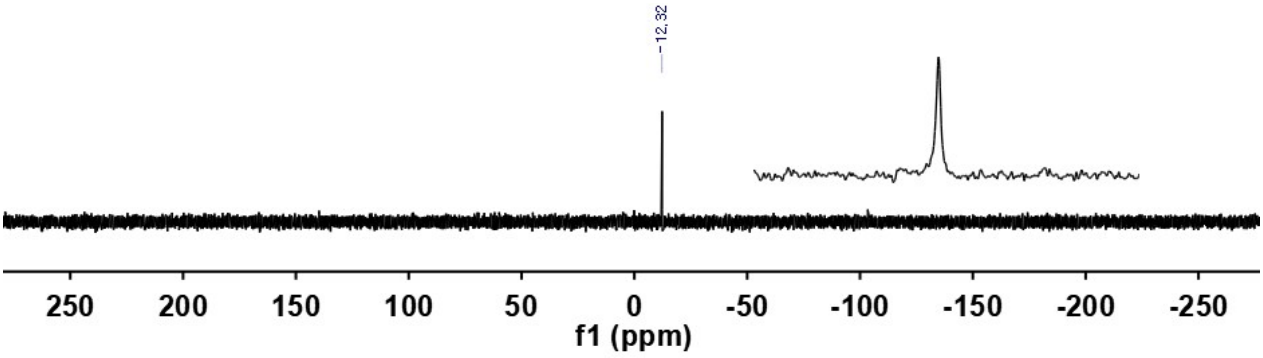


Figure S5. ^{31}P NMR spectrum (C_6D_6, 162 MHz) of (PNP)Ni($O^{15}NO_2$) (**1-$O^{15}NO_2$**) at room temperature.

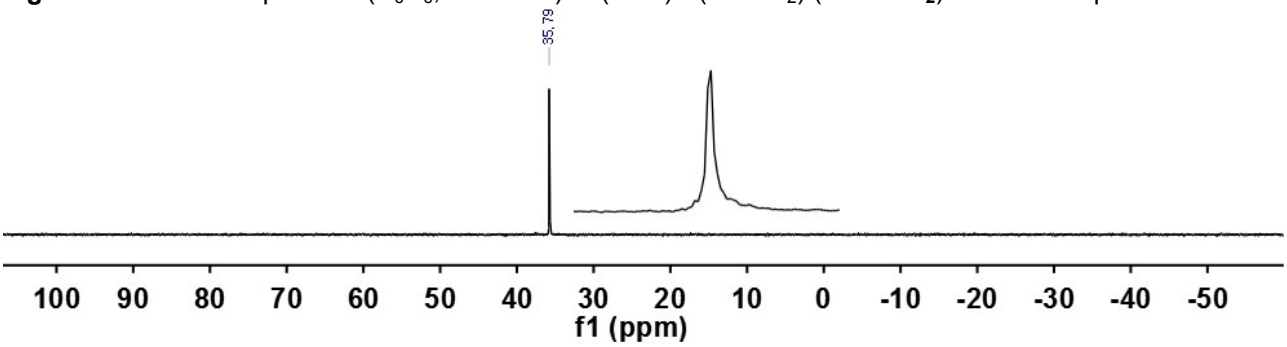


Figure S6. ^{1}H NMR spectrum (C_6D_6, 400 MHz) of (PNP)Ni(NO_2) (**2**) at room temperature.

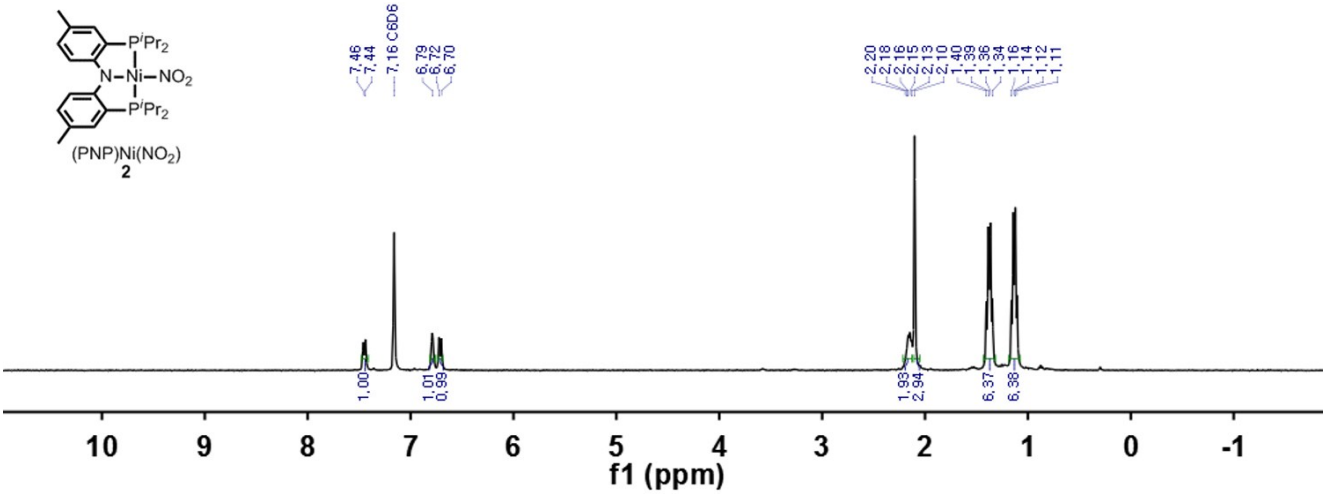


Figure S7. ^{13}C NMR spectrum (C_6D_6, 151 MHz) of (PNP)Ni(NO_2) (**2**) at room temperature.

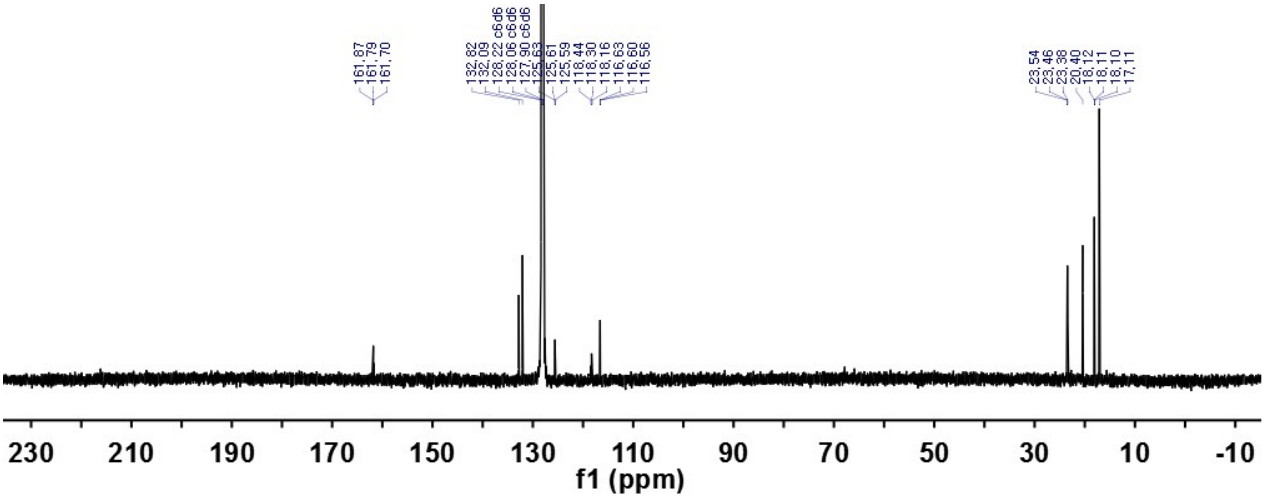


Figure S8. ^{31}P NMR spectrum (C_6D_6, 162 MHz) of (PNP)Ni(NO_2) (**2**) at room temperature.

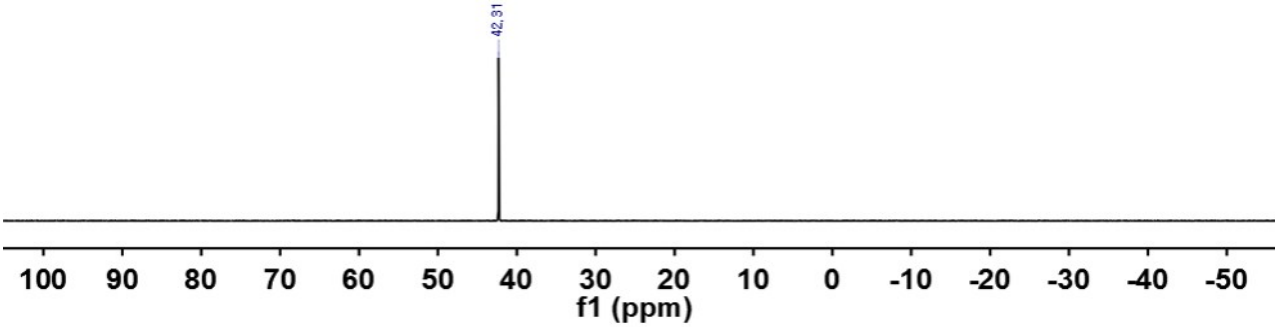


Figure S9. ^{15}N NMR spectrum (C_6D_6, 61 MHz) of (PNP)Ni($^{15}NO_2$) (**2-$^{15}NO_2$**) at room temperature.

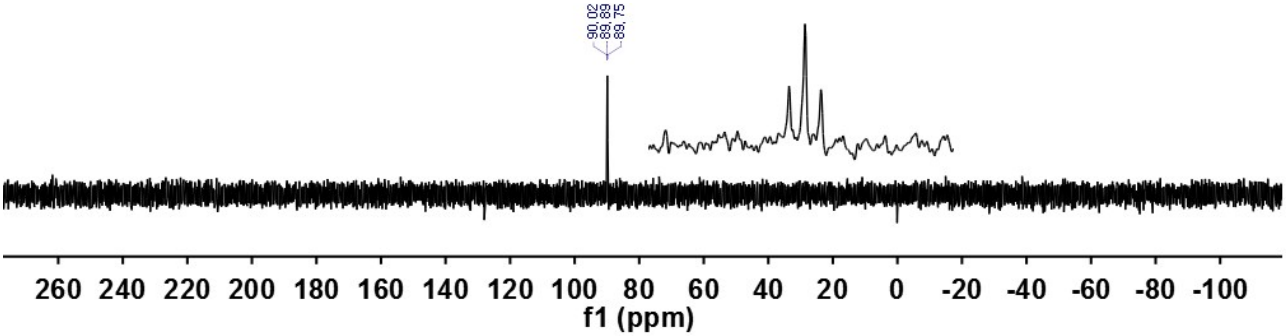


Figure S10. ^{31}P NMR spectrum (C_6D_6, 162 MHz) of (PNP)Ni($^{15}NO_2$) (**2-$^{15}NO_2$**) at room temperature.

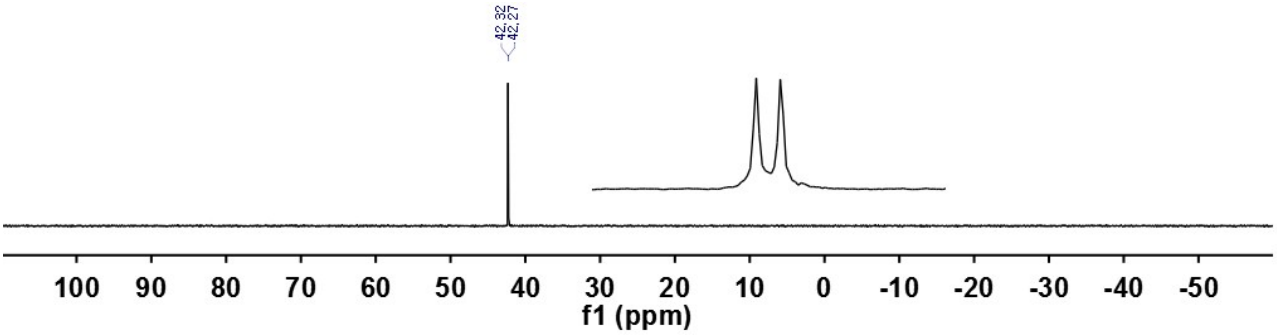


Figure S11. ^{1}H NMR spectrum (C_6D_6, 400 MHz) of (PNP)Ni(NO) (**3**) at room temperature.

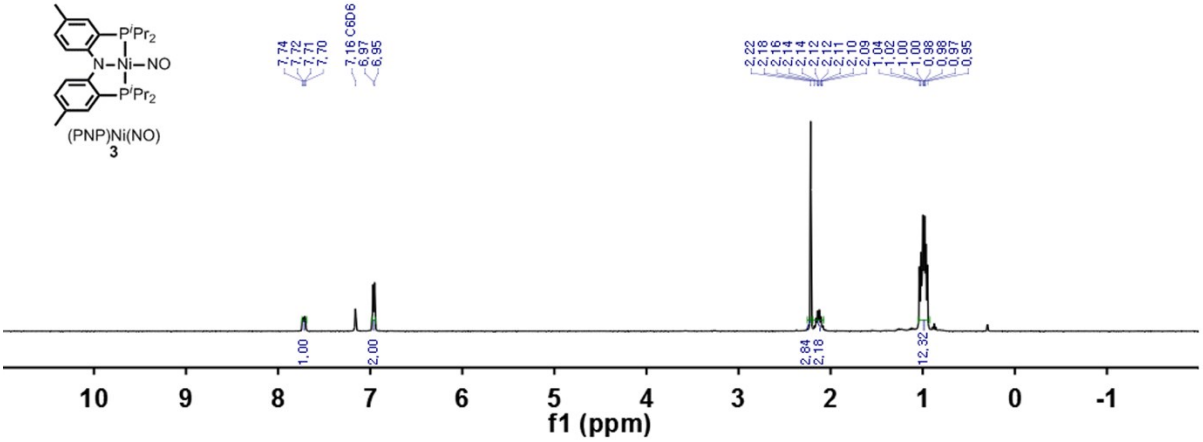


Figure S12. ^{13}C NMR spectrum (C_6D_6, 151 MHz) of (PNP)Ni(NO) (**3**) at room temperature.

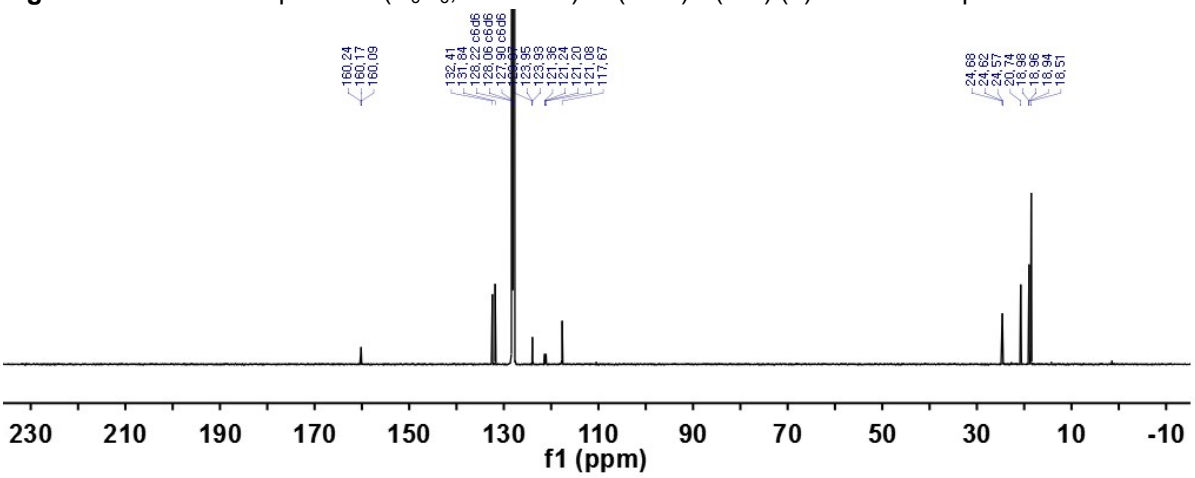


Figure S13. ^{31}P NMR spectrum (C_6D_6, 162 MHz) of (PNP)Ni(NO) (**3**) at room temperature.

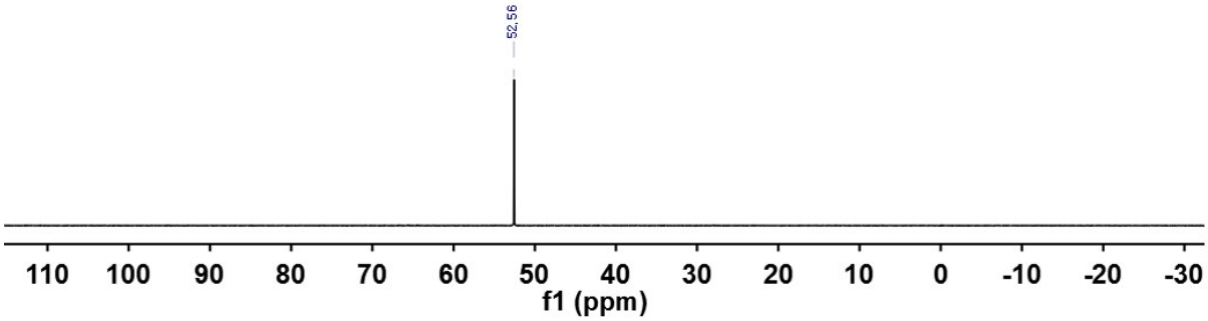


Figure S14. ^{15}N NMR spectrum (C_6D_6, 61 MHz) of (PNP)Ni(^{15}NO) (**3-^{15}NO**) at room temperature.

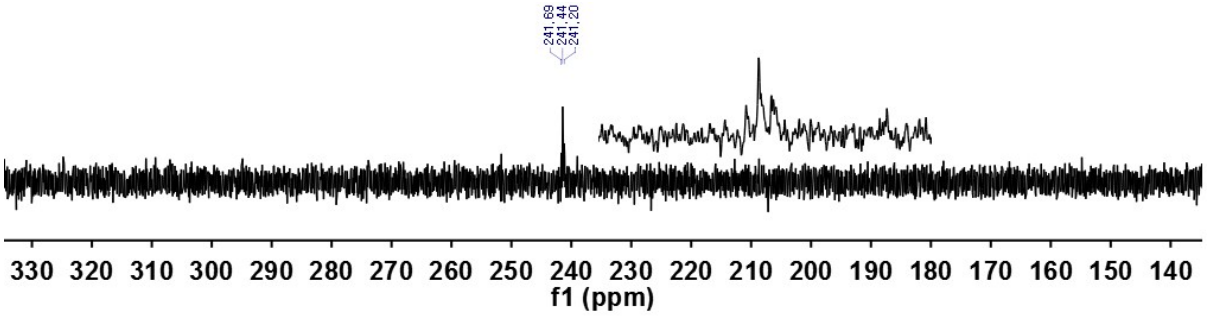


Figure S15. ^{31}P NMR spectrum (C_6D_6, 162 MHz) of (PNP)Ni($^{15}NO_2$) (**3-^{15}NO**) at room temperature.

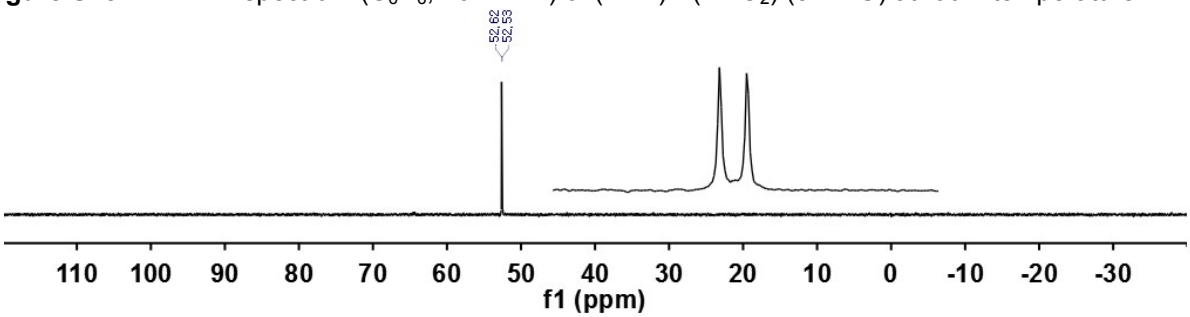
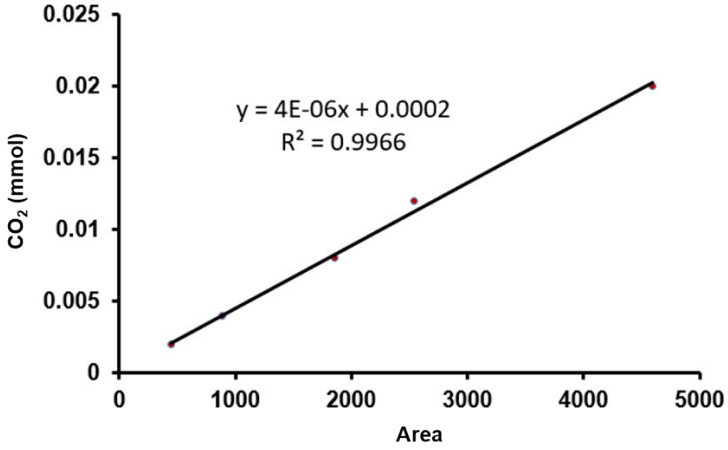
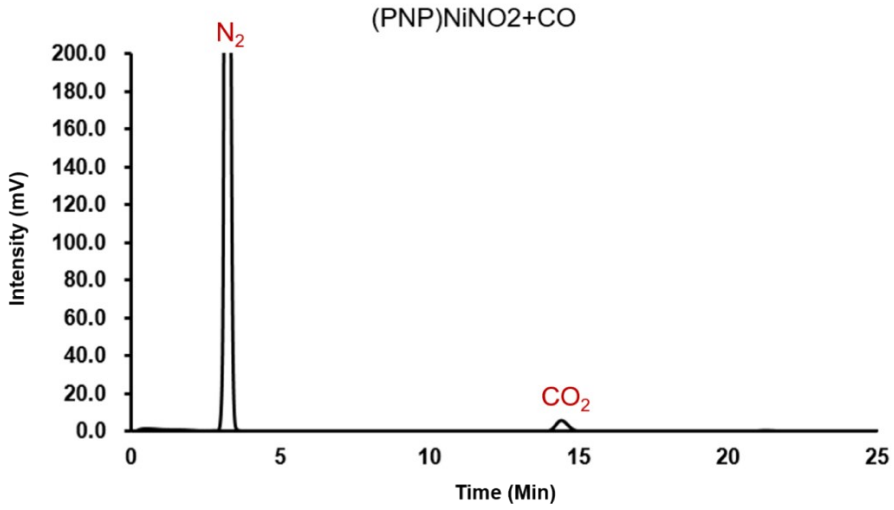


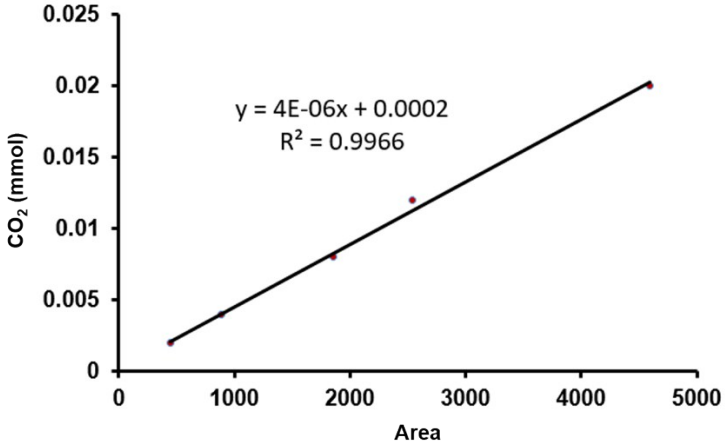
Figure S16. Gas chromatogram of the head space gases formed during the reaction (PNP)Ni(NO_2) (**2**) and 1 equivalents of carbon monoxide gas after 2 hours. A 1 mL volume of the head space was sampled using a gas-tight syringe and a GC trace was collected. The first major peak is N_2 (retention time 3.2 min) and the second peak is CO_2 (retention time 14.4 min; area 141.03 mVsec). The amount of CO_2 was determined using an CO_2 calibration curve with the linear relationship: $y = (4.0 \times 10^{-6})x + 0.0002$ (y: mmol of CO_2, and x: area).

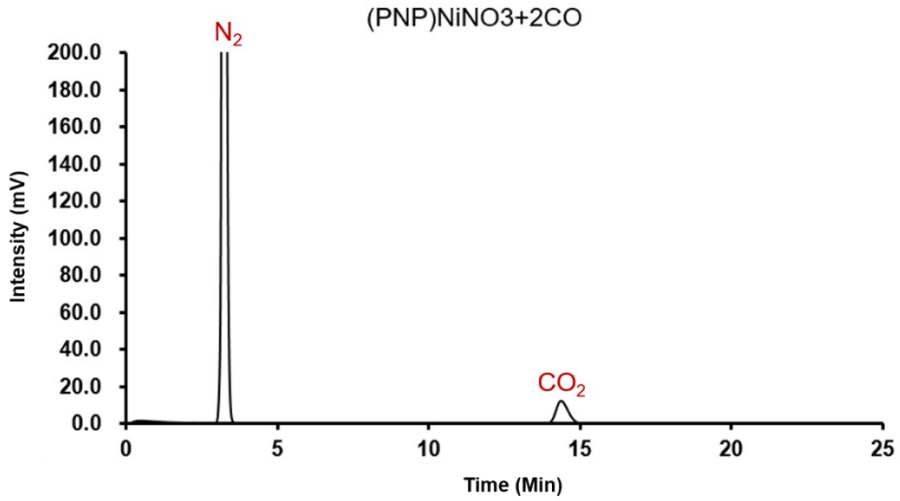




Ostwald coefficient: $L_c = [CO_2]_l/[CO_2]_g$[S7, S8]	2.43 (for benzene at 1atm and 298.15 K)
Moles of CO_2 in the headspace	4.97×10^{-3} mmol
$[CO_2]_g$ in headspace (6.5 mL)	0.76×10^{-3} mol L^{-1}
$[CO_2]_l$ in solution (5 mL)	1.86×10^{-3} mol L^{-1}
Moles of CO_2 in the solution	0.93×10^{-2} mmol
Total moles of CO_2 and yield	0.0143 mmol (60%)

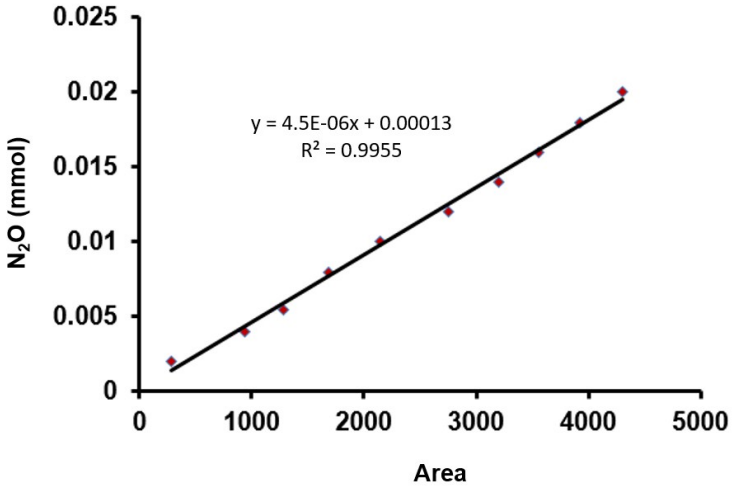
Figure S17. Gas chromatogram of the head space gases formed during the reaction (PNP)Ni(ONO_2) (**1**) and 2 equivalents of carbon monoxide gas after 4 hours. A 1 mL volume of the head space was sampled using a gas-tight syringe and a GC trace was collected. The first major peak is N_2 (retention time 3.2 min) and the second peak is CO_2 (retention time 14.4 min; area 335.18 mVsec). The amount of CO_2 was determined using an CO_2 calibration curve with the linear relationship: $y = (4.0 \times 10^{-6})x + 0.0002$ (y: mmol of CO_2, and x: area).

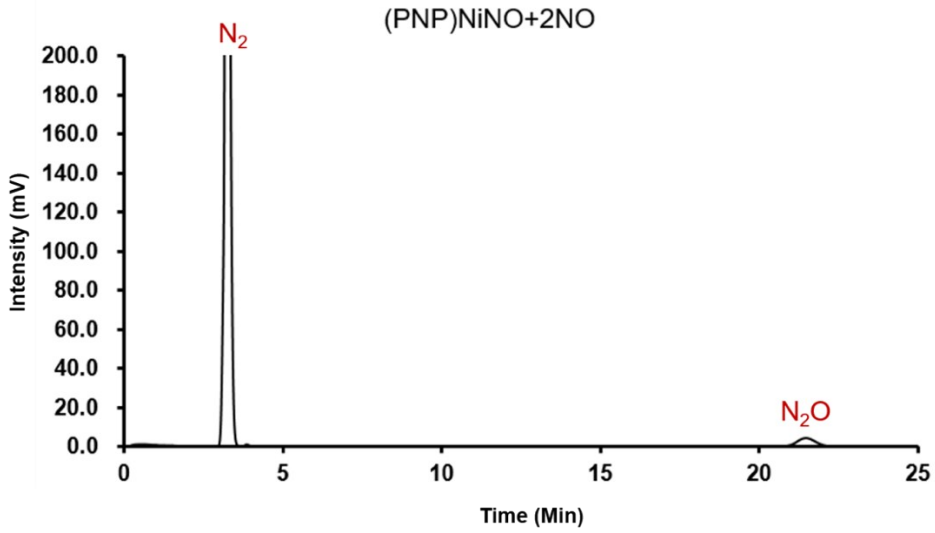




Ostwald coefficient: $L_c = [CO_2]_l/[CO_2]_g$ [S7, S8]	2.43 (for benzene at 1atm and 298.15 K)
Moles of CO_2 in the headspace	1.00×10^{-2} mmol
$[CO_2]_g$ in headspace (6.5 mL)	1.54×10^{-3} mol L^{-1}
$[CO_2]_l$ in solution (5 mL)	3.74×10^{-3} mol L^{-1}
Moles of CO_2 in the solution	1.87×10^{-2} mmol
Total moles of CO_2 and yield	0.0287 mmol (119%)

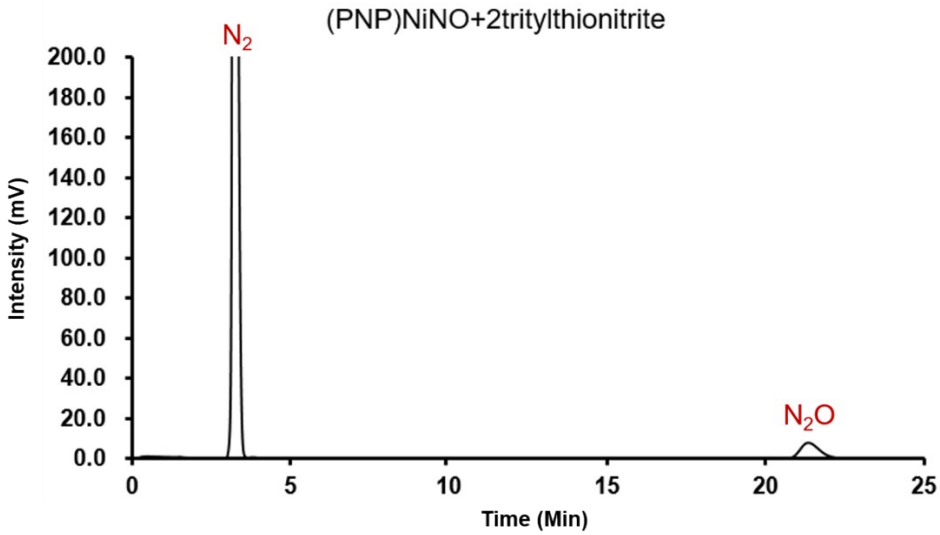
Figure S18. Gas chromatogram of the head space gases formed during the reaction (PNP)Ni(NO) (**3**) and 2 equivalents of nitric oxide gas after 2 hours. A 1 mL volume of the head space was sampled using a gas-tight syringe and a GC trace was collected. The first major peak is N_2 (retention time 3.2 min) and the second peak is N_2O (retention time 21.5 min; area 129.52 mVsec). The amount of N_2O was determined using an N_2O calibration curve with the linear relationship: $y = (4.5 \times 10^{-6})x + 0.00013$ (y: mmol of N_2O, and x: area).





Ostwald coefficient: $L_c = [N_2O]_l/[N_2O]_g$ [S7, S9]	3.686 (for benzene at 1atm and 298.15 K)
Moles of N_2O in the headspace	4.63×10^{-3} mmol
$[N_2O]_g$ in headspace (6.5 mL)	0.71×10^{-3} mol L^{-1}
$[N_2O]_l$ in solution (5 mL)	2.63×10^{-3} mol L^{-1}
Moles of N_2O in the solution	1.32×10^{-2} mmol
Total moles of N_2O and yield	0.0178 mmol (54%)

Figure S19. Gas chromatogram of the head space gases formed during the reaction (PNP)Ni(NO) (**3**) and 2 equivalents of tritylthionitrite after 4 hours. A 1 mL volume of the head space was sampled using a gas-tight syringe and a GC trace was collected. The first major peak is N_2 (retention time 3.2 min) and the second peak is N_2O (retention time 21.5 min; area 263.9 mVsec). The amount of N_2O was determined using an N_2O calibration curve with the linear relationship: $y = (4.5 \times 10^{-6})x + 0.00013$ (y: mmol of N_2O, and x: area).



Ostwald coefficient: $L_c = [N_2O]_l/[N_2O]_g$ [S7, S9]	3.686 (for benzene at 1atm and 298.15 K)
Moles of N_2O in the headspace	8.56×10^{-3} mmol
$[N_2O]_g$ in headspace (6.5 mL)	1.32×10^{-3} mol L^{-1}
$[N_2O]_l$ in solution (5 mL)	4.87×10^{-3} mol L^{-1}
Moles of N_2O in the solution	2.44×10^{-2} mmol
Total moles of N_2O and yield	0.0330 mmol (56%)

Figure S20. Gas chromatogram of the head space gases formed during the reaction (PNP)Ni(NO) (**3**), 10 equivalents of carbon monoxide and 20 equivalents of nitric oxide after 140 min.

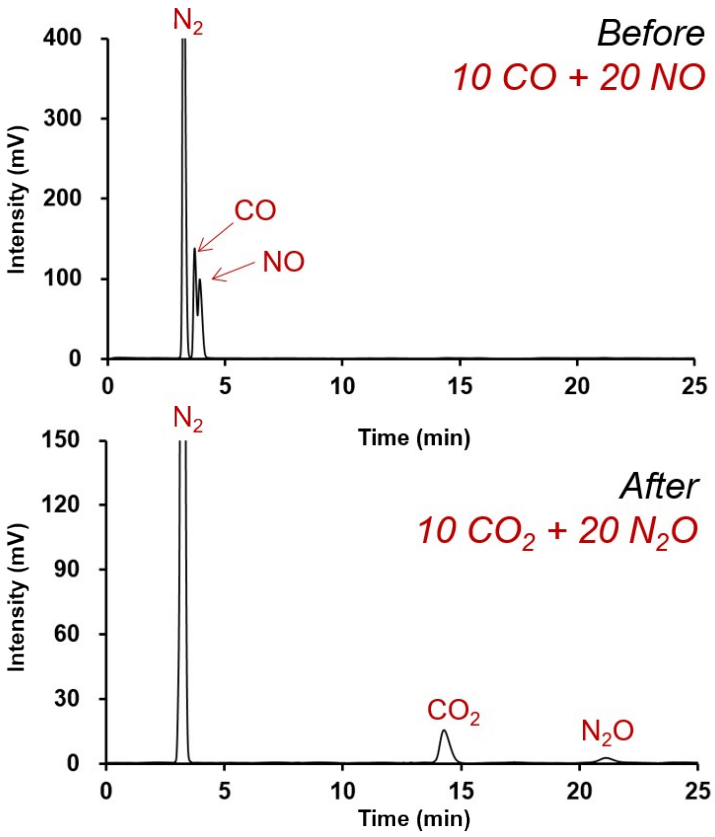
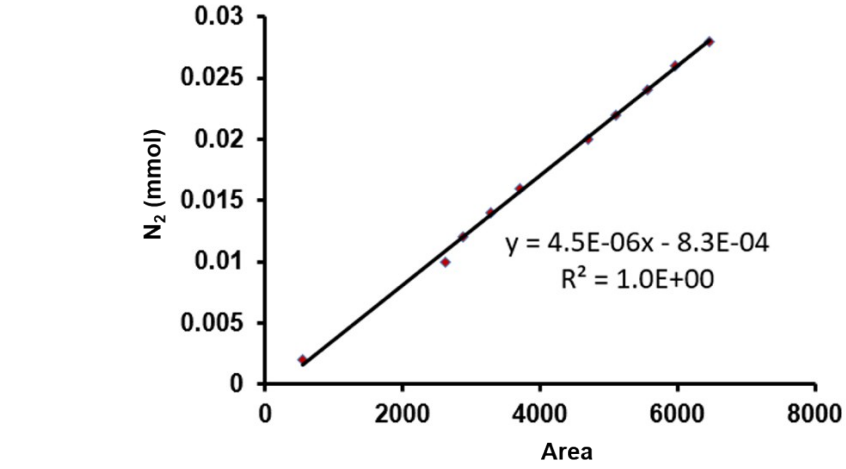
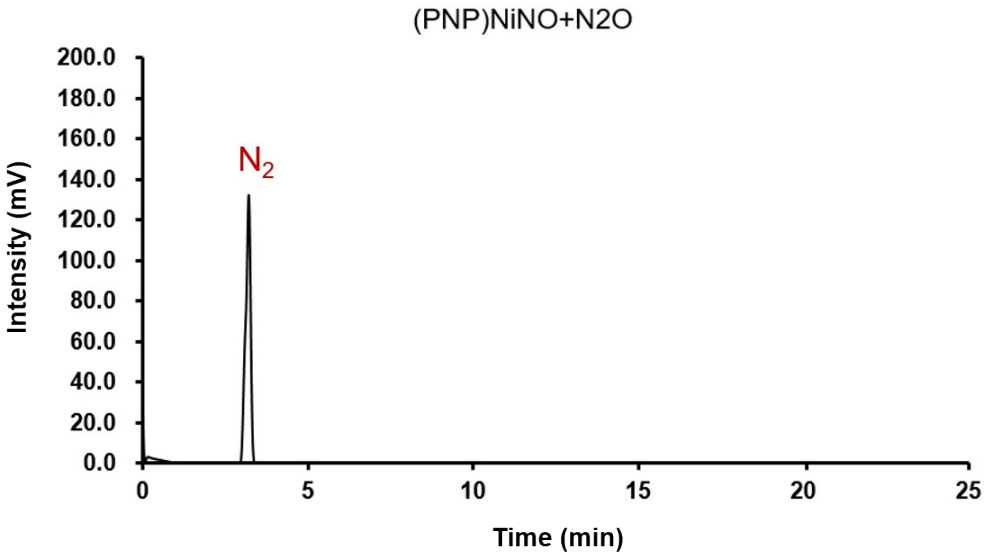


Figure S21. Gas chromatogram of the head space gases formed during the reaction (PNP)Ni(NO) (**3**) and 1 equivalents of N_2O after 72 hours. A 1 mL volume of the head space was sampled using a gas-tight syringe and a GC trace was collected. The first major peak is N_2 (retention time 3.2 min) and the second peak is N_2O (retention time 21.5 min; area 263.9 mVsec). The amount of N_2O was determined using an N_2O calibration curve with the linear relationship: $y = (4.5 \times 10^{-6})x - 0.00083$ (y: mmol of N_2, and x: area).





Reaction sample N_2 area	1436.16 mVsec
Control sample N_2 area (only **3**)	982.37 mVsec
Ostwald coefficient: $L_c = [N_2]_l/[N_2]_g$ [S7, S10]	0.1159 (for benzene at 1atm and 298.15 K)
Moles of N_2 in the headspace	7.88×10^{-3} mmol
$[N_2]_g$ in headspace (6.5 mL)	1.21×10^{-3} mol L^{-1}
$[N_2]_l$ in solution (5 mL)	1.40×10^{-4} mol L^{-1}
Moles of N_2 in the solution	7.01×10^{-4} mmol
Total moles of N_2 and yield	0.0086 mmol (41%)

Figure S22. Solid-state structure of (PNP)Ni(ONO_2) (**1**). Hydrogen atoms are omitted for clarity.

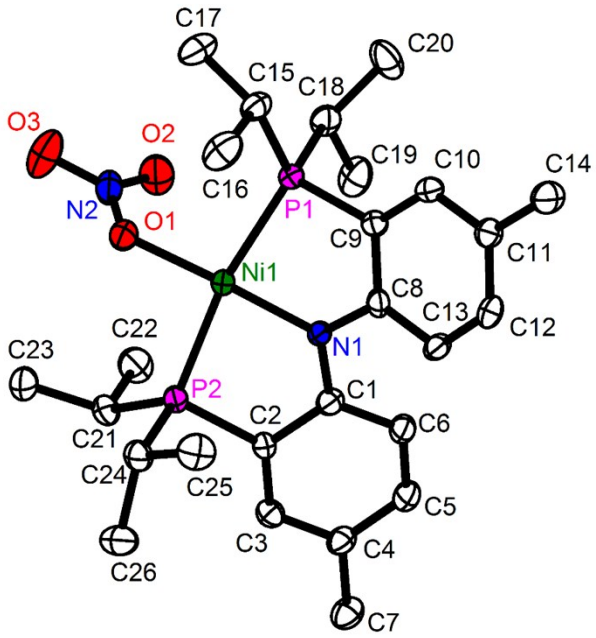


Table S1. Selected bond distances and angles for (PNP)Ni(ONO_2) (**1**) (Å and °).

Distance	(PNP)Ni(ONO_2)	Angle	(PNP)Ni(ONO_2)
d_{N2-O1}	1.272(4)	∠O1-N2-O2	121.3(3)
d_{N2-O2}	1.235(4)	∠O2-N2-O3	120.9(3)
d_{N2-O3}	1.249(4)	∠O3-N2-O1	117.7(3)
d_{Ni1-O1}	1.897(2)	∠Ni1-O1-N2	115.8(2)
d_{Ni1-N1}	1.887(3)	∠N1-Ni1-O1	175.41(12)
d_{Ni1-P1}	2.2199(10)	∠P1-Ni1-P2	169.27(4)
d_{Ni1-P2}	2.2152(10)		
		∠N1-Ni1-P1	84.39(9)
		∠O1-Ni1-P1	97.04(8)
		∠N1-Ni1-P2	84.89(9)
		∠O1-Ni1-P2	93.66(8)

Figure S23. Solid-state structure of (PNP)Ni(NO_2) (**2**). Hydrogen atoms are omitted for clarity.

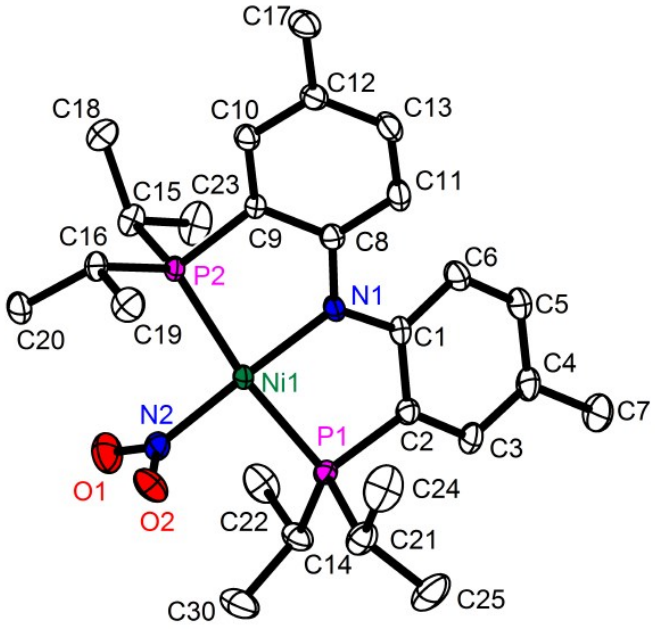


Table S2. Selected bond distances and angles for (PNP)Ni(NO_2) (**2**) (Å and °).

