

Mechanical rupture of mono- and bivalent transition metal complexes in experiment and theory

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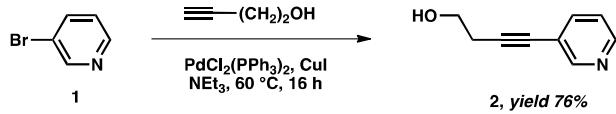
General Information

Reactions were generally performed under argon in dried flasks. Solvents and reagents were added by syringes. Solvents were dried using standard procedures. Triethylamine was distilled from CaH and stored over potassium hydroxide under an atmosphere of argon. Pyridine was distilled from potassium hydroxide and stored over potassium hydroxide under an atmosphere of argon. Dichloromethane and tetrahydrofuran (THF) were dried with activated alumina using an MBraun solvent system model MB SPS-800. Other reagents were purchased and were used as received without further purification unless otherwise stated. Reactions were monitored by thin-layer chromatography (TLC). Products were purified by flash chromatography on silica gel (32-63 µm). Yields refer to chromatographically and spectroscopically (¹H- NMR) homogeneous materials, unless otherwise stated. NMR spectra were recorded on Bruker (AM 250, AC500, AVIII 700) and JEOL (ECX 400, Eclipse 500) instruments. Integrals are in accordance with assignments, and coupling constants are given in Hz. Chemical shifts are reported relative to TMS (¹H: δ = 0.00 ppm) and CDCl₃ (¹³C: δ = 77.0 ppm). Integrals are in accordance with assignments; coupling constants are given in Hz. All ¹³C NMR spectra are proton-decoupled. For detailed peak-assignment 2D spectra were measured (COSY, HMQC, HMBC). Multiplicity is indicated as follows: s (singlet), d (doublet), t (triplet), m (multiplet), m_c (centered multiplet), dd (doublet of doublet), br s (broad singlet). IR spectra were measured with a Nexus FT-IR spectrometer equipped with a Nicolet Smart DuraSampleIR ATR. MS and HRMS analyses were performed with Varian Ionspec QFT-7 (ESI-FT ICRMS) instrument. Elemental analyses were carried out with Vario EL III. Melting points were measured with a Reichert apparatus Thermovar and are uncorrected.

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Experimental Procedures

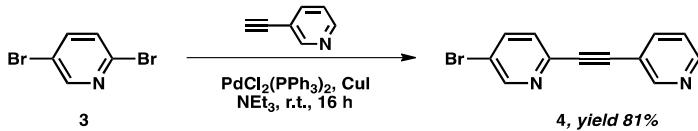
4-(Pyridin-3-yl)but-3-yn-1-ol (**2**)



A reaction tube was charged with 3-bromopyridine (**1**) (401 mg, 2.54 mmol), $\text{PdCl}_2(\text{PPh}_3)_2$ (90 mg, 0.13 mmol) and CuI (24 mg, 0.13 mmol). NEt_3 (12 mL) was added and the resulting mixture was degassed before but-3-yn-1-ol (195 mg, 2.78 mmol) was added. The reaction mixture was stirred at 60 °C for 16 h. After complete consumption of the starting materials (as indicated by TLC) the mixture was filtered through celite and then partitioned between EtOAc and water. The organic layer was separated and the aqueous phase was extracted with EtOAc (3 x 30 mL). The combined organic layers were dried with Na_2SO_4 , filtered and the solvent was evaporated under reduced pressure. The crude material was purified by flash column chromatography (silica gel, $\text{EtOAc}/\text{hexane} = 9:1$) to afford **2** (237 mg, 76%) as a colorless oil.

^1H NMR (500 MHz, CD_3OD): δ = 2.66, 3.75 (2 t, J = 6.6 Hz, 2 H each, 2-H/1-H), 7.38 (dd, J = 5.0, 7.9 Hz, 1 H, 5'-H), 7.83 (m_c, 1 H, 4'-H), 8.44 (d, J = 5.0 Hz, 1 H, 6'-H), 8.55 (s, 1 H, 2'-H) ppm. ^{13}C NMR (101 MHz, CD_3OD): δ = 23.0, 60.2 (2 t, C-1/C-2), 78.8, 92.9 (2 s, C≡C) 121.6 (s, C-3'), 123.6, 139.3, 147.7, 151.2 (4 d, C-5'/C-4'/C-6'/C-2') ppm. IR (ATR): ν = 3220 (OH), 3200-2820 (=C-H, -C-H), 2220 (C≡C), 1690-1440 (C=C) cm^{-1} . HRMS (ESI-TOF): *m/z* calcd for $\text{C}_9\text{H}_{10}\text{NO} [\text{M}+\text{H}]^+$: 148.0757, found: 148.0755.

5-Bromo-2-(pyridin-3-ylethynyl)pyridine (**4**)



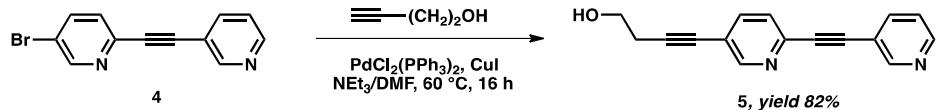
A flame dried Schlenk-flask was charged with 2,5-dibromopyridine (**3**) (2.36 g, 10.0 mmol), $\text{PdCl}_2(\text{PPh}_3)_2$ (350 mg, 0.50 mmol), CuI (80 mg, 0.50 mmol) and 3-ethynylpyridine (1.03 g, 10.0 mmol). The reaction vessel was evacuated and backfilled with argon before NEt_3 (50 mL) was added. The mixture was degassed by three pump-freeze-thaw cycles and stirred

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under an atmosphere of argon at r.t. for 16 h. After complete consumption of the starting materials (as indicated by TLC) the reaction mixture was filtered through a short plug of silica. The obtained solution was partitioned between EtOAc and water. The organic layer was separated and the aqueous layer was extracted with EtOAc (3 x 100 mL). The combined organic layers were dried with Na₂SO₄, filtered and the solvent was removed under reduced pressure. The crude material was purified by flash column chromatography on silica gel (hexane/EtOAc = 1:1) to provide **4** (2.09 g, 81%) as a colorless, crystalline solid; mp 116-117 °C.

¹H NMR (400 MHz, CDCl₃): δ = 7.27 (m_c, 1 H, Pyr), 7.43-7.46, 7.83-7.90, 8.59-8.62, 8.70-8.61 (4 m, 1 H, 2 H, 1 H, 1 H, Pyr), 8.83 (br. s, 1 H, Pyr) ppm. ¹³C NMR (101 MHz, CDCl₃): δ = 86.9, 90.8 (2 s, C≡C), 120.7, 126.1, 128.3, 130.0, 139.0, 139.1, 141.1, 149.5, 151.5, 152.6 (7 d, 3 s, Pyr) ppm. IR (KBr): ν = 3080-2850 (=C-H, C-H), 2220 (C≡C), 1560-1450 (C=C) cm⁻¹. HRMS (ESI-TOF): *m/z* calcd for C₁₂H₈BrN₂ [M+H]⁺: 258.9871, found 258.9894. Anal. calcd for C₁₂H₇BrN₂ (259.1): C, 55.63, H, 2.72, N, 10.81, found: C, 55.35, H, 2.65, N, 10.93.

4-[6-(Pyridin-3-ylethynyl)pyridin-3-yl]but-3-yn-1-ol (**5**)



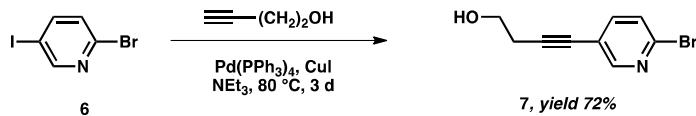
A reaction tube was charged with pyridine derivative **4** (504 mg, 1.96 mmol), PdCl₂(PPh₃)₂ (68 mg, 0.085 mmol) and CuI (17 mg, 0.085 mmol). NEt₃ (0.8 mL), DMF (1.7 mL) and but-3-yn-1-ol (39 mg, 0.55 mmol) were added and argon was bubbled through the solution for 15 min before the reaction mixture was heated to 60 °C for 16 h. After complete consumption of the starting materials the mixture was filtered through celite and concentrated to dryness. The crude material was partitioned between EtOAc and water. The organic layer was separated and the aqueous layer was extracted with EtOAc (3 x 20 mL). The combined organic layers were dried with Na₂SO₄, filtered and the solvent was removed under reduced pressure. Flash column chromatography on silica gel (EtOAc) provided **5** (400 mg, 82%) as a colorless oil.

¹H NMR (700 MHz, CD₃OD/DMF): δ = 2.69, 3.78 (2 t, *J* = 6.7 Hz, 2 H each, 1-H, 2-H), 7.45, 7.56, 7.80, 7.98 (4 m_c, 1 H each, Pyr), 8.53-8.56 (m, 2 H, Pyr), 8.75 (s, 1 H, Pyr) ppm. ¹³C NMR (175 MHz, CD₃OD+DMF): δ = 22.6, 59.4 (2 t, CH₂), 76.8, 86.1, 90.3, 92.9 (4 s, C≡C),

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118.9, 120.4 (2 s, Pyr), 123.0, 126.1, 138.6, 138.8 (4 d, Pyr), 139.3 (s, Pyr), 148.0, 150.8, 151.3 (3 d, Pyr) ppm. IR (ATR): ν = 3280 (OH), 3050-2880 (-C-H, =C-H), 2260-2185 (C≡C), 1540-1405 (C=C) cm^{-1} . HRMS (ESI-TOF): m/z calcd for $\text{C}_{16}\text{H}_{13}\text{N}_2\text{O} [\text{M}+\text{H}]^+$: 249.1022, found: 249.1035.

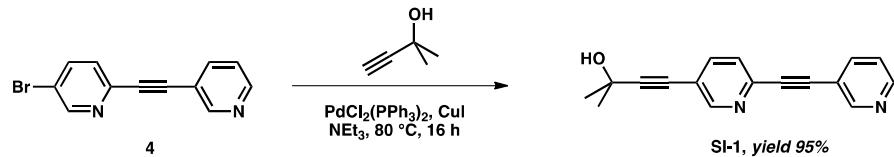
4-(6-Bromopyridin-3-yl)but-3-yn-1-ol (7)



5-Iodo-2-bromopyridine (**6**) (200 mg, 0.69 mmol) was dissolved in NEt₃ (3 mL) and the resulting mixture was degassed by three pump-freeze-thaw cycles before Pd(PPh₃)₄ (40 mg, 0.04 mmol), Cul (15 mg, 0.08 mmol) and but-3-yn-1-ol (55 mg, 0.79 mmol) were added. The mixture was stirred under an atmosphere of argon at 80 °C for 3 days. After completion the reaction mixture was filtered through a short plug of silica (EtOAc) and the resulting solution was concentrated to dryness under reduced pressure. Flash column chromatography on silica gel (EtOAc/hexane = 1:1) provided **7** (113 mg, 72%) as a colorless solid; mp 56–57 °C.

¹H NMR (500 MHz, CDCl₃): δ = 2.70, 3.85 (2 t, J = 6.4 Hz, 2 H each, 1-H/2-H), 2.98 (br. s, 1 H, OH), 7.41(d, J = 8.2 Hz, 1 H, 5'-H), 7.53 (dd, J = 2.3, 8.2 Hz, 1 H, 4'-H), 8.37 (d, J = 2.3 Hz, 1 H, 2'-H) ppm. ¹³C NMR (101 MHz, CDCl₃): δ = 23.7, 60.6 (2 t, C-1/C-2), 77.5, 92.1 (2 s, C≡C), 119.9 (s, C-3'), 127.5 (d, C-5'), 140.4 (s, C-6'), 140.8 (d, C-4'), 152.3 (d, C-2') ppm. IR (ATR): ν = 3310 (OH), 3035-2880 (-C=H, -C-H), 2240 (C≡C), 1570-1460 (C=C) cm⁻¹. HRMS (ESI-TOF): *m/z* calcd for C₉H₉BrNO [M+H]⁺: 225.9862, found: 225.9869. Anal. calcd for C₉H₇BrNO (226.1): C, 47.82; H, 3.57; N, 6.20, found: C, 47.59, H, 3.58; N, 6.46.

2-Methyl-4-[6-(pyridin-3-ylethynyl)pyridin-3-yl]but-3-yn-2-ol (**SI-1**)



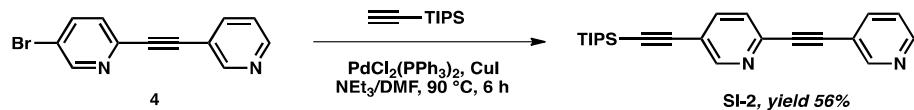
Pyridine derivative **4** (68 mg, 0.26 mmol), 2-methylbut-3-yn-2-ol (24 mg, 0.29 mmol), PdCl₂(PPh₃)₂ (9 mg, 0.01 mmol) and Cul (3 mg, 0.01 mmol) were dissolved in NEt₃ (2.6 mL)

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and the solution was degassed by three pump-freeze-thaw cycles. The mixture was heated to 80 °C for 16 h until complete consumption of the starting materials (TLC). After the mixture was cooled to r.t. water and EtOAc were added (20 mL each), the organic layer was separated and the aqueous layer was extracted with EtOAc (3 x 20 mL). The combined organic layers were dried with Na₂SO₄, filtered and the solvent was removed under reduced pressure. The crude product was purified by flash column chromatography on silica gel (hexane/EtOAc = 3:7) to afford 65 mg (95%) of **SI-1** as a colorless oil.

¹H NMR (400 MHz, CDCl₃): δ = 1.60 (s, 6 H, CH₃), 7.28-7.32, 7.43-7.45, 7.68-7.70, 7.84-7.87, 8.54-8.55, 8.61-8.62 (6 m, 1 H each, pyr), 8.78 (s, 1 H, pyr) ppm; the OH signal was not detected. ¹³C NMR (101 MHz, CDCl₃): δ = 31.3 (q, CH₃), 65.1 (s, C-2), 78.3, 87.1, 91.4, 100.0 (4 s, C≡C), 119.6, 123.2, 126.6, 128.4, 132.0, 138.7, 138.9, 141.0, 149.1, 152.4 (7 d, 3 s, Pyr) ppm. IR (ATR): ν = 3230-3000 (O-H, =C-H, C-H), 2230 (C≡C), 1585-1540 (C=C) cm⁻¹. HRMS (ESI-TOF): *m/z* calcd for C₁₇H₁₅N₂O [M+H]⁺: 263.1184, found: 263.1089. *m/z* calcd for C₁₇H₁₃N₂ [M+H-H₂O]⁺: 245.1079, found: 245.1061.

2-(Pyridin-3-ylethynyl)-5-[(triisopropylsilyl)ethynyl]pyridine (**SI-2**)



A reaction tube was charged with pyridine derivative **4** (200 mg, 0.77 mmol), PdCl₂(PPh₃)₂ (27 mg, 0.04 mmol) and CuI (7 mg, 0.04 mmol). Anhydrous DMF (2 mL), NEt₃ (1 mL) and (triisopropylsilyl)acetylene (169 mg, 0.93 mmol) were added and the resulting mixture was stirred under an atmosphere of argon at 90 °C for 6 h. After complete consumption of the starting materials (as indicated by TLC) saturated aqueous NH₄Cl solution was added. The organic layer was separated and the aqueous layer was extracted with EtOAc (3 x 20 mL). The combined organic layers were dried with Na₂SO₄, filtered and the solvent was removed under reduced pressure. The crude material was purified by flash column chromatography on silica gel (hexane/EtOAc = 7:3) to provide **SI-2** as a colorless oil (156 mg, 56%).

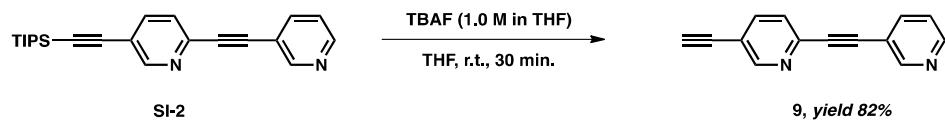
¹H NMR (500 MHz, CDCl₃): δ = 1.12 (s, 21 H, TIPS), 7.29, 7.47, 7.74, 7.86, 8.57, 8.67, 8.81 (7 m_c, 1 H each, Pyr) ppm. ¹³C NMR (101 MHz, CDCl₃): δ = 11.2, 18.6 (d, q, TIPS), 87.3, 91.5, 97.4, 103.0 (4 s, C≡C), 119.3, 120.1 (2 s, Pyr), 123.1, 126.4, 138.9, 139.0 (4 d, Pyr), 141.2 (s,

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Pyr), 149.3, 152.6, 152.9 (3 d, Pyr) ppm. IR (ATR): ν = 3090-2840 (=C-H, C-H), 2220 (C≡C), 1560-1450 (C=C) cm⁻¹. HRMS (ESI-TOF): *m/z* calcd for C₂₃H₂₉N₂Si [M+H]⁺: 316.2100, found: 316.2055. Anal. calcd for C₂₃H₂₈N₂Si (360.6): C, 76.61; H, 7.83; N, 7.77, found: C, 76.40; H, 7.56; N, 7.69.

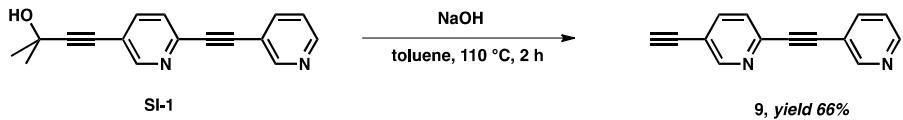
5-Ethynyl-2-(pyridin-3-ylethynyl)pyridine (9)

By proto-desilylation from **SI-2**:



To a solution of pyridine derivative **SI-2** (150 mg, 0.42 mmol) in THF (4 mL) was added TBAF (1.0 M solution in THF, 0.5 mL, 0.50 mmol). The resulting mixture was stirred at r.t. for 30 min. until the starting material had been consumed. The mixture was diluted with THF and water was added. The organic layer was separated and the aqueous layer was extracted with EtOAc (3 x 20 mL). The combined organic layers were dried with Na_2SO_4 , filtered and the solvent was removed under reduced pressure. The crude material was purified by flash column chromatography on silica gel (hexane/EtOAc = 1:1) to provide **9** as a beige solid (70 mg, 82%). Due to rapid decomposition, **9** has to be stored in the dark at -20 °C; mp 114-115 °C.

By elimination from **SI-1**:

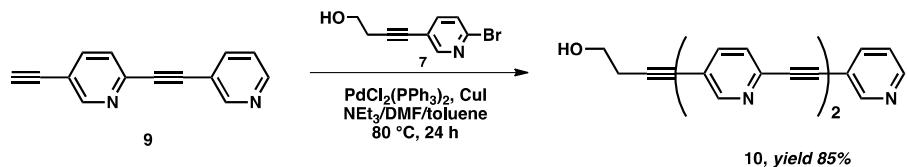


SI-1 (96 mg, 0.37 mmol) was dissolved in toluene (3.7 mL) and NaOH (44 mg, 1.83 mmol) was added. The mixture was heated to 100 °C for 2 h until complete consumption of the starting material was observed by TLC. The mixture was cooled to r.t. and CH₂Cl₂ and water were added. The organic layer was separated and the aqueous layer was extracted with CH₂Cl₂. The combined organic layers were dried with Na₂SO₄, filtered and all volatiles were removed under reduced pressure. The residual material was purified by flash column chromatography on silica gel (hexane:EtOAc = 1:1) to provide **9** as a brownish solid (50 mg, 66%); mp 114-115 °C.

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¹H NMR (400 MHz, CDCl₃): δ = 3.32 (s, 1 H, ≡CH), 7.40-7.52, 7.61-7.68, 7.72-7.75, 7.71-7.76, 8.52-8.56, 8.68-8.72, 8.78-8.81 (7 m, 1 H each, Pyr) ppm. ¹³C NMR (101 MHz, CDCl₃): δ = 79.9, 82.5 (s, d, C≡C), 87.5, 91.2 (2 s, C≡C), 118.7, 119.1 (2 s, Pyr), 123.0, 126.4, 138.8, 139.2 (4 d, Pyr), 141.8 (s, Pyr), 149.3, 152.5, 153.0 (3 d, Pyr) ppm. IR (KBr): ν = 3200-2920 (≡C-H, C-H), 2220-2100 (C≡C), 1575-1455 (C=C) cm⁻¹. HRMS (ESI-TOF): *m/z* calcd for C₁₄H₉N₂ [M+H]⁺: 205.0776, found: 205.0766. Anal. calcd for C₁₄H₈N₂ (204.2): C, 82.33; H, 3.95; N, 13.72, found: C, 81.58; H, 3.65; N, 13.57.

4-{6-[(6-(Pyridin-3-ylethynyl)pyridin-3-yl)ethynyl]pyridin-3-yl}but-3-yn-1-ol (**10**)



A Schlenk flask was charged with pyridine derivative **7** (44 mg, 0.20 mmol), ethynyl pyridine **9** (40 mg, 0.20 mmol), $\text{PdCl}_2(\text{PPh}_3)_2$ (14 mg, 0.02 mmol) and CuI (7 mg, 0.04 mmol). NEt_3 (2 mL), pyridine (0.5 mL) and toluene (0.5 mL) were added and the resulting solution was heated to 80 °C under an atmosphere of argon for 24 h until complete consumption of the starting materials had been indicated by TLC. The mixture was filtered through a short plug of silica (EtOAc) and concentrated to dryness. The residue was purified by flash column chromatography (silica gel, 15% MeOH in CH_2Cl_2). The obtained solid was recrystallized from pyridine to provide pyridine derivative **10** in pure form (58 mg, 85%) as a colorless solid; mp > 300 °C.

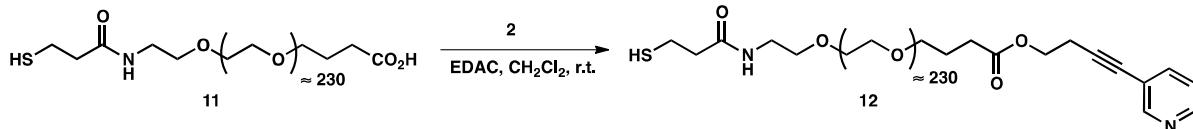
¹H NMR (700 MHz, CDCl₃/benzene-d₆): δ = 2.56, 3.71 (2 t, J = 6.3 Hz, 2 H each, 1-H/2-H), 7.09 (ddd, J = 0.7, 4.9, 7.8 Hz, 1 H), 7.32 (dd, J = 0.7, 8.0 Hz, 1 H), 7.36 (dd, J = 0.8, 8.1 Hz, 1 H), 7.54 (dd, J = 2.1, 8.0 Hz, 1 H), 7.70 (dd, J = 2.1, 8.1 Hz, 1 H), 7.74-7.72 (m, 1 H), 8.46 (dd, J = 4.7, 1.4 Hz, 1 H), 8.60-8.61 (m, 1 H), 8.75-8.78 (m, 2 H) ppm; the OH signal could not be detected. ¹³C NMR (175 MHz, CDCl₃/benzene-d₆): δ = 28.8, 60.8 (2 t, C-1/C-2), 78.8, 86.9, 87.9, 91.5, 92.8, 93.3 (6 s, C≡C), 118.8, 119.2, 120.37 (3 s, Pyr), 123.1, 126.50, 126.54, 138.7, 138.8, 138.9 (6 d, Pyr), 140.8, 142.1 (2 s, Pyr), 149.4, 152.6, 152.8, 152.9 (e d, Pyr) ppm. IR (ATR): ν = 3350 (OH), 3045-2680 (=C-H, -C-H), 2490-2220 (C≡C), 1540-1360 (C=C) cm⁻¹. HRMS (ESI-TOF): m/z calcd for C₂₃H₁₆N₃O [M+H]⁺: 350.1288, found: 350.1280.

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Synthesis of pyridine-PEG conjugates

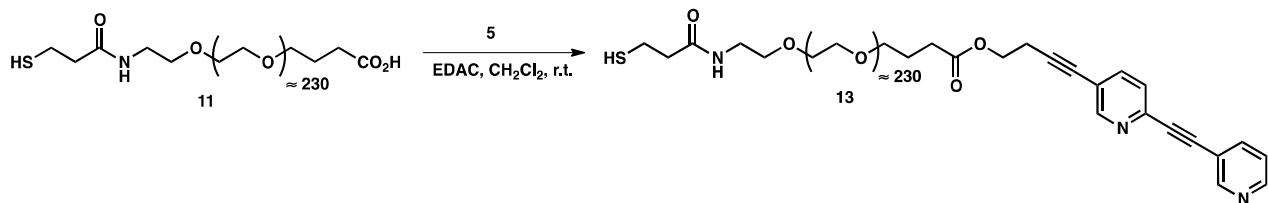
Monovalent pyridine-PEG conjugate (12)



To a solution of **11** (18.6 mg, 1.9 μ mol) and pyridyl-alcohol **2** (5.6 mg, 0.038 mmol) in anhydrous CH_2Cl_2 (0.3 mL) was added EDAC (0.8 mg, 0.0042 mmol) and the resulting mixture was stirred at r.t. under an atmosphere of argon for 3 days. The solvent was evaporated and the residue was purified by dialysis (MW cut-off: 1000 g/mol) against MeOH to provide the pyridine-PEG conjugate **12** (14 mg, 75%) as a colorless solid; mp 127 °C.

^1H NMR (700 MHz, CDCl_3): δ = 2.59 (t, J = 6.7 Hz, 2 H, CH_2), 2.63 (t, J = 8.9 Hz, 2 H, CH_2), 2.97 (t, J = 6.9 Hz, 2 H, CH_2), 3.13 (t, J = 6.7 Hz, 2 H, CH_2), 3.64 (s, - $\text{OCH}_2\text{CH}_2\text{O}-$, \approx 460 H), 7.45, 7.68, 8.51, 8.62 (4 m_c, 1 H each, Pyr) ppm.

Bivalent pyridine-PEG conjugate (13)

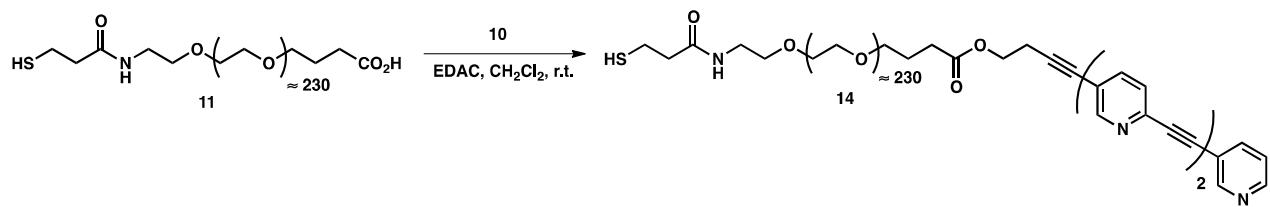


To a solution of **11** (53.2 mg, 5.3 μ mol) and pyridyl-alcohol **5** (12.4 mg, 0.056 mmol) in anhydrous CH_2Cl_2 (0.3 mL) was added EDAC (1.1 mg, 0.0076 mmol) and the resulting mixture was stirred at r.t. under an atmosphere of argon for 3 days. The solvent was evaporated and the residue was purified by dialysis (MW cut-off: 1000 g/mol) against MeOH to provide the pyridine-PEG conjugate **13** (37 mg, 74%) as a yellowish solid; mp 127 °C.

^1H NMR (500 MHz, CDCl_3): δ = 2.58 (t, J = 7.1 Hz, 2 H, CH_2), 2.72 (t, J = 6.4 Hz, 2 H, CH_2), 2.95 (t, J = 7.1 Hz, 2 H, CH_2), 3.64 (s, - $\text{OCH}_2\text{CH}_2\text{O}-$, \approx 460 H), 7.29 (dd, J = 4.9, 8.0 Hz, 1 H, Pyr), 7.46 (d, J = 8.0 Hz, 1 H, Pyr), 7.71-7.66 (m, 1 H, Pyr), 7.85 (d, J = 7.8 Hz, 1 H, Pyr), 8.57 (d, J = 4.9 Hz, 1 H, Pyr), 8.63, 8.80 (2 s, 1 H each, Pyr) ppm.

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Trivalent pyridine-PEG conjugate (14)



To a solution of **11** (49.0 mg, 0.0049 mmol) and pyridyl-alcohol **10** (17.0 mg, 0.049 mmol) in anhydrous CH_2Cl_2 (0.3 mL) was added EDAC (2.8 mg, 0.0146 mmol) and the resulting mixture was stirred at r.t. under an atmosphere of argon for 3 days. The solvent was evaporated and the residue was purified by dialysis (MW cut-off: 1000 g/mol) against MeOH to provide the pyridine-PEG conjugate **14** (31 mg, 63%) as a yellowish solid; mp 127 °C.

¹H NMR (700 MHz, CDCl₃): δ = 2.41 (m_c 2 H, CH₂), 2.60, 2.98 (2 t, J = 7.2 Hz, 2 H CH₂), 3.64 (s, -OCH₂CH₂O-, ≈ 460 H), 6.63 (m_c, 2 H, Pyr), 7.32, 7.55, 7.81, 7.89, 8.61, 8.80, 8.88 (7 m_c, 1 H each, Pyr) ppm.

Measurements in pure H₂O

We measured saw-tooth signals in pure H₂O (without additional metal ions) or saturated solutions of EDTA as well. Over the measured range of loading rates and according to the first and second maximum, respectively, the most probable rupture forces f^* of these measurements were smaller than those for the experiments in metal containing solvents. Applying the BKE model (Figure 1) we calculated larger rupture lengths than for the metal containing interactions. We attribute this kind of interaction to dipol-dipol interactions between pyridines in a parallel displaced configuration.^{1,2} This interaction is characterized by a quite flat energy surface, leading to relatively long rupture lengths.³

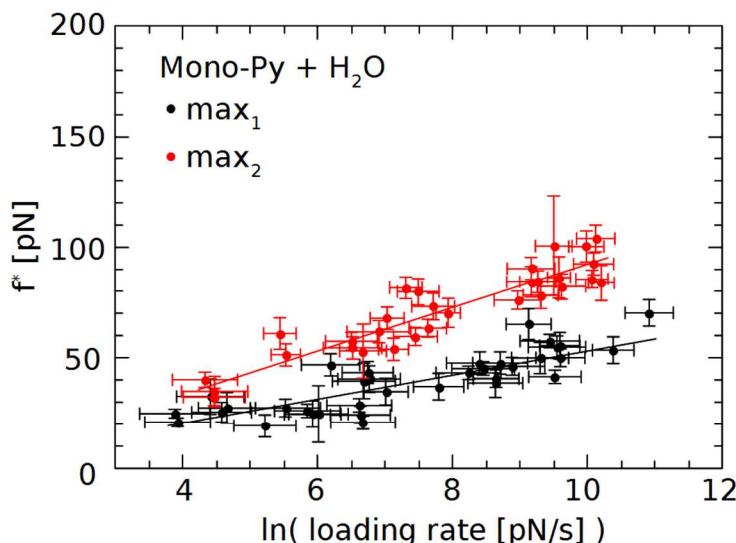


Figure 1: KBE plot for monovalent pyridine in H₂O, considering the first (max₁) and second maximum (max₂). Continuous lines represent fits according to the KBE model with (black) $r_b = 7.6 \pm 0.5 \text{ \AA}$, $k_{\text{off}} = 0.23 \pm 0.10 \text{ s}^{-1}$, (red) $r_b = 4.2 \pm 0.2 \text{ \AA}$, $k_{\text{off}} = 0.19 \pm 0.07 \text{ s}^{-1}$.

(1) Hohenstein, E. G.; Sherrill, C. D. *J. Phys. Chem. A* **2009**, *113*, 878.

(2) Ninkovic, D. B.; Janjic, G. V.; Zaric, S. D. *Cryst Growth Des* **2012**, *12*, 1060.

(3) Piacenza, M.; Grimme, S. *ChemPhysChem* **2005**, *6*, 1554.

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Contour lengths of non-modified PEG

If rupture signals in SMFS experiments show a pronounced accumulation at certain tip-sample-separations, a separate analysis according to the expected tether length is possible. Therefore we designed the experiment such, that surfaces as well as cantilever tips were coated by pyridine end-modified polymers. Using the double tether approach, only signals around twice the contour length would be selected for further investigation.^{1,2} Unfortunately, we detected rupture events at higher contour lengths as well. Therefore we utilized the coordination of Fe²⁺ with carboxylic acids in an octahedral coordination with additional aqua ligands^{3,4} in order to measure contour lengths of the non-modified polymers with COOH end modification.

In Figure 2 rupture forces of last-peak saw tooth signals are plotted over their corresponding tip-sample-separation. Red lines are worm-like chain plots using a persistence length of 0.38 nm⁵ and multiples of the polymer contour length (assuming an all-trans configuration under force with 0.36 nm⁶ per repeat unit). At a pulling angle of 90° normal to the surface and cantilever modification at the tip apex, all rupture points would accumulate along this plots. A shift of rupture points to a lower tip-sample-separation may be due to a worn tip without any modifications left at the apex. Thus, already the purchased polymer shows accumulation of data points for doubles and triples of the contour length and the double tether approach was not applicable here.

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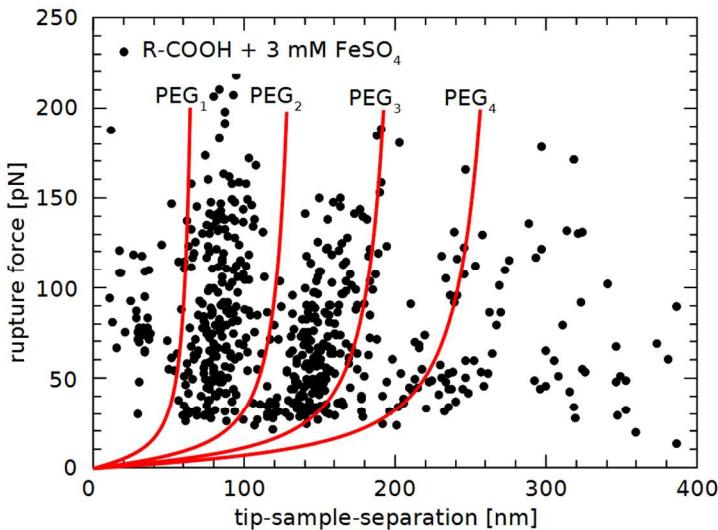


Figure 2: Force vs. tip-sample-separation plot of all last-peak rupture events in a blank experiment using non-modified PEG in 3 mM FeSO_4 (black circles). Red lines are WLC plots according to the analyzed polymer ($l_p = 0.38 \text{ nm}$, $L_{c1} = 72.7 \text{ nm}$, $L_{c2} = 145.4 \text{ nm}$, $L_{c3} = 218.2 \text{ nm}$, $L_{c4} = 290.9 \text{ nm}$)

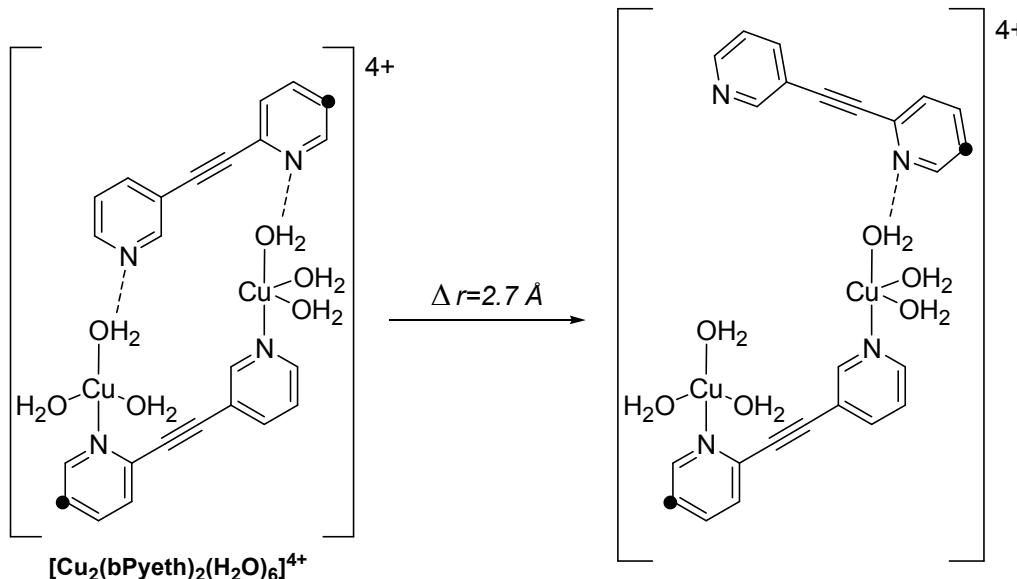
Sample Preparation: UV/ozone cleaned gold coated cantilevers and freshly template-stripped gold surfaces were incubated for 12 to 24 hours with a 0.1 mM aqueous solution of thiol end-modified $\text{HS-C}_2\text{H}_4\text{-CONH-PEG-O-C}_3\text{H}_6\text{-COOH}$ (Rapp Polymere GmbH, Tübingen, M = 9040 Da, PDI = 1.04). Afterwards, cantilevers and surfaces were rinsed thoroughly with water and immediately used for force-spectroscopy measurements in freshly prepared 3 mM FeSO_4 solution.

- (1) Ratto, T. V.; Langry, K. C.; Rudd, R. E.; Balhorn, R. L.; Allen, M. J.; McElfresh, M. W. *Biophys J* **2004**, 86, 2430.
- (2) Ray, C.; Akhremitchev, B. B. *J Am Chem Soc* **2005**, 127, 14739.
- (3) Ohtaki, H.; Radnai, T. *Chem. Rev.* **1993**, 93, 1157.
- (4) Mandado, M.; Cordeiro, M. N. D. S. *J. Comp. Chem.* **2010**, 31, 2735.
- (5) Kienberger, F. P.; Kada, G.; Gruber, H. J.; Riener, C.; Schindler, H. S.; Hinterdorfer, P. *Single Mol* **2000**, 1, 123.
- (6) Oesterhelt, F.; Rief, M.; Gaub, H. E. *New J Phys* **1999**, 1.

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Optimization issues for $[\text{Cu}_2(\text{bPyeth})_2(\text{H}_2\text{O})_6]^{4+}$ complex

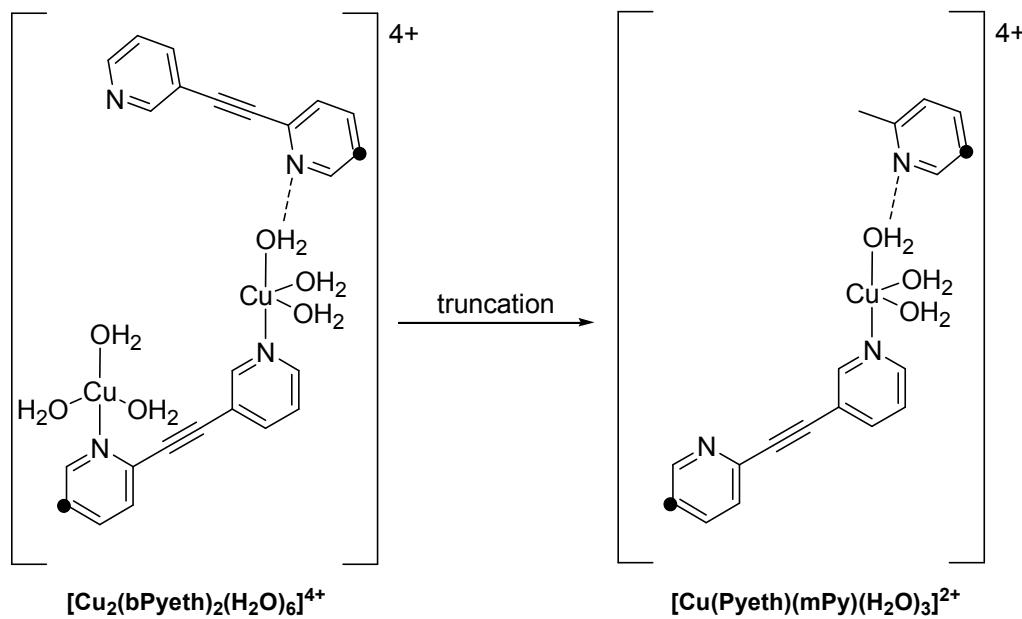
During the optimization of $[\text{Cu}_2(\text{bPyeth})_2(\text{H}_2\text{O})_6]^{4+}$ complex at $\Delta r = 2.7 \text{ \AA}$, where the rupture of the hydrogen bond in the outer shell of one of the copper centers takes place, the QM program arrives to a convergency problem.



HB-form

To avoid this problem the original $[\text{Cu}_2(\text{bPyeth})_2(\text{H}_2\text{O})_6]^{4+}$ structure was truncated to smaller model $[\text{Cu}(\text{bPyeth})(\text{mPy})(\text{H}_2\text{O})_3]^{2+}$, where the molecular groups essential for the further computations were conserved. The energies of the truncated model were normalized to original $[\text{Cu}_2(\text{bPyeth})_2(\text{H}_2\text{O})_6]^{4+}$.

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Additional parameters derived from COGEF approach for gas-phase models $[\text{Zn}(\text{Py})_2(\text{H}_2\text{O})_4]^{2+}$ and $[\text{Cu}(\text{Py})_2(\text{H}_2\text{O})_4]^{2+}$

In COGEF approach the energy curves in vacuum can be represented by Morse potential function:

$$V_f = D_e(1 - e^{-\beta r})^2,$$

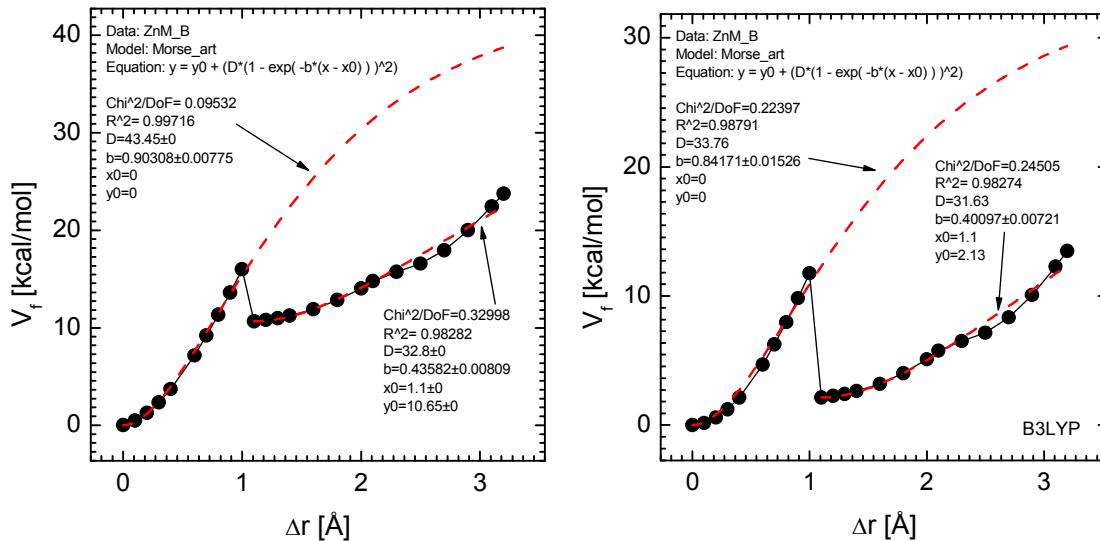
$$\beta = 2f_{\max} / D_e,$$

$$D_e = V_f(r \rightarrow \infty) - V_f(r_{eq})$$

By fitting Morse potential to the energy curves two relevant parameters can be identified, namely the maximal value of the force f_{\max} along the curve and the length (r_{max}) corresponding to maximal force. Another parameter, which we are interested in, is a distance r_b at which the bond breaks during the DFT-calculation.

$[\text{Zn}(\text{Py})_2(\text{H}_2\text{O})_4]^{2+}$ in gas-phase

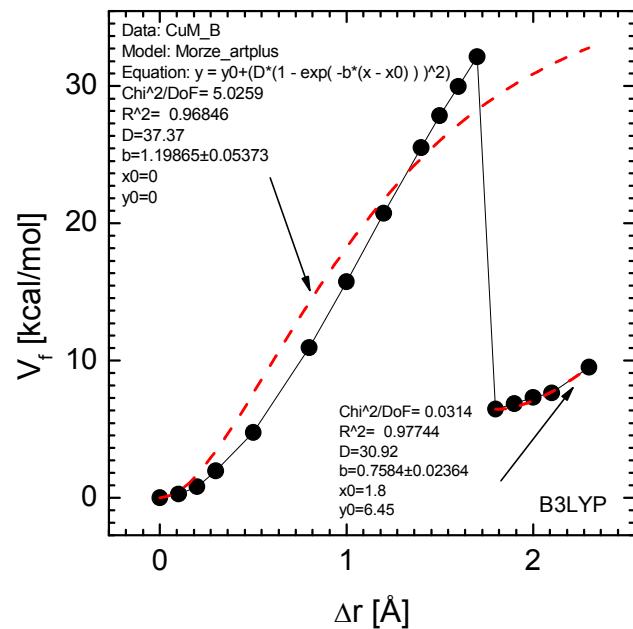
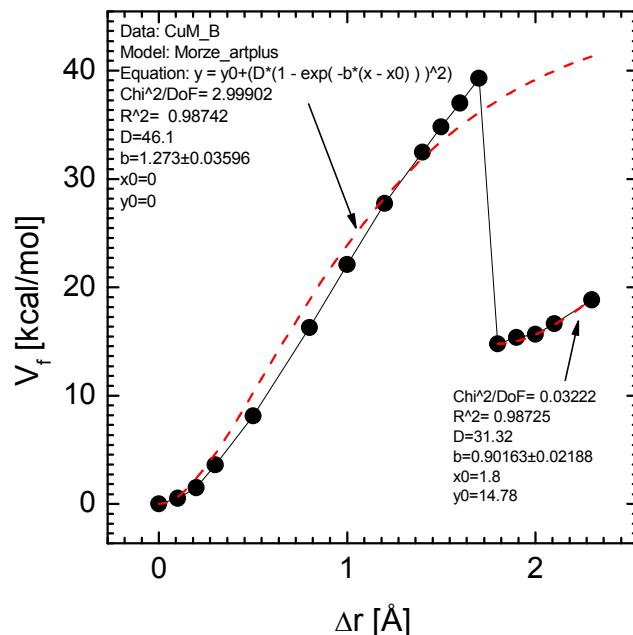
	f_{\max}, nN	$r_{max}, \text{\AA}$	$r_b, \text{\AA}$	$D_e, \text{kcal/mol}$
M06D3	1.362	0.77	1.1	43.45
	0.496	2.69	3.3	32.80
B3LYP	0.987	0.83	1.1	33.76
	0.440	2.83	3.3	31.63



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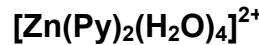
$[\text{Cu}(\text{Py})_2(\text{H}_2\text{O})_4]^{2+}$ in gas-phase

	$f_{max, \text{nN}}$	$r_{max, \text{\AA}}$	$r_b, \text{\AA}$	$D_e, \text{kcal/mol}$
M06D3	2.033	0.55	1.8	46.10
	0.981	2.56	2.5	31.32
B3LYP	1.556	0.58	1.8	37.37
	0.814	2.82	2.5	30.92



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Optimized geometries for gas-phase models.



$\Delta r=0.0 \text{ \AA}$

Atom	X	Y	Z
H1	1.3916078380	7.3860469076	-1.3196551380
C2	2.5812907414	10.3594895768	0.7657303850
C3	3.2466051060	9.1395107292	0.7437807715
N4	2.8263842768	8.0891373829	0.0025852480
C5	1.7122730412	8.2496835962	-0.7471360657
C6	0.9961885632	9.4400308729	-0.7861504957
C7	1.4351119764	10.5169100305	-0.0146341151
H8	2.9591391239	11.1687645523	1.3810623307
H9	4.1505164388	8.9858948221	1.3232206759
H10	0.11074466362	9.5165200822	-1.4077868607
H11	0.8953884997	11.4588344731	-0.0214067549
C12	6.3555856705	1.9257830912	0.0352878574
C13	6.9655346543	3.0921382037	-0.4285558077
C14	6.2433918638	4.2794300998	-0.4141441419
N15	4.9660168688	4.3548090803	0.0242049689
C16	4.3818383813	3.2183474196	0.4680407675
C17	5.0392355400	1.9942148505	0.4936497946
H18	6.8946601597	0.9835293909	0.0396385364
H19	7.9867826871	3.0867513317	-0.7938607763
H20	6.6903019554	5.2088563535	-0.7504104126
H21	3.3529975141	3.3065827611	0.8001186862
H22	4.5249103783	1.1136795643	0.8632961455
O23	5.8123946045	7.3223333669	0.3536932704
O24	1.9821426207	5.1232389192	-0.3283109207
O25	3.6148640005	6.0694136443	2.1878027256
O26	4.1923915866	6.3781211337	-2.1580036724
Zn27	3.8971777154	6.2230385739	0.0143283394
H28	3.9218342406	5.3496942485	2.7565381182
H29	3.1390717299	6.6936402089	2.7531527589
H30	6.4233366288	7.1961538812	1.0927256354
H31	6.1881025706	8.0159186762	-0.2062104460
H32	4.6556666443	5.7431930652	-2.7217869113
H33	3.8906400689	7.0971840017	-2.7302435422
H34	1.7896232074	4.5199785000	-1.0593546713
H35	1.1867770389	5.1616620468	0.2209644439

$\Delta r=0.1 \text{ \AA}$

Atom	X	Y	Z
H1	1.3455178994	7.2801772453	-1.1324451372
C2	2.5813000036	10.3594999877	0.7656999996
C3	3.2471325638	9.1378676923	0.7919264382
N4	2.8125416500	8.0483638776	0.1166965845
C5	1.6793677212	8.1715092829	-0.6124442369
C6	0.9602805144	9.3577646994	-0.6951248282
C7	1.4160314835	10.4746810217	0.0068099693
H8	2.9736824833	11.1994393327	1.3288048077
H9	4.1639051380	9.0149796602	1.3586165989
H10	0.0590597693	9.4004520820	-1.2972649833
H11	0.8743526300	11.4144690639	-0.0366283836
C12	6.3955067299	1.8684254847	0.0636005415
C13	7.0021230508	3.0643193087	-0.3234864258
C14	6.2653527396	4.2414292106	-0.2684454115
N15	4.9760193483	4.2829068519	0.1398111534
C16	4.3965300630	3.1174633631	0.5111690348
C17	5.0673999964	1.8985000123	0.4905000004
H18	6.9462759869	0.9334124058	0.0334934963
H19	8.0326291574	3.0892630281	-0.6612195507
H20	6.7104055673	5.1907264739	-0.5462921406
H21	3.3593234570	3.1772814116	0.8231374811

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H22	4.5537950962	0.9953082119	0.8019097651
O23	5.7966229238	7.2734623883	0.5076149040
O24	1.9830179539	5.0530537378	-0.1725073019
O25	3.6079500916	6.0114015884	2.3212931029
O26	4.1872210150	6.3211268993	-2.0089552758
Zn27	3.8911077577	6.1644212343	0.1589153691
H28	3.8945392960	5.2808295762	2.8867909965
H29	3.1516093971	6.6483006342	2.8885572613
H30	6.3885289351	7.1730460034	1.2661272826
H31	6.1860789975	7.9472455578	-0.0668419137
H32	4.6672180933	5.6964666361	-2.5701591708
H33	3.8654184290	7.0301772441	-2.5827387533
H34	1.7811123344	4.4690789649	-0.9167839993
H35	1.1995874837	5.0675085211	0.3948259608

$\Delta r=0.2 \text{ \AA}$			
Atom	X	Y	Z
H1	1.3071510425	7.1918478243	-0.9550482370
C2	2.5813000042	10.3594999856	0.7656999995
C3	3.2488619218	9.1383380222	0.8351675728
N4	2.8032090972	8.0153987762	0.2231931541
C5	1.6526210366	8.1056940866	-0.4842776492
C6	0.9297409523	9.2862671378	-0.6064482628
C7	1.3989966536	10.4368177995	0.0293683969
H8	2.9863419970	11.2245854179	1.2793625909
H9	4.1770603788	9.0432858945	1.3885564098
H10	0.0145633913	9.2989122691	-1.1886545673
H11	0.8542155525	11.3726896791	-0.0473517994
C12	6.4334934506	1.8072761009	0.0923465888
C13	7.0340310146	3.0270720715	-0.2233387706
C14	6.2824240697	4.1925007270	-0.1328968049
N15	4.9825607542	4.2041619567	0.2448107337
C16	4.4105851482	3.0145548493	0.5480510898
C17	5.0955999958	1.8026000144	0.4874000004
H18	6.9967687598	0.8811929845	0.0321857032
H19	8.0720729538	3.0792280587	-0.5337749562
H20	6.7243902279	5.1570071286	-0.3575303633
H21	3.3661851729	3.0482568804	0.8395909458
H22	4.5840601433	0.8814942281	0.7446996464
O23	5.7790661489	7.2158936095	0.6560388543
O24	1.9847216023	4.9915814210	-0.0220409605
O25	3.6025701738	5.9533046288	2.4446761038
O26	4.1807681654	6.2629403115	-1.8680971094
Zn27	3.8851373717	6.1058882658	0.2925653375
H28	3.8625319067	5.2088355665	3.0049973559
H29	3.1731488581	6.6053804291	3.0157895023
H30	6.3523138663	7.1315123073	1.4307307233
H31	6.1856777019	7.8718348195	0.0728445419
H32	4.6557277704	5.6345184605	-2.4294696342
H33	3.8617278238	6.9746639331	-2.4401989932
H34	1.7661704968	4.4304644121	-0.7791216314
H35	1.2164620847	4.9852727041	0.5658913427

$\Delta r=0.3 \text{ \AA}$			
Atom	X	Y	Z
H1	1.2877107163	7.1331974687	-0.8306561234
C2	2.5813000031	10.3594999893	0.7656999996
C3	3.2558945073	9.1409967781	0.8587491329
N4	2.8050921603	7.9953552036	0.2920643211
C5	1.6395538824	8.0614106031	-0.3939206834
C6	0.9088215815	9.2347937580	-0.5376817059
C7	1.3841152328	10.4075794408	0.0517532241
H8	2.9937032785	11.2410617167	1.2441456443
H9	4.1951096583	9.0675755239	1.3971131819
H10	-0.0179171800	9.2249666674	-1.1013401241

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H11	0.8323467212	11.3375870124	-0.0436138144
C12	6.4691908184	1.7345656554	0.1175452463
C13	7.0647042905	2.9687719498	-0.1486049043
C14	6.3020776176	4.1253983281	-0.0393920812
N15	4.9942141849	4.1186603324	0.3109014740
C16	4.4278969409	2.9140357841	0.5664397884
C17	5.1237999969	1.7067000107	0.4843000003
H18	7.0422893800	0.8157734200	0.0411596038
H19	8.1084029296	3.0386243346	-0.4356870655
H20	6.7423383590	5.0984736119	-0.2273166195
H21	3.3776901846	2.9304926872	0.8387744261
H22	4.6134837841	0.7752499846	0.7038858049
O23	5.7742536757	7.1581222750	0.7466379333
O24	1.9983272863	4.9415647124	0.0723780542
O25	3.6102801124	5.9014815640	2.5190587175
O26	4.1867737936	6.2095055021	-1.7753931181
Zn27	3.8917527253	6.0530766822	0.3755868115
H28	3.8518292617	5.1480105113	3.0756852094
H29	3.1990547208	6.5633747742	3.0923584229
H30	6.3330351163	7.0867011906	1.5331325371
H31	6.1953114215	7.7974214375	0.1552655637
H32	4.6618324443	5.5801858678	-2.3357307603
H33	3.8667334612	6.9214490382	-2.3467233616
H34	1.7660110494	4.4003379049	-0.6950079574
H35	1.2419972906	4.9192931481	0.6752435342

$\Delta r=0.4 \text{ \AA}$			
Atom	X	Y	Z
H1	1.2640402930	7.0907165302	-0.7253695263
C2	2.5813000026	10.3594999913	0.7656999997
C3	3.2611794409	9.1424668476	0.8733241227
N4	2.8040437315	7.9799483185	0.3447314747
C5	1.6236890418	8.0290453251	-0.3175165058
C6	0.8866207610	9.1969895155	-0.4739933123
C7	1.3695438760	10.3859419484	0.0760482293
H8	3.0021259456	11.2527059187	1.2141627681
H9	4.2109870336	9.0848727114	1.3951592104
H10	-0.0517749812	9.1707091146	-1.0175816255
H11	0.8120175873	11.3113025156	-0.0310586266
C12	6.5047484045	1.6605279768	0.1461328951
C13	7.0928108405	2.9066611619	-0.0787901317
C14	6.3166542799	4.0537129980	0.0384259450
N15	5.0008277129	4.0297409845	0.3587390327
C16	4.4428833916	2.8123533185	0.5739731672
C17	5.1519999975	1.6108000087	0.4812000003
H18	7.0895506632	0.7497099872	0.0625286185
H19	8.1420263082	2.9930557917	-0.3403038737
H20	6.7535016402	5.0338164968	-0.1188961829
H21	3.3869391192	2.8123515912	0.8243618546
H22	4.6448409435	0.6707338867	0.6686301350
O23	5.7664670456	7.0969873801	0.8131736728
O24	2.0059535115	4.8952477927	0.1419039511
O25	3.6120892364	5.8485046224	2.5708990264
O26	4.1865694948	6.1560919787	-1.7047229309
Zn27	3.8923930011	5.9998546357	0.4356937938
H28	3.8382254411	5.0875960783	3.1239792202
H29	3.2161295708	6.5180768646	3.1461300972
H30	6.3118737334	7.0371816248	1.6100041798
H31	6.2019899673	7.7194614446	0.2143339672
H32	4.6608009738	5.5254435323	-2.2643888284
H33	3.8663985424	6.8690230484	-2.2748618102
H34	1.7616822141	4.3718190980	-0.6340714907
H35	1.2596124491	4.8600501191	0.7565065903

$\Delta r=0.6 \text{ \AA}$			
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Atom	X	Y	Z
H1	1.2482142701	7.0290528788	-0.5765256765
C2	2.5813000053	10.3594999818	0.7656999994
C3	3.2767176873	9.1476960210	0.8874891223
N4	2.8172216357	7.9605356015	0.4135202368
C5	1.6143448948	7.9816856413	-0.2089965087
C6	0.8604519384	9.1375240919	-0.3772130752
C7	1.3471531588	10.3495011704	0.1171049947
H8	3.0094730608	11.2692950229	1.1714421348
H9	4.2436754057	9.1169606991	1.3803654669
H10	-0.0953571939	9.0843897307	-0.8874928991
H11	0.7746565771	11.2642571220	-0.0013983257
C12	6.5717682624	1.4959134314	0.1935495786
C13	7.1510396995	2.7558101128	0.0287321367
C14	6.3579373535	3.8910115812	0.1499927303
N15	5.0309120566	3.8480716286	0.4190225509
C16	4.4829915562	2.6151624773	0.5759627725
C17	5.2083999947	1.4190000182	0.4750000006
H18	7.1722702954	0.5958405465	0.1049777852
H19	8.2082782301	2.8615711736	-0.1898624551
H20	6.7923256933	4.8784530134	0.0366633020
H21	3.4183372918	2.5951678500	0.7881645661
H22	4.7034795432	0.4696991547	0.6152254895
O23	5.7788910654	6.9756170373	0.8828974452
O24	2.0403683825	4.8184561234	0.2252618387
O25	3.6422599531	5.7531665758	2.6304858570
O26	4.2069845974	6.0543416446	-1.6110717618
Zn27	3.9169351072	5.9016444041	0.5099779444
H28	3.8461924135	4.9822012388	3.1785129130
H29	3.2693778761	6.4341089280	3.2080190555
H30	6.3058083587	6.9383210860	1.6934254516
H31	6.2351567708	7.5673191224	0.2685138348
H32	4.6761446022	5.4187997816	-2.1696699390
H33	3.8890103094	6.7700330182	-2.1791889495
H34	1.7837303257	4.3146427103	-0.5596540357
H35	1.3044863129	4.7708022235	0.8515418308

$\Delta r=0.7 \text{ \AA}$			
Atom	X	Y	Z
H1	1.2279160815	7.0024522499	-0.4918152972
C2	2.5813000010	10.3594999966	0.7656999999
C3	3.2852664625	9.1504891021	0.8858886741
N4	2.8203387501	7.9530558677	0.4422091787
C5	1.6007267435	7.9614537801	-0.1473943423
C6	0.8369023880	9.1115317069	-0.3117094696
C7	1.3302846306	10.3334332822	0.1510660190
H8	3.0166850133	11.2765195761	1.1464969541
H9	4.2648007071	9.1314588659	1.3542797538
H10	-0.1322407842	9.0464697079	-0.7947500718
H11	0.7494826337	11.2432129106	0.0344664611
C12	6.6062459004	1.4123079680	0.2274716791
C13	7.1814717430	2.6778530006	0.0934770695
C14	6.3788371400	3.8074220633	0.2077869520
N15	5.0455394691	3.7554938892	0.4416961836
C16	4.5023606362	2.5161526078	0.5685437978
C17	5.2365999990	1.3231000034	0.4719000001
H18	7.2150522225	0.5173743332	0.1436625789
H19	8.2434355332	2.7922852612	-0.0960469776
H20	6.8115055887	4.7981428111	0.1172096875
H21	3.4326961163	2.4871531373	0.7536224448
H22	4.7331124163	0.3698165066	0.5869609374
O23	5.7780129160	6.9109658002	0.9138488197
O24	2.0493095476	4.7759769810	0.2529065346
O25	3.6433528827	5.6970700445	2.6488907151
O26	4.2093347290	6.0010255126	-1.5769276115
Zn27	3.9196225477	5.8482089142	0.5344563708
H28	3.8418750246	4.9231826423	3.1948577373
H29	3.2746489600	6.3799794174	3.2268883107

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H30	6.2959466099	6.8790546940	1.7303305102
H31	6.2427279480	7.4944889297	0.2980138331
H32	4.6795502025	5.3650601597	-2.1343125182
H33	3.8889317365	6.7158843832	-2.1448726537
H34	1.7804679981	4.2955053579	-0.5424894988
H35	1.3266642555	4.7049130984	0.8921975367

$\Delta r=0.8 \text{ \AA}$			
Atom	X	Y	Z
H1	1.2270785483	6.9847091869	-0.4466609954
C2	2.5813000010	10.3594999966	0.7656999999
C3	3.2919300050	9.1526395137	0.8866432339
N4	2.8277038545	7.9479532702	0.4597465518
C5	1.6008535511	7.9476580026	-0.1144214313
C6	0.8301158691	9.0932285745	-0.2791780932
C7	1.3229937894	10.3217317388	0.1668097235
H8	3.0179548222	11.2812351986	1.1334747809
H9	4.2772587648	9.1425962302	1.3435707414
H10	-0.1445874319	9.0197433156	-0.7496824015
H11	0.7360728057	11.2274710478	0.0492524839
C12	6.6368119892	1.3247494447	0.2419724274
C13	7.2075611525	2.5942188244	0.1245147819
C14	6.3988347907	3.7198078846	0.2371286201
N15	5.0628780553	3.6622987621	0.4538201512
C16	4.5246308641	2.4185256447	0.5646037319
C17	5.2647999990	1.2272000034	0.4688000002
H18	7.2511357329	0.4334832917	0.1589232469
H19	8.2713286437	2.7145532595	-0.0509110891
H20	6.8297859556	4.7125508111	0.1587791063
H21	3.4527862848	2.3829027109	0.7368069124
H22	4.7632614107	0.2714188223	0.5707723998
O23	5.7902880740	6.8481411296	0.9283009057
O24	2.0673528046	4.7458296280	0.2703389552
O25	3.6597501840	5.6506565992	2.6599198559
O26	4.2246043606	5.9539940600	-1.5501330696
Zn27	3.9353103676	5.8019586878	0.5525833350
H28	3.8489244822	4.8725334484	3.2033604337
H29	3.3007335190	6.3378252777	3.2391261371
H30	6.2997305300	6.8266693062	1.7504809765
H31	6.2649355497	7.4166007957	0.3059628838
H32	4.6883494434	5.3133938566	-2.1077496955
H33	3.9110555720	6.6735658331	-2.1160670812
H34	1.7945944487	4.2725355141	-0.5280284614
H35	1.3475406627	4.6718208636	0.9125015398

$\Delta r=0.9 \text{ \AA}$			
Atom	X	Y	Z
H1	1.2341388554	6.9745491382	-0.4293838222
C2	2.5813000004	10.3594999985	0.7656999999
C3	3.2992701222	9.1551426902	0.8817746608
N4	2.8386236667	7.9462782819	0.4615861236
C5	1.6066484137	7.9396869086	-0.1015427725
C6	0.8283056392	9.0809865771	-0.2613242513
C7	1.3179751230	10.3132289907	0.1782084616
H8	3.0169081952	11.2838237775	1.1280104253
H9	4.2886885275	9.1517917872	1.3303441775
H10	-0.1501506801	9.0014274431	-0.7230079406
H11	0.7245659468	11.2151705030	0.0642976006
C12	6.6662390848	1.2367538401	0.2505151153
C13	7.2308452766	2.5095671974	0.1379822328
C14	6.4153125500	3.6310749472	0.2440424996
N15	5.0778797778	3.5679182385	0.4495282647
C16	4.5461780297	2.3203989938	0.5552376910
C17	5.2929999996	1.1313000015	0.4657000000
H18	7.2864352598	0.3491115931	0.1726046508

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H19	8.2954281006	2.6354853748	-0.0284624910
H20	6.8429019181	4.6257345366	0.1693380597
H21	3.4729617713	2.2784991078	0.7185979956
H22	4.7949634824	0.1732595498	0.5631850369
O23	5.8034014947	6.7817145316	0.9193918671
O24	2.0811423507	4.7189087159	0.2620782563
O25	3.6721498015	5.6032752752	2.6489737854
O26	4.2382256226	5.9072821549	-1.5479991379
Zn27	3.9479168490	5.7557779451	0.5473593973
H28	3.8511166565	4.8206886737	3.1895600138
H29	3.3228915878	6.2941535777	3.2298281984
H30	6.3101563009	6.7614930586	1.7432649939
H31	6.2819404218	7.3446946586	0.2950649593
H32	4.6958932297	5.2625261022	-2.1059807487
H33	3.9309148567	6.6308555847	-2.1123924649
H34	1.8065750531	4.2505403800	-0.5385832130
H35	1.3632105454	4.6421210346	0.9060056625

$\Delta r=1.0 \text{ \AA}$			
Atom	X	Y	Z
H1	1.2163739105	6.9625086320	-0.3768172401
C2	2.5813000010	10.3594999966	0.7656999999
C3	3.3061913175	9.1570346165	0.8692411468
N4	2.8402556231	7.9434949191	0.4679396429
C5	1.5940928660	7.9303043925	-0.0625942199
C6	0.8073627644	9.0680005261	-0.2079439765
C7	1.3033063693	10.3047447447	0.2117860011
H8	3.0231759976	11.2871114931	1.1114611943
H9	4.3067502189	9.1602226340	1.2927126126
H10	-0.1825246647	8.9823341227	-0.6434970057
H11	0.7032320565	11.2035473080	0.1082740869
C12	6.6992412722	1.1493174845	0.2866505555
C13	7.2597505921	2.4256231493	0.1951590982
C14	6.4358514457	3.5427082043	0.2826807088
N15	5.0937185643	3.4733109251	0.4506963547
C16	4.5666300158	2.2219090173	0.5363407673
C17	5.3211999990	1.03540000034	0.4626000001
H18	7.3264310452	0.2655152880	0.2223470554
H19	8.3278363433	2.5575596836	0.0585586640
H20	6.8612859773	4.5394143787	0.2215754087
H21	3.4893837144	2.1733116138	0.6697044142
H22	4.8250347035	0.0747919273	0.5420633049
O23	5.8093071352	6.7165004714	0.9000633127
O24	2.0887178179	4.6888550257	0.2439881980
O25	3.6793020777	5.5507480310	2.6313218670
O26	4.2409689025	5.8583268533	-1.5527095971
Zn27	3.9523712492	5.7081190823	0.5358175525
H28	3.8580884880	4.7652982829	3.1678442241
H29	3.3342463055	6.2414255875	3.2149564210
H30	6.3072165243	6.7117488675	1.7295377282
H31	6.2931620627	7.2683351457	0.2699485249
H32	4.6974039319	5.2127564077	-2.1107393888
H33	3.9354598530	6.5836687329	-2.1158445665
H34	1.8073233102	4.2393378778	-0.5649413241
H35	1.3831721905	4.5853315229	0.8978252624

$\Delta r=1.1 \text{ \AA}$			
Atom	X	Y	Z
H1	0.9883555313	8.4863637271	-2.1668490442
C2	2.5813002916	10.3594990076	0.7656999678
C3	3.0027185193	9.0964928089	0.3647574446
N4	2.4353748251	8.4315580705	-0.6693576011
C5	1.4205518168	9.0351361479	-1.3351346284
C6	0.9441929662	10.2938922471	-0.9931741572
C7	1.5321174147	10.9703319513	0.0775032382

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H8	3.0694868210	10.8491101730	1.6013162110
H9	3.8216504058	8.5970699236	0.8743327068
H10	0.1292858260	10.7327930319	-1.5587322992
H11	1.1807460702	11.9555936899	0.3680389395
C12	6.7409073692	1.0276325737	0.3898881361
C13	7.3242831497	2.2377386354	0.0086095884
C14	6.4967554424	3.3125301810	-0.2909494984
N15	5.1471437436	3.2426137863	-0.2283551973
C16	4.5942897278	2.0653531127	0.1457595497
C17	5.3493997084	0.9396009924	0.4595000323
H18	7.3601756075	0.1687607598	0.6295095454
H19	8.4013111409	2.3479588839	-0.0552285113
H20	6.9168958423	4.2698643852	-0.5889246223
H21	3.5087732118	2.0356139511	0.1918759543
H22	4.8552835771	0.0197103276	0.7525881067
O23	4.3534068861	7.4886048256	-2.7454615924
O24	1.1808744038	5.8380328330	-1.7374056586
O25	3.9945935885	5.7123906188	0.3761976392
O26	3.7650141324	4.7017254647	-2.1796597831
Zn27	3.1284104190	6.5337103391	-1.3099380094
H28	4.3990100681	4.8367841766	0.2944620821
H29	3.8121079510	5.8940590335	1.3092366393
H30	5.0392378506	7.0926560041	-3.3012108047
H31	4.4218487021	8.4490552617	-2.8378345220
H32	4.2531750141	4.0957490704	-1.6042927695
H33	3.8629470285	4.4129216159	-3.0980678912
H34	1.0407855011	4.9590410840	-2.1159608551
H35	0.3522773223	6.1132281881	-1.3205934010

$\Delta r=1.2 \text{ \AA}$			
Atom	X	Y	Z
H1	1.0199467552	8.4098127859	-2.1337311614
C2	2.5813000011	10.3594999962	0.76569999999
C3	3.0055467763	9.0850256945	0.4039514021
N4	2.4500607838	8.3927951817	-0.6187837521
C5	1.4442685900	8.9803621111	-1.3127965300
C6	0.9656237549	10.2484232976	-1.0106295470
C7	1.5416744338	10.9530467858	0.0483867606
H8	3.0602416252	10.8705202519	1.5938597884
H9	3.8166102456	8.5987883607	0.9381715095
H10	0.1577808462	10.6724595888	-1.5972653295
H11	1.1882504633	11.9462055543	0.3081598964
C12	6.7682316836	0.9486737620	0.3968356585
C13	7.3398256228	2.1731801628	0.0446460187
C14	6.5023459500	3.2448553190	-0.2373804060
N15	5.1530944100	3.1598011599	-0.1841628672
C16	4.6119676887	1.9682409422	0.1622204239
C17	5.3775999989	0.8437000038	0.4564000001
H18	7.3960735574	0.0921177541	0.6216496056
H19	8.4158425600	2.2969420603	-0.0103259593
H20	6.9147850472	4.2122449342	-0.5135053346
H21	3.5265501787	1.9251781201	0.2011811715
H22	4.8913916344	-0.0870979478	0.7267589095
O23	4.3880026516	7.4250503957	-2.6555283279
O24	1.1931730457	5.7896810866	-1.6424452709
O25	4.0100240144	5.6460852502	0.4565283879
O26	3.7644717701	4.6467507054	-2.1017170182
Zn27	3.1456842601	6.4813607487	-1.2240090005
H28	4.4041160170	4.7658454603	0.3743150745
H29	3.8500630500	5.8371331121	1.3917948451
H30	5.0735712607	7.0226980155	-3.2068623390
H31	4.4634942273	8.3847496307	-2.7505889127
H32	4.2535980677	4.0363023787	-1.5318321960
H33	3.8585663211	4.3644111970	-3.0225204876
H34	1.0548569893	4.9060402453	-2.0107583384
H35	0.3662306039	6.0652990229	-1.2226403233

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 $\Delta r=1.3 \text{ \AA}$

Atom	X	Y	Z
H1	1.0694058786	8.2922037301	-2.0773780207
C2	2.5813000017	10.3594999942	0.76569999998
C3	3.0240311939	9.0786649312	0.4520804550
N4	2.4868281669	8.3453664810	-0.5516503689
C5	1.4793681583	8.8959878106	-1.2732394089
C6	0.9830743991	10.1675104595	-1.0189334750
C7	1.5414150398	10.9153535812	0.0195194098
H8	3.0460438346	10.9040862535	1.5804256854
H9	3.8354993286	8.6212150836	1.0107389471
H10	0.1757366742	10.5612409373	-1.6269453810
H11	1.1742309242	11.9125813173	0.2416303402
C12	6.7969622390	0.8432882804	0.3874608491
C13	7.3765179419	2.0717255435	0.0625441085
C14	6.5454936243	3.1565025070	-0.1880264696
N15	5.1960877996	3.0803081411	-0.1273100555
C16	4.6472831199	1.8854724633	0.1937958808
C17	5.4057999983	0.7478000058	0.4533000002
H18	7.4193040259	-0.0237605233	0.5864595726
H19	8.4532764321	2.1880455714	0.0034222664
H20	6.9631675268	4.1269987227	-0.4443077646
H21	3.5619937360	1.8503999116	0.2397577384
H22	4.9146083191	-0.1861189073	0.7035772636
O23	4.4684312179	7.3594099486	-2.5272828926
O24	1.2492136958	5.7130368197	-1.4737284905
O25	4.0972673493	5.5768426624	0.5484923587
O26	3.7943229479	4.5930589652	-2.0125535906
Zn27	3.2058786842	6.4269330477	-1.1064428029
H28	4.4711382279	4.6890354516	0.4535256338
H29	3.9882621588	5.7813241127	1.4882478099
H30	5.1597717593	6.9510607138	-3.0669436908
H31	4.5462143786	8.3182515330	-2.6299128943
H32	4.2898901353	3.9730679169	-1.4587130554
H33	3.8744262863	4.3257292458	-2.9391578712
H34	1.1135674395	4.8229415164	-1.8274255451
H35	0.4300309846	5.9847889136	-1.0364563827

 $\Delta r=1.4 \text{ \AA}$

Atom	X	Y	Z
H1	1.1093935986	8.1891568975	-2.0205345983
C2	2.5813000011	10.3594999964	0.76569999999
C3	3.0405633165	9.0742076717	0.4939384260
N4	2.5181358793	8.3043821339	-0.4906557486
C5	1.5092152913	8.8223216006	-1.2342809737
C6	0.9975603956	10.0952089884	-1.0220149614
C7	1.5406111622	10.8808013387	-0.0037641803
H8	3.0347145955	10.9331476157	1.5668116731
H9	3.8522823102	8.6429202745	1.0728689182
H10	0.1896765080	10.4606906801	-1.6464810358
H11	1.1609951365	11.8800578488	0.1855339688
C12	6.8250579793	0.7412673042	0.3784231736
C13	7.4089946416	1.9730815692	0.0750255395
C14	6.5823337317	3.0670203976	-0.1495060243
N15	5.2328038536	2.9974259751	-0.0829032405
C16	4.6803084131	1.7989338456	0.2176345329
C17	5.4339999989	0.6519000036	0.4502000001
H18	7.4440132356	-0.1326882218	0.5562858569
H19	8.4860353898	2.0853586875	0.0124961831
H20	7.0043851049	4.0400031769	-0.3890074415
H21	3.5951678956	1.7683270027	0.2690156374
H22	4.9385078733	-0.2839182894	0.6841235973
O23	4.5275135184	7.3061254847	-2.4238784792
O24	1.2961571314	5.6523331656	-1.3422202650
O25	4.1636536948	5.5139130320	0.6334337268
O26	3.8252747093	4.5465438978	-1.9297908874
Zn27	3.2556028322	6.3782876567	-1.0061527503