Distance	(PNP)Ni(NO_2)	Angle	(PNP)Ni(NO_2)
d_{N2-O1} d_{N2-O2}	1.230(5) 1.224(5)	∠O1-N2-O2	121.4(4)
d_{Ni1-N2}	1.860(4)	∠Ni1-N2-O1 ∠Ni1-N2-O2	117.5(3) 121.1(3)
d_{Ni1-N1} d_{Ni1-P1} d_{Ni1-P2}	1.907(4) 2.1919(13) 2.1934(12)	∠N1-Ni1-N2 ∠P1-Ni1-P2	176.12(17) 170.46(2)
		∠N1-Ni1-P1 ∠N2-Ni1-P1 ∠N1-Ni1-P2 ∠N2-Ni1-P2	85.53(11) 95.18(12) 86.23(11) 93.37(12)

Figure S24. Solid-state structure of (PNP)Ni(NO) (**3**). Hydrogen atoms are omitted for clarity.

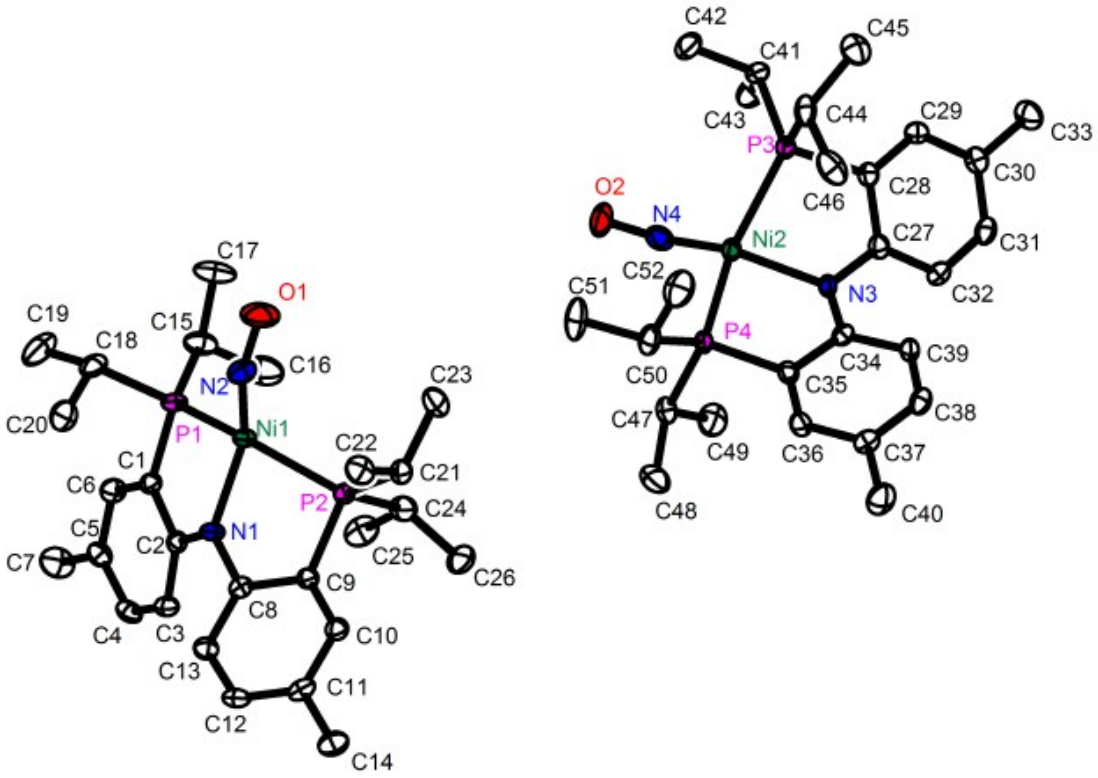


Table S3. Selected bond distances and angles for (PNP)Ni(NO) (**3**) (Å and °).

Distance	(PNP)Ni(NO)	Angle	(PNP)Ni(NO)
d_{N2-O1}	1.174(6)	∠Ni1-N2-O1	145.4(4)
d_{N4-O2}	1.179(6)	∠Ni2-N4-O2	144.6(5)
d_{Ni1-N2}	1.694(4)	∠N1-Ni1-N2	148.5(2)
d_{Ni2-N4}	1.698(4)	∠N3-Ni2-N4	148.7(2)
d_{Ni1-N1}	1.999(4)		
d_{Ni2-N3}	1.997(4)		
d_{Ni1-P1}	2.2228(13)	∠P1-Ni1-P2	142.53(5)
d_{Ni2-P3}	2.2483(14)	∠P3-Ni2-P4	142.72(5)
d_{Ni1-P2}	2.2442(13)		
d_{Ni2-P4}	2.2182(13)		
		∠N1-Ni1-P1	84.35(12)
		∠N3-Ni2-P3	82.45(12)
		∠N2-Ni1-P1	102.71(15)
		∠N4-Ni2-P3	107.24(15)
		∠N1-Ni1-P2	82.44(13)
		∠N3-Ni2-P4	84.46(12)
		∠N2-Ni1-P2	106.82(15)
		∠N4-Ni2-P4	101.99(15)

Figure S25. IR spectrum of (PNP)Ni(ONO_2) (**1**) (KBr pellet).

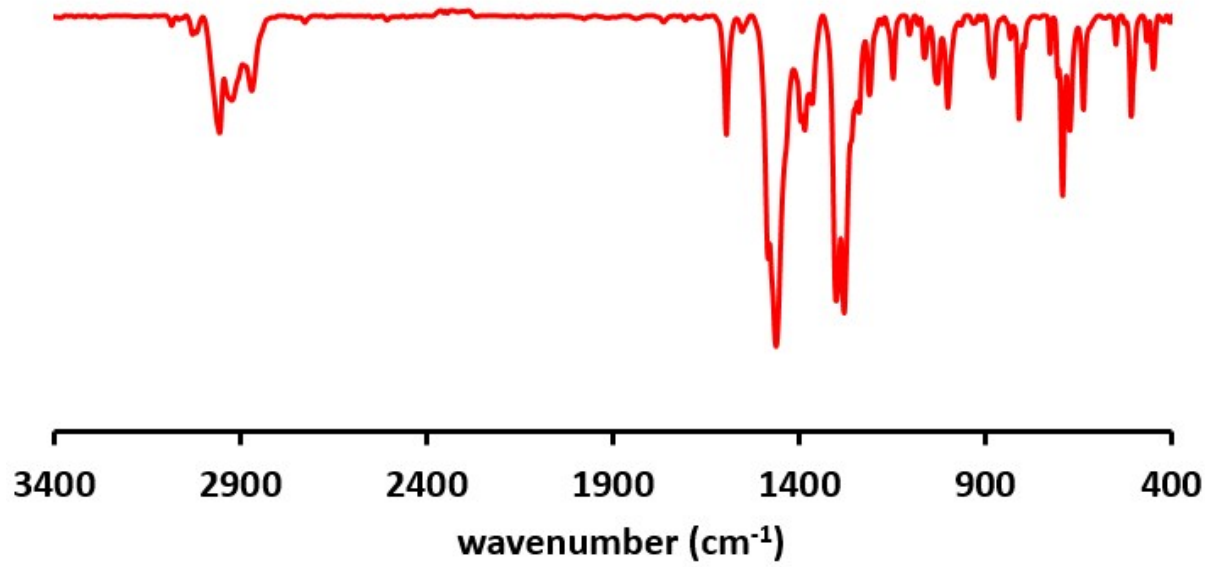


Figure S26. IR spectrum of (PNP)Ni(NO_2) (**2**) (KBr pellet).

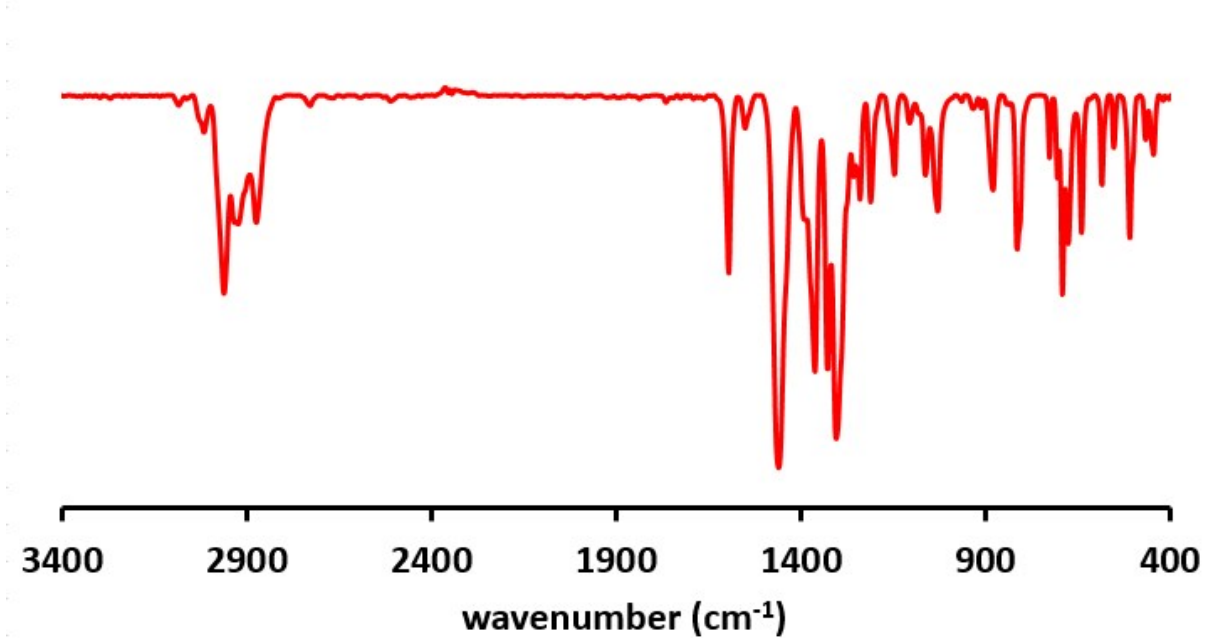


Figure S27. IR spectra of (PNP)Ni(ONO_2) (**1**, blue) and (PNP)Ni(NO) (**3**, red) (KBr pellet).

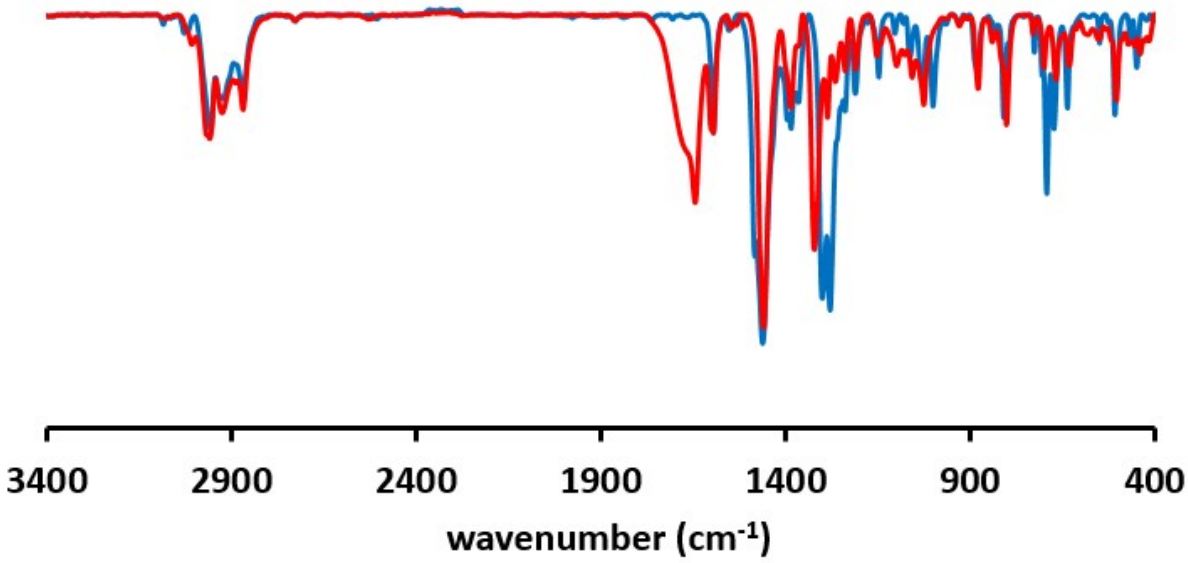


Figure S28. IR spectra of (PNP)Ni(NO_2) (**2**, blue) and (PNP)Ni(NO) (**3**, red) (KBr pellet).

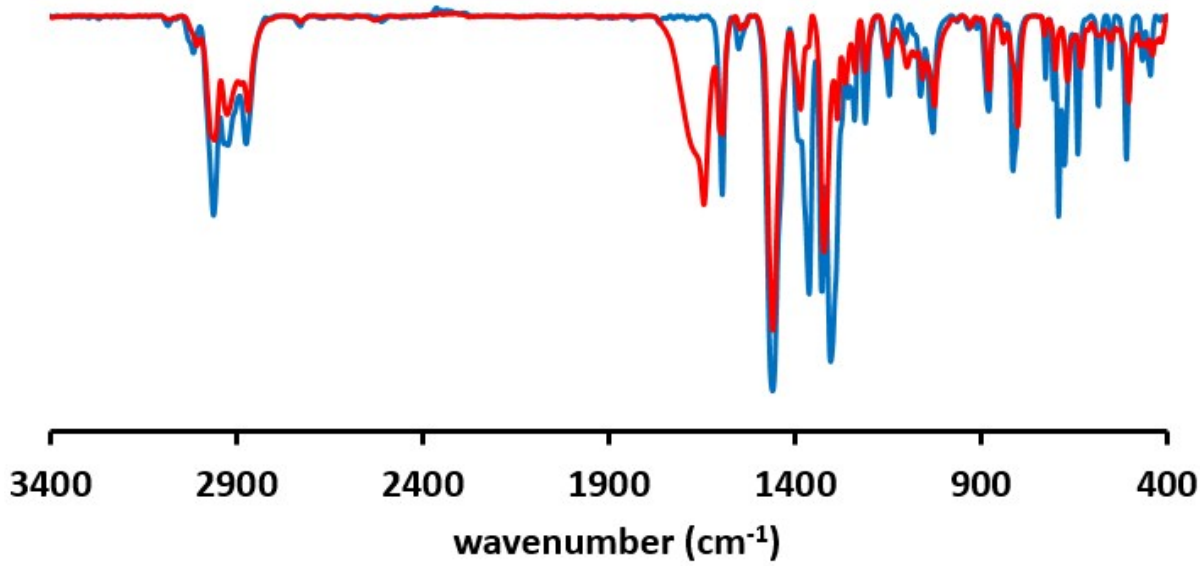


Figure S29. IR spectra of (PNP)Ni(NO_2) (**2**, blue) and (PNP)Ni(ONO_2) (**1**, red) (KBr pellet).

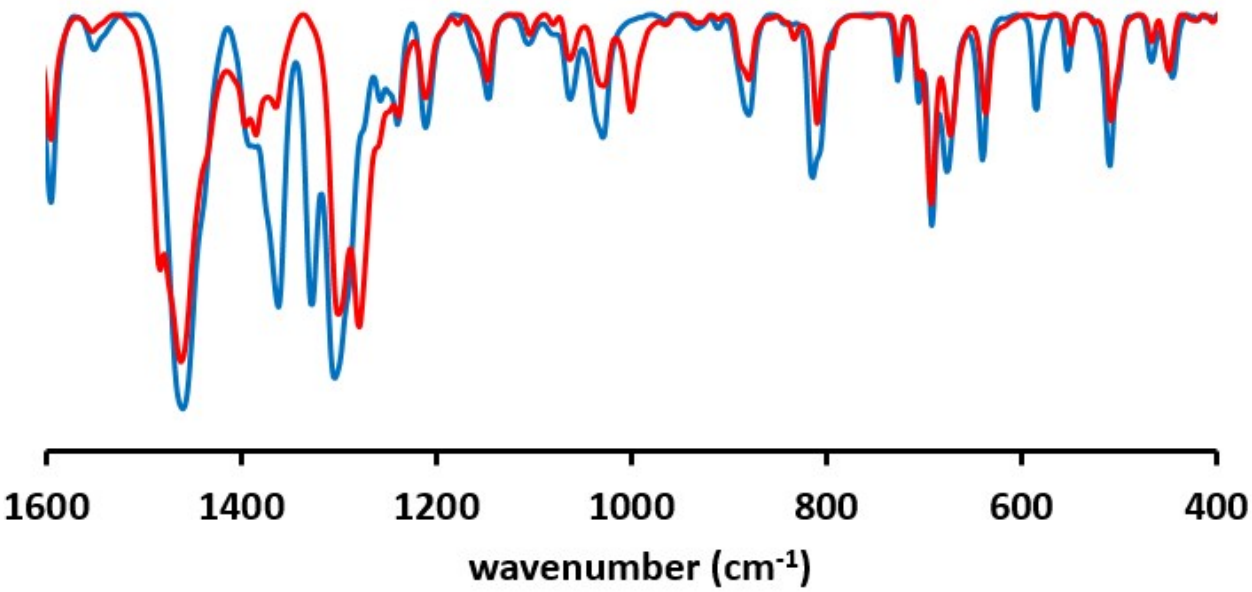


Figure S30. IR spectra of (PNP)Ni(ONO_2) (**1**, blue) and (PNP)Ni($O^{15}NO_2$) (**1-$O^{15}NO_2$**, red) (KBr pellet).

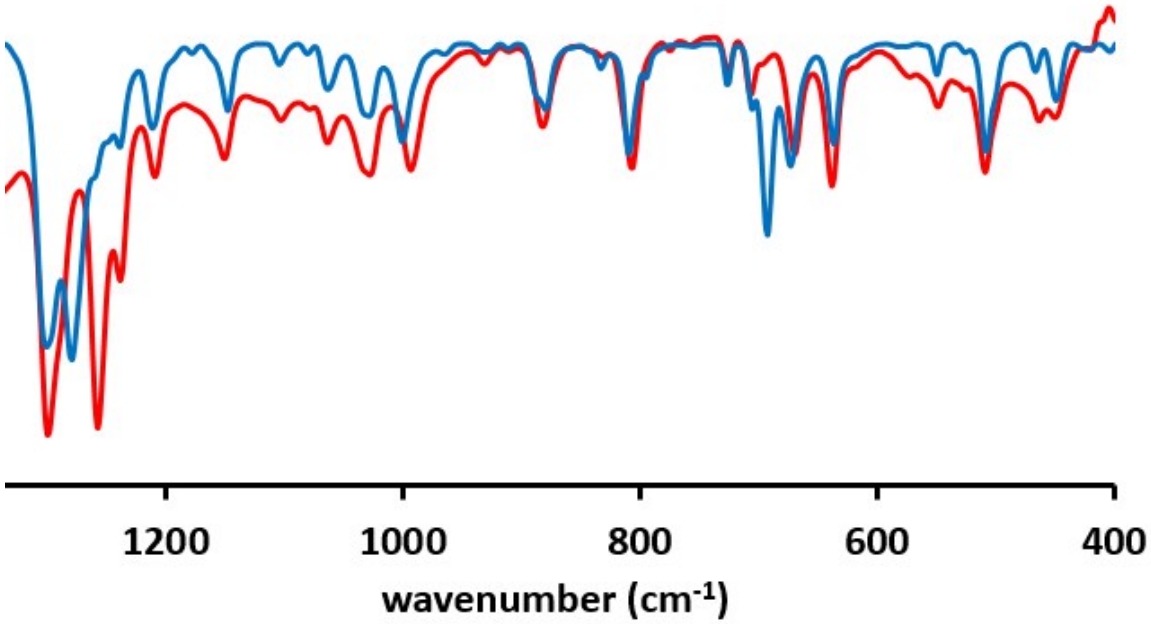


Figure S31. IR spectra of (PNP)Ni(NO_2) (**2**, blue) and (PNP)Ni($^{15}NO_2$) (**2-$^{15}NO_2$**, red) (KBr pellet).

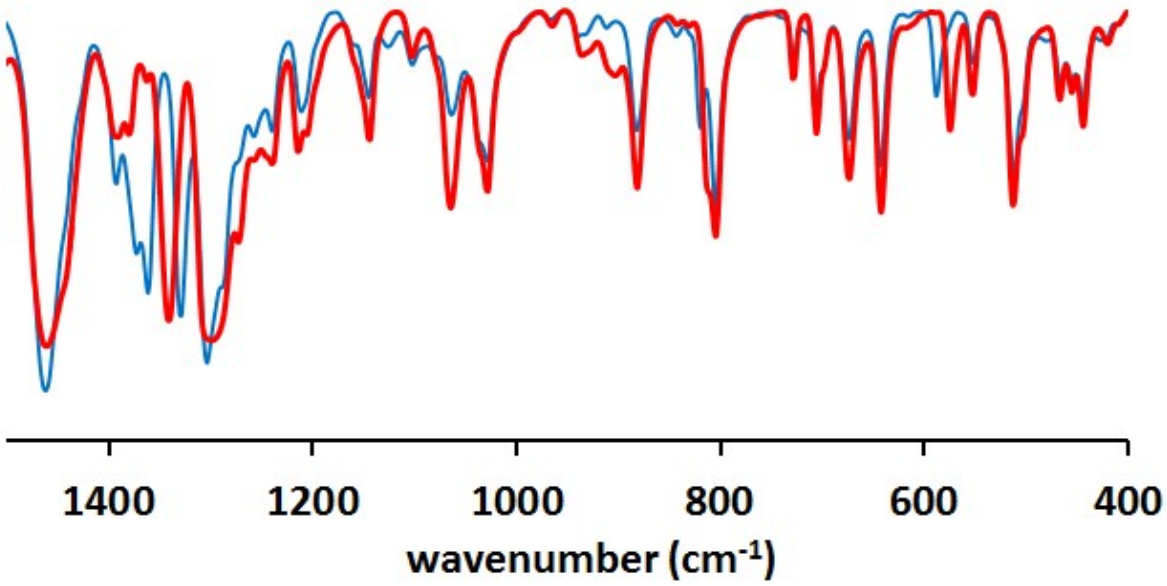


Figure S32. IR spectra of (PNP)Ni(NO) (**3**, blue) and (PNP)Ni(^{15}NO) (**3-^{15}NO**, red) (KBr pellet).

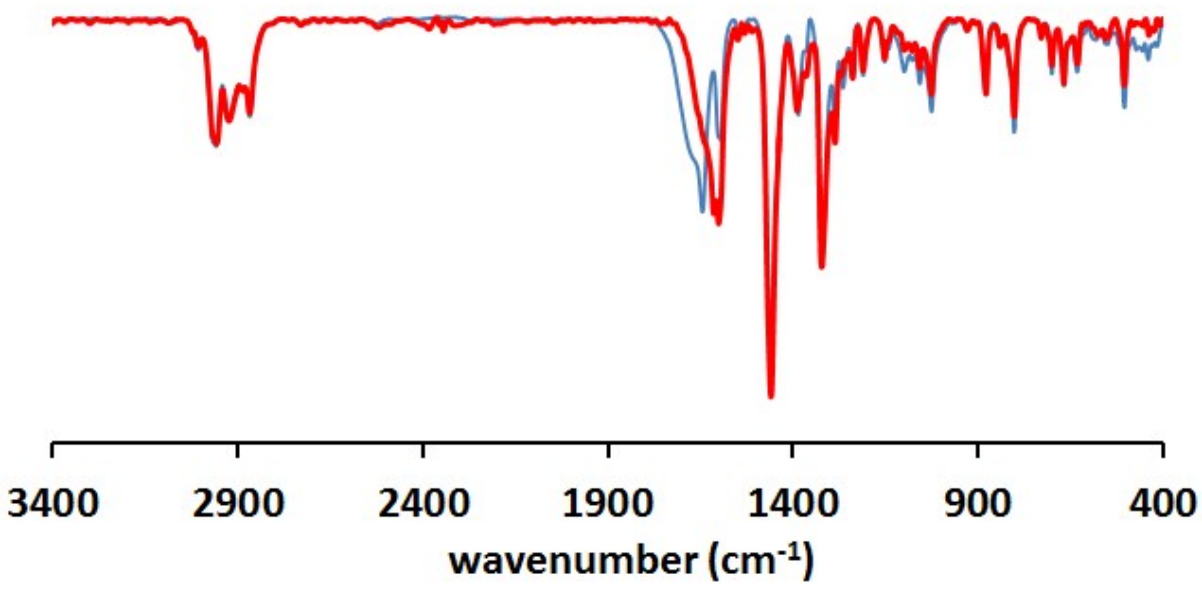


Figure S33. Solution IR spectrum of (PNP)Ni(NO) (**3**) (THF solution).

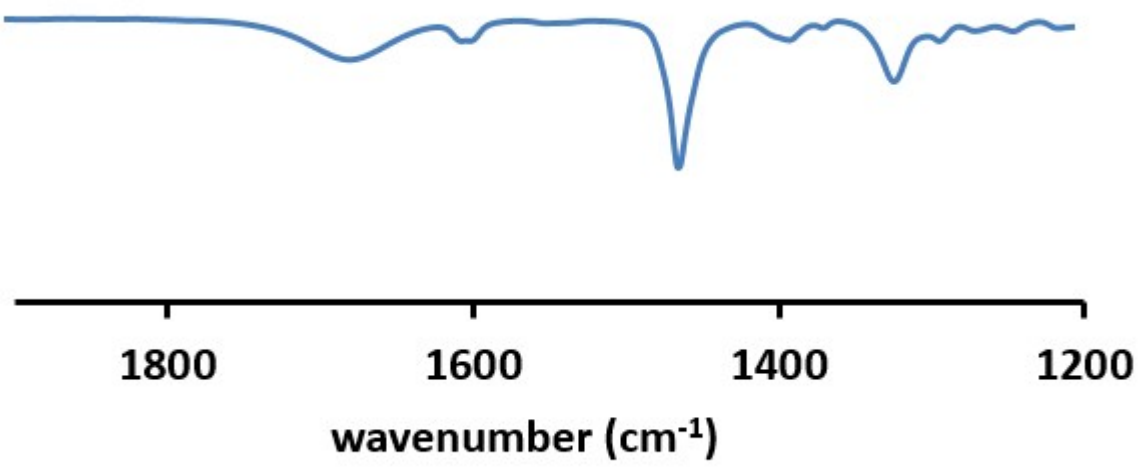


Figure S34. UV-Vis spectrum of (PNP)Ni(ONO_2) (**1**) in THF at room temperature.

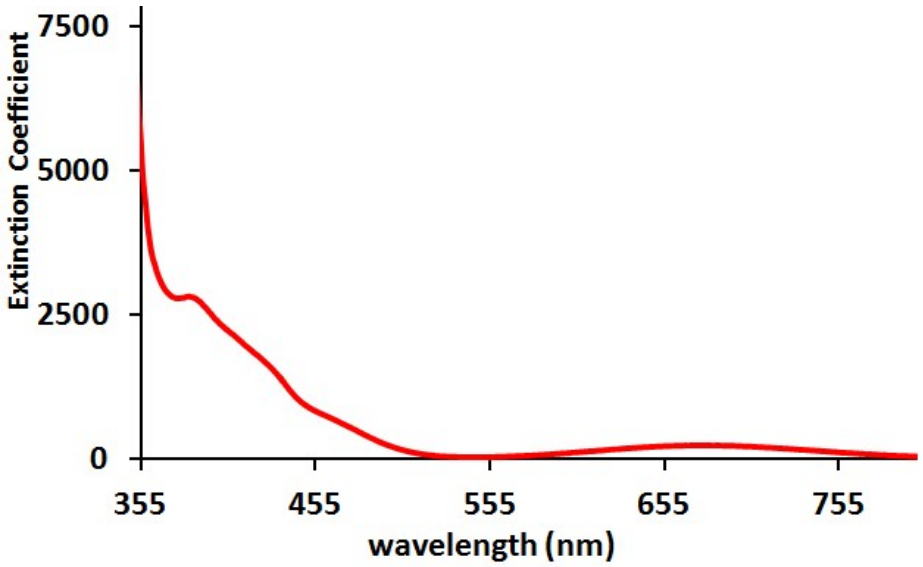


Figure S35. UV-Vis spectrum of (PNP)Ni(NO_2) (**2**) in THF at room temperature.

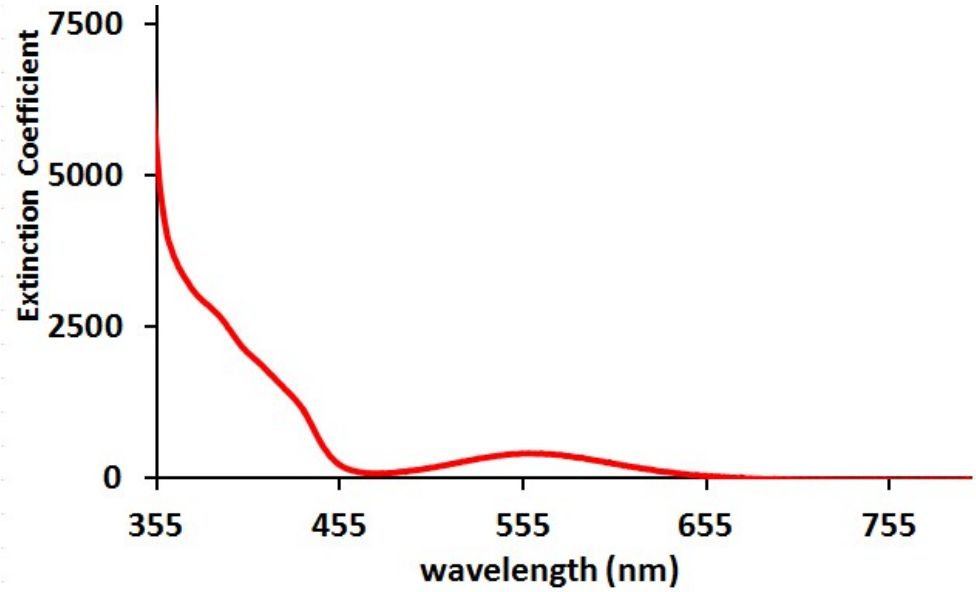
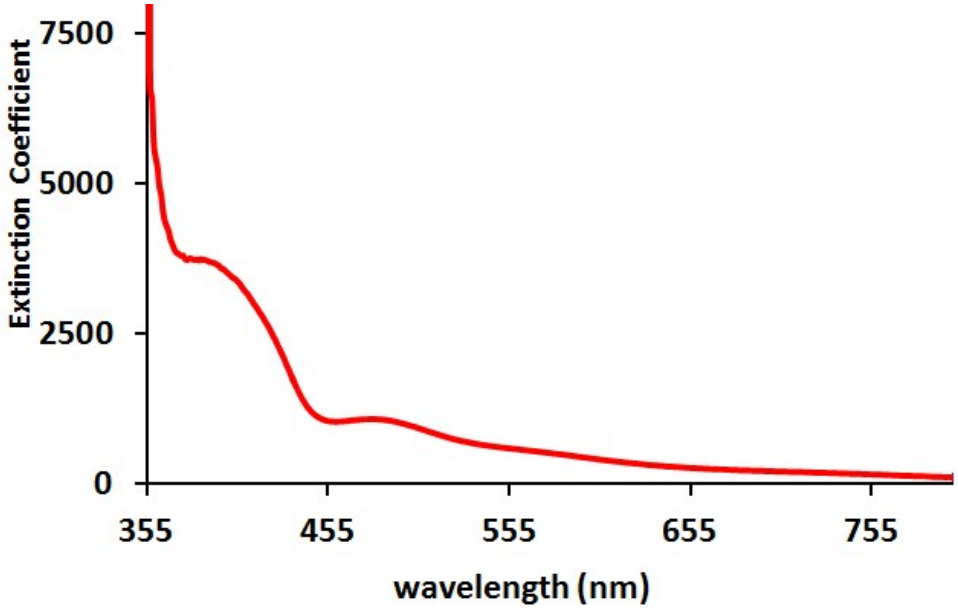


Figure S36. UV-Vis spectrum of (PNP)Ni(NO) (**3**) in THF at room temperature.



2. Computational section

2.1 Computational details

All geometry optimizations and frequency calculations except for the complex **3** in Fig. S41, Table2, and Table S7 were performed using DFT[S11] as implemented in the Jaguar 9.1[S12] suite of *ab initio* quantum chemistry programs. Geometry optimizations were carried out with the B3LYP[S13–S17] functional and the 6-31G** basis set[S18] with D3 dispersion correction[S19]. Nickel was represented using the Los Alamos LACVP** basis[S20–S22] that includes effective core potentials. This basis set combination is represented as B1. The energies of the optimized structures were reevaluated by additional single-point calculations on each optimized geometry using Dunning's correlation consistent triple-ζ basis set cc-pVTZ(-f)[S23] that includes a double set of polarization functions. For Ni, a modified version of LACVP, designated LACV3P, in which the exponents were decontracted to match the effective core potential with triple-ζ quality. We represent this basis set combination as B2. Analytical vibrational frequencies within the harmonic approximation were computed with the 6-31G**/LACVP** basis to confirm proper convergence to well-defined minima on the potential energy surface. Solvation energies were evaluated by a self-consistent reaction field (SCRF) approach based on accurate numerical solutions of the Poisson−Boltzmann equation[S24,S25]. In the results reported, solvation calculations were carried out with the 6-31G**/LACVP** basis at the optimized gas-phase geometry employing the dielectric constant of ε = 2.284 for benzene. The free energy in solution-phase G(sol) has been calculated as follows:

$$G(sol) = G(gas) + \Delta G^{solv} \quad (1)$$

$$G(gas) = H(gas) - TS(gas) \quad (2)$$

$$H(gas) = E(SCF) + ZPE \quad (3)$$

$$\Delta E(SCF) = \Sigma E(SCF) \text{ for products} - \Sigma E(SCF) \text{ for reactants} \quad (4)$$

$$\Delta G(sol) = \Sigma G(sol) \text{ for products} - \Sigma G(sol) \text{ for reactants} \quad (5)$$

G(gas) is the free energy in the gas phase; G(sol) is the free energy of solvation as computed using the continuum solvation model; H(gas) is the enthalpy in gas phase; T is the temperature (298.15K); S(gas) is the entropy in the gas phase; E(SCF) is the self-consistent field energy, i.e., raw electronic energy as computed from the SCF procedure; and ZPE is the zero-point energy. Note that by entropy here we refer specifically to the vibrational/rotational/translational entropy of the solute(s); the entropy of the solvent is incorporated implicitly in the continuum solvation model. Transition state structures were obtained from the quadratic synchronous transit search methods (QST)[S26] and transition state optimization.

For structures of the complex **3** depending on spin-state in in Fig. S41, Table2, and Table S7, we used B3LYP[S13–S17] functional and the remaining process follow the same protocol. To obtain the accurate energy of small molecules, such as NO_3^-, NO_2^-, and N_2, we carried out the ccCA-CC(2,3) calculation implemented in GAMESS program [S27,S28]. The ccCA-CC(2,3) is a composite method utilizing the correlation consistent basis sets [S29,S30].

2.2 Selected computed structures

Figure S37. Optimized structure of (PNP)Ni(ONO_2) **(1)**. Hydrogen atoms are omitted for clarity.

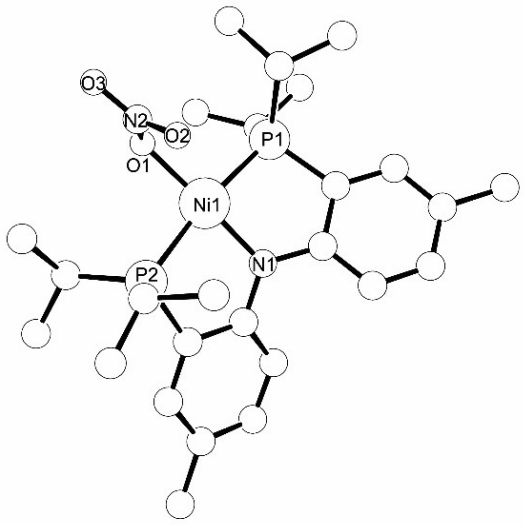


Table S4. Selected bond distances and angles for (PNP)Ni(ONO_2) **(1)** (the units are Å and °). The values in brackets mean measured values.

Distance	(PNP)Ni(NO_3)	Angle	(PNP)Ni(NO_3)
d_{N2-O1} d_{N2-O2} d_{N2-O3}	1.321 [1.272(4)] 1.245 [1.235(4)] 1.228 [1.249(4)]	∠O1–N2–O2 ∠O2–N2–O3 ∠O3–N2–O1	118.1 [121.3(3)] 124.8 [120.9(3)] 117.2 [117.7(3)]
d_{Ni1-O1}	1.907 [1.897(2)]	∠Ni1–O1–N2	114.2 [115.8(2)]
d_{Ni1-N1} d_{Ni1-P1} d_{Ni1-P2}	1.900 [1.887(3)] 2.262 [2.2199(10)] 2.261 [2.2152(10)]	∠N1–Ni1–O1 ∠P1–Ni1–P2	175.95 [175.41(12)] 171.06 [169.27(4)]
		∠N1–Ni1–P1 ∠O1–Ni1–P1 ∠N1–Ni1–P2 ∠O1–Ni1–P2	85.87 [84.39(9)] 94.66 [97.04(8)] 85.72 [84.89(9)] 93.89 [93.66(8)]

Figure S38. Optimized structure of (PNP)Ni(NO_2) **(2)**. Hydrogen atoms are omitted for clarity.

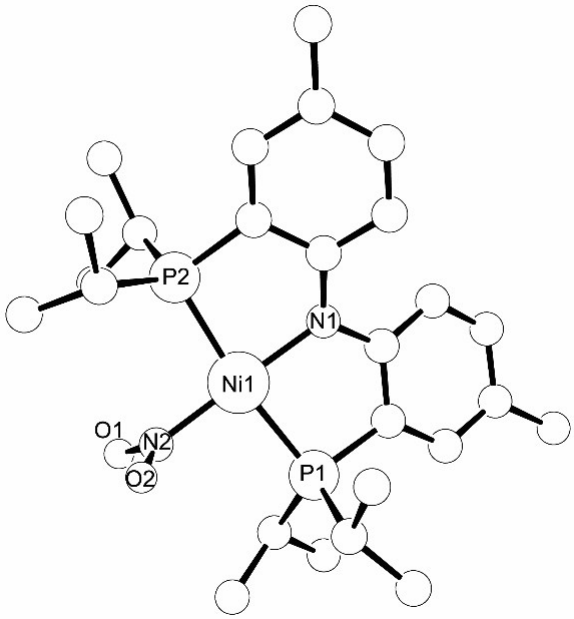


Table S5. Selected bond distances and angles for (PNP)Ni(NO_2) **(2)** (the units are Å and °). The values in brackets mean measured values.

Distance	(PNP)Ni(NO_2)	Angle	(PNP)Ni(NO_2)
$d_{N2–O1}$ $d_{N2–O2}$	1.242 [1.230(5)] 1.241 [1.224(5)]	∠O1–N2–O2	121.6 [121.4(4)]
$d_{Ni1–N2}$	1.868 [1.860(4)]	∠Ni1–N2–O1 ∠Ni1–N2–O2	118.1 [117.5(3)] 120.3 [121.1(3)]
$d_{Ni1–N1}$ $d_{Ni1–P1}$ $d_{Ni1–P2}$	1.911 [1.907(4)] 2.243 [2.1919(13)] 2.254 [2.1934(12)]	∠N1–Ni1–N2 ∠P1–Ni1–P2	178.23 [176.12(17)] 172.13 [170.46(2)]
		∠N1–Ni1–P1 ∠N2–Ni1–P1 ∠N1–Ni1–P2 ∠N2–Ni1–P2	85.85 [85.53(11)] 95.00 [95.18(12)] 86.37 [86.23(11)] 92.81 [93.37(12)]

Figure S39. Optimized structure of (PNP)Ni(NO) **(3)**. Hydrogen atoms are omitted for clarity.

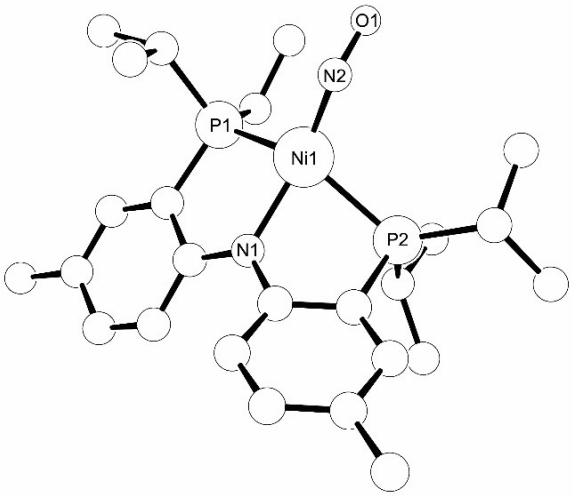


Table S6. Selected bond distances and angles for (PNP)Ni(NO) **(3)** (the units are Å and °). The values in brackets mean measured values.

Distance	(PNP)Ni(NO)	Angle	(PNP)Ni(NO)
d_{N2-O1}	1.187 [1.174(6)]	∠Ni1–N2–O1	142.7 [145.4(4)]
d_{Ni1-N2}	1.740 [1.694(4)]	∠N1–Ni1–N2	151.9 [148.5(2)]
d_{Ni1-N1} d_{Ni1-P1} d_{Ni1-P2}	2.025 [1.999(4)] 2.280 [2.2228(13)] 2.333 [2.2442(13)]	∠P1–Ni1–P2	135.7 [142.53(5)]
		∠N1–Ni1–P1 ∠N2–Ni1–P1 ∠N1–Ni1–P2 ∠N2–Ni1–P2	84.6 [84.35(12)] 104.4 [102.71(15)] 79.2 [82.44(13)] 109.2 [106.82(15)]

Figure S40. Frontier orbitals of (PNP)Ni(NO) (**3**).

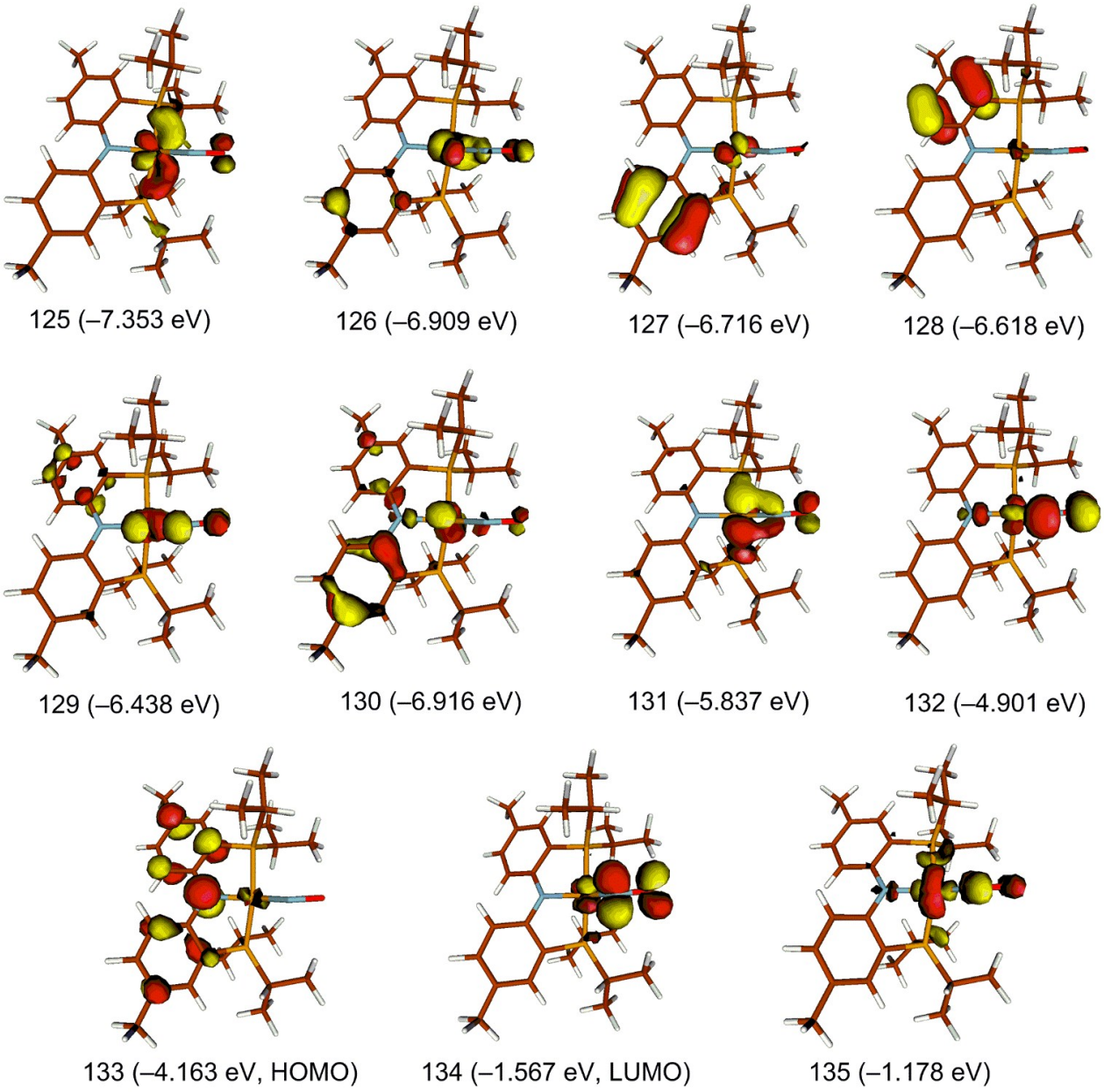


Figure S41. Optimized structures of (PNP)Ni(NO) (**3**) depending on spin-state. **a.** closed singlet spin-state like a nitrosyl radical. **b.** closed singlet spin-state like a nitrosyl anion. **c.** triplet spin-state.