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H28	4.5256394346	4.6218129620	0.5331138394
H29	4.0853690677	5.7228887780	1.5752075830
H30	5.2226980767	6.8946916706	-2.9561863453
H31	4.6078020814	8.2645306573	-2.5291499831
H32	4.3224630013	3.9192383434	-1.3856253634
H33	3.9003825891	4.2868051906	-2.8589845939
H34	1.1652737319	4.7584123146	-1.6879717820
H35	0.4803593157	5.9189076174	-0.8955439713

$\Delta r=1.6 \text{ \AA}$			
Atom	X	Y	Z
H1	1.1807853695	7.9742469445	-1.8782749053
C2	2.5813000058	10.3594999804	0.7656999994
C3	3.0720039938	9.0692177386	0.5833847646
N4	2.5766428550	8.2227840000	-0.3519011819
C5	1.5618078377	8.6677010341	-1.1349151645
C6	1.0200345277	9.9400034638	-1.0115261669
C7	1.5363934111	10.8044978720	-0.0444503260
H8	3.0143501099	10.9944016262	1.5309075637
H9	3.8861695039	8.6958949723	1.1978998544
H10	0.2091745274	10.2439938434	-1.6646250078
H11	1.1325314647	11.8050873215	0.0747254179
C12	6.8819921913	0.5472976329	0.3782442697
C13	7.4710474052	1.7899033473	0.1347990076
C14	6.6495152761	2.8966779840	-0.0389729826
N15	5.2995970550	2.8310495775	0.0231390170
C16	4.7421161701	1.6213569994	0.2664299266
C17	5.4903999942	0.4601000196	0.4440000006
H18	7.4972937209	-0.3366310686	0.5148039253
H19	8.5485511272	1.9005101057	0.0792393413
H20	7.0767055237	3.8775619250	-0.2325320008
H21	3.6567876207	1.5928902093	0.3161482882
H22	4.9903036093	-0.4835234715	0.6324664342
O23	4.6851109249	7.2002162892	-2.1473894255
O24	1.3947985021	5.5194434449	-1.0311872836
O25	4.2827993009	5.3673657635	0.8240233551
O26	3.8843113089	4.4608036531	-1.7541532338
Zn27	3.3539979200	6.2833969279	-0.7747065145
H28	4.6188013203	4.4684183402	0.6980460128
H29	4.2711232651	5.5764379299	1.769845371
H30	5.3963246201	6.7809170937	-2.6516309952
H31	4.7743691570	8.1574260972	-2.2562430103
H32	4.3843931380	3.8124136262	-1.2380376136
H33	3.9472064255	4.2366038152	-2.6934483861
H34	1.2712813437	4.6212993920	-1.3686045945
H35	0.5903130887	5.7728434934	-0.5571221681

$\Delta r=1.8 \text{ \AA}$			
Atom	X	Y	Z
H1	1.2221951817	7.7960037863	-1.7293449561
C2	2.5813000060	10.3594999795	0.7656999993
C3	3.0941251024	9.0677186610	0.6607041929
N4	2.6142637061	8.1568422487	-0.2217968849
C5	1.5917302504	8.5381742495	-1.0287763331
C6	1.0288367569	9.8062319328	-0.9816990533
C7	1.5293739318	10.7365803054	-0.0690902109
H8	3.0031879829	11.0456489009	1.4919824004
H9	3.9135572624	8.7465357072	1.2973947947
H10	0.2137214106	10.0563123222	-1.6520725331
H11	1.1081330469	11.7353557741	-0.0103671712
C12	6.9374281015	0.3803235062	0.3994055436
C13	7.5093850674	1.6416634039	0.2186780439
C14	6.6728572191	2.7419816978	0.0772194298
N15	5.3232966221	2.6544014442	0.1146878201
C16	4.7828827983	1.4260532971	0.2975831751

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C17	5.5467999940	0.2683000205	0.4378000007
H18	7.5653375788	-0.4985020929	0.5087744912
H19	8.5857274074	1.7715338870	0.1856657739
H20	7.0883811544	3.7361495937	-0.0688864202
H21	3.6975705721	1.3779720899	0.3279637006
H22	5.0581979835	-0.6896953637	0.5772657818
O23	4.8056200782	7.0979314727	-1.8827493516
O24	1.4528694591	5.4230896241	-0.7654114383
O25	4.3357936945	5.2283125932	1.0119407544
O26	3.9126515888	4.3764183144	-1.5730923788
Zn27	3.4133006593	6.1992721357	-0.5648514216
H28	4.6404161907	4.3202443294	0.8719757833
H29	4.3586798691	5.4310494534	1.9580997838
H30	5.5318585420	6.6677660293	-2.3553707293
H31	4.9048639133	8.0533430878	-1.9984347426
H32	4.4024930137	3.7048274027	-1.0771023945
H33	3.9716990764	4.1743748059	-2.5175554574
H34	1.3314152103	4.5225980337	-1.0971318208
H35	0.6572725818	5.6714252105	-0.2739262599

$\Delta r=2.0 \text{ \AA}$			
Atom	X	Y	Z
H1	1.2931686721	7.6440010670	-1.6047842252
C2	2.5813000156	10.3594999469	0.7656999983
C3	3.1077301966	9.0673509581	0.7436936181
N4	2.6552578255	8.1014329257	-0.0953181952
C5	1.6456401569	8.4281658272	-0.9423274837
C6	1.0716311180	9.6916651215	-0.9789975712
C7	1.5444944924	10.6780012381	-0.1112271745
H8	2.9820444660	11.0886437758	1.4612804498
H9	3.9155731981	8.7907073066	1.4150831438
H10	0.2681980029	9.8949209542	-1.6787811022
H11	1.1128958174	11.6741160067	-0.1189756246
C12	6.9912742092	0.2167705174	0.4062377242
C13	7.5387217602	1.4948252663	0.2735713640
C14	6.6817922231	2.5832440529	0.1641204371
N15	5.3338728419	2.4707514221	0.1901095440
C16	4.8178723830	1.2255513186	0.3270934537
C17	5.6031999844	0.0765000531	0.4316000017
H18	7.6360387475	-0.6527819385	0.4883766101
H19	8.6124874469	1.6465373279	0.2523130623
H20	7.0808136258	3.5887840927	0.0532798057
H21	3.7336163658	1.1550822569	0.3484538594
H22	5.1313181344	-0.8944777556	0.5336244911
O23	4.9221933876	6.9913355135	-1.6133984550
O24	1.4979165133	5.3443356548	-0.4887142603
O25	4.3827753391	5.0945076571	1.2049904409
O26	3.9204059640	4.2989133659	-1.3857446601
Zn27	3.4638640678	6.1203767082	-0.3476910164
H28	4.6643049687	4.1817351917	1.0481902753
H29	4.4397206565	5.2851128417	2.1522670935
H30	5.6511389372	6.5429787987	-2.0645720878
H31	5.0451705153	7.9438616984	-1.7300460349
H32	4.3988275634	3.5996697843	-0.9176230243
H33	3.9582704214	4.1209774179	-2.3361500121
H34	1.3701747428	4.4380696088	-0.8018457145
H35	0.7106280280	5.6042791747	0.0100950443

$\Delta r=2.1 \text{ \AA}$			
Atom	X	Y	Z
H1	1.3217609254	7.5741966121	-1.5388822726
C2	2.5813000103	10.3594999651	0.7656999989
C3	3.1171970497	9.0702601807	0.7788563886
N4	2.6756453988	8.0791525693	-0.0369330555
C5	1.6676003359	8.3776205751	-0.8963809001

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C6	1.0852965893	9.6357912402	-0.9682392729
C7	1.5468203398	10.6477856068	-0.1242101922
H8	2.9737595788	11.1086781947	1.4445173516
H9	3.9229901120	8.8167961093	1.4617736518
H10	0.2837419518	9.8150635692	-1.6765768559
H11	1.1081395386	11.6401901674	-0.1596881721
C12	7.0189646411	0.1271256760	0.4138892751
C13	7.5614281470	1.4097963411	0.3058640128
C14	6.7002855915	2.4966519249	0.2092924362
N15	5.3528820725	2.3791221929	0.2254535625
C16	4.8422199404	1.1292505167	0.3381095416
C17	5.6313999897	-0.0193999651	0.4285000011
H18	7.6675009585	-0.7406211196	0.4851857253
H19	8.6347637208	1.5665284335	0.2933376748
H20	7.0969894787	3.5051889915	0.1171513757
H21	3.7582822105	1.0537552209	0.3514216763
H22	5.1626881151	-0.9935704569	0.5113486594
O23	4.9651281130	6.9486380816	-1.5083347466
O24	1.5312642287	5.3084950747	-0.3645188238
O25	4.4152097862	5.0594046380	1.3065423236
O26	3.9435386419	4.2626416653	-1.2813029556
Zn27	3.4951432474	6.0920306715	-0.2492716876
H28	4.6853947050	4.1426230682	1.1531017511
H29	4.4815808203	5.2503914596	2.2531479414
H30	5.6966386164	6.4940740075	-1.9489178026
H31	5.0871865676	7.8995245097	-1.6390560810
H32	4.4184163210	3.5534975844	-0.8247170097
H33	3.9686373788	4.0899538753	-2.2330875749
H34	1.4057383365	4.3976465511	-0.6647446907
H35	0.7463513947	5.5718625265	0.1362727091

$\Delta r=2.3 \text{ \AA}$			
Atom	X	Y	Z
H1	1.1728539076	7.2065610074	-0.8875135774
C2	2.5813000705	10.3594997601	0.7656999922
C3	3.2489746352	9.1397418189	0.7816278255
N4	2.7474153915	8.0226892187	0.1992443474
C5	1.5482390131	8.1135570529	-0.4247155252
C6	0.8238934935	9.2972073362	-0.4845780352
C7	1.3455005483	10.4415122974	0.1211126848
H8	3.0252539866	11.2226173073	1.2497527289
H9	4.2150161565	9.0432418219	1.2694262457
H10	-0.1304777005	9.3172604685	-0.9995202377
H11	0.8002282247	11.3797678849	0.0903228515
C12	7.0137618322	-0.1993123680	0.8545283887
C13	7.6597041130	1.0281199918	1.0100634857
C14	6.9554176756	2.1931002380	0.7260092200
N15	5.6729187336	2.1963494408	0.3140566771
C16	5.0594923782	1.0057122312	0.1664227714
C17	5.6876999295	-0.2110997601	0.4223000078
H18	7.5356624318	-1.1280350682	1.0629321214
H19	8.6918102041	1.0833723223	1.3390783920
H20	7.4362946785	3.1641673679	0.8228717535
H21	4.0279680651	1.0314758042	-0.1757611835
H22	5.1467259556	-1.1406891585	0.2832328444
O23	5.1529025432	7.1317394964	-1.2587305606
O24	2.0432857679	5.0568296852	0.2806104797
O25	4.7307549328	6.1939240503	2.0590104944
O26	4.6463922369	4.4421808260	-0.5556981395
Zn27	3.8345908113	6.2041881961	0.1629321333
H28	5.4104945052	5.5662992540	2.3437966492
H29	4.3771187012	6.6131838641	2.8565719174
H30	6.0551893272	6.8773681092	-1.4974032284
H31	4.9934213258	8.0081516257	-1.6364811556
H32	4.9824002683	3.6250807056	-0.1603719380
H33	4.8451223996	4.3848783915	-1.5009847477
H34	2.0720291763	4.1274972532	0.0138720928
H35	1.2353060374	5.1939454098	0.7950191665

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 $\Delta r=2.5 \text{ \AA}$

Atom	X	Y	Z
H1	1.1535485676	7.1523600737	-0.7667927705
C2	2.5813000553	10.3594998118	0.7656999939
C3	3.2387972994	9.1336369609	0.8334562063
N4	2.7324164631	7.9960141381	0.2944008267
C5	1.5364961913	8.0734008302	-0.3387634692
C6	0.8226347404	9.2597845424	-0.4501129501
C7	1.3496903656	10.4242233599	0.1115977581
H8	3.0309243666	11.2370757093	1.2172137631
H9	4.2016184239	9.0494933488	1.3297976296
H10	-0.1289930231	9.2664360692	-0.9705606850
H11	0.8112263669	11.3641754580	0.0395997681
C12	7.0528114144	-0.3508919577	0.8946438624
C13	7.6288761962	0.8960973226	1.1425180599
C14	6.8759082547	2.0398291228	0.9006907115
N15	5.6088985769	2.0076731795	0.4439692399
C16	5.0631491564	0.7971194449	0.2084837105
C17	5.7440999447	-0.4028998118	0.4161000061
H18	7.6149077129	-1.2630393814	1.0688778512
H19	8.6451720635	0.9826503912	1.5114845542
H20	7.3044105904	3.0251064762	1.0721291331
H21	4.0424140085	0.7919580643	-0.1654478241
H22	5.2542733113	-1.3472678675	0.2057177481
O23	5.0962736815	6.9502253394	-1.1498864153
O24	1.9773419419	5.0363422690	0.5189248393
O25	4.7023225519	6.2056986219	2.2114990084
O26	4.5443544792	4.3045351791	-0.3275114948
Zn27	3.7814651726	6.1363875711	0.3311703575
H28	5.3879837184	5.5948236201	2.5175797506
H29	4.3604431523	6.6654758867	2.9917587856
H30	5.9891055841	6.6615458201	-1.3850604138
H31	4.9573136592	7.8163205276	-1.5585361869
H32	4.8770252344	3.4789591887	0.0527059571
H33	4.7131641654	4.2303351553	-1.2774350329
H34	1.9946293938	4.0913119293	0.3135716712
H35	1.1729359234	5.2181792332	1.0250217385

 $\Delta r=2.7 \text{ \AA}$

Atom	X	Y	Z
H1	1.2324637630	7.0226673179	-0.5491073410
C2	2.5813000446	10.3594998481	0.7656999950
C3	3.2705648166	9.1559740283	0.9099964979
N4	2.7943481384	7.9713599291	0.4476008957
C5	1.5946761477	7.9786688715	-0.1843860090
C6	0.8506149844	9.1367591779	-0.3696308678
C7	1.3476832060	10.3491464777	0.1129705207
H8	3.0096887411	11.2750085506	1.1586844634
H9	4.2359385473	9.1296290413	1.4078601138
H10	-0.1020092583	9.0847308658	-0.8856012250
H11	0.7842667861	11.2677708799	-0.0183423728
C12	7.0761787577	-0.5640557348	0.9713618231
C13	7.6142920350	0.6674237352	1.3487511407
C14	6.8591972117	1.8181150862	1.1488404426
N15	5.6232314317	1.8107214584	0.6119876172
C16	5.1146100903	0.6131352919	0.2524385175
C17	5.8004999553	-0.5946998481	0.4099000049
H18	7.6420519396	-1.4798076554	1.1112885762
H19	8.6040430164	0.7371861178	1.7870074595
H20	7.2609564407	2.7906461705	1.4253482071
H21	4.1184789237	0.6241272250	-0.1827587141
H22	5.3378140259	-1.5246351133	0.0984443225
O23	5.1589741651	6.8349360750	-0.9623354169
O24	2.0963541237	5.0090073827	0.8632651735

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O25	4.8429257212	6.2962726920	2.4289758241
O26	4.6304294731	4.2329847376	-0.0276896604
Zn27	3.8745687460	6.1191486248	0.5863604411
H28	5.5617878620	5.7263121540	2.7379462592
H29	4.5125926476	6.7830033623	3.1978406219
H30	6.0616450837	6.5562464114	-1.1703639150
H31	5.0040067083	7.6732024530	-1.4202641978
H32	4.9158100615	3.3775060482	0.3235075389
H33	4.7977418483	4.1665484758	-0.9784272082
H34	2.1271648063	4.0560766177	0.7006426978
H35	1.3005552383	5.2010247138	1.3791311140

$\Delta r=2.9 \text{ \AA}$			
Atom	X	Y	Z
H1	1.3642658544	7.0270589235	-0.6854732221
C2	2.5813000129	10.3594999562	0.7656999986
C3	3.2822935754	9.1620626959	0.9262480266
N4	2.8548936110	7.9770633729	0.4171375873
C5	1.6923313487	7.9803140755	-0.2825334412
C6	0.9404960569	9.1298434045	-0.4889100466
C7	1.3871714705	10.3411296220	0.0438411488
H8	2.9722993141	11.2733063161	1.1992379930
H9	4.2182477664	9.1430020571	1.4776498146
H10	0.0197702869	9.0721047727	-1.0594963216
H11	0.8154132486	11.2523644956	-0.1026015805
C12	7.1702329161	-0.7253153318	0.8673024334
C13	7.7138790221	0.5218270447	1.1811140504
C14	6.9274993201	1.6575905843	1.0186169012
N15	5.6548577200	1.6250577596	0.5761124015
C16	5.1424914175	0.4111983588	0.2773182509
C17	5.8568999871	-0.7864999562	0.4037000014
H18	7.7605466832	-1.6291703961	0.9815247767
H19	8.7321398595	0.6147109391	1.5432967033
H20	7.3345342819	2.6398570667	1.2499589316
H21	4.1160642567	0.3981638284	-0.0806021846
H22	5.3856334241	-1.7280340945	0.1444274559
O23	5.2107904658	6.7259519774	-0.9709551101
O24	2.1256387126	5.0088048111	0.7885859280
O25	4.8698914314	6.2345911923	2.4235239853
O26	4.6481533074	4.1290564236	0.0029180586
Zn27	3.9147919646	6.0906323543	0.5774758937
H28	5.5652386430	5.6371679596	2.7345129816
H29	4.5473654609	6.7250455090	3.1932382060
H30	6.0965148648	6.3952451461	-1.1753844151
H31	5.1068160683	7.5761162967	-1.4214502210
H32	4.9180807607	3.2670379064	0.3503920581
H33	4.7797001447	4.0370531939	-0.9512689594
H34	2.1645042099	4.0515517452	0.6559421150
H35	1.3036454538	5.2202910303	1.2531415668

$\Delta r=3.1 \text{ \AA}$			
Atom	X	Y	Z
H1	1.2911693802	7.2131066684	-1.0058745596
C2	2.5813000596	10.3594997972	0.7656999934
C3	3.1834389049	9.1058493795	0.9111806923
N4	2.7303225578	7.9844820991	0.2902578511
C5	1.6412313522	8.1133405533	-0.5094077000
C6	0.9889507289	9.3232545077	-0.7069157001
C7	1.4617325873	10.4673331297	-0.0597184243
H8	2.9903768386	11.2157728282	1.2902616360
H9	4.0609076479	8.9885578435	1.5409165697
H10	0.1240227664	9.3643409038	-1.3601587237
H11	0.9666081122	11.4234460619	-0.1985521722
C12	7.2831639248	-0.7973646473	0.5809324220
C13	7.7796659645	0.5033694062	0.6874778304

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C14	6.8919339722	1.5714394091	0.6047814108
N15	5.5632075378	1.4266342228	0.4303108969
C16	5.0985932504	0.1611434981	0.3310326176
C17	5.9132999404	-0.9782997972	0.3975000066
H18	7.9525807744	-1.6499975547	0.6395835277
H19	8.8389503204	0.6888859361	0.8301266362
H20	7.2616826331	2.5923764038	0.6795857541
H21	4.0258572794	0.0550206472	0.1905571186
H22	5.4726368061	-1.9649447090	0.3079452146
O23	4.9874907500	6.4965598201	-1.1018298027
O24	1.8050246148	4.9845274458	0.3359249061
O25	4.4627470053	5.9784670606	2.3029330709
O26	4.3190879016	3.9131188444	-0.1030380770
Zn27	3.6229890629	5.9964603953	0.4030524764
H28	5.0802497650	5.3071657776	2.6271163358
H29	4.1475633039	6.4761710280	3.0709737786
H30	5.7985669193	6.0187793308	-1.3244365227
H31	5.0280226061	7.3659018444	-1.5249584994
H32	4.6731426222	3.0884893035	0.2595228491
H33	4.3369068540	3.7489914026	-1.0564522459
H34	1.8679952033	4.0217817328	0.2687702542
H35	0.9352550632	5.2148643969	0.6917652325

Atom	X	Y	Z
H1	1.3129146654	7.1679442377	-0.9413021747
C2	2.5813000216	10.3594999264	0.76569999976
C3	3.1816634695	9.1097674013	0.9504342725
N4	2.7369342904	7.9724305768	0.3521748420
C5	1.6572536529	8.0804592588	-0.4635911064
C6	1.0071948319	9.2847221264	-0.6994956212
C7	1.4719200626	10.4454055029	-0.0760753263
H8	2.9838490643	11.2288120419	1.2736479154
H9	4.0506864620	9.0090862606	1.5945808318
H10	0.1501226169	9.3087044270	-1.3639003128
H11	0.9781884643	11.3973772947	-0.2454616757
C12	7.3128829656	-0.8867059255	0.5577561068
C13	7.8024163211	0.4156925172	0.6751908050
C14	6.9065399255	1.4788866777	0.6229524004
N15	5.5760035914	1.3285665364	0.4678619004
C16	5.1186404912	0.0611189568	0.3580859646
C17	5.9414999784	-1.0741999264	0.3944000024
H18	7.9889117849	-1.7353851720	0.5930099712
H19	8.8626575107	0.6063275439	0.8033770313
H20	7.2712342607	2.5009449705	0.7076111925
H21	4.0443922384	-0.0503853106	0.2339256167
H22	5.5053857963	-2.0621484077	0.2979092267
O23	5.0211767075	6.4358889046	-0.9685943534
O24	1.8260338098	4.9523764750	0.4226650289
O25	4.4445101920	5.9581454132	2.4175330205
O26	4.3181505598	3.8565315732	0.0045075665
Zn27	3.6238432141	5.9859401279	0.5135831000
H28	5.0491793605	5.2784432181	2.7485303205
H29	4.1337391645	6.4657964790	3.1808695609
H30	5.8220729014	5.9310287649	-1.1671096828
H31	5.0960866087	7.2991355874	-1.3994245419
H32	4.6705515954	3.0258942563	0.3545685660
H33	4.3266401891	3.6983936239	-0.9501275550
H34	1.9170806292	3.9915269909	0.3614976710
H35	0.9475020993	5.1632801780	0.7688278832

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[Cu(Py)₂(H₂O)₄]²⁺

Δr=0.0 Å

Atom	X	Y	Z
H1	1.5616067162	7.3065195864	-1.4417021919
C2	2.5977420558	10.1971992865	0.8424213281
C3	3.2673155345	8.9796654229	0.8198300626
N4	2.8917512331	7.9695389165	0.0036538875
C5	1.8344443313	8.1502775753	-0.8192190749
C6	1.1237220426	9.3439146721	-0.8552040712
C7	1.5084081866	10.3860829224	-0.0098406481
H8	2.9310317471	10.9804478709	1.5147617336
H9	4.1299564520	8.7928230999	1.4481297580
H10	0.2827069178	9.4475463572	-1.5323700722
H11	0.9690734757	11.3282824331	-0.0151387817
C12	6.2806512811	2.0553125829	0.0374303802
C13	6.8526030317	3.1965843143	-0.5271236473
C14	6.1349078175	4.3866242812	-0.5137037279
N15	4.8967078610	4.4719909279	0.0220227711
C16	4.3407862410	3.3661114334	0.5655186030
C17	5.0037572586	2.1450540048	0.5942370577
H18	6.8201326444	1.1131991382	0.0432539681
H19	7.8425122520	3.1717117604	-0.9698148780
H20	6.5446748191	5.3023829359	-0.9226588794
H21	3.3412591083	3.4801667466	0.9676710820
H22	4.5216372588	1.2829559810	1.0424028355
O23	5.8561509561	7.3453007024	0.3784558840
O24	1.9345750618	5.0914975714	-0.3478472334
O25	3.5869382734	6.0563485088	2.1843353196
O26	4.2031762211	6.3873443819	-2.1594926964
Cu27	3.8940777366	6.2217961906	0.0122181160
H28	4.0293722066	5.4389591258	2.7826480230
H29	2.9983998668	6.6014922821	2.7240912818
H30	6.4826124679	7.1967628321	1.1003405353
H31	6.2353860770	8.0407800382	-0.1765378335
H32	4.5157073974	5.6897033988	-2.7514126688
H33	4.0318270812	7.1667515816	-2.7053718688
H34	1.7448991765	4.4739919100	-1.0677034947
H35	1.1405710810	5.1239522819	0.2034806694

Δr=0.1 Å

Atom	X	Y	Z
H1	1.5017540118	7.1894329740	-1.2554924145
C2	2.5977000048	10.1971999840	0.8423999995
C3	3.2623898993	8.9749806865	0.8726939823
N4	2.8686596711	7.9218268290	0.1205707903
C5	1.7918278701	8.0636858520	-0.6854733850
C6	1.0833990811	9.2562032382	-0.7699819496
C7	1.4900924038	10.3430303762	0.0060112051
H8	2.9488709387	11.0138856475	1.4638630796
H9	4.1375648907	8.8200993563	1.4923302879
H10	0.2269265613	9.3248710397	-1.4320678085
H11	0.9533726172	11.2856244429	-0.0402192918
C12	6.3205484971	2.0051704907	0.0560693748
C13	6.8864939901	3.1825905322	-0.4363479347
C14	6.1524278902	4.3609886463	-0.3763213651
N15	4.9024054694	4.4053111648	0.1381433265
C16	4.3536807862	3.2638234971	0.6132035717
C17	5.0324999952	2.0489000160	0.5913000005
H18	6.8733368400	1.0713689980	0.0231939256
H19	7.8851619614	3.1943458895	-0.8595606134
H20	6.5588410303	5.3008072974	-0.7295673106
H21	3.3449492326	3.3430247971	1.0010512627
H22	4.5528296731	1.1595856492	0.9856945871
O23	5.8363738808	7.2983638008	0.5436119852
O24	1.9255235156	5.0114602743	-0.2036712374
O25	3.5637377687	5.9921142932	2.3090202434

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O26	4.1945873871	6.3372196528	-2.0092462738
Cu27	3.8803590493	6.1616620944	0.1545823993
H28	3.9734056381	5.3481488341	2.9024468808
H29	3.0066278970	6.5666616947	2.8514954402
H30	6.4401492665	7.1687910333	1.2880838350
H31	6.2346975839	7.9763307419	-0.0196311663
H32	4.5379479938	5.6521487299	-2.5988179110
H33	3.9880158714	7.1075553592	-2.5558180889
H34	1.7305077819	4.4119076559	-0.9371327334
H35	1.1420948254	5.0170688290	0.3635947028

$\Delta r=0.2 \text{ \AA}$			
Atom	X	Y	Z
H1	1.4463052440	7.0917639812	-1.0792200698
C2	2.5977000055	10.1971999815	0.8423999994
C3	3.2719379890	8.9781843962	0.9007461811
N4	2.8608453834	7.8876878476	0.2114964487
C5	1.7538072629	7.9910204077	-0.5597279611
C6	1.0347913552	9.1750836230	-0.6705737292
C7	1.4601138732	10.2986509083	0.0408745041
H8	2.9668150790	11.0414136786	1.4146476591
H9	4.1708969816	8.8565802567	1.4933536881
H10	0.1543219476	9.2088460798	-1.3033171971
H11	0.9144187337	11.2347148691	-0.0282607678
C12	6.3700076291	1.9463147728	0.1052468739
C13	6.9407439643	3.1504178376	-0.3114683665
C14	6.1917420251	4.3183349573	-0.2318940358
N15	4.9203112857	4.3312396726	0.2308532682
C16	4.3682258102	3.1624581656	0.6339179928
C17	5.0610999945	1.9531000185	0.5883000005
H18	6.9355404810	1.0209874843	0.0542977632
H19	7.9557884616	3.1908053361	-0.6918552900
H20	6.6038326434	5.2753908820	-0.5275495151
H21	3.3435210913	3.2142632332	0.9824470335
H22	4.5743392104	1.0438132774	0.9238072076
O23	5.8395861016	7.2589768410	0.6719296545
O24	1.9192020307	4.9423215426	-0.0731057665
O25	3.5670663751	5.9378813476	2.3855873063
O26	4.1983012749	6.2779066156	-1.8797362520
Cu27	3.8844837165	6.1067930105	0.2554533605
H28	3.9380730657	5.2624992445	2.9693956695
H29	3.0605460614	6.5505910528	2.9357645398
H30	6.4155239647	7.1443799464	1.4406108222
H31	6.2653813648	7.9178521485	0.1059433674
H32	4.5530200556	5.5937168146	-2.4635720041
H33	3.9661677716	7.0383994174	-2.4298239562
H34	1.6897814049	4.3631184135	-0.8131005380
H35	1.1624903292	4.9306555005	0.5294014775

$\Delta r=0.3 \text{ \AA}$			
Atom	X	Y	Z
H1	1.2430924168	6.9525179347	-0.6776235690
C2	2.5977000136	10.1971999546	0.8423999986
C3	3.2814150641	8.9829723265	0.9160325958
N4	2.7984360730	7.8411163100	0.3674622172
C5	1.6047322519	7.8890992624	-0.2708695126
C6	0.8705999820	9.0636801717	-0.3848758149
C7	1.3714233339	10.2388538271	0.1786117292
H8	3.0282309769	11.0817680506	1.2989166041
H9	4.2420715505	8.9028487777	1.4108532506
H10	-0.0804241359	9.0500140445	-0.9065177167
H11	0.8150385432	11.1680517970	0.1024398606
C12	6.4137748502	1.9028238657	0.1489702327
C13	6.9693581038	3.1384104290	-0.1897346213
C14	6.1920497658	4.2852467517	-0.0802265313

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N15	4.9050457815	4.2524487898	0.3377648468
C16	4.3684177194	3.0513472951	0.6630410227
C17	5.0896999865	1.8574000454	0.5853000014
H18	7.0027915545	0.9939482398	0.0732686409
H19	7.9951986571	3.2190173950	-0.5330951654
H20	6.5943494081	5.2619133958	-0.3191795644
H21	3.3310908898	3.0632373683	0.9758351389
H22	4.6111068480	0.9238078768	0.8600529269
O23	5.8074219908	7.2037049715	1.0020981269
O24	1.8584256260	4.8141514505	-0.0421935178
O25	3.2858174997	5.7257542662	2.4155384393
O26	4.3603579231	6.3792928682	-1.6273819006
Cu27	3.8409127674	6.0442649410	0.3981006871
H28	3.7980607450	5.1459988447	2.9975612928
H29	2.9738207550	6.4673497660	2.9543024102
H30	6.4110413722	7.0543864613	1.7435155091
H31	6.2871563930	7.7670554699	0.3782338789
H32	4.5407623941	5.6467566463	-2.2340781495
H33	3.9167898159	7.0722508085	-2.1376842087
H34	1.5768273186	4.2314921242	-0.7614853494
H35	1.2023910957	4.7103842667	0.6615980520

$\Delta r=0.5 \text{ \AA}$			
Atom	X	Y	Z
H1	1.1926652854	6.8170007771	-0.3047673276
C2	2.5977000177	10.1971999408	0.8423999982
C3	3.3209679092	8.9999169413	0.9268955855
N4	2.8231595815	7.8053947869	0.5132039780
C5	1.5692739072	7.7861847073	-0.0003614418
C6	0.7940279971	8.9340604778	-0.1193858056
C7	1.3108158896	10.1597069096	0.3063921179
H8	3.0486092435	11.1198034363	1.1906673524
H9	4.3279747389	8.9771249418	1.3265354250
H10	-0.2035476052	8.8608981065	-0.5392567373
H11	0.7193153249	11.0662848620	0.2220752310
C12	6.5237844553	1.7521942988	0.3753005233
C13	7.1081927490	3.0145645810	0.2470778773
C14	6.3099310586	4.1499131947	0.3262334798
N15	4.9706439254	4.0855392419	0.5198955737
C16	4.4083261179	2.8555925127	0.6434300008
C17	5.1468999823	1.6658000592	0.5794000019
H18	7.1327142747	0.8551563669	0.3171250766
H19	8.1757653521	3.1249320008	0.0891931395
H20	6.7352510943	5.1426380552	0.2462689471
H21	3.3341941850	2.8426046681	0.7847145256
H22	4.6391727788	0.7137616375	0.6867041756
O23	5.8840753950	7.1964119498	1.0672586020
O24	1.8622515620	4.6753805998	0.1884879695
O25	3.3664944867	5.6606449471	2.5405683339
O26	4.3955307884	6.2338038493	-1.4272716601
Cu27	3.8911291238	5.9418609024	0.5579825414
H28	3.8747501664	5.0507737463	3.0953425176
H29	3.1312143033	6.4255524494	3.0861892996
H30	6.4717913501	7.2297282836	1.8355420395
H31	6.3407165450	7.6803165728	0.3642966743
H32	4.6182951921	5.4785334011	-1.9910116845
H33	3.9001370639	6.8675094621	-1.9666555592
H34	1.4728486157	4.1744174663	-0.5422532583
H35	1.2726046155	4.5471960159	0.9451579791

$\Delta r=0.8 \text{ \AA}$			
Atom	X	Y	Z
H1	1.1036336859	6.7152512969	0.1969299863
C2	2.5977000170	10.1971999433	0.8423999982
C3	3.3536181718	9.0097903604	0.8869732841

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N4	2.8273309713	7.7761405594	0.6570915464
C5	1.5048305424	7.7068464407	0.3727421951
C6	0.6916969694	8.8335472566	0.3081080988
C7	1.2392446139	10.0970806457	0.5449224331
H8	3.0817942891	11.1474351411	1.0371387872
H9	4.4138843930	9.0297352365	1.1129239944
H10	-0.3610635216	8.7148556459	0.0744507257
H11	0.6151498542	10.9843580265	0.4979606664
C12	6.6198865843	1.4994570193	0.6415844252
C13	7.1824766858	2.7756861479	0.7236587635
C14	6.3554219355	3.8938080708	0.7337946404
N15	5.0056859810	3.8050390861	0.6644677145
C16	4.4648148526	2.5590843415	0.5835881360
C17	5.2327999831	1.3785000567	0.5705000016
H18	7.2543456107	0.6183793378	0.6337504083
H19	8.2573507262	2.9106176072	0.7814893950
H20	6.7664708772	4.8940794915	0.8055610843
H21	3.3827517390	2.5231450984	0.5243169073
H22	4.7357031999	0.4172946116	0.5052425895
O23	5.9410027029	7.0631163774	1.1328977921
O24	1.8693466020	4.5159642595	0.2752041402
O25	3.4084579682	5.5270389297	2.6196716796
O26	4.4160222284	6.0543665117	-1.2637993194
Cu27	3.9120263449	5.7882434211	0.6770134407
H28	3.9176387995	4.9046792715	3.1603255929
H29	3.2095154133	6.3042895054	3.1630107333
H30	6.4598848857	7.2904621005	1.9173906459
H31	6.4304159450	7.4211109855	0.3787598799
H32	4.6276147591	5.2811066890	-1.8079956883
H33	3.9044652451	6.6732232807	-1.8062468824
H34	1.4146391546	4.1457361751	-0.4944739350
H35	1.3317567102	4.2760189749	1.0432004227

Δr=1.0 Å			
Atom	X	Y	Z
H1	1.1614764568	6.6515717443	0.4440921996
C2	2.5977000257	10.1971999140	0.8423999973
C3	3.3865792560	9.0265225422	0.8933466840
N4	2.8825950885	7.7693039126	0.7525660140
C5	1.5475763536	7.6584700920	0.5556185812
C6	0.7017439326	8.7614708813	0.4937567371
C7	1.2269999737	10.0483128734	0.6374936045
H8	3.0688061405	11.1660493007	0.9630911216
H9	4.4583217705	9.0846983373	1.0528789218
H10	-0.3599049301	8.6064380110	0.3328492635
H11	0.5760167990	10.9160428820	0.5898777200
C12	6.6689229527	1.2960390571	0.7400951025
C13	7.2311689218	2.5638894082	0.9146654763
C14	6.4138753314	3.6898932142	0.9111042740
N15	5.0723214154	3.6173306268	0.7437774347
C16	4.5316164211	2.3783872397	0.5742022377
C17	5.2899999743	1.1869000860	0.5646000027
H18	7.2989827973	0.4117150731	0.7420087456
H19	8.3000704276	2.6860621869	1.0544568291
H20	6.8264602795	4.6836479867	1.0467451650
H21	3.4552968193	2.3547679772	0.4419328105
H22	4.7912610921	0.2347899343	0.4241838162
O23	6.0255516587	6.9245589471	1.2059148734
O24	1.9642813265	4.4505213986	0.3670764339
O25	3.5029999937	5.4411852910	2.7116245924
O26	4.4994948796	5.9575906565	-1.1589482846
Cu27	4.0083538247	5.6916868802	0.7772126099
H28	4.0011817226	4.8140199597	3.2570871568
H29	3.3075056338	6.2220763209	3.2512099751
H30	6.5173911140	7.2128013412	1.9876046922
H31	6.5282060072	7.2403967823	0.4418551477
H32	4.6861074270	5.1813219976	-1.7082434112
H33	3.9894218675	6.5878676525	-1.6898171614

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H34	1.4845047890	4.1401406177	-0.4137293880
H35	1.4494796436	4.1547701154	1.1311489911

$\Delta r=1.2 \text{ \AA}$			
Atom	X	Y	Z
H1	1.1691077136	6.6526171034	0.4470076642
C2	2.5977000451	10.1971998490	0.8423999953
C3	3.3925237356	9.0297709468	0.8675744759
N4	2.8914712206	7.7726214994	0.7294204023
C5	1.5543620318	7.6590354623	0.5609502040
C6	0.7004855881	8.7573142270	0.5268412945
C7	1.2234881717	10.0447739769	0.6680991216
H8	3.0672109286	11.1673829061	0.9589095552
H9	4.4676733661	9.0948062846	1.0028708664
H10	-0.3635081529	8.5980388161	0.3865653001
H11	0.5686300386	10.9105094172	0.6413696334
C12	6.7277764240	1.0973280218	0.7263749012
C13	7.2991254887	2.3629278057	0.8859220515
C14	6.4872259216	3.4935298955	0.8752190533
N15	5.1463106239	3.4261416569	0.7136446689
C16	4.5982888990	2.1910504822	0.5594299936
C17	5.3471999549	0.9954001510	0.5587000046
H18	7.3520418879	0.2089052123	0.7336764305
H19	8.3694973996	2.4799367675	1.0191964958
H20	6.9076597855	4.4853527783	1.0007889579
H21	3.5208959243	2.1704699681	0.4305359938
H22	4.8418092499	0.0451253283	0.4299734911
O23	6.0645969449	6.7439163898	1.1720298035
O24	2.0623988954	4.4264729856	0.3260032515
O25	3.5752149608	5.3430494721	2.6731717897
O26	4.5380437631	5.8654951612	-1.1814955059
Cu27	4.0617861864	5.5965545329	0.7459885601
H28	4.0738677985	4.7052784042	3.2062412400
H29	3.4058172596	6.1274437653	3.2170315966
H30	6.5480902420	7.0287192290	1.9600283743
H31	6.5701169246	7.0669267415	0.4129617469
H32	4.6995396733	5.0877371943	-1.7369772274
H33	4.0350311592	6.5113988869	-1.7006254882
H34	1.5846396779	4.1222223532	-0.4582830414
H35	1.5554128037	4.1138013233	1.0885005056

$\Delta r=1.4 \text{ \AA}$			
Atom	X	Y	Z
H1	1.1358330336	6.6655672862	0.4279498005
C2	2.5977000064	10.1971999786	0.8423999994
C3	3.3785900236	9.0218602802	0.8660115902
N4	2.8660451536	7.7724786698	0.7195481420
C5	1.5302836700	7.6694598651	0.5440003318
C6	0.6869798836	8.7768018598	0.5084236042
C7	1.2229542864	10.0583192925	0.6588560088
H8	3.0755070539	11.1624828819	0.9656689609
H9	4.4538580403	9.0778151821	1.0074940690
H10	-0.3782121736	8.6296573789	0.3638189108
H11	0.5765633064	10.9304193721	0.6331200083
C12	6.7832805360	0.9232423974	0.7204931899
C13	7.3394720650	2.1966243615	0.8685048596
C14	6.5125730646	3.3164772711	0.8465341288
N15	5.1733751933	3.2328759195	0.6860293163
C16	4.6409924261	1.9909514181	0.5420708777
C17	5.4043999936	0.8038000214	0.5528000007
H18	7.4178238718	0.0422225168	0.7362235529
H19	8.4083163779	2.3275654703	1.0009861084
H20	6.9222442024	4.3144916969	0.9614871781
H21	3.5634766299	1.9523011380	0.4136723823
H22	4.9110693182	-0.1540420313	0.4327321599

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O23	5.9833148617	6.5827955438	1.1140497474
O24	2.0835714964	4.4074733593	0.3147674276
O25	3.5628080916	5.2531774359	2.6328833675
O26	4.5064063208	5.7492389260	-1.2071091351
Cu27	4.0393920399	5.4920922158	0.7127095592
H28	4.0757191332	4.6271584215	3.1668883659
H29	3.3827467942	6.0396295140	3.1707210682
H30	6.4464156626	6.8831126664	1.9082774187
H31	6.4862704673	6.9164985302	0.3578246233
H32	4.6819561189	4.9675603191	-1.7532699699
H33	3.9893611888	6.3802825819	-1.7312728058
H34	1.6263111839	4.0916004171	-0.4768285401
H35	1.5785088516	4.0828497750	1.0735588801

$\Delta r=1.5 \text{ \AA}$			
Atom	X	Y	Z
H1	1.2011740343	6.6405614018	0.4610654996
C2	2.5977000036	10.1971999879	0.8423999996
C3	3.4017563826	9.0377468294	0.8671169261
N4	2.9139690068	7.7773317557	0.7341329417
C5	1.5791336465	7.6514767535	0.5713554428
C6	0.7119117705	8.7400905127	0.5399464670
C7	1.2239281893	10.0322441963	0.6759137271
H8	3.0579088461	11.1725402205	0.9534103612
H9	4.4772100349	9.1183943137	0.9972162625
H10	-0.3513194297	8.5702402244	0.4063716219
H11	0.5614255627	10.8921985388	0.6513908354
C12	6.8145796667	0.8040998961	0.7116220874
C13	7.3910065020	2.0673008790	0.8682323921
C14	6.5804240999	3.1993058174	0.8604278499
N15	5.2389546476	3.1377940604	0.7061844276
C16	4.6887376361	1.9055069735	0.5540349154
C17	5.4329999964	0.7081000121	0.5498000004
H18	7.4350133343	-0.0870038301	0.7164611527
H19	8.4623112137	2.1812500039	0.9965971204
H20	7.0071207183	4.1901162787	0.9785570234
H21	3.6100535834	1.8822582457	0.4302378847
H22	4.9246700561	-0.2409304572	0.4224506824
O23	6.0815417992	6.4739893589	1.1568561138
O24	2.1949118574	4.3743959815	0.3427688835
O25	3.6725538933	5.1642142477	2.6652371757
O26	4.6037809762	5.6909507984	-1.1633846636
Cu27	4.1427327334	5.4205419697	0.7509685930
H28	4.1867430340	4.5313104568	3.1900982727
H29	3.4976560343	5.9465458329	3.2112331257
H30	6.5350842820	6.7739708492	1.9566761634
H31	6.5815233831	6.8230904304	0.4056046332
H32	4.7797890736	4.9148721506	-1.7174810696
H33	4.0847074767	6.3276290368	-1.6790568371
H34	1.7475967148	4.0587451118	-0.4545135984
H35	1.6868698835	4.0426110266	1.0964913357

$\Delta r=1.6 \text{ \AA}$			
Atom	X	Y	Z
H1	1.1134948681	6.6779573444	0.4219173498
C2	2.5977000029	10.1971999904	0.8423999997
C3	3.3714438954	9.0197192963	0.8556146133
N4	2.8513127775	7.7757241652	0.7077098616
C5	1.5145638855	7.6793964177	0.5415570993
C6	0.6753376813	8.7905175283	0.5173686570
C7	1.2203447579	10.0677772686	0.6693562148
H8	3.0807791652	11.1599900206	0.9653975784
H9	4.4482467894	9.0725064753	0.9892380215
H10	-0.3917041942	8.6498396753	0.3798563732
H11	0.5795393932	10.9442206983	0.6527612429

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C12	6.8421170920	0.7471255091	0.6883091382
C13	7.3859143485	2.0271023170	0.8180795198
C14	6.5424604224	3.1349084626	0.8038306702
N15	5.2027929733	3.0335057161	0.6674610294
C16	4.6838414462	1.7866779214	0.5408549771
C17	5.4617999971	0.6119000096	0.5468000003
H18	7.4860557837	-0.1270793736	0.6975659513
H19	8.4551963394	2.1723662554	0.9305777645
H20	6.9412490910	4.1386410060	0.9078775366
H21	3.6045113119	1.7294614877	0.4310829502
H22	4.9794297822	-0.3534390701	0.4422570978
O23	5.9602924332	6.4117532193	1.1040832460
O24	2.0874596070	4.3988564697	0.2722385222
O25	3.5485356457	5.1476386745	2.5967760627
O26	4.4972450318	5.6685167078	-1.2193246627
Cu27	4.0235565605	5.4047232623	0.6884497401
H28	4.0621366460	4.5132576728	3.1209206760
H29	3.3691660158	5.9282338138	3.1439082853
H30	6.3845809303	6.7381934919	1.9095757579
H31	6.4481733722	6.7875417430	0.3576695551
H32	4.6807888917	4.8914747649	-1.7700866877
H33	3.9796230166	6.3023102111	-1.7402082934
H34	1.6832194415	4.0411835054	-0.5303262502
H35	1.5954341054	4.0331592887	1.0210026628

$\Delta r=1.7 \text{ \AA}$			
Atom	X	Y	Z
H1	1.2295152139	6.6220164713	0.5474071966
C2	2.5977000017	10.1971999944	0.8423999998
C3	3.4106959517	9.0482698466	0.8907917229
N4	2.9320271802	7.7833730755	0.7866482038
C5	1.5978203995	7.6389713907	0.6322459646
C6	0.7216218378	8.7195852105	0.5769342802
C7	1.2246089826	10.0180708754	0.6826242045
H8	3.0490101204	11.1790774982	0.9306722520
H9	4.4856349355	9.1434360139	1.0173464823
H10	-0.3407744062	8.5386891137	0.4514398551
H11	0.5556264672	10.8723108131	0.6411533813
C12	6.8743093482	0.6027394058	0.6889404358
C13	7.4580341229	1.8601217166	0.8600913076
C14	6.6480963926	2.9931504670	0.8815990154
N15	5.3065391803	2.9399482213	0.7424748757
C16	4.7516712746	1.7144448894	0.5770748115
C17	5.4902999983	0.5165000056	0.5439000001
H18	7.4900675439	-0.2914014905	0.6697222558
H19	8.5313778995	1.9678020830	0.9769562791
H20	7.0816998924	3.9795209233	1.0169893613
H21	3.6707960660	1.6921212499	0.4672713638
H22	4.9785379843	-0.4296670133	0.4084911994
O23	6.1086833350	6.3380905285	1.2515956578
O24	2.2657886737	4.4168631354	0.4104242279
O25	3.7010951675	5.1512754964	2.7307007809
O26	4.6408392918	5.7076548756	-1.0741563795
Cu27	4.1663312849	5.4439698222	0.8281413474
H28	4.2095256143	4.4943422193	3.2321156198
H29	3.5163731723	5.9089842570	3.3075307005
H30	6.5261984573	6.6475172253	2.0674066133
H31	6.6151516658	6.7072227539	0.5140728474
H32	4.8171769499	4.9285284184	-1.6249487337
H33	4.1196229157	6.3438037043	-1.5891694409
H34	1.8998538901	4.0265332961	-0.3953720527
H35	1.7978947991	4.0162624806	1.1569407710

$\Delta r=1.8 \text{ \AA}$			
Atom	X	Y	Z

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H1	1.4960293391	6.9947713193	-0.9373354880
C2	2.5977002239	10.1971992507	0.8423999769
C3	3.4193680200	9.0792018797	0.7168372624
N4	3.0332230834	7.9439334898	0.0895056010
C5	1.7857483050	7.9128376933	-0.4317508098
C6	0.8989877289	8.9788277098	-0.3462452735
C7	1.3124624091	10.1450255632	0.3011601226
H8	2.9617686422	11.0821907770	1.3525390616
H9	4.4262340785	9.0853487535	1.1256382776
H10	-0.0914035460	8.8972133335	-0.7807746661
H11	0.6450925097	10.9975815481	0.3803809803
C12	6.7781853705	0.0808102495	0.0429074496
C13	7.5467060547	1.0618098101	-0.5862222562
C14	7.0381773993	2.3500161204	-0.6978120962
N15	5.8161926978	2.6781888947	-0.2172990111
C16	5.0674755437	1.7293521623	0.3905880149
C17	5.5188997761	0.4208007493	0.5409000231
H18	7.1546877111	-0.9324831152	0.1442746870
H19	8.5294596672	0.8400146568	-0.9881682770
H20	7.6102976224	3.1425744698	-1.1683709755
H21	4.0934325803	2.0348666249	0.7593891024
H22	4.8894307896	-0.3080983990	1.0396913948
O23	6.9710907339	5.2848851102	0.0969951041
O24	3.6638866410	3.9364734865	-1.8057928637
O25	3.5944341864	5.1284743335	0.9127269700
O26	4.9243079080	6.4596990925	-1.2031033214
Cu27	5.1681614975	4.5567422037	-0.5357893868
H28	3.4597457241	4.8473242540	1.8316041021
H29	3.3469361990	6.0650760564	0.8632941492
H30	7.3949221736	5.0543143480	0.9353078743
H31	7.0678651203	6.2370290792	-0.0470184805
H32	4.8033682715	6.5857248451	-2.1575828791
H33	4.2685821661	7.0123040709	-0.7490657587
H34	3.7332246417	3.1375496733	-2.3466455552
H35	2.7825100391	3.9423829149	-1.4060261416

$\Delta r=1.9 \text{ \AA}$			
Atom	X	Y	Z
H1	1.5014143442	6.9751683665	-0.9057482876
C2	2.5977000015	10.197199948	0.8423999998
C3	3.4131877718	9.0713249732	0.7465318916
N4	3.0287795990	7.9289940399	0.1309294075
C5	1.7891826913	7.8983925572	-0.4084263677
C6	0.9087728538	8.9717328516	-0.3528322298
C7	1.3204680057	10.1451631852	0.2826423618
H8	2.9603675850	11.0874358226	1.3442842120
H9	4.4140385069	9.0773056147	1.1698090226
H10	-0.0752543897	8.8903662044	-0.8016562212
H11	0.6580511983	11.0034148020	0.3380770787
C12	6.8014197954	0.0142717322	0.0078725226
C13	7.5458393910	1.0203945252	-0.6107551935
C14	7.0198212048	2.3044659757	-0.6804034063
N15	5.8022521058	2.6047420490	-0.1694000605
C16	5.0764777691	1.6312183454	0.4289923948
C17	5.5474999985	0.3250000051	0.5379000001
H18	7.1924738090	-0.9962569787	0.0766755018
H19	8.5235830852	0.8211354609	-1.0359852719
H20	7.5738302712	3.1154814253	-1.1406910049
H21	4.1063026153	1.9149201481	0.8244978673
H22	4.9373416588	-0.4243119116	1.0305394857
O23	6.9209234762	5.2037669718	0.2434446450
O24	3.5858182171	3.8900179709	-1.6366521561
O25	3.5504727181	5.1131175709	1.0028562898
O26	4.9283461636	6.4037271550	-1.1074301735
Cu27	5.1360740853	4.4899311433	-0.4342494330
H28	3.3921383423	4.8418755227	1.9208808349
H29	3.3196023098	6.0532429250	0.9412992969
H30	7.3284648314	4.9529338018	1.0841437333

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H31	7.0195198509	6.1588578804	0.1222803701
H32	4.8427387854	6.5373356520	-2.0646095296
H33	4.2682258951	6.9672447865	-0.6736039615
H34	3.6086859781	3.0806838506	-2.1660344342
H35	2.7272105449	3.9297745693	-1.1918226640

$\Delta r=2.0 \text{ \AA}$			
Atom	X	Y	Z
H1	1.5567343507	6.9527856236	-0.8987119451
C2	2.5977000016	10.1971999946	0.8423999998
C3	3.4170701995	9.0709644671	0.7835576015
N4	3.0519515479	7.9202907394	0.1713041008
C5	1.8284345154	7.8818437569	-0.4031413566
C6	0.9454860201	8.9543745125	-0.3855875688
C7	1.3370597656	10.1360425558	0.2472290974
H8	2.9452261534	11.0939208767	1.3434293535
H9	4.4054503523	9.0835443150	1.2350746165
H10	-0.0250742447	8.8661924467	-0.8615108598
H11	0.6720558070	10.9936912980	0.2732791966
C12	6.8118300306	-0.0635082897	-0.0450617384
C13	7.5284091802	0.9590554888	-0.6696856535
C14	6.9938084558	2.2411609778	-0.6950032610
N15	5.7932269785	2.5247479860	-0.1358996107
C16	5.0942682983	1.5347290645	0.4676811108
C17	5.5760999984	0.2292000054	0.5349000001
H18	7.2107593410	-1.0726624196	-0.0099116148
H19	8.4915683908	0.7739264841	-1.1329082414
H20	7.5285541337	3.0641006109	-1.1571219475
H21	4.1374171381	1.8044555059	0.9032693360
H22	4.9874472877	-0.5328009746	1.0340286364
O23	6.9067493684	5.1039054544	0.3644365708
O24	3.5231259614	3.8654317312	-1.4740824074
O25	3.5248987995	5.0899898544	1.0901819218
O26	4.9586558258	6.3513258644	-1.0019424473
Cu27	5.1277504001	4.4229754194	-0.3404720463
H28	3.3553565709	4.8328674289	2.0102231797
H29	3.3112751819	6.0333989185	1.0177824322
H30	7.3127716545	4.8236397315	1.1965796710
H31	7.0114008136	6.0615224577	0.2714571445
H32	4.9057205334	6.4974966051	-1.9596689901
H33	4.3004303933	6.9285469744	-0.5833178877
H34	3.4910834104	3.0513124341	-1.9955595099
H35	2.7008522551	3.9332736534	-0.9682280975

$\Delta r=2.1 \text{ \AA}$			
Atom	X	Y	Z
H1	1.5535234625	6.9613807706	-0.9140027862
C2	2.5977000165	10.1971999447	0.8423999983
C3	3.4096596403	9.0641396726	0.7914803539
N4	3.0441643913	7.9160246191	0.1741885328
C5	1.8271252643	7.8878420433	-0.4144913135
C6	0.9522145548	8.9670628039	-0.4070433568
C7	1.3442724214	10.1455847292	0.2314092933
H8	2.9462699388	11.0904770378	1.3487623314
H9	4.3925335011	9.0695771637	1.2550297027
H10	-0.0128700679	8.8862276685	-0.8953342130
H11	0.6849214594	11.0078058183	0.2494801686
C12	6.8431678786	-0.1308240421	-0.0558662032
C13	7.5384559018	0.9112694665	-0.6726925534
C14	6.9809969671	2.1838977069	-0.6833367199
N15	5.7776972054	2.4409511280	-0.1170735517
C16	5.0997703435	1.4316951113	0.4797058099
C17	5.6046999835	0.1334000552	0.5319000017
H18	7.2606333983	-1.1328693506	-0.0326770031
H19	8.5030334573	0.7484250946	-1.1414471994

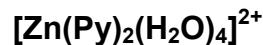
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H20	7.4999005565	3.0202351677	-1.1393213434
H21	4.1401753377	1.6792342483	0.9225248354
H22	5.0311129527	-0.6435911701	1.0255146892
O23	6.8493696411	5.0330121238	0.4065775001
O24	3.4839428208	3.7659470422	-1.4247234647
O25	3.4733395430	5.0349110739	1.1174470550
O26	4.9085564378	6.2732425523	-0.9707678017
Cu27	5.0834982711	4.3378063472	-0.3063859512
H28	3.2844240803	4.7719578646	2.0320952144
H29	3.2727221502	5.9816539317	1.0518657340
H30	7.2539345531	4.7576039611	1.2409731134
H31	6.9436948472	5.9915861360	0.3126278215
H32	4.8651262313	6.4233211834	-1.9283343646
H33	4.2684739408	6.8722119486	-0.5545048583
H34	3.4458256056	2.9382154898	-1.9240384546
H35	2.6581250138	3.8610822211	-0.9293270635

$\Delta r=2.3 \text{ \AA}$			
Atom	X	Y	Z
H1	1.7947509471	6.9446424719	-1.0103950684
C2	2.5977000116	10.1971999609	0.8423999988
C3	3.4105229821	9.0637514677	0.9067438626
N4	3.1295180029	7.9096562490	0.2562911648
C5	2.0004594436	7.8759481681	-0.4874607581
C6	1.1328564994	8.9549167259	-0.6045342211
C7	1.4361999187	10.1388053744	0.0715705365
H8	2.8764466805	11.0941337086	1.3842251205
H9	4.3234917931	9.0730284512	1.4959455662
H10	0.2406583435	8.8692564592	-1.2153146693
H11	0.7791821621	10.9997432460	-0.0037354489
C12	6.7916147048	-0.3446394402	-0.2423153605
C13	7.4187638887	0.6887137860	-0.9420487584
C14	6.9046927531	1.9762893911	-0.8541715102
N15	5.8055261389	2.2568006728	-0.1133755046
C16	5.1936469557	1.2556610948	0.5638029996
C17	5.6618999883	-0.0580999610	0.5260000012
H18	7.1792304403	-1.3574954191	-0.2947653714
H19	8.2983856501	0.5071941534	-1.5502642910
H20	7.3770040721	2.8038986723	-1.3736540581
H21	4.3184143246	1.5218281651	1.1482135594
H22	5.1440136077	-0.8265115933	1.0894251111
O23	6.9576378676	4.7698787540	0.5777934477
O24	3.4093094332	3.7968109786	-0.9831993610
O25	3.3307827737	5.0877949327	1.3174523141
O26	5.0555623910	6.1730128353	-0.6967130561
Cu27	5.1890565453	4.1946797690	-0.1670213457
H28	3.0357712785	4.8725125960	2.2164240259
H29	3.1948364598	6.0415092328	1.2044950579
H30	7.4028034094	4.3605405206	1.3328030888
H31	7.0840250690	5.7287079812	0.6140603043
H32	5.1101322792	6.3833200234	-1.6422355760
H33	4.4046950442	6.7821912422	-0.3131662784
H34	3.1426649260	2.9359297713	-1.3348009728
H35	2.7956898884	4.0794883747	-0.2903830416

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Optimized geometries for solvation models.



$\Delta r=0.0 \text{ \AA}$			
Atom	X	Y	Z
H1	0.9863877961	7.2715548555	-0.5612717073
C2	2.7403315670	10.5718269987	0.3083886876
C3	3.4008064576	9.3398249343	0.3163613708
N4	2.7716735110	8.1732147531	0.0038578296
C5	1.4514834497	8.2200599654	-0.3283622614
C6	0.7290997334	9.4162448302	-0.3613504530
C7	1.3810853648	10.6150183624	-0.0372316648
H8	3.2845418857	11.4754871475	0.5670920964
H9	4.4502073110	9.2620112437	0.5677495259
H10	-0.3221890094	9.4029099395	-0.6351912196
H11	0.8433250380	11.5592230928	-0.0531445713
C12	6.4144308144	1.8247959267	0.0129261705
C13	7.1041011260	3.0448584297	0.0709624028
C14	6.3748294578	4.2376007763	0.0748612663
N15	5.0133634994	4.2621946103	0.0237772753
C16	4.3486141305	3.0748117193	-0.0320772295
C17	5.0122179469	1.8444742858	-0.0387552629
H18	6.9556537369	0.8823926085	0.0091306797
H19	8.1894517011	3.0769847513	0.1131739535
H20	6.8664107025	5.2002520829	0.1252624169
H21	3.2685564255	3.1361532469	-0.0718562217
H22	4.4380320347	0.9236060961	-0.0843736734
O23	5.7462541458	7.2847363519	0.3636600095
O24	2.0365493686	5.1563304333	-0.2953476091
O25	3.6132840399	6.0807524714	2.1468528694
O26	4.1742302940	6.3744250256	-2.0955433601
Zn27	3.8936636217	6.2203568721	0.0274936046
H28	3.9144755007	5.3328846968	2.7021974915
H29	3.2172519812	6.7746547159	2.7128781186
H30	6.1734874416	7.4065865631	1.2359258201
H31	6.2935730154	7.7151355114	-0.3239262853
H32	4.6723518851	5.7434939897	-2.6536638337
H33	3.7920187117	7.0783126524	-2.6591100703
H34	1.7126660763	4.8284666496	-1.1589325239
H35	1.3989193756	4.9054468696	0.4033199068

$\Delta r=0.3 \text{ \AA}$			
Atom	X	Y	Z
H1	0.9370188961	7.2289471797	-0.2888259018
C2	2.7403000081	10.5717999690	0.3083999988
C3	3.4012234928	9.3334543086	0.3222306745
N4	2.7593686642	8.1484622881	0.1073560447
C5	1.4177629524	8.1856599298	-0.1276987223
C6	0.6916165189	9.3801837257	-0.1591642910
C7	1.3594834111	10.5948229847	0.0620873956
H8	3.3009016894	11.4849062449	0.4861678191
H9	4.4665533073	9.2667482630	0.5042932197
H10	-0.3771316720	9.3547650026	-0.3525603595
H11	0.8159257209	11.5357982196	0.0434360825
C12	6.4803572198	1.5801022658	0.1127938265
C13	7.1177864559	2.8193957291	0.2783028194
C14	6.3499011801	3.9877935212	0.2750981094
N15	4.9960466347	3.9777652610	0.1181812959
C16	4.3831605842	2.7693160647	-0.0412487299
C17	5.0877999919	1.5543000310	-0.0502999988
H18	7.0555575438	0.6579446100	0.1109729090
H19	8.1944838453	2.8841813683	0.4075878741
H20	6.8052365376	4.9618419230	0.3983894637
H21	3.3071855487	2.7969580575	-0.1622023339

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H22	4.5492946332	0.6202708362	-0.1818557927
O23	5.6887480615	7.0725681760	0.4486854656
O24	2.0055692465	5.0228735399	-0.1794476819
O25	3.5435527847	5.9026627303	2.2180203097
O26	4.0765879939	6.1901424003	-1.9849012447
Zn27	3.8454483400	6.0492824065	0.1211432058
H28	3.7409141435	5.1160785172	2.7654185479
H29	3.1752373991	6.6158719748	2.7789408285
H30	6.0532182787	7.2875250995	1.3307595921
H31	6.2754046174	7.4385963344	-0.2434930433
H32	4.4154856113	5.4802188866	-2.5673319216
H33	3.8336791941	6.9717418289	-2.5214434060
H34	1.6457493279	4.7562242825	-1.0490353069
H35	1.4172526726	4.6960125640	0.5303371925

$\Delta r=0.6 \text{ \AA}$			
Atom	X	Y	Z
H1	1.0523037157	7.1791535936	-0.3520573621
C2	2.7403000195	10.5717999250	0.3083999970
C3	3.4390733979	9.3500405138	0.3191862768
N4	2.8401830625	8.1442729723	0.0844000195
C5	1.5013868348	8.1473688833	-0.1715285518
C6	0.7382212661	9.3189655831	-0.2002437874
C7	1.3631507146	10.5524357356	0.0432116980
H8	3.2715359196	11.4990354197	0.5017674157
H9	4.5039002989	9.3156283334	0.5178745439
H10	-0.3263151064	9.2614881023	-0.4095016108
H11	0.7896316927	11.4754144775	0.0263981744
C12	6.5607042958	1.2842972313	0.0573059160
C13	7.2124154768	2.5224647761	0.1715018923
C14	6.4554778644	3.6984525882	0.1647958483
N15	5.0972365179	3.7007525131	0.0493198730
C16	4.4718676050	2.4904289720	-0.0624097110
C17	5.1632999805	1.2641000750	-0.0617999970
H18	7.1295320889	0.3583032962	0.0610904472
H19	8.2931607616	2.5809623175	0.2648801135
H20	6.9249728074	4.6701156159	0.2545459635
H21	3.3925694381	2.5236809510	-0.1548047250
H22	4.6120440853	0.3329717308	-0.1531371348
O23	5.8068433069	6.8893258299	0.3966703479
O24	2.1323917747	4.9457028960	-0.2598815451
O25	3.6849177564	5.7423695500	2.1433342157
O26	4.2327298587	6.0961846866	-2.0169505360
Zn27	3.9724662337	5.9160542626	0.0622258099
H28	3.9283796225	4.9595779906	2.6784236871
H29	3.2782071966	6.4246485586	2.7160611621
H30	6.1846655429	7.0847587037	1.2772773823
H31	6.3848837589	7.2631647040	-0.2980864793
H32	4.6189221369	5.4091301187	-2.5978624116
H33	3.9671399861	6.8722028120	-2.5510855609
H34	1.7843066322	4.6824247324	-1.1353552386
H35	1.5295245967	4.6310671476	0.4431250533

$\Delta r=0.7 \text{ \AA}$			
Atom	X	Y	Z
H1	1.0375795417	7.1750041418	-0.2996117116
C2	2.7403000047	10.5717999819	0.3083999993
C3	3.4373016381	9.3481961864	0.3234561797
N4	2.8341961132	8.1412766321	0.1054018410
C5	1.4924791948	8.1439172303	-0.1346720593
C6	0.7309322893	9.3167127519	-0.1669673507
C7	1.3603818517	10.5514133452	0.0572340200
H8	3.2738940711	11.5003216657	0.4890437373
H9	4.5040706721	9.3147304102	0.5132286783
H10	-0.3360040199	9.2590534742	-0.3639839513

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H11	0.7877308722	11.4749194461	0.0370725545
C12	6.5835412050	1.1969854719	0.0776848724
C13	7.2243583425	2.4389405316	0.2121759831
C14	6.4590401196	3.6096602618	0.2011423810
N15	5.1030320015	3.6036116153	0.0637248351
C16	4.4886747015	2.3898061744	-0.0680473511
C17	5.1884999953	1.1674000181	-0.0655999993
H18	7.1590088048	0.2750404487	0.0841026921
H19	8.3030532208	2.5038113075	0.3245825830
H20	6.9220456918	4.5833116753	0.3041543562
H21	3.4104998613	2.4164042842	-0.1770316827
H22	4.6453760802	0.2331817915	-0.1733712732
O23	5.8039753208	6.8255548019	0.4099423331
O24	2.1350613500	4.9103716654	-0.2395397099
O25	3.6844050065	5.7082943966	2.1570163690
O26	4.2316103596	6.0421375784	-1.9928098863
Zn27	3.9700558776	5.8669699062	0.0829161080
H28	3.8929172843	4.9145081859	2.6910488087
H29	3.3103571340	6.4075449570	2.7308233786
H30	6.1871888997	7.0203272314	1.2885945515
H31	6.3779233881	7.1976072146	-0.2891972793
H32	4.5976487179	5.3469376454	-2.5768781227
H33	3.9877525628	6.8276544666	-2.5235021157
H34	1.7850659678	4.6531909133	-1.1159093889
H35	1.5366568044	4.5860168505	0.4629505466

$\Delta r=0.8 \text{ \AA}$			
Atom	X	Y	Z
H1	1.0369403379	7.1789504292	-0.3179509986
C2	2.7403000035	10.5717999864	0.3083999995
C3	3.4313437795	9.3446741109	0.3446198519
N4	2.8284321188	8.1390542225	0.1199125320
C5	1.4928076676	8.1464386606	-0.1491548030
C6	0.7373320940	9.3223261737	-0.2067886598
C7	1.3665260014	10.5558381002	0.0254961447
H8	3.2744299518	11.4986662664	0.4958804621
H9	4.4939594426	9.3082648062	0.5559236912
H10	-0.3250604626	9.2675591962	-0.4278900431
H11	0.7983299916	11.4815480912	-0.0127974142
C12	6.6113626400	1.1095341343	0.0401867875
C13	7.2473615708	2.3559168343	0.1552506943
C14	6.4749017063	3.5220373708	0.1580099549
N15	5.1161937461	3.5081267602	0.0516229032
C16	4.5070866401	2.2895867780	-0.0608310645
C17	5.2135999965	1.0707000136	-0.0694999995
H18	7.1927123686	0.1912672468	0.0365896723
H19	8.3279814192	2.4275907378	0.2422440841
H20	6.9350284037	4.4983432337	0.2481827983
H21	3.4265294829	2.3083740341	-0.1453561486
H22	4.6735513864	0.1329183455	-0.1608439127
O23	5.8075253500	6.7573016581	0.4201385453
O24	2.1373505803	4.8801351643	-0.2381964697
O25	3.6939154331	5.6411659488	2.1607724110
O26	4.2445988809	5.9994815222	-1.9801676127
Zn27	3.9733280090	5.8186299687	0.0890823862
H28	3.8810640102	4.8347410651	2.6829611540
H29	3.3519364236	6.3461506884	2.7471688203
H30	6.1829933929	6.9589036400	1.3003553159
H31	6.3870302044	7.1217917409	-0.2786531033
H32	4.5810161188	5.2934844827	-2.5687929600
H33	4.0395729275	6.7996290774	-2.5051459054
H34	1.7895905069	4.6247018885	-1.1161184282
H35	1.5336619334	4.5609557800	0.4622381032

$\Delta r=0.9 \text{ \AA}$			
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Atom	X	Y	Z
H1	0.9034975742	7.2462023750	-0.2753781142
C2	2.7403000171	10.5717999341	0.3083999974
C3	3.4022466538	9.3395226431	0.2726428459
N4	2.7427263834	8.1631619178	0.0663741408
C5	1.3914239345	8.1989010224	-0.1126741253
C6	0.6684297133	9.3934072654	-0.0899978696
C7	1.3499756425	10.6010069455	0.1242288330
H8	3.3074054888	11.4824589651	0.4760688996
H9	4.4744573224	9.2704409513	0.4107962017
H10	-0.4072188789	9.3722621400	-0.2373550322
H11	0.8101706508	11.5434915388	0.1472174858
C12	6.6355080859	1.0042868535	0.0644237912
C13	7.2774015964	2.2469979195	0.1884140647
C14	6.5033839807	3.4128998910	0.1719499458
N15	5.1492174621	3.3999420557	0.0387018387
C16	4.5385041993	2.1884672021	-0.0829508309
C17	5.2387999828	0.9740000659	-0.0732999974
H18	7.2097573194	0.0819512009	0.0749357813
H19	8.3567081254	2.3152175280	0.2972957717
H20	6.9586087417	4.3918709901	0.2698730971
H21	3.4606158490	2.2081565867	-0.1902023185
H22	4.7001603121	0.0355316995	-0.1721417510
O23	5.7356392791	6.8729792416	0.3604892458
O24	2.1287224239	5.0264920223	-0.3741139877
O25	3.6116578112	5.7723493392	2.0630128776
O26	4.2371579233	6.2114406489	-2.0363761795
Zn27	3.7785214613	6.2311196655	0.0188626646
H28	3.8574379043	4.9101875291	2.4554756778
H29	3.3257738474	6.3954582090	2.7627509751
H30	6.1557931046	6.9876206754	1.2362330119
H31	6.3549892684	7.1421701809	-0.3473073077
H32	4.7070624705	5.4900669017	-2.5027683516
H33	4.0349929118	6.9386567102	-2.6607573809
H34	1.8711804492	4.7228187651	-1.2677895532
H35	1.5822866236	4.5828864848	0.3047825475

$\Delta r=1.0 \text{ \AA}$			
Atom	X	Y	Z
H1	0.0826070047	7.8271078918	0.6918553616
C2	2.7403000346	10.5717998670	0.3083999948
C3	3.0166083930	9.3383168559	0.8928716985
N4	2.0694937030	8.3674134725	1.0167905658
C5	0.8093412781	8.6179769853	0.5604582975
C6	0.4658970813	9.8331747930	-0.0358940975
C7	1.4453526569	10.8286021087	-0.1668407260
H8	3.5260706414	11.3169523738	0.2275946746
H9	4.0028133855	9.0978422202	1.2644042678
H10	-0.5491010175	9.9912091949	-0.3879829741
H11	1.2054823569	11.7826499372	-0.6272383665
C12	6.5634867627	1.1362460562	0.3852984645
C13	6.8811782210	2.4232358342	0.8457554134
C14	5.8900824125	3.4076663304	0.8276114178
N15	4.6335128849	3.1544635430	0.3788991513
C16	4.3222062521	1.9099896047	-0.0649723706
C17	5.2638999653	0.8773001330	-0.0771999946
H18	7.3135441692	0.3502812767	0.3872903746
H19	7.8752029400	2.6603117636	1.2127721978
H20	6.0824418333	4.4187274631	1.1689242347
H21	3.3042286938	1.7548042502	-0.4077574928
H22	4.9823306275	-0.1065755771	-0.4399453668
O23	4.7233532129	6.8774553068	1.8426560540
O24	0.5999989615	5.8152305436	2.1332976436
O25	2.6737206756	6.8221713772	3.9434516430
O26	2.8503509100	5.0510687147	0.3908180955
Zn27	2.6164830343	6.4618685122	1.8636433945
H28	2.7158510281	6.0994443192	4.6042961299
H29	2.6662071860	7.6909577555	4.3932631605

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H30	5.2372409842	7.1130710853	2.6418979377
H31	5.2816733386	6.9719655260	1.0447330693
H32	3.5768771865	4.2819738125	0.3824495245
H33	2.2970855586	5.0436835320	-0.4154388225
H34	0.1247732097	5.1698368318	1.5713372654
H35	0.0507857518	6.0520898913	2.9082179501

$\Delta r=1.1 \text{ \AA}$			
Atom	X	Y	Z
H1	0.3620348215	7.5637095731	0.1691607960
C2	2.7403000522	10.5717997995	0.3083999920
C3	3.0831893253	9.3249948090	0.8241991528
N4	2.2345268473	8.2614907102	0.7605099439
C5	1.0113322759	8.4288075465	0.1820359262
C6	0.6083885525	9.6517121388	-0.3573216533
C7	1.4854927036	10.7440315392	-0.2953276954
H8	3.4460504567	11.3942108362	0.3787227306
H9	4.0447954182	9.1512423333	1.2875530935
H10	-0.3736429618	9.7403769260	-0.8122011029
H11	1.1986782399	11.7074959409	-0.7059235864
C12	6.6432581307	1.0265245841	0.1950504565
C13	7.0802336715	2.3517399518	0.3501188108
C14	6.1489480706	3.3864934859	0.2265998062
N15	4.8422081772	3.1426910282	-0.0495480913
C16	4.4142051142	1.8636497674	-0.1992103337
C17	5.2890999478	0.7806002005	-0.0809999920
H18	7.3437267528	0.2013811902	0.2884119127
H19	8.1194758936	2.5799113728	0.5664673868
H20	6.4352686106	4.4252892307	0.3463267078
H21	3.3592868692	1.7244672841	-0.4132416095
H22	4.9166871454	-0.2317954444	-0.2047555422
O23	4.9141300768	6.8950877835	1.6313151589
O24	0.8418002359	5.6497755755	1.7251836537
O25	2.8797178743	6.5250407524	3.6457693160
O26	3.1097428886	5.0593078738	-0.0296395370
Zn27	2.8486384307	6.3506484273	1.5422642495
H28	2.5547956100	5.8095944541	4.2314229049
H29	3.3386592229	7.2087718565	4.1757093338
H30	5.4574544458	6.8821673319	2.4459659509
H31	5.4637045056	7.1769944394	0.8725951814
H32	3.8329421884	4.2789574544	-0.0673093050
H33	2.6778655235	5.2017879676	-0.8958813223
H34	0.4997764487	4.8817015343	1.2233384243
H35	0.1760991985	5.9468663320	2.3786080197

$\Delta r=1.2 \text{ \AA}$			
Atom	X	Y	Z
H1	0.2697620869	7.6361690681	0.4135783234
C2	2.7403000124	10.5717999524	0.3083999981
C3	3.0807388276	9.3248781016	0.8294827007
N4	2.1986607535	8.2864194348	0.8549734087
C5	0.9424348642	8.4814188626	0.3614191090
C6	0.5377652614	9.7055493383	-0.1743124869
C7	1.44961110097	10.7710984569	-0.2039947989
H8	3.4752786742	11.3712887090	0.3064752885
H9	4.0683719568	9.1278141490	1.2231282853
H10	-0.4719881334	9.8156185778	-0.5582799300
H11	1.1620115363	11.7338115884	-0.6160959973
C12	6.6382494513	0.9138670744	0.3210616571
C13	7.0320858784	2.2180794544	0.6595915514
C14	6.0911144589	3.2494589809	0.5805397672
N15	4.8124177933	3.0264362018	0.1819685117
C16	4.4275767368	1.7648033733	-0.1438992113
C17	5.3141999876	0.6839000476	-0.0848999981
H18	7.3479019333	0.0929614947	0.3740216661