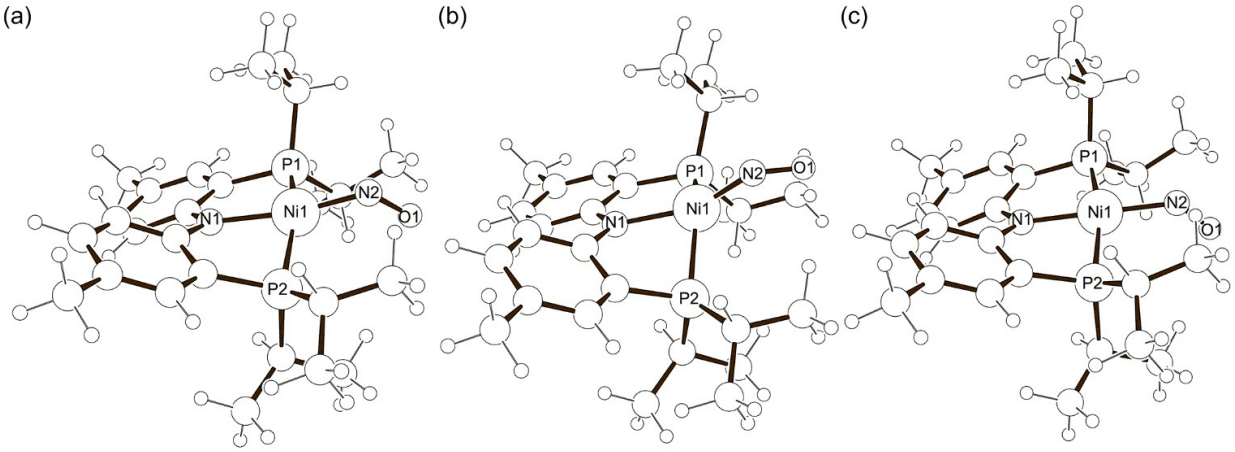


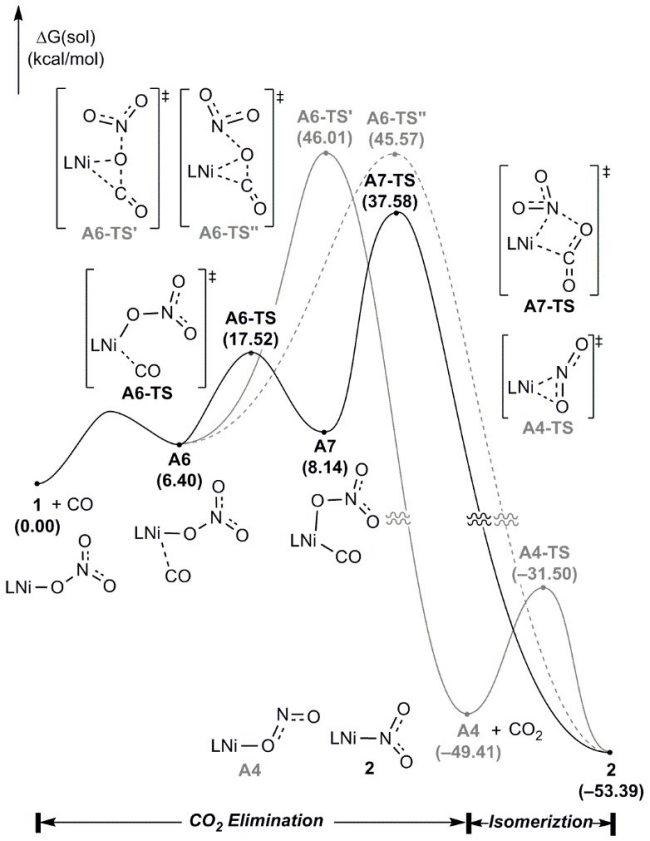
Table S7. Selected bond distances, angles, ν(CO, cm^{-1}), and relative free energies for (PNP)Ni(NO) **(3)** depending on spin-state.

	Antiferromagnetic	***Closed Singlet[a]***	***Closed Singlet[a]***	***Triplet***	***Measured***
	(PNP)Ni–N=O (0.57, 0.16, −0.43, −0.31)	(PNP)Ni–N=O (0.00, 0.00)	(PNP)Ni–N=O (0.00, 0.00)	(PNP)Ni–N=O (0.98, 0.10, 0.29, 0.62)	
Ni1–P2/P1(Å)	2.333/2.280	2.315/2.253	2.296/2.263	2.311/2.265	2.223(1)/2.244(1)
Ni1–N1(Å)	2.025	2.008	2.018	1.961	1.999(4)
Ni1–N2(Å)	1.740	1.701	1.771	1.894	1.694(4)
N5–O1(Å)	1.187	1.191	1.206	1.222	1.176(6)
P1–Ni1–P2(°)	136.7	137.4	157.7	166.5	142.5(5)
N1–Ni1–N2(°)	151.9	153.6	170.7	177.6	148.5(2)
Ni1–N2–O1(°)	142.7	140.8	124.5	128.7	145.4(4)
ν(NO, cm^{-1})	1675.79	1662.56	1577.81	1498.56	1664 (Ref)
ΔG(kcal/mol)	0.00	1.99	5.04	6.79	

a) These two closed singlet structures are structural isomer.

2.3. Mechanistic Studies

Figure S42. Calculated monometallic pathway of from (PNP)Ni(NO_3) (**1**) to (PNP)Ni(NO_2) (**2**).



The calculated energy profile of the transformation from (PNP)Ni(NO_3) (**1**) to (PNP)Ni(NO_2) (**2**) is described in Fig. S42. The reaction begins with approaching CO to the complex **1** and affords an adduct **A6** with a slightly high energy of 6.4 kcal/mol. After the formation of the adduct **A6**, CO_2 is generated via three possible pathways exist with O- and N-bound intermediate and reorientation of ligands. First, we investigated a reorientation pathway of two ligands. The CO is traversing into the PNP plane, and NO_3 moiety moves to the axial position of the complex by slightly elongating the Ni–O bond and forms the intermediate **A7** which is located at a free energy of 8.14 kcal/mol via **A6-TS**. Compared to the intermediate **A6**, the five-coordinated intermediate **A7** is sterically crowded which is confirmed in energy profile, and liberates CO_2 via **A7-TS** with a barrier of 37.6 kcal/mol. Unfortunately, this barrier is too high relative to the given experimental condition. This high barrier might be related to the destabilization of the negative charge of the NO_2 fragment. When the NO_2 moiety is generated, the negative charge should be stabilized, however, in this pathway, there is no an appropriate source to stabilize the negative charge of NO_2. Compared to this step, the remaining step is negligible. Next, we examined the O- and N-bound pathways instead of the reorientation pathway. The O-bound pathway forms the intermediate **A4** via **A6-TS'** with a barrier of 46.0 kcal/mol, and the N-bound pathway has a nearly same barrier of 45.6 kcal/mol via **A6-TS"**. In each TS, the Ni–O bond cleavage and a highly negative charge of NO_2 moiety should be compensated, however, these two pathways are not sufficient. The computed results give rise to some interpretation: (i) as expected in the simple deoxygenation of NO_3^- to NO_2^-, the reaction is exergonic; (ii) at the transition states, a positive charge source should be needed to reduce the negative charge of the NO_2 analogue. Based on this theoretical insight, we needed to consider an alternative pathway, such as a bimetallic pathway.

Figure S43. Calculated energy profile of the O-bound pathway at the deoxygenation of (PNP)Ni(NO_2) (**2**) to (PNP)Ni(NO) (**3**).

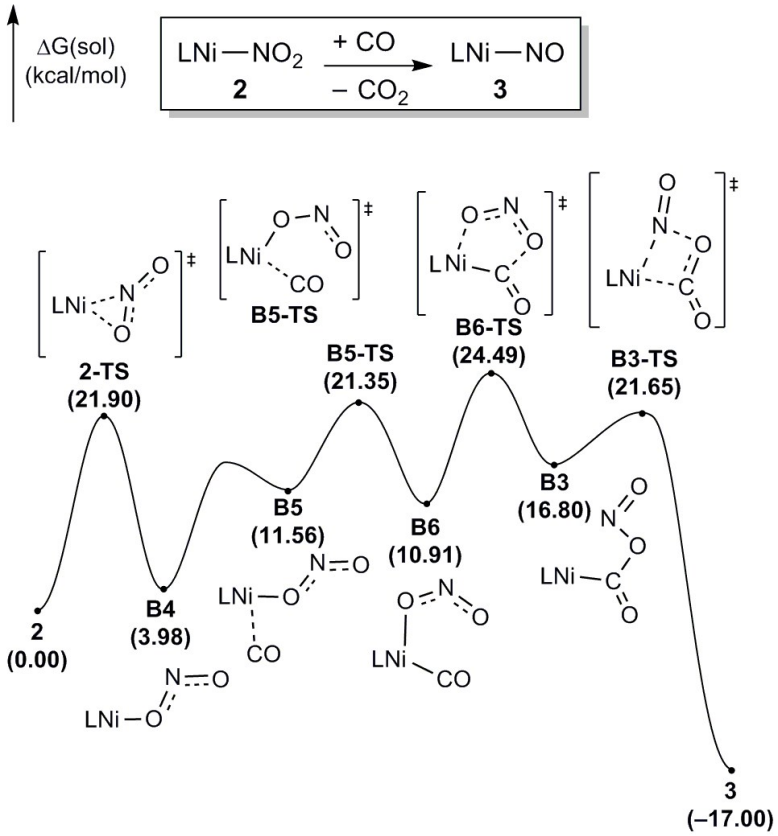
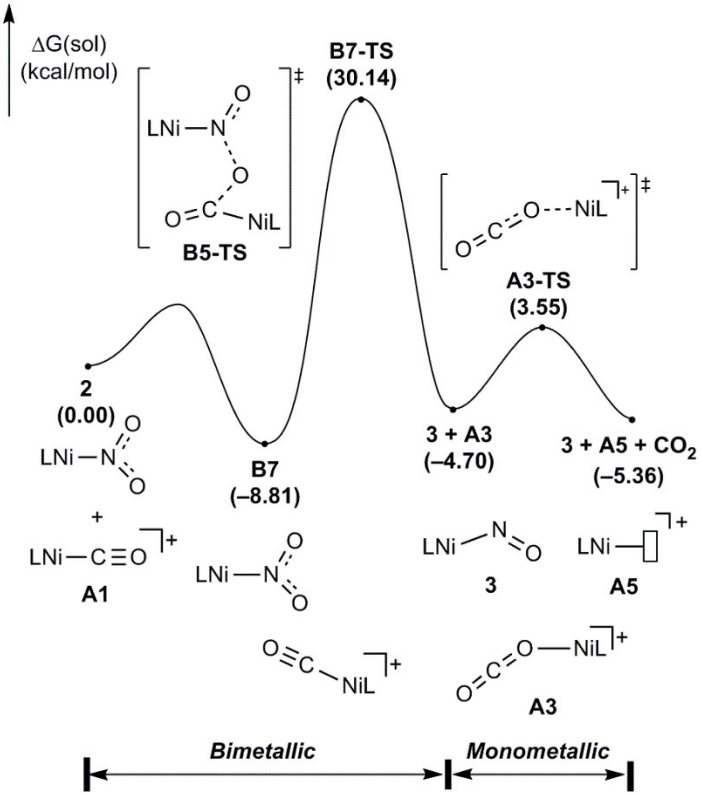


Fig. S43 displays the calculated energy profile of the deoxygenation of the nitro moiety via the O-bound intermediate **B4**. In contrast to the N-bound pathway in Fig. 6, the proposed mechanism starts with isomerization of the nitro moiety affording the intermediate **B4** via **2-TS** with a barrier of 21.9 kcal/mol. The Ni-nitrito complex **B4** generates an adduct **B5** approaching CO which was located at a slightly higher than **B4** by 7.6 kcal/mol. Following the similar route of the formation of **A7**, the CO is traversing into the PNP plane and ONO ligand changes from equatorial position to the axial position of the complex by slightly elongating the Ni–O bond. This reorientation affords the five-coordinated intermediate **B6** via **B5-TS** with a barrier of 21.4 kcal/mol. In contrast to the N–bound pathway, reorganization of the nitrito ligand at transition state **B6-TS** was higher by 2.9 kcal/mol than the extraction of the oxygen atom from the nitro group at **B3-TS**. In this proposed mechanism, the overall barrier was 24.5 kcal/mol, which was higher than the N-bound pathway. Although this overall barrier seemed to be relevant, this barrier was slightly higher than the N–bound pathway compared to the experimental result. Therefore, we concluded that the N-bound pathway is more relevant.

Figure S44. Calculated energy profile of the bimetallic pathway from **2** to **3**.



As mentioned the bimetallic pathway of the first step in Fig. 4, we also considered the bimetallic pathway at the second step. The calculated energy profile of the transformation from (PNP)Ni(NO_2) (**2**) to (PNP)Ni(NO) (**3**) following the bimetallic pathway is described in Fig. S44. The transition state for this bimetallic mechanism was located at 39.0 kcal/mol which is too high to proceed under room temperature. The remaining step was negligible because of the higher barrier of **B7-TS**. Thus, we were able to rule out the bimetallic pathway at the second step.

Scheme S1. Possible pathways of the formation of **C2** depending on the direction of a nitric oxide radical.

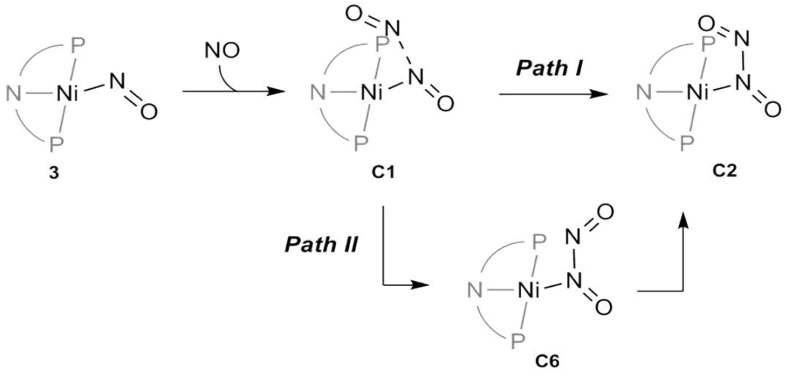
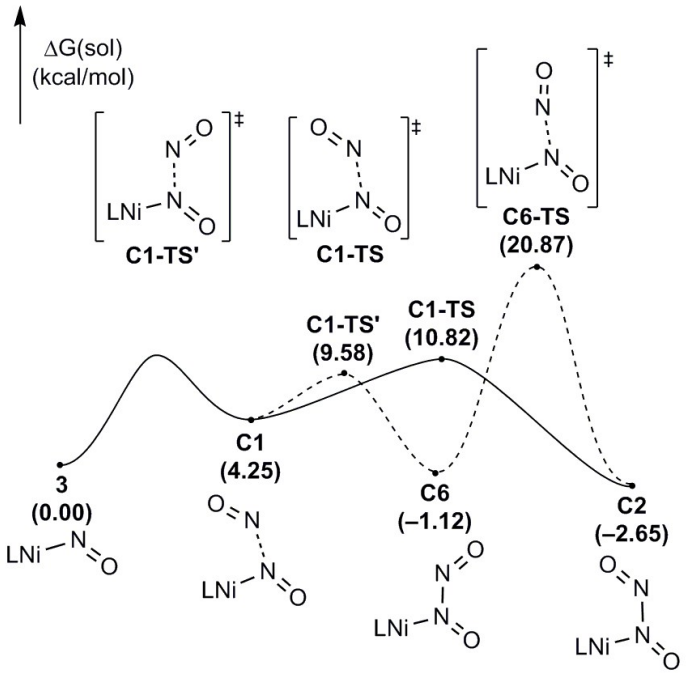
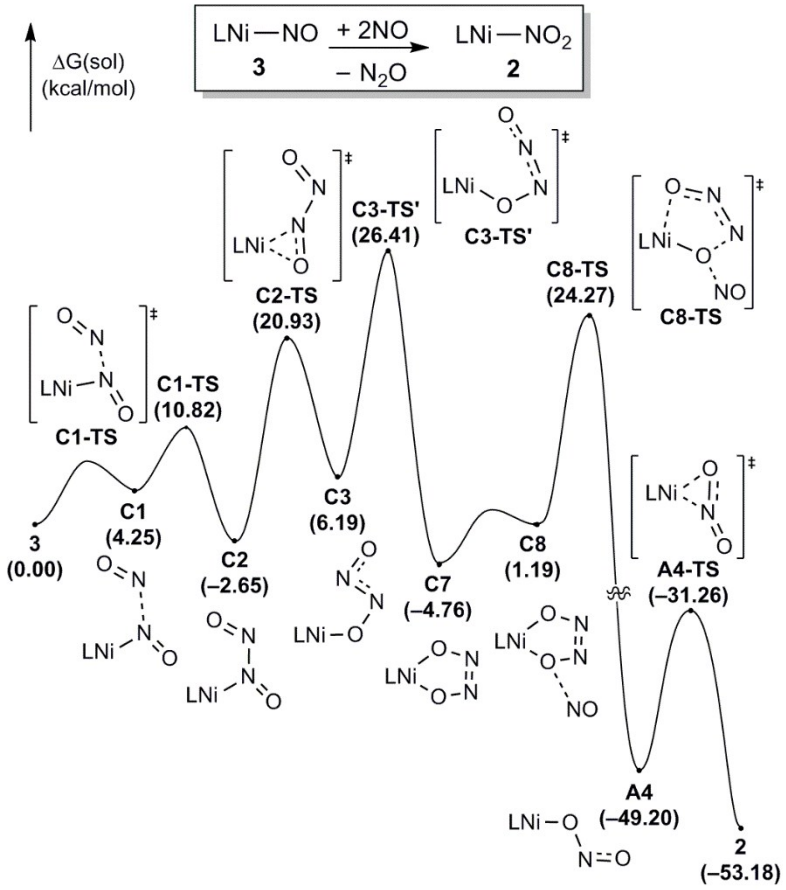


Figure S45. Calculated energy profile of Scheme S1.



Scheme S1 shows two possible pathways depending on the direction of a nitric oxide radical. The calculated energy profiles of Scheme S1 is described in Fig. S45. In Path I, to generate the intermediate **C2**, an adduct **C1** proceed through association of a nitric oxide radical at **C1-TS** with a barrier of 10.8 kcal/mol. Whereas, in Path II the intermediate **C1** produces the complex **C6** by forming the N–N bond via **C1-TS'** and the barrier of this transition state is slightly lower than **C1-TS** by 1.2 kcal/mol. Although the formation of **C6** is viable, to make the intermediate **C2**, **C6** passes through isomerization at **C6-TS**, however, this barrier is higher compared to **C1-TS** by 11.2 kcal/mol. Based on the calculated results, we concluded that the Path I is a suitable pathway.

Figure S46. Calculated energy profile of N_2O formation via five-membered ring formation.



Following the four-membered ring formation pathway, we investigated a five-membered ring formation pathway as shown in Fig. S46. The front stage of the pathway before the intermediate **C3** was the same as the four-membered ring pathway. To form the five-membered ring intermediate, the intermediate **C7** proceeds via **C3-TS'** which has a barrier of 29.1 kcal/mol. Although the intermediate **C7** is more stable than the intermediate **C4** due to less steric hindrance, the barrier of 29.1 kcal/mol of **C3-TS'** is fairly high to occur at room temperature. Next, a nitric oxide radical approaches the intermediate **C7** affording an adduct **C8** with a free energy of 1.2 kcal/mol. The Ni-nitrito complex **A4** is generated by liberating N_2O via **19-TS** with a barrier of 29.0 kcal/mol, however, this transition state is also too high to proceed at room temperature. Namely, the calculated overall barrier is 29.1 kcal/mol which means that in this pathway the reaction needs harsher conditions than what we performed. In addition, the stability of the intermediate **C7** showed that may disturb the reproducing of the complex **2** by increasing the barrier of N_2O elimination.

Table S8. Computed energy components of ccCA-CC(2,3) calculations.

	E(ccCA-CC(2,3), 0K)//(a.u.)	E(ccCA-CC(2,3), 298K)//(a.u.)	H(ccCA-CC(2,3))//(a.u.)	H(ccCA-CC(2,3))//(a.u.)
NO_3^-	-280.543692	-280.543692	-280.543692	-280.543692
NO_2^-	-205.277998	-205.275071	-205.274126	-205.301669
NO^-	-129.965203	-129.962837	-129.961893	-129.985764
· NO	-129.965926	-129.963565	-129.962621	-129.985914
N^-	-54.588734	-54.587318	-54.586374	-54.588734
CO	-113.377870	-113.375510	-113.374565	-113.396989
CO_2	-188.691870	-188.689254	-188.688310	-188.713215
N_2O	-184.759493	-184.756828	-184.755884	-184.780787
N_2	-109.585187	-109.582826	-109.581882	-109.603615

Table S9. Computed energy components of all DFT-computed structures.

	E(SCF)/(eV)	ZPE/(kcal/mol)	S(gas)/(cal/mol·K)	G(solv)/(kcal/mol)
	cc-pVTZ(-f)/LACV3P**	6-31G**/LACVP**	6-31G**/LACVP**	6-31G**/LACVP**
CO	-3084.529	3.16	47.24	0.00
CO_2	-5133.565	7.28	51.16	-1.26
NO	-3535.739	2.85	49.06	0.00
N_2O	-5026.663	7.02	52.51	-1.65
1	-59937.605	391.70	232.16	-5.95
2	-57890.930	388.85	226.19	-5.52
2-TS	-57889.898	387.90	227.94	-5.95
3	-55843.086	384.37	229.48	-3.46
A1	-55386.523	386.89	223.19	-20.97
A2	-115324.953	779.26	404.40	-20.53
A2-TS	-115324.047	777.50	410.11	-18.73

A3	-57434.348	389.20	236.02	-21.19
A3-TS	-57433.996	388.59	235.19	-20.70
A4	-57890.590	387.52	233.68	-5.81
A4-TS	-57889.898	387.90	227.94	-5.95
A5	-52300.246	380.19	221.63	-20.29
A6	-63022.336	395.94	247.46	-5.49
A6-TS	-63021.781	395.23	248.27	-6.22
A6-TS’	-63020.609	394.62	246.20	-4.76
A6-TS’’	-63020.605	394.56	248.28	-4.62
A7	-63022.246	396.78	244.35	-7.60
A7-TS	-63021.156	396.33	234.49	-5.78
B1	-60975.691	393.01	244.63	-5.17
B1-TS	-60975.105	392.44	237.79	-5.93
B2	-60975.184	393.04	239.01	-6.93
B2-TS	-60975.059	392.79	236.59	-7.76
B3	-60975.266	393.35	238.78	-4.84
B3-TS	-60975.105	393.05	233.53	-4.97
B4	-57890.590	387.52	233.68	-5.81
B5	-60975.238	391.71	252.14	-5.10
B5-TS	-60975.004	392.22	238.59	-5.25
B6	-60975.426	392.95	239.10	-6.55
B6-TS	-60974.957	392.49	235.41	-4.42
B7	-113278.836	776.70	400.90	-18.82
B7-TS	-113277.164	775.59	395.06	-19.06
C1	-59379.098	388.29	246.13	-3.64
C1-TS	-59378.867	388.63	240.23	-4.50
C1-TS’	-59379.000	388.98	235.88	-4.32
C2	-59379.586	390.53	233.10	-5.42

C2-TS	-59378.488	389.22	234.00	-5.57
C3	-59379.113	389.74	239.02	-4.93
C3-TS	-59379.098	390.34	229.58	-7.16
C3-TS’	-59378.184	388.50	239.74	-4.67
C4	-59379.160	390.88	232.05	-6.97
C5	-62914.875	393.90	254.32	-6.39
C5-TS	-62914.656	393.87	245.26	-6.51
C6	-59379.426	389.88	236.87	-5.80
C6-TS	-59378.563	389.15	233.42	-4.01
C7	-59379.617	390.66	231.93	-7.29
C8	-62915.758	395.79	238.25	-7.09
C8-TS	-62914.781	394.32	239.61	-4.66
3-AF	-55840.277	383.22	233.23	-3.32
3-Triplet	-55839.930	383.13	234.93	-3.94
3-Singlet-1	-55840.234	383.70	230.72	-3.56
3-Singlet-2	-55840.102	383.71	229.79	-3.84

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4. Cartesian coordinates of the optimized geometries

Table S10. Cartesian coordinates of the optimized geometries.

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 ================================
CO
================================
  C   0.177062765   0.319277823  -1.355465889
  O   0.177062765   0.319277823  -2.492726564

================================
CO2
================================
  C   0.177062884   0.319277793  -1.182494640
  O   0.177062720   0.319277823  -2.352298975
  O   0.177062720   0.319277823  -0.012693036

================================
NO
================================
  N   0.177062765   0.319277823  -1.332735538
  O   0.177062765   0.319277823  -2.490964890

================================
N2O
================================
  N   0.177063167   0.319278032  -1.172076821
  O   0.177062586   0.319277734  -2.365479231
  N   0.177062571   0.319277734  -0.036489628

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1
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  C  -1.448456883  -0.595071852  -2.770339966
 Ni  -2.224115849   1.212431431  -0.689626038
  P  -2.465215683   0.061833177   1.211741090
  C  -2.875970840  -1.556839824   0.503192484
  C  -2.670670748  -1.605737686  -0.904142976
  N  -2.104655743  -0.500381112  -1.541881323
  C  -1.305085182   0.576702118  -3.565246582
  P  -1.924887538   2.065160275  -2.734138250
  C  -3.370326757  -2.670712233   1.195997953
  C  -3.123070478  -2.769878626  -1.570128679
  C  -0.850193799  -1.777100682  -3.270586491
  C  -0.726251543   0.512163937  -4.840182781
  C  -3.748907566  -3.840553999   0.537205577
  C  -3.640830278  -3.845856667  -0.862688184
  C  -0.257617652  -1.806996226  -4.525632381
  C  -0.206883013  -0.675298512  -5.356251240
  H  -3.478405476  -2.621717691   2.274615765
  H  -3.982399940  -4.718301773  -1.416664600
  H   0.188058168  -2.737943411  -4.870646477
  H  -0.660964549   1.413033366  -5.442345619
  H  -3.082044363  -2.816460609  -2.652023554
  H  -0.843743265  -2.672310114  -2.660102844
  C  -3.855486393   0.730885208   2.285140753
  H  -4.496272087   1.208763123   1.533478260
  C  -3.333457470   1.835676074   3.221344471
  C  -4.696599960  -0.299873024   3.050384521
  H  -5.151860237  -1.034746289   2.383213043
  H  -4.105456352  -0.834237993   3.801542759
  H  -5.504581928   0.218724981   3.579658508
  H  -2.650020599   1.434492350   3.977093458
  H  -4.181043148   2.282539845   3.753092289
  H  -2.830302000   2.640503883   2.683377266
  C  -0.905069590  -0.120432466   2.217177391
  H  -0.705323398   0.892305434   2.585426807
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  H  -1.796872139  -0.808050334   4.106100559
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  C  -0.617282629   3.410104752  -2.701328993
  H   0.000912859   3.069248915  -1.861709833
  C  -1.230920911   4.764806747  -2.301241159
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  H   0.820639253   2.627346754  -4.157498360
  H  -0.304704577   3.822623730  -4.833173752
  H   1.007578135   4.341842175  -3.770599127
  H  -1.780751109   5.213175297  -3.135160446
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  C  -3.476937771   2.587307453  -3.639189959
  H  -3.968576431   1.612569332  -3.761826754
  C  -3.250824928   3.195210695  -5.030372143
  C  -4.381132603   3.460880995  -2.751926661
  H  -4.472543240   3.044513226  -1.744451404
  H  -3.994297028   4.478275299  -2.655152798
  H  -5.381264210   3.526317358  -3.195570707
  H  -2.733018160   4.157280922  -4.968296051
  H  -4.215793133   3.372763872  -5.520117760
  H  -2.668856859   2.530987501  -5.675671101
  C   0.428895116  -0.738394976  -6.724709988
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H	0.282484591	0.194733649	-7.277642727
C	-4.271045685	-5.044112206	1.284719706
H	-5.194065094	-5.426955700	0.833653152
H	-3.545995951	-5.867936611	1.278483868
H	-4.486520290	-4.804443359	2.330640554
O	-2.461288929	2.943977118	0.178651467
N	-1.373975396	3.395378590	0.774799168
O	-1.483027935	4.424255371	1.435124278
O	-0.316840410	2.750503063	0.638112068

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2

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C	-1.898123503	-0.258603126	-2.774412394
Ni	-2.602130651	1.519582272	-0.669095278
P	-2.839922905	0.361336917	1.204061151
C	-3.365081072	-1.216903448	0.475488037
C	-3.163579702	-1.264583468	-0.934206486
N	-2.576394796	-0.170282915	-1.562543750
C	-1.695968390	0.934189379	-3.528795481
P	-2.328435421	2.416523218	-2.685168266
C	-3.903945684	-2.314147711	1.162029982
C	-3.646479130	-2.414315701	-1.604486942
C	-1.329718947	-1.443888783	-3.298833609
C	-1.079573274	0.889965355	-4.785749435
C	-4.323910236	-3.466134071	0.496386737
C	-4.204702854	-3.473334312	-0.902839601
C	-0.692510486	-1.450991154	-4.532303333
C	-0.572400808	-0.296097636	-5.319738865
H	-4.009553432	-2.268576145	2.240978003
H	-4.569901943	-4.333969116	-1.460389256
H	-0.267011106	-2.385321856	-4.894021511
H	-0.974002182	1.803508162	-5.361610413
H	-3.599888802	-2.459090710	-2.686388493
H	-1.376781344	-2.360036850	-2.722097397
C	-4.110644817	1.114276767	2.363811493
H	-4.713720798	1.703294754	1.662234426
C	-3.432173729	2.110770226	3.322508097
C	-5.033156872	0.146441445	3.115078926
H	-5.583626747	-0.506248116	2.433949947
H	-4.479666710	-0.480325907	3.822747946
H	-5.765108585	0.723058760	3.692649603
H	-2.834322929	1.592251062	4.079771996
H	-4.204741478	2.683457613	3.846877098
H	-2.792083979	2.826651096	2.801123381
C	-1.244614363	0.052655373	2.121840954
H	-0.983130634	1.030096054	2.543334484
C	-0.169690803	-0.336566329	1.092562079
C	-1.362922430	-0.987956703	3.243897200
H	-2.103478193	-0.705675840	3.998300791
H	-1.643768907	-1.965479612	2.838287592
H	-0.397779495	-1.102904558	3.751225710
H	-0.433985323	-1.268454671	0.580737352
H	0.792995214	-0.485271811	1.594645977
H	-0.049758777	0.441671133	0.333198279
C	-1.063828945	3.804404020	-2.658329964
H	-0.460453272	3.509745836	-1.790628910
C	-1.728048444	5.149784088	-2.311457634
C	-0.140960753	3.942860842	-3.876085043
H	0.445326447	3.038553238	-4.050300598
H	-0.700771630	4.175825596	-4.788263798
H	0.560411990	4.767494678	-3.702192783
H	-2.287540674	5.545741558	-3.165220261
H	-0.948006094	5.877598763	-2.063209534
H	-2.400945425	5.084118366	-1.454343200
C	-3.903859377	2.876909256	-3.585687399
H	-4.377392769	1.887445092	-3.648005247
C	-3.695528746	3.406312943	-5.011181355
C	-4.819985867	3.782780647	-2.744549751
H	-4.864939690	3.459294081	-1.700878978
H	-4.477415562	4.820725918	-2.751595497
H	-5.832438469	3.767256498	-3.164542675
H	-3.187552452	4.376121998	-5.007474899
H	-4.666494846	3.546648741	-5.500984669
H	-3.111944675	2.712204218	-5.622609138
O	-3.633023262	3.759560823	0.463257551
N	-2.577884436	3.142114401	0.246883228
O	-1.482107162	3.561267614	0.653441727
C	0.128351659	-0.328931183	-6.658133984
H	1.218199968	-0.393541127	-6.541857719
H	-0.181860328	-1.195042014	-7.253470421
H	-0.084335893	0.570869446	-7.244006157
C	-4.897222519	-4.652187347	1.236473083
H	-5.840347767	-4.987262249	0.788728356
H	-4.211987019	-5.509323120	1.217222571
H	-5.094563961	-4.413403511	2.286183596

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C	-1.878353834	-0.218951836	-2.773193121
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P	-2.886263609	0.348905802	1.233900189
C	-3.486988783	-1.160922527	0.425002038
C	-3.240685940	-1.167939067	-0.974810123
N	-2.522017717	-0.116148748	-1.535832405
C	-1.682936311	0.966132462	-3.533318043
P	-2.298654795	2.423018456	-2.635354280

C	-4.151163578	-2.233190775	1.039275408
C	-3.805481195	-2.232081175	-1.719065666
C	-1.364309549	-1.420313954	-3.308906555
C	-1.121090651	0.908238649	-4.813421726
C	-4.646936893	-3.311562777	0.306262434
C	-4.480094910	-3.266450167	-1.087623239
C	-0.775383592	-1.445729017	-4.567893982
C	-0.662291288	-0.293682009	-5.360547066
H	-4.304311275	-2.220232725	2.113533020
H	-4.903057575	-4.062855721	-1.697261453
H	-0.387626439	-2.389810324	-4.945285320
H	-1.033202648	1.814469218	-5.402548313
H	-3.722795486	-2.232313871	-2.799631596
H	-1.420870781	-2.332832098	-2.726507187
C	-4.258317947	1.177581787	2.213648081
H	-4.729303360	1.792448521	1.437260866
C	-3.660247326	2.134689569	3.257701159
C	-5.324173450	0.257632226	2.823256731
H	-5.806820393	-0.368295282	2.069387674
H	-4.908420086	-0.395784765	3.597842693
H	-6.099176884	0.872075498	3.296358109
H	-3.158448696	1.588668466	4.064136982
H	-4.466432095	2.722156286	3.711125374
H	-2.957441092	2.833371401	2.799802542
C	-1.477983594	-0.121820696	2.360783577
H	-1.185550094	0.825334787	2.830014467
C	-0.319130480	-0.606663644	1.472506642
C	-1.832517505	-1.147271752	3.446027517
H	-2.645849705	-0.806015730	4.093523026
H	-2.127457619	-2.101411581	2.997972250
H	-0.958510280	-1.336368322	4.080243587
H	-0.595492005	-1.522016764	0.937157154
H	0.561313689	-0.825475216	2.086917400
H	-0.048109610	0.150264487	0.730380774
C	-1.225626945	3.942522287	-2.848502398
H	-0.420154423	3.742331266	-2.131963968
C	-1.977552652	5.191712379	-2.350750923
C	-0.605172873	4.178126335	-4.233408928
H	0.085829534	3.380174875	-4.512794018
H	-1.364954352	4.274116516	-5.015812874
H	-0.036223579	5.114979744	-4.212055683
H	-2.759060383	5.489827633	-3.057519674
H	-1.268615961	6.022490978	-2.272127151
H	-2.422222853	5.042217731	-1.364017725
C	-4.037457466	2.658290625	-3.292512655
H	-4.373621941	1.612485766	-3.290643215
C	-4.107259750	3.189822912	-4.730261326
C	-4.938202858	3.435680866	-2.318712473
H	-4.829313755	3.061936855	-1.296227574
H	-4.702799797	4.502435207	-2.305347443
H	-5.985898018	3.327301264	-2.622914314
H	-3.783803225	4.233932495	-4.787733078
H	-5.140429497	3.145455599	-5.095236778
H	-3.487711430	2.597237587	-5.411041260
O	-2.708259821	3.554332018	0.459425539
N	-1.446421981	3.270945311	0.394845247
O	-0.645955861	4.188024521	0.499006689
C	-0.024036113	-0.346114010	-6.728469372
H	1.067137003	-0.443884850	-6.659902096
H	-0.387305796	-1.201663852	-7.308805943
H	-0.235320210	0.560743868	-7.303731441
C	-5.343727112	-4.475738525	0.969407320
H	-6.250586033	-4.763027668	0.424785614
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H	-5.633358479	-4.238761902	1.997857332

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C	-1.322068810	-0.585020900	-2.974586725
Ni	-1.786031246	1.156751156	-0.673519731
P	-2.979798079	0.061235212	0.884500444
C	-3.185130835	-1.560448766	0.104054540
C	-2.608537674	-1.672707558	-1.203316212
N	-1.899411798	-0.610309899	-1.706188202
C	-1.442107558	0.634464800	-3.697560072
P	-2.371310234	1.890955210	-2.754585266
C	-3.892075777	-2.632772923	0.673574686
C	-2.895522356	-2.876113176	-1.908046246
C	-0.561716497	-1.614024282	-3.566467524
C	-0.834495366	0.794882536	-4.944858074
C	-4.107491016	-3.828768253	-0.007249550
C	-3.610673189	-3.906404018	-1.320906997
C	0.025477158	-1.436452150	-4.816563606
C	-0.095107026	-0.237537563	-5.533573627
H	-4.306050301	-2.522883892	1.671416402
H	-3.800217867	-4.806546211	-1.903927803
H	0.611975551	-2.249197006	-5.241238594
H	-0.926179171	1.738036036	-5.476246357
H	-2.563599825	-2.984474421	-2.933480024
H	-0.405188769	-2.540258169	-3.024173260
C	-4.660076141	0.833307207	1.187287450
H	-4.950205803	1.099853873	0.163078398
C	-4.463984013	2.138830900	1.976798773
C	-5.773693562	-0.046245806	1.769131660
H	-5.951740742	-0.928131044	1.149442673
H	-5.548549652	-0.382149190	2.785344601
H	-6.707454205	0.527849674	1.812712550
H	-4.194693089	1.934522629	3.019219637
H	-5.393841267	2.718901396	1.985956907

H	-3.675998926	2.761570930	1.539879203
C	-2.068565130	-0.152417704	2.506827354
H	-1.926469684	0.879811764	2.853564739
C	-0.686875165	-0.746912301	2.179844856
C	-2.772021532	-0.957519710	3.607324123
H	-3.730543852	-0.519611478	3.897278547
H	-2.944988489	-1.990464211	3.290809870
H	-2.139508247	-0.991660833	4.502802849
H	-0.787452638	-1.764355421	1.786588907
H	-0.070710823	-0.790172696	3.085066795
H	-0.160939679	-0.146634877	1.431050181
C	-1.939647913	3.559663534	-3.487845659
H	-0.860114038	3.456274033	-3.662688017
C	-2.145591497	4.664649487	-2.435408354
C	-2.616578579	3.932571173	-4.817269325
H	-2.520367861	3.154373646	-5.578127384
H	-3.683534384	4.128873825	-4.674551487
H	-2.167696238	4.850288391	-5.215919971
H	-3.206572533	4.793540478	-2.196906090
H	-1.775682092	5.622882366	-2.818907022
H	-1.619038582	4.443027496	-1.504243255
C	-4.183194637	1.467764854	-3.025933743
H	-4.244978905	0.547796726	-2.431047440
C	-4.593377113	1.126550078	-4.464797497
C	-5.103519440	2.517543077	-2.384977818
H	-4.791049004	2.764018774	-1.364652872
H	-5.120496273	3.446656466	-2.964298725
H	-6.132391930	2.141491175	-2.342808008
H	-4.624711514	2.013062477	-5.103774071
H	-5.596820354	0.683995605	-4.466378689
H	-3.905895233	0.404959053	-4.914614677
O	-1.113523841	3.374645710	0.828712881
N	-0.936647177	2.380124092	0.201803803
C	0.573028445	-0.063475221	-6.876838207
H	1.665413260	-0.018895106	-6.781216621
H	0.344567418	-0.897589445	-7.550572395
H	0.248911187	0.858995736	-7.368848801
C	-4.857811928	-4.983259201	0.611521244
H	-5.680227757	-5.321232796	-0.031363409
H	-4.205248356	-5.850744724	0.775173664
H	-5.287090302	-4.708894730	1.580536127

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C	-2.267545223	-1.432446718	-3.057182789
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P	-3.454059124	-0.412882149	0.753529191
C	-2.989907026	-2.134519577	0.481805742
C	-2.822760344	-2.437112808	-0.889817834
N	-2.953049421	-1.399130464	-1.833218098
C	-2.710225344	-0.589639664	-4.105959415
P	-3.944121838	0.621038437	-3.595362186
C	-2.806063175	-3.113361597	1.471517444
C	-2.602267981	-3.789088488	-1.223476529
C	-1.127096653	-2.223062277	-3.317939758
C	-2.145286560	-0.667819500	-5.387652397
C	-2.519218922	-4.436528683	1.137081504
C	-2.457132816	-4.750462532	-0.231051624
C	-0.562841654	-2.262963057	-4.586030483
C	-1.076843143	-1.520094752	-5.662088394
H	-2.888614416	-2.845993996	2.518630266
H	-2.293795586	-5.783589840	-0.528409898
H	0.312357008	-2.888035774	-4.746834278
H	-2.518025160	-0.028333049	-6.180805683
H	-2.560208797	-4.086679935	-2.264314413
H	-0.681283414	-2.807194710	-2.522273064
C	-4.860772610	-0.193215877	1.980728030
H	-5.744826317	-0.329950631	1.345288157
C	-4.869670868	1.247987986	2.525421858
C	-4.944195271	-1.217569232	3.122268677
H	-5.057099819	-2.237159729	2.749933004
H	-4.069091320	-1.176089764	3.777645588
H	-5.821995258	-0.987432480	3.735374928
H	-4.050902843	1.408182979	3.233293056
H	-5.807368755	1.423092127	3.061697483
H	-4.796108723	2.008689642	1.743049145
C	-1.948967814	0.533278644	1.325744987
H	-2.300134182	1.559089065	1.487387180
C	-0.898541212	0.535377324	0.201370254
C	-1.378338695	-0.026308928	2.638770819
H	-2.098342657	0.015956318	3.460882425
H	-1.056794882	-1.064724803	2.513516903
H	-0.503203809	0.561588764	2.935269833
H	-0.582830191	-0.483025908	-0.046101436
H	-0.015592881	1.096638441	0.523240149
H	-1.282593727	0.996619761	-0.714502156
C	-3.197201967	2.341761112	-3.759240866
H	-2.530321598	2.365092993	-2.885907412
C	-4.246032238	3.456112146	-3.598544836
C	-2.343437195	2.568913221	-5.017215729
H	-1.514941692	1.862414241	-5.084858894
H	-2.938350201	2.498535156	-5.932334900
H	-1.920682192	3.578477859	-4.977282047
H	-4.914917946	3.504744768	-4.462162495
H	-3.732919693	4.420767307	-3.531975985
H	-4.859432697	3.351815224	-2.701490164
C	-5.499471188	0.393529415	-4.607090473
H	-5.565444469	-0.701514304	-4.649185658
C	-5.408030987	0.932549238	-6.044878006

C	-6.743243217	0.921371996	-3.871077299
H	-6.856418610	0.454604924	-2.888268232
H	-6.713646889	2.006482601	-3.737932920
H	-7.639155865	0.686321080	-4.454643726
H	-5.332134247	2.022995234	-6.067255020
H	-6.317888737	0.655983508	-6.588216782
H	-4.561048985	0.514443994	-6.593608856
C	-0.472188473	-1.620457768	-7.040571213
H	0.621585786	-1.585332513	-6.999505997
H	-0.747002780	-2.565649748	-7.523764133
H	-0.810242951	-0.807453334	-7.689461231
C	-2.293105841	-5.493118763	2.190186977
H	-2.843388796	-6.410689831	1.957031846
H	-1.232048512	-5.761638641	2.257976532
H	-2.611907959	-5.152152538	3.179213524
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O	-5.858105659	2.208990097	-0.627369881