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H19	8.0465904967	2.4339398429	0.9809289418
H20	6.3439719388	4.2721405267	0.8397872469
H21	3.3950331284	1.6346081868	-0.4512509958
H22	4.9735529585	-0.3120868239	-0.3514214166
O23	4.8882354139	6.8543783525	1.6484944074
O24	0.7999846383	5.6693399147	1.8261639219
O25	2.8561581204	6.6290098391	3.7113614547
O26	3.0890921845	4.9939748098	0.1140417721
Zn27	2.8118937511	6.3618667289	1.6249309153
H28	2.8310696786	5.8770425270	4.3396870485
H29	2.9336992672	7.4753230869	4.1960582542
H30	5.3955375157	7.0368535645	2.4655414163
H31	5.4383703856	7.0547379216	0.8645041675
H32	3.7964173541	4.2073466827	0.1311688560
H33	2.6161877629	5.0420081202	-0.7404804916
H34	0.4099054108	4.9214129507	1.3295316102
H35	0.1836057848	5.9645820384	2.5269645053

$\Delta r=1.4 \text{ \AA}$			
Atom	X	Y	Z
H1	0.7543319113	7.3015829710	-0.0088245602
C2	2.7403001091	10.5717995810	0.3083999833
C3	3.2079417475	9.3582012880	0.8148339078
N4	2.4986894619	8.1998694694	0.6928863368
C5	1.2928791423	8.2373038654	0.0566290059
C6	0.7693964682	9.4168785695	-0.4762462086
C7	1.5025374074	10.6061568209	-0.3506009716
H8	3.3387738170	11.4698090052	0.4298200799
H9	4.1611759661	9.2865099898	1.3200467951
H10	-0.1940434705	9.3981047835	-0.9770202844
H11	1.1184567631	11.5377806348	-0.7554704968
C12	6.7243488421	0.5542999046	0.2509794052
C13	7.3167245152	1.8080796202	0.4695680860
C14	6.5313845821	2.9575583352	0.3398485137
N15	5.2163544919	2.8922567882	0.0070109167
C16	4.6403261926	1.6815238077	-0.2075301342
C17	5.3645998909	0.4905004190	-0.0925999833
H18	7.3107114751	-0.3553099164	0.3472656800
H19	8.3654010386	1.8949890434	0.7374058174
H20	6.9409301460	3.9494833062	0.5035641794
H21	3.5876125214	1.6837003259	-0.4719053415
H22	4.8734504375	-0.4616708870	-0.2692311536
O23	5.2688576145	7.1255439089	1.6525154469
O24	1.3714375203	5.3976542209	1.5142067919
O25	3.1652928936	6.4758914860	3.5497995073
O26	3.7971256472	5.0795922986	-0.0965492416
Zn27	3.2969491315	6.3290107204	1.4487277298
H28	2.7352180246	5.7955724091	4.1093497440
H29	3.6019535589	7.1448393281	4.1146006167
H30	5.7852952454	7.1843928178	2.4819595569
H31	5.8175245128	7.4304384314	0.9018490050
H32	4.3812850123	4.1983399535	-0.0563124097
H33	3.6627737255	5.3728755905	-1.0196110678
H34	1.1599967635	4.5874003774	1.0072306149
H35	0.6250942809	5.6295897897	2.1036551547

$\Delta r=1.6 \text{ \AA}$			
Atom	X	Y	Z
H1	1.0129108785	7.1716671825	-0.1343776937
C2	2.7403001117	10.5717995707	0.3083999829
C3	3.3315388793	9.3694038979	0.7122348153
N4	2.7124225312	8.1616093793	0.5541144944
C5	1.4781009070	8.1418384884	-0.0292943397
C6	0.8363364779	9.3029288148	-0.4625049019
C7	1.4731242915	10.5410406706	-0.2909301483

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H8	3.2717011985	11.5066333601	0.4605757791
H9	4.3119402638	9.3501086198	1.1689413605
H10	-0.1445344003	9.2320644091	-0.9232916701
H11	0.9936166289	11.4592766611	-0.6165108808
C12	6.7524054105	0.2274252893	0.3203188126
C13	7.4536263535	1.4182658576	0.5652847622
C14	6.7965885872	2.6390747459	0.3843362216
N15	5.5018081198	2.7053475226	-0.0215626746
C16	4.8224351434	1.5537702230	-0.2623255391
C17	5.4149998883	0.2971004293	-0.1002999829
H18	7.2380366774	-0.7350832491	0.4548120504
H19	8.4889696119	1.4040650317	0.8922761948
H20	7.2977908992	3.5838289568	0.5647844274
H21	3.7912877734	1.6570677427	-0.5846459704
H22	4.8406733959	-0.6024732051	-0.3004543100
O23	5.5623630527	7.1232608201	1.5555842794
O24	1.7836601053	5.2198914368	1.1357947383
O25	3.4179723635	6.3382635943	3.3137319408
O26	4.3340253482	5.0482638192	-0.2874874181
Zn27	3.6437780989	6.2703326904	1.2163594989
H28	3.0493859476	5.6034628510	3.8477339846
H29	3.8314467184	6.9996308513	3.9042956124
H30	6.0779645463	6.9530350215	2.3700698212
H31	6.1652800207	7.3965872073	0.8349871127
H32	4.8078180510	4.1090274004	-0.1736818942
H33	4.4338616409	5.3789524809	-1.2022839604
H34	1.6065433212	4.5123502037	0.4828474974
H35	1.0044412604	5.3427680978	1.7154246796

$\Delta r=1.8 \text{ \AA}$			
Atom	X	Y	Z
H1	1.1049987189	7.1220917877	-0.1290393354
C2	2.7403002329	10.5717991053	0.3083999644
C3	3.3696420808	9.3813359385	0.6990035602
N4	2.7861873648	8.1550479203	0.5429441253
C5	1.5457188726	8.1038543628	-0.0258202974
C6	0.8651930920	9.2487170570	-0.4438868469
C7	1.4667887833	10.5048268694	-0.2743895368
H8	3.2472968205	11.5202624448	0.4595723659
H9	4.3564817700	9.3884424542	1.1426253372
H10	-0.1193772886	9.1512133324	-0.8919690821
H11	0.9546587711	11.4090706288	-0.5895390294
C12	6.7316146748	-0.0077396301	0.4873354953
C13	7.3953509864	1.1574224522	0.9030733235
C14	6.7732582318	2.3948946014	0.7123123527
N15	5.5457446965	2.5039990412	0.1395331199
C16	4.9045534592	1.3760301480	-0.2681648208
C17	5.4652997671	0.1037008947	-0.1079999644
H18	7.1915247646	-0.9822708560	0.6251601629
H19	8.3762997868	1.1105732502	1.3666166331
H20	7.2459244859	3.3202863395	1.0240957885
H21	3.9292150783	1.5084765673	-0.7243950996
H22	4.9214035205	-0.7740567361	-0.4438379040
O23	5.6842459397	7.0974371537	1.5003864279
O24	1.9292818367	5.1755051607	1.1649071287
O25	3.5224652319	6.4704637524	3.3069115065
O26	4.4642346979	4.9064439879	-0.2066863593
Zn27	3.7671133597	6.2439809419	1.2200256074
H28	3.2122833509	5.7475257438	3.8918053858
H29	3.9357083847	7.1769966010	3.8426979106
H30	6.2355976209	6.8135253049	2.2577906194
H31	6.2586600699	7.3391396434	0.7460164936
H32	4.8975612067	3.9557077726	-0.0391988521
H33	4.6060100238	5.1876424079	-1.1324448353
H34	1.7881009379	4.3926518125	0.5941924660
H35	1.1383016920	5.3432626363	1.7167739058

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$\Delta r=1.9 \text{ \AA}$

Atom	X	Y	Z
H1	1.1326735346	7.0940195817	-0.0096000853
C2	2.7403000020	10.5717999923	0.3083999997
C3	3.3953079820	9.3946957373	0.7050308786
N4	2.8237098044	8.1558830282	0.5914812374
C5	1.5650365620	8.0825440106	0.0648930351
C6	0.8577296204	9.2112077985	-0.3520167371
C7	1.4495190047	10.4775559583	-0.2304382166
H8	3.2404480159	11.5287121134	0.4242691411
H9	4.3951660830	9.4247667321	1.1183768601
H10	-0.1396056260	9.0936156343	-0.7654339607
H11	0.9170273584	11.3687126487	-0.5488788281
C12	6.7218877528	-0.1242772303	0.5488408191
C13	7.3653840958	1.0277041518	1.0286095687
C14	6.7591147293	2.2721083839	0.8327415072
N15	5.5633888480	2.4025841487	0.1985557060
C16	4.9411399983	1.2859179639	-0.2680249461
C17	5.4904999980	0.0070000077	-0.1117999997
H18	7.1703377842	-1.1039120934	0.6876697961
H19	8.3191420642	0.9646504370	1.5442156133
H20	7.2217862161	3.1866191166	1.1892272691
H21	3.9910502594	1.4349373581	-0.7706485526
H22	4.9621787715	-0.8590174824	-0.4988436561
O23	5.7688427447	7.0239189552	1.5336409729
O24	2.0424751652	5.0900147143	1.1823401070
O25	3.5690938973	6.4784928834	3.3244503811
O26	4.5330693686	4.8756097276	-0.1830569337
Zn27	3.8251871192	6.2362932134	1.2418348259
H28	3.2709631289	5.7619402072	3.9233922457
H29	3.9636640191	7.2047156775	3.8477791519
H30	6.3165115141	6.7104040569	2.2820147148
H31	6.3472904140	7.2535514108	0.7784881875
H32	4.9384509487	3.9143190508	-0.0061153453
H33	4.7147755208	5.1543575721	-1.1025044218
H34	1.9444115241	4.3096530579	0.5993898711
H35	1.2465179984	5.2030774528	1.7409996238

$\Delta r=2.0 \text{ \AA}$

Atom	X	Y	Z
H1	1.2515307363	7.1274837800	1.1023664820
C2	2.7403002205	10.5717991529	0.3083999663
C3	3.4995287532	9.4026751579	0.2805848225
N4	2.9618707424	8.1841455150	0.5658654110
C5	1.6382776752	8.1127981503	0.8835076177
C6	0.8217939768	9.2444408814	0.9304575922
C7	1.3790004089	10.4981308782	0.6384264262
H8	3.2118032781	11.5218822397	0.0744166161
H9	4.5468614758	9.4145089476	0.0147868690
H10	-0.2278518817	9.1389751862	1.1879900002
H11	0.7670141142	11.3950768554	0.6653901113
C12	4.3966344697	-0.5657987491	0.5849479542
C13	3.4970979555	0.3570365939	1.1410589987
C14	3.7457814691	1.7227441421	0.9769983233
N15	4.8297733664	2.1795271535	0.2988175805
C16	5.7024645568	1.2897069976	-0.2395436993
C17	5.5156997795	-0.0896991529	-0.1156999663
H18	4.2297634227	-1.6336452396	0.6952733215
H19	2.6200523343	0.0277791424	1.6903561080
H20	3.0830527865	2.4760445285	1.3859444393
H21	6.5543872904	1.7009183394	-0.7716281530
H22	6.2328859784	-0.7745232563	-0.5585869683
O23	5.6946684068	7.4622446740	-0.7097078074
O24	2.6193392046	5.1421714557	1.1910031125
O25	5.1399548386	6.7100816256	2.3080113746
O26	5.2610285788	4.7311407874	-0.0733370788
Zn27	4.1974561023	6.3966941948	0.4477521835

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H28	5.8272876651	6.1165143360	2.6772166083
H29	5.0006372440	7.4712923130	2.9064318181
H30	6.5979806249	7.6831230166	-0.4038717001
H31	5.6086587171	7.6639826346	-1.6633810369
H32	5.0748571951	3.7045936265	0.1034825751
H33	6.0292660304	4.8774484364	-0.6602838054
H34	1.9369158303	4.7404201272	0.6154112618
H35	2.3640572861	5.0488384230	2.1315091132

$\Delta r=2.12 \text{ \AA}$			
Atom	X	Y	Z
H1	0.8309279545	7.3447662629	1.1415513226
C2	2.7403002162	10.5717991696	0.3083999670
C3	3.2105077475	9.3037462502	-0.0432487462
N4	2.5288073981	8.1624602916	0.2601011630
C5	1.3436592751	8.2718300713	0.9240779456
C6	0.8135325064	9.5076845074	1.3034569232
C7	1.5208808931	10.6795078110	0.9932859269
H8	3.3208099334	11.4514984652	0.0459138432
H9	4.1379428935	9.1756504998	-0.5828613105
H10	-0.1358072839	9.5458966744	1.8294148512
H11	1.1297395342	11.6523852865	1.2766389678
C12	4.3515879232	-0.8928554508	0.1469445008
C13	3.1363978988	-0.1887603502	0.1184006178
C14	3.1530007950	1.1781698017	-0.1771521189
N15	4.3076314166	1.8440979448	-0.4382555690
C16	5.4847988026	1.1636592112	-0.4089751752
C17	5.5458997838	-0.2057991696	-0.1202999670
H18	4.3665672848	-1.9553542860	0.3734673011
H19	2.1935495087	-0.6881784635	0.3207165435
H20	2.2409104074	1.7651253838	-0.2070843438
H21	6.3817430647	1.7363205811	-0.6211045881
H22	6.5049598456	-0.7148904716	-0.1065187131
O23	4.6424280823	7.1277065142	-1.7330917114
O24	1.6868806944	5.1384501042	0.5236957349
O25	4.5877962082	6.1784730366	1.3762529368
O26	4.1979050682	4.4300424170	-1.0561810307
Zn27	3.3249511631	6.1753487008	-0.3190119374
H28	5.1765734193	5.4343169902	1.6224724815
H29	4.6777706561	6.9062058805	2.0237480076
H30	5.6196081609	7.1439125083	-1.6772544511
H31	4.3501610701	7.4998442668	-2.5896875418
H32	4.2229707188	3.4101396821	-0.7755291056
H33	4.6592852133	4.5627978943	-1.9080976493
H34	0.8653382476	4.9730938033	0.0175794879
H35	1.5751115226	4.8539739122	1.4537343354

$\Delta r=2.2 \text{ \AA}$			
Atom	X	Y	Z
H1	1.2202234054	7.1727035207	1.2468336345
C2	2.7403001379	10.5717994703	0.3083999789
C3	3.3650098756	9.3571103662	0.0105951721
N4	2.8200615840	8.1534082595	0.3483904925
C5	1.6225401013	8.1452762170	1.0001791602
C6	0.9441622349	9.3214768757	1.3296631408
C7	1.5088259375	10.5578109781	0.9791405508
H8	3.2145879553	11.5042654741	0.0168132357
H9	4.3108393614	9.3208034554	-0.5119162376
H10	-0.0077391788	9.2637567256	1.8492946728
H11	1.0012489998	11.4869437489	1.2216562241
C12	4.3114813420	-0.8233450742	0.1966623032
C13	3.1963021793	0.0276951717	0.2510705762
C14	3.3716781152	1.3891876352	-0.0160111079
N15	4.5839873761	1.9156132031	-0.3277820686
C16	5.6653832108	1.0919235393	-0.3800226222

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C17	5.5660998621	-0.2830994703	-0.1233999789
H18	4.2040134324	-1.8852737504	0.3997876384
H19	2.2099115477	-0.3547076426	0.4966316754
H20	2.5427916895	2.0869975872	0.0177386600
H21	6.6150644287	1.5534242941	-0.6313547026
H22	6.4522814326	-0.9085401851	-0.1744472186
O23	5.2092351115	7.2628792882	-1.4380596748
O24	2.1718919476	5.0651801633	0.5001227794
O25	4.9270656088	6.2318523927	1.6282821879
O26	4.7719304692	4.5235010113	-0.8539957313
Zn27	3.8138821023	6.2341464919	-0.1583696816
H28	5.5584226894	5.5213038482	1.8681986201
H29	4.9070191543	6.9161284731	2.3270702436
H30	6.1636819977	7.3903351176	-1.2618566842
H31	4.9941020017	7.5637274251	-2.3440790315
H32	4.6818441845	3.4946846772	-0.6237433329
H33	5.3726862795	4.6695952183	-1.6116279109
H34	1.3826719428	4.9295722399	-0.0630562649
H35	2.0059692712	4.7240778354	1.4026247011

$\Delta r=2.4 \text{ \AA}$			
Atom	X	Y	Z
H1	1.3621644717	7.2045814800	1.5479999164
C2	2.7403000336	10.5717998709	0.3083999949
C3	3.2388144904	9.3381134067	-0.1341549157
N4	2.7548070160	8.1433357060	0.3168595860
C5	1.7387841401	8.1662159765	1.2260721100
C6	1.1963860951	9.3577473757	1.7148229589
C7	1.7023521715	10.5822048666	1.2519377824
H8	3.1602477086	11.4932326014	-0.0839705450
H9	4.0306187707	9.2854116268	-0.8693026794
H10	0.3864637238	9.3210818363	2.4376176082
H11	1.2931372503	11.5212952170	1.6134054293
C12	4.4547564939	-1.1928849602	-0.4591343141
C13	3.3371230034	-0.4948439732	-0.9448067131
C14	3.4112309340	0.8950310034	-1.0860124623
N15	4.5346184542	1.5954036349	-0.7771422630
C16	5.6176250949	0.9157451151	-0.3064316463
C17	5.6164999664	-0.4764998710	-0.1310999949
H18	4.4204233896	-2.2722812427	-0.3395563019
H19	2.4216345401	-1.0157349424	-1.2093927416
H20	2.5693061852	1.4682190778	-1.4591255372
H21	6.4952082542	1.5086780857	-0.0711474185
H22	6.5026550056	-0.9770417810	0.2478133782
O23	4.4370862390	7.0610189689	-2.0907468280
O24	1.9501302753	5.0316273701	0.4264688188
O25	4.9506489635	6.0933155881	1.0666832725
O26	4.4721311516	4.3200925693	-1.1736884971
Zn27	3.4969705691	6.1042115829	-0.4634783553
H28	5.6390479428	5.3964578528	1.1059287522
H29	5.0500042599	6.7120288366	1.8178007949
H30	5.4003245540	7.1670911481	-2.2295563976
H31	3.9442355463	7.4058779997	-2.8625985616
H32	4.4685260608	3.2844554050	-0.9568280023
H33	4.8223333399	4.4462989609	-2.0779528318
H34	1.0847925578	4.9001570945	-0.0120792931
H35	1.9742601976	4.5628991391	1.2855903872

$\Delta r=2.6 \text{ \AA}$			
Atom	X	Y	Z
H1	1.6277837903	7.1357952195	1.6275641911
C2	2.7403000916	10.5717996479	0.3083999860
C3	3.2981552201	9.3646683150	-0.1449021541
N4	2.9028454759	8.1442324986	0.3267661177
C5	1.9245754006	8.1159485126	1.2776793397

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C6	1.3278257618	9.2761016668	1.7776488910
C7	1.7376050409	10.5248030591	1.2877759830
H8	3.0908203425	11.5137525446	-0.1027007655
H9	4.0696810523	9.3560105769	-0.9042062824
H10	0.5528088372	9.1964212514	2.5344310987
H11	1.2844064455	11.4392040800	1.6599616070
C12	4.7122282890	-1.3564101044	-0.9048157985
C13	3.7830257787	-0.6183005298	-1.6555968632
C14	3.8325642722	0.7797310586	-1.6194266835
N15	4.7525434083	1.4596280684	-0.8818266062
C16	5.6543471982	0.7362671199	-0.1549516118
C17	5.6667999083	-0.6698996479	-0.1387999860
H18	4.6925470217	-2.4426107546	-0.9176545317
H19	3.0304541096	-1.1148463405	-2.2615180815
H20	3.1303979775	1.3790761845	-2.1886885210
H21	6.3760226676	1.3060922259	0.4210163710
H22	6.4043330076	-1.1998133342	0.4567886319
O23	4.3278995672	7.0710970577	-2.2219665997
O24	2.3531127026	4.9777768694	0.6395353261
O25	5.3802770565	6.1766390679	0.7525806126
O26	4.5227349170	4.2790412764	-1.3462028799
Zn27	3.6950911405	6.1094563582	-0.4733869505
H28	6.0832484086	5.4940232621	0.7237981305
H29	5.6267563261	6.8990276039	1.3643191600
H30	5.2418075868	7.1137691959	-2.5701848167
H31	3.72241102497	7.5706593260	-2.8063947860
H32	4.6094303515	3.2639558370	-1.0605244803
H33	4.7345757124	4.3598234175	-2.2974771378
H34	1.5112445740	4.6737439997	0.2430481273
H35	2.5665636150	4.4450273248	1.4325894392

$\Delta r=2.8 \text{ \AA}$			
Atom	X	Y	Z
H1	1.8621979338	7.1290187750	1.7834543239
C2	2.7403000427	10.5717998359	0.3083999935
C3	3.3120020226	9.3757657414	-0.1534424427
N4	3.0004359169	8.1549006236	0.3747115810
C5	2.0912578117	8.1112348909	1.3909024855
C6	1.4830138673	9.2606937612	1.9022214121
C7	1.8091995998	10.5116999551	1.3558631634
H8	3.0242430067	11.5149411910	-0.1489866601
H9	4.0279134166	9.3763819957	-0.9651323651
H10	0.7655725848	9.1718755810	2.7127846841
H11	1.3463769175	11.4173944768	1.7374131685
C12	4.9138234396	-1.4611027045	-1.1294622102
C13	4.1404561109	-0.6410966576	-1.9666554152
C14	4.1925825461	0.7468489066	-1.7977817481
N15	4.9677206496	1.3421470605	-0.8500509400
C16	5.7161900678	0.5377673237	-0.0399842847
C17	5.7171999573	-0.8632998359	-0.1464999935
H18	4.8901528289	-2.5415446285	-1.2414841261
H19	3.5062925323	-1.0668862719	-2.7392875833
H20	3.6068114578	1.4082135621	-2.4270683391
H21	6.3243335197	1.0386625421	0.7056131878
H22	6.3318121710	-1.4570669671	0.5237659789
O23	4.2901241067	7.0607042030	-2.2399765011
O24	2.7688897831	4.9755474550	0.9058241754
O25	5.6408589548	6.4584291718	0.6260288045
O26	4.7701442131	4.2971676674	-1.2156399622
Zn27	3.8642484889	6.1481395712	-0.4089849628
H28	6.3698073524	5.8030907784	0.6234923399
H29	5.8858050990	7.2404926809	1.1600502967
H30	5.1737746435	7.2449088751	-2.6188037805
H31	3.5924675259	7.4240009278	-2.8222518268
H32	4.8272979751	3.2804137152	-0.9287400035
H33	5.1795181648	4.3900420632	-2.0989231865
H34	1.9608004803	4.4937737906	0.6349543082
H35	3.0918525106	4.6425714911	1.7679655716

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 $\Delta r=3.0 \text{ \AA}$

Atom	X	Y	Z
H1	2.1367341304	7.2633304183	2.1753354866
C2	2.7403001588	10.5717993901	0.3083999757
C3	3.3017196322	9.3517533973	-0.1020908969
N4	3.0940342884	8.1782643607	0.5676545115
C5	2.3000959695	8.2095971084	1.6768936172
C6	1.7110821440	9.3868650366	2.1454252440
C7	1.9318168430	10.5883368888	1.4545021193
H8	2.9383509762	11.4738035806	-0.2628118329
H9	3.9311762019	9.2922020380	-0.9806647841
H10	1.0882610632	9.3562773372	3.0347988486
H11	1.4819194635	11.5145081679	1.8005703448
C12	4.8852205795	-1.5944295888	-1.1036942201
C13	4.0566710223	-0.7252747623	-1.8296279095
C14	4.1342769181	0.6506442065	-1.5869446220
N15	4.9837980974	1.1885122715	-0.6689347807
C16	5.7848286922	0.3357236356	0.0328862022
C17	5.7675998412	-1.0566993901	-0.1541999757
H18	4.8435445733	-2.6663839175	-1.2753556775
H19	3.3610317501	-1.1040662938	-2.5734353144
H20	3.5102757247	1.3489440344	-2.1337529035
H21	6.4512214138	0.7932680708	0.7569704031
H22	6.4280285249	-1.6901809708	0.4306282387
O23	4.6226406433	6.9267787858	-1.9116698640
O24	2.6477933921	5.0298608317	1.1061327337
O25	5.5824317749	6.3030503362	1.1194921375
O26	4.8379210556	4.2236379015	-0.8520432385
Zn27	3.9209949380	6.1207411896	-0.1134413572
H28	6.2678428294	5.6036882901	1.1622000372
H29	5.7942446803	7.0355674792	1.7322507835
H30	5.5149057986	7.2930574060	-2.0791441459
H31	4.0677092600	7.0157089026	-2.7128243649
H32	4.8678264150	3.1926282811	-0.6162640790
H33	5.3391692673	4.3582439471	-1.6809404171
H34	1.7785072599	4.7130270646	0.7862091135
H35	2.9100248142	4.5424551623	1.9137283329

 $\Delta r=3.2 \text{ \AA}$

Atom	X	Y	Z
H1	2.1815424824	7.2929069498	2.2394788859
C2	2.7403000382	10.5717998533	0.3083999942
C3	3.2809404319	9.3459272632	-0.1038770505
N4	3.0879274289	8.1860617250	0.5897447802
C5	2.3322721932	8.2324464704	1.7241867087
C6	1.7678355541	9.4197332945	2.1977508772
C7	1.9720905141	10.6096432155	1.4818466297
H8	2.9229147588	11.4654780714	-0.2807557754
H9	3.8771818290	9.2692630510	-1.0040096482
H10	1.1756281483	9.4058754095	3.1081671265
H11	1.5393880171	11.5434921483	1.8293706963
C12	5.0175362720	-1.8139712631	-1.1670001309
C13	4.2088209277	-0.9691795314	-1.9432012923
C14	4.2266543094	0.4069260731	-1.6910071918
N15	4.9982144934	0.9691457929	-0.7196964056
C16	5.7795753836	0.1392016133	0.0290938490
C17	5.8179999618	-1.2500998533	-0.1618999942
H18	5.0233364280	-2.8861806008	-1.3417931370
H19	3.5746673360	-1.3660725840	-2.7312381490
H20	3.6131010199	1.0869595906	-2.2722482465
H21	6.3841608862	0.6113525408	0.7963545714
H22	6.4592845455	-1.8649685770	0.4633576873
O23	4.6018595439	6.9434286625	-1.9050101018
O24	2.6431387051	5.0512900710	1.1257544796

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O25	5.5578559133	6.3540980313	1.1214099382
O26	4.8246290265	4.2528691266	-0.8591966724
Zn27	3.8917141531	6.1560341537	-0.1078011593
H28	6.2432510038	5.6581088570	1.2017192098
H29	5.7618312057	7.1063677975	1.7126544889
H30	5.4888308989	7.3264370790	-2.0630737228
H31	4.0630465425	6.9934961191	-2.7203334924
H32	4.8397411203	3.2218160600	-0.6223190676
H33	5.3268011351	4.3745994075	-1.6895574206
H34	1.7780056946	4.7164964593	0.8128611723
H35	2.9166140914	4.5773093232	1.9375911774

$\Delta r=3.3 \text{ \AA}$			
Atom	X	Y	Z
H1	2.0457060626	7.4464885803	2.4369396828
C2	2.7403000351	10.5717998651	0.3083999946
C3	3.2871054363	9.3178363462	0.0116640227
N4	3.0460301315	8.2126787747	0.7762203619
C5	2.2369962750	8.3450476017	1.8656603657
C6	1.6684413398	9.5684082976	2.2282604882
C7	1.9201461571	10.7016013089	1.4393749871
H8	2.9600987327	11.4192421546	-0.3339492252
H9	3.9296182330	9.1721552981	-0.8468489138
H10	1.0357716872	9.6246700351	3.1093216890
H11	1.4844021479	11.6623251045	1.6982666162
C12	4.8039633327	-1.9751796205	-0.8687806755
C13	3.7328248897	-1.1957101434	-1.3324932736
C14	3.7392470268	0.1803028667	-1.0786855537
N15	4.7392381096	0.8010591419	-0.3944527954
C16	5.7738217441	0.0353155324	0.0514140498
C17	5.8431999649	-1.3467998651	-0.1656999946
H18	4.8276913748	-3.0459444074	-1.0507388931
H19	2.9073947244	-1.6415609064	-1.8808592766
H20	2.9277442308	0.8127336011	-1.4222149137
H21	6.5589684379	0.5522954578	0.5925803951
H22	6.6913649509	-1.9120573609	0.2109047180
O23	4.9972729458	6.9267989326	-1.3413095733
O24	2.2766208737	5.1884125801	1.2059990734
O25	5.2101559191	6.1998438592	1.8227280996
O26	4.7306591775	4.2747523407	-0.4316412464
Zn27	3.8395540785	6.1758497009	0.2516598578
H28	5.8049901403	5.4487782256	2.0293918684
H29	5.3384813796	6.9211230249	2.4711532157
H30	5.9039671806	7.2889798490	-1.2705510520
H31	4.6813135720	6.9894834205	-2.2653645712
H32	4.6922646006	3.2422269091	-0.2037504956
H33	5.3201738174	4.3904489747	-1.2034356933
H34	1.4016076157	5.0741208057	0.7821068127
H35	2.3590729363	4.5910474242	1.9772668724

$\Delta r=3.4 \text{ \AA}$			
Atom	X	Y	Z
H1	2.1309494049	7.4292195479	2.4363215868
C2	2.7403000333	10.5717998721	0.3083999949
C3	3.3798384599	9.3510820548	0.0552982823
N4	3.1679672211	8.2393826556	0.8197160475
C5	2.2968933466	8.3324722806	1.8645976787
C6	1.6351182065	9.5209325922	2.1822428357
C7	1.8557277197	10.6597810291	1.3937512146
H8	2.9391350913	11.4262522519	-0.3314712994
H9	4.0746139258	9.2389384114	-0.7666122523
H10	0.9558537665	9.5458989206	3.0292383222
H11	1.3481276838	11.5934380022	1.6186347940
C12	4.7808013495	-2.0414433838	-0.8253995386
C13	3.7106829827	-1.2321419621	-1.2344990872

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C14	3.7662238241	0.1413981235	-0.9737848431
N15	4.8149630598	0.7329518703	-0.3381258272
C16	5.8477531803	-0.0617638528	0.0547572401
C17	5.8683999667	-1.4434998721	-0.1694999949
H18	4.7676314537	-3.1112020317	-1.0129951263
H19	2.8491108788	-1.6541519437	-1.7450521142
H20	2.9569988035	0.7975632588	-1.2767405846
H21	6.6714107263	0.4331922847	0.5581126008
H22	6.7186967144	-2.0318769372	0.1643179017
O23	5.3119416634	7.0684480353	-1.1807584334
O24	2.6066457831	5.1708131610	1.3072879501
O25	5.4502656803	6.3931202561	1.9419446724
O26	5.0396266928	4.3750374438	-0.2839542415
Zn27	4.1076866217	6.2595217072	0.3504130846
H28	6.0822038704	5.6829996111	2.1804729170
H29	5.5313136913	7.1404139448	2.5682594438
H30	6.1909193763	7.4819678798	-1.0595489517
H31	5.0480039589	7.1123300637	-2.1221188085
H32	4.9112255292	3.3443925907	-0.0815676975
H33	5.6961175840	4.4686548003	-1.0028452975
H34	1.7453800005	4.9813807982	0.8821793385
H35	2.7133279933	4.6216544589	2.1108054210

$\Delta r=3.5 \text{ \AA}$			
Atom	X	Y	Z
H1	1.7986009109	7.4345757165	2.3218767051
C2	2.7403003214	10.5717987654	0.3083999509
C3	3.0863513468	9.2783230831	-0.1006336070
N4	2.7575734920	8.1682183983	0.6221098907
C5	2.0617410132	8.3347705089	1.7822045931
C6	1.6889236007	9.5957144043	2.2538393748
C7	2.0312840129	10.7344090633	1.5081793912
H8	3.0236088746	11.4232348690	-0.3029901230
H9	3.6359541760	9.1066697880	-1.0168308147
H10	1.1381681832	9.6776452922	3.1863993619
H11	1.7498922766	11.7251255271	1.8532199808
C12	5.0907147239	-2.5848396382	-0.6565735729
C13	3.8317048930	-2.2769245058	-1.1934877824
C14	3.4238425437	-0.9384898764	-1.2267717738
N15	4.1972328644	0.0782782316	-0.7615492870
C16	5.4137622756	-0.2302804768	-0.2431860417
C17	5.8935996786	-1.5401987654	-0.1732999509
H18	5.4378730906	-3.6131778516	-0.6152853370
H19	3.1767854876	-3.0545427218	-1.5777816318
H20	2.4567771013	-0.6613526468	-1.6330011537
H21	6.0104558845	0.5984568198	0.1204725845
H22	6.8752476964	-1.7359740741	0.2509101529
O23	4.5201034401	6.7618580210	-1.5902847387
O24	1.5969785654	5.2234751251	0.8105536000
O25	4.6126581048	5.8373562196	1.5295436098
O26	4.0309052889	4.0618653541	-0.7381510094
Zn27	3.2739311940	6.0798713667	-0.0476979252
H28	5.0851939884	4.9956749515	1.6991079915
H29	4.8249669989	6.4940204793	2.2231661773
H30	5.4015313583	7.1723408456	-1.4762305863
H31	4.2297789262	6.8364900579	-2.5218199637
H32	3.7678341503	3.0407311687	-0.6505743179
H33	4.7157478640	4.1390249702	-1.4320403662
H34	0.6877972043	5.3785877700	0.4825640157
H35	1.5866556044	4.5704210715	1.5398832917

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[Cu(Py)₂(H₂O)₄]²⁺

Δr=0.0 Å			
Atom	X	Y	Z
H1	1.1562624626	7.1345260727	-0.7743712986
C2	2.7973653190	10.3797825180	0.4635830002
C3	3.4655631439	9.1530646189	0.4560111935
N4	2.8675320232	8.0143674637	0.0088253170
C5	1.5851719499	8.0716037409	-0.4452909860
C6	0.8657249773	9.2688364356	-0.4672088567
C7	1.4770250703	10.4438320842	-0.0055952396
H8	3.3090785823	11.2653018959	0.8292627706
H9	4.4896321038	9.0532013232	0.7898003794
H10	-0.1547995590	9.2727640606	-0.8389771584
H11	0.9375334203	11.3871277969	-0.0113432216
C12	6.3048104888	2.0026974463	0.0461437322
C13	6.9957663131	3.2185815055	-0.0632628622
C14	6.2745371639	4.4150940899	-0.0694454606
N15	4.9166777460	4.4333275532	0.0236186158
C16	4.2416125537	3.2556962684	0.1260810253
C17	4.9056969363	2.0267137696	0.1431297789
H18	6.8433954820	1.0589168617	0.0550989113
H19	8.0787001288	3.2468358760	-0.1412668649
H20	6.7594680572	5.3800351596	-0.1332665778
H21	3.1634915054	3.3285594996	0.1740014740
H22	4.3309131211	1.1090731736	0.2281247712
O23	6.0200623866	7.4483374968	0.3667036769
O24	1.7850596447	5.0020995913	-0.4177361148
O25	3.6356205066	6.0828645111	2.0373690434
O26	4.1528814193	6.3640808583	-2.0094935411
Cu27	3.8941342860	6.2237923524	0.0141202083
H28	4.0342436129	5.3893448453	2.6006547776
H29	3.1285624857	6.7227243791	2.5766120797
H30	6.5353065138	7.4980028494	1.1995543846
H31	6.4866919091	7.9761823119	-0.3153901490
H32	4.5605470707	5.6703615865	-2.5654635593
H33	3.8685126494	7.1261367092	-2.5529116417
H34	1.5693632181	4.6156897012	-1.2926459414
H35	1.0455499023	4.8091593722	0.1967206373

Δr=0.4 Å			
Atom	X	Y	Z
H1	1.0719386269	6.9655344872	0.0161263070
C2	2.7974000211	10.3797999164	0.4635999968
C3	3.4980320086	9.1584095932	0.4832395287
N4	2.8748729543	7.9524056596	0.3238204761
C5	1.5239839541	7.9410499157	0.1417192777
C6	0.7676661855	9.1160725208	0.1135296709
C7	1.4080169039	10.3548127566	0.2754022062
H8	3.3404313530	11.3111087024	0.5936995925
H9	4.5699840500	9.1177900853	0.6273586418
H10	-0.3068435561	9.0551183563	-0.0343109507
H11	0.8356065187	11.2784500166	0.2551138979
C12	6.3902607309	1.6604095165	0.3358807342
C13	7.0277753653	2.8961614729	0.5312565638
C14	6.2717724598	4.0720292044	0.5158016867
N15	4.9235565471	4.0642708112	0.3160341671
C16	4.3037698538	2.8611370533	0.1242437759
C17	5.0034999789	1.6391000836	0.1283000032
H18	6.9625652629	0.7365215524	0.3454976652
H19	8.1001840040	2.9544387674	0.6946841320
H20	6.7228687505	5.0454255238	0.6606386223
H21	3.2339133684	2.9058819905	-0.0333331392
H22	4.4626090287	0.7105600950	-0.0282179037
O23	5.9432135451	7.1744113903	0.6812576577
O24	1.8619532945	4.8407442142	-0.0948294800
O25	3.6468633767	5.8696668061	2.3183525263

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O26	4.1560463886	6.1514667051	-1.6691515779
Cu27	3.8993910196	6.0096541299	0.3247738714
H28	3.9096414079	5.0935949859	2.8529191517
H29	3.3414726724	6.6043193782	2.8869991311
H30	6.2957014867	7.4436035487	1.5551606274
H31	6.5147789438	7.5605232284	-0.0150535148
H32	4.4888220299	5.4281498768	-2.2367819156
H33	3.9498695229	6.9492198802	-2.1960408082
H34	1.5548798487	4.6241645406	-0.9998285926
H35	1.2373554679	4.4428267584	0.5475844239

$\Delta r=0.7 \text{ \AA}$			
Atom	X	Y	Z
H1	1.1192688955	6.9492091424	-0.0730410973
C2	2.7974000099	10.3797999606	0.4635999985
C3	3.5101216440	9.1601953186	0.4748881008
N4	2.9091017686	7.9458069250	0.2833959771
C5	1.5621715958	7.9264676849	0.0737617207
C6	0.7923594956	9.0937306404	0.0494452684
C7	1.4127112296	10.3384781537	0.2459799913
H8	3.3277839352	11.3140036094	0.6214565875
H9	4.5804189657	9.1311340999	0.6386659421
H10	-0.2781830737	9.0225964311	-0.1217183603
H11	0.8276701609	11.2543099571	0.2296436842
C12	6.4679328451	1.3918778631	0.2913746839
C13	7.0947790120	2.6384404598	0.4508467571
C14	6.3253675874	3.8061411637	0.4338707820
N15	4.9729690115	3.7849949766	0.2659234405
C16	4.3646448679	2.5687932561	0.1096713366
C17	5.0768999901	1.3485000394	0.1172000015
H18	7.0529281839	0.4759659989	0.3031174499
H19	8.1701476605	2.7104951915	0.5881172180
H20	6.7689428541	4.7866255199	0.5561405515
H21	3.2899754665	2.5969503172	-0.0224453534
H22	4.5418934001	0.4123435030	-0.0106400801
O23	5.9730997769	6.9808886760	0.6342548914
O24	1.9183551039	4.7391890728	-0.0940676225
O25	3.6333076749	5.7095899842	2.2310756040
O26	4.2349459938	6.0192144325	-1.6777200385
Cu27	3.9358001065	5.8599186991	0.2764721529
H28	3.8427433584	4.9139698316	2.7596898660
H29	3.3544042944	6.4541791762	2.8004298661
H30	6.3450616840	7.2397980072	1.5028112312
H31	6.5231697502	7.3736403792	-0.0746569187
H32	4.6124926244	5.3120528906	-2.2372701485
H33	4.0201779270	6.8157084925	-2.2031355729
H34	1.5596587354	4.4613763765	-0.9624271747
H35	1.3456956901	4.3796894370	0.6145556774

$\Delta r=1.0 \text{ \AA}$			
Atom	X	Y	Z
H1	0.9975054992	7.0598805166	-0.2366586222
C2	2.7974003028	10.3797988005	0.4635999540
C3	3.4460681698	9.1375487340	0.4979673736
N4	2.8045114699	7.9625163687	0.2470900709
C5	1.4763977525	8.0126329417	-0.0452652045
C6	0.7583607118	9.2122076478	-0.0983232999
C7	1.4279735273	10.4183178661	0.1596542970
H8	3.3559884182	11.2882979010	0.6710172350
H9	4.5023072027	9.0627706555	0.7284062906
H10	-0.3016140400	9.1975612751	-0.3369408456
H11	0.8955426229	11.3651310051	0.1251959720
C12	6.5473883232	1.0444711982	0.2368135147
C13	7.2260142726	2.2663274999	0.3622819575
C14	6.4893920216	3.4558260884	0.3531100691

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N15	5.1346402161	3.4822279346	0.2287375632
C16	4.4843968722	2.2918283784	0.1071304815
C17	5.1502996972	1.0578011995	0.1061000460
H18	7.0936767937	0.1049293887	0.2409467116
H19	8.3071532552	2.3013296703	0.4658956976
H20	6.9752847969	4.4193064993	0.4470679319
H21	3.4060238588	2.3471686140	0.0097324585
H22	4.5837785959	0.1362012355	0.0058977453
O23	5.7238446694	6.6444844887	0.5464423740
O24	2.2080699930	4.8075872506	-0.0426179310
O25	3.7136698493	5.5787564139	2.2569767766
O26	4.2233950004	5.8833452989	-1.7505006967
Cu27	3.9611793969	5.7362555687	0.2544036731
H28	4.0452953628	4.8325492758	2.7965599407
H29	3.3360048030	6.2810737682	2.8242427947
H30	6.1015006499	6.8429592324	1.4262898555
H31	6.2562652992	7.0507809545	-0.1657554598
H32	4.6619028957	5.2049538616	-2.3030124362
H33	3.9216974650	6.6394866060	-2.2932059417
H34	1.8888205980	4.5042886106	-0.9156659090
H35	1.6312056847	4.4824794300	0.6769004909

$\Delta r=1.2 \text{ \AA}$

Atom	X	Y	Z
H1	1.0190942041	7.0204057266	-0.1001465643
C2	2.7974000196	10.3797999225	0.4635999970
C3	3.4634472403	9.1449769377	0.5051203678
N4	2.8310540217	7.9544005168	0.3038185011
C5	1.4933672422	7.9824607876	0.0538070367
C6	0.7579954825	9.1715861411	-0.0042978597
C7	1.4186074441	10.3925305072	0.2034667202
H8	3.3502049964	11.2999038998	0.6311654669
H9	4.5281109348	9.0895929458	0.7026092676
H10	-0.3086857787	9.1373522641	-0.2087160037
H11	0.8719423706	11.3309881925	0.1637157132
C12	6.5936416398	0.8501711315	0.2551507731
C13	7.2687318790	2.0703729149	0.4155703348
C14	6.5314602252	3.2598666803	0.4142811597
N15	5.1790190587	3.2891025877	0.2655942252
C16	4.5327881329	2.0992869631	0.1104217284
C17	5.1991999804	0.86400000775	0.0987000030
H18	7.1410506473	-0.0887332089	0.2525289145
H19	8.3477917431	2.1036977395	0.5399524214
H20	7.0154123517	4.2216938580	0.5349769851
H21	3.4561452993	2.1553902440	-0.0049893157
H22	4.6350892086	-0.0556548716	-0.0286215967
O23	5.7692734762	6.5259474090	0.6262504248
O24	2.2552091462	4.7307223862	0.0132832162
O25	3.7440644835	5.4752910064	2.3116211643
O26	4.2801680927	5.7936841268	-1.6691436796
Cu27	4.0094128962	5.6344083654	0.3215891838
H28	4.0589571587	4.7212339550	2.8499240121
H29	3.3660701190	6.1788544949	2.8768918500
H30	6.1420766169	6.7243817146	1.5082706806
H31	6.3155400688	6.9202746167	-0.0824247435
H32	4.6995473749	5.1089657420	-2.2283823808
H33	3.9973336227	6.5624387652	-2.2042929836
H34	1.9216395825	4.4653957491	-0.8667834772
H35	1.6831613365	4.3831191541	0.7261867948

$\Delta r=1.4 \text{ \AA}$

Atom	X	Y	Z
H1	1.0627701230	7.0088108279	-0.1625518972
C2	2.7974000012	10.3797999954	0.4635999998
C3	3.4808385356	9.1527353459	0.4781048106

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N4	2.8659429715	7.9565824993	0.2551313125
C5	1.5271893756	7.9723475279	0.0100609100
C6	0.7744570406	9.1519132344	-0.0217114730
C7	1.4177541814	10.3778263244	0.2084395867
H8	3.3378308297	11.3041092094	0.6476659528
H9	4.5471944799	9.1091614485	0.6705878515
H10	-0.2924131803	9.1065803765	-0.2231757423
H11	0.8573203928	11.3087885281	0.1894692237
C12	6.6412242650	0.6575034900	0.2577905278
C13	7.3167829185	1.8796096352	0.4012646512
C14	6.5814733621	3.0701654928	0.3756683441
N15	5.2301385978	3.1001601216	0.2149946558
C16	4.5842938215	1.9077236857	0.0746364796
C17	5.2480999988	0.6702000046	0.0913000002
H18	7.1875859067	-0.2817961528	0.2749695133
H19	8.3951063968	1.9136788609	0.5315611368
H20	7.0701850429	4.0316366072	0.4826444343
H21	3.5087356141	1.9627398530	-0.0531576488
H22	4.6831389814	-0.2505338788	-0.0236841426
O23	5.8246448602	6.4138077598	0.5293707535
O24	2.3029873670	4.6754682726	-0.0712432706
O25	3.8015746716	5.3789540249	2.2174423742
O26	4.3228355325	5.7101076872	-1.7471428746
Cu27	4.0610091105	5.5476374749	0.2352657583
H28	4.1135765788	4.6200574462	2.7509743647
H29	3.4159544720	6.0760047611	2.7855897203
H30	6.1947537607	6.6294492630	1.4085460427
H31	6.3744711072	6.7883072311	-0.1873951789
H32	4.7143068216	5.0170581667	-2.3160204412
H33	4.0569924578	6.4915833245	-2.2733763449
H34	1.9658098529	4.4195863934	-0.9529352441
H35	1.7263609516	4.3340043125	0.6409711272

Δr=1.6 Å			
Atom	X	Y	Z
H1	1.0770472611	6.9930867431	-0.1166175443
C2	2.7974000032	10.3797999872	0.4635999995
C3	3.4857771739	9.1577382233	0.4840994813
N4	2.8762631832	7.9560913997	0.2784056825
C5	1.5350830380	7.9613843724	0.0467317663
C6	0.7745272756	9.1359054437	0.0139706158
C7	1.4145361220	10.3674969982	0.2249604487
H8	3.3348019886	11.3087243542	0.6320497742
H9	4.5532907135	9.1245041543	0.6692772592
H10	-0.2941846702	9.0825641306	-0.1752151940
H11	0.8489568581	11.2952873221	0.2041613072
C12	6.6898174002	0.4647605586	0.2523796535
C13	7.3615962132	1.6862203376	0.4144891627
C14	6.6235179370	2.8747607507	0.4037535329
N15	5.2718490992	2.9047195365	0.2423503775
C16	4.6288298279	1.7117187752	0.0853287333
C17	5.2969999968	0.4764000128	0.0839000005
H18	7.2385298996	-0.4731711579	0.2566883471
H19	8.4395257515	1.7221376231	0.5473288829
H20	7.1102881425	3.8339633018	0.5268918277
H21	3.5530711196	1.7648455299	-0.0412651356
H22	4.7342882799	-0.4437431132	-0.0453048014
O23	5.8438960243	6.2095827251	0.5783935169
O24	2.3122838853	4.5452373270	-0.0246318371
O25	3.8114695637	5.2201513879	2.2584476852
O26	4.3518737353	5.5337938097	-1.7027255922
Cu27	4.0936714061	5.3443143851	0.2759026031
H28	4.1102355499	4.4682971224	2.8093398607
H29	3.4303676434	5.9352479660	2.8085435542
H30	6.2178853716	6.4110786924	1.4595881175
H31	6.4165043862	6.5464650315	-0.1387660660
H32	4.7681815594	4.8558153992	-2.2719374694
H33	4.0548688349	6.3055336640	-2.2274053723

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H34	1.9564161641	4.3027727995	-0.9029219678
H35	1.7332567394	4.2253407128	0.6957211088

$\Delta r=1.8 \text{ \AA}$			
Atom	X	Y	Z
H1	1.1617596838	6.9658969223	-0.1978208580
C2	2.7974000013	10.3797999950	0.4635999998
C3	3.5161980386	9.1730200071	0.4659280558
N4	2.9383001748	7.9605120977	0.2291816267
C5	1.5998708400	7.9406409311	-0.0167451892
C6	0.8126223601	9.0979434047	-0.0395662402
C7	1.4189426871	10.3398046557	0.2049272828
H8	3.3097361076	11.3175539543	0.6592604188
H9	4.5830830775	9.1605264456	0.6614402943
H10	-0.2521180306	9.0231325218	-0.2438235610
H11	0.8313470276	11.2539616694	0.1948017986
C12	6.7387051077	0.2446586521	0.2411863774
C13	7.4371543716	1.4548004865	0.3755406817
C14	6.7229613108	2.6580711338	0.3425381884
N15	5.3714655868	2.7134771591	0.1864064468
C16	4.7054468254	1.5311229497	0.0547412247
C17	5.3458999987	0.2826000050	0.0765000002
H18	7.2671408129	-0.7046552616	0.2635944178
H19	8.5160881108	1.4705353454	0.5041101062
H20	7.2292788329	3.6102571289	0.4443147782
H21	3.6308417314	1.6023619367	-0.0697575296
H22	4.7634000549	-0.6278456396	-0.0321772955
O23	5.9606305148	6.1776599337	0.4502467775
O24	2.4356080279	4.5187614124	-0.1353062864
O25	3.9334480295	5.2102585092	2.1361471897
O26	4.4698145453	5.4703460555	-1.8199834340
Cu27	4.2097230203	5.3226615976	0.1579592203
H28	4.2312160210	4.4614628889	2.6925817803
H29	3.5539484511	5.9290406099	2.6805556800
H30	6.3330959078	6.3914832704	1.3290957158
H31	6.5375082516	6.4976527047	-0.2719236214
H32	4.8709530668	4.7727111580	-2.3780216490
H33	4.1868396653	6.2372287207	-2.3581925486
H34	2.0811023913	4.2812064966	-1.0157349281
H35	1.8631622488	4.1865801273	0.5850039067

$\Delta r=1.9 \text{ \AA}$			
Atom	X	Y	Z
H1	1.3689486257	6.8363401660	0.1944214395
C2	2.7974000679	10.3797997311	0.4635999896
C3	3.5714492036	9.2309475957	0.6514022899
N4	3.0627206791	7.9731688250	0.5554777902
C5	1.7414135783	7.8501497871	0.2669351029
C6	0.8952657575	8.9474255372	0.0680818386
C7	1.4334843394	10.2393179775	0.1664683883
H8	3.2545792770	11.3619495549	0.5511111471
H9	4.6280864996	9.3036540670	0.8844255585
H10	-0.1551089989	8.7890751237	-0.1628672873
H11	0.8083784720	11.1151262084	0.0154518346
C12	6.7574442711	0.0524949025	0.2381814372
C13	7.5172462330	1.1932076768	0.5412019088
C14	6.8716792129	2.4280573014	0.6616415874
N15	5.5270966200	2.5698194230	0.5000636828
C16	4.7952196512	1.4557032532	0.2157128687
C17	5.3702999321	0.1857002689	0.0728000103
H18	7.2355767211	-0.9177849284	0.1357699757
H19	8.5931917650	1.1315987430	0.6792856062
H20	7.4241740302	3.3320622587	0.8870395219
H21	3.7273843073	1.6024353002	0.1021100442
H22	4.7424435768	-0.6695455564	-0.1599286062

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O23	6.2781403109	5.7480236686	0.9163851696
O24	2.7066093026	4.1573688066	0.4811915417
O25	4.3032871637	4.7696462487	2.6639174131
O26	4.6842215611	5.1048211206	-1.3157506026
Cu27	4.5699976879	4.7924271146	0.6688839815
H28	4.5438768054	4.0148178656	3.2394293993
H29	3.9193818533	5.5018783611	3.1881187971
H30	6.5811344533	6.0852291188	1.7837060891
H31	6.7806248710	6.1452620212	0.1776196674
H32	4.9382852066	4.4093286161	-1.9565977408
H33	4.3788285226	5.9127964354	-1.7760898562
H34	2.3130700767	3.8129811491	-0.3453290862
H35	2.1763711226	3.8964735318	1.2623043860

$\Delta r=2.0 \text{ \AA}$			
Atom	X	Y	Z
H1	1.0790446245	7.0289746637	-0.2918617442
C2	2.7974000652	10.3797997419	0.4635999901
C3	3.4322324882	9.1447142391	0.6193562342
N4	2.8205033017	7.9592031050	0.3541241096
C5	1.5348176950	7.9919856735	-0.0847654538
C6	0.8251970617	9.1852517433	-0.2661738893
C7	1.4674342431	10.4020390585	0.0132921382
H8	3.3315645563	11.2989391112	0.6896061978
H9	4.4586101541	9.0892471248	0.9651403966
H10	-0.2032156667	9.1580209570	-0.6177889914
H11	0.9449749165	11.3456924421	-0.1172241623
C12	6.7801992350	0.1474621815	0.2805362151
C13	7.3969404952	1.4038620516	0.3770424314
C14	6.6120330004	2.5548219524	0.2618019848
N15	5.2657840168	2.5055507621	0.0602409802
C16	4.6726611076	1.2837782713	-0.0347577235
C17	5.3946999348	0.0888002581	0.0691000099
H18	7.3647383992	-0.7643827226	0.3663677670
H19	8.4671672438	1.4958199865	0.5393715293
H20	7.0480313325	3.5432296190	0.3284902991
H21	3.6006646199	1.2817677301	-0.1954778432
H22	4.8766007186	-0.8625207813	-0.0125436718
O23	5.7591524180	5.6501034070	0.0994446468
O24	2.2288266340	3.9973914807	-0.3238450079
O25	3.7777289435	4.7069544689	1.8846683633
O26	4.2811564905	4.6797879740	-2.0846658312
Cu27	4.1134471438	4.5459702593	-0.0842674673
H28	4.0237651903	4.0279236060	2.5458755188
H29	3.3204088252	5.4646968910	2.3029582403
H30	6.0523962196	6.0489341748	0.9436390684
H31	6.2134097412	6.0547791674	-0.6660534546
H32	4.5637976303	3.9225872523	-2.6374966760
H33	3.9831314629	5.4263315807	-2.6429680668
H34	1.8262576451	3.7978130787	-1.1926034556
H35	1.6352517588	3.7454449919	0.4134445854

$\Delta r=2.1 \text{ \AA}$			
Atom	X	Y	Z
H1	6.3239864495	10.7569312478	1.9291207796
C2	2.7974007497	10.3797970293	0.4635998861
C3	3.6526452464	9.2942324320	0.6592251202
N4	4.9018984293	9.4304663905	1.1781501662
C5	5.3245326817	10.6791098675	1.5141450090
C6	4.5287142346	11.8171877933	1.3437707673
C7	3.2403452827	11.6661368612	0.8095385793
H8	1.8064052616	10.2192844011	0.0469464909
H9	3.3417012156	8.2890702492	0.3965550174
H10	4.9124894453	12.7943979975	1.6245215784
H11	2.5969142484	12.5291884213	0.6663994386

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C12	4.2115993501	0.1479109442	-0.6319097931
C13	3.6501982847	1.4290108224	-0.7505405203
C14	4.3058444811	2.5168675041	-0.1708274033
N15	5.4766062120	2.3568165329	0.5066997563
C16	6.0286652839	1.1186084949	0.6256515759
C17	5.4190992503	-0.0080970293	0.0654001139
H18	3.7159182632	-0.7115818284	-1.0741859513
H19	2.7174717111	1.5883611264	-1.2824839726
H20	3.9026656573	3.5212812562	-0.2367845055
H21	6.9536208863	1.0514350807	1.1830140186
H22	5.8853164374	-0.9817102226	0.1800197692
O23	4.9286719063	4.0157059524	2.7556339617
O24	7.5353770466	4.2513948275	-0.2419576239
O25	6.7237145111	5.9464261086	1.8649751400
O26	7.9034232668	2.9360273134	2.5062588478
Cu27	6.3503503124	3.9973392860	1.3512736269
H28	7.4076692537	6.1815792749	2.5250140317
H29	6.2602386005	6.7491963647	1.5505264719
H30	4.7546668883	4.8099900401	3.3002403626
H31	4.2326365433	3.3387553598	2.8715369320
H32	7.7565302427	2.4340094626	3.3340287174
H33	8.7955668302	2.7329862023	2.1587410504
H34	8.1659350619	4.9961899112	-0.3071071628
H35	7.6865888472	3.5865209478	-0.9451671068

$\Delta r=2.2 \text{ \AA}$			
Atom	X	Y	Z
H1	5.2097324397	8.1195916759	-1.4965702808
C2	2.7974009693	10.3797961594	0.4635998528
C3	2.7486665873	8.9820590259	0.5323870172
N4	3.6090405318	8.1898709392	-0.1621083927
C5	4.5448527659	8.7815105470	-0.9519244961
C6	4.6563941431	10.1709215641	-1.0679926277
C7	3.7683018357	10.9853348188	-0.3484458091
H8	2.0906580197	10.9746293249	1.0346897444
H9	2.0132389535	8.4749181887	1.1483957630
H10	5.4207972363	10.6013784865	-1.7083928261
H11	3.8306492881	12.0676791571	-0.4194956557
C12	5.4677392327	-0.7161090722	1.3252367166
C13	5.0680717754	0.0214688162	2.4505854978
C14	4.6539070600	1.3455950414	2.2875886094
N15	4.6274777113	1.9345290447	1.0615978039
C16	5.0173551611	1.2251028541	-0.0361527417
C17	5.4435990307	-0.1049961594	0.0617001472
H18	5.7921942534	-1.7476047582	1.4309274259
H19	5.0744837615	-0.4179898916	3.4434744914
H20	4.3401960489	1.9553692884	3.1258214110
H21	4.9820324653	1.7367089525	-0.9915365459
H22	5.7459989760	-0.6391439270	-0.8334903282
O23	3.6091785461	4.5369157274	2.9143880159
O24	2.0951312685	3.2369429745	0.6774939817
O25	3.4760904124	5.4767128790	-0.2813669682
O26	5.8788002630	4.5311414252	0.8428061610
Cu27	3.9828487074	3.8827955405	0.8608388122
H28	3.0554015223	5.2621905108	-1.1391505467
H29	3.5345271402	6.4450199198	-0.1502942029
H30	2.7247624336	4.5015033233	3.3318988115
H31	4.2100564231	5.0677702648	3.4740389920
H32	6.6269500069	4.0922771731	1.2971987055
H33	6.1207599815	5.4219892421	0.5175067112
H34	1.3484288381	3.8574906945	0.5600111613
H35	1.7826150658	2.3438176068	0.9304126526

$\Delta r=2.29 \text{ \AA}$			
Atom	X	Y	Z

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H1	6.0369995299	8.3089056144	0.4219158682
C2	2.7974000681	10.3797997302	0.4635999896
C3	2.8468659052	9.0358912789	0.8627070782
N4	3.9961400578	8.3020111291	0.8469530045
C5	5.1367459026	8.9139622182	0.4242923487
C6	5.1692698173	10.2501320035	0.0119592841
C7	3.9806248970	10.9974021183	0.0305138199
H8	1.8551521852	10.9193299839	0.4947629137
H9	1.9540068042	8.5227244388	1.2040472944
H10	6.1059233554	10.6921013283	-0.3163480194
H11	3.9777063696	12.0367874138	-0.2854340973
C12	5.6223128514	-1.0981692652	1.1184491220
C13	5.5153666002	-0.6314363148	2.4379468050
C14	5.2537187643	0.7213164618	2.6677213869
N15	5.0981655837	1.6044300076	1.6418805873
C16	5.2051142003	1.1543404465	0.3565340432
C17	5.4655999319	-0.1921997301	0.0584000103
H18	5.8236245926	-2.1471793954	0.9207820914
H19	5.6314426615	-1.3027125348	3.2836275780
H20	5.1619323730	1.1154315893	3.6725520797
H21	5.0775686486	1.8868142972	-0.4320380560
H22	5.5409155820	-0.5070764594	-0.9776310660
O23	4.6105426129	3.8730166276	4.2722558557
O24	2.7182510039	3.1994603463	2.1867714016
O25	4.1532357860	5.3874912239	1.0961672873
O26	6.5904219633	4.0763372367	2.1223765901
Cu27	4.6555664098	3.6140661604	2.1407393635
H28	3.7338422426	5.1903256712	0.2335813723
H29	4.1449502586	6.3572484310	1.2292293225
H30	3.7963328638	3.8114532518	4.8117730362
H31	5.3508311519	4.1874778380	4.8283914881
H32	7.2922717805	3.4144514282	2.2903949197
H33	6.9268158558	4.9882768988	2.2368939299
H34	2.0731376860	3.9114408465	2.3692547383
H35	2.3546232581	2.3192166649	2.4156097098

$\Delta r=2.4 \text{ \AA}$			
Atom	X	Y	Z
H1	6.0855622816	8.4486960840	0.9432179327
C2	2.7974001009	10.3797996004	0.4635999847
C3	2.8445703474	8.9856302760	0.6029683585
N4	4.0117785446	8.3030735427	0.7740748121
C5	5.1713306574	9.0165578836	0.8090499562
C6	5.2039649730	10.4089437131	0.6843218362
C7	3.9976935572	11.1044448272	0.5071326144
H8	1.8415946096	10.8772093776	0.3271900703
H9	1.9373383121	8.3911201402	0.5789734520
H10	6.1545981295	10.9330952855	0.7239307933
H11	3.9942899398	12.1859659370	0.4057655082
C12	5.6157349415	-1.0669252954	1.2223900459
C13	5.4755683830	-0.4409239311	2.4712334480
C14	5.2153311736	0.9307063726	2.5253587297
N15	5.0882740021	1.6761139002	1.3934400397
C16	5.2266304546	1.0732927288	0.1758726396
C17	5.4924998991	-0.2987996004	0.0543000153
H18	5.8179136982	-2.1325964730	1.1610736812
H19	5.5673013763	-1.0027659580	3.3958473329
H20	5.1062136338	1.4542065452	3.4673336900
H21	5.1208549978	1.7030497103	-0.6996559458
H22	5.5961972495	-0.7406647034	-0.9317027355
O23	4.8050982948	4.0922385636	3.7035807071
O24	2.7043092483	3.2927853753	1.7964123006
O25	4.0897833663	5.4601725756	0.6193498360
O26	6.5583937499	4.1513458885	1.2044382182
Cu27	4.6409856698	3.7052622978	1.5627701276
H28	3.6657667925	5.2986736164	-0.2484004298
H29	4.0988400679	6.4207385437	0.8075901801
H30	4.0378998934	4.1263404852	4.3101830831

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H31	5.6076615593	4.3849201148	4.1791974954
H32	7.3057600280	3.5365690694	1.3536337543
H33	6.8690686611	5.0564394705	0.9990228965
H34	2.0623952258	4.0133424032	1.9549410008
H35	2.3586844549	2.4322650147	2.1115162220

$\Delta r=2.5 \text{ \AA}$			
Atom	X	Y	Z
H1	1.2655239845	8.2735702765	3.2829974707
C2	2.7974000782	10.3797996901	0.4635999881
C3	3.1169479920	9.0344565297	0.6624334257
N4	2.5761235239	8.2869469551	1.6622110637
C5	1.6836271432	8.8904708003	2.4948152902
C6	1.3094316161	10.2321439976	2.3609017259
C7	1.8760901997	10.9926519243	1.3269632291
H8	3.2593574364	10.9325340794	-0.3502295828
H9	3.8237106354	8.5306499242	0.0124026218
H10	0.5910691986	10.6657029141	3.0512521014
H11	1.6068096437	12.0368027471	1.1966605142
C12	6.6636994903	-0.9195428927	0.6650125706
C13	7.3733348864	-0.1236963049	1.5778562852
C14	6.9222387551	1.1685848152	1.8551828362
N15	5.8073271165	1.6815520283	1.2622149233
C16	5.1147484636	0.9113846259	0.3710042807
C17	5.5168999218	-0.3955996901	0.0506000119
H18	6.9976993218	-1.9278334739	0.4377160343
H19	8.2652074410	-0.4941731501	2.0740960008
H20	7.4484425539	1.8045908732	2.5564180158
H21	4.2340572957	1.3545159668	-0.0806035163
H22	4.9375951389	-0.9742771565	-0.6618109270
O23	6.1140756059	4.8991738049	3.2386973622
O24	4.1142252697	2.7991326674	3.2895187424
O25	3.5906662631	4.9359065010	1.3761598315
O26	6.2543259050	4.4446136255	0.3675360532
Cu27	5.2008286814	3.6021476466	1.8362272041
H28	2.8691864559	4.6413907909	0.7832948052
H29	3.3917503474	5.8298613605	1.7219485479
H30	5.8548457879	4.9642523646	4.1801254814
H31	6.7298440984	5.6250463258	3.0151493943
H32	7.0905549136	4.0848045264	0.0068354831
H33	6.1084767738	5.3709312024	0.0871907800
H34	3.4443211128	3.3187778211	3.7771127856
H35	4.3451308044	1.9762345179	3.7678262308

$\Delta r=2.6 \text{ \AA}$			
Atom	X	Y	Z
H1	0.8795069458	9.0950616651	3.5265760939
C2	2.7974000317	10.3797998742	0.4635999951
C3	2.9345756941	9.0792287255	0.9495686772
N4	2.2551439091	8.6240993929	2.0334992195
C5	1.4102557145	9.4837525283	2.6640995806
C6	1.2167325315	10.8030201724	2.2396195492
C7	1.9228323010	11.2610958429	1.1177118735
H8	3.3634651707	10.6956583541	-0.4093055691
H9	3.6028640080	8.3750920979	0.4681466686
H10	0.5303019144	11.4514679390	2.7776152273
H11	1.7961573980	12.2792092223	0.7617729429
C12	6.8074750073	-0.8866166048	0.5052592563
C13	7.5330460901	-0.0215858459	1.3396254472
C14	6.9803764133	1.2102563753	1.6967665474
N15	5.7501802431	1.5960546579	1.2546941674
C16	5.0411316544	0.7580635314	0.4417020288
C17	5.5413999682	-0.4924998741	0.0469000048
H18	7.2208544325	-1.8492876381	0.2183979297
H19	8.5156220714	-0.2929107453	1.7137377798

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H20	7.5160270210	1.8981690772	2.3390050232
H21	4.0677111522	1.1013194612	0.1118548179
H22	4.9457642992	-1.1278974833	-0.6007299928
O23	5.9727234280	4.7208893609	3.3315162355
O24	4.0496025178	2.5302283054	3.3842684911
O25	3.3414946316	4.7599519258	1.6350322905
O26	5.9581330573	4.3786323372	0.4357621708
Cu27	5.0257167548	3.4472687805	1.9236826819
H28	2.6118778667	4.4780547390	1.0461245217
H29	3.1378902512	5.6311238717	2.0322740769
H30	5.7842766802	4.7162643470	4.2917886476
H31	6.6123063687	5.4306816067	3.1235108877
H32	6.6986514331	4.0022993223	-0.0826942407
H33	5.8482258722	5.3359990413	0.2647178285
H34	3.3490014702	2.9759762380	3.9009607549
H35	4.3882618501	1.7381919584	3.8503570400

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[Zn₂(bPyeth)₂(H₂O)₈]⁴⁺

Δr=0.0 Å			
Atom	X	Y	Z
N1	3.0866973749	1.0453552732	0.0537510003
C2	4.4178751307	0.9968069591	-0.2342043055
C3	5.0912693599	-0.2119962300	-0.4341188696
C4	4.3817496361	-1.4145065830	-0.3637600794
C5	2.9970706738	-1.3747889471	-0.0798906063
C6	2.3958294104	-0.1174508295	0.1370053742
C7	2.2094372914	-2.5657601712	-0.0385245138
C8	1.5266959367	-3.5781138522	-0.0213846466
C9	0.8172120437	-4.8179078395	0.0104398333
N10	-0.5581810814	-4.8083096543	-0.0459547285
C11	-1.2066256773	-6.0016881562	-0.0019693150
C12	-0.5463733238	-7.2303579932	0.0930208424
C13	0.8532804515	-7.2414195762	0.1481718825
C14	1.5409019562	-6.0240963767	0.1067132960
Zn15	-1.9552215382	-2.9681983278	-0.1372628499
O16	-2.7771711190	-3.5941675694	-2.0413129576
Zn17	1.9417842260	3.0145370988	0.1522798367
O18	3.5756962122	4.0292058993	-0.7749737338
N19	-3.0968976821	-1.0186221023	0.0896485435
C20	-2.4250046290	0.1512664104	-0.0256416547
C21	-3.0252273769	1.4004051897	0.2318384613
C22	-4.3885768835	1.4241968173	0.6051876840
C23	-5.0783665634	0.2128420261	0.7169279846
C24	-4.4077230643	-0.9871082837	0.4629238927
C25	-2.2498585412	2.5941874589	0.1235731600
C26	-1.5675713706	3.6021900089	0.0326100185
C27	-0.8601939144	4.8364786644	-0.0949574081
N28	0.5158046551	4.8288851125	-0.0670160777
C29	1.1616165789	6.0150331702	-0.2131625712
C30	0.4981758947	7.2339969214	-0.3832922083
C31	-0.9023305561	7.2429912758	-0.4059194458
C32	-1.5877015689	6.0325325513	-0.2608485011
O33	-0.6047864893	-1.8944679081	-1.4363915226
O34	-3.5919059252	-4.0578276572	0.7048350116
O35	-1.2336411793	-2.5698594356	1.8191260957
O36	1.2323078734	2.4854192412	-1.7816921632
O37	2.7280163778	3.9133145864	1.9625447135
O38	0.6260341532	2.0075335841	1.5216961061
H39	-1.3911017036	0.0849926612	-0.3361410375
H40	-4.8843650209	2.3690584983	0.8080478758
H41	-6.1244844803	0.1936216104	1.0074480468
H42	-4.9013416620	-1.9438854034	0.5683951938
H43	1.0726600268	8.1481380779	-0.4989728478
H44	2.2418163078	5.9686037255	-0.2139893766
H45	-2.6726142930	5.9971152189	-0.2793786539
H46	-1.4512659404	8.1709266549	-0.5386380794
H47	1.3999115517	-8.1767778324	0.2262822594
H48	-1.1226065167	-8.1500696077	0.1284809463
H49	-2.2870664021	-5.9556795514	-0.0204659072
H50	2.6250725017	-5.9920115342	0.1519557561
H51	4.9273641628	1.9472601106	-0.3187534749
H52	6.1543753074	-0.2057018824	-0.6550573081
H53	4.8780271563	-2.3659763692	-0.5311964811
H54	1.3458484005	-0.0388324472	0.3848715621
H55	-3.7013374876	-4.2636321880	1.6558583735
H56	-4.3017779502	-4.4887654427	0.1873581467
H57	3.7168709820	4.1165915672	-1.7396514411
H58	4.2572606098	4.5366270235	-0.2901045179
H59	-0.6764132424	-3.1805401667	2.3423391142
H60	-1.5406554540	-1.8362018282	2.3885047835
H61	3.4777121395	3.5903747595	2.5028859002
H62	2.1633405471	4.4993265364	2.5084772348
H63	0.3195753824	-2.1725469787	-1.5916552257
H64	-0.9788635237	-1.5302385292	-2.2644193492
H65	-0.3003539641	2.2745552999	1.6854253176
H66	1.0045921685	1.6138721011	2.3340888990

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H67	-2.3064298795	-4.2277538285	-2.6220088213
H68	-3.4138056994	-3.0706429238	-2.5696920378
H69	0.6478357283	3.0459432704	-2.3310085753
H70	1.5828873621	1.7504563585	-2.3230395042

$\Delta r=0.4 \text{ \AA}$			
Atom	X	Y	Z
N1	3.0104548346	1.1362687078	-0.0549687264
C2	4.3408983127	1.0755935850	-0.3431592540
C3	5.0072817543	-0.1382065170	-0.5354011389
C4	4.2908398119	-1.3351657595	-0.4500046952
C5	2.9055773296	-1.2897499295	-0.1630134882
C6	2.3112365827	-0.0230686349	0.0393102399
C7	2.1350481714	-2.4957222062	-0.1013193085
C8	1.4963478205	-3.5376304293	-0.0719994597
C9	0.8058754924	-4.7932321688	-0.0281615125
N10	-0.5709245364	-4.7954025386	-0.0732116550
C11	-1.2106259052	-5.9955936187	-0.0087738651
C12	-0.5463999959	-7.2303999434	0.0929999981
C13	0.8555657596	-7.2203473706	0.1301487473
C14	1.5351499075	-5.9960949460	0.0704941382
Zn15	-1.9307027623	-2.8054267550	-0.2194850167
O16	-2.8936742708	-3.4117153740	-2.0554208673
Zn17	1.9496328796	3.2391769261	0.0785747199
O18	3.5849721707	4.2169340271	-0.8343298197
N19	-2.9783552560	-0.7463533964	-0.0467035200
C20	-2.2895327879	0.4154038013	-0.1814951180
C21	-2.8881647988	1.6813451286	0.0080622040
C22	-4.2671925939	1.7244626607	0.3229435214
C23	-4.9732695729	0.5248016254	0.4490633270
C24	-4.3024434560	-0.6885775573	0.2706171341
C25	-2.1233865342	2.8882904542	-0.0896870999
C26	-1.4877298470	3.9310138331	-0.1467696997
C27	-0.8052888832	5.1893649901	-0.2211362570
N28	0.5702921521	5.2044565476	-0.1518488676
C29	1.2004237639	6.4080799408	-0.2435536140
C30	0.5269999959	7.6328999434	-0.3963999981
C31	-0.8735094574	7.6094998429	-0.4595486956
C32	-1.5431416646	6.3814238845	-0.3729148684
O33	-0.5830048832	-1.8586995409	-1.5805725337
O34	-3.5493695824	-3.8186470089	0.6863087244
O35	-1.1367768821	-2.3770837224	1.6935526996
O36	1.1980135454	2.7654615929	-1.8322807308
O37	2.8595349605	3.9561533511	1.8971753194
O38	0.6215347995	2.2842827165	1.4362019564
H39	-1.2463551160	0.3276296677	-0.4547905040
H40	-4.7624938422	2.6798400982	0.4698133689
H41	-6.0313366200	0.5250526842	0.6933870996
H42	-4.8109286984	-1.6360878914	0.3924186859
H43	1.0901987244	8.5585146329	-0.4631309733
H44	2.2816221406	6.3756057431	-0.2053051318
H45	-2.6267755502	6.3339741945	-0.4258766770
H46	-1.4397056023	8.5293018651	-0.5767641205
H47	1.4159831632	-8.1479100819	0.2075307040
H48	-1.1162287592	-8.1530753369	0.1411290818
H49	-2.2921264036	-5.9517497770	-0.0261086366
H50	2.6200226782	-5.9603136311	0.1038994816
H51	4.8584959399	2.0219810420	-0.4313239367
H52	6.0704060069	-0.1405394547	-0.7570614794
H53	4.7833289508	-2.2905111623	-0.6062652943
H54	1.2623642486	0.0676270717	0.2890825228
H55	-3.6618334619	-3.9863204796	1.6439206439
H56	-4.2575313291	-4.2659440772	0.1809644212
H57	3.7356341448	4.3094228447	-1.7966632621
H58	4.2597758024	4.7214817113	-0.3377745324
H59	-0.5820625440	-2.9894778654	2.2171742644
H60	-1.3935453887	-1.6098754848	2.2432400618
H61	3.6152143539	3.5488630445	2.3684508552

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H62	2.3395229282	4.4952838591	2.5286572120
H63	0.3225258444	-2.1836153358	-1.7565403489
H64	-0.9796508687	-1.5389976025	-2.4175558238
H65	-0.2917784605	2.5912659309	1.6027107571
H66	1.0058916676	1.9347606579	2.2667089123
H67	-2.4723072390	-4.0461823504	-2.6717911481
H68	-3.5569072393	-2.8812038871	-2.5443833060
H69	0.6595427806	3.3729824154	-2.3783616525
H70	1.4652235978	1.9902854917	-2.3647766186