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C	-3.915212154	-1.472844005	-3.349856377
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C	-2.261873245	0.175994396	-2.616164446
N	-3.535808802	-0.410258949	-2.514221191
C	-5.028763294	-2.258442640	-2.967048645
P	-6.094429016	-1.457594156	-1.762979507
C	-0.838065863	2.153917313	-2.275331736
C	-1.113294482	-0.484002888	-3.109926939
C	-3.310580969	-1.811114430	-4.582503319
C	-5.375829220	-3.428946972	-3.654097319
C	0.259591967	1.528092384	-2.859910727
C	0.099815927	0.180692270	-3.225088120
C	-3.684097290	-2.960870504	-5.268998623
C	-4.687366486	-3.826654673	-4.799565315
H	-0.731977463	3.173663616	-1.921103001
H	0.957585812	-0.368301779	-3.606705904
H	-3.178837061	-3.195371389	-6.202908039
H	-6.215483189	-4.026314735	-3.304438353
H	-1.167371988	-1.530645728	-3.380687475
H	-2.542453051	-1.174717069	-5.003632545
C	-2.917109489	2.638813257	0.578171909
H	-2.995935678	1.698511124	1.138519406
C	-3.907940388	3.650673866	1.179386020
C	-1.472837329	3.142684221	0.714119136
H	-0.744484663	2.408836603	0.364867806
H	-1.313863993	4.079378605	0.170743838
H	-1.269992709	3.340524435	1.772165179
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H	-3.683772802	3.781339407	2.243196249
H	-4.950552464	3.337917089	1.104819536
C	-4.281690598	3.523326397	-2.029342890
H	-5.053355217	3.861837149	-1.329162717
C	-4.963327408	2.995552540	-3.302795172
C	-3.325728893	4.687324047	-2.332121372
H	-2.843107462	5.080267429	-1.432314396
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H	-3.883073092	5.508786201	-2.795840740
H	-4.227098942	2.578197002	-3.997951269
H	-5.484056473	3.813338280	-3.812227249
H	-5.696679592	2.214481592	-3.076461792
C	-7.379310608	-0.608664095	-2.851657629
H	-6.698654652	-0.119398184	-3.563164711
C	-8.183294296	0.472602755	-2.120985985
C	-8.293653488	-1.555683374	-3.643774271
H	-7.740135193	-2.361027956	-4.133178711
H	-9.063673019	-1.991841435	-3.003676891
H	-8.802816391	-0.982273936	-4.426617146
H	-8.783768654	0.078468457	-1.301732183
H	-8.857365608	0.961406946	-2.832646370
H	-7.539108753	1.249845624	-1.699981809
C	-6.692175388	-2.751627684	-0.538530290
H	-6.175658226	-3.649689436	-0.898916543
C	-8.204134941	-3.020987034	-0.525983870
C	-6.157335281	-2.424345255	0.868415833
H	-5.087872505	-2.185739040	0.852214813
H	-6.705613136	-1.587337971	1.307412028
H	-6.297789097	-3.292383671	1.521313429
H	-8.773719788	-2.123106480	-0.278457731
H	-8.416872978	-3.767274618	0.247762829
H	-8.555357933	-3.425934315	-1.478079200
C	-5.021492958	-5.105648994	-5.525949955
H	-5.050496101	-4.954400063	-6.610218525
H	-4.269210339	-5.878322124	-5.327410221
H	-5.991787434	-5.503963470	-5.215083122
C	1.572255731	2.243386269	-3.063868284
H	2.415585518	1.629731059	-2.729159117
H	1.739720345	2.470461369	-4.123604298
H	1.605919600	3.188544750	-2.514039516
O	-8.640811920	-0.211435080	1.121746898
N	-9.191827774	0.855415761	1.438312292
O	-9.700233459	1.559861183	0.459627181
O	-9.275719643	1.274783134	2.597885370
C	-5.685392380	0.794669628	0.192549780
O	-6.184965134	1.182978034	1.145187974
C	-11.518065453	5.846300125	0.788974941
Ni	-10.846029282	3.084360123	0.857209742
P	-12.622529984	1.857758641	0.309699565

C	-13.931069374	3.047230482	0.660882115
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C	-10.158526421	6.077189922	1.135751843
P	-9.248272896	4.554914474	1.501566887
C	-15.307015419	2.772619724	0.705037773
C	-14.360966682	5.251423359	1.539339423
C	-12.230326653	6.945772171	0.249854729
C	-9.615508080	7.371303082	1.083991647
C	-16.229972839	3.719980955	1.143056631
C	-15.716129303	4.953468800	1.582806826
C	-11.657347679	8.207587242	0.175924242
C	-10.348847389	8.462447166	0.622603297
H	-15.665144920	1.796222687	0.393598795
H	-16.401058197	5.697486877	1.983811259
H	-12.240570068	9.022706985	-0.247168168
H	-8.595409393	7.533093929	1.415573716
H	-14.016041756	6.206468582	1.918118358
H	-13.236636162	6.798531055	-0.124310464
C	-12.759463310	0.385760099	1.447267652
H	-11.844858170	-0.177712083	1.214125872
C	-13.973101616	-0.523435950	1.209115267
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H	-11.768708229	1.442515612	3.086821795
H	-13.545308113	1.512896895	3.142396688
H	-12.697917938	0.019964514	3.586471319
H	-14.907533646	-0.003664385	1.440756679
H	-13.912339211	-1.395184040	1.870750189
H	-14.024884224	-0.893458664	0.180931598
C	-12.693096161	1.226096749	-1.452052474
H	-12.260028839	0.218122050	-1.394214749
C	-11.783135414	2.108928680	-2.323181152
C	-14.112198830	1.139130950	-2.033019781
H	-14.758657455	0.463270783	-1.466892123
H	-14.587970734	2.124251604	-2.048124313
H	-14.066644669	0.769862175	-3.063831091
H	-12.148481369	3.141790152	-2.348107815
H	-11.759538651	1.734818101	-3.353369713
H	-10.762693405	2.121897697	-1.932016611
C	-7.766080379	4.463792324	0.354937732
H	-7.268463612	3.539960623	0.675699651
C	-6.778945923	5.634917259	0.436178327
C	-8.265798569	4.262050152	-1.085394382
H	-8.891850471	3.370227098	-1.164261580
H	-8.850825310	5.125273705	-1.420578599
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H	-7.240897655	6.557021141	0.076018438
H	-5.912636280	5.440219402	-0.205873668
H	-6.408551693	5.808137417	1.449773431
C	-8.634918213	4.562671661	3.282028198
H	-9.469157219	4.079067707	3.804716349
C	-8.434805870	5.964822769	3.877142429
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H	-7.518813133	2.681857109	3.068828344
H	-6.504292965	4.143492699	3.012483358
H	-7.177601814	3.586858273	4.544721603
H	-7.600338459	6.492377281	3.402160168
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H	-9.327323914	6.587000847	3.777886629
C	-9.768362999	9.855664253	0.585972071
H	-9.949561119	10.339941978	-0.380402595
H	-10.217067719	10.496937752	1.354688525
H	-8.687397957	9.845459938	0.756873727
C	-17.713478088	3.442050457	1.161767364
H	-18.163417816	3.732911587	2.117588997
H	-18.234191895	4.005098343	0.377235413
H	-17.925914764	2.380793095	1.001273036

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C	-2.456188679	-0.737830222	0.737407148
C	-2.065286160	-1.438000917	-0.437877595
N	-2.596733093	-1.034384012	-1.662882328
C	-2.823155403	-1.379801989	-4.051833153
P	-4.529751301	-0.873830259	-3.706411839
C	-1.877279520	-1.030557275	1.980939984
C	-1.194897056	-2.538521528	-0.253283292
C	-0.634699047	-1.645049810	-3.073927164
C	-2.304325104	-1.777148128	-5.292756557
C	-0.953731239	-2.063893318	2.135207653
C	-0.659044862	-2.828156948	0.993809879
C	-0.137166634	-2.000439644	-4.320923328
C	-0.959436357	-2.111427546	-5.453449249
H	-2.170045137	-0.458497763	2.855508566
H	0.005485241	-3.684425831	1.089365363
H	0.928387702	-2.196575642	-4.420238018
H	-2.956239223	-1.824319601	-6.158108234
H	-0.949607074	-3.175583839	-1.094595075
H	0.047833435	-1.557560682	-2.236967087
C	-5.249137402	0.137828499	1.576589465
H	-5.845602036	-0.546016693	0.960469306
C	-6.079583645	1.413677812	1.793534756
C	-4.944106579	-0.552129090	2.912660837
H	-4.403304577	-1.490978837	2.778221369
H	-4.357717037	0.090383895	3.578291178
H	-5.887860775	-0.776695669	3.422830343

H	-5.558895111	2.115335941	2.451822042
H	-7.026201248	1.149996161	2.277265072
H	-6.326869011	1.925431132	0.861001670
C	-3.116885424	2.184211731	0.726659834
H	-3.986601353	2.830635786	0.567496240
C	-2.083024025	2.480864286	-0.373179942
C	-2.542716980	2.423419237	2.129800320
H	-3.267685652	2.212962866	2.922059536
H	-1.661236405	1.797500134	2.299181223
H	-2.230111361	3.468980551	2.233538151
H	-1.228819370	1.798892736	-0.302931279
H	-1.706797123	3.505240440	-0.269869030
H	-2.521916866	2.368639708	-1.369265079
C	-5.166014671	0.370057940	-4.962586880
H	-4.734894276	1.299778819	-4.570108891
C	-6.699411392	0.498139262	-4.894310474
C	-4.700056553	0.195996210	-6.415100574
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H	-5.031836033	-0.757178724	-6.839081764
H	-5.132390499	0.995586693	-7.027626991
H	-7.186306000	-0.365404129	-5.357656479
H	-7.009472370	1.389128089	-5.450502872
H	-7.080693245	0.594091535	-3.876102448
C	-5.522599220	-2.461952686	-3.669610739
H	-4.857126713	-3.080147028	-3.051584959
C	-5.678025246	-3.134715557	-5.040630341
C	-6.859079838	-2.321879625	-2.922955275
H	-6.740975857	-1.795960903	-1.971960545
H	-7.601156235	-1.778510809	-3.513451099
H	-7.266057968	-3.318782330	-2.719595909
H	-6.310227871	-2.542795420	-5.710266590
H	-6.156165123	-4.113366127	-4.918518066
H	-4.712353230	-3.296670914	-5.527438641
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H	0.544880748	-2.071412325	-7.010024071
H	-0.209516108	-3.647834778	-6.780193329
H	-1.097939134	-2.359753132	-7.601134777
C	-0.315972865	-2.373669863	3.467901945
H	-0.343893290	-3.447542191	3.684133768
H	0.738313675	-2.070603609	3.485766172
H	-0.821870148	-1.854443312	4.287603378
O	-5.404164791	2.164193630	-2.061999083
N	-6.617777824	3.311129093	-2.063945293
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O	-6.759590149	3.836520672	-0.948076069
C	-5.843607426	0.948965788	-1.639812350
O	-6.986936569	0.706419766	-1.322521687
C	-8.926357269	7.846961021	0.084507138
Ni	-8.127975464	5.200983524	-0.536737204
P	-9.929855347	4.050889015	-1.266865849
C	-11.157831192	4.916237354	-0.266890287
C	-10.664651871	6.117662430	0.300413102
N	-9.360792160	6.520326614	-0.019393910
C	-7.544540405	8.099328041	0.281704992
P	-6.568126202	6.587913036	0.294151187
C	-12.448241234	4.454397678	0.019065218
C	-11.505630493	6.789423466	1.212561727
C	-9.767364502	8.972533226	-0.060980003
C	-7.051966190	9.406606674	0.399031252
C	-13.291362762	5.143670082	0.890939116
C	-12.780745506	6.309132576	1.486186028
C	-9.255721092	10.259846687	0.047063205
C	-7.894743443	10.512351036	0.296443492
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H	-13.397471428	6.848399639	2.201824427
H	-9.932891846	11.101526260	-0.079132564
H	-5.991995811	9.565738678	0.574422300
H	-11.147450447	7.675330639	1.724300861
H	-10.819276810	8.831466675	-0.281580716
C	-9.825282097	2.251277685	-0.793616951
H	-8.903588295	1.920024991	-1.282399058
C	-10.963803291	1.338741541	-1.269672394
C	-9.604068756	2.162827492	0.725049913
H	-8.768551826	2.796224594	1.044442654
H	-10.496654510	2.475229025	1.276267648
H	-9.367423058	1.130567908	1.002547979
H	-11.924047470	1.604293346	-0.817936480
H	-10.738011360	0.306685209	-0.977745831
H	-11.075123787	1.352572680	-2.357467651
C	-10.373269081	4.219302177	-3.073975801
H	-9.814230919	3.414876699	-3.568822145
C	-9.848628998	5.578075409	-3.572087288
C	-11.875937462	4.067416191	-3.357816458
H	-12.274871826	3.103255987	-3.033499956
H	-12.447271347	4.854449272	-2.856369019
H	-12.054142952	4.156923294	-4.435258389
H	-10.325701714	6.402543068	-3.030951977
H	-10.068931580	5.699822426	-4.638149738
H	-8.767508507	5.665815353	-3.430834293
C	-5.117832661	6.681030273	-0.879211485
H	-4.724348545	5.655792236	-0.850817084
C	-3.986309767	7.651316643	-0.510319412
C	-5.658623219	6.957165718	-2.293334723
H	-6.422764301	6.229753494	-2.588827610
H	-6.107847691	7.953806877	-2.352310658
H	-4.843297005	6.907823086	-3.022775173
H	-4.329020500	8.689695358	-0.523702860
H	-3.179237366	7.565104008	-1.247023106
H	-3.558222294	7.440497398	0.472388297
C	-5.986533642	6.222009182	2.031115055

H	-6.923828125	5.918526649	2.516423464
C	-5.419239998	7.423704147	2.799367428
C	-5.035449982	5.017783642	2.015209913
H	-5.468027592	4.178672791	1.465314031
H	-4.073714733	5.268878460	1.554801702
H	-4.831325531	4.681910515	3.037363291
H	-4.471415043	7.770577431	2.378577709
H	-5.231706142	7.133343220	3.839138031
H	-6.118644238	8.263422012	2.805872917
C	-7.376849651	11.923118591	0.438876778
H	-7.728733063	12.562395096	-0.378315628
H	-7.719555855	12.379900932	1.375249028
H	-6.283159733	11.951782227	0.438745320
C	-14.690283775	4.662263870	1.190314889
H	-14.903087616	4.694856644	2.264374495
H	-15.440987587	5.289337635	0.693950415
H	-14.842584610	3.633865833	0.849545956

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A3

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C	-1.472430348	-0.736669064	-2.896391630
Ni	-2.948270321	0.909168482	-1.137508631
P	-3.177302361	-0.166782677	0.850248754
C	-3.206926823	-1.842409968	0.186092332
C	-2.780812740	-1.892772198	-1.165250421
N	-2.306042910	-0.720445156	-1.768581152
C	-1.526857972	0.341555804	-3.811202049
P	-2.643100500	1.645322919	-3.256468773
C	-3.600209236	-3.006514311	0.862889647
C	-2.892862558	-3.133105040	-1.828883410
C	-0.538156211	-1.760909677	-3.158791304
C	-0.777835846	0.317720234	-4.997754574
C	-3.647095680	-4.242814541	0.219095975
C	-3.309566498	-4.267342091	-1.144412041
C	0.215848088	-1.747981906	-4.324762821
C	0.096419036	-0.729298770	-5.285612583
H	-3.889984608	-2.949839115	1.906612158
H	-3.384163380	-5.205475807	-1.689477801
H	0.924907446	-2.554647684	-4.495676517
H	-0.868582726	1.130698323	-5.709951401
H	-2.653207541	-3.203451395	-2.883323431
H	-0.408578932	-2.565629721	-2.444294214
C	-4.790600300	0.301830411	1.695824623
H	-5.409063339	0.630009294	0.848183155
C	-4.566297054	1.500802040	2.636859655
C	-5.553904057	-0.823879123	2.408637285
H	-5.803800583	-1.639953613	1.728273630
H	-4.984775543	-1.232475042	3.248972416
H	-6.490510941	-0.422438741	2.810926437
H	-4.057081223	1.188488245	3.553294182
H	-5.530761242	1.929609179	2.926330090
H	-3.962682247	2.297024965	2.188464642
C	-1.763524771	-0.026951753	2.058752060
H	-1.811870098	1.002655387	2.434357405
C	-0.453080982	-0.206723332	1.272360563
C	-1.859408617	-1.006278157	3.238552332
H	-2.766880989	-0.862199008	3.831963301
H	-1.836691976	-2.042540550	2.888118029
H	-1.001940846	-0.862575531	3.904903173
H	-0.390483350	-1.211773038	0.842736304
H	0.403044522	-0.069242038	1.940283060
H	-0.371294230	0.512166560	0.450945646
C	-1.810394049	3.331033468	-3.324870586
H	-1.188271523	3.302237749	-2.420136929
C	-2.823652983	4.479830265	-3.171700001
C	-0.886762917	3.581910610	-4.527667046
H	-0.064759023	2.865596533	-4.566404819
H	-1.431456685	3.544934988	-5.475872993
H	-0.450724840	4.583017349	-4.437529087
H	-3.443183422	4.592328072	-4.065407753
H	-2.282959700	5.421017170	-3.029327154
H	-3.487052679	4.353177071	-2.313538551
C	-4.179036140	1.548064828	-4.318917751
H	-4.309875011	0.459249347	-4.374950409
C	-4.007286549	2.089704752	-5.745607853
C	-5.408185482	2.128769159	-3.599893808
H	-5.537011623	1.670553684	-2.611809254
H	-5.344192982	3.213914871	-3.479105473
H	-6.313271046	1.917407274	-4.178431511
H	-3.867071629	3.174423933	-5.756132603
H	-4.904823780	1.868686080	-6.333596230
H	-3.157674789	1.625854850	-6.254435062
C	0.915856779	-0.757160485	-6.553126335
H	1.984902620	-0.643547654	-6.337388992
H	0.794219375	-1.707490325	-7.084236622
H	0.628142416	0.046747323	-7.236673832
C	-4.055984020	-5.502737522	0.942316771
H	-4.799525738	-6.067503452	0.369712859
H	-3.197046280	-6.166647911	1.097076297
H	-4.484900475	-5.283407211	1.924231052
O	-3.691906214	2.682090759	-0.429848164
C	-4.750248432	3.169149876	-0.248066470
O	-5.776968479	3.668496609	-0.060291070

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C	-1.637175560	-0.782814324	-3.017292023
Ni	-3.100283861	0.862143874	-1.274309754

P	-3.428782463	-0.196467564	0.717599094
C	-3.218803883	-1.884389400	0.119140714
C	-2.841039181	-1.973286510	-1.238590002
N	-2.581889153	-0.807634354	-1.981784105
C	-1.688100338	0.287392467	-3.951383114
P	-2.712131977	1.664710045	-3.386216879
C	-3.531490803	-3.039751768	0.857391238
C	-2.872484684	-3.253997564	-1.835497022
C	-0.646297455	-1.765890479	-3.218024969
C	-0.920413256	0.252641916	-5.118594170
C	-3.515259504	-4.304713726	0.278213382
C	-3.199591398	-4.376747131	-1.090456963
C	0.123937055	-1.766653419	-4.375740528
C	-0.020433007	-0.788290918	-5.371607780
H	-3.791451693	-2.950258493	1.906401634
H	-3.223759413	-5.343136787	-1.588669896
H	0.864204824	-2.551827431	-4.509740353
H	-1.007501483	1.055893183	-5.843136311
H	-2.666436434	-3.356553078	-2.894340515
H	-0.497938335	-2.543269634	-2.477798462
C	-5.163506031	-0.042459995	1.413477659
H	-5.751533031	-0.611605763	0.681576073
C	-5.625728130	1.423999071	1.374736547
C	-5.379600525	-0.641756892	2.811136484
H	-5.140181065	-1.705755830	2.856502295
H	-4.785481930	-0.117031038	3.566464186
H	-6.433304787	-0.532128572	3.090271473
H	-5.077610970	2.031365156	2.105428219
H	-6.685863495	1.486920714	1.640451193
H	-5.500601768	1.871124387	0.383824944
C	-2.152675867	0.187517360	2.032423973
H	-2.569302082	1.027542710	2.601786137
C	-0.861127794	0.644564331	1.328590989
C	-1.870160460	-0.980956078	2.990434408
H	-2.759162903	-1.304310322	3.536199808
H	-1.471179485	-1.842340589	2.446990252
H	-1.122285008	-0.670847833	3.728030682
H	-0.449760824	-0.160409138	0.709475696
H	-0.103484899	0.921993911	2.068238020
H	-1.028223276	1.508709908	0.674897492
C	-1.707419395	3.249193430	-3.398570299
H	-0.996109843	3.056011200	-2.582366943
C	-2.641183853	4.392914295	-2.956878662
C	-0.902778089	3.588392258	-4.660353184
H	-0.134354204	2.840630054	-4.869475842
H	-1.540985584	3.693449259	-5.542243958
H	-0.395151019	4.547864437	-4.504652977
H	-3.285846710	4.725019932	-3.776726007
H	-2.061301708	5.253655434	-2.607816696
H	-3.267237425	4.026109219	-2.143000126
C	-4.248003483	1.754526734	-4.450239182
H	-4.459183693	0.686039507	-4.592754364
C	-4.060019493	2.405408621	-5.827793121
C	-5.421665668	2.367759943	-3.664877653
H	-5.553592205	1.874255657	-2.694081068
H	-5.282196045	3.437974453	-3.486301899
H	-6.351486683	2.244165421	-4.230796337
H	-3.864149332	3.478466988	-5.742367744
H	-4.975623131	2.285540104	-6.417706966
H	-3.241974354	1.946817756	-6.391214371
C	0.781334996	-0.849067569	-6.647617340
H	1.830401778	-1.092283130	-6.448931694
H	0.391970307	-1.624457479	-7.318679333
H	0.751585245	0.100700974	-7.189068794
C	-3.834408283	-5.551039696	1.066900730
H	-4.569019318	-6.173278809	0.544177830
H	-2.938827991	-6.166148186	1.214701653
H	-4.239224911	-5.311804771	2.054295540
O	-3.469576836	3.424227238	0.047358233
C	-3.017452002	3.491966724	1.128771067
O	-2.576335192	3.549623489	2.204653502

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C	-1.952901483	-0.280823261	-2.830605268
Ni	-2.533460855	1.502878785	-0.659215569
P	-2.847750902	0.327140421	1.204453468
C	-3.288562298	-1.272805214	0.474452853
C	-3.130551577	-1.297515273	-0.940297067
N	-2.560320377	-0.194471523	-1.575908303
C	-1.786015868	0.909188151	-3.596105576
P	-2.311724663	2.394714832	-2.695868254
C	-3.788442373	-2.388289213	1.161986828
C	-3.638715506	-2.436584949	-1.611442566
C	-1.425754547	-1.469048858	-3.390467405
C	-1.260952711	0.860830605	-4.893711567
C	-4.215659142	-3.536741495	0.495654583
C	-4.156730652	-3.514273643	-0.907734990
C	-0.879971147	-1.482176900	-4.667185307
C	-0.809508741	-0.329890311	-5.465222836
H	-3.864072084	-2.355486631	2.244258881
H	-4.539341927	-4.366430759	-1.466669798
H	-0.488448322	-2.420243263	-5.056566238
H	-1.185659051	1.775602937	-5.473083019
H	-3.640260220	-2.461402655	-2.694722414
H	-1.436067104	-2.384538651	-2.811262846
C	-4.260454178	1.016358614	2.232543468
H	-4.889326572	1.469831347	1.455454230
C	-3.750684023	2.150264263	3.138946533

C	-5.114167690	0.006180691	3.010611534
H	-5.561546803	-0.743710697	2.354770184
H	-4.535012722	-0.511853456	3.782183170
H	-5.928204060	0.538856924	3.516241550
H	-3.105645180	1.765484571	3.936482668
H	-4.605487347	2.640168905	3.618391275
H	-3.204088211	2.908208370	2.575135946
C	-1.327334523	0.117211126	2.261784077
H	-1.140159249	1.122885227	2.657054424
C	-0.163406640	-0.260169864	1.329574585
C	-1.477312565	-0.876670837	3.421065092
H	-2.275994301	-0.592304587	4.112437248
H	-1.687915087	-1.883862615	3.046982050
H	-0.543512285	-0.925087154	3.993607283
H	-0.348154306	-1.223819613	0.842000842
H	0.766828656	-0.341250688	1.902845383
H	-0.024669509	0.494644016	0.549786210
C	-0.996427357	3.731693268	-2.733896971
H	-0.322640032	3.378369093	-1.941921473
C	-1.576933384	5.081828117	-2.274852276
C	-0.184063494	3.882696629	-4.027098179
H	0.350932747	2.966229916	-4.284469128
H	-0.815642715	4.166758060	-4.875387669
H	0.559655368	4.676884651	-3.891546249
H	-2.206408024	5.526954651	-3.052015543
H	-0.753470719	5.777668953	-2.081002474
H	-2.158592701	4.988566875	-1.356139421
C	-3.918215036	2.940826893	-3.487306356
H	-4.423901558	1.970369458	-3.584025383
C	-3.778334618	3.554526329	-4.887204647
C	-4.755846024	3.812305450	-2.536069155
H	-4.800952911	3.374167442	-1.534388185
H	-4.344686508	4.819841862	-2.436879873
H	-5.777100563	3.905031443	-2.923612833
H	-3.257858515	4.516498566	-4.854085922
H	-4.771410465	3.733186245	-5.316856384
H	-3.236513853	2.892220736	-5.568803787
O	-2.506730795	3.194479704	0.240828320
N	-1.313165665	3.517078161	0.746243179
O	-1.302574635	4.613914490	1.264030933
C	-0.215338856	-0.371612579	-6.852615356
H	0.878833175	-0.456586689	-6.821041584
H	-0.586465240	-1.230416059	-7.423147202
H	-0.456371576	0.533399403	-7.419049740
C	-4.740684986	-4.743428230	1.235467434
H	-5.688081741	-5.094520569	0.809566796
H	-4.037257195	-5.584517002	1.185784817
H	-4.913366318	-4.522507191	2.293352365

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C	-1.878353834	-0.218951836	-2.773193121
Ni	-2.378351688	1.535025358	-0.587962985
P	-2.886263609	0.348905802	1.233900189
C	-3.486988783	-1.160922527	0.425002038
C	-3.240685940	-1.167939067	-0.974810123
N	-2.522017717	-0.116148748	-1.535832405
C	-1.682936311	0.966132462	-3.533318043
P	-2.298654795	2.423018456	-2.635354280
C	-4.151163578	-2.233190775	1.039275408
C	-3.805481195	-2.232081175	-1.719065666
C	-1.364309549	-1.420313954	-3.308906555
C	-1.121090651	0.908238649	-4.813421726
C	-4.646936893	-3.311562777	0.306262434
C	-4.480094910	-3.266450167	-1.087623239
C	-0.775383592	-1.445729017	-4.567893982
C	-0.662291288	-0.293682009	-5.360547066
H	-4.304311275	-2.220232725	2.113533020
H	-4.903057575	-4.062855721	-1.697261453
H	-0.387626439	-2.389810324	-4.945285320
H	-1.033202648	1.814469218	-5.402548313
H	-3.722795486	-2.232313871	-2.799631596
H	-1.420870781	-2.332832098	-2.726507187
C	-4.258317947	1.177581787	2.213648081
H	-4.729303360	1.792448521	1.437260866
C	-3.660247326	2.134689569	3.257701159
C	-5.324173450	0.257632226	2.823256731
H	-5.806820393	-0.368295282	2.069387674
H	-4.908420086	-0.395784765	3.597842693
H	-6.099176884	0.872075498	3.296358109
H	-3.158448696	1.588668466	4.064136982
H	-4.466432095	2.722156286	3.711125374
H	-2.957441092	2.833371401	2.799802542
C	-1.477983594	-0.121820696	2.360783577
H	-1.185550094	0.825334787	2.830014467
C	-0.319130480	-0.606663644	1.472506642
C	-1.832517505	-1.147271752	3.446027517
H	-2.645849705	-0.806015730	4.093523026
H	-2.127457619	-2.101411581	2.997972250
H	-0.958510280	-1.336368322	4.080243587
H	-0.595492005	-1.522016764	0.937157154
H	0.561313689	-0.825475216	2.086917400
H	-0.048109610	0.150264487	0.730380774
C	-1.225626945	3.942522287	-2.848502398
H	-0.420154423	3.742331266	-2.131963968
C	-1.977552652	5.191712379	-2.350750923
C	-0.605172873	4.178126335	-4.233408928
H	0.085829534	3.380174875	-4.512794018
H	-1.364954352	4.274116516	-5.015812874

H	-0.036223579	5.114979744	-4.212055683
H	-2.759060383	5.489827633	-3.057519674
H	-1.268615961	6.022490978	-2.272127151
H	-2.422222853	5.042217731	-1.364017725
C	-4.037457466	2.658290625	-3.292512655
H	-4.373621941	1.612485766	-3.290643215
C	-4.107259750	3.189822912	-4.730261326
C	-4.938202858	3.435680866	-2.318712473
H	-4.829313755	3.061936855	-1.296227574
H	-4.702799797	4.502435207	-2.305347443
H	-5.985898018	3.327301264	-2.622914314
H	-3.783803225	4.233932495	-4.787733078
H	-5.140429497	3.145455599	-5.095236778
H	-3.487711430	2.597237587	-5.411041260
O	-2.708259821	3.554332018	0.459425539
N	-1.446421981	3.270945311	0.394845247
O	-0.645955861	4.188024521	0.499006689
C	-0.024036113	-0.346114010	-6.728469372
H	1.067137003	-0.443884850	-6.659902096
H	-0.387305796	-1.201663852	-7.308805943
H	-0.235320210	0.560743868	-7.303731441
C	-5.343727112	-4.475738525	0.969407320
H	-6.250586033	-4.763027668	0.424785614
H	-4.698346138	-5.362974167	1.005951166
H	-5.633358479	-4.238761902	1.997857332

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C	-1.529565573	-0.813653290	-2.987745523
Ni	-3.065992355	0.800827742	-1.230128884
P	-3.360690594	-0.157870561	0.812920928
C	-3.188751936	-1.858527422	0.192191854
C	-2.737954855	-1.938072681	-1.160044193
N	-2.204564571	-0.784795463	-1.749467492
C	-1.690664053	0.249914110	-3.905591965
P	-2.761968613	1.571307063	-3.304910660
C	-3.557996511	-3.017895937	0.878949702
C	-2.847829580	-3.186475992	-1.808200002
C	-0.592889369	-1.817098141	-3.314579010
C	-1.015605688	0.246358871	-5.137180805
C	-3.561817408	-4.274360657	0.259038568
C	-3.233797789	-4.321614742	-1.104519129
C	0.081951208	-1.784981489	-4.527300835
C	-0.128887609	-0.771778286	-5.479106426
H	-3.865227222	-2.949660778	1.917073607
H	-3.288711071	-5.271178722	-1.630857944
H	0.800519228	-2.571872473	-4.743791103
H	-1.182433844	1.055409431	-5.841680050
H	-2.612039566	-3.268196344	-2.862357855
H	-0.384298831	-2.608650684	-2.604129076
C	-5.087964535	0.148278385	1.479899049
H	-5.682778358	0.177633315	0.556962788
C	-5.117285728	1.551369905	2.114962101
C	-5.702992916	-0.907506287	2.408928394
H	-5.808646202	-1.874052405	1.912824154
H	-5.119537354	-1.044818163	3.323420286
H	-6.704961300	-0.578701019	2.706623793
H	-4.573438168	1.571201682	3.065124035
H	-6.152058601	1.840575576	2.323912859
H	-4.684154034	2.315958500	1.458968639
C	-2.067601204	0.163656577	2.117070198
H	-2.259348631	1.195444584	2.438931465
C	-0.690670967	0.110682972	1.430608749
C	-2.132296801	-0.769436598	3.334557295
H	-3.071147919	-0.671683311	3.885312080
H	-2.010071039	-1.815286279	3.036057234
H	-1.317972660	-0.526249170	4.025752068
H	-0.477367818	-0.896112084	1.057097912
H	0.092195183	0.380147129	2.146641970
H	-0.632623613	0.799179375	0.581232846
C	-1.809352756	3.180181980	-3.228371382
H	-1.060294032	2.935333967	-2.462193727
C	-2.714533091	4.292792797	-2.671113968
C	-1.061356306	3.618919134	-4.495771408
H	-0.332262337	2.871129274	-4.814077377
H	-1.740688801	3.822549582	-5.327034950
H	-0.513081431	4.543419838	-4.282682896
H	-3.452254534	4.617915630	-3.410592318
H	-2.108268261	5.164539337	-2.406328440
H	-3.253908157	3.977058649	-1.769485235
C	-4.309479713	1.658476233	-4.350259304
H	-4.489833355	0.593945444	-4.549776077
C	-4.153513908	2.389981985	-5.691365242
C	-5.492378712	2.199022532	-3.526717186
H	-5.614503384	1.643338203	-2.589561462
H	-5.368509293	3.257857323	-3.281528234
H	-6.420213699	2.098610878	-4.099423409
H	-4.001087189	3.463526964	-5.546230316
H	-5.067725182	2.265998840	-6.281774521
H	-3.322302341	1.998140574	-6.283902645
C	0.605081320	-0.782249629	-6.797597408
H	1.686330318	-0.684295714	-6.647664547
H	0.438082576	-1.720879793	-7.337307930
H	0.283018470	0.038140811	-7.444988728
C	-3.920098066	-5.525800228	1.019487262
H	-4.574501991	-6.176701546	0.430658579
H	-3.021615267	-6.106269836	1.262488842
H	-4.428017139	-5.295693874	1.960215569

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C	-1.518459797	-0.530261815	-2.746882915
Ni	-2.194300175	1.282822371	-0.627143502
P	-2.457776546	0.150585413	1.283339858
C	-2.800792217	-1.490153670	0.596349955
C	-2.626587868	-1.551238894	-0.813798726
N	-2.102771759	-0.439824015	-1.479827404
C	-1.404354930	0.644078016	-3.541829824
P	-1.909514070	2.148699999	-2.669245958
C	-3.265357971	-2.601609707	1.313385606
C	-3.096967220	-2.723299742	-1.455193400
C	-0.963546693	-1.714455366	-3.291664600
C	-0.916495264	0.579132020	-4.854337692
C	-3.648275614	-3.782709122	0.678563535
C	-3.584757090	-3.797536135	-0.723738134
C	-0.462908447	-1.746626854	-4.585929871
C	-0.460180730	-0.612876296	-5.415420055
H	-3.351189137	-2.538812876	2.393384218
H	-3.940510273	-4.674829960	-1.260731578
H	-0.052723147	-2.681144953	-4.963695049
H	-0.871862292	1.485756636	-5.450078011
H	-3.100095510	-2.776623011	-2.536965132
H	-0.916244626	-2.611048937	-2.685800552
C	-3.927653551	0.778523386	2.270662308
H	-4.585752010	1.137316465	1.468843341
C	-3.517096281	1.981666923	3.137739420
C	-4.709139824	-0.259605676	3.088748455
H	-5.105529785	-1.060020089	2.460895538
H	-4.098094940	-0.708028078	3.878843307
H	-5.558160782	0.235408813	3.574775696
H	-2.822142601	1.685868621	3.931081772
H	-4.408385277	2.394009352	3.623957396
H	-3.063176394	2.783347130	2.554030657
C	-0.936805606	0.049588900	2.358295202
H	-0.767069221	1.085338950	2.673741341
C	0.238232836	-0.372686684	1.459910274
C	-1.072335124	-0.858913004	3.587485790
H	-1.872600675	-0.536815703	4.259804249
H	-1.265910149	-1.895119429	3.291150331
H	-0.136239007	-0.849710882	4.158186913
H	0.083454944	-1.381003380	1.060130715
H	1.167200565	-0.375264674	2.040703297
H	0.356438160	0.320610970	0.623852849
C	-0.498451144	3.387612343	-2.631729126
H	0.106021948	2.984655857	-1.810079813
C	-0.989530802	4.782329082	-2.200292110
C	0.371668786	3.468800306	-3.892593622
H	0.824194431	2.506066084	-4.139523506
H	-0.198865354	3.816400528	-4.760459900
H	1.182341695	4.187137127	-3.722706079
H	-1.514182687	5.290376186	-3.015625715
H	-0.125102639	5.398975372	-1.932191968
H	-1.654684186	4.746684074	-1.336309671
C	-3.424942493	2.826357603	-3.532533646
H	-3.972750902	1.897972822	-3.733290434
C	-3.169721842	3.535913467	-4.869370937
C	-4.273493767	3.671276331	-2.565752745
H	-4.422771454	3.152791739	-1.614094615
H	-3.805238008	4.633579254	-2.343833923
H	-5.254096508	3.871564150	-3.012949228
H	-2.594245434	4.456631184	-4.737435818
H	-4.127076149	3.810005426	-5.328981400
H	-2.636352777	2.894856691	-5.576905251
C	0.048543856	-0.684266686	-6.835378170
H	1.072709560	-1.074441433	-6.877739429
H	-0.572799802	-1.346332431	-7.451231003
H	0.049746897	0.301892549	-7.310094357
C	-4.133937359	-4.983440399	1.454412699
H	-5.046233654	-5.402790546	1.014546990
H	-3.385131121	-5.785715103	1.465869784
H	-4.354267120	-4.725779057	2.495104074
O	-2.398702145	3.023769379	0.225640863
N	-1.311452866	3.461403370	0.834365129
O	-1.415501237	4.493466854	1.489474535
O	-0.261507601	2.803834438	0.708725452
C	-5.063481331	0.146491349	-2.058737040
O	-5.520694256	0.165251076	-1.001809359

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C	-1.443426251	-0.694615424	-2.600304842
Ni	-2.260331631	1.219379663	-0.631062806
P	-2.296996832	0.012678546	1.254950881
C	-2.959484816	-1.543964624	0.586219013
C	-2.852801085	-1.599326015	-0.828020811
N	-2.281513214	-0.523791373	-1.505795121
C	-1.097503066	0.451201499	-3.370045662
P	-1.845106244	1.967594862	-2.713094234
C	-3.476705074	-2.630746603	1.305291533
C	-3.381595373	-2.740394115	-1.472890615
C	-0.855827034	-1.922687054	-2.991933823
C	-0.291351706	0.339231223	-4.509687424
C	-3.962160587	-3.771239758	0.664164841
C	-3.919893026	-3.789030075	-0.739704132
C	-0.034928430	-1.998749971	-4.109117508
C	0.255141377	-0.881175458	-4.908520222
H	-3.504332542	-2.592733860	2.388298273

H	-4.328532219	-4.646338463	-1.271230459
H	0.403860867	-2.960988283	-4.367028713
H	-0.083953425	1.222186208	-5.105103970
H	-3.376233578	-2.784510851	-2.556807756
H	-1.031931162	-2.814977407	-2.402596474
C	-3.307828188	0.719551623	2.691379786
H	-3.847795963	1.534076810	2.202279806
C	-2.428877592	1.361461759	3.780026913
C	-4.340498447	-0.232178599	3.310804605
H	-4.991062164	-0.689343452	2.561605215
H	-3.861211300	-1.030501962	3.887688637
H	-4.971870422	0.335805357	4.003496170
H	-1.860066533	0.611283839	4.337739468
H	-3.084055901	1.873706222	4.493319035
H	-1.734990478	2.109408855	3.393757105
C	-0.564052045	-0.344336241	1.851014495
H	-0.248474360	0.581846833	2.343522310
C	0.348713517	-0.579713583	0.636489928
C	-0.512667418	-1.518586516	2.839172602
H	-1.160620570	-1.369126916	3.708374262
H	-0.815696239	-2.449269056	2.348721981
H	0.511425078	-1.649434328	3.206511497
H	0.016262937	-1.440347552	0.046813149
H	1.371327400	-0.776283145	0.978305101
H	0.362383395	0.296822608	-0.015319937
C	-0.648078978	3.397006273	-2.669705629
H	0.095619142	3.004026651	-1.966032743
C	-1.306701779	4.620136261	-1.999101639
C	0.047794655	3.791504145	-3.979563713
H	0.661953330	2.984191179	-4.382936954
H	-0.670304477	4.100821018	-4.745893478
H	0.709965289	4.644776344	-3.790368557
H	-1.907782674	5.188845634	-2.713896036
H	-0.523568451	5.286818504	-1.623189211
H	-1.939617395	4.340874672	-1.154248357
C	-3.346006155	2.277010202	-3.799246788
H	-3.967842579	1.420490384	-3.502994537
C	-3.078206062	2.174633503	-5.308772087
C	-4.107244015	3.567775726	-3.460634232
H	-4.227731705	3.720431805	-2.385380268
H	-3.597239971	4.444437981	-3.869938612
H	-5.106171608	3.530515909	-3.909089565
H	-2.445332050	2.995567799	-5.661448479
H	-4.028401375	2.236613750	-5.852154732
H	-2.598374128	1.230941772	-5.576561928
C	1.138761878	-1.000275254	-6.127648830
H	2.152869225	-1.323405862	-5.860960484
H	0.745666802	-1.736006737	-6.839883327
H	1.225574255	-0.044522431	-6.653958321
C	-4.517832279	-4.942366600	1.439521313
H	-5.494970322	-5.252151966	1.050739288
H	-3.856536388	-5.815846920	1.376893640
H	-4.643460274	-4.699678421	2.499138594
O	-0.982725024	2.501501322	0.232731983
N	-1.356230140	3.283191919	1.216389656
O	-2.555929184	3.595907211	1.320833325
O	-0.480330974	3.656160355	2.000312328
C	-4.130905151	2.016043186	-0.365250200
O	-5.226568699	2.098580599	-0.048851408

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C	-1.480135918	-0.777062774	-2.692163706
Ni	-3.033084393	0.892580271	-0.966576457
P	-3.134202719	-0.195013061	1.000931740
C	-3.171273947	-1.895933867	0.365925014
C	-2.789987803	-1.957323432	-1.001007199
N	-2.400571108	-0.780829430	-1.645299077
C	-1.429645896	0.353984624	-3.552754164
P	-2.573855639	1.670366406	-3.042412519
C	-3.506751776	-3.061498880	1.067504287
C	-2.886213303	-3.214619637	-1.639501810
C	-0.540647089	-1.807939887	-2.934490919
C	-0.570965350	0.369399697	-4.660083294
C	-3.549614429	-4.308821201	0.442538708
C	-3.256273270	-4.348937988	-0.929736376
C	0.319076538	-1.753003955	-4.023147106
C	0.308747679	-0.680132270	-4.928978443
H	-3.744968414	-3.000851631	2.123723269
H	-3.327954531	-5.297070026	-1.459172249
H	1.028781772	-2.564635754	-4.170651913
H	-0.570906103	1.227172971	-5.324464798
H	-2.681945324	-3.288961887	-2.701772213
H	-0.482462496	-2.648696184	-2.253052711
C	-4.623977184	0.211125955	2.067429543
H	-5.375475883	0.462367266	1.309960008
C	-4.344328403	1.484182954	2.887183428
C	-5.199356556	-0.907493949	2.947759390
H	-5.537109852	-1.759148121	2.353934765
H	-4.479816437	-1.264899015	3.690893650
H	-6.066934109	-0.518563509	3.493659258
H	-3.601715565	1.302792668	3.671353817
H	-5.269029617	1.808595657	3.376059771
H	-4.000583172	2.310195684	2.262564898
C	-1.573398590	-0.032533210	2.017711639
H	-1.564556956	1.014987946	2.338780880
C	-0.368462682	-0.259118617	1.088579059
C	-1.525696039	-0.955657542	3.242931604
H	-2.326163054	-0.743248761	3.957100630

H	-1.600187659	-2.006644964	2.944056034
H	-0.571477413	-0.827235341	3.767375946
H	-0.365307361	-1.279859662	0.691617846
H	0.562269628	-0.107892171	1.646688581
H	-0.383509815	0.434955060	0.245192081
C	-1.673467755	3.313667059	-2.934021235
H	-1.141543865	3.189624786	-1.983178735
C	-2.678544283	4.467879295	-2.764137745
C	-0.634939075	3.631797791	-4.019228458
H	0.169766411	2.894255161	-4.041471004
H	-1.082200289	3.689683199	-5.016228199
H	-0.184677243	4.608508110	-3.804736614
H	-3.191709518	4.690113068	-3.705223322
H	-2.141779184	5.374144077	-2.462544203
H	-3.425581694	4.249084949	-1.999034047
C	-3.927824259	1.687368155	-4.342403889
H	-4.100230694	0.608929455	-4.459891796
C	-3.509943247	2.261577368	-5.703985691
C	-5.230823040	2.318059921	-3.827894449
H	-5.526938915	1.893811464	-2.865427494
H	-5.137028217	3.400062084	-3.700869083
H	-6.035228252	2.138025761	-4.550558090
H	-3.321515322	3.337803125	-5.643156052
H	-4.318470478	2.112221718	-6.429529667
H	-2.615471125	1.774741054	-6.101459503
C	1.222756624	-0.662472546	-6.131019592
H	2.252739906	-0.918702006	-5.856823921
H	0.903616667	-1.387489319	-6.890664577
H	1.240983605	0.323310912	-6.606249332
C	-3.903318167	-5.566036224	1.200911522
H	-4.655668736	-6.157943726	0.666820645
H	-3.027214527	-6.212151527	1.340194345
H	-4.303543568	-5.336924553	2.193372488
O	-1.330618143	2.842793226	0.481457204
N	-2.393815756	3.437370062	0.516579688
O	-3.706608057	2.588304758	-0.246756449
O	-2.657033920	4.488976955	1.040015101
C	-5.285579681	2.456032276	-0.360152155
O	-6.036001682	3.147139072	0.208420023

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C	-1.422479630	-0.627472818	-2.721018553
Ni	-2.830468178	1.059594750	-0.907219410
P	-3.077115059	-0.054449264	1.017658234
C	-3.109034061	-1.742942333	0.359581202
C	-2.715634346	-1.798037291	-1.005513906
N	-2.303042650	-0.625214458	-1.637300014
C	-1.393252015	0.507878184	-3.576776266
P	-2.515740633	1.824640989	-3.016602993
C	-3.476459265	-2.907130957	1.048986197
C	-2.831501722	-3.050862789	-1.652622581
C	-0.507326126	-1.666769981	-3.006749630
C	-0.584221184	0.519509017	-4.719984531
C	-3.531351328	-4.149307251	0.416780204
C	-3.224963188	-4.183142662	-0.953546882
C	0.309032410	-1.613467813	-4.128923416
C	0.274977535	-0.536858201	-5.027775288
H	-3.738803387	-2.844794512	2.100033045
H	-3.308037043	-5.125936031	-1.490855813
H	1.000707269	-2.434005022	-4.310164928
H	-0.610734820	1.375592947	-5.385388851
H	-2.624876976	-3.123187780	-2.714341164
H	-0.433125705	-2.514268160	-2.335324287
C	-4.667518139	0.393114299	1.909188151
H	-5.287580490	0.744010806	1.075281024
C	-4.429723263	1.586275101	2.851892710
C	-5.415080070	-0.744350851	2.617039680
H	-5.670877457	-1.555735230	1.932214618
H	-4.837120056	-1.161841154	3.448223352
H	-6.349005222	-0.350461602	3.034666777
H	-3.860179424	1.284942985	3.737648010
H	-5.395857811	1.969770789	3.196861506
H	-3.900597334	2.407081366	2.364355087
C	-1.637159705	0.073628299	2.200027704
H	-1.677338243	1.105890512	2.568723917
C	-0.341057867	-0.113164619	1.392254114
C	-1.710836887	-0.895509720	3.388356209
H	-2.611116886	-0.748736262	3.992138386
H	-1.693036795	-1.934480786	3.043978214
H	-0.843645751	-0.747804940	4.042560577
H	-0.298594773	-1.115236163	0.951885462
H	0.528230965	0.007268743	2.048155069
H	-0.266707838	0.618111014	0.583151162
C	-1.677760005	3.500805378	-3.066042900
H	-1.067291021	3.445256948	-2.158560276
C	-2.712573051	4.621109009	-2.858445883
C	-0.751182735	3.810026169	-4.250893593
H	0.090462796	3.116483450	-4.300482273
H	-1.277936339	3.789645672	-5.209924221
H	-0.339514047	4.818714142	-4.124585152
H	-3.335174561	4.765139103	-3.747291565
H	-2.188522100	5.565015316	-2.670879841
H	-3.361063957	4.425141811	-2.003268719
C	-3.973690987	1.716949463	-4.196421623
H	-4.106263638	0.627372265	-4.239247322
C	-3.683329105	2.225306273	-5.615890503
C	-5.261198044	2.322189808	-3.618144512
H	-5.467746735	1.936517358	-2.617001057

H	-5.205863953	3.411979914	-3.547952652
H	-6.107523441	2.074521303	-4.269662380
H	-3.541336060	3.310394764	-5.630558968
H	-4.533340454	1.998091340	-6.270380497
H	-2.797130823	1.753340364	-6.049005508
C	1.164845109	-0.507530630	-6.247559547
H	2.220782757	-0.388176262	-5.973282814
H	1.087012649	-1.436385512	-6.824423313
H	0.903198481	0.320309669	-6.913971424
C	-3.912912846	-5.405803680	1.162237048
H	-4.647701263	-5.996428967	0.603011787
H	-3.043072701	-6.053451538	1.331210613
H	-4.345720768	-5.176023006	2.140826702
O	-0.787840128	3.087772608	0.136323079
N	-1.825937867	3.343720436	0.715374529
O	-3.277035475	2.764835119	-0.057273328
O	-1.981727719	3.927886963	1.759830236
C	-4.841982841	3.003897667	-0.287360847
O	-5.414943695	3.940984726	0.105154060

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A7

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C	-1.321530819	-0.608845353	-2.629384041
Ni	-2.180360794	1.221544504	-0.633016765
P	-2.412015915	0.045710020	1.254454970
C	-3.080472231	-1.463385940	0.504221857
C	-2.750366449	-1.552663922	-0.875786901
N	-2.059403658	-0.494088113	-1.455109835
C	-1.155851722	0.547406912	-3.436001778
P	-1.949347496	2.020270586	-2.724272013
C	-3.756910563	-2.501991510	1.154641271
C	-3.211138964	-2.694633722	-1.570318699
C	-0.687666118	-1.794413686	-3.063458204
C	-0.491914481	0.470813155	-4.666996956
C	-4.183108330	-3.639908791	0.466864258
C	-3.907420635	-3.697525024	-0.908415616
C	-0.008256016	-1.838249087	-4.274126053
C	0.087179184	-0.718081772	-5.115581512
H	-3.958552599	-2.428360701	2.217948437
H	-4.257404804	-4.553796768	-1.481899619
H	0.470986396	-2.768106937	-4.573342800
H	-0.406186819	1.354968190	-5.289620399
H	-3.039645433	-2.777527332	-2.637448549
H	-0.722509325	-2.676584721	-2.434234142
C	-3.541270971	0.864072204	2.506885529
H	-4.239852428	1.412925482	1.864022970
C	-2.715153456	1.894219518	3.305207729
C	-4.377257824	-0.040700696	3.423717737
H	-5.070578575	-0.662684739	2.852445841
H	-3.758072615	-0.692305744	4.045945644
H	-4.971918583	0.587797821	4.097211838
H	-2.078521490	1.398450375	4.044340611
H	-3.393628120	2.561983109	3.846736670
H	-2.069305658	2.512571573	2.673044443
C	-0.813073695	-0.451007992	2.087858915
H	-0.342460573	0.487682939	2.395895720
C	0.109194085	-1.134247422	1.065278769
C	-1.044020057	-1.350066185	3.313142061
H	-1.597554445	-0.847848594	4.110584736
H	-1.579554081	-2.265909195	3.039152145
H	-0.072761104	-1.646999359	3.725004196
H	-0.333139360	-2.066905499	0.697349727
H	1.057595611	-1.376974344	1.556513190
H	0.319951773	-0.472198844	0.225617588
C	-0.827068746	3.520689487	-2.756248236
H	-0.224984154	3.319158554	-1.863678098
C	-1.608138919	4.825351238	-2.521372795
C	0.109338127	3.649824381	-3.966051817
H	0.779113710	2.792341709	-4.052869320
H	-0.438051105	3.768023252	-4.907590866
H	0.731170297	4.543026447	-3.834911346
H	-2.209738970	5.105749130	-3.392061234
H	-0.892281830	5.634806156	-2.342918158
H	-2.260436535	4.780144215	-1.647907734
C	-3.512717724	2.258571148	-3.728919983
H	-3.862655401	1.220707655	-3.807289839
C	-3.269801140	2.796418905	-5.147361279
C	-4.584363937	3.058724880	-2.972435236
H	-4.774600029	2.629429579	-1.984520435
H	-4.300232410	4.105850220	-2.839476109
H	-5.524077415	3.039919138	-3.536022902
H	-2.901025295	3.826338768	-5.130897999
H	-4.210519791	2.792764664	-5.710493565
H	-2.552392006	2.181699276	-5.697936058
C	0.827088356	-0.789937794	-6.430429935
H	1.905508041	-0.922511280	-6.277780533
H	0.482892931	-1.633912325	-7.039452076
H	0.688433111	0.122651845	-7.018492222
C	-4.908775806	-4.765629768	1.164404750
H	-5.816579819	-5.054974556	0.622146368
H	-4.281153679	-5.662603378	1.240354538
H	-5.203723431	-4.484347343	2.180056572
O	0.108352296	1.731706977	-0.303035617
N	0.223640904	2.479773283	0.733882785
O	-0.565949023	3.464107037	0.860585093
O	1.077187300	2.223514080	1.594138026
C	-2.762469053	2.783833504	0.042932183
O	-3.365595818	3.688374758	0.406477958

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C	-1.696656823	-0.267376155	-2.786059618
Ni	-2.376937151	1.651806593	-0.738441050
P	-2.186793566	0.706699193	1.276097298
C	-2.542660952	-0.999239802	0.750303090
C	-2.510304928	-1.184708834	-0.664522886
N	-2.083230019	-0.125250503	-1.459592223
C	-1.690106869	0.885064185	-3.626780272
P	-1.886371613	2.471006632	-2.757931232
C	-2.882560492	-2.059577703	1.601412892
C	-3.009077549	-2.420181274	-1.148688674
C	-1.233008981	-1.474393606	-3.368602753
C	-1.419282556	0.762421668	-4.996161461
C	-3.289663076	-3.300279617	1.112097621
C	-3.383258581	-3.435986042	-0.282905489
C	-0.943624437	-1.558787227	-4.721734524
C	-1.071825624	-0.454921424	-5.580667496
H	-2.842434883	-1.914992452	2.674776793
H	-3.768103600	-4.364033699	-0.701121449
H	-0.603686929	-2.510106564	-5.126381874
H	-1.456541538	1.645770073	-5.625406742
H	-3.134395599	-2.564136982	-2.214268446
H	-1.091647625	-2.347644806	-2.744002581
C	-3.329355001	1.322808027	2.635250568
H	-4.157551289	1.719450116	2.041480541
C	-2.671195030	2.503443241	3.374246836
C	-3.908341169	0.296298862	3.617182732
H	-4.491430283	-0.471281737	3.104722261
H	-3.135167122	-0.191733018	4.220067024
H	-4.580380440	0.815747261	4.310317516
H	-1.858898878	2.169688225	4.029101849
H	-3.423545122	2.987040281	4.006929398
H	-2.286777496	3.261213779	2.687128782
C	-0.429135263	0.723199606	1.914064169
H	-0.257730335	1.760259748	2.225102901
C	0.533155560	0.388034493	0.764201343
C	-0.218018457	-0.215271890	3.111893892
H	-0.858969271	0.040545978	3.960244656
H	-0.420417666	-1.254013896	2.831062317
H	0.822588921	-0.157788604	3.452379942
H	0.342685819	-0.615955710	0.371280044
H	1.568855762	0.426352113	1.119574547
H	0.425789803	1.092658520	-0.064882398
C	-0.131632432	3.130222559	-2.568006992
H	0.270438284	2.401615858	-1.850611567
C	-0.123210102	4.510768890	-1.891009331
C	0.759456754	3.088402033	-3.817498922
H	0.772138417	2.098156452	-4.279257774
H	0.443584800	3.815674782	-4.569643021
H	1.787458301	3.340334415	-3.530910730
H	-0.503158033	5.286368847	-2.564241648
H	0.907286882	4.781999588	-1.632903337
H	-0.722998917	4.525436401	-0.977725744
C	-2.953837872	3.615836143	-3.791408300
H	-3.709441185	2.922959805	-4.180750370
C	-2.248482943	4.306218147	-4.971266747
C	-3.666965961	4.658560276	-2.911001921
H	-4.314679623	4.185122490	-2.175095558
H	-2.955962420	5.296097279	-2.377449036
H	-4.283963680	5.303941727	-3.547125101
H	-1.525886059	5.048356056	-4.619843960
H	-2.995461941	4.838514805	-5.571066380
H	-1.725626469	3.614501715	-5.634662151
O	-5.045355797	0.730203688	-0.050102383
N	-4.634064198	1.539805412	-0.850135505
O	-4.950654984	1.742249727	-2.001473427
O	-4.344794273	3.137884378	-0.004338849
C	-3.012930632	3.264127016	-0.004861890
O	-2.478289843	4.260002136	0.454956353
C	-0.772934020	-0.572660685	-7.055722237
H	0.301217049	-0.702482343	-7.240145206
H	-1.281762600	-1.435881495	-7.499495983
H	-1.094502568	0.319689125	-7.601457119
C	-3.657850266	-4.438598156	2.033067703
H	-4.697388649	-4.754493713	1.881614208
H	-3.026877642	-5.318572521	1.857881188
H	-3.547963619	-4.155653000	3.084459066

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B1

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C	-1.910521030	-0.247449085	-2.717561007
Ni	-2.724909306	1.531884432	-0.650258422
P	-2.816463709	0.370355815	1.242047787
C	-3.341017485	-1.220140696	0.534072697
C	-3.163040400	-1.268475175	-0.877730191
N	-2.604879856	-0.163965702	-1.516462445
C	-1.716837049	0.942602456	-3.477131605
P	-2.374070883	2.430158615	-2.661630392
C	-3.862863302	-2.319929361	1.228203773
C	-3.647035360	-2.419335127	-1.542770624
C	-1.312685609	-1.428396702	-3.221413136
C	-1.067159295	0.898348331	-4.718535423
C	-4.289302826	-3.472646236	0.566584110
C	-4.191051960	-3.481550694	-0.833537102
C	-0.649507165	-1.435921431	-4.440951347
C	-0.528833807	-0.282463014	-5.231561184
H	-3.950780153	-2.277072906	2.308662653

H	-4.560777664	-4.343900681	-1.385376334
H	-0.202199474	-2.365778685	-4.787116051
H	-0.954321563	1.811096430	-5.294664383
H	-3.613057852	-2.462175131	-2.625413656
H	-1.358004928	-2.340526819	-2.638157606
C	-4.007031918	1.070906639	2.508819818
H	-4.674107552	1.647153139	1.860365391
C	-3.280236483	2.066175461	3.431583881
C	-4.851781368	0.069043420	3.305349112
H	-5.449390888	-0.568750918	2.650160074
H	-4.238272667	-0.571083367	3.948670149
H	-5.541583061	0.620076954	3.955394268
H	-2.619040728	1.552018881	4.137625694
H	-4.025253296	2.615025997	4.017895699
H	-2.693175554	2.801759481	2.875731230
C	-1.150430799	0.091648608	2.036043882
H	-0.881790698	1.068775892	2.453682661
C	-0.137318283	-0.262329429	0.934456050
C	-1.174452066	-0.963896692	3.150527954
H	-1.859549046	-0.697422981	3.961048841
H	-1.476974010	-1.939002156	2.754569292
H	-0.173422709	-1.075323582	3.583554745
H	-0.410790890	-1.196678877	0.432564914
H	0.859818578	-0.389445871	1.370728135
H	-0.087802008	0.522224307	0.173820764
C	-1.057363868	3.765303373	-2.539710283
H	-0.537281156	3.450671196	-1.626549959
C	-1.680909157	5.143315315	-2.254315138
C	-0.040961422	3.846432209	-3.685761452
H	0.495554864	2.905896902	-3.826353550
H	-0.516747952	4.119308949	-4.634071350
H	0.697618246	4.623102188	-3.454564333
H	-2.147989273	5.558805943	-3.153319597
H	-0.889145195	5.834006310	-1.944612145
H	-2.422713757	5.117544651	-1.454113245
C	-3.862672567	2.973215818	-3.658787489
H	-4.416280746	2.025953054	-3.701196909
C	-3.549179077	3.420112133	-5.093462467
C	-4.737378597	3.997277975	-2.912130356
H	-4.823571682	3.770598650	-1.847426772
H	-4.335506439	5.009259701	-3.006553173
H	-5.742587566	3.998652935	-3.348228931
H	-2.939551830	4.329732895	-5.104652882
H	-4.483374119	3.645340681	-5.621540070
H	-3.026858330	2.644854546	-5.659745693
O	-3.929193020	3.710238695	0.430031091
N	-2.828872681	3.166315317	0.245725051
O	-1.775084019	3.665936708	0.672766685
C	-5.498435020	1.142879605	-0.630136669
O	-5.993400574	1.296087980	-1.644467235
C	0.206126973	-0.311054319	-6.550505638
H	1.293056488	-0.363990337	-6.405009747
H	-0.080110006	-1.181870699	-7.150998116
H	-0.001082796	0.585351884	-7.143525600
C	-4.850559711	-4.658756256	1.313887715
H	-5.802994251	-4.988984585	0.882513583
H	-4.167781830	-5.517193794	1.277966619
H	-5.027090549	-4.422187805	2.367772102

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C	-1.978787065	-0.308713645	-2.696700573
Ni	-2.642776966	1.634607673	-0.647263765
P	-2.910953045	0.285584003	1.124783516
C	-3.787616491	-1.095368385	0.324129343
C	-3.625003099	-1.098823667	-1.087117672
N	-2.888916016	-0.080668829	-1.675817132
C	-1.410679817	0.837075472	-3.321710110
P	-2.159792423	2.367939472	-2.706688881
C	-4.477377892	-2.133809566	0.964632154
C	-4.256954193	-2.134242296	-1.810100675
C	-1.500817895	-1.566702247	-3.127962112
C	-0.415375769	0.722707033	-4.291557789
C	-5.075886726	-3.170146704	0.243826002
C	-4.962834835	-3.134645700	-1.154969692
C	-0.509813964	-1.655712247	-4.101056576
C	0.061462812	-0.526041269	-4.702964306
H	-4.547692776	-2.148445845	2.046126604
H	-5.447084427	-3.910225153	-1.745286345
H	-0.152420282	-2.643038511	-4.388074398
H	0.018713951	1.616803885	-4.728081226
H	-4.196573257	-2.131071091	-2.893527508
H	-1.876396179	-2.473673820	-2.668943405
C	-3.886821032	1.025822282	2.547801018
H	-4.639785290	1.622585416	2.020331621
C	-2.975434542	1.994904757	3.323085785
C	-4.641272545	0.074325539	3.489808559
H	-5.427982807	-0.475140333	2.969162226
H	-3.979911327	-0.644854307	3.980246067
H	-5.120133400	0.667235374	4.278165817
H	-2.221502781	1.451132536	3.903018475
H	-3.580018044	2.573421001	4.030444622
H	-2.459746599	2.691296101	2.657354593
C	-1.285939455	-0.396577835	1.749533772
H	-0.754438758	0.485038847	2.126728296
C	-0.505789697	-0.966810346	0.551448047
C	-1.431435108	-1.433296442	2.872481823
H	-1.863574982	-1.007578254	3.781883478
H	-2.054150581	-2.275733232	2.552234411

H	-0.444078356	-1.832882881	3.131550550
H	-1.023622870	-1.831411958	0.123388804
H	0.483017325	-1.296638846	0.888528466
H	-0.367975384	-0.220535949	-0.232157320
C	-1.001584411	3.813859463	-2.923411846
H	-0.059261668	3.398808718	-2.547582626
C	-1.407613754	4.987351418	-2.009179831
C	-0.815991759	4.303463459	-4.370436192
H	-0.563288152	3.506109715	-5.072042942
H	-1.719122410	4.798799038	-4.739521980
H	-0.005835514	5.041143417	-4.397671223
H	-2.330686808	5.462503910	-2.354749203
H	-0.619019866	5.747629642	-2.029340744
H	-1.546258569	4.680642605	-0.972036600
C	-3.731790543	2.571286917	-3.712414503
H	-4.343974590	1.778417230	-3.263588428
C	-3.563058853	2.268380880	-5.209841251
C	-4.432408333	3.919209957	-3.487262487
H	-4.552825451	4.162672043	-2.429295301
H	-3.885959864	4.739064217	-3.963455439
H	-5.431770802	3.891001701	-3.935682774
H	-2.969487906	3.037128210	-5.713774681
H	-4.549023628	2.246178150	-5.688632011
H	-3.081521034	1.302198529	-5.377598286
O	-1.069802403	3.338546276	1.018538356
N	-1.000039697	2.481091976	0.123867087
O	0.095209636	2.139592409	-0.348267138
C	-4.012007713	2.891032219	-0.196238846
O	-4.542199612	3.798115492	0.267918885
C	1.176119566	-0.646943152	-5.714853764
H	2.157412291	-0.717407405	-5.227529049
H	1.059249759	-1.541368127	-6.336236477
H	1.208204389	0.220980212	-6.382172108
C	-5.803786278	-4.296549797	0.938360512
H	-6.714756966	-4.577563286	0.398354232
H	-5.179523945	-5.197178364	1.005372882
H	-6.091521740	-4.021411896	1.957831383

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B2

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C	-1.860470653	-0.320767939	-2.697652102
Ni	-2.614800215	1.605912685	-0.669433594
P	-2.959301472	0.308922261	1.113013268
C	-3.801134825	-1.081557035	0.312253684
C	-3.491131783	-1.152446508	-1.073894382
N	-2.724889755	-0.141010866	-1.626441360
C	-1.448278785	0.846283972	-3.392361164
P	-2.229418516	2.347146511	-2.740231514
C	-4.560022831	-2.079015255	0.936644971
C	-4.036493778	-2.238311529	-1.797425508
C	-1.296472549	-1.544772625	-3.114351749
C	-0.532840610	0.785055697	-4.442459106
C	-5.080202579	-3.156896830	0.216817871
C	-4.810079098	-3.199930191	-1.161259651
C	-0.384244829	-1.584077239	-4.164694309
C	0.021723034	-0.432250708	-4.853129864
H	-4.746201992	-2.025885105	2.004108667
H	-5.227264404	-4.011296749	-1.754918218
H	0.044515893	-2.544011116	-4.446124077
H	-0.220678031	1.697166443	-4.942760944
H	-3.867196083	-2.302039862	-2.866796494
H	-1.545780182	-2.458976984	-2.587918043
C	-3.951418877	1.126525879	2.471251726
H	-4.683007240	1.709443212	1.900442004
C	-3.016553640	2.110325336	3.203141689
C	-4.742633820	0.235769033	3.441236258
H	-5.532653332	-0.317077845	2.927335978
H	-4.109520912	-0.478009164	3.973413944
H	-5.223067760	0.873000383	4.193245411
H	-2.350445747	1.578451753	3.890650272
H	-3.613643885	2.812510729	3.794516325
H	-2.385741711	2.676726818	2.510836840
C	-1.369646192	-0.380588681	1.818620682
H	-0.806804717	0.509945393	2.115266323
C	-0.596462786	-1.114473820	0.707736254
C	-1.592165112	-1.298365116	3.030230522
H	-1.993499398	-0.763516247	3.894491911
H	-2.268683672	-2.124796152	2.784563303
H	-0.633863330	-1.736968398	3.331162930
H	-1.128691077	-2.020391226	0.398387522
H	0.384123534	-1.412289500	1.094171643
H	-0.438801020	-0.489801377	-0.171372741
C	-1.074126601	3.804902315	-2.910618305
H	-0.111606702	3.345062017	-2.662853479
C	-1.383474946	4.870018959	-1.842078805
C	-1.001579762	4.434123993	-4.311689377
H	-0.796435654	3.706672668	-5.100306988
H	-1.928595424	4.955838203	-4.567497730
H	-0.195482925	5.176246166	-4.327667713
H	-2.374877930	5.312773705	-1.985679865
H	-0.647080004	5.678175449	-1.912224650
H	-1.329716921	4.456350803	-0.833607078
C	-3.815678358	2.557359457	-3.717342615
H	-4.386627674	1.701845288	-3.332367182
C	-3.655583858	2.386471033	-5.236633301
C	-4.575142860	3.845953941	-3.368005753
H	-4.744548798	3.954551697	-2.294661045
H	-4.043662071	4.735475540	-3.719661713
H	-5.555209637	3.837275982	-3.857786894

H	-3.136701822	3.236727953	-5.687672138
H	-4.646924973	2.322377920	-5.699832439
H	-3.105229139	1.476465940	-5.487512112
O	-0.444279045	2.680245161	0.971400321
N	-0.609790325	2.076759100	-0.109378785
O	0.365553290	1.821677089	-0.836284280
C	-3.607275248	2.992961407	-0.113432504
O	-4.161080837	3.910799265	0.306955159
C	1.055567741	-0.495605856	-5.951439381
H	2.073966265	-0.531656086	-5.542673588
H	0.926348925	-1.387468576	-6.574314594
H	0.999514759	0.380233556	-6.606185913
C	-5.885290146	-4.243888378	0.886536360
H	-6.759642124	-4.522031307	0.287254572
H	-5.291175365	-5.156130791	1.028544545
H	-6.243124485	-3.929780006	1.871888399

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C	-2.041534424	-0.290542781	-2.675644159
Ni	-2.815582275	1.573847651	-0.684592962
P	-3.164540052	0.338312775	1.127268314
C	-3.959984064	-1.089358926	0.340751976
C	-3.653590679	-1.147767901	-1.045143366
N	-2.913330555	-0.112515450	-1.603338838
C	-1.649451852	0.871262789	-3.390529633
P	-2.402508259	2.386042595	-2.727064371
C	-4.675909996	-2.118775845	0.964535594
C	-4.166845798	-2.244736671	-1.772807360
C	-1.453853369	-1.512071371	-3.060942173
C	-0.736273885	0.797825992	-4.442962646
C	-5.157925606	-3.212700129	0.243002310
C	-4.898470402	-3.238970995	-1.137051702
C	-0.543353260	-1.561204433	-4.112570286
C	-0.162919506	-0.418705523	-4.828609943
H	-4.857194424	-2.077980995	2.033146858
H	-5.287528992	-4.063050747	-1.732033849
H	-0.095212817	-2.519021273	-4.369339943
H	-0.435055733	1.702255249	-4.962270737
H	-4.000810623	-2.297316074	-2.843262434
H	-1.683475494	-2.417291403	-2.510879040
C	-4.189494133	1.162142873	2.462122679
H	-4.849104881	1.811030626	1.873269320
C	-3.268852234	2.062059879	3.312377214
C	-5.080340385	0.266878754	3.335126400
H	-5.835570812	-0.253897965	2.741978168
H	-4.503436089	-0.476032853	3.893154383
H	-5.604789257	0.891961932	4.067439556
H	-2.691874981	1.467126369	4.026934624
H	-3.879894495	2.766942263	3.886151314
H	-2.559311867	2.634839535	2.709069967
C	-1.569817066	-0.299154222	1.869055867
H	-1.044366241	0.608412623	2.185422421
C	-0.738066018	-1.001000762	0.780892372
C	-1.798956156	-1.231612802	3.068828821
H	-2.292504787	-0.733292878	3.906861305
H	-2.398245573	-2.102455616	2.780669689
H	-0.832434475	-1.601963282	3.428938150
H	-1.245451093	-1.904444098	0.426006705
H	0.225464299	-1.298633218	1.208602309
H	-0.537641585	-0.350605667	-0.070256032
C	-1.183375955	3.788558245	-2.958396435
H	-0.233114660	3.286561966	-2.739505768
C	-1.376822352	4.913536549	-1.925847054
C	-1.141833305	4.376002312	-4.380886078
H	-1.058930397	3.622463942	-5.166673183
H	-2.035602570	4.974545002	-4.583693981
H	-0.276852965	5.043193340	-4.466101170
H	-2.374212265	5.360853195	-1.992986083
H	-0.648618996	5.708082199	-2.124627113
H	-1.210714340	4.563724518	-0.906852841
C	-3.997915268	2.645406723	-3.670535803
H	-4.560444355	1.773091197	-3.311053276
C	-3.895736933	2.554502964	-5.199769974
C	-4.723944187	3.914494991	-3.200057745
H	-4.816890717	3.948791504	-2.110050678
H	-4.201372623	4.820174694	-3.525086880
H	-5.733336926	3.947419643	-3.624705315
H	-3.432867289	3.445560694	-5.631288052
H	-4.901093483	2.466418743	-5.627822876
H	-3.318337679	1.680063844	-5.513276577
O	-0.829770982	3.012714148	0.874716401
N	-0.559085011	2.166779041	-0.047758792
O	0.626035750	1.898029685	-0.252094030
C	-3.141609192	3.159399748	0.138862029
O	-3.570681334	4.124345303	0.586126924
C	0.873283386	-0.484377205	-5.925343037
H	1.890604019	-0.448436320	-5.514889240
H	0.790271878	-1.411520123	-6.502409458
H	0.774595976	0.354326844	-6.622339249
C	-5.915427208	-4.334217072	0.913054764
H	-6.828815460	-4.587223530	0.362369865
H	-5.311382294	-5.248874664	0.968790710
H	-6.204951763	-4.069276810	1.934594393

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C	-1.852352142	-0.421535790	-2.794619560

Ni	-2.601529121	1.431069016	-0.727638006
P	-3.082901001	0.299451739	1.113380551
C	-3.610402822	-1.263620734	0.347071290
C	-3.261647224	-1.353158355	-1.031064391
N	-2.568151951	-0.297867537	-1.607361436
C	-1.643772483	0.750656605	-3.576640844
P	-2.360108137	2.228810310	-2.783914089
C	-4.265206814	-2.322549105	0.992461205
C	-3.722499371	-2.498687267	-1.727469802
C	-1.266435027	-1.617626905	-3.267920971
C	-1.005417705	0.674170315	-4.819754124
C	-4.666145802	-3.469673872	0.307535976
C	-4.400510788	-3.514739513	-1.070739269
C	-0.600381851	-1.656830311	-4.486344814
C	-0.476477623	-0.524995506	-5.304571629
H	-4.483222961	-2.249008656	2.052577496
H	-4.744117260	-4.371023178	-1.648570538
H	-0.161078095	-2.598062038	-4.811915398
H	-0.912452400	1.563433766	-5.432464123
H	-3.564257622	-2.572396040	-2.797060966
H	-1.327020407	-2.516505003	-2.664896965
C	-4.442545891	1.090921044	2.137422562
H	-4.933165073	1.721014142	1.386028767
C	-3.835062265	2.030814886	3.194059849
C	-5.493148804	0.158853933	2.753445864
H	-5.981025696	-0.462351769	1.999171734
H	-5.062843323	-0.498862386	3.516382933
H	-6.265955448	0.763707697	3.241977453
H	-3.360519886	1.468055367	4.004899979
H	-4.631663322	2.640174627	3.633900404
H	-3.099623919	2.719066620	2.770549059
C	-1.625443578	-0.114056468	2.208329439
H	-1.340742946	0.842268109	2.663559914
C	-0.475542337	-0.593038738	1.305480480
C	-1.939063191	-1.134333968	3.311404467
H	-2.745641232	-0.803159952	3.972624540
H	-2.226988792	-2.096714735	2.876820326
H	-1.048728228	-1.301596880	3.928845406
H	-0.748897910	-1.518895388	0.787717283
H	0.417167544	-0.791873872	1.909191847
H	-0.226197496	0.154941499	0.547986031
C	-1.283861756	3.749593973	-3.010959864
H	-0.530245602	3.594853163	-2.228955984
C	-2.075574636	5.023258209	-2.660490751
C	-0.546772659	3.922295570	-4.347543716
H	0.171029568	3.119377136	-4.523718834
H	-1.237115741	3.967973232	-5.195706844
H	0.011082993	4.865935802	-4.327684879
H	-2.773865700	5.281177998	-3.462938309
H	-1.378121853	5.860393524	-2.549964190
H	-2.640282154	4.936545849	-1.730670571
C	-4.037714481	2.400268555	-3.604571342
H	-4.363184929	1.352365375	-3.551532507
C	-3.983359575	2.820080996	-5.078966141
C	-5.031617165	3.238608360	-2.785439253
H	-5.009167671	2.973834038	-1.725300550
H	-4.820762157	4.308608055	-2.861501932
H	-6.046053410	3.074620008	-3.167383671
H	-3.657646656	3.859953403	-5.186701775
H	-4.981611252	2.742140770	-5.525620461
H	-3.308611393	2.182467222	-5.657458305
O	-1.541077971	3.753434896	0.628419757
N	-0.408721447	2.963683367	0.390180409
O	0.570481181	3.476680994	0.823563397
C	-2.761255026	3.100169897	0.117062114
O	-3.750753164	3.754405499	0.330945909
C	0.245653272	-0.592909694	-6.630855560
H	1.333770633	-0.647253752	-6.495672703
H	-0.050067559	-1.478471518	-7.204720974
H	0.036837395	0.287489086	-7.246971607
C	-5.364705086	-4.614577293	1.004709244
H	-6.251696110	-4.941583633	0.449143499
H	-4.708631039	-5.489265919	1.101600170
H	-5.688862324	-4.335041046	2.012147188

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C	-1.987756491	-0.198294058	-2.604784966
Ni	-3.168030977	1.503057957	-0.603919029
P	-3.710781097	0.283287197	1.181424975
C	-3.889775276	-1.337097645	0.364878863
C	-3.374612331	-1.368585706	-0.963485599
N	-2.811603546	-0.213635385	-1.482283115
C	-1.955010414	1.005037665	-3.362854481
P	-3.083071232	2.261083841	-2.687556505
C	-4.431629181	-2.492271900	0.947952569
C	-3.541124582	-2.579235554	-1.681851625
C	-1.110379338	-1.230106950	-3.001421928
C	-1.097001195	1.149174929	-4.454864502
C	-4.544842720	-3.694023132	0.247386381
C	-4.106270790	-3.697556257	-1.086653709
C	-0.265274554	-1.064377069	-4.093898296
C	-0.236219779	0.118487753	-4.846759319
H	-4.791708469	-2.455305099	1.970557451
H	-4.219140053	-4.604159355	-1.678802490
H	0.410398334	-1.875524759	-4.358924866
H	-1.079963088	2.083611250	-5.008868217
H	-3.241613865	-2.626320839	-2.722467899
H	-1.063920736	-2.146444082	-2.423710108

C	-5.315617085	0.855870128	1.970191836
H	-5.754445553	1.437090874	1.150250077
C	-5.031882763	1.846196771	3.113881826
C	-6.312359333	-0.229489312	2.395629644
H	-6.565380573	-0.900495470	1.571525335
H	-5.933075905	-0.834228218	3.226526022
H	-7.238163471	0.248551726	2.736649275
H	-4.619530678	1.341292739	3.993420124
H	-5.971290112	2.322598457	3.414284945
H	-4.349543571	2.643545151	2.812211752
C	-2.402732849	0.051165331	2.497637033
H	-2.276185036	1.051027536	2.930802584
C	-1.092753291	-0.364130974	1.806548119
C	-2.777791262	-0.946821094	3.603178263
H	-3.711479187	-0.688176036	4.109703541
H	-2.878735781	-1.956600666	3.193799257
H	-1.984962463	-0.976513207	4.359804630
H	-1.197309852	-1.353503466	1.348585606
H	-0.281646460	-0.414450884	2.541679859
H	-0.809573770	0.341119349	1.022490621
C	-2.509486437	3.933522701	-3.299413204
H	-1.416834116	3.837388277	-3.247665882
C	-2.938133001	5.067961693	-2.351204872
C	-2.906280518	4.258757114	-4.750358582
H	-2.675657034	3.455262423	-5.453935623
H	-3.977480888	4.470026970	-4.821172237
H	-2.373364210	5.158461094	-5.078593731
H	-4.025265217	5.114860058	-2.239718199
H	-2.601433516	6.027622223	-2.760323763
H	-2.506360531	4.954395771	-1.356799483
C	-4.787844181	1.810567379	-3.332697153
H	-4.919485092	0.848839939	-2.820514679
C	-4.898752213	1.554340005	-4.842428684
C	-5.853184700	2.783882856	-2.804255962
H	-5.765270710	2.935209274	-1.723858833
H	-5.777552128	3.761941195	-3.292137623
H	-6.852888584	2.388931513	-3.020159721
H	-4.901232243	2.482852221	-5.418420315
H	-5.842732430	1.037286758	-5.052014351
H	-4.082443714	0.923436463	-5.207207203
O	-0.503630400	3.304988861	-0.366864830
N	-1.315212131	2.724683285	0.231824905
O	-2.517519474	3.765161514	0.701874316
C	-3.621934891	3.121050835	0.257152289
O	-4.729644775	3.612211227	0.397850126
C	0.720699012	0.283890069	-6.003386497
H	1.749911308	0.438974977	-5.654520035
H	0.730437219	-0.602978468	-6.646954060
H	0.453162640	1.144024014	-6.625144482
C	-5.135506153	-4.934260845	0.875969231
H	-6.003383636	-5.297989368	0.311827570
H	-4.408422470	-5.755479813	0.907021165
H	-5.464465141	-4.746258736	1.902785778

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B4

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C	-1.952901483	-0.280823261	-2.830605268
Ni	-2.533460855	1.502878785	-0.659215569
P	-2.847750902	0.327140421	1.204453468
C	-3.288562298	-1.272805214	0.474452853
C	-3.130551577	-1.297515273	-0.940297067
N	-2.560320377	-0.194471523	-1.575908303
C	-1.786015868	0.909188151	-3.596105576
P	-2.311724663	2.394714832	-2.695868254
C	-3.788442373	-2.388289213	1.161986828
C	-3.638715506	-2.436584949	-1.611442566
C	-1.425754547	-1.469048858	-3.390467405
C	-1.260952711	0.860830605	-4.893711567
C	-4.215659142	-3.536741495	0.495654583
C	-4.156730652	-3.514273643	-0.907734990
C	-0.879971147	-1.482176900	-4.667185307
C	-0.809508741	-0.329890311	-5.465222836
H	-3.864072084	-2.355486631	2.244258881
H	-4.539341927	-4.366430759	-1.466669798
H	-0.488448322	-2.420243263	-5.056566238
H	-1.185659051	1.775602937	-5.473083019
H	-3.640260220	-2.461402655	-2.694722414
H	-1.436067104	-2.384538651	-2.811262846
C	-4.260454178	1.016358614	2.232543468
H	-4.889326572	1.469831347	1.455454230
C	-3.750684023	2.150264263	3.138946533
C	-5.114167690	0.006180691	3.010611534
H	-5.561546803	-0.743710697	2.354770184
H	-4.535012722	-0.511853456	3.782183170
H	-5.928204060	0.538856924	3.516241550
H	-3.105645180	1.765484571	3.936482668
H	-4.605487347	2.640168905	3.618391275
H	-3.204088211	2.908208370	2.575135946
C	-1.327334523	0.117211126	2.261784077
H	-1.140159249	1.122885227	2.657054424
C	-0.163406640	-0.260169864	1.329574585
C	-1.477312565	-0.876670837	3.421065092
H	-2.275994301	-0.592304587	4.112437248
H	-1.687915087	-1.883862615	3.046982050
H	-0.543512285	-0.925087154	3.993607283
H	-0.348154306	-1.223819613	0.842000842
H	0.766828656	-0.341250688	1.902845383
H	-0.024669509	0.494644016	0.549786210
C	-0.996427357	3.731693268	-2.733896971

H	-0.322640032	3.378369093	-1.941921473
C	-1.576933384	5.081828117	-2.274852276
C	-0.184063494	3.882696629	-4.027098179
H	0.350932747	2.966229916	-4.284469128
H	-0.815642715	4.166758060	-4.875387669
H	0.559655368	4.676884651	-3.891546249
H	-2.206408024	5.526954651	-3.052015543
H	-0.753470719	5.777668953	-2.081002474
H	-2.158592701	4.988566875	-1.356139421
C	-3.918215036	2.940826893	-3.487306356
H	-4.423901558	1.970369458	-3.584025383
C	-3.778334618	3.554526329	-4.887204647
C	-4.755846024	3.812305450	-2.536069155
H	-4.800952911	3.374167442	-1.534388185
H	-4.344686508	4.819841862	-2.436879873
H	-5.777100563	3.905031443	-2.923612833
H	-3.257858515	4.516498566	-4.854085922
H	-4.771410465	3.733186245	-5.316856384
H	-3.236513853	2.892220736	-5.568803787
O	-2.506730795	3.194479704	0.240828320
N	-1.313165665	3.517078161	0.746243179
O	-1.302574635	4.613914490	1.264030933
C	-0.215338856	-0.371612579	-6.852615356
H	0.878833175	-0.456586689	-6.821041584
H	-0.586465240	-1.230416059	-7.423147202
H	-0.456371576	0.533399403	-7.419049740
C	-4.740684986	-4.743428230	1.235467434
H	-5.688081741	-5.094520569	0.809566796
H	-4.037257195	-5.584517002	1.185784817
H	-4.913366318	-4.522507191	2.293352365

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B5

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C	-1.898971796	-0.494528621	-2.769603968
Ni	-3.014655113	1.345235229	-0.825335324
P	-2.988725424	0.381220162	1.192350030
C	-2.974529028	-1.356247425	0.669073939
C	-2.794288874	-1.517956853	-0.733064294
N	-2.497109413	-0.395241976	-1.510613680
C	-1.977229118	0.609348357	-3.665528774
P	-2.565634251	2.129240036	-2.871376991
C	-3.178879976	-2.467000246	1.500437856
C	-3.014203072	-2.819888592	-1.246550560
C	-1.133441925	-1.603520751	-3.209828377
C	-1.446406126	0.524267375	-4.961163044
C	-3.300564289	-3.759815931	0.992918015
C	-3.252078533	-3.896666050	-0.403739333
C	-0.612905085	-1.657850027	-4.494608879
C	-0.785046995	-0.614239633	-5.418772221
H	-3.265789747	-2.319145679	2.571774721
H	-3.412096500	-4.878456593	-0.845510721
H	-0.042126052	-2.536931276	-4.788295746
H	-1.539325833	1.373992085	-5.629979134
H	-3.013430834	-2.980379820	-2.317593575
H	-0.937111437	-2.422874689	-2.529495478
C	-4.488947392	0.782609463	2.260459185
H	-5.161202431	1.218097210	1.511309624
C	-4.170701027	1.875605106	3.296231508
C	-5.202625275	-0.406982392	2.916257143
H	-5.461070061	-1.186004162	2.195646286
H	-4.593498230	-0.857887983	3.707619905
H	-6.130357742	-0.052973971	3.380986452
H	-3.516231775	1.497864246	4.089033127
H	-5.103632927	2.202866077	3.768492699
H	-3.702968121	2.753293753	2.845981121
C	-1.423885107	0.688235939	2.169187307
H	-1.529479504	1.712491632	2.543593407
C	-0.233225182	0.640509784	1.196426034
C	-1.225395083	-0.276046723	3.347921133
H	-2.071581602	-0.270994455	4.042240620
H	-1.086519003	-1.300861835	2.989665508
H	-0.328610599	0.004404499	3.913192272
H	-0.149898916	-0.346180320	0.727717280
H	0.700884163	0.842497349	1.732807994
H	-0.342512637	1.380969882	0.397758245
C	-1.035610437	3.226953030	-2.809995174
H	-0.260895401	2.480189323	-2.590430737
C	-1.081097126	4.218667030	-1.635790706
C	-0.668524623	3.921355486	-4.129780769
H	-0.570645928	3.214250803	-4.957274437
H	-1.409369946	4.677518368	-4.405285835
H	0.294821769	4.433216572	-4.017429829
H	-1.884586573	4.951951504	-1.744756579
H	-0.132095426	4.765453815	-1.582164526
H	-1.235885262	3.705563068	-0.683900714
C	-3.973370552	2.929671526	-3.806149244
H	-4.799092293	2.268995285	-3.519994497
C	-3.867753267	2.920803070	-5.337682724
C	-4.271631718	4.331687450	-3.245255232
H	-4.369019508	4.318819046	-2.156812906
H	-3.492391825	5.049005985	-3.522953272
H	-5.214302540	4.695838451	-3.669600725
H	-3.023321867	3.516433001	-5.697346687
H	-4.780632973	3.355769157	-5.762060642
H	-3.769321918	1.905937076	-5.731113434
O	-3.887957811	2.958584309	-0.323464364
N	-3.422279119	3.738035679	0.651059389
O	-4.066025734	4.756998062	0.780467033
C	-5.527864933	0.176093131	-2.070034266