Δr=0.6 Å			
Atom	X	Y	Z
N1	2.9893167343	1.1884242033	0.1804436565
C2	4.3203777184	1.1247632407	-0.1046584050
C3	4.9811521649	-0.0902314128	-0.3105746782
C4	4.2576750557	-1.2846980056	-0.2497931916
C5	2.8697217821	-1.2404944790	0.0279597074
C6	2.2845897475	0.0285373233	0.2556174464
C7	2.0995365441	-2.4524153728	0.0529097638
C8	1.4775314535	-3.5067048401	0.0439511063
C9	0.7941208794	-4.7713493936	0.0454023349
N10	-0.5838151907	-4.7832693080	0.0032381175
C11	-1.2156708914	-5.9915338527	0.0309363229
C12	-0.5463999996	-7.2303999943	0.0929999998
C13	0.8562181849	-7.2064605526	0.1273892588
C14	1.5280433655	-5.9746590448	0.1049363909
Zn15	-1.9187358826	-2.7379486139	-0.0793018843
O16	-2.9796322235	-3.2749126289	-1.8878492947
Zn17	1.9903755681	3.4031285345	0.3365953780
O18	3.6651881909	4.3230297109	-0.5449341411
N19	-2.9129106138	-0.5816842553	0.1400236597
C20	-2.2188334057	0.5759790291	-0.0077877123
C21	-2.7988266403	1.8472282256	0.2114623535
C22	-4.1680008840	1.8969493040	0.5679079784
C23	-4.8792221985	0.7026384641	0.7117508864
C24	-4.2244941660	-0.5147976691	0.5035746240
C25	-2.0374571378	3.0564438657	0.0921639428
C26	-1.4206090042	4.1096039375	0.0130645169
C27	-0.7543216572	5.3749364707	-0.1097255348
N28	0.6197618606	5.4177410181	-0.0138687954
C29	1.2308180334	6.6265802286	-0.1634640699
C30	0.5413999996	7.8321999943	-0.4029999998
C31	-0.8571496607	7.7779386753	-0.4881980125
C32	-1.5074446550	6.5444946737	-0.3420077520
O33	-0.6040986627	-1.8126500110	-1.4679379880
O34	-3.5337794797	-3.7151038857	0.8490327385
O35	-1.0930154640	-2.3320131411	1.8121764480
O36	1.2854491497	2.9084325921	-1.5673699510
O37	2.9040005841	4.0996412210	2.1618277369
O38	0.6362753583	2.4858678519	1.6917563593
H39	-1.1866073668	0.4789563524	-0.3171426393
H40	-4.6517554828	2.8545603927	0.7356904364
H41	-5.9286186959	0.7106354381	0.9909864625
H42	-4.7370841033	-1.4589294177	0.6363139326
H43	1.0911553762	8.7614100563	-0.5145985579
H44	2.3118100401	6.6141982781	-0.0979487010
H45	-2.5890340767	6.4764109578	-0.4123055730
H46	-1.4377842935	8.6782709104	-0.6698151178
H47	1.4260066258	-8.1304195442	0.1745493886
H48	-1.1113534665	-8.1568763516	0.1123248792
H49	-2.2979633934	-5.9524490995	0.0157178841
H50	2.6128359430	-5.9355810721	0.1393209553
H51	4.8435118188	2.0698027350	-0.1782780168
H52	6.0454435595	-0.0962742194	-0.5265826760
H53	4.7474125449	-2.2386343575	-0.4214826051
H54	1.2365717722	0.1199588353	0.5087662078
H55	-3.6341762034	-3.8861565812	1.8073550035
H56	-4.2544146583	-4.1486497279	0.3496241946

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H57	3.8451932813	4.3849113861	-1.5045498463
H58	4.3313738730	4.8339334079	-0.0432352696
H59	-0.5383602261	-2.9543772552	2.3238521607
H60	-1.3195172055	-1.5584095201	2.3659118424
H61	3.6672771914	3.6893741541	2.6193117916
H62	2.3734286696	4.6016185455	2.8152500523
H63	0.2899394887	-2.1467685188	-1.6812945730
H64	-1.0221136435	-1.4692291698	-2.2850230091
H65	-0.2632760809	2.8212885220	1.8788239111
H66	1.0233525084	2.1177159751	2.5130446127
H67	-2.5871927614	-3.8752878266	-2.5551286928
H68	-3.6803644848	-2.7373961412	-2.3127253037
H69	0.7857722790	3.5112848576	-2.1534669499
H70	1.5247660815	2.0938469783	-2.0524208615

Δr=0.8 Å			
Atom	X	Y	Z
N1	2.8769556250	1.2412849661	0.0739248173
C2	4.2134502264	1.1904139359	-0.1888797643
C3	4.8965242488	-0.0182226567	-0.3534740821
C4	4.1910725235	-1.2219871608	-0.2726398635
C5	2.7986336502	-1.1941690807	-0.0152566919
C6	2.1892948418	0.0716224912	0.1683987168
C7	2.0513242140	-2.4206188740	0.0268264047
C8	1.4548840937	-3.4897744697	0.0295163685
C9	0.7824207852	-4.7610413020	0.0414613540
N10	-0.5949155051	-4.7790181900	-0.0127619474
C11	-1.2207370237	-5.9912543441	0.0193424074
C12	-0.5463999986	-7.2303999812	0.0929999994
C13	0.8559897451	-7.1962099650	0.1392965008
C14	1.5215265762	-5.9602187258	0.1157226053
Zn15	-1.8975358507	-2.6518983299	-0.1213690111
O16	-3.0044379631	-3.1910231574	-1.9027326042
Zn17	1.8864906836	3.4769405746	0.1826604641
O18	3.5662086940	4.3644532859	-0.7013137077
N19	-2.8974020405	-0.4128221271	0.0331281156
C20	-2.2180073964	0.7512227249	-0.1451817123
C21	-2.8117973192	2.0240404255	0.0406817199
C22	-4.1823624622	2.0643752321	0.3950220300
C23	-4.8798100900	0.8652849092	0.5669366623
C24	-4.2101600977	-0.3501065335	0.3933140089
C25	-2.0652050308	3.2451389094	-0.0862886916
C26	-1.4618921100	4.3094266394	-0.1492880711
C27	-0.7856629640	5.5763925226	-0.2310981117
N28	0.5881389005	5.5965228799	-0.1208872351
C29	1.2206130979	6.8019584139	-0.2143334390
C30	0.5557999986	8.0315999812	-0.4095999994
C31	-0.8434772278	7.9969773318	-0.5139573946
C32	-1.5157582723	6.7674895740	-0.4259231128
O33	-0.5989676803	-1.7607623531	-1.5316669742
O34	-3.4933441529	-3.5792392364	0.8593385228
O35	-1.0424848624	-2.1699738604	1.7319629561
O36	1.1459428402	3.0176912100	-1.7141202241
O37	2.8318086540	4.1222285770	2.0118121028
O38	0.5270814783	2.6107443962	1.5580134507
H39	-1.1849371911	0.6593730494	-0.4535070160
H40	-4.6780881793	3.0198877899	0.5386159494
H41	-5.9299152307	0.8684924043	0.8439065744
H42	-4.7126885027	-1.2959829006	0.5532479531
H43	1.1214314864	8.9555579569	-0.4748989949
H44	2.3007134909	6.7676954138	-0.1397278639
H45	-2.5977381782	6.7220889193	-0.5099555900
H46	-1.4109789283	8.9113024940	-0.6649310452
H47	1.4316009319	-8.1161374834	0.1965459399
H48	-1.1070067511	-8.1593601211	0.1139802300
H49	-2.3034804446	-5.9572106748	-0.0073044423
H50	2.6058883494	-5.9160436194	0.1569071411
H51	4.7226353546	2.1412872078	-0.2793405354

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H52	5.9641986643	-0.0123381191	-0.5524392426
H53	4.6986559888	-2.1720197618	-0.4104039817
H54	1.1352266772	0.1499029357	0.4008858202
H55	-3.5741613489	-3.7221740263	1.8239779456
H56	-4.2177606077	-4.0373400620	0.3883439634
H57	3.7309785209	4.4460689223	-1.6622505051
H58	4.2451100586	4.8582187840	-0.1994649879
H59	-0.4997180806	-2.7777391723	2.2734106860
H60	-1.2256551884	-1.3521230448	2.2348651526
H61	3.5865822394	3.6905016437	2.4623041035
H62	2.3141977997	4.6281290457	2.6726805961
H63	0.2967712414	-2.0887134215	-1.7474922502
H64	-1.0159710454	-1.4056067555	-2.3437009878
H65	-0.3691207179	2.9582577488	1.7389002056
H66	0.9262520453	2.2925164680	2.3949042808
H67	-2.6263459254	-3.7831652838	-2.5855356305
H68	-3.7291384099	-2.6673307560	-2.3028557170
H69	0.6438144369	3.6358560378	-2.2821935489
H70	1.3698775236	2.2097509921	-2.2156320454

$\Delta r=0.9 \text{ \AA}$			
Atom	X	Y	Z
N1	2.8991698929	1.2207941126	0.0091584182
C2	4.2351098890	1.1671619002	-0.2554814449
C3	4.9218840292	-0.0423047105	-0.3969486047
C4	4.2196439782	-1.2458883690	-0.2921908492
C5	2.8273401392	-1.2150663282	-0.0357417810
C6	2.2149661439	0.0520535039	0.1248661707
C7	2.0795450278	-2.4393778126	0.0200849135
C8	1.4793171118	-3.5058855321	0.0257534545
C9	0.8001217490	-4.7723129351	0.0402099236
N10	-0.5752175660	-4.7797673000	-0.0511633912
C11	-1.2099166100	-5.9878817673	-0.0182510092
C12	-0.5463999995	-7.2303999926	0.0929999998
C13	0.8541914722	-7.2056689795	0.1772573102
C14	1.5288060896	-5.9748278222	0.1523145149
Zn15	-1.8561207476	-2.6105724267	-0.2204590847
O16	-2.9429295101	-3.1113382910	-2.0231831514
Zn17	1.8886354232	3.5070410905	0.0801827714
O18	3.5435324793	4.3575443726	-0.8722483273
N19	-2.8231487653	-0.3468433682	-0.0522373020
C20	-2.1545307539	0.8230484727	-0.2365272988
C21	-2.7542732985	2.0904206469	-0.0320940941
C22	-4.1183518446	2.1204055543	0.3468758509
C23	-4.8051316214	0.9163838026	0.5222096653
C24	-4.1305681534	-0.2929792400	0.3295415325
C25	-2.0201370303	3.3190394070	-0.1565888137
C26	-1.4338943814	4.3924572582	-0.2122084340
C27	-0.7673856778	5.6651915367	-0.2777927016
N28	0.6085301054	5.6856348172	-0.1997717916
C29	1.2349287755	6.8963482540	-0.2706659363
C30	0.5629999995	8.1312999926	-0.4128999998
C31	-0.8384363851	8.0934683142	-0.4839456175
C32	-1.5048818042	6.8591808555	-0.4179777145
O33	-0.5043913898	-1.7699218205	-1.6078214117
O34	-3.4979794186	-3.4994098333	0.7146127484
O35	-1.0400507809	-2.1688394942	1.6490195730
O36	1.0869237578	2.9285794686	-1.7582422475
O37	2.8636265562	4.1917605079	1.8755450305
O38	0.5536723391	2.6618890622	1.4806135199
H39	-1.1246100844	0.7424513672	-0.5595192249
H40	-4.6168530734	3.0720005482	0.5061356410
H41	-5.8502061980	0.9104410260	0.8173053906
H42	-4.6244117700	-1.2427983806	0.4911448597
H43	1.1245142369	9.0585418018	-0.4635929331
H44	2.3167481712	6.8639024746	-0.2198482947
H45	-2.5885991882	6.8128843667	-0.4756454881
H46	-1.4129057365	9.0094792793	-0.5919316351

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H47	1.4209482492	-8.1285908888	0.2650658043
H48	-1.1146637944	-8.1547766806	0.1123679122
H49	-2.2912922277	-5.9481863347	-0.0758391277
H50	2.6121730092	-5.9373736339	0.2191962175
H51	4.7436154433	2.1167034930	-0.3647833048
H52	5.9892037291	-0.0370207965	-0.5975357845
H53	4.7286360509	-2.1973819019	-0.4129842173
H54	1.1609426283	0.1315967917	0.3567596704
H55	-3.6075831711	-3.6317012062	1.6778558518
H56	-4.2153628774	-3.9495278270	0.2254739139
H57	3.6878510671	4.4100488419	-1.8388551657
H58	4.2303784291	4.8699512365	-0.4006764517
H59	-0.5230335770	-2.7902194706	2.1995145947
H60	-1.2196089038	-1.3493443880	2.1514217433
H61	3.6227311446	3.7701751736	2.3287506739
H62	2.3575362382	4.7185862221	2.5289618530
H63	0.3938315575	-2.1134444915	-1.7864424217
H64	-0.8905709413	-1.4253649132	-2.4395128914
H65	-0.3421170289	3.0084407735	1.6653218465
H66	0.9562824902	2.3417987036	2.3148272915
H67	-2.5641805298	-3.7019019822	-2.7072722224
H68	-3.6567774249	-2.5745475663	-2.4251799715
H69	0.5729044693	3.5072246952	-2.3566370882
H70	1.2774302774	2.0743853422	-2.1947217428

$\Delta r=1.0 \text{ \AA}$			
Atom	X	Y	Z
N1	2.9189067782	1.2272729919	0.0332198016
C2	4.2563567339	1.1577789347	-0.2208714867
C3	4.9323013275	-0.0597854308	-0.3425620561
C4	4.2177932449	-1.2552879343	-0.2297076663
C5	2.8236901073	-1.2090579608	0.0163707678
C6	2.2229299849	0.0659409064	0.1584073218
C7	2.0688073563	-2.4299074686	0.0759788414
C8	1.4691439675	-3.4976663115	0.0735108430
C9	0.7923193097	-4.7667383308	0.0742738474
N10	-0.5823335811	-4.7789179752	-0.0322945637
C11	-1.2128816762	-5.9894754747	-0.0160550565
C12	-0.5463999999	-7.2303999988	0.0930000000
C13	0.8530249765	-7.2009152781	0.1942076964
C14	1.5237053543	-5.9675615529	0.1865509937
Zn15	-1.8646124122	-2.5879524616	-0.1898283738
O16	-2.9514123229	-3.0487367746	-1.9984102547
Zn17	1.9490339474	3.4987747724	0.1183356588
O18	3.6159282174	4.3239671446	-0.8253407967
N19	-2.8148485198	-0.2495969685	-0.0176488036
C20	-2.1380192463	0.9155074820	-0.1991185554
C21	-2.7265024126	2.1867815364	0.0128473591
C22	-4.0900794612	2.2246901911	0.3939468324
C23	-4.7862136080	1.0253106156	0.5664775767
C24	-4.1208245311	-0.1882172589	0.3674457419
C25	-1.9851231541	3.4107302780	-0.1150981450
C26	-1.4019618409	4.4851233491	-0.1776033296
C27	-0.7422365766	5.7603807276	-0.2554804351
N28	0.6329703192	5.7880672233	-0.1791928723
C29	1.2508736186	7.0018325028	-0.2637858898
C30	0.5701999999	8.2309999988	-0.4162000000
C31	-0.8306662357	8.1851860072	-0.4870451696
C32	-1.4888111126	6.9473078564	-0.4082022534
O33	-0.5095096256	-1.7480779115	-1.5668768904
O34	-3.5198269730	-3.4590876274	0.7273193113
O35	-1.0777540518	-2.1384921683	1.6878445637
O36	1.1314770901	3.0084268536	-1.7365866324
O37	2.9774659326	4.0608053898	1.9221827357
O38	0.5833311648	2.6692011516	1.4959531943
H39	-1.1099244824	0.8274373947	-0.5256653842
H40	-4.5816468616	3.1790080016	0.5580080303
H41	-5.8309512904	1.0269286274	0.8631054725

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H42	-4.6206961637	-1.1357422116	0.5264509828
H43	1.1257447113	9.1612789120	-0.4769625574
H44	2.3332878508	6.9779698334	-0.2147161183
H45	-2.5721449778	6.8925428199	-0.4662710364
H46	-1.4101369309	9.0970781085	-0.6034395748
H47	1.4220488347	-8.1225476761	0.2808807767
H48	-1.1111229655	-8.1570809153	0.0985928173
H49	-2.2936469547	-5.9521434514	-0.0859434518
H50	2.6061097281	-5.9268742399	0.2671084132
H51	4.7737771202	2.1011842157	-0.3381875250
H52	6.0011665143	-0.0669548994	-0.5344422801
H53	4.7184525208	-2.2130097586	-0.3352591733
H54	1.1693631720	0.1611013457	0.3836898741
H55	-3.6357682164	-3.6019592766	1.6881500481
H56	-4.2416146814	-3.8925637161	0.2296602291
H57	3.7537820611	4.3977231108	-1.7913348957
H58	4.3162313953	4.8102335006	-0.3456591661
H59	-0.5660686666	-2.7541294402	2.2500911390
H60	-1.2676816488	-1.3128849044	2.1762367947
H61	3.7276873924	3.5845991194	2.3352027686
H62	2.5087581073	4.5756809057	2.6119992370
H63	0.3893111050	-2.0908477418	-1.7420958548
H64	-0.8892189363	-1.3848606458	-2.3935373073
H65	-0.3089087231	3.0257089577	1.6846187155
H66	0.9746993572	2.3322241413	2.3292152325
H67	-2.5735061616	-3.6267810988	-2.6933936451
H68	-3.6647459787	-2.5021549364	-2.3880992237
H69	0.6358711044	3.6206059195	-2.3169098605
H70	1.2952590625	2.1619079159	-2.1978856701

$\Delta r=1.1 \text{ \AA}$			
Atom	X	Y	Z
N1	4.0143915018	0.5847665040	1.0026896162
C2	5.2642378482	0.4695535689	0.4657281347
C3	5.7268737064	-0.7257805405	-0.0879503393
C4	4.8864404971	-1.8411530288	-0.1134016671
C5	3.5826991966	-1.7358201225	0.4279486761
C6	3.1948011469	-0.4988284615	0.9886354578
C7	2.6873296990	-2.8534627649	0.3748594444
C8	1.9484330684	-3.8240621418	0.2882790898
C9	1.1096330449	-4.9848391777	0.2020435442
N10	-0.2529315843	-4.8070917958	0.2795036696
C11	-1.0413608816	-5.9170280209	0.2300436496
C12	-0.5463999962	-7.2303999477	0.0929999983
C13	0.8437888567	-7.3953419081	0.0023488730
C14	1.6765101581	-6.2679288705	0.0594031342
Zn15	-1.3223178598	-2.4263374220	0.4819311521
O16	-2.6513843174	2.6318277556	-1.1947671514
Zn17	3.4980818690	2.5815976950	1.8595417774
O18	5.2639187814	3.5641107098	1.3211909001
N19	-2.1338306168	-0.2914844674	0.9771109132
C20	-1.5114503519	0.8769347405	0.6642263720
C21	-2.0379183552	2.1384331690	1.0281870628
C22	-3.2676710665	2.1649775535	1.7310514792
C23	-3.9033567271	0.9615096788	2.0450425253
C24	-3.3119775422	-0.2450236146	1.6619857459
C25	-1.3793723817	3.3712227984	0.7053905259
C26	-0.9128659409	4.4746083689	0.4564697453
C27	-0.4266893843	5.7937210165	0.1602800942
N28	0.9292657614	5.9699113930	0.0554609602
C29	1.4044937370	7.2113720654	-0.2261656266
C30	0.5773999962	8.3306999477	-0.4194999983
C31	-0.8101056106	8.1453977552	-0.3101086018
C32	-1.3187888764	6.8711360691	-0.0180583157
O33	-0.0088323673	-1.6444623555	-0.9612991192
O34	-2.8185121943	-3.4279640843	1.5570192452
O35	-0.1208996582	-2.1820100107	2.2123705416
O36	2.4636006908	3.5157587726	0.2935353852

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O37	4.4000357548	2.1905806814	3.7402798988
O38	1.6805708309	2.1953825178	2.8509062324
H39	-0.5857382819	0.7993616912	0.1071073889
H40	-3.7048614869	3.1154152952	2.0217060775
H41	-4.8455585236	0.9541602416	2.5848110145
H42	-3.7668011944	-1.1972622284	1.9025760556
H43	1.0095427762	9.3006942199	-0.6449934396
H44	2.4833461995	7.3013070119	-0.2978401560
H45	-2.3890115364	6.7054591114	0.0685416784
H46	-1.4910269791	8.9804450609	-0.4498239252
H47	1.2797775764	-8.3844647777	-0.1074392352
H48	-1.2317978528	-8.0714060475	0.0603177598
H49	-2.1060533865	-5.7370347410	0.3149517110
H50	2.7560713939	-6.3719177173	0.0004478362
H51	5.8825723410	1.3571410751	0.4886100464
H52	6.7307179022	-0.7742849269	-0.4985675228
H53	5.2194610745	-2.7792559657	-0.5472811397
H54	2.2160731439	-0.3751291375	1.4325708273
H55	-2.7485965272	-3.7745095193	2.4698070061
H56	-3.6352773040	-3.7595056190	1.1324829537
H57	5.3791965429	4.0958142607	0.5068971335
H58	6.0118541081	3.7137699304	1.9352106376
H59	0.4139436219	-2.8876108074	2.6292611805
H60	-0.0988107349	-1.3746648889	2.7660460570
H61	4.8078290678	1.3499399046	4.0312269467
H62	4.3933172314	2.8352814938	4.4781945083
H63	0.9024854307	-1.9469089147	-1.1439901116
H64	-0.3694656841	-1.1965828340	-1.7543453379
H65	0.8800498619	2.7362851411	2.7004260165
H66	1.7113232812	1.8911163145	3.7820344593
H67	-2.4347902311	-3.1754622065	-1.9805989564
H68	-3.3273218404	-1.9658171751	-1.4392455118
H69	1.9925558456	4.4041168757	0.3121457695
H70	2.4854047840	3.1699010956	-0.6217359577

$\Delta r=1.2 \text{ \AA}$			
Atom	X	Y	Z
N1	3.6576032100	0.7335580271	-0.9981425169
C2	4.7413801807	0.5955986223	-1.8157326343
C3	5.1124524066	-0.6390157056	-2.3531504799
C4	4.3542831444	-1.7725564130	-2.0538980802
C5	3.2189047631	-1.6433083659	-1.2168667083
C6	2.9076447443	-0.3628573578	-0.7099035963
C7	2.4152416975	-2.7858424822	-0.9056889423
C8	1.7623286884	-3.7922914431	-0.6786186089
C9	1.0038808814	-4.9800961385	-0.4193469641
N10	-0.3499904241	-4.8393970580	-0.2539719878
C11	-1.0965934508	-5.9437846723	-0.0030723226
C12	-0.5463999844	-7.2303997838	0.0929999929
C13	0.8389165403	-7.3749404423	-0.0807762167
C14	1.6242627827	-6.2424461701	-0.3382165611
Zn15	-2.3114718415	-1.4545191226	-2.3243066292
O16	-3.1658098129	-0.8582053619	-4.1694178657
Zn17	3.2387671905	2.7440482084	-0.1662542892
O18	4.8669796527	3.6537078370	-1.1740192738
N19	-3.1205549280	0.2666821640	-1.2409024831
C20	-2.4228754173	1.4248068648	-1.1546531505
C21	-2.9314001793	2.5610550208	-0.4941115316
C22	-4.2094268067	2.4719771761	0.1056425041
C23	-4.9199056978	1.2717588542	0.0152167328
C24	-4.3546908232	0.1908859270	-0.6648528348
C25	-2.1658052363	3.7634618927	-0.4468898875
C26	-1.5264923500	4.8018751724	-0.4211830413
C27	-0.8273535647	6.0473477938	-0.4036048549
N28	0.5130799558	6.0295418579	-0.6884551579
C29	1.1946518628	7.1998590043	-0.6937193041
C30	0.5845999844	8.4302997838	-0.4227999921
C31	-0.7853334091	8.4514489339	-0.1235428165

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C32	-1.5021615171	7.2487773679	-0.1117895901
O33	-0.5510402126	-0.5739291875	-3.1137933026
O34	-3.9334046640	-2.7610927223	-1.9739322947
O35	-1.2743338285	-2.2459897283	-0.6952354924
O36	1.8770369584	3.7638801736	-1.3332746668
O37	4.4913067066	2.6410816750	1.5166856224
O38	1.6246560531	2.1122511437	1.0990450516
H39	-1.4471942326	1.4455177973	-1.6261651606
H40	-4.6279153214	3.3282603035	0.6258507863
H41	-5.9030294734	1.1714453226	0.4641947254
H42	-4.8777270531	-0.7514415581	-0.7644559021
H43	1.1727631333	9.3427240868	-0.4423055083
H44	2.2536037875	7.1374746686	-0.9202364166
H45	-2.5644572086	7.2290557804	0.1132364919
H46	-1.2887924464	9.3884595945	0.0961301583
H47	1.3030254910	-8.3549526639	-0.0163375869
H48	-1.1850323117	-8.0844081136	0.2961363571
H49	-2.1617725422	-5.7828850009	0.1264813124
H50	2.6992015575	-6.3251252222	-0.4707568255
H51	5.3019308136	1.4962356137	-2.0235244337
H52	5.9840207911	-0.7041712804	-2.9971176724
H53	4.6234575321	-2.7445666106	-2.4564699857
H54	2.0633446177	-0.2101799811	-0.0491308328
H55	-4.0456876091	-3.3470479716	-1.1974169089
H56	-4.6258365412	-2.9496759751	-2.6415622844
H57	4.8143937757	4.1698253887	-2.0044872236
H58	5.7350673941	3.7976777703	-0.7443166529
H59	-1.0065914711	-3.2191592565	-0.5278836377
H60	-0.9392364272	-1.6604967334	0.0123259414
H61	4.9709498280	1.8550522025	1.8484202741
H62	4.6294331614	3.4025495758	2.1176732943
H63	0.3415968491	-0.9616874664	-3.0269518147
H64	-0.5920463352	-0.0416104319	-3.9358795288
H65	0.7241449117	2.4945050204	1.0518293056
H66	1.8213337676	1.8548758915	2.0249489807
H67	-2.8761438014	-1.2437489353	-5.0228961027
H68	-3.5772360058	0.0171240683	-4.3258769614
H69	1.3625152158	4.6093364287	-1.0556286105
H70	1.8321903562	3.6490096696	-2.3045916413

$\Delta r=1.3 \text{ \AA}$			
Atom	X	Y	Z
N1	4.0306484138	0.5227930928	-0.6546114487
C2	5.1359094913	0.4086275305	-1.4461999938
C3	5.5088697734	-0.8072593971	-2.0256159418
C4	4.7317001905	-1.9460000351	-1.7989931305
C5	3.5784345455	-1.8416625315	-0.9841213700
C6	3.2714350475	-0.5810468172	-0.4292728087
C7	2.7389479581	-2.9774384971	-0.7424354437
C8	2.0362926938	-3.9612111568	-0.5637301848
C9	1.1926077120	-5.1024458389	-0.3522699706
N10	-0.1333111635	-4.8545327405	-0.1066270927
C11	-0.9711291332	-5.8967730761	0.1109000728
C12	-0.5463999959	-7.2303999435	0.0929999981
C13	0.8097775737	-7.4885406754	-0.1678263496
C14	1.6903449248	-6.4196756459	-0.3914890754
Zn15	-2.0024138926	-1.4851822565	-1.9945891680
O16	-3.0524361889	-0.8123664562	-3.6962362585
Zn17	3.5390130079	2.4952984742	0.2710045400
O18	5.2227181243	3.4543161710	-0.5449514930
N19	-2.7375221026	0.1783227377	-0.7927989484
C20	-2.0761449474	1.3609458408	-0.7597446396
C21	-2.5205942844	2.4554132957	0.0076569545
C22	-3.6959643806	2.2950969941	0.7786415062
C23	-4.3679534647	1.0693835461	0.7464177383
C24	-3.8708774493	0.0332032066	-0.0473837481
C25	-1.8072707538	3.6915512122	-0.0266160259
C26	-1.2232453094	4.7617669821	-0.0851160938

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C27	-0.6125965509	6.0517550964	-0.1756438837
N28	0.7370086376	6.1115791494	-0.4125107425
C29	1.3132297935	7.3331052924	-0.5335289307
C30	0.5917999959	8.5299999435	-0.4260999981
C31	-0.7850838420	8.4676407882	-0.1723437540
C32	-1.3971473286	7.2147705343	-0.0431247330
O33	-0.2518897747	-0.8633038219	-2.9941833613
O34	-3.4684329903	-2.9202255803	-1.5242333984
O35	-0.8149698801	-2.2520138451	-0.4395425224
O36	2.2532050112	3.6788505789	-0.8873296773
O37	4.6071546270	2.2343357061	2.0526389834
O38	1.8038338607	1.7486189137	1.2552545859
H39	-1.1837066941	1.4438697084	-1.3682148051
H40	-4.0662104368	3.1165467970	1.3843980311
H41	-5.2721021764	0.9143064547	1.3268755898
H42	-4.3727004040	-0.9239215787	-0.1069893739
H43	1.1040473941	9.4811663593	-0.5365270407
H44	2.3810945784	7.3438793386	-0.7230052442
H45	-2.4624546523	7.1269746518	0.1501710893
H46	-1.3725088923	9.3762132984	-0.0769297677
H47	1.1796403015	-8.5095145105	-0.1956986317
H48	-1.2523336003	-8.0347944369	0.2748724179
H49	-2.0083465179	-5.6464949440	0.3067678886
H50	2.7428578347	-6.5951969098	-0.5952743466
H51	5.7099442827	1.3116451842	-1.6038431626
H52	6.3963306409	-0.8540472153	-2.6492150712
H53	5.0010994199	-2.9002925330	-2.2417248004
H54	2.4111594713	-0.4448188016	0.2126499466
H55	-3.4332715139	-3.5821319836	-0.8040372700
H56	-4.2152733951	-3.1210226848	-2.1236630493
H57	5.2284972359	3.9988844966	-1.3588897036
H58	6.0513185673	3.5920126130	-0.0415916953
H59	-0.6255847651	-3.1979284200	-0.2750222299
H60	-0.3131924605	-1.6725601326	0.1698995936
H61	5.0570030684	1.4216966200	2.3607854348
H62	4.6750141909	2.9378323573	2.7313634720
H63	0.5678398696	-1.3956202368	-2.9882009538
H64	-0.2812911185	-0.3240643646	-3.8113949112
H65	0.9262146992	2.1396105310	1.0733381695
H66	1.8666005774	1.4920992291	2.1990480913
H67	-2.8203840016	-1.1045873170	-4.6022241717
H68	-3.5104617454	0.0527517005	-3.7405109150
H69	1.7985096546	4.5344724926	-0.6182066277
H70	2.1823050987	3.5621863912	-1.8563888916

$\Delta r=1.4 \text{ \AA}$			
Atom	X	Y	Z
N1	4.0881033032	0.4626194016	-0.9218405270
C2	5.1860748005	0.3166347404	-1.7204644421
C3	5.5576100068	-0.9209439003	-2.2521663038
C4	4.7851733883	-2.0512769655	-1.9731048980
C5	3.6380305332	-1.9166837279	-1.1540400817
C6	3.3365381529	-0.6355398399	-0.6452542370
C7	2.7912038105	-3.0399369394	-0.8777036859
C8	2.0804773376	-4.0143653774	-0.6815717031
C9	1.2178827098	-5.1358355300	-0.4368091088
N10	-0.1186846385	-4.8641766148	-0.2824289201
C11	-0.9650072659	-5.8943648588	-0.0187634905
C12	-0.5463999755	-7.2303996601	0.0929999888
C13	0.8207199712	-7.5033137314	-0.0807197412
C14	1.7119698890	-6.4518897104	-0.3452655258
Zn15	-1.8493792562	-1.4465384138	-2.4246682277
O16	-2.8418430590	-0.7457898662	4.1548906782
Zn17	3.6180387985	2.5041483861	-0.0913809872
O18	5.2568609213	3.4071916835	-1.0481879198
N19	-2.5813383986	0.2424535934	-1.2390412905
C20	-1.9693255768	1.4509588135	-1.1911055861
C21	-2.4505270403	2.5088136889	-0.3947637889

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C22	-3.6178590218	2.2939274407	0.3743519691
C23	-4.2473114230	1.0475753684	0.3157137257
C24	-3.7086908791	0.0453745898	-0.4939522642
C25	-1.7622672641	3.7584507308	-0.3707899200
C26	-1.1953674116	4.8380557096	-0.3496307291
C27	-0.5979092287	6.1369735276	-0.3478693796
N28	0.7544241421	6.2168629411	-0.5564207868
C29	1.3277018267	7.4444254615	-0.5944413603
C30	0.5989999754	8.6296996601	-0.4293999888
C31	-0.7817479232	8.5467496398	-0.2022756871
C32	-1.3904258347	7.2863541438	-0.1591157914
O33	-0.0415148351	-1.0003027480	-3.4226900846
O34	-3.3433591690	-2.8433572828	-1.9656513447
O35	-0.6546709624	-2.1693480757	-0.8504295812
O36	2.2954577034	3.7982326248	-1.1256124780
O37	4.7715020954	2.3515567089	1.6411602685
O38	1.9106082848	1.8344412321	0.9866559347
H39	-1.0894471670	1.5860452586	-1.8071742973
H40	-4.0113544608	3.0899291395	0.9992415033
H41	-5.1449441579	0.8482575563	0.8928985380
H42	-4.1669916674	-0.9328340265	-0.5573347359
H43	1.1076012221	9.5881230056	-0.4732413985
H44	2.3992196506	7.4673398200	-0.7636094237
H45	-2.4589158056	7.1829518590	0.0068863070
H46	-1.3750033027	9.4459474741	-0.0634598347
H47	1.1925692800	-8.5214218248	-0.0071477962
H48	-1.2640092928	-8.0164484550	0.3061564685
H49	-2.0108470003	-5.6343158344	0.1054187947
H50	2.7739511965	-6.6406537235	-0.4755743841
H51	5.7540628315	1.2137942648	-1.9244279210
H52	6.4395126753	-0.9906250659	-2.8817236478
H53	5.0516117812	-3.0216488461	-2.3812750244
H54	2.4822398798	-0.4705887145	-0.0038553317
H55	-3.3116033609	-3.4980648114	-1.2387529468
H56	-4.1006904957	-3.0320856056	-2.5558136037
H57	5.2296019597	3.9291402328	-1.8763682572
H58	6.1075927941	3.5539222780	-0.5859366638
H59	-0.4912618891	-3.1053223892	-0.6161021051
H60	-0.1285005573	-1.5421155343	-0.3131066856
H61	5.2405315509	1.5599490914	1.9743190745
H62	4.8830895419	3.1001195859	2.2636394979
H63	0.7540341568	-1.5624146530	-3.3425690006
H64	-0.0325507655	-0.5302646187	-4.2820552529
H65	1.0335606573	2.2262356902	0.8037042416
H66	1.9941707837	1.6305419495	1.9415109875
H67	-2.6798274120	-1.1134010298	-5.0485650053
H68	-3.2145438405	0.1569088010	-4.2362441274
H69	1.8394906829	4.6302344793	-0.7923176262
H70	2.1967774632	3.7571967385	-2.0984324903

Δr=1.5 Å			
Atom	X	Y	Z
N1	4.0056652121	0.6615545927	0.2028597844
C2	5.1357101539	0.5199307016	-0.5517385117
C3	5.5288346133	-0.7090764831	-1.0843509852
C4	4.7325015421	-1.8354426789	-0.8730075441
C5	3.5477509812	-1.7117375623	-0.1063562819
C6	3.2394056198	-0.4421193790	0.4325748585
C7	2.6786609142	-2.8426186342	0.0486915347
C8	1.9701254389	-3.8385112991	0.0862822763
C9	1.1473950451	-5.0161944537	0.1001110151
N10	-0.2088282797	-4.8313451750	0.1756739584
C11	-1.0223616802	-5.9161380496	0.1780549779
C12	-0.5463999967	-7.2303999537	0.0929999985
C13	0.8428362957	-7.4211782815	0.0037590972
C14	1.6995229733	-6.3098028730	0.0091375959
Zn15	-2.3065822424	-1.2187036418	-1.3164846139
O16	-3.4516320830	-0.5256240703	-2.9448720498

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Zn17	3.5358442036	2.7782685415	0.8892860683
O18	5.2006790200	3.5965763975	-0.0980053731
N19	-2.9149655435	0.4899996936	-0.0863097244
C20	-2.2713119745	1.6794220124	-0.1743302079
C21	-2.5954038761	2.7802573379	0.6413332445
C22	-3.6593003260	2.6389296335	1.5617412318
C23	-4.3278177100	1.4126246959	1.6396607831
C24	-3.9323995846	0.3583554733	0.8132969506
C25	-1.8695678916	4.0030979058	0.4988647175
C26	-1.2659298694	5.0539008931	0.3538921957
C27	-0.6359251907	6.3194058193	0.1294997192
N28	0.7104443433	6.3269024958	-0.1292853615
C29	1.3057877392	7.5149194343	-0.4011502155
C30	0.6061999967	8.7293999537	-0.4326999985
C31	-0.7672286736	8.7215539897	-0.1522356392
C32	-1.3976775271	7.5044409348	0.1347153396
O33	-0.6059011111	-0.8169680873	-2.4917548543
O34	-3.8057387072	-2.5706428950	-0.7397808985
O35	-0.9726373511	-2.0803946798	0.0853089157
O36	2.2632325163	3.9793614357	-0.3077527718
O37	4.6433688911	2.7514795154	2.6509551162
O38	1.7962946421	2.3079469607	2.0171933747
H39	-1.4937588341	1.7662149720	-0.9218921050
H40	-3.9436658004	3.4694302092	2.2007676370
H41	-5.1484401779	1.2692131235	2.3355685730
H42	-4.4236882435	-0.6051187767	0.8517875218
H43	1.1313249407	9.6514495344	-0.6632313085
H44	2.3715132423	7.4810358972	-0.6017093144
H45	-2.4626161640	7.4589875344	0.3437362238
H46	-1.3394245755	9.6447544107	-0.1602644724
H47	1.2569094356	-8.4227222259	-0.0704702195
H48	-1.2372974436	-8.0678332130	0.0956523621
H49	-2.0859169752	-5.7134265571	0.2440821215
H50	2.7759369390	-6.4343006192	-0.0689946474
H51	5.7124708374	1.4178538313	-0.7221886032
H52	6.4395750470	-0.7713807938	-1.6721644833
H53	5.0064421245	-2.7976941033	-1.2948780692
H54	2.3590577769	-0.2962010227	1.0453050213
H55	-3.7481742154	-3.2457094911	-0.0333827371
H56	-4.6257060678	-2.7007166140	-1.2576432152
H57	5.1964008921	4.0646022179	-0.9582226051
H58	6.0428499319	3.7653427254	0.3723123505
H59	-0.7562459244	-3.0316033314	0.1632126317
H60	-0.3836748923	-1.5387289377	0.6498255393
H61	5.0880532481	1.9798764302	3.0566520743
H62	4.7664820714	3.5477076851	3.2085862086
H63	0.1996618480	-1.3692656489	-2.4567063842
H64	-0.6731022204	-0.3730321253	-3.3622607853
H65	0.9357087495	2.7124977695	1.7894746485
H66	1.8651729758	2.1944025561	2.9880541642
H67	-3.4050311834	-0.9232113056	-3.8391021487
H68	-3.8005002964	0.3879758607	-3.0081840273
H69	1.7335016380	4.7985977849	-0.0638554340
H70	2.2566199271	3.8969418521	-1.2829070342