O	-5.941733837	-0.401736885	-1.174538612
C	-0.236134976	-0.713060260	-6.819556236
H	0.854198873	-0.836320937	-6.818902969
H	-0.655121803	-1.574369073	-7.354038239
H	-0.467921942	0.182694197	-7.403868675
C	-3.538597345	-4.948691845	1.889448881
H	-4.568934917	-5.317795753	1.804663062
H	-2.876930714	-5.784121037	1.633524537
H	-3.365761757	-4.697473526	2.940485716

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C	-1.842468143	-0.358536810	-2.529521704
Ni	-3.332453966	1.469584227	-0.815676808
P	-3.301488638	0.415901482	1.152141333
C	-3.531485796	-1.293232799	0.567246735
C	-3.195341110	-1.430716872	-0.807185173
N	-2.764651537	-0.308478862	-1.500795960
C	-1.706168890	0.780681074	-3.371563911
P	-2.783143759	2.162196398	-2.887592793
C	-3.906506777	-2.411340475	1.325295687
C	-3.373765945	-2.708859205	-1.388036728
C	-0.969412386	-1.447306871	-2.787271261
C	-0.827530265	0.764454067	-4.464510441
C	-4.039587021	-3.677308083	0.753184140
C	-3.785878420	-3.790905476	-0.623483002
C	-0.087376744	-1.422946334	-3.857553720
C	-0.008027361	-0.330498815	-4.738394260
H	-4.098723888	-2.301835299	2.386043549
H	-3.920337915	-4.755597591	-1.109243870
H	0.567836881	-2.277915478	-4.014041901
H	-0.778654993	1.625693202	-5.122343063
H	-3.198008776	-2.836270571	-2.450505257
H	-0.979498684	-2.306975126	-2.127511024
C	-4.584039211	0.969372451	2.428476810
H	-5.275773525	1.548654914	1.811004281
C	-3.984049797	1.936641932	3.464264154
C	-5.385166645	-0.142166764	3.120634079
H	-5.864604950	-0.816045344	2.407312632
H	-4.759469032	-0.736177325	3.795400143
H	-6.172413349	0.318103671	3.728791475
H	-3.287276506	1.430385828	4.139189720
H	-4.797447205	2.342523575	4.076068401
H	-3.478038311	2.782282591	2.998095036
C	-1.611936331	0.460306704	1.951719999
H	-1.532459497	1.468381763	2.371309042
C	-0.528774083	0.299166590	0.873271406
C	-1.465216637	-0.588739514	3.064360857
H	-2.223825932	-0.486933738	3.846715212
H	-1.538338423	-1.600580931	2.653407335
H	-0.482633442	-0.489195257	3.539525032
H	-0.611139953	-0.668484390	0.368386120
H	0.461990118	0.356296301	1.338904977
H	-0.608236492	1.086190224	0.120862611
C	-1.828168273	3.768480539	-2.831663609
H	-1.169901490	3.563502550	-1.980009556
C	-2.746455908	4.937852383	-2.426568508
C	-0.970077634	4.140013218	-4.049070358
H	-0.177418873	3.412405491	-4.231790543
H	-1.567993760	4.243943214	-4.960407257
H	-0.490586847	5.108439445	-3.862306833
H	-3.271291256	5.347760201	-3.294162989
H	-2.137410879	5.741463661	-1.999344349
H	-3.486001968	4.653038502	-1.675944567
C	-4.185248375	2.174989462	-4.137966633
H	-4.673213482	1.225847602	-3.875482321
C	-3.747623205	2.099918842	-5.608440876
C	-5.199082851	3.310842752	-3.925207138
H	-5.453335285	3.464841366	-2.874494076
H	-4.820288658	4.256546497	-4.321679592
H	-6.124605179	3.077361345	-4.462902069
H	-3.227575541	3.012158632	-5.919036388
H	-4.632835865	1.994909167	-6.246721268
H	-3.093219519	1.246932507	-5.798729420
O	-2.232716322	2.973734856	0.038301405
N	-2.816945791	3.900346994	0.721888244
O	-4.039975643	3.832763910	0.812181711
C	-5.225736618	1.844731212	-0.804844439
O	-6.349077225	2.028216124	-0.664037704
C	0.948868513	-0.336684942	-5.906869888
H	1.994536042	-0.337221980	-5.573534012
H	0.812632501	-1.225774884	-6.534272194
H	0.807942510	0.542301178	-6.543813229
C	-4.467971325	-4.875672340	1.566906810
H	-5.454926014	-5.241168022	1.255952001
H	-3.767184496	-5.711173534	1.452016830
H	-4.526982784	-4.636197090	2.633184195

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C	-1.681759119	-0.326181799	-2.634896994
Ni	-2.754580736	1.473689318	-0.704199314
P	-3.091197252	0.319428682	1.166692615
C	-3.520562649	-1.277883768	0.424699605
C	-3.098665237	-1.363171577	-0.930909812
N	-2.491640568	-0.256903827	-1.504445076
C	-1.590669990	0.828582942	-3.451134682
P	-2.556045771	2.226727486	-2.811093092

C	-4.101850986	-2.377632856	1.070334554
C	-3.385366201	-2.570370436	-1.613439441
C	-0.886329234	-1.434020877	-2.997661114
C	-0.782317102	0.845840573	-4.591102600
C	-4.349294186	-3.575032234	0.398370951
C	-3.994457245	-3.631917000	-0.959784865
C	-0.086273931	-1.393765926	-4.133687496
C	-0.019203452	-0.263657451	-4.962488174
H	-4.369010925	-2.305109501	2.118906260
H	-4.209366798	-4.537299633	-1.524507880
H	0.522540987	-2.262869358	-4.375290871
H	-0.725649238	1.743227601	-5.199319363
H	-3.146741629	-2.657392979	-2.667271614
H	-0.876295388	-2.314735651	-2.365603924
C	-4.423296452	1.011774778	2.294104099
H	-5.101977348	1.486242056	1.575517297
C	-3.819142580	2.117723703	3.182932615
C	-5.251329422	0.014203703	3.116763830
H	-5.803673267	-0.678069174	2.477640867
H	-4.635188103	-0.566796362	3.808941364
H	-5.982223034	0.569674909	3.716323853
H	-3.234589338	1.687250018	4.001426220
H	-4.629173756	2.705144167	3.628530979
H	-3.167269468	2.799043417	2.632286310
C	-1.524497986	0.039302059	2.145576954
H	-1.203394294	1.048566699	2.424285412
C	-0.461662143	-0.590353966	1.227222323
C	-1.741316438	-0.821483433	3.399505854
H	-2.418092489	-0.359498739	4.122397423
H	-2.137717962	-1.807672501	3.133755922
H	-0.779647768	-0.978482425	3.901277065
H	-0.756038666	-1.604203463	0.935128927
H	0.486950815	-0.656096995	1.771342993
H	-0.301100135	0.003993174	0.327507704
C	-1.553684235	3.785679817	-3.088853121
H	-0.541170955	3.422310352	-2.879959583
C	-1.886672497	4.877062321	-2.058185816
C	-1.613164067	4.362169266	-4.514094353
H	-1.401642799	3.627152205	-5.293104172
H	-2.593518257	4.801275730	-4.723533630
H	-0.871938109	5.164036274	-4.605888367
H	-2.927528620	5.208068848	-2.137254238
H	-1.250331759	5.750359535	-2.241296291
H	-1.701841950	4.541500092	-1.038027644
C	-4.179889679	2.241124868	-3.745790005
H	-4.632833958	1.323318958	-3.346901655
C	-4.072741508	2.097971678	-5.271353245
C	-5.061385155	3.430058718	-3.333051920
H	-5.168594360	3.504893541	-2.247321606
H	-4.655096054	4.378195763	-3.699840307
H	-6.063281059	3.316066265	-3.761658669
H	-3.699131727	3.011414528	-5.741249084
H	-5.066399574	1.896996021	-5.688585281
H	-3.415126085	1.271756530	-5.554427147
O	-0.544242382	2.100884914	-0.524867773
N	-0.303419769	2.870468378	0.455013365
O	-1.296515107	3.288437843	1.092209816
C	-3.506338596	2.962941408	-0.059098598
O	-4.109894753	3.865769148	0.320064813
C	0.875883639	-0.236837104	-6.178720951
H	1.936387777	-0.230393663	-5.897186756
H	0.717611015	-1.115800381	-6.814335823
H	0.693613827	0.652432919	-6.790336132
C	-4.980443001	-4.761157513	1.088046908
H	-5.883966446	-5.097012043	0.564491451
H	-4.295547485	-5.617594242	1.125000715
H	-5.264486790	-4.521786213	2.117553949

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C	-1.782743216	-0.247079372	-2.662876129
Ni	-2.839846611	1.531040311	-0.669191778
P	-3.303036451	0.363577873	1.152714849
C	-3.658755064	-1.239370465	0.366139740
C	-3.220413208	-1.308819175	-0.988104939
N	-2.614312887	-0.194607571	-1.545714736
C	-1.639500260	0.948765576	-3.419767380
P	-2.651675463	2.303334236	-2.748789787
C	-4.241156101	-2.353255510	0.988497734
C	-3.497511387	-2.510498762	-1.685911775
C	-0.992335737	-1.349142432	-3.054344416
C	-0.762117207	1.019426823	-4.503376961
C	-4.469127655	-3.547502279	0.303454876
C	-4.101155758	-3.586358070	-1.051789522
C	-0.125977024	-1.255698919	-4.139237881
C	0.012281595	-0.079669289	-4.889994621
H	-4.535490036	-2.290320396	2.030868292
H	-4.302424908	-4.487376690	-1.628811836
H	0.480529994	-2.121806622	-4.398004532
H	-0.656584084	1.950910807	-5.052146435
H	-3.253509760	-2.581396341	-2.739748478
H	-1.027769446	-2.266747475	-2.478224754
C	-4.770872593	1.051613331	2.099209785
H	-5.265745163	1.642822862	1.319254875
C	-4.294410229	2.037104845	3.182406187
C	-5.779998302	0.041545514	2.659175873
H	-6.176229000	-0.614693344	1.880979061
H	-5.344028473	-0.581908464	3.447094440
H	-6.622839928	0.585141361	3.101774216

H	-3.832811356	1.512799859	4.025577068
H	-5.157711029	2.589930773	3.568126440
H	-3.583320379	2.771869421	2.798013926
C	-1.878899932	0.061802473	2.325945616
H	-1.659683704	1.049715877	2.747866392
C	-0.666669369	-0.402642667	1.501219869
C	-2.193081856	-0.929243147	3.455780983
H	-3.044453621	-0.616584301	4.066899300
H	-2.408893585	-1.922769427	3.050497055
H	-1.324644685	-1.024065137	4.118187904
H	-0.864237309	-1.373751640	1.035060525
H	0.208508998	-0.508607090	2.151981115
H	-0.423746079	0.307936698	0.707899630
C	-1.897919655	3.921139956	-3.314123392
H	-0.822896659	3.718742371	-3.219933748
C	-2.251979351	5.082187176	-2.368142605
C	-2.204357147	4.304471493	-4.773180008
H	-2.034642935	3.491601944	-5.482897282
H	-3.243679523	4.629908085	-4.878743649
H	-1.567551970	5.146815777	-5.067061901
H	-3.332813025	5.234132290	-2.296894789
H	-1.809167981	6.008461952	-2.752563000
H	-1.866388321	4.916343212	-1.363221407
C	-4.373845577	2.045445204	-3.451007128
H	-4.620680332	1.095304966	-2.959693670
C	-4.467427254	1.827809572	-4.967532635
C	-5.344318390	3.118612528	-2.933213234
H	-5.264893055	3.247638464	-1.849162936
H	-5.155365467	4.088685513	-3.406057835
H	-6.375272751	2.834165573	-3.174090862
H	-4.352383137	2.760750771	-5.524645329
H	-5.454291344	1.418877959	-5.214997292
H	-3.712171793	1.119400382	-5.321391582
O	-0.121565603	3.338401794	-0.286178529
N	-0.716764152	3.006335020	0.675727785
O	-1.958663583	3.771245956	0.831384122
C	-3.119397879	3.166586399	0.198718280
O	-4.140051842	3.791903973	0.342715889
C	0.988934457	0.004482322	-6.039083481
H	2.028021097	0.001738534	-5.685406208
H	0.881162524	-0.845882833	-6.722331047
H	0.843660951	0.919476926	-6.621918201
C	-5.100062847	-4.745758533	0.972878158
H	-5.994563103	-5.082954884	0.434663564
H	-4.409269333	-5.597701073	1.009227753
H	-5.398736000	-4.519814968	2.001353502

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C	-1.587104440	0.306857407	-4.026398182
Ni	-4.053226948	0.262832195	-2.572182417
P	-3.642374039	-0.275165558	-0.422151148
C	-2.093650103	-1.166297674	-0.671959102
C	-1.586783648	-1.049262047	-1.988658667
N	-2.239660978	-0.191504925	-2.889162779
C	-2.368436337	0.742031932	-5.124496937
P	-4.135751724	0.818532526	-4.768310070
C	-1.422708631	-1.921370625	0.302334398
C	-0.481129676	-1.867165446	-2.313169718
C	-0.186787203	0.461040467	-4.148331642
C	-1.769138217	1.131511688	-6.332088470
C	-0.277298748	-2.652891874	-0.004606819
C	0.146485418	-2.637466431	-1.343367100
C	0.387241811	0.874823749	-5.343446732
C	-0.383915126	1.177997947	-6.478644371
H	-1.803757071	-1.951578021	1.316989303
H	0.994652927	-3.252311230	-1.636294961
H	1.468987107	0.973456979	-5.396953583
H	-2.390936375	1.431796670	-7.169142723
H	-0.121369928	-1.907682776	-3.333840609
H	0.451964378	0.257816583	-3.297424078
C	-4.965867519	-1.357296228	0.367940575
H	-5.403431892	-1.853438258	-0.508282363
C	-6.055164337	-0.497245580	1.034915686
C	-4.464360237	-2.451248646	1.322251081
H	-3.761986971	-3.132711411	0.838984668
H	-3.988123178	-2.029848814	2.212953568
H	-5.323925495	-3.039874792	1.661157370
H	-5.677106857	-0.017053865	1.942727208
H	-6.887595177	-1.145653248	1.328350067
H	-6.445037365	0.287475199	0.387688100
C	-3.289619684	1.228911400	0.609810233
H	-4.254444122	1.737536192	0.670729935
C	-2.308150291	2.115983725	-0.175601348
C	-2.762858868	0.894933701	2.013119221
H	-3.454941034	0.270102710	2.584741592
H	-1.796191096	0.384390503	1.962140560
H	-2.618394136	1.823666334	2.576171637
H	-1.367920637	1.591987967	-0.377035588
H	-2.072562695	3.012258291	0.407897323
H	-2.737581015	2.429082394	-1.132037640
C	-4.736671925	2.587623835	-4.961912155
H	-4.382782459	3.040874481	-4.029352188
C	-6.271067619	2.669383287	-4.959587574
C	-4.141576767	3.370959759	-6.141658783
H	-3.052365780	3.418099642	-6.094614029
H	-4.430960655	2.947469473	-7.108382702
H	-4.522196293	4.397943974	-6.105506420
H	-6.706243992	2.231551409	-5.862494469

H	-6.565248013	3.721410275	-4.932049751
H	-6.715324402	2.189315557	-4.087062359
C	-5.010200500	-0.384760261	-5.908413887
H	-4.307857037	-1.228434563	-5.901070118
C	-5.158194065	0.107502423	-7.357828140
C	-6.346265793	-0.873122096	-5.323122025
H	-6.207537651	-1.328902602	-4.338361263
H	-7.075631618	-0.063899547	-5.226871014
H	-6.780345917	-1.632061958	-5.982906342
H	-5.835060596	0.962996006	-7.430505276
H	-5.578319073	-0.697356880	-7.971254826
H	-4.198942661	0.388005376	-7.799565315
C	0.264744490	1.565381050	-7.785164356
H	1.080733657	2.279505253	-7.630365849
H	0.693702579	0.690584242	-8.289030075
H	-0.454250604	2.021198273	-8.472402573
C	0.469340205	-3.441641808	1.043456912
H	0.717147052	-4.446917057	0.685807168
H	1.414648175	-2.952436924	1.308687091
H	-0.116103888	-3.547176123	1.961587071
O	-5.343424320	3.209555626	-1.899796009
N	-6.051124573	3.431636333	-0.894577086
O	-6.193237782	2.545538187	-0.031647138
C	-5.792234421	0.508379638	-2.291293383
O	-6.928495407	0.533305645	-2.153391600
C	-6.969436169	7.911277771	-0.237936303
Ni	-6.912212849	5.088176250	-0.612718761
P	-8.894699097	4.411905289	-1.396565557
C	-9.914452553	5.717625618	-0.676698744
C	-9.153218269	6.799412727	-0.160563931
N	-7.766139030	6.766348839	-0.309838116
C	-5.603597164	7.761338711	0.118372746
P	-5.126103878	6.034712791	0.328752637
C	-11.311225891	5.690182209	-0.560039520
C	-9.866946220	7.801076412	0.538361728
C	-7.396427155	9.216455460	-0.571619034
C	-4.746214390	8.865770340	0.211096019
C	-12.010529518	6.703895569	0.094205610
C	-11.250246048	7.746942520	0.651618600
C	-6.525046349	10.294920921	-0.486919135
C	-5.188340187	10.156832695	-0.075828686
H	-11.865731239	4.855600834	-0.979185820
H	-11.759275436	8.532752991	1.205654621
H	-6.891397476	11.281911850	-0.761974990
H	-3.711372614	8.716767311	0.505554140
H	-9.326812744	8.610400200	1.015935183
H	-8.409785271	9.376997948	-0.921748459
C	-9.372064590	2.736601591	-0.727395117
H	-8.530289650	2.109084129	-1.042843819
C	-10.667387009	2.108752012	-1.258215427
C	-9.347120285	2.814784765	0.808760703
H	-8.381215096	3.185944557	1.163067222
H	-10.137706757	3.472010851	1.184069991
H	-9.500138283	1.816073060	1.232524753
H	-11.548427582	2.702752352	-0.998199642
H	-10.799287796	1.117264152	-0.809181392
H	-10.647468567	1.975917459	-2.343522310
C	-9.087531090	4.461694241	-3.254817486
H	-8.685957909	3.502394676	-3.606486797
C	-8.196496964	5.604355812	-3.776507616
C	-10.534813881	4.633316040	-3.742595434
H	-11.193524361	3.826315165	-3.414589405
H	-10.953894615	5.577929974	-3.383320093
H	-10.552991867	4.653814316	-4.838389397
H	-8.533121109	6.568775654	-3.381087542
H	-8.244010925	5.654694080	-4.870302677
H	-7.152870655	5.471519947	-3.473607779
C	-3.565759420	5.660795689	-0.623946249
H	-3.538243771	4.566757202	-0.606431246
C	-2.242235184	6.193483353	-0.059132550
C	-3.788465023	6.095110416	-2.083711863
H	-4.690248966	5.631562710	-2.494015932
H	-3.883500099	7.182632446	-2.163298130
H	-2.937193155	5.779230118	-2.697824955
H	-2.214560747	7.286777496	-0.045837000
H	-1.415163279	5.855094433	-0.694700837
H	-2.046145201	5.833763123	0.954171896
C	-4.927041531	5.685211182	2.155021667
H	-5.969995499	5.746678352	2.493971109
C	-4.110280514	6.730511665	2.927917242
C	-4.434742451	4.247935772	2.384677649
H	-5.078154087	3.521075010	1.881765246
H	-3.409793854	4.115040302	2.021026373
H	-4.433736324	4.021079540	3.456558704
H	-3.053045750	6.715035439	2.648223162
H	-4.170175552	6.516985416	4.001127243
H	-4.492347717	7.741346836	2.764763832
C	-4.278816700	11.356589317	0.036450911
H	-4.347388744	11.995224953	-0.851383567
H	-4.543136120	11.978763580	0.900450885
H	-3.232439280	11.058552742	0.153287053
C	-13.515709877	6.687157631	0.211705148
H	-13.839468956	6.902033806	1.236269951
H	-13.975661278	7.444131851	-0.435620755
H	-13.930525780	5.715225220	-0.072325088

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C	-2.044522285	0.330723077	-4.519727707

Ni	-3.933616877	0.589186430	-2.392668962
P	-3.245011806	-0.403766602	-0.530053735
C	-1.694486737	-1.119893909	-1.117400408
C	-1.496548772	-0.974626541	-2.520466566
N	-2.341485739	-0.125498354	-3.228106022
C	-3.126981735	0.732506096	-5.351331234
P	-4.708920956	0.599601150	-4.474506855
C	-0.797267556	-1.857992291	-0.333423942
C	-0.461583793	-1.757221818	-3.090552568
C	-0.743305087	0.509752214	-5.039151669
C	-2.904976130	1.158242464	-6.666024685
C	0.289497554	-2.528196335	-0.893482685
C	0.405035734	-2.490824461	-2.293930769
C	-0.547356248	0.975710750	-6.333535671
C	-1.616393089	1.277628064	-7.190224171
H	-0.964365602	-1.936916828	0.736821473
H	1.195401430	-3.064174652	-2.773747683
H	0.471682429	1.113036752	-6.689107418
H	-3.746641159	1.398840666	-7.303630829
H	-0.341679901	-1.787685156	-4.166507244
H	0.117381155	0.317079067	-4.410410404
C	-4.393381119	-1.860563159	-0.231829002
H	-4.518637180	-2.220106125	-1.261702776
C	-5.761248589	-1.387290835	0.281157166
C	-3.829181194	-3.018920660	0.602980554
H	-2.892688274	-3.398922682	0.189112544
H	-3.654417038	-2.731907368	1.643592596
H	-4.551620483	-3.843426704	0.607727647
H	-5.688430786	-1.035050631	1.315214038
H	-6.470305443	-2.222652912	0.272964060
H	-6.175823689	-0.580344796	-0.330002397
C	-2.968322992	0.618851721	1.007687449
H	-3.917940140	1.160865188	1.100405335
C	-1.858243346	1.635649562	0.686745524
C	-2.711776018	-0.122612461	2.326099157
H	-3.538166285	-0.785655856	2.594377995
H	-1.794343829	-0.716176987	2.288329363
H	-2.592532635	0.605101585	3.137962103
H	-0.901009202	1.127441525	0.533460498
H	-1.733498693	2.337778568	1.519872427
H	-2.092163563	2.206786394	-0.215209931
C	-5.997399330	1.830352187	-5.051133633
H	-5.672682762	2.749871731	-4.547628403
C	-7.356526375	1.410031676	-4.462857246
C	-6.122991562	2.133960009	-6.553419590
H	-5.249959469	2.664619684	-6.936651230
H	-6.272128105	1.230402470	-7.150625229
H	-6.994175434	2.780401945	-6.716153145
H	-7.740927696	0.519793153	-4.967759132
H	-8.086882591	2.207003832	-4.629321098
H	-7.304796219	1.214034200	-3.388376713
C	-5.241628170	-1.171823978	-4.810644150
H	-4.283547401	-1.672463894	-4.618868828
C	-5.651935577	-1.442942023	-6.263927937
C	-6.259094715	-1.718212724	-3.795641184
H	-5.997670650	-1.429615498	-2.773011684
H	-7.272138596	-1.359187841	-3.992174149
H	-6.282194138	-2.812524319	-3.849507570
H	-6.619716644	-0.989004970	-6.500697613
H	-5.750124931	-2.522349119	-6.427342892
H	-4.907182217	-1.065321326	-6.971369743
C	-1.377885222	1.713750958	-8.615932465
H	-0.583969116	2.466400385	-8.676999092
H	-1.068896174	0.869797230	-9.245224953
H	-2.280369997	2.142767429	-9.062000275
C	1.283840895	-3.284870863	-0.047634702
H	1.532628298	-4.254568100	-0.492418826
H	2.223651886	-2.727414131	0.053577285
H	0.899627388	-3.466795921	0.960720181
O	-4.233692646	2.705134392	-1.391492486
N	-4.494746208	4.169006348	-0.246368498
O	-3.429677486	4.625787735	-0.095254138
C	-5.153835297	1.770610690	-1.515716672
O	-6.308169365	1.805808663	-1.113043904
C	-8.457159042	6.318933964	0.264939129
Ni	-6.124968052	4.652870655	0.350030363
P	-6.079167843	3.433442831	2.240923882
C	-7.262050152	4.384916306	3.198068142
C	-7.866701603	5.440516949	2.472157955
N	-7.649696827	5.524278164	1.088059902
C	-7.952239037	6.765434265	-0.985090196
P	-6.562757015	5.775189400	-1.547942758
C	-7.513374805	4.189418793	4.564330101
C	-8.594950676	6.381495953	3.238299608
C	-9.806732178	6.642257214	0.542958736
C	-8.705589294	7.606935501	-1.821522236
C	-8.324268341	5.062038422	5.285675049
C	-8.818148613	6.181087494	4.594044685
C	-10.536901474	7.465610504	-0.302011013
C	-9.996637344	8.003661156	-1.483372211
H	-7.061224461	3.345933914	5.077552795
H	-9.394475937	6.925514698	5.138910294
H	-11.570916176	7.686217785	-0.046461605
H	-8.286938667	7.934111595	-2.767766476
H	-8.978422165	7.279989719	2.772207022
H	-10.289870262	6.224061489	1.417166829
C	-4.396987915	3.576186180	3.045819998
H	-3.722412109	3.102279425	2.322666883
C	-4.205279827	2.914272308	4.418108463
C	-4.058356285	5.078794003	3.126830101

H	-4.176626205	5.587821484	2.166073322
H	-4.707277298	5.579063892	3.852385759
H	-3.020561695	5.205158234	3.451741457
H	-4.862545013	3.362162828	5.168173790
H	-3.173741102	3.078423500	4.749357700
H	-4.380268574	1.838526487	4.403329849
C	-6.705910206	1.694362402	2.001368999
H	-6.085997105	1.295061946	1.196132302
C	-8.146991730	1.799193144	1.473664403
C	-6.630517006	0.776565492	3.229779720
H	-5.603651524	0.516356945	3.494793892
H	-7.116182327	1.220703125	4.104039192
H	-7.158911705	-0.157097116	3.006825686
H	-8.826880455	2.144948959	2.258417130
H	-8.477431297	0.812516809	1.134458423
H	-8.217532158	2.485110044	0.628557324
C	-7.306438923	4.572436333	-2.779170275
H	-6.520855427	3.825244904	-2.926892519
C	-7.683331966	5.221372604	-4.120568752
C	-8.522960663	3.885523796	-2.136723757
H	-8.238204956	3.347088814	-1.232997179
H	-9.306435585	4.609095097	-1.894942045
H	-8.939723969	3.155531645	-2.835239649
H	-8.490150452	5.948249817	-3.990132570
H	-8.052256584	4.448320389	-4.803509712
H	-6.844467640	5.718483925	-4.612112999
C	-5.128612041	6.701378345	-2.307682753
H	-4.534695148	6.968290329	-1.422845483
C	-5.510746479	8.002038956	-3.030488491
C	-4.276852608	5.770536900	-3.195933342
H	-4.052060604	4.806813717	-2.732288361
H	-4.773912907	5.570611954	-4.149627209
H	-3.325100899	6.262823582	-3.420676708
H	-6.118371487	7.810002327	-3.919936895
H	-4.599071980	8.512911797	-3.358370543
H	-6.060163498	8.682916641	-2.375624418
C	-10.802419662	8.932246208	-2.358426809
H	-11.835018158	8.582604408	-2.465129852
H	-10.846479416	9.941473007	-1.931267023
H	-10.371246338	9.017519951	-3.360356569
C	-8.646674156	4.835985661	6.742268562
H	-8.500120163	5.747694492	7.331537724
H	-9.692633629	4.532519817	6.872817039
H	-8.019768715	4.051380634	7.176244259

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C1

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C	-1.126738310	-0.340975165	-2.973349571
Ni	-1.603474021	1.352197289	-0.625648022
P	-2.797971964	0.220593289	0.903960228
C	-2.825896978	-1.437156677	0.165926218
C	-2.283762217	-1.516205788	-1.157623410
N	-1.633882999	-0.415839344	-1.669717789
C	-1.350847244	0.875231445	-3.673357248
P	-2.283102512	2.093600750	-2.681311846
C	-3.426446438	-2.556223392	0.763160348
C	-2.486784458	-2.743354797	-1.843743682
C	-0.337619066	-1.319533467	-3.609562159
C	-0.823769212	1.072393179	-4.953210354
C	-3.558923960	-3.773265123	0.098121144
C	-3.096978188	-3.824515581	-1.227924943
C	0.167024881	-1.106293678	-4.889142990
C	-0.065404095	0.085159056	-5.590652466
H	-3.823714018	-2.468437672	1.769793391
H	-3.221446514	-4.745154381	-1.795733213
H	0.777874649	-1.880896211	-5.348788738
H	-0.993781269	2.011994600	-5.470645428
H	-2.168085337	-2.837686777	-2.874249697
H	-0.087399580	-2.229253769	-3.076487064
C	-4.568472862	0.833320737	0.989474654
H	-4.784485340	0.970746636	-0.076345876
C	-4.583627701	2.218106508	1.656797767
C	-5.639370441	-0.107403211	1.555293918
H	-5.645285130	-1.067092299	1.033142567
H	-5.501525402	-0.299783856	2.622734785
H	-6.628873825	0.349428266	1.430279613
H	-4.405558586	2.141016006	2.735229969
H	-5.560269833	2.695951939	1.518490314
H	-3.816518545	2.876692057	1.234846354
C	-2.060500622	0.197411940	2.623370647
H	-2.070323467	1.263011575	2.891661644
C	-0.595329225	-0.254941314	2.513303041
C	-2.801274776	-0.591670156	3.711352587
H	-3.829251051	-0.250038713	3.852727413
H	-2.819253445	-1.661108136	3.481769562
H	-2.279019117	-0.474101454	4.668545246
H	-0.533372104	-1.308875203	2.226747513
H	-0.093986474	-0.131228939	3.479949951
H	-0.050019208	0.324163944	1.762911558
C	-1.921246052	3.788151264	-3.400848627
H	-0.846449852	3.716681242	-3.616342068
C	-2.116870403	4.866308212	-2.319351435
C	-2.656181812	4.173609257	-4.695989609
H	-2.567843199	3.418041706	-5.479971409
H	-3.721927404	4.338856220	-4.511726856
H	-2.245352983	5.112185478	-5.086985588
H	-3.171082497	4.960662365	-2.038075447
H	-1.788632631	5.841480732	-2.698081732
H	-1.548699737	4.642495155	-1.413673639

C	-4.091435909	1.634207726	-2.917075396
H	-4.124942303	0.710658789	-2.324762583
C	-4.525803566	1.285317183	-4.347017288
C	-5.018680573	2.669638872	-2.261129379
H	-4.685221672	2.938980341	-1.253896475
H	-5.074721336	3.589401722	-2.852408409
H	-6.036553383	2.269772291	-2.184291363
H	-4.582812309	2.170454979	-4.985781670
H	-5.522819996	0.828809023	-4.327738762
H	-3.837637901	0.573362947	-4.810639858
O	-1.064134717	3.572336197	0.920757949
N	-0.822789192	2.607444048	0.271402836
N	0.616733789	-1.109552264	-0.556522012
O	0.366708815	-2.123630524	-0.032196272
C	0.507969320	0.299258143	-6.971697330
H	1.603584051	0.353048593	-6.948409557
H	0.241992205	-0.521439731	-7.648395538
H	0.141926154	1.229244709	-7.417996883
C	-4.193191528	-4.978670597	0.748930752
H	-5.065587521	-5.331109524	0.184226409
H	-3.490794659	-5.819490433	0.808172107
H	-4.526142120	-4.755301476	1.767440438

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C	-1.646672726	-0.548103750	-3.160926104
Ni	-2.086540699	1.202450633	-0.854463935
P	-2.597127438	-0.010699289	0.940583110
C	-2.747223616	-1.659900427	0.207426086
C	-2.563496590	-1.698004842	-1.207700849
N	-2.146207809	-0.552878678	-1.859133601
C	-1.729392529	0.669628918	-3.892387390
P	-2.430235624	2.027930737	-2.918957472
C	-3.100127220	-2.816406965	0.920784593
C	-2.898699760	-2.922334909	-1.846190333
C	-0.962738216	-1.613889575	-3.790724993
C	-1.205530047	0.782146931	-5.183749676
C	-3.340025425	-4.034030914	0.287052333
C	-3.262129545	-4.043044090	-1.116767645
C	-0.449611515	-1.479100823	-5.075944901
C	-0.568703473	-0.290199429	-5.812011719
H	-3.221775770	-2.758980513	1.997883201
H	-3.506947756	-4.957842827	-1.653919935
H	0.081937440	-2.321499825	-5.515028954
H	-1.273498774	1.729448676	-5.711353779
H	-2.888557673	-2.978364944	-2.927844286
H	-0.795009196	-2.537250519	-3.249399662
C	-4.280598640	0.490236402	1.619025707
H	-4.793442249	0.811543107	0.702557087
C	-4.146346092	1.713661313	2.540877581
C	-5.120077133	-0.620839238	2.264723778
H	-5.279166698	-1.460907221	1.585448146
H	-4.657509804	-1.004791141	3.179674864
H	-6.101634502	-0.215923414	2.538936853
H	-3.626544237	1.457755804	3.470452785
H	-5.143431187	2.077201366	2.814148188
H	-3.610782146	2.533250093	2.057893991
C	-1.326390505	-0.010408076	2.304944515
H	-1.310715556	1.039260507	2.626325846
C	0.035249334	-0.343770236	1.670730233
C	-1.618818998	-0.903439283	3.518323660
H	-2.582357645	-0.678889871	3.984255314
H	-1.608701944	-1.961047053	3.238606453
H	-0.841024816	-0.758820236	4.277379990
H	0.044111203	-1.373412371	1.296763539
H	0.829306662	-0.247520611	2.419617653
H	0.268891484	0.322733581	0.835922837
C	-1.788750410	3.634310961	-3.638239145
H	-0.761696219	3.365158796	-3.917139769
C	-1.719516873	4.742847919	-2.572756767
C	-2.525745392	4.133872986	-4.893064499
H	-2.645828962	3.365138531	-5.660146713
H	-3.520603895	4.511440754	-4.637244225
H	-1.965342522	4.965979099	-5.334823608
H	-2.702916622	4.951568604	-2.139683247
H	-1.358728051	5.668756962	-3.035691738
H	-1.037501574	4.483711243	-1.761823773
C	-4.296043396	1.882244706	-3.070757389
H	-4.432785988	0.909995377	-2.579598188
C	-4.868760109	1.775396466	-4.490363121
C	-4.992201328	2.952380180	-2.215653419
H	-4.573771000	2.991859674	-1.203758836
H	-4.892627239	3.948719978	-2.659803867
H	-6.063642502	2.735164642	-2.136267662
H	-4.886835575	2.741010904	-5.001346588
H	-5.902113438	1.411598086	-4.440823078
H	-4.294337273	1.072248936	-5.101274967
O	-2.240254879	3.573876619	0.522183359
N	-1.584850669	2.718404531	0.000233226
N	0.390575528	3.000808716	-0.241632089
O	0.830295086	2.086468220	-0.858643293
C	0.002857168	-0.170711443	-7.204690933
H	1.089493394	-0.322188228	-7.207677841
H	-0.426991910	-0.918067098	-7.882815361
H	-0.193224788	0.816842735	-7.634346485
C	-3.698956251	-5.281304359	1.057847023
H	-4.578264236	-5.778458595	0.630948722
H	-2.880708694	-6.012876034	1.046059608
H	-3.921394587	-5.055306911	2.105631351

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C	-1.290332437	-0.773603857	-2.947508335
Ni	-2.267061472	1.094050765	-0.907123208
P	-2.735979319	-0.059549950	0.951963663
C	-2.909539938	-1.725547194	0.251568645
C	-2.528090477	-1.820736885	-1.120485783
N	-1.990606904	-0.706728458	-1.746495366
C	-1.227326155	0.396947622	-3.753920317
P	-2.042111397	1.842938900	-3.013561964
C	-3.381904125	-2.850099802	0.946449876
C	-2.797826529	-3.059896469	-1.758891940
C	-0.542685151	-1.888720036	-3.398166895
C	-0.518998265	0.408515126	-4.961140633
C	-3.568453550	-4.082945824	0.323116720
C	-3.295493841	-4.144474030	-1.053512454
C	0.153236240	-1.851802349	-4.599402428
C	0.171855271	-0.714207232	-5.420908928
H	-3.625890493	-2.760302544	1.999823570
H	-3.487762213	-5.071812630	-1.590433598
H	0.716313183	-2.732578516	-4.902894974
H	-0.491274059	1.317119956	-5.556313038
H	-2.634469509	-3.155624628	-2.825546265
H	-0.486160159	-2.778450727	-2.782380819
C	-4.299064159	0.526149452	1.819975734
H	-4.806438446	1.067009211	1.010243654
C	-3.973145723	1.549875021	2.922686100
C	-5.243696213	-0.566542685	2.338146210
H	-5.515592098	-1.282606006	1.559476018
H	-4.800498486	-1.120410800	3.172950029
H	-6.164244175	-0.099912807	2.707750797
H	-3.457536221	1.078620672	3.765687466
H	-4.909293175	1.971881151	3.304739237
H	-3.363474846	2.380979776	2.565117836
C	-1.315461755	-0.104676344	2.165395260
H	-1.280001044	0.911114156	2.574743271
C	-0.022384373	-0.349575698	1.368283391
C	-1.480104804	-1.128372073	3.297052622
H	-2.401539087	-0.979952574	3.868565321
H	-1.485783458	-2.148116827	2.899457932
H	-0.638731897	-1.049396992	3.995607138
H	-0.055997308	-1.314609528	0.850698471
H	0.839785337	-0.355013579	2.044731617
H	0.132753983	0.430716395	0.616935968
C	-0.974981427	3.334927320	-3.424135923
H	0.028234450	2.889098406	-3.437103510
C	-1.025093675	4.373836517	-2.291309357
C	-1.227338433	3.998161077	-4.787834644
H	-1.181542158	3.294730425	-5.622350216
H	-2.203319311	4.491530895	-4.815069675
H	-0.467216641	4.768857479	-4.960328102
H	-2.029436350	4.794416904	-2.175017834
H	-0.342233628	5.200597286	-2.519160032
H	-0.733565867	3.945047855	-1.330004334
C	-3.751889229	1.949136376	-3.772418976
H	-4.192511082	1.032915115	-3.355457067
C	-3.820919752	1.855297327	-5.302322388
C	-4.527293205	3.149242401	-3.205765247
H	-4.518321991	3.155464172	-2.112165213
H	-4.108631611	4.099331856	-3.554647207
H	-5.570455074	3.109969854	-3.539782286
H	-3.486632109	2.778161764	-5.783117771
H	-4.859343052	1.683934450	-5.609738827
H	-3.215879679	1.027857304	-5.683964729
O	-3.529199123	3.241499901	0.093852356
N	-2.475629807	2.674053192	-0.027302627
N	-1.194806218	3.508692265	1.396517754
O	-1.884331822	4.334459782	1.882072091
C	0.951513648	-0.696787179	-6.714289188
H	2.033257723	-0.650697768	-6.533241749
H	0.764094234	-1.598520398	-7.308395863
H	0.686377287	0.167971939	-7.330717564
C	-4.062549114	-5.294990063	1.076264858
H	-4.900883675	-5.775887012	0.557985961
H	-3.276072741	-6.053261757	1.182529807
H	-4.402083397	-5.031527996	2.082921267

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C	-1.802443266	-0.535165370	-3.010735989
Ni	-2.650937796	1.196635604	-0.887310803
P	-2.762188673	0.005535683	0.988532424
C	-3.095886946	-1.627478004	0.271053582
C	-2.898399353	-1.661113620	-1.137152553
N	-2.464164257	-0.507501602	-1.780678153
C	-1.835263014	0.644001722	-3.800625086
P	-2.746786356	1.987777114	-2.990567207
C	-3.483149290	-2.779451132	0.970667303
C	-3.222293377	-2.872804880	-1.795641541
C	-1.023631334	-1.607284188	-3.499610662
C	-1.159584403	0.719864309	-5.021381855
C	-3.746924162	-3.983673811	0.318152428
C	-3.629696369	-3.990260363	-1.081423521
C	-0.358624876	-1.509126306	-4.717235088
C	-0.414855927	-0.355629355	-5.513455391
H	-3.593906879	-2.737177134	2.049185514
H	-3.875768423	-4.898686409	-1.628288031

H	0.243498221	-2.352250099	-5.050931931
H	-1.194304943	1.639642954	-5.598728180
H	-3.170443773	-2.921621323	-2.877190590
H	-0.911296189	-2.505729437	-2.903755665
C	-4.150919437	0.591412425	2.112919092
H	-4.784364223	1.138848424	1.403954983
C	-3.634481192	1.607684016	3.147677183
C	-4.996834755	-0.501368701	2.779653311
H	-5.416652679	-1.199054003	2.051630974
H	-4.417608261	-1.074352622	3.511934519
H	-5.829346180	-0.032097526	3.316631317
H	-3.001885891	1.126702070	3.900865078
H	-4.489693642	2.051080465	3.669218063
H	-3.071475267	2.425462246	2.693248510
C	-1.167477846	-0.124180898	1.948356032
H	-1.020673513	0.877588928	2.367000580
C	-0.034071624	-0.401345283	0.946040273
C	-1.199891925	-1.165943146	3.075409651
H	-2.001990557	-0.982025802	3.796868324
H	-1.330245256	-2.173805475	2.668838978
H	-0.249892443	-1.149208784	3.622209549
H	-0.183016405	-1.362676024	0.442035258
H	0.926099300	-0.438581169	1.472805500
H	0.015639290	0.384632617	0.188526571
C	-2.008252382	3.603701591	-3.587431431
H	-0.947176814	3.343641043	-3.695129633
C	-2.128069639	4.702396870	-2.517556906
C	-2.528337717	4.102556229	-4.946330547
H	-2.481675863	3.343785763	-5.730956554
H	-3.565047979	4.443516254	-4.869537830
H	-1.925962806	4.958597183	-5.271322250
H	-3.169974327	4.888863564	-2.239068747
H	-1.712096214	5.639110088	-2.906022787
H	-1.579530954	4.440680981	-1.612859488
C	-4.536878586	1.781087995	-3.512353182
H	-4.748460293	0.819749236	-3.024770737
C	-4.793548584	1.614009619	-5.016270638
C	-5.426746845	2.851991415	-2.862502337
H	-5.250829697	2.923915386	-1.784837484
H	-5.250716209	3.839495897	-3.303056717
H	-6.482516766	2.606144190	-3.025342941
H	-4.716414928	2.562770128	-5.552885056
H	-5.810042381	1.233007550	-5.170699120
H	-4.095923901	0.903213680	-5.469447136
O	-4.039186001	3.342615366	0.254974723
N	-2.917976379	2.820980310	0.069833577
N	-1.863829851	3.434584618	0.717137158
O	-0.797513068	2.830078840	0.488142520
C	0.320037395	-0.279593468	-6.831057072
H	1.389843583	-0.487566024	-6.707472324
H	-0.067058012	-1.010950089	-7.551465511
H	0.226321533	0.711749792	-7.285414219
C	-4.146205425	-5.228639603	1.073726058
H	-4.991307259	-5.735612869	0.593811870
H	-3.322840452	-5.953118324	1.120345592
H	-4.437660694	-4.997505188	2.103034735

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C	-1.813319683	-0.550358951	-3.081213713
Ni	-2.548568249	1.167111874	-0.915980935
P	-2.761223793	-0.025364252	0.979031205
C	-2.999997854	-1.665105104	0.248328656
C	-2.832762241	-1.682269812	-1.163736343
N	-2.409965754	-0.523539186	-1.812689185
C	-1.881596565	0.623107016	-3.876552343
P	-2.707431555	1.985989094	-3.015169859
C	-3.358705997	-2.829860687	0.942357421
C	-3.175242662	-2.884087563	-1.829325557
C	-1.064144254	-1.628527403	-3.600037336
C	-1.274284124	0.683188915	-5.133854389
C	-3.623193264	-4.030106068	0.282999635
C	-3.550685406	-4.015610218	-1.119317770
C	-0.468039364	-1.546453953	-4.854070663
C	-0.566247821	-0.401231706	-5.658059597
H	-3.455597162	-2.795843363	2.022816658
H	-3.806873322	-4.917604446	-1.671909213
H	0.111150622	-2.395728588	-5.211497784
H	-1.335812092	1.599088192	-5.715012550
H	-3.158638954	-2.917997837	-2.912391186
H	-0.921749115	-2.521005154	-3.001913786
C	-4.294150352	0.515895009	1.920806527
H	-4.910229683	0.927479446	1.111826897
C	-3.956047058	1.671094298	2.877921343
C	-5.087888241	-0.593886733	2.623653412
H	-5.397116661	-1.380450130	1.931763768
H	-4.515501499	-1.055015564	3.435497284
H	-5.992163658	-0.160639614	3.066984177
H	-3.309673548	1.340649247	3.698069096
H	-4.883267879	2.049992561	3.322615147
H	-3.477621555	2.500467539	2.354180813
C	-1.277566791	-0.055752914	2.104139566
H	-1.220844388	0.961584926	2.505657911
C	-0.032418136	-0.278484911	1.229988456
C	-1.362954497	-1.064824343	3.257211685
H	-2.238241434	-0.899525642	3.892967463
H	-1.399023414	-2.091847897	2.880323887
H	-0.472284734	-0.975828290	3.890058041
H	-0.073129043	-1.247918367	0.720436990

H	0.866987109	-0.256481916	1.854783297
H	0.059560657	0.510176599	0.478225440
C	-1.983964205	3.596348286	-3.634073257
H	-0.929307222	3.329702139	-3.783696175
C	-2.058023453	4.694234371	-2.557821751
C	-2.554241657	4.101024628	-4.970921040
H	-2.546488047	3.344140053	-5.759041309
H	-3.583846807	4.450673580	-4.850875378
H	-1.958973169	4.953199387	-5.318415642
H	-3.091448784	4.917810440	-2.278889894
H	-1.604471684	5.613056660	-2.947925806
H	-1.527888298	4.403770447	-1.650351167
C	-4.533647537	1.824927568	-3.410971880
H	-4.746214390	0.879438460	-2.893632650
C	-4.893625259	1.640511632	-4.891903877
C	-5.345052719	2.936675072	-2.727581263
H	-5.061916828	3.050324202	-1.677571535
H	-5.196356297	3.901046753	-3.224954844
H	-6.414661884	2.703199148	-2.781687737
H	-4.802287102	2.572596550	-5.454974174
H	-5.935722828	1.309261322	-4.974071980
H	-4.262182236	0.885748982	-5.370231152
O	-3.222076654	2.985169649	-0.031692248
N	-1.921496987	2.817095041	0.167825118
N	-1.349493742	3.358089924	1.174446464
O	-0.207327873	3.075061798	1.574905276
C	0.091027945	-0.341433167	-7.016635418
H	1.173556328	-0.503756821	-6.946959019
H	-0.305880219	-1.111513138	-7.689362049
H	-0.067672603	0.629579127	-7.495936394
C	-3.985839128	-5.288485050	1.034191132
H	-4.828099728	-5.808378696	0.563528061
H	-3.146906614	-5.995778561	1.061232209
H	-4.264377594	-5.071280479	2.070056915

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C	-1.323195815	-0.679638505	-3.072677135
Ni	-2.350317478	1.158113956	-1.098913193
P	-2.709051371	0.038979854	0.816452861
C	-2.954144001	-1.619354606	0.119165309
C	-2.599590540	-1.710210681	-1.256192923
N	-2.071742773	-0.590969384	-1.894680142
C	-1.274494648	0.461788386	-3.917308569
P	-2.170135260	1.875398517	-3.221865892
C	-3.435016632	-2.741460800	0.810268581
C	-2.875112057	-2.940830946	-1.902659655
C	-0.535379231	-1.787372708	-3.457574368
C	-0.521912158	0.462719619	-5.094628811
C	-3.643198013	-3.966905355	0.178920552
C	-3.374742985	-4.026278973	-1.198558807
C	0.205846995	-1.763266683	-4.633841515
C	0.224989176	-0.650364578	-5.487597466
H	-3.668835878	-2.655297518	1.866418481
H	-3.571985483	-4.951610565	-1.737063766
H	0.807598770	-2.634025812	-4.887763977
H	-0.497996300	1.354770422	-5.714951515
H	-2.706382990	-3.032519579	-2.969188929
H	-0.482781589	-2.657976389	-2.814256191
C	-4.255790234	0.665189445	1.685919881
H	-4.756113529	1.193294406	0.864926815
C	-3.900798082	1.709915280	2.757899523
C	-5.212371826	-0.400681704	2.236596107
H	-5.509675503	-1.122822165	1.472687483
H	-4.770030022	-0.950240850	3.074554920
H	-6.119388103	0.089241922	2.610028267
H	-3.404618025	1.249595404	3.618533134
H	-4.822762012	2.177377462	3.121603012
H	-3.259056568	2.503363371	2.368726254
C	-1.293188810	-0.068256810	2.029473066
H	-1.189926028	0.947970688	2.425353050
C	-0.018435156	-0.407527864	1.239161849
C	-1.521908879	-1.052811742	3.185075521
H	-2.432542324	-0.833372712	3.750987053
H	-1.588186979	-2.080450535	2.814802647
H	-0.677608430	-1.005336285	3.882783890
H	-0.097330011	-1.397431135	0.776357472
H	0.846031487	-0.411908597	1.911894202
H	0.165805370	0.325867921	0.450052053
C	-1.277583718	3.433761597	-3.749327421
H	-0.230727792	3.102895498	-3.758728027
C	-1.423474669	4.540451527	-2.691393137
C	-1.635306835	3.962293863	-5.148716450
H	-1.565692663	3.201757193	-5.930084229
H	-2.650101662	4.370955467	-5.166189194
H	-0.951426923	4.777224064	-5.412343502
H	-2.467532158	4.838894844	-2.561104774
H	-0.855635464	5.423270226	-3.007919312
H	-1.048539639	4.218888760	-1.719676018
C	-3.920328379	1.792125463	-3.886370420
H	-4.247669220	0.859542608	-3.406419277
C	-4.076011181	1.621179819	-5.403308868
C	-4.761435032	2.944093943	-3.313287973
H	-4.618241787	3.045563698	-2.232590437
H	-4.497426033	3.899577141	-3.779094934
H	-5.824867725	2.766556025	-3.510164022
H	-3.873498440	2.549109459	-5.943486691
H	-5.106689453	1.326235890	-5.633917809
H	-3.409631729	0.844304860	-5.790572166

O	-2.826221943	2.880479813	-0.364927411
N	-2.006865978	3.403036118	0.533334672
N	-0.831600606	2.911046267	0.563806951
O	0.032435283	3.100516558	1.435377359
C	1.052552938	-0.647598028	-6.751080513
H	2.127040148	-0.670611382	-6.529049397
H	0.836397529	-1.522104979	-7.376033306
H	0.861052692	0.245857373	-7.353687286
C	-4.163710594	-5.173127651	0.924184561
H	-5.116157532	-5.524659634	0.507923305
H	-3.461663723	-6.014285564	0.868558586
H	-4.328328609	-4.950227737	1.983020067

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C	-2.303707361	-1.474319458	-3.062692165
Ni	-3.391501904	0.313639402	-1.092688560
P	-3.745918512	-0.806946516	0.813701630
C	-3.986436129	-2.459158421	0.088416412
C	-3.623787642	-2.549998999	-1.285143137
N	-3.108052254	-1.419335604	-1.918933153
C	-2.199635506	-0.296713203	-3.853405952
P	-3.157446623	1.103400826	-3.194955826
C	-4.459733963	-3.583318710	0.778963566
C	-3.879157543	-3.781150818	-1.931143403
C	-1.501079559	-2.571368933	-3.439313889
C	-1.361047268	-0.253198028	-4.969986916
C	-4.657562733	-4.810837269	0.144210100
C	-4.378614426	-4.870934486	-1.229609728
C	-0.673601925	-2.502764702	-4.555739403
C	-0.587384939	-1.353086710	-5.352125168
H	-4.697031021	-3.499410629	1.834450841
H	-4.563917160	-5.798485756	-1.767881155
H	-0.059740867	-3.366412878	-4.803709030
H	-1.287929773	0.661173344	-5.550982475
H	-3.699190378	-3.870635509	-2.996246099
H	-1.496904850	-3.467497349	-2.830157042
C	-5.261153698	-0.172915414	1.715664864
H	-5.784816265	0.339716852	0.901023746
C	-4.860870838	0.901594222	2.741599798
C	-6.184615135	-1.232991934	2.329183340
H	-6.522371292	-1.963427186	1.590313911
H	-5.701822758	-1.771139503	3.152266741
H	-7.071205616	-0.736091673	2.739896536
H	-4.330131054	0.468556404	3.595943213
H	-5.769264698	1.379411578	3.124853849
H	-4.239730358	1.682291508	2.297154665
C	-2.274756193	-0.902116656	1.949242830
H	-2.147240639	0.125137359	2.307987452
C	-1.041744351	-1.264890194	1.104028583
C	-2.468138218	-1.861505866	3.131719351
H	-3.345159531	-1.612990141	3.737204313
H	-2.572438717	-2.894260168	2.783800602
H	-1.589700460	-1.819727421	3.785984993
H	-1.164323807	-2.242057800	0.624148965
H	-0.158607796	-1.311709166	1.750938654
H	-0.857837200	-0.506358325	0.340399653
C	-2.326977015	2.688891172	-3.738200188
H	-1.262816548	2.429357767	-3.665537119
C	-2.613446712	3.845357895	-2.763546705
C	-2.635339499	3.113795042	-5.185962200
H	-2.485907316	2.316247463	-5.917341709
H	-3.666849613	3.465200663	-5.279521465
H	-1.980432868	3.948286772	-5.461119652
H	-3.683968067	4.056471348	-2.692302227
H	-2.114117861	4.751105309	-3.126822948
H	-2.249943972	3.633207798	-1.758818388
C	-4.890310287	0.932259560	-3.898869038
H	-5.224820614	0.038959116	-3.353907108
C	-4.967532158	0.622213721	-5.400858879
C	-5.786569595	2.109813452	-3.482504845
H	-5.698419571	2.319372654	-2.413112640
H	-5.530304909	3.019527912	-4.035922527
H	-6.831832409	1.872861385	-3.713040590
H	-4.727849483	1.497103095	-6.010519981
H	-5.989633083	0.316868395	-5.653959751
H	-4.292238712	-0.190163389	-5.684286118
O	-4.466018200	1.920803070	-0.495638371
N	-3.430554152	2.499751806	0.138837814
N	-2.411433220	1.739413023	0.009809805
O	-1.272338867	1.912011147	0.500127375
C	0.337886661	-1.292838335	-6.543971539
H	1.389433861	-1.251303792	-6.233036041
H	0.226675257	-2.175573349	-7.183705807
H	0.141970068	-0.408897102	-7.158682346
C	-5.176190376	-6.017838955	0.889445066
H	-6.103509903	-6.397565365	0.443589509
H	-4.451603413	-6.841158867	0.873265266
H	-5.385138988	-5.782069683	1.937449574

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C	-1.327028513	-0.679488897	-3.109536409
Ni	-2.318876743	1.151604533	-1.106160283
P	-2.711835623	0.009948747	0.779997766
C	-2.996905327	-1.631374717	0.058278635
C	-2.628131628	-1.711774588	-1.314380884
N	-2.069315195	-0.596155465	-1.927502036

C	-1.278433800	0.468837142	-3.944689751
P	-2.192604780	1.867260337	-3.237872601
C	-3.511161089	-2.750817060	0.729542851
C	-2.919125319	-2.929525852	-1.978878856
C	-0.545414686	-1.787253499	-3.504619598
C	-0.521394312	0.479622036	-5.119053841
C	-3.736980677	-3.963919163	0.080147684
C	-3.450409651	-4.012502193	-1.294342399
C	0.199610963	-1.754086256	-4.678705692
C	0.226274222	-0.631349862	-5.518944740
H	-3.758256435	-2.672438145	1.783214808
H	-3.659018993	-4.927183151	-1.846557975
H	0.798059404	-2.624655485	-4.940801620
H	-0.493922502	1.376249433	-5.731988907
H	-2.736206293	-3.012683153	-3.043914795
H	-0.499420971	-2.664457560	-2.869409561
C	-4.258283615	0.669088006	1.620183229
H	-4.747165203	1.178735375	0.781002879
C	-3.896486044	1.744373322	2.658029318
C	-5.229322433	-0.369809866	2.195838451
H	-5.542371750	-1.099646568	1.445842981
H	-4.793839455	-0.912376344	3.041842461
H	-6.126769066	0.141818151	2.563478708
H	-3.391969442	1.312349200	3.528698206
H	-4.815246105	2.222776175	3.015658379
H	-3.262758970	2.523925304	2.232143164
C	-1.327065229	-0.164318815	2.020848989
H	-1.169389606	0.850912333	2.402664185
C	-0.065090567	-0.596041143	1.255503297
C	-1.627590895	-1.112197161	3.190565109
H	-2.523712873	-0.823837817	3.747765541
H	-1.759716988	-2.138673782	2.835077286
H	-0.784824669	-1.111964107	3.891874313
H	-0.201702341	-1.587499619	0.810302615
H	0.787758410	-0.643273592	1.941316724
H	0.177512839	0.111705638	0.459777564
C	-1.366951466	3.443437338	-3.821200848
H	-0.306543112	3.157924891	-3.817329645
C	-1.562447071	4.587224007	-2.811264753
C	-1.743627429	3.905290127	-5.239730358
H	-1.655089259	3.116970301	-5.990919590
H	-2.770870447	4.281142712	-5.268072128
H	-1.086548686	4.730094910	-5.539052010
H	-2.616387367	4.864997387	-2.718065739
H	-1.009665489	5.471002579	-3.151408195
H	-1.209952116	4.317103386	-1.816769361
C	-3.955094337	1.723205328	-3.859632969
H	-4.243145943	0.789112687	-3.358376741
C	-4.142529488	1.525271058	-5.369538784
C	-4.814485073	2.858952522	-3.281668663
H	-4.636101723	2.987730265	-2.208801031
H	-4.598589897	3.811990738	-3.776639938
H	-5.877754688	2.643031597	-3.437116623
H	-3.977607965	2.449839592	-5.928245068
H	-5.170027733	1.199451923	-5.571290970
H	-3.464502096	0.760762632	-5.761275768
O	-2.765199423	2.833439350	-0.348848313
N	-1.855667233	3.523479462	0.488024414
N	-0.764448762	3.032674789	0.674502313
O	0.360364825	2.590474606	0.904749930
C	1.061329722	-0.615867019	-6.777442455
H	2.134662628	-0.628011167	-6.548976421
H	0.858063519	-1.490672708	-7.406176567
H	0.863665760	0.277437210	-7.378231525
C	-4.290338039	-5.168649197	0.803763151
H	-5.222929001	-5.521102905	0.345811903
H	-3.586182356	-6.009820461	0.781899512
H	-4.501996517	-4.943381310	1.853695273

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C4

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C	-2.426731348	-1.568637490	-3.093466043
Ni	-3.466004610	0.244010240	-1.119398355
P	-3.740521193	-0.838526368	0.828159213
C	-3.905472994	-2.520999432	0.157610103
C	-3.644908190	-2.628176451	-1.237828851
N	-3.202762365	-1.498821020	-1.930459619
C	-2.310074329	-0.398076892	-3.894210815
P	-3.172571421	1.064763904	-3.230662823
C	-4.275109291	-3.647391319	0.905909538
C	-3.914767504	-3.878839970	-1.839151263
C	-1.654136658	-2.684778452	-3.483877420
C	-1.512465596	-0.392222226	-5.042648315
C	-4.471960068	-4.894101620	0.311398566
C	-4.311955452	-4.972292423	-1.080042124
C	-0.864112318	-2.649937868	-4.628108978
C	-0.782822132	-1.513920665	-5.442725658
H	-4.427777767	-3.549808264	1.975779057
H	-4.508560181	-5.916268826	-1.584577799
H	-0.279800832	-3.531359196	-4.885130882
H	-1.438197732	0.513851643	-5.636076927
H	-3.822741985	-3.982321739	-2.914001465
H	-1.646058559	-3.574815273	-2.866785049
C	-5.247871876	-0.288708568	1.796615958
H	-5.823301792	0.206105694	1.005895257
C	-4.869927883	0.777718365	2.840460539
C	-6.098310947	-1.403960228	2.418606520
H	-6.415379047	-2.144541979	1.680956721
H	-5.568737507	-1.922775626	3.225665092

H	-6.999325752	-0.957315922	2.854467869
H	-4.311007500	0.343705654	3.676728725
H	-5.790085316	1.210633516	3.247938395
H	-4.286121368	1.595666051	2.412720442
C	-2.210987568	-0.745621145	1.880501628
H	-2.228384018	0.277117580	2.272429466
C	-0.984744847	-0.867552578	0.960404336
C	-2.195367336	-1.762479305	3.029063463
H	-3.071149349	-1.669863462	3.679853678
H	-2.163573265	-2.786826849	2.643959284
H	-1.303871274	-1.609521151	3.648074150
H	-0.998117208	-1.803538561	0.391279876
H	-0.068396412	-0.847210526	1.561141729
H	-0.948884785	-0.024031587	0.264937192
C	-2.134090900	2.571953535	-3.638880491
H	-1.112909794	2.176842690	-3.560143948
C	-2.315502644	3.669366837	-2.573318005
C	-2.327607393	3.146061897	-5.053853035
H	-2.212043047	2.401841402	-5.844961166
H	-3.314440250	3.602941990	-5.165297031
H	-1.583077312	3.931935549	-5.224737167
H	-3.362975121	3.970754147	-2.476989508
H	-1.738751411	4.554138184	-2.867336750
H	-1.964511633	3.347145796	-1.591864347
C	-4.854629993	1.116281629	-4.063151836
H	-5.343897820	0.274498641	-3.555206537
C	-4.834736824	0.829045236	-5.571564674
C	-5.636197090	2.393717527	-3.718431950
H	-5.687848568	2.536041737	-2.637374163
H	-5.189588547	3.279245138	-4.181466103
H	-6.657634735	2.304647684	-4.106413841
H	-4.410630703	1.663405418	-6.137206078
H	-5.863358974	0.685655832	-5.922477245
H	-4.266400814	-0.073204845	-5.812481403
O	-5.073007107	1.513438582	-0.760293663
N	-4.297107697	2.346656084	-0.046333287
N	-3.119250298	1.854843378	-0.018759683
O	-2.121530056	2.305475712	0.603036761
C	0.092144571	-1.490944386	-6.671725273
H	1.156835198	-1.494389176	-6.406215191
H	-0.084965773	-2.367023706	-7.305896282
H	-0.093563803	-0.598187506	-7.276978493
C	-4.878939629	-6.102381229	1.118730903
H	-5.873576164	-6.461935520	0.827503204
H	-4.180181980	-6.934659004	0.973149717
H	-4.908696651	-5.876095295	2.188985348

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C5

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C	-2.728479147	-1.571593523	-3.229208231
Ni	-3.669175386	0.120384492	-1.148376942
P	-4.217266083	-0.998753428	0.684084833
C	-4.003641129	-2.684677839	0.076569803
C	-3.707772017	-2.761279345	-1.315330982
N	-3.426671743	-1.593341708	-2.016463041
C	-2.836874962	-0.402057856	-4.033100128
P	-3.783550024	0.918491960	-3.236768723
C	-4.203519344	-3.844041824	0.838339150
C	-3.788258553	-4.049761295	-1.901038885
C	-1.835532546	-2.568091631	-3.680825233
C	-2.124360323	-0.274650753	-5.228516102
C	-4.175336838	-5.114984989	0.266683251
C	-4.000615597	-5.181300640	-1.126486421
C	-1.136010170	-2.418341875	-4.874005318
C	-1.268422842	-1.280519962	-5.682783127
H	-4.409678459	-3.749483347	1.901103735
H	-4.041351795	-6.150635242	-1.619004011
H	-0.441932589	-3.201403856	-5.171597958
H	-2.213893175	0.638498425	-5.810595036
H	-3.691100597	-4.153875351	-2.974931479
H	-1.648895383	-3.440607071	-3.067420006
C	-6.064039707	-0.710148931	0.883434176
H	-6.382212639	-0.675319612	-0.168152630
C	-6.352357864	0.664769173	1.510760784
C	-6.838202000	-1.844510198	1.571705103
H	-6.681722164	-2.805641890	1.076261640
H	-6.555774689	-1.951879978	2.622995377
H	-7.910439014	-1.617798686	1.541181326
H	-6.106344223	0.674234927	2.577689171
H	-7.422196865	0.886172533	1.421965837
H	-5.783528328	1.460806847	1.026611209
C	-3.296158552	-0.667719185	2.264814138
H	-3.296283007	0.429288089	2.299185276
C	-1.845279813	-1.158014417	2.114109039
C	-3.942046642	-1.211731672	3.548738480
H	-4.952943802	-0.830014944	3.706794262
H	-3.983311176	-2.305595160	3.548460484
H	-3.336606979	-0.909242749	4.410880089
H	-1.810604930	-2.250376463	2.042616844
H	-1.270650744	-0.857864976	2.997383118
H	-1.351075053	-0.738351047	1.234720826
C	-3.154549599	2.564874411	-3.857631922
H	-2.081140995	2.368395567	-3.975113869
C	-3.330847740	3.674934149	-2.807393312
C	-3.730854273	3.003788710	-5.215637207
H	-3.671280146	2.230642796	-5.985901833
H	-4.779389858	3.300775290	-5.116189003
H	-3.178006411	3.879604101	-5.573925018
H	-4.383212566	3.837503910	-2.560183764

H	-2.931715488	4.614173889	-3.208007813
H	-2.806345701	3.446361542	-1.881000042
C	-5.597168922	0.644165218	-3.626052856
H	-5.742941380	-0.325782418	-3.131084442
C	-5.962206364	0.473702401	-5.107201099
C	-6.463662624	1.688199162	-2.902564049
H	-6.166636944	1.802611113	-1.854859352
H	-6.386578083	2.670818329	-3.379689932
H	-7.517720222	1.389538884	-2.935928345
H	-5.948546410	1.424776435	-5.644672394
H	-6.976707458	0.065380186	-5.188162327
H	-5.279830456	-0.217764378	-5.611042500
O	-3.904993773	1.791976094	-0.174857676
N	-2.572788000	1.980996370	0.032029506
N	-1.966085792	1.012139320	-0.534596205
O	-0.734549761	0.808843195	-0.557764530
N	-4.841534138	4.114428520	0.122926176
O	-3.877319336	4.735115528	0.306293309
C	-0.464367598	-1.117805004	-6.950684071
H	0.573748827	-0.836588144	-6.730860710
H	-0.430905670	-2.047285080	-7.529250145
H	-0.884194016	-0.337905109	-7.593954086
C	-4.340251446	-6.364935875	1.096449018
H	-4.993529320	-7.092838287	0.602426469
H	-3.376129150	-6.861435890	1.266516209
H	-4.769729137	-6.141344070	2.078055620

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C	-1.114636540	-0.951893806	-2.862332582
Ni	-2.333590508	0.800931334	-1.001938105
P	-2.628741026	-0.381988406	0.869172275
C	-2.974797726	-2.000931263	0.127127677
C	-2.580526114	-2.045344353	-1.234576941
N	-2.039807320	-0.899790585	-1.814397335
C	-0.983474791	0.202586740	-3.675711155
P	-2.087837934	1.538720012	-3.131712675
C	-3.484856367	-3.141467810	0.763414860
C	-2.807176828	-3.252291203	-1.935370445
C	-0.253065288	-2.034032345	-3.131230831
C	-0.055492267	0.248458490	-4.717330933
C	-3.671680212	-4.341622829	0.076266296
C	-3.336651802	-4.360013962	-1.288272738
C	0.663317621	-1.966954470	-4.176721096
C	0.785049200	-0.835173428	-4.994914055
H	-3.743356228	-3.097648144	1.816202164
H	-3.502935886	-5.270250797	-1.861365080
H	1.321633220	-2.816462994	-4.348037243
H	0.036672324	1.148668408	-5.317964077
H	-2.574043274	-3.306396008	-2.993079901
H	-0.284130633	-2.916357994	-2.502123594
C	-4.055827141	0.276822865	1.891477108
H	-4.653513432	0.789894223	1.127350211
C	-3.549431086	1.336803555	2.885336876
C	-4.948962688	-0.765201986	2.577824354
H	-5.382724762	-1.466876149	1.861812115
H	-4.402224064	-1.336540461	3.335115194
H	-5.772899151	-0.251713336	3.086748362
H	-2.978292227	0.876936972	3.698437452
H	-4.407138348	1.849766970	3.333571434
H	-2.919602394	2.090697765	2.408187866
C	-1.106185079	-0.594303668	1.927484989
H	-0.910743177	0.400981337	2.340144157
C	0.070436858	-0.966505826	1.008522987
C	-1.289332747	-1.609060407	3.065081835
H	-2.103639126	-1.338818550	3.744370937
H	-1.489477515	-2.609774113	2.668636084
H	-0.368527949	-1.664976954	3.656938314
H	-0.126095131	-1.902088404	0.473489821
H	0.972528934	-1.103889108	1.614790916
H	0.274514735	-0.172490850	0.287805229
C	-1.296729326	3.171486855	-3.593201160
H	-0.236206695	2.975222588	-3.387572050
C	-1.765540481	4.304978848	-2.664033175
C	-1.447721839	3.582988501	-5.068220615
H	-1.164348483	2.796184301	-5.770879745
H	-2.478565454	3.875052452	-5.290041447
H	-0.812437654	4.453963757	-5.265815258
H	-2.843328476	4.476758480	-2.750012159
H	-1.261040807	5.236435890	-2.944514036
H	-1.533916593	4.098402023	-1.619346857
C	-3.706083536	1.246925831	-4.035481453
H	-4.012457848	0.310614645	-3.549956799
C	-3.596584558	0.985928297	-5.544368267
C	-4.744949341	2.326122046	-3.695136786
H	-4.840862751	2.474689245	-2.615526915
H	-4.487797737	3.288860321	-4.149556160
H	-5.726023197	2.033042908	-4.085876465
H	-3.392370701	1.901952624	-6.104292870
H	-4.547074318	0.582120776	-5.912490368
H	-2.811405897	0.259878486	-5.773946762
O	-2.820584297	2.554085255	-0.132161736
N	-1.442723632	3.209460735	0.698075056
N	-0.662708104	2.294422150	0.404308915
O	0.530201793	2.246958494	0.823806942
N	-3.984886408	3.246678114	-0.276126176
O	-4.012842655	4.319102764	0.243223727
C	1.814178586	-0.774964571	-6.098265171
H	2.829448700	-0.672665715	-5.694438457

H	1.801688313	-1.684636831	-6.709212303
H	1.638707399	0.075907230	-6.763909817
C	-4.219572067	-5.573603630	0.756572187
H	-5.121899605	-5.942579269	0.253928244
H	-3.490749359	-6.393547535	0.748547971
H	-4.480010509	-5.373476028	1.800440669

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C	-1.335194588	-0.729341924	-2.915296078
Ni	-2.261938334	1.081859231	-0.877839208
P	-2.720204353	-0.052677535	0.976004660
C	-2.974309206	-1.698652625	0.259762228
C	-2.637161732	-1.765793324	-1.121521950
N	-2.081072092	-0.646732211	-1.734776974
C	-1.226427674	0.440453947	-3.713674784
P	-2.071395636	1.867456913	-2.980318785
C	-3.471937180	-2.823191643	0.935646534
C	-2.958342791	-2.973365784	-1.791073680
C	-0.600391686	-1.858124137	-3.343492746
C	-0.475565404	0.449358732	-4.892393112
C	-3.718241453	-4.028162003	0.280023307
C	-3.475667238	-4.061017513	-1.103358150
C	0.141199827	-1.825731039	-4.519404888
C	0.214315251	-0.683674216	-5.329900265
H	-3.691467047	-2.752993345	1.996104717
H	-3.709382772	-4.966863155	-1.659908414
H	0.697683930	-2.715400934	-4.808487415
H	-0.409915775	1.361536503	-5.479480743
H	-2.813402891	-3.044154167	-2.862573624
H	-0.587986708	-2.754426718	-2.734786749
C	-4.282251358	0.598704636	1.801711202
H	-4.746098042	1.152345896	0.975675523
C	-3.954336166	1.618300557	2.907266140
C	-5.271999836	-0.463386297	2.298744678
H	-5.552553177	-1.168875933	1.513542771
H	-4.865956783	-1.032438874	3.142340660
H	-6.183998585	0.033769820	2.648887157
H	-3.467494011	1.139518023	3.763439417
H	-4.889549255	2.061244965	3.267075300
H	-3.325046062	2.437937737	2.557376146
C	-1.330724478	-0.143556967	2.215575457
H	-1.297340751	0.860753834	2.652527332
C	-0.022736680	-0.378362387	1.441851735
C	-1.541062593	-1.187566400	3.320935011
H	-2.475903034	-1.034529686	3.869524240
H	-1.550897479	-2.199278355	2.903641701
H	-0.718339682	-1.133855939	4.043361187
H	-0.053807378	-1.327197790	0.894854665
H	0.823275328	-0.413723737	2.137396812
H	0.153907955	0.427172154	0.723006248
C	-1.109121919	3.402869940	-3.459513903
H	-0.078741670	3.025248766	-3.492341995
C	-1.196812510	4.470882893	-2.355312586
C	-1.451494336	4.001368999	-4.833961964
H	-1.410728931	3.269594193	-5.644194126
H	-2.450422764	4.447194576	-4.832370281
H	-0.737900972	4.799754620	-5.067626476
H	-2.230055571	4.779025078	-2.167788267
H	-0.629576981	5.359188080	-2.656157732
H	-0.783633590	4.107018948	-1.413094044
C	-3.812032461	1.855818629	-3.681184292
H	-4.177184582	0.925164104	-3.225330830
C	-3.929642439	1.712985396	-5.204890251
C	-4.641181469	3.021296740	-3.119763613
H	-4.567275524	3.082498550	-2.030071020
H	-4.314944267	3.980479240	-3.536339760
H	-5.695278645	2.890378237	-3.390702963
H	-3.686474323	2.644071817	-5.722602844
H	-4.962831020	1.454691887	-5.465769768
H	-3.278216124	0.922886848	-5.590216160
O	-3.550205469	3.347802162	0.092152484
N	-2.481926918	2.712221622	0.050777692
N	-1.385596514	3.129289389	0.880154014
O	-1.641845584	4.122241974	1.553267837
C	1.038985729	-0.673324466	-6.595327377
H	2.114111900	-0.699893713	-6.376409054
H	0.818625689	-1.542983055	-7.225115776
H	0.847473025	0.224878713	-7.190803528
C	-4.254452229	-5.239543438	1.005576491
H	-5.193398952	-5.591672897	0.560796022
H	-3.547855616	-6.077923775	0.965910017
H	-4.448924541	-5.021647453	2.060348749

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C	-1.778091192	-0.566291928	-3.066529512
Ni	-2.537009716	1.211151719	-0.880820811
P	-2.755756617	0.010725600	0.995037973
C	-3.035070658	-1.626261473	0.253713757
C	-2.818567753	-1.667936444	-1.152492404
N	-2.358591795	-0.525777459	-1.795051336
C	-1.861494660	0.599511862	-3.873369932
P	-2.701696873	1.963564634	-3.023193836
C	-3.443879366	-2.774077892	0.948803306
C	-3.158691883	-2.876763582	-1.810540318
C	-1.028761268	-1.645503640	-3.586492300
C	-1.266708136	0.651849389	-5.137558460

C	-3.711654663	-3.978491783	0.299176961
C	-3.584790707	-3.988363266	-1.099359274
C	-0.446820557	-1.571860790	-4.847313404
C	-0.558241248	-0.433340490	-5.659669876
H	-3.578243256	-2.724858046	2.024112940
H	-3.838778496	-4.893713474	-1.647865653
H	0.130573004	-2.422318935	-5.205434799
H	-1.340441823	1.560551763	-5.728663445
H	-3.103071928	-2.929027557	-2.891548872
H	-0.877505064	-2.532749414	-2.982248068
C	-4.250861645	0.569595516	1.994872332
H	-4.769058704	1.197424412	1.260354042
C	-3.837830305	1.491414309	3.153161287
C	-5.205015659	-0.533841014	2.468919992
H	-5.528330326	-1.184217691	1.653044939
H	-4.749652386	-1.159319878	3.244740009
H	-6.096689224	-0.069390669	2.906123161
H	-3.299557209	0.944478810	3.934894085
H	-4.739307880	1.917304635	3.607397795
H	-3.221441031	2.321830750	2.807397127
C	-1.261580467	-0.140909225	2.106949091
H	-1.204321742	0.827032447	2.611961842
C	-0.024223777	-0.301280081	1.208266854
C	-1.350929737	-1.260224819	3.152969360
H	-2.244789124	-1.176855326	3.779539108
H	-1.359577298	-2.244008064	2.674685717
H	-0.476691425	-1.218489051	3.813405991
H	-0.084697276	-1.222973228	0.619009018
H	0.884349346	-0.346781373	1.819175482
H	0.069219790	0.535513878	0.509015918
C	-2.022058010	3.563873053	-3.723005772
H	-0.969353020	3.306278706	-3.900247574
C	-2.073935747	4.697054386	-2.683664083
C	-2.641751289	4.021776199	-5.054744244
H	-2.656105518	3.238543510	-5.816318512
H	-3.669359446	4.368005753	-4.909321308
H	-2.065928936	4.865867615	-5.451854229
H	-3.101797819	4.919094086	-2.380661726
H	-1.646287560	5.609415054	-3.116192818
H	-1.513018727	4.449810028	-1.781542420
C	-4.532330990	1.752121329	-3.378712177
H	-4.699649811	0.796456158	-2.863495588
C	-4.932049751	1.567666173	-4.849033833
C	-5.352103233	2.833151817	-2.655522823
H	-5.073037624	2.918381929	-1.599928617
H	-5.217044830	3.815064192	-3.122701406
H	-6.419611931	2.590206385	-2.712031603
H	-4.909096718	2.509520531	-5.402508736
H	-5.957346916	1.182320952	-4.902085781
H	-4.278068542	0.852560639	-5.357702732
O	-3.801862955	3.316065788	0.539791942
N	-2.757534027	2.895592690	-0.029860802
N	-1.469669461	3.592328548	0.629735768
O	-1.146927953	3.061582088	1.639305949
C	0.086733662	-0.382073551	-7.024751186
H	1.176404119	-0.492935628	-6.960495949
H	-0.278921038	-1.187650442	-7.673141003
H	-0.118762717	0.567050397	-7.529701233
C	-4.133761883	-5.215497494	1.054943562
H	-4.985478401	-5.709531307	0.572970867
H	-3.322758436	-5.953560352	1.106109023
H	-4.425211430	-4.977642536	2.082820892

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C7

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C	-1.276861310	-0.655609369	-3.034967899
Ni	-2.291284084	1.170089602	-1.072453737
P	-2.674107075	0.015164088	0.845311701
C	-2.979428768	-1.617739439	0.111435860
C	-2.612265348	-1.689335465	-1.258868933
N	-2.052788496	-0.565306008	-1.870749950
C	-1.214776278	0.482314795	-3.878329754
P	-2.150840044	1.889230847	-3.216555357
C	-3.499279737	-2.738282442	0.774163783
C	-2.901824951	-2.896665573	-1.935677052
C	-0.483580917	-1.765489817	-3.389448404
C	-0.429127008	0.480080545	-5.033857822
C	-3.733655930	-3.943846464	0.111034214
C	-3.443125963	-3.983400583	-1.261646032
C	0.290356547	-1.746292353	-4.545496464
C	0.330767095	-0.635171950	-5.399642467
H	-3.743496418	-2.667545795	1.829013109
H	-3.654741764	-4.892137051	-1.821940303
H	0.899022877	-2.617206573	-4.780638695
H	-0.388226986	1.368153095	-5.657752514
H	-2.712485075	-2.971436501	-3.000310183
H	-0.452287227	-2.632548332	-2.739680529
C	-4.162984848	0.697926521	1.754407287
H	-4.648805618	1.264452934	0.950825632
C	-3.728350401	1.716200352	2.822777510
C	-5.146883011	-0.335907072	2.316862822
H	-5.500258446	-1.030719161	1.551274896
H	-4.704701424	-0.918152750	3.132805109
H	-6.019200325	0.187543005	2.725162983
H	-3.231507778	1.229056597	3.668241978
H	-4.619238377	2.221884251	3.211457253
H	-3.067116499	2.483513832	2.413975477
C	-1.213390589	-0.153429165	1.989731669
H	-1.053980947	0.862357795	2.368760109

C	0.014540400	-0.567388535	1.161125422
C	-1.463231802	-1.119980454	3.157367229
H	-2.337990761	-0.848301709	3.755456924
H	-1.601323485	-2.142564058	2.791807175
H	-0.592159450	-1.122938514	3.822793722
H	-0.144517481	-1.541482687	0.685073018
H	0.886052370	-0.653310359	1.820122957
H	0.227226928	0.178625047	0.393660426
C	-1.280452967	3.460093737	-3.723834515
H	-0.226313218	3.159129143	-3.674098492
C	-1.509059429	4.588946819	-2.704537630
C	-1.595928192	3.937867880	-5.152140617
H	-1.483870983	3.157804966	-5.909121513
H	-2.616588593	4.326416969	-5.218382835
H	-0.917180002	4.757859707	-5.412823200
H	-2.568827868	4.840854168	-2.608136654
H	-0.978286862	5.487198353	-3.041329622
H	-1.134442329	4.319108009	-1.719663501
C	-3.887610197	1.760336876	-3.896849632
H	-4.207987309	0.831140995	-3.404911995
C	-4.010963917	1.561774135	-5.413624287
C	-4.754856110	2.910926819	-3.359414101
H	-4.625127792	3.039060116	-2.280222893
H	-4.501388073	3.858099937	-3.847491264
H	-5.811678886	2.708068848	-3.567076683
H	-3.789441347	2.479723454	-5.963835239
H	-5.038689613	1.270297289	-5.660789013
H	-3.341430902	0.774502635	-5.773372173
O	-3.119952440	2.726422310	-0.393654644
N	-2.286348820	3.472012520	0.394301295
N	-1.073376894	3.158639431	0.399008065
O	-0.685054302	2.133867264	-0.379763544
C	1.193916082	-0.635450244	-6.638588428
H	2.260896206	-0.649585903	-6.383512020
H	1.001008034	-1.516757727	-7.261250973
H	1.013860464	0.251929134	-7.253060818
C	-4.298116207	-5.149701118	0.823345840
H	-5.220812798	-5.502424240	0.346766770
H	-3.591456175	-5.988741398	0.813178539
H	-4.529665470	-4.925568581	1.869085908

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C	-0.993089497	-0.619734466	-2.944968939
Ni	-2.116544485	1.203184247	-1.048343182
P	-2.244616985	0.078034580	0.910098970
C	-2.655626059	-1.545692325	0.225191414
C	-2.296461582	-1.657672405	-1.147609353
N	-1.764446974	-0.551710129	-1.793984175
C	-0.966149151	0.495704114	-3.825899124
P	-1.890775084	1.938598633	-3.220441818
C	-3.197308064	-2.634025812	0.924246490
C	-2.584917068	-2.892158270	-1.779144645
C	-0.192954123	-1.732935786	-3.291000128
C	-0.266424835	0.425590187	-5.038884163
C	-3.443048239	-3.856153965	0.300049126
C	-3.137069702	-3.947364807	-1.068984032
C	0.509137750	-1.765401840	-4.487211704
C	0.472751200	-0.701398730	-5.401935101
H	-3.432411671	-2.529380322	1.978342175
H	-3.353033543	-4.874188423	-1.597128034
H	1.114059448	-2.640784502	-4.715677738
H	-0.282822937	1.272330403	-5.716312408
H	-2.392767191	-3.005095482	-2.839746952
H	-0.119744413	-2.567728519	-2.603216410
C	-3.559915543	0.846686125	1.993040562
H	-4.166645527	1.373669505	1.246489763
C	-2.939464331	1.921710134	2.902838469
C	-4.460263252	-0.125705287	2.766365051
H	-4.972757816	-0.824869037	2.101215601
H	-3.900868654	-0.701974511	3.510663986
H	-5.225102901	0.447542548	3.302875519
H	-2.329747438	1.481567860	3.698072433
H	-3.747459888	2.485424042	3.382049799
H	-2.329470158	2.630129576	2.338703871
C	-0.646138787	-0.125859335	1.848508954
H	-0.346395701	0.895576596	2.107567549
C	0.423254848	-0.746254444	0.933805108
C	-0.842638731	-0.967991412	3.120689631
H	-1.566323042	-0.535538852	3.816180944
H	-1.170495152	-1.981709123	2.867143869
H	0.114698716	-1.053888798	3.647260904
H	0.132982031	-1.756153703	0.624805152
H	1.364817381	-0.821539462	1.489601374
H	0.582766175	-0.127036065	0.051131845
C	-0.840006530	3.480360508	-3.278999090
H	-0.134093806	3.252290964	-2.474888086
C	-1.658507705	4.717318058	-2.871315241
C	-0.041085616	3.738063574	-4.564208031
H	0.675940752	2.941443205	-4.770831108
H	-0.685943186	3.867146492	-5.439625740
H	0.527156830	4.667401791	-4.438381195
H	-2.278700352	5.072895050	-3.700868845
H	-0.969068646	5.525605679	-2.605486155
H	-2.292055607	4.517997742	-2.005249262
C	-3.445374012	2.057693481	-4.253057480
H	-3.850247860	1.045298934	-4.117267609
C	-3.215071201	2.284166336	-5.753901482
C	-4.459044456	3.061301470	-3.675046921

H	-4.541136742	2.992715120	-2.586737394
H	-4.186379910	4.089722157	-3.922692299
H	-5.447950840	2.867410421	-4.105270386
H	-2.794427395	3.275939941	-5.946882248
H	-4.172345638	2.224510193	-6.285441875
H	-2.547732115	1.533020496	-6.183477402
O	-2.435843468	2.861533403	-0.246960118
N	-1.294501066	3.435412407	0.261908889
N	-0.209879965	2.876700878	0.023403654
O	-0.231492400	1.753179908	-0.729530394
N	-4.074606895	1.029452085	-1.210343242
O	-4.533174992	0.070733324	-1.702713966
C	1.243222833	-0.761173666	-6.699257851
H	2.326019764	-0.717056870	-6.526123047
H	1.043203235	-1.692289829	-7.242057800
H	0.981792212	0.071566835	-7.359443188
C	-4.024768353	-5.033105850	1.046802759
H	-4.955813885	-5.382012367	0.583542466
H	-3.333537579	-5.884975910	1.056173801
H	-4.248251438	-4.777714729	2.087193966

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C	-1.245573640	-0.534068167	-2.832710743
Ni	-2.688810587	1.207967401	-1.014444113
P	-2.566235542	0.172295257	0.971757710
C	-2.829311609	-1.513232112	0.356153488
C	-2.476065636	-1.618088603	-1.018846989
N	-2.001798630	-0.478784591	-1.668223977
C	-1.265695214	0.571318746	-3.725819349
P	-2.183167219	2.015096664	-3.101713419
C	-3.293415070	-2.625455618	1.069613218
C	-2.712217808	-2.866229296	-1.643067598
C	-0.406828582	-1.622693062	-3.173192024
C	-0.584825158	0.500625432	-4.951144218
C	-3.490030289	-3.861174107	0.452777624
C	-3.207248211	-3.943242550	-0.920732319
C	0.274831265	-1.653064966	-4.380671978
C	0.180929065	-0.607616723	-5.313831806
H	-3.514977694	-2.527840614	2.126750231
H	-3.390269041	-4.880611897	-1.442787886
H	0.906697154	-2.510332108	-4.605404377
H	-0.629144371	1.341954231	-5.634384632
H	-2.528222084	-2.976525307	-2.705442667
H	-0.293459147	-2.444262505	-2.474870920
C	-3.849806786	0.805273712	2.172188282
H	-4.485999584	1.366095066	1.474915504
C	-3.236891508	1.825097322	3.149971485
C	-4.695841789	-0.243410125	2.903768301
H	-5.194370270	-0.922306359	2.207813740
H	-4.098546028	-0.837237179	3.605862856
H	-5.471550465	0.268026263	3.485623598
H	-2.584161520	1.345691562	3.888191938
H	-4.046001434	2.321587324	3.696793318
H	-2.667948008	2.604602575	2.637493372
C	-0.878441215	0.178042814	1.768248916
H	-0.756113052	1.197643638	2.146224022
C	0.203879222	-0.073635764	0.706891656
C	-0.789342940	-0.834819198	2.921094894
H	-1.534391880	-0.650998890	3.701678514
H	-0.931195676	-1.855855942	2.551294327
H	0.201433241	-0.782114446	3.387536287
H	0.090568028	-1.063143969	0.252427816
H	1.193275452	-0.027968554	1.176640153
H	0.159001082	0.673769176	-0.087486692
C	-0.975355327	3.451791763	-3.011955023
H	-0.447115839	3.207702160	-2.083424091
C	-1.698412299	4.793511391	-2.795617819
C	0.058231167	3.566267252	-4.143346786
H	0.689919412	2.678102255	-4.216526508
H	-0.409932256	3.741451502	-5.118374825
H	0.711321950	4.422905922	-3.936744690
H	-2.110391378	5.172566414	-3.737796783
H	-0.977687299	5.534918308	-2.432034254
H	-2.506737709	4.729369640	-2.064812660
C	-3.620370626	2.348873377	-4.246472836
H	-4.124977589	1.373209834	-4.213668823
C	-3.261170626	2.671398878	-5.703102589
C	-4.583765984	3.391114473	-3.643000126
H	-4.700279236	3.258221626	-2.564016581
H	-4.230826855	4.408899307	-3.828888893
H	-5.565262794	3.293162584	-4.120716095
H	-2.697711706	3.608135462	-5.775362015
H	-4.179976463	2.797910452	-6.288356304
H	-2.676760674	1.875895500	-6.171994686
O	-3.996861219	2.419271469	-0.490784973
N	-3.280764341	3.850331068	0.249567345
N	-2.104202747	3.706675053	0.334305912
O	-1.267391920	2.794999838	0.019183941
N	-4.758187294	0.899418831	-1.411278963
O	-5.333567142	0.197808072	-0.686846137
C	0.921577632	-0.669770479	-6.628811836
H	2.008269548	-0.694038093	-6.478347778
H	0.656749308	-1.570217013	-7.196089745
H	0.695284128	0.196642548	-7.257956982
C	-4.010138988	-5.057671070	1.213645577
H	-4.961170673	-5.413786888	0.798507273
H	-3.307743549	-5.899097443	1.171849012
H	-4.179064751	-4.819075108	2.268240929

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C	-1.384362936	-0.573909819	-2.953924417
Ni	-1.880919337	1.165022254	-0.698257446
P	-2.967371464	0.038706027	0.960388005
C	-3.179918766	-1.580715299	0.159152746
C	-2.654574633	-1.671134949	-1.171869874
N	-2.007617235	-0.585081875	-1.708703995
C	-1.466285110	0.637617111	-3.700191498
P	-2.428638697	1.933003306	-2.832220793
C	-3.837723017	-2.679029942	0.742442369
C	-2.925026417	-2.883544683	-1.869072556
C	-0.604704142	-1.615709901	-3.502693176
C	-0.801978052	0.769641876	-4.923679352
C	-4.044315815	-3.877643108	0.062771209
C	-3.588680029	-3.938100815	-1.265562892
C	0.037477899	-1.462114334	-4.727988243
C	-0.044642087	-0.274193376	-5.466796398
H	-4.217259884	-2.590388298	1.755840540
H	-3.769042730	-4.840847969	-1.847435594
H	0.636000633	-2.286124945	-5.112442017
H	-0.863781512	1.703902245	-5.474693298
H	-2.623172760	-2.977843761	-2.905087471
H	-0.474300534	-2.536005020	-2.944131136
C	-4.656158447	0.774463534	1.374150753
H	-4.994334698	1.089190483	0.378136396
C	-4.468592644	2.044320345	2.223778248
C	-5.737740517	-0.150161952	1.950345993
H	-5.917182446	-1.012570500	1.304589510
H	-5.483568192	-0.517712295	2.949140072
H	-6.680694103	0.403938234	2.037555695
H	-4.161166191	1.800595403	3.246723175
H	-5.414590836	2.594006300	2.290390968
H	-3.717787266	2.716526031	1.796080112
C	-1.980924129	-0.189342529	2.548910141
H	-1.860480309	0.837710202	2.918935776
C	-0.586900532	-0.728933454	2.180945396
C	-2.617640972	-1.037265182	3.660209417
H	-3.585659266	-0.647644222	3.985980749
H	-2.753925323	-2.074445248	3.339963198
H	-1.957421899	-1.051504374	4.536224842
H	-0.656303704	-1.741937876	1.770813346
H	0.046607792	-0.769123316	3.074656963
H	-0.090162426	-0.097499162	1.438767195
C	-1.898637772	3.588914156	-3.559624434
H	-0.814729869	3.448966026	-3.669839144
C	-2.124503374	4.721214771	-2.540003061
C	-2.479181528	3.979645252	-4.930031300
H	-2.363465786	3.199598789	-5.685778618
H	-3.545222282	4.216809750	-4.856297016
H	-1.972856164	4.879844666	-5.299270153
H	-3.191292524	4.890037060	-2.357712984
H	-1.705933213	5.658809185	-2.924986124
H	-1.650354028	4.509163380	-1.579552531
C	-4.231011391	1.552030802	-3.244295359
H	-4.353445053	0.611719668	-2.692315578
C	-4.553326130	1.271013498	-4.719842434
C	-5.186040878	2.589479685	-2.632439137
H	-4.973078251	2.765680552	-1.572832346
H	-5.128209114	3.552252054	-3.151906013
H	-6.222001553	2.239870071	-2.713793993
H	-4.542214394	2.181458712	-5.325474262
H	-5.558145046	0.838052452	-4.799245358
H	-3.847891569	0.560025573	-5.158004761
O	-1.093322873	3.379830837	0.784340322
N	-0.972690642	2.393199921	0.134875000
C	0.676377535	-0.120721504	-6.785520077
H	1.765326738	-0.092676647	-6.652074814
H	0.458137661	-0.953853786	-7.463953495
H	0.384599477	0.804192841	-7.292799473
C	-4.746113777	-5.052162170	0.702219307
H	-5.605702400	-5.384150505	0.106420510
H	-4.078807831	-5.917258263	0.807565033
H	-5.115389824	-4.799645901	1.701243401

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3-Triplet

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C	-1.647808433	-0.666134059	-2.873917818
Ni	-2.463469267	1.181751966	-0.799546778
P	-2.876928568	0.005690198	1.091394663
C	-3.209678411	-1.618454099	0.343180537
C	-2.910083294	-1.675796628	-1.050266266
N	-2.353715897	-0.568749309	-1.675570369
C	-1.537840366	0.492914230	-3.693336010
P	-2.312680960	1.974771023	-2.965064287
C	-3.729784489	-2.741577387	1.008211732
C	-3.279320478	-2.869607210	-1.724520326
C	-0.944598913	-1.816257596	-3.306012630
C	-0.808382988	0.457872003	-4.887965679
C	-4.029312611	-3.930629969	0.344727874
C	-3.814985037	-3.951145649	-1.043832183
C	-0.226021260	-1.820756435	-4.494619370
C	-0.146721929	-0.692767382	-5.324028015
H	-3.920101404	-2.684541941	2.075299025
H	-4.084684372	-4.841529369	-1.609665394
H	0.304130346	-2.728133440	-4.779416084
H	-0.737086236	1.355086327	-5.496517658

H	-3.154631138	-2.931698084	-2.799349308
H	-0.942730844	-2.705640078	-2.686521053
C	-4.375880718	0.644602418	2.047902107
H	-4.930689335	1.163735986	1.256638646
C	-3.953704119	1.710807085	3.074554443
C	-5.312412262	-0.397063881	2.675160170
H	-5.677196980	-1.118392944	1.940923333
H	-4.830858231	-0.949467957	3.489325285
H	-6.182709694	0.116349809	3.101395369
H	-3.409931898	1.268780947	3.916395187
H	-4.849706650	2.193230391	3.481217623
H	-3.336801529	2.490386963	2.623352528
C	-1.430497646	-0.177206099	2.276136637
H	-1.326060295	0.820676923	2.719608545
C	-0.159002006	-0.478153169	1.464174390
C	-1.630348682	-1.207273245	3.397801638
H	-2.509603024	-0.993442833	4.012802124
H	-1.736656904	-2.216755629	2.988707781
H	-0.756198585	-1.210231066	4.060376644
H	-0.240844145	-1.438736081	0.944683731
H	0.709101975	-0.529894114	2.131645918
H	0.031863231	0.294306636	0.713580847
C	-1.240957618	3.446294546	-3.466300488
H	-0.239134341	2.996610165	-3.467510223
C	-1.264228821	4.544559479	-2.387842417
C	-1.495774150	4.054886341	-4.856079102
H	-1.478396773	3.318261147	-5.662398338
H	-2.459782124	4.571087360	-4.893903255
H	-0.720856845	4.800484180	-5.071083546
H	-2.254501104	5.002462387	-2.297656536
H	-0.553757191	5.335989475	-2.655823469
H	-0.996857226	4.152457237	-1.404910326
C	-4.050962925	2.088099003	-3.687615395
H	-4.505196095	1.201393008	-3.224945784
C	-4.172616482	1.929469824	-5.210407734
C	-4.795973301	3.327108860	-3.161942482
H	-4.716596127	3.424660444	-2.075191498
H	-4.411050320	4.248368263	-3.612576723
H	-5.858836174	3.258964062	-3.422495365
H	-3.817266703	2.814326286	-5.745457649
H	-5.226259708	1.786399245	-5.479853630
H	-3.614516973	1.061822891	-5.573299408
O	-3.645711660	3.510951519	0.274105191
N	-2.636437416	2.850159168	0.079453655
C	0.651466608	-0.714356005	-6.606803417
H	1.731654286	-0.752380908	-6.414128780
H	0.406883121	-1.589519620	-7.220127583
H	0.459485441	0.177150905	-7.212077141
C	-4.580967426	-5.136205673	1.069355488
H	-5.515905857	-5.488309383	0.616086721
H	-3.879741669	-5.980339050	1.046561360
H	-4.788214684	-4.911293983	2.120234251

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3-Singlet-1

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C	-1.616270542	-0.623162448	-3.008809566
Ni	-1.870431662	1.088917017	-0.708798349
P	-2.931584835	0.038314495	0.978456020
C	-3.316574574	-1.548830628	0.177890107
C	-2.880196810	-1.652970076	-1.182402492
N	-2.184231997	-0.606730640	-1.737293601
C	-1.617852092	0.608235359	-3.725306273
P	-2.416104794	1.962405920	-2.782020330
C	-4.017916679	-2.605293751	0.785965085
C	-3.282088041	-2.825942278	-1.881588340
C	-0.963051319	-1.719284058	-3.611914158
C	-0.996826589	0.708828211	-4.973667145
C	-4.353095055	-3.772004843	0.101371929
C	-3.985402584	-3.840141296	-1.253501058
C	-0.359604776	-1.594999194	-4.860474110
C	-0.360952646	-0.386969864	-5.569397926
H	-4.329574108	-2.507447481	1.821456313
H	-4.268881798	-4.715259552	-1.836333156
H	0.143939704	-2.460615396	-5.287145138
H	-0.994392693	1.657869577	-5.502312660
H	-3.052063704	-2.920712471	-2.935913801
H	-0.895813048	-2.661056280	-3.078758478
C	-4.530745506	0.904354215	1.481237173
H	-4.894030571	1.251466990	0.505180120
C	-4.199080467	2.149338722	2.324137211
C	-5.648983479	0.060857628	2.109671593
H	-5.927774429	-0.780550241	1.471355796
H	-5.372717857	-0.332109779	3.092767000
H	-6.540377617	0.685451806	2.247550964
H	-3.859134197	1.873934388	3.328657866
H	-5.095282078	2.769346714	2.442876816
H	-3.421437740	2.764052153	1.860232234
C	-1.880380273	-0.275309980	2.507972479
H	-1.660115361	0.737288356	2.871746063
C	-0.554983556	-0.919444442	2.062740564
C	-2.521559477	-1.077020407	3.650766850
H	-3.435878277	-0.613516629	4.030299664
H	-2.757531643	-2.098115683	3.336660862
H	-1.817467570	-1.149284482	4.488817692
H	-0.724990487	-1.921986818	1.656209111
H	0.121039227	-1.013055921	2.920559168
H	-0.052559089	-0.323714584	1.295430303
C	-1.757754922	3.582244158	-3.484120131
H	-0.695137680	3.346663237	-3.631918907

C	-1.848222256	4.704724789	-2.433021784
C	-2.339737177	4.059137821	-4.826417446
H	-2.325333357	3.289989233	-5.601808071
H	-3.374105692	4.398159504	-4.711810112
H	-1.758641005	4.913953781	-5.193345070
H	-2.888937712	4.966592789	-2.214339972
H	-1.356285930	5.608686447	-2.811604261
H	-1.367992520	4.427953243	-1.492575645
C	-4.264014721	1.768411160	-3.125192881
H	-4.458727360	0.841833234	-2.570960045
C	-4.669587612	1.527532697	-4.587420464
C	-5.086103439	2.892181873	-2.474425793
H	-4.813248634	3.042423964	-1.424707174
H	-4.955425739	3.846461058	-2.996198416
H	-6.153830528	2.646103621	-2.512953997
H	-4.595540524	2.435399055	-5.192065716
H	-5.713694096	1.193275332	-4.626789570
H	-4.054008007	0.753999114	-5.054326057
O	-0.975190163	3.195772648	0.778887808
N	-0.891580880	2.223170042	0.096547864
C	0.324860364	-0.264905304	-6.909531116
H	1.417691946	-0.258653045	-6.806782246
H	0.069279246	-1.101419330	-7.569873810
H	0.038966436	0.660311699	-7.419684410
C	-5.094141483	-4.906447887	0.767071128
H	-5.965955734	-5.218759537	0.179275677
H	-4.457631111	-5.792496204	0.889234066
H	-5.450933456	-4.620107174	1.761464596

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3-Singlet-2

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C	-1.146962404	-0.617123783	-2.821632862
Ni	-1.633099318	1.296236277	-0.653467238
P	-2.233962059	0.145660639	1.200499415
C	-2.700321198	-1.440564394	0.444526643
C	-2.394490719	-1.541065454	-0.948414028
N	-1.747270823	-0.495664418	-1.573479414
C	-1.050065637	0.553510487	-3.626694441
P	-1.745797276	2.036634445	-2.823830605
C	-3.322279930	-2.506502867	1.118133783
C	-2.864811897	-2.710975170	-1.607968688
C	-0.535983264	-1.788278222	-3.330957174
C	-0.410852879	0.519450068	-4.871401787
C	-3.718101740	-3.674324036	0.468906403
C	-3.495913744	-3.731955290	-0.918034196
C	0.091881521	-1.794568658	-4.570377350
C	0.165459827	-0.649378955	-5.376826286
H	-3.519015312	-2.418220758	2.181896448
H	-3.837230921	-4.603917599	-1.474186182
H	0.554832935	-2.717435837	-4.916206837
H	-0.345723778	1.425801516	-5.467340946
H	-2.743113756	-2.798657894	-2.681035757
H	-0.530367732	-2.691272736	-2.731213331
C	-3.701050758	0.927111328	2.106455326
H	-4.142623425	1.539762378	1.309562445
C	-3.228708029	1.890969276	3.210139990
C	-4.792889118	-0.018614143	2.626253843
H	-5.173140049	-0.678566933	1.843633652
H	-4.437293053	-0.640788436	3.454807758
H	-5.633796692	0.576179981	3.003408670
H	-2.801326990	1.351492763	4.062021255
H	-4.087189198	2.461780548	3.582549810
H	-2.490514278	2.610384941	2.848560810
C	-0.863934278	-0.182844669	2.445361137
H	-0.682094574	0.797449291	2.903822184
C	0.405207485	-0.596378207	1.680269718
C	-1.201444268	-1.195946932	3.549381495
H	-2.092546940	-0.916378617	4.119925976
H	-1.364857674	-2.192695856	3.128875017
H	-0.365733922	-1.268661618	4.256175995
H	0.253890246	-1.542805433	1.150392413
H	1.238393307	-0.731830239	2.379863501
H	0.694806159	0.159206003	0.944250226
C	-0.805139184	3.510753155	-3.539103270
H	0.194580153	3.082171679	-3.688915491
C	-0.676448822	4.647059917	-2.509444952
C	-1.298325539	4.059391975	-4.889494419
H	-1.409992456	3.287276506	-5.654071331
H	-2.260957241	4.569262981	-4.785148621
H	-0.579923511	4.798193455	-5.264754772
H	-1.650937557	5.074912071	-2.251576662
H	-0.061026592	5.453495502	-2.926194906
H	-0.206143707	4.304634094	-1.584950447
C	-3.575388193	2.073723555	-3.287636757
H	-3.914487600	1.174205065	-2.757472754
C	-3.922348022	1.891871452	-4.772808552
C	-4.282852650	3.285763025	-2.658462286
H	-4.055868149	3.381302834	-1.591751814
H	-3.995983601	4.221991539	-3.149781466
H	-5.369153976	3.182904482	-2.765992403
H	-3.717972279	2.791894674	-5.358695030
H	-4.992668629	1.673229337	-4.873596668
H	-3.369402885	1.059535742	-5.217504501
O	-2.076865673	3.612715960	0.546991765
N	-1.253932476	2.812112570	0.179189011
C	-4.372232914	-4.819581032	1.204694510
H	-5.295748234	-5.143459320	0.709225237
H	-3.716001034	-5.698269844	1.258046508
H	-4.628767967	-4.541190147	2.231716633

C 0.870471001 -0.673840702 -6.712605476
H 1.961265802 -0.723391473 -6.597007751
H 0.573749065 -1.544009686 -7.309539318
H 0.645561576 0.222262025 -7.299607754

5. Vibrational frequencies of the optimized geometries

Table S11. Vibrational frequencies (in cm^{-1}) of the optimized geometries.

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CO
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2214.25

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CO2
==========
644.23 644.33 1369.91 2434.62

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NO
==========
1995.19

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N2O
==========
604.56 605.05 1342.42 2360.01

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1
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23.51 26.05 44.36 53.46 57.56 62.80
66.06 68.85 71.52 74.95 81.37 83.38
88.37 97.81 106.06 107.95 119.13 126.09
133.02 142.94 146.38 165.47 170.74 195.70
208.50 214.01 221.28 225.39 234.30 242.61
246.86 255.36 259.62 262.68 266.53 271.09
277.67 286.60 288.81 291.44 303.51 306.05
312.00 323.39 329.95 341.90 348.84 357.65
364.93 383.31 395.34 403.27 412.72 414.88
435.61 457.03 471.80 486.41 500.45 505.37
521.23 533.03 542.86 554.02 561.39 581.95
615.02 632.87 662.42 666.89 705.15 707.19
715.99 743.76 750.22 788.12 812.23 831.22
855.74 859.20 867.48 891.46 894.69 895.94
898.80 901.32 921.96 926.98 928.56 946.58
947.16 954.78 959.27 969.67 982.14 982.28
984.04 984.75 992.31 1022.20 1025.33 1031.78
1063.80 1064.61 1065.19 1066.64 1076.61 1078.98
1083.22 1095.50 1113.37 1118.45 1120.67 1125.58
1189.46 1190.12 1192.13 1195.11 1195.96 1197.51
1240.78 1243.11 1246.16 1285.14 1288.92 1293.12
1297.40 1318.27 1319.75 1327.06 1328.57 1335.87
1336.22 1337.09 1340.60 1346.53 1356.30 1416.15
1418.28 1419.10 1420.98 1427.06 1429.29 1434.40
1435.21 1436.25 1443.61 1444.13 1446.18 1496.57
1497.30 1499.40 1500.05 1503.38 1504.62 1505.62
1506.81 1507.63 1509.35 1510.88 1512.38 1512.77
1516.36 1519.16 1519.93 1522.39 1523.27 1525.29
1526.66 1534.08 1541.10 1583.84 1594.37 1602.83
1653.46 1660.43 3028.24 3028.83 3033.78 3038.49
3039.88 3041.07 3041.64 3042.58 3046.10 3046.28
3050.11 3050.45 3057.97 3070.68 3082.79 3083.17
3103.26 3103.63 3105.36 3107.50 3109.24 3110.61
3113.60 3113.68 3113.75 3117.64 3126.01 3131.56
3141.96 3142.00 3142.16 3142.97 3156.59 3164.14
3166.47 3170.58 3194.95 3200.38 3212.50 3220.08

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2
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26.29 28.51 52.28 55.51 60.11 65.32
68.02 75.21 78.81 82.11 86.30 92.00
96.79 104.04 108.25 119.89 127.62 139.27
144.77 150.91 160.13 167.54 176.05 205.48
216.66 222.09 231.23 232.01 240.22 255.25
256.50 263.71 269.71 274.51 278.50 282.49
284.94 290.09 294.28 297.74 300.59 310.94
322.30 326.98 338.32 347.61 361.83 366.41
378.29 389.54 401.31 412.80 413.45 433.78
456.93 472.69 486.24 497.44 504.25 519.99
532.06 540.92 554.30 562.42 576.90 596.93
618.91 633.17 662.04 666.21 704.32 714.08
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A4

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A4-TS

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A5

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A6

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3166.80 3191.32 3199.73 3216.75 3219.36 3231.33

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B1

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19.77 27.16 42.99 51.09 59.11 60.82
62.43 67.08 70.35 76.23 77.67 83.69
87.87 92.37 99.01 102.13 103.53 107.56
121.01 122.21 132.77 138.75 141.83 150.55
155.61 161.68 171.50 183.29 209.71 223.25
224.66 232.45 235.30 243.30 258.88 261.14
268.00 272.20 276.76 284.31 284.79 290.85
291.76 299.33 301.10 307.17 311.65 326.38
329.66 340.95 350.68 360.99 367.26 378.25
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473.08 488.05 498.11 503.63 520.49 532.61
542.21 555.06 563.23 575.95 593.98 620.38
634.50 662.60 665.95 704.59 714.30 746.27
751.91 821.73 831.45 855.48 858.51 868.93
892.79 896.90 898.84 901.19 902.57 921.94
926.99 929.43 951.31 953.89 957.37 958.47
969.67 981.92 984.68 985.84 987.70 990.08
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1077.04 1081.53 1085.77 1096.94 1114.95 1117.98
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1429.15 1435.71 1437.06 1440.21 1446.50 1447.51
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3082.34 3083.50 3085.57 3100.66 3101.88 3104.61
3105.97 3111.03 3111.27 3112.47 3113.41 3113.92
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B1-TS

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172.07 175.69 197.30 207.09 216.66 218.92
226.35 229.19 237.09 245.29 249.07 259.56
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284.89 291.47 298.49 305.30 313.08 321.45
323.71 328.09 339.97 341.34 354.39 373.28
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626.88 665.23 675.19 693.46 711.06 734.40
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B2
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627.73 668.41 674.37 700.53 711.93 735.82
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912.76 924.58 950.38 957.06 958.89 964.58
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1116.44 1124.11 1185.19 1186.91 1193.43 1193.96
1194.74 1196.56 1238.48 1242.93 1247.00 1278.81
1286.84 1291.99 1295.72 1313.72 1321.78 1325.93
1334.38 1343.58 1344.59 1348.21 1357.50 1370.06
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3047.82 3048.54 3048.96 3053.12 3062.49 3083.27
3084.31 3084.83 3089.71 3103.85 3109.42 3111.66
3112.49 3113.82 3114.86 3115.06 3115.92 3116.92
3120.75 3126.82 3133.10 3138.48 3144.73 3150.04
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3205.77 3207.84 3215.55

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B2-TS
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166.84 176.20 194.47 209.93 214.38 219.75
226.77 229.82 236.27 242.28 253.57 256.56
265.33 269.98 274.17 276.41 279.84 283.22
287.04 291.12 299.19 308.37 316.22 322.06
337.18 339.40 352.71 360.70 376.99 387.26
395.64 414.90 419.04 436.36 446.01 458.68
466.00 480.39 489.88 493.99 511.89 518.50
532.48 543.26 552.70 559.46 584.46 615.16
629.29 665.53 672.18 700.73 712.27 739.73
747.97 784.29 830.02 850.22 854.61 867.24
889.49 892.85 893.86 894.88 896.65 900.53
914.26 925.83 950.47 957.87 962.00 963.04
966.47 980.36 981.94 983.99 984.97 989.94
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1120.15 1121.86 1185.32 1187.93 1193.70 1194.13
1196.19 1197.59 1238.46 1242.63 1246.32 1261.56
1280.56 1287.23 1292.55 1297.74 1315.43 1323.90
1327.75 1334.27 1336.53 1340.96 1346.05 1353.39
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3207.37 3209.06 3216.88

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B3
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91.32 98.67 107.26 110.40 113.30 120.34
136.72 144.68 146.47 153.87 159.83 164.95
165.02 193.91 210.09 215.57 223.93 234.29
235.29 242.86 253.27 259.13 265.15 271.07
273.89 278.01 278.93 283.16 288.77 295.96
297.95 311.43 327.49 330.82 337.45 339.73
347.84 362.49 365.07 367.73 387.30 398.14

411.73 414.34 428.73 456.38 471.69 482.40
488.21 497.59 501.92 518.12 530.38 540.17
552.88 562.63 578.04 608.89 620.48 631.89
642.89 662.60 666.92 701.14 711.05 741.15
751.45 776.77 831.47 842.34 854.72 863.85
891.15 894.31 896.96 899.97 900.56 917.49
925.33 927.48 948.52 952.92 955.43 956.53
969.10 982.00 984.11 985.62 987.14 990.38
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1448.38 1497.98 1498.34 1498.62 1501.62 1504.57
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3120.31 3127.64 3127.83 3133.52 3140.13 3141.33
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3209.05 3215.17 3217.50

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B3-TS

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173.74 200.94 210.34 221.02 223.62 228.81
236.35 238.14 245.88 252.27 256.05 264.69
270.26 273.55 279.28 283.13 285.63 292.74
298.59 303.33 307.51 321.04 328.18 336.05
343.43 362.14 368.39 389.38 391.98 399.67
401.88 414.40 416.98 433.27 459.14 463.60
473.86 499.74 503.02 516.92 529.06 537.76
553.62 561.55 581.45 605.13 623.17 628.77
640.32 660.05 673.79 701.28 709.76 739.84
741.44 750.57 831.47 843.86 854.96 861.74
893.26 895.14 897.50 899.32 900.61 902.72
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1076.01 1079.13 1082.78 1083.68 1096.86 1111.08
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3203.19 3208.62 3216.68

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B4

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209.25 219.20 221.24 229.28 234.55 241.85
248.38 257.24 263.05 265.86 266.43 278.43
280.78 288.57 289.77 292.05 304.71 308.96
311.07 320.51 328.19 342.55 350.20 359.41
365.56 384.22 393.85 400.31 411.51 412.85
435.11 457.36 471.72 486.42 500.82 505.15
521.44 532.87 543.40 554.24 561.83 581.80
614.89 633.49 662.71 667.12 705.80 716.84
745.74 751.15 829.60 831.13 857.77 860.26
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3106.39 3108.16 3110.28 3112.24 3113.71 3113.85
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B5

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B5-TS

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628.76 655.87 667.42 699.08 711.43 736.72
747.52 825.50 828.41 838.57 853.53 861.59
889.63 893.42 897.00 898.81 899.80 913.02
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969.12 982.13 982.35 983.97 986.30 988.24
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3208.28 3216.55 3218.38

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B6

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27.96 31.28 44.28 46.88 59.92 64.58
66.39 69.15 77.16 82.99 83.90 88.54
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170.84 182.11 201.02 211.22 220.04 226.32

232.22 234.91 239.60 248.28 250.44 255.25
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B6-TS

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B7

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B7-TS

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C3

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C3-TS

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C4
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C5
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C6

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1516.46 1517.76 1519.15 1522.64 1524.75 1525.37
1530.17 1531.32 1533.24 1585.23 1595.87 1653.00
1660.48 1711.81 3026.14 3028.16 3032.26 3034.23
3036.26 3037.68 3038.78 3039.83 3041.78 3043.09
3046.53 3047.15 3059.80 3080.95 3081.48 3098.68
3099.94 3100.09 3104.23 3106.84 3109.52 3110.86
3111.90 3112.43 3112.60 3115.96 3119.47 3121.48
3131.00 3137.41 3138.15 3140.31 3162.13 3162.75
3163.14 3168.60 3184.28 3202.08 3210.04 3217.51

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C7

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24.58 28.53 39.48 43.06 54.05 62.30
64.79 69.42 77.68 80.22 85.98 93.48
98.69 107.21 117.08 122.79 133.27 139.85
146.46 154.94 164.89 170.94 173.25 186.74
202.40 216.55 220.81 224.17 235.62 236.55
244.32 261.52 264.14 269.53 272.96 273.53
276.70 282.10 290.60 291.83 304.91 311.65
327.08 329.03 332.76 340.19 350.64 362.00
370.23 387.77 397.27 409.86 413.26 417.91
433.98 457.56 466.21 472.11 497.53 501.99
514.33 527.75 540.97 550.42 552.40 559.10
567.93 585.69 614.95 629.36 664.70 677.60
705.87 715.07 741.03 749.02 833.00 847.59
856.46 862.21 865.18 891.96 894.22 895.44
898.02 898.68 900.91 926.83 928.64 946.83
952.71 956.48 957.64 965.09 969.03 980.95
981.82 986.46 986.83 989.22 992.54 1022.38
1025.30 1059.82 1064.28 1065.54 1071.30 1079.25
1082.73 1087.12 1094.92 1110.54 1115.63 1123.39
1126.05 1187.36 1189.42 1190.96 1195.98 1197.73
1200.49 1234.77 1244.43 1245.50 1281.17 1288.77
1297.81 1306.10 1311.45 1320.62 1325.98 1329.23
1329.94 1332.74 1335.35 1341.37 1346.95 1414.89
1419.62 1420.86 1421.39 1427.53 1429.11 1433.62
1436.25 1436.71 1443.73 1445.77 1446.70 1457.46
1496.76 1496.96 1497.59 1502.46 1502.77 1504.98
1506.89 1507.27 1508.72 1509.96 1511.21 1511.25
1513.53 1515.22 1518.10 1520.42 1523.11 1527.55
1530.84 1532.27 1532.30 1532.86 1589.14 1600.71
1651.38 1657.44 3026.40 3029.86 3031.61 3037.28
3038.51 3039.13 3042.10 3042.86 3045.70 3045.96
3050.95 3051.19 3058.60 3072.97 3083.57 3087.03
3102.23 3103.41 3105.27 3109.06 3109.32 3111.65
3113.55 3115.79 3116.02 3122.85 3127.62 3127.94
3135.50 3135.98 3140.22 3146.27 3159.81 3165.77
3167.38 3190.18 3201.52 3203.14 3211.64 3217.98

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C8

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17.50 34.87 47.62 56.21 59.49 63.55
65.57 67.72 77.39 79.50 85.33 94.65
101.03 104.66 113.75 119.82 125.83 138.80
140.53 146.92 154.09 157.98 174.74 184.05
189.35 208.22 214.52 217.59 227.94 233.02
235.00 239.18 244.51 249.44 253.39 257.31
265.35 269.53 270.63 275.60 276.54 287.76
293.06 308.33 315.87 322.12 325.89 334.81
338.26 341.69 353.51 375.46 376.68 387.73

396.00 411.84 415.65 429.41 434.63 456.75
473.53 485.58 494.65 495.49 514.86 525.79
536.22 540.07 541.30 551.56 557.65 574.92
587.79 618.18 633.63 669.98 671.71 704.07
713.72 741.61 747.30 830.14 851.24 856.53
858.60 867.87 890.60 896.51 897.33 900.77
902.55 918.14 924.36 930.89 951.62 952.95
957.51 961.10 964.25 970.97 979.86 984.49
986.54 987.84 989.59 1006.46 1022.29 1025.47
1064.03 1065.10 1065.27 1072.40 1077.86 1082.02
1083.67 1096.87 1108.88 1114.80 1121.03 1123.45
1189.32 1190.43 1195.23 1195.42 1197.14 1199.65
1242.54 1243.21 1251.36 1279.98 1285.86 1297.76
1312.57 1314.21 1318.84 1326.96 1328.24 1332.59
1337.89 1341.03 1362.05 1369.08 1413.42 1415.93
1420.68 1422.38 1427.01 1429.32 1433.05 1435.20
1436.49 1444.06 1444.95 1446.02 1496.34 1497.25
1497.34 1501.23 1501.87 1503.41 1506.64 1507.69
1509.91 1510.24 1511.40 1512.42 1513.79 1515.03
1518.92 1520.37 1522.80 1523.44 1525.40 1529.39
1533.98 1535.86 1538.08 1583.04 1593.73 1652.59
1659.73 1779.94 3028.84 3029.64 3033.34 3040.36
3041.09 3041.89 3043.33 3044.59 3045.66 3049.42
3050.12 3052.84 3076.79 3081.99 3084.91 3092.64
3103.81 3105.76 3106.66 3109.09 3111.97 3114.55
3114.86 3115.31 3115.55 3120.51 3133.42 3137.67
3139.50 3143.63 3147.99 3154.14 3157.90 3165.24
3166.26 3171.78 3203.43 3205.97 3211.75 3218.99

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C8-TS

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-499.93 23.54 33.74 45.79 49.37 57.02
57.91 68.39 70.03 79.82 81.23 87.14
89.15 96.32 102.41 110.93 112.56 120.12
129.30 138.31 144.48 156.57 160.18 167.28
174.53 177.26 186.39 194.34 209.73 221.40
227.57 232.69 241.67 244.28 255.22 260.64
267.12 272.46 277.89 278.73 283.65 285.12
291.14 297.41 309.37 311.59 323.65 328.14
333.23 339.82 341.34 350.39 354.99 359.80
371.86 387.12 402.90 416.36 419.20 432.34
454.43 469.55 478.83 490.26 494.14 498.30
515.20 529.37 542.03 543.52 554.35 555.32
561.46 576.35 619.49 634.09 665.13 668.16
704.30 714.99 719.57 742.57 751.32 831.78
849.05 858.44 865.90 892.13 896.44 897.99
899.66 901.73 914.85 929.81 931.91 953.56
957.45 959.08 959.77 970.37 981.12 984.92
986.53 986.87 990.09 1021.85 1024.97 1064.91
1065.44 1068.16 1071.24 1078.70 1083.79 1089.96
1098.38 1109.92 1112.99 1115.19 1120.77 1125.99
1189.01 1189.34 1194.27 1196.49 1197.65 1200.02
1241.46 1243.04 1247.31 1286.74 1288.19 1296.78
1317.78 1319.05 1322.05 1327.39 1329.92 1333.70
1337.84 1344.61 1355.22 1368.09 1417.01 1418.25
1420.04 1421.92 1426.76 1429.16 1435.08 1436.30
1438.63 1442.89 1446.01 1447.72 1496.50 1496.84
1497.54 1501.69 1504.71 1505.64 1507.04 1509.28
1509.47 1509.83 1511.52 1511.79 1512.82 1516.52
1517.17 1520.58 1523.10 1524.24 1528.60 1529.26
1532.39 1546.96 1584.05 1593.78 1652.20 1659.05
1784.89 1811.14 3028.45 3028.78 3030.27 3033.08
3035.74 3037.30 3038.55 3040.80 3042.56 3043.97
3045.01 3049.55 3069.15 3081.86 3082.24 3087.74
3095.78 3096.85 3100.94 3105.01 3105.38 3108.12
3112.50 3114.39 3114.65 3118.10 3122.22 3135.64
3135.77 3139.21 3143.89 3145.09 3153.24 3156.42
3164.31 3165.03 3203.62 3209.49 3210.14 3217.67

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3-AF

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21.10 25.55 38.25 43.00 55.28 57.03
59.21 65.96 69.27 70.68 73.19 75.02
84.13 86.44 95.08 103.14 115.59 126.92
132.63 151.25 152.11 171.98 187.53 196.79
213.00 218.79 219.47 223.87 230.05 235.52
241.00 242.89 251.03 254.92 260.22 267.64
271.64 277.05 278.11 285.36 293.12 297.28
311.75 318.82 332.97 351.08 355.51 368.70
376.27 381.09 403.61 404.17 420.89 451.29
458.49 467.18 488.66 491.31 502.46 506.20
518.18 528.35 551.49 557.72 568.37 596.75
625.15 642.88 655.52 696.69 707.10 739.79
747.60 822.81 832.75 847.66 858.49 886.48
889.22 890.69 892.06 895.36 898.11 917.42
923.30 937.28 937.73 939.32 940.53 963.50
972.49 974.53 975.07 976.31 983.87 1016.97
1020.40 1047.51 1054.71 1063.94 1065.62 1067.49
1068.58 1075.17 1083.75 1111.04 1113.30 1117.50
1120.49 1171.41 1182.69 1189.53 1189.82 1191.43
1191.54 1234.82 1240.27 1240.68 1275.30 1284.03
1286.36 1287.42 1302.88 1315.77 1318.60 1326.85
1334.89 1337.22 1343.30 1350.30 1382.16 1411.25
1412.50 1414.30 1416.91 1424.66 1427.13 1430.20
1430.89 1435.01 1436.47 1439.84 1443.10 1496.83
1497.28 1497.43 1498.15 1500.67 1501.27 1504.64
1505.27 1505.41 1507.51 1508.37 1510.51 1510.90
1514.64 1514.98 1515.60 1520.19 1521.36 1523.71

1524.37 1526.63 1527.58 1576.83 1592.07 1648.06
1659.52 1743.48 3025.62 3030.17 3035.50 3035.91
3036.47 3036.92 3039.01 3039.46 3040.47 3041.59
3042.83 3043.94 3045.43 3050.73 3075.37 3083.52
3100.30 3102.82 3102.85 3105.11 3107.48 3108.95
3110.83 3110.96 3111.04 3113.58 3115.02 3119.39
3128.18 3136.37 3138.24 3140.30 3144.18 3150.23
3157.99 3163.62 3187.51 3193.40 3209.92 3223.69

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3-Triplet

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16.94 23.07 43.18 48.23 49.85 61.20
65.07 67.40 70.10 71.32 73.43 83.57
87.36 89.80 99.62 111.01 124.77 132.89
137.57 148.94 158.96 168.13 185.32 199.04
206.35 214.67 219.98 224.51 228.89 234.68
242.50 247.53 249.39 252.65 259.04 264.71
268.95 274.77 278.26 282.78 293.03 301.94
306.72 311.98 324.37 338.10 354.62 358.10
373.89 386.09 401.51 405.97 418.35 437.05
451.00 463.07 467.92 491.78 495.02 509.04
519.03 532.05 551.24 556.89 568.65 603.40
624.84 645.60 653.47 701.49 711.08 740.61
749.53 830.18 839.10 850.91 862.00 889.40
890.93 893.13 895.36 895.55 898.27 919.70
924.14 937.86 939.33 941.33 942.39 967.83
973.63 974.80 978.17 978.33 990.54 1017.41
1020.65 1049.67 1057.97 1063.65 1065.26 1071.97
1072.90 1077.95 1084.64 1110.18 1114.00 1118.86
1122.43 1180.37 1181.54 1190.08 1190.18 1193.46
1193.65 1234.30 1239.79 1241.47 1277.06 1282.69
1289.89 1297.30 1304.30 1316.72 1320.64 1332.76
1335.23 1335.58 1340.00 1343.21 1355.86 1412.48
1414.65 1415.83 1417.32 1424.82 1427.46 1431.31
1433.80 1434.67 1436.93 1442.69 1443.24 1493.63
1496.37 1497.12 1497.88 1501.38 1501.72 1503.38
1505.17 1506.02 1507.12 1507.28 1509.62 1510.81
1514.07 1514.64 1515.94 1519.27 1519.71 1521.41
1524.34 1525.04 1527.43 1559.38 1581.20 1592.53
1651.96 1659.83 3027.81 3028.37 3033.19 3038.42
3038.77 3039.16 3039.96 3040.64 3042.27 3043.15
3045.65 3045.93 3050.74 3055.25 3078.21 3081.50
3100.12 3102.31 3104.66 3106.63 3108.24 3109.70
3110.23 3113.21 3113.45 3113.53 3125.97 3129.03
3129.06 3138.01 3139.42 3141.91 3149.63 3152.87
3160.63 3161.74 3187.27 3198.52 3211.54 3219.49

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3-Singlet-1

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23.19 26.44 41.25 46.14 57.49 60.92
64.45 68.12 73.34 73.96 76.69 80.23
86.95 87.54 96.55 106.68 116.42 129.03
135.35 152.59 155.05 177.32 193.76 205.16
214.86 219.65 220.10 227.02 229.30 235.97
239.96 243.34 252.35 253.49 262.83 265.67
269.69 276.90 279.35 286.17 295.26 301.49
313.87 318.88 334.02 353.80 360.11 375.09
379.17 402.87 404.18 416.11 423.61 452.71
459.86 467.90 489.48 491.66 508.39 518.71
529.18 551.68 557.57 567.64 598.16 606.05
627.82 647.27 656.69 697.46 708.01 741.58
748.83 826.17 834.50 848.29 859.73 886.78
889.57 890.49 892.18 895.91 898.95 916.83
924.57 937.87 938.23 940.08 940.36 964.45
972.75 974.88 975.06 976.82 985.62 1017.83
1021.20 1048.12 1055.21 1064.20 1066.52 1067.87
1069.36 1075.74 1083.82 1110.68 1113.32 1117.59
1120.86 1172.53 1183.26 1189.99 1190.08 1191.36
1191.95 1236.59 1240.81 1241.13 1275.21 1284.84
1286.66 1288.41 1303.02 1317.84 1320.36 1328.61
1334.19 1337.09 1342.83 1349.80 1383.27 1411.43
1412.48 1415.18 1417.33 1425.36 1427.51 1430.37
1431.54 1435.69 1437.29 1440.42 1444.18 1497.44
1497.56 1497.81 1499.23 1501.03 1501.51 1504.69
1505.73 1506.44 1507.72 1508.59 1510.82 1511.13
1515.38 1515.51 1516.05 1520.66 1522.29 1523.76
1523.94 1526.34 1527.45 1577.95 1593.87 1648.02
1659.01 1730.03 3026.19 3029.82 3036.35 3036.39
3037.14 3038.26 3039.81 3039.95 3041.11 3041.91
3043.15 3044.41 3046.16 3051.06 3077.48 3084.96
3100.68 3102.50 3103.64 3105.40 3108.39 3109.13
3111.34 3111.44 3111.61 3114.17 3115.83 3123.62
3129.38 3136.48 3138.53 3140.76 3143.82 3154.56
3158.92 3164.35 3188.75 3193.14 3210.63 3223.67

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3-Singlet-2

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17.28 23.32 41.27 53.31 57.37 61.69
62.91 66.76 70.42 73.59 81.55 83.62
87.07 93.73 107.27 121.03 127.79 134.43
141.50 152.83 160.86 177.11 194.73 209.65
214.08 220.81 223.30 231.83 239.79 245.17
248.42 254.08 257.69 261.17 265.72 268.63
274.81 278.67 280.42 284.75 298.70 308.29
310.38 327.68 335.06 351.05 356.12 372.58
376.16 389.79 402.18 405.99 422.86 449.85
463.22 464.94 491.89 495.61 506.96 517.36

529.73 551.09 557.14 562.65 577.47 603.52
626.25 644.61 653.19 699.99 709.77 738.96
749.68 828.62 831.42 851.09 861.14 889.04
889.78 892.58 895.21 897.06 898.15 919.80
924.53 937.77 938.81 941.03 941.38 967.03
974.75 974.93 976.52 977.77 988.91 1017.39
1020.58 1049.92 1058.47 1063.63 1065.45 1070.67
1071.26 1076.99 1084.00 1108.26 1115.45 1119.56
1121.47 1177.56 1182.84 1190.04 1190.49 1192.35
1193.15 1236.66 1240.51 1242.52 1276.68 1283.87
1288.56 1294.95 1304.56 1318.82 1319.95 1333.15
1334.40 1338.15 1339.76 1347.13 1372.00 1412.30
1414.14 1415.59 1416.85 1425.34 1427.66 1431.37
1431.83 1435.14 1437.72 1440.42 1444.22 1496.78
1497.01 1497.28 1498.23 1502.34 1503.42 1504.10
1505.28 1505.71 1507.63 1507.84 1510.00 1510.86
1514.81 1515.09 1515.87 1519.96 1521.57 1522.01
1524.93 1526.23 1526.82 1577.86 1590.05 1633.38
1651.15 1661.20 3025.61 3028.12 3036.36 3037.16
3037.88 3038.40 3039.82 3040.85 3041.33 3041.50
3043.10 3044.90 3045.69 3050.24 3075.95 3082.17
3098.72 3101.17 3103.65 3104.61 3108.21 3108.30
3109.07 3111.43 3111.59 3113.11 3118.16 3126.28
3129.29 3137.63 3139.75 3141.58 3142.20 3143.94
3158.07 3161.02 3184.38 3197.68 3211.56 3220.91