$\Delta r=1.6 \text{ \AA}$			
Atom	X	Y	Z
N1	3.9756984927	0.6526932640	0.2059896900
C2	5.1039340448	0.5438521681	-0.5564100243
C3	5.4993444011	-0.6650427415	-1.1331623603
C4	4.7075088213	-1.8015684491	-0.9581925396
C5	3.5268737441	-1.7066454487	-0.1818361740
C6	3.2175361779	-0.4597346302	0.4035356466
C7	2.6665008190	-2.8435223587	-0.0361979030
C8	1.9605428439	-3.8398987039	0.0128780063
C9	1.1377256390	-5.0154800567	0.0491879594
N10	-0.2127465778	-4.8305318609	0.1970027777
C11	-1.0225332273	-5.9183134132	0.2167744300

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C12	-0.5463999931	-7.2303999048	0.0929999969
C13	0.8368690520	-7.4183282545	-0.0610108013
C14	1.6895569469	-6.3053095600	-0.0831542486
Zn15	-2.3399889434	-1.1630116171	-1.2004724001
O16	-3.5086542922	-0.5562303760	-2.8465038077
Zn17	3.4697015903	2.7440814260	0.9558632204
O18	5.1592518853	3.6055524343	0.0579902046
N19	-2.9397372048	0.5873541934	-0.0278664969
C20	-2.3113395188	1.7835662399	-0.1482571051
C21	-2.6607745395	2.9057765295	0.6291141497
C22	-3.7339383675	2.7753220614	1.5411349796
C23	-4.3869341962	1.5434164291	1.6498851038
C24	-3.9667799024	0.4692066150	0.8624678745
C25	-1.9517956359	4.1384938318	0.4755446423
C26	-1.3516587614	5.1917596296	0.3296835328
C27	-0.6970962828	6.4470399628	0.1106228518
N28	0.6586088415	6.4278144719	-0.0987842936
C29	1.2864943145	7.6009776482	-0.3634639475
C30	0.6133999931	8.8290999048	-0.4359999969
C31	-0.7698194064	8.8483448565	-0.2057787300
C32	-1.4347141413	7.6466061622	0.0727690796
O33	-0.6618690444	-0.8176179420	-2.4325119346
O34	-3.8206857503	-2.5017673437	-0.5555412578
O35	-0.9926726655	-2.0238412443	0.1812379486
O36	2.2342197280	3.9861627722	-0.2419655476
O37	4.5183353233	2.6512336307	2.7507668244
O38	1.6835914360	2.2301950676	1.9913153224
H39	-1.5209479797	1.8512102615	-0.8847337297
H40	-4.0374144607	3.6212497691	2.1507817857
H41	-5.2130747205	1.4102233769	2.3414147179
H42	-4.4534191510	-0.4957877370	0.9156367798
H43	1.1642297963	9.7380349037	-0.6586333009
H44	2.3579862970	7.5443410590	-0.5237545628
H45	-2.5071381032	7.6257227567	0.2443015320
H46	-1.3243770140	9.7815124532	-0.2457315799
H47	1.2479945636	-8.4184237972	-0.1650608009
H48	-1.2342859130	-8.0701219744	0.1136457405
H49	-2.0826291018	-5.7220647894	0.3359386383
H50	2.7627788856	-6.4258507558	-0.2013937219
H51	5.6760360159	1.4498290670	-0.6978197370
H52	6.4083596411	-0.7038501962	-1.7256756369
H53	4.9816665217	-2.7468294960	-1.4166481928
H54	2.3473497464	-0.3449788140	1.0356666208
H55	-3.7448559393	-3.1519411759	0.1720960404
H56	-4.6545011957	-2.6482881983	-1.0461534082
H57	5.1835414786	4.1081051937	-0.7821510154
H58	5.9838924447	3.7571555764	0.5637160445
H59	-0.7810523550	-2.9775562255	0.2388877084
H60	-0.3991561722	-1.5040236621	0.7612639854
H61	4.9454699447	1.8623039746	3.1417440013
H62	4.6333157366	3.4267817819	3.3383979840
H63	0.1586060149	-1.3434533167	-2.3578829466
H64	-0.7511304829	-0.4615159128	-3.3406120559
H65	0.8216721442	2.6225579833	1.7477433889
H66	1.7167147939	2.0718603563	2.9578085879
H67	-3.4820177924	-1.0035151096	-3.7177545316
H68	-3.8621456947	0.3516418943	-2.9524038987
H69	1.6899398345	4.7984897167	-0.0073545350
H70	2.2736346913	3.9309703835	-1.2182186300

$\Delta r=1.8 \text{ \AA}$			
Atom	X	Y	Z
N1	3.9758896551	0.6506744023	0.0314060259
C2	5.1215297268	0.5310995299	-0.7018227122
C3	5.5263275461	-0.6851388228	-1.2564911139
C4	4.7324183393	-1.8192856527	-1.0783185670
C5	3.5365269701	-1.7138457752	-0.3265993254
C6	3.2083377213	-0.4560800818	0.2262108654

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C7	2.6822923117	-2.8543004248	-0.1701659126
C8	1.9816114962	-3.8541363755	-0.0998770213
C9	1.1493718465	-5.0217994367	-0.0298067816
N10	-0.2019329131	-4.8204623676	0.0999863113
C11	-1.0148876729	-5.9081234648	0.1598457266
C12	-0.5463999984	-7.2303999774	0.0929999993
C13	0.8378795740	-7.4264878486	-0.0433778065
C14	1.6953643269	-6.3180346885	-0.1049988181
Zn15	-2.3782790820	-1.0755452187	-1.4717467423
O16	-3.5772372835	-0.4776546184	-3.0975393491
Zn17	3.4695635137	2.7337878020	0.7841495992
O18	5.1852448148	3.5830625399	-0.0781009496
N19	-2.8749507271	0.7126882760	-0.3091832315
C20	-2.2469026996	1.9108944893	-0.4383202119
C21	-2.5941086237	3.0322946130	0.3462960244
C22	-3.6590642662	2.8940797228	1.2681691480
C23	-4.3093387192	1.6629362083	1.3827506930
C24	-3.8933512583	0.5922446295	0.5910550165
C25	-1.8960780405	4.2738432488	0.2155288611
C26	-1.3106343018	5.3406598860	0.1097457469
C27	-0.6649864147	6.6099088420	-0.0534806144
N28	0.6947460913	6.6129787872	-0.2343887395
C29	1.3138158731	7.8052556089	-0.4235865411
C30	0.6277999984	9.0284999774	-0.4425999993
C31	-0.7601592811	9.0218655899	-0.2430101796
C32	-1.4174377397	7.8003756791	-0.0441681927
O33	-0.7159450404	-0.7750160479	-2.7387108739
O34	-3.8912241984	-2.3308992784	-0.7269199390
O35	-1.0082700580	-1.9137948303	-0.0997762159
O36	2.2731438455	4.0155947507	-0.4134111113
O37	4.4956138076	2.5934797228	2.5907636722
O38	1.6792174850	2.1833102038	1.7960641254
H39	-1.4768839216	1.9879513440	-1.1947876683
H40	-3.9571681852	3.7363555143	1.8850913551
H41	-5.1291274542	1.5281398883	2.0814307550
H42	-4.3828881410	-0.3709753440	0.6426819383
H43	1.1727358671	9.9535237333	-0.6060000430
H44	2.3891646747	7.7687891210	-0.5626569443
H45	-2.4913200106	7.7600428730	0.1150769248
H46	-1.3229531467	9.9509177385	-0.2428158986
H47	1.2482858454	-8.4306813279	-0.1008285652
H48	-1.2395089943	-8.0643429874	0.1465322730
H49	-2.0752503453	-5.7042432832	0.2659520662
H50	2.7687706569	-6.4484631426	-0.2122968514
H51	5.7002742384	1.4338696312	-0.8373807299
H52	6.4476221079	-0.7325833072	-1.8290184828
H53	5.0174544681	-2.7722852881	-1.5136673448
H54	2.3176424130	-0.3202196438	0.8266371736
H55	-3.8119306851	-2.9711450742	0.0090863814
H56	-4.7572156378	-2.4366983541	-1.1699080147
H57	5.2305357042	4.0883599153	-0.9157471922
H58	6.0000911552	3.7271734228	0.4452896359
H59	-0.8429880663	-2.8714373163	0.0152835354
H60	-0.3730345947	-1.3687477273	0.4083909364
H61	4.9022467111	1.7902047405	2.9742540172
H62	4.6245735515	3.3584666895	3.1892772018
H63	0.1055811339	-1.3006451260	-2.6749937607
H64	-0.8137784933	-0.4185337609	-3.6457712130
H65	0.8092292270	2.5587508479	1.5544961562
H66	1.7108211974	1.9965228178	2.7575153347
H67	-3.6093929827	-0.9654234367	-3.9465547880
H68	-3.8956009238	0.4394718356	-3.2313767299
H69	1.7203124207	4.8215843455	-0.1770022235
H70	2.3224977916	3.9673638120	-1.3895278075

Δr=2.0 Å			
Atom	X	Y	Z
N1	4.2227611582	0.5005932118	-0.1207788453

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C2	5.3857488500	0.3232314988	-0.8144612704
C3	5.7462016597	-0.9115522842	-1.3587082276
C4	4.8928630265	-2.0058655159	-1.2051509087
C5	3.6789669527	-1.8411982607	-0.4937189599
C6	3.3948434422	-0.5669611304	0.0446797815
C7	2.7782971390	-2.9455364674	-0.3405081442
C8	2.0532954956	-3.9262383650	-0.2542540189
C9	1.1965292529	-5.0732900088	-0.1452207746
N10	-0.1444767289	-4.8357317132	0.0166618511
C11	-0.9808153285	-5.8984523745	0.1301640072
C12	-0.5463999983	-7.2303999834	0.0929999995
C13	0.8279203388	-7.4687294416	-0.0751448203
C14	1.7103352498	-6.3844348306	-0.1956731091
Zn15	-2.1364041824	-0.8810509460	-1.8074686412
O16	-3.2758984605	-0.0862085751	-3.3892964696
Zn17	3.8090413021	2.5918685638	0.6506060444
O18	5.6186488666	3.3584571355	-0.0847368375
N19	-2.5796638776	0.8127708099	-0.5029493472
C20	-2.0077993335	2.0397187406	-0.6138488131
C21	-2.3515274368	3.1077024069	0.2422230635
C22	-3.3337942556	2.8783199397	1.2349217583
C23	-3.9161206183	1.6129757184	1.3404309457
C24	-3.5187595011	0.6022746999	0.4642195735
C25	-1.7217190153	4.3843031888	0.1137440191
C26	-1.1878199617	5.4780871423	0.0181272794
C27	-0.5839302525	6.7703346435	-0.1159466284
N28	0.7685421399	6.8079933969	-0.3364808192
C29	1.3544264366	8.0211661843	-0.4970081288
C30	0.6421999988	9.2277999834	-0.4491999995
C31	-0.7385580177	9.1842345330	-0.2086906537
C32	-1.3628137775	7.9413022012	-0.0378283293
O33	-0.4265204540	-0.5519497603	-2.9952934501
O34	-3.7168983501	-2.1276229527	-1.2022479228
O35	-0.8136604243	-1.8969581927	-0.5025461051
O36	2.7429290118	3.9851103748	-0.5461963273
O37	4.7045130936	2.3211751843	2.5120633402
O38	1.9346606675	2.1536109886	1.5444031108
H39	-1.2902794117	2.1828115907	-1.4130193783
H40	-3.6264959459	3.6806585647	1.9054752825
H41	-4.6695618425	1.4063893347	2.0940679430
H42	-3.9600915201	-0.3840915485	0.5045794376
H43	1.1626405211	10.1705298529	-0.5911564322
H44	2.4261438929	8.0155274012	-0.6690563825
H45	-2.4306881283	7.8699661498	0.1494024461
H46	-1.3204918128	10.0999403069	-0.1571256933
H47	1.2108700581	-8.4846264246	-0.1114548702
H48	-1.2578974108	-8.0449525310	0.1892312662
H49	-2.0326981815	-5.6650947553	0.2583708777
H50	2.77787875088	-6.5440164858	-0.3131035483
H51	6.0153524888	1.1947825242	-0.9259452006
H52	6.6819208901	-1.0053499114	-1.9013789636
H53	5.1458525342	-2.9725737204	-1.6298113771
H54	2.4916648495	-0.3894343653	0.6148268425
H55	-3.6834870568	-2.8448499782	-0.5371843097
H56	-4.5824703046	-2.1323255980	-1.6584953519
H57	5.7425685833	3.8851233414	-0.9009601840
H58	6.4094763731	3.4349021257	0.4875588889
H59	-0.6863504459	-2.8670260824	-0.4850156490
H60	-0.1780707095	-1.4331112921	0.0803582414
H61	5.0310126852	1.4783130007	2.8871207440
H62	4.8437988584	3.0543295598	3.1470061623
H63	0.3623201578	-1.1270055927	-2.9464990972
H64	-0.4783242195	-0.1165605425	-3.8711123178
H65	1.1146078944	2.5953408960	1.2466465858
H66	1.8866759874	1.9586071345	2.5034931626
H67	-3.3206246832	-0.5007551815	-4.2758275498
H68	-3.5552788411	0.8512318324	-3.4485036920
H69	2.2333822996	4.8076672320	-0.2725703326
H70	2.7992232795	3.9718594046	-1.5230229123

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$\Delta r=2.1 \text{ \AA}$			
Atom	X	Y	Z
N1	4.0321647466	0.6160028705	0.0406847217
C2	5.2038949060	0.4799548887	-0.6479519514
C3	5.6036540908	-0.7383354558	-1.2023397329
C4	4.7818053848	-1.8588651798	-1.0659927670
C5	3.5608092756	-1.7378714200	-0.3579848239
C6	3.2366752774	-0.4780506668	0.1914653496
C7	2.6871061078	-2.8664209922	-0.2233299563
C8	1.9845045373	-3.8652155640	-0.1591610426
C9	1.1532329499	-5.0338825494	-0.0802794840
N10	-0.1908850964	-4.8291755152	0.0988864830
C11	-1.0060302020	-5.9104017411	0.1811512596
C12	-0.5463999998	-7.2303999966	0.0929999999
C13	0.8309725043	-7.4366843977	-0.0921204606
C14	1.6919841900	-6.3321940955	-0.1799337201
Zn15	-2.2672543949	-0.7671289055	-1.5909281713
O16	-3.4431935243	0.0155592924	-3.1511142545
Zn17	3.5525643298	2.6891796750	0.8227267303
O18	5.3519409536	3.5096654135	0.1231301480
N19	-2.6600378900	0.9434329845	-0.2885803249
C20	-2.0759082236	2.1617820947	-0.4293859608
C21	-2.3796640406	3.2449963656	0.4217111526
C22	-3.3379060831	3.0448152524	1.4432393389
C23	-3.9346044992	1.7891011220	1.5805558322
C24	-3.5753584777	0.7608571202	0.7073909470
C25	-1.7331789788	4.5091912504	0.2526456360
C26	-1.1919288688	5.5961812988	0.1254067604
C27	-0.5827378252	6.8824824968	-0.0446697456
N28	0.7650372252	6.9091632774	-0.2939272558
C29	1.3535473289	8.1159672437	-0.4903309790
C30	0.6493999998	9.3274999966	-0.4524999999
C31	-0.7267172106	9.2953981722	-0.1837999749
C32	-1.3536358895	8.0593949409	0.0249404586
O33	-0.5911207351	-0.4867926515	-2.8371414402
O34	-3.8428626068	-1.9856424224	-0.9169909441
O35	-0.9112629524	-1.7904272385	-0.3241702935
O36	2.4715735961	4.0622070421	-0.3877102633
O37	4.4250976480	2.4219069395	2.6956381276
O38	1.6714459154	2.2202199183	1.6874148678
H39	-1.3764648016	2.2858634824	-1.2477753601
H40	-3.5985061858	3.8606821045	2.1108263796
H41	-4.6713067988	1.6029878742	2.3558354183
H42	-4.0300669734	-0.2179389104	0.7742402469
H43	1.1714497077	10.2645402791	-0.6231607272
H44	2.4213473120	8.1011277563	-0.6844700935
H45	-2.4186163839	7.9976558464	0.2312369267
H46	-1.3032023037	10.2148767007	-0.1389119794
H47	1.2322611517	-8.4433215864	-0.1673051948
H48	-1.2413140143	-8.0615752085	0.1657807047
H49	-2.0611200256	-5.7020820736	0.3253687279
H50	2.7621492484	-6.4669414677	-0.3121007869
H51	5.8079784723	1.3708410940	-0.7471289184
H52	6.5444137372	-0.7989157593	-1.7410387081
H53	5.0651579557	-2.8127349700	-1.5003320559
H54	2.3257627421	-0.3339088720	0.7581104955
H55	-3.7985835706	-2.6933052001	-0.2424769264
H56	-4.7224572262	-1.9857259553	-1.3457198078
H57	5.4747958211	4.0476230319	-0.6859047909
H58	6.1320029346	3.6000513879	0.7081265082
H59	-0.7749737388	-2.7594739472	-0.3219901140
H60	-0.2556964052	-1.3326400830	0.2411027665
H61	4.7666687012	1.5833933939	3.0670299820
H62	4.5361468331	3.1513450225	3.3402514004
H63	0.1903452686	-1.0724765785	-2.7969903164
H64	-0.6630288265	-0.0719263632	-3.7214475123
H65	0.8480579464	2.6483477407	1.3790537805
H66	1.6122805431	2.0221332545	2.6452577267
H67	-3.5138077257	-0.4094392735	-4.0309326697
H68	-3.7204396906	0.9533763725	-3.2137357170

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H69	1.9358816404	4.8693454782	-0.1181186398
H70	2.5465679918	4.0573160721	-1.3633301120

$\Delta r=2.3 \text{ \AA}$			
Atom	X	Y	Z
N1	3.9871785237	0.6618492601	-0.0687885513
C2	5.1629301525	0.5022523668	-0.7457006273
C3	5.5605593736	-0.7286567920	-1.2704941179
C4	4.7336313051	-1.8415822841	-1.1137971322
C5	3.5079276305	-1.7020484451	-0.4173287601
C6	3.1852158209	-0.4268904439	0.1006081844
C7	2.6400647703	-2.8338661302	-0.2676462027
C8	1.9473558802	-3.8390261208	-0.1906949343
C9	1.1312685957	-5.0181703715	-0.0986447722
N10	-0.2166999371	-4.8286261969	0.0600747545
C11	-1.0217072638	-5.9155657686	0.1522892651
C12	-0.5463999998	-7.2303999972	0.0929999999
C13	0.8354751954	-7.4242445683	-0.0720604777
C14	1.6856292243	-6.3119283385	-0.1688763940
Zn15	-2.2953609245	-0.6030591591	-1.7300657399
O16	-3.4565691329	0.1762154208	-3.3019852222
Zn17	3.5512190982	2.7622082926	0.6666598510
O18	5.3749588270	3.5270216866	-0.0311387552
N19	-2.6785349324	1.1285018967	-0.4492537224
C20	-2.0888411602	2.3457663387	-0.5900518838
C21	-2.3970535234	3.4336051207	0.2563564840
C22	-3.3659766168	3.2353019048	1.2690211247
C23	-3.9684562864	1.9826286509	1.4040404692
C24	-3.6039570119	0.9512426242	0.5378909290
C25	-1.7490112074	4.7004777687	0.1059847989
C26	-1.2051812591	5.7893702239	0.0020293325
C27	-0.5892438637	7.0778963020	-0.1322518719
N28	0.7614326007	7.1042677360	-0.3619617601
C29	1.3598117822	8.3118823389	-0.5192869623
C30	0.6637999998	9.5268999972	-0.4590999999
C31	-0.7163603791	9.4951200471	-0.2100007535
C32	-1.3538143155	8.2577267378	-0.0425647692
O33	-0.6153235615	-0.3829286439	-2.9826140630
O34	-3.8823007588	-1.8063520221	-1.0531705419
O35	-0.9502623970	-1.6098302960	-0.4360881192
O36	2.5225013501	4.1417896842	-0.5842359997
O37	4.3997007000	2.5084320649	2.5523076924
O38	1.6485393611	2.3815742998	1.5281710414
H39	-1.3812176575	2.4635038546	-1.4021741544
H40	-3.618581954	4.0522952721	1.9332715764
H41	-4.7129691716	1.8014345935	2.1729535241
H42	-4.0609832067	-0.0265519875	0.6037900342
H43	1.1938398979	10.4646120094	-0.5985215244
H44	2.4300360063	8.2951055225	-0.6989946784
H45	-2.4211522553	8.1979355164	0.1522940668
H46	-1.2886748365	10.4162254796	-0.1483868330
H47	1.2488249185	-8.4273543471	-0.1243784902
H48	-1.2325521567	-8.0682628810	0.1725870335
H49	-2.0805995440	-5.7155898961	0.2794336763
H50	2.7583622281	-6.4369705390	-0.2895557454
H51	5.7732617847	1.3867256412	-0.8613264570
H52	6.5050364765	-0.8052233193	-1.8004891729
H53	5.0155519538	-2.8060834869	-1.5248276527
H54	2.2703059076	-0.2666227652	0.6566954213
H55	-3.8472526300	-2.5104828975	-0.3744093549
H56	-4.7604718393	-1.8013436920	-1.4847609959
H57	5.5178405005	4.0466441025	-0.8487567542
H58	6.1517892333	3.6096258636	0.5593392205
H59	-0.8088860957	-2.5778903183	-0.4114010754
H60	-0.2944146219	-1.1501229553	0.1271920480
H61	4.7166945257	1.6685728426	2.9420026644
H62	4.523344819	3.2465968703	3.1846117215
H63	0.1519791437	-0.9861426114	-2.9314483716

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H64	-0.6778147561	0.0173558724	-3.8743344601
H65	0.8423421388	2.8297823546	1.2036760978
H66	1.5768018014	2.2093742594	2.4902051877
H67	-3.5287444456	-0.2571219567	-4.1775318237
H68	-3.7238376341	1.1162222411	-3.3752637060
H69	2.0070461508	4.9683309512	-0.3348276371
H70	2.6082118373	4.1173815005	-1.5586600978

$\Delta r=2.5 \text{ \AA}$			
Atom	X	Y	Z
N1	4.2641110739	0.4844414477	-0.0263620120
C2	5.4385439783	0.2891749751	-0.6963021044
C3	5.8029455172	-0.9568528605	-1.2115455231
C4	4.9429990085	-2.0448727068	-1.0518982632
C5	3.7200619112	-1.8639648385	-0.3595637323
C6	3.4315225773	-0.5785205721	0.1476842085
C7	2.8093670636	-2.9597433166	-0.2057004491
C8	2.0785739920	-3.9369948379	-0.1327822748
C9	1.2168372556	-5.0830923427	-0.0553378490
N10	-0.1222997215	-4.8417609724	0.1078592936
C11	-0.9678492952	-5.8995090672	0.1798070708
C12	-0.5463999995	-7.2303999927	0.0929999998
C13	0.8265040280	-7.4758618714	-0.0769279330
C14	1.7198477291	-6.3962410204	-0.1515933341
Zn15	-2.1426036306	-0.4335171520	-1.6455852464
O16	-3.3149429585	0.3088755657	-3.2260487710
Zn17	3.8738064203	2.5960212583	0.6989649825
O18	5.7240971508	3.3140962799	0.0233762037
N19	-2.5726568991	1.3044032047	-0.3865079490
C20	-2.0110267426	2.5331203267	-0.5378674957
C21	-2.3507636461	3.6234148733	0.2918032876
C22	-3.3227163238	3.4179785823	1.3001037493
C23	-3.8979532225	2.1533292224	1.4457566253
C24	-3.5026605145	1.1190189613	0.5956113248
C25	-1.7250756407	4.8994814069	0.1274249219
C26	-1.1968481439	5.9949128958	0.0158423749
C27	-0.58774488151	7.2859692205	-0.1255315988
N28	0.7638412372	7.3080622317	-0.3459998360
C29	1.3690643343	8.5097043693	-0.5102750050
C30	0.6781999995	9.7262999927	-0.4656999998
C31	-0.7043348999	9.7018321096	-0.2259421569
C32	-1.3489657610	8.4688139225	-0.0517857785
O33	-0.4589205168	-0.2039029098	-2.8896691771
O34	-3.6924508383	-1.6855282753	-0.9698709867
O35	-0.7830439228	-1.4020715687	-0.3343744744
O36	2.9013165641	3.9967297628	-0.5744014105
O37	4.6915349464	2.3254891264	2.5956363256
O38	1.9458366943	2.2790287438	1.5306566718
H39	-1.3018521992	2.6583364072	-1.3471882728
H40	-3.6115333346	4.2382691524	1.9506090844
H41	-4.6445954773	1.9646553212	2.2107659329
H42	-3.9388345577	0.1323269754	0.6699959820
H43	1.2119123087	10.6612770083	-0.6098478114
H44	2.4403496400	8.4858894982	-0.6824373926
H45	-2.4178870745	8.4147983818	0.1368908174
H46	-1.2733289093	10.6256824885	-0.1765772485
H47	1.1993245630	-8.4934017867	-0.1503543500
H48	-1.2656478771	-8.0415421684	0.1571261043
H49	-2.0188360613	-5.6618820822	0.3110906555
H50	2.7862588702	-6.5613412711	-0.2810778963
H51	6.0729993392	1.1561321310	-0.8141985666
H52	6.7471174521	-1.0641339000	-1.7366249201
H53	5.1989297188	-3.0196841954	-1.4555736174
H54	2.5197058350	-0.3888493449	0.6993975479
H55	-3.6367068723	-2.3900322344	-0.2929793544
H56	-4.5707475338	-1.7038143810	-1.4009154541
H57	5.8901871464	3.8298414843	-0.7923629013
H58	6.4956969879	3.3762528271	0.6230289492

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H59	-0.6448715319	-2.3706472563	-0.3144347715
H60	-0.1416678089	-0.9234116076	0.2298569605
H61	4.9822232049	1.4789863527	2.9913035096
H62	4.8260405158	3.0616454357	3.2280931463
H63	0.3170791332	-0.7945278954	-2.8248028561
H64	-0.5206248526	0.1830893271	-3.7872797906
H65	1.1582112899	2.7490736833	1.1917674463
H66	1.8538200119	2.1132739387	2.4920598156
H67	-3.3754754769	-0.1328509287	-4.0982573116
H68	-3.6024786684	1.2422050916	-3.3071246090
H69	2.4037280473	4.8366991637	-0.3337773608
H70	3.0024383766	3.9688269499	-1.5473278785

$\Delta r=2.6 \text{ \AA}$			
Atom	X	Y	Z
N1	4.1791929621	0.5881976676	0.4039846525
C2	5.4021119621	0.3917210606	-0.1740578586
C3	5.7851030959	-0.8411927098	-0.7042322895
C4	4.9012048999	-1.9197161876	-0.6504329058
C5	3.6291196542	-1.7493180802	-0.0487150785
C6	3.3167974428	-0.4692777132	0.4687683666
C7	2.7203615123	-2.8617147866	0.0029517086
C8	2.0154943127	-3.8631246435	0.0041782028
C9	1.1814603732	-5.0383577465	0.0222649813
N10	-0.1546830912	-4.8422123028	0.2427182097
C11	-0.9844841015	-5.9139877589	0.2810778614
C12	-0.5463999972	-7.2303999618	0.0929999987
C13	0.8261278439	-7.4333985990	-0.1398865704
C14	1.7013875269	-6.3345217148	-0.1753715727
Zn15	-2.6241146904	-0.3929599008	-1.0937043868
O16	-4.0128531314	0.2186518257	-2.5563456908
Zn17	3.8117779929	2.7024812778	1.1500370243
O18	5.7679971144	3.3424658385	0.7796772506
N19	-2.8130515574	1.4870180068	0.0585084496
C20	-2.2422513513	2.6912393364	-0.2141935521
C21	-2.4725653960	3.8342116410	0.5814339341
C22	-3.3545243357	3.7164950646	1.6820311412
C23	-3.9506563985	2.4827474073	1.9472781218
C24	-3.6584267899	1.3916230144	1.1280309091
C25	-1.8149860041	5.0766166015	0.3110250645
C26	-1.2704963403	6.1567155041	0.1409455875
C27	-0.6303755690	7.4265601241	-0.0536809727
N28	0.7080538893	7.4099340535	-0.3391523857
C29	1.3385956129	8.5912375045	-0.5415472595
C30	0.6853999972	9.8258999618	-0.4689999987
C31	-0.6841902053	9.8425952303	-0.1634803558
C32	-1.3550466386	8.6301538384	0.0481664234
O33	-1.2425158258	-0.5491502169	-2.6608271367
O34	-4.1493924252	-1.4213266231	-0.1192279994
O35	-1.0434919174	-1.3080719216	0.0541663555
O36	3.2081973253	4.2807218475	-0.1966127235
O37	4.3643146083	2.3509595586	3.1263316326
O38	1.8077952595	2.8456261718	1.8412970048
H39	-1.5870871822	2.7429418737	-1.0752147193
H40	-3.5591138020	4.5798144123	2.3078433964
H41	-4.6321026048	2.3590649379	2.7834069526
H42	-4.1021599950	0.4229768998	1.3071208957
H43	1.2350838554	10.7463957793	-0.6445202642
H44	2.3988845118	8.5361196724	-0.7674009612
H45	-2.4142759706	8.6088219869	0.2908820709
H46	-1.2219536411	10.7835178816	-0.0920455616
H47	1.2153623574	-8.4360730543	-0.2920969336
H48	-1.2483505418	-8.0582970674	0.1287631140
H49	-2.0323715876	-5.7007702627	0.4656564001
H50	2.7665085715	-6.4755146817	-0.3390081794
H51	6.0637362885	1.2454407444	-0.2033956332
H52	6.7654538759	-0.9459625424	-1.1592897525
H53	5.1759472333	-2.8839184726	-1.0667655260

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H54	2.3582226434	-0.2808055712	0.9344763335
H55	-4.0876696217	-2.0539255078	0.6248395078
H56	-5.0647943008	-1.4010750780	-0.4643889399
H57	6.0783084571	3.9120030220	0.0459200217
H58	6.4618002342	3.2751756670	1.4673289953
H59	-0.8941178544	-2.2742729592	0.0965997450
H60	-0.2812840961	-0.8286445785	0.4388048977
H61	4.5568078091	1.4861659670	3.5419345182
H62	4.4770186776	3.0718171880	3.7802826206
H63	-0.5011911915	-1.1859718668	-2.6512171458
H64	-1.4728797833	-0.3087494884	-3.5819143199
H65	1.1300029549	3.4239392392	1.4384165327
H66	1.6371930312	2.7426928357	2.8007291956
H67	-4.2350743437	-0.3234892108	-3.3413329064
H68	-4.2981023086	1.1443473056	-2.7055010382
H69	2.6769010133	5.1041866703	0.0286075062
H70	3.5664879273	4.3747372613	-1.1023295922

$\Delta r=2.7 \text{ \AA}$			
Atom	X	Y	Z
N1	4.1062232792	0.6306156185	0.5000067820
C2	5.3450187178	0.4453800858	-0.0469174974
C3	5.7629750362	-0.7923122247	-0.5412277033
C4	4.8972796456	-1.8865391209	-0.4886578723
C5	3.6079211593	-1.7264590200	0.0785523798
C6	3.2653212809	-0.4436508496	0.5643947650
C7	2.6986004089	-2.8398329826	0.1299557293
C8	1.9955608840	-3.8425091948	0.1164455387
C9	1.1641415297	-5.0207461153	0.1032018417
N10	-0.1783453844	-4.8382552065	0.3038886126
C11	-0.9973761117	-5.9201622206	0.3019154509
C12	-0.5463999997	-7.2303999964	0.0929999999
C13	0.8317754194	-7.4158570162	-0.1179049039
C14	1.6971499984	-6.3087046162	-0.1126185137
Zn15	-2.6671799011	-0.3369959891	-1.0149709528
O16	-4.1077107806	0.2997495869	-2.4162332030
Zn17	3.6725890478	2.7787584064	1.1601071282
O18	5.6291153117	3.4380863823	0.8279897186
N19	-2.7885956240	1.5491318819	0.1511739982
C20	-2.1995580014	2.7446887464	-0.1337582075
C21	-2.3877686684	3.8937398960	0.6672672174
C22	-3.2499366053	3.7898919792	1.7860776827
C23	-3.8631905050	2.5670877979	2.0643316139
C24	-3.6116142605	1.4698818151	1.2390339065
C25	-1.7264425371	5.1354416428	0.3860802599
C26	-1.1919829727	6.2206919515	0.2056727079
C27	-0.5758744175	7.5030065233	-0.0078061116
N28	0.7586814185	7.5084990316	-0.3124431376
C29	1.3652219670	8.6989609576	-0.5382684776
C30	0.6925999997	9.9255999964	-0.4722999999
C31	-0.6736184684	9.9207920964	-0.1500620069
C32	-1.3193240188	8.6971645030	0.0865687463
O33	-1.3714658135	-0.4946664742	-2.6534198591
O34	-4.1582613902	-1.3550178510	0.0155607693
O35	-1.0817183168	-1.2833205346	0.1078108046
O36	3.1147070172	4.3778972120	-0.2057671087
O37	4.1868574092	2.4372383978	3.1517684088
O38	1.6677187902	2.9860902319	1.8435997523
H39	-1.5684737133	2.7850979166	-1.0135989059
H40	-3.4235470799	4.6553030733	2.4186950590
H41	-4.5294375105	2.4566634197	2.9144531947
H42	-4.0760561169	0.5115860484	1.4233002118
H43	1.2250338064	10.8525552745	-0.6656950020
H44	2.4228738336	8.6589243302	-0.7788399408
H45	-2.3770280065	8.6609952474	0.3343871461
H46	-1.2285003534	10.8520437905	-0.0831199068
H47	1.2333128824	-8.4113275580	-0.2850901736
H48	-1.2421047749	-8.0642619796	0.0970751737

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H49	-2.0503952943	-5.7205996052	0.4718533909
H50	2.7654823970	-6.4372556242	-0.2666476919
H51	5.9904810042	1.3111813188	-0.0801503997
H52	6.7552869047	-0.8883789550	-0.9715609630
H53	5.2011391157	-2.8534192308	-0.8775778935
H54	2.2942112144	-0.2775184579	1.0068660738
H55	-4.0719882115	-1.9929433379	0.7526377485
H56	-5.0865694458	-1.3239285402	-0.2923513939
H57	5.9533600391	3.9887796193	0.0859108157
H58	6.3039134677	3.4010938825	1.5364814241
H59	-0.9454352237	-2.2511841831	0.1560543183
H60	-0.3146637990	-0.8039775686	0.4827081857
H61	4.3780034111	1.5744143296	3.5720736403
H62	4.2839180243	3.1608730579	3.8051458266
H63	-0.6374311327	-1.1390082200	-2.6873151708
H64	-1.6458678128	-0.2443162656	-3.5596923609
H65	0.9897890316	3.5419227396	1.4104327992
H66	1.4994838577	2.9393638120	2.8077858248
H67	-4.3741241856	-0.2414608970	-3.1880452211
H68	-4.3836711086	1.2297594803	-2.5556880909
H69	2.5593365636	5.1929208200	-0.0096876314
H70	3.5266191626	4.4882898551	-1.0864766132

$\Delta r=2.8 \text{ \AA}$			
Atom	X	Y	Z
N1	4.1702417771	0.5683054910	0.6869609271
C2	5.3980306214	0.3773625728	0.1157949532
C3	5.8031583909	-0.8557169006	-0.3988988864
C4	4.9322235042	-1.9443394508	-0.3466022554
C5	3.6532469572	-1.7765210804	0.2376825325
C6	3.3207864588	-0.4994054747	0.7466581070
C7	2.7370705839	-2.8819613724	0.2683908807
C8	2.0247114824	-3.8773475246	0.2313251756
C9	1.1830063999	-5.0441518273	0.1821030832
N10	-0.1617540804	-4.8474974305	0.3502957359
C11	-0.9911999888	-5.9201520136	0.3101276334
C12	-0.5463999995	-7.2303999932	0.0929999998
C13	0.8338744666	-7.4304942682	-0.0842254563
C14	1.7098054242	-6.3336355405	-0.0388281916
Zn15	-2.5895009917	-0.3043107131	-0.8591595313
O16	-4.0322264217	0.3320984631	-2.2596034329
Zn17	3.7918457621	2.7398069608	1.3535764019
O18	5.7390670717	3.3583393718	0.9075002969
N19	-2.6942803817	1.6100395536	0.2785817310
C20	-2.0963847918	2.7972116107	-0.0233050248
C21	-2.2759187506	3.9593624253	0.7595513115
C22	-3.1374087386	3.8794509219	1.8807165453
C23	-3.7576483283	2.6650389299	2.1790483620
C24	-3.5155524727	1.5539100002	1.3694016392
C25	-1.6140395813	5.1941030202	0.4491314517
C26	-1.0927544313	6.2819591256	0.2491949239
C27	-0.5056273134	7.5744736556	0.0149684364
N28	0.8296682195	7.6120437419	-0.2837704803
C29	1.4047283945	8.8156903482	-0.5236307685
C30	0.6997999995	10.0252999932	-0.4755999998
C31	-0.6676755931	9.9857922363	-0.1604769894
C32	-1.2812423055	8.7487961714	0.0890338782
O33	-1.3064822563	-0.4955858115	-2.5019411425
O34	-4.0843768902	-1.2863812831	0.1961272296
O35	-1.0126257166	-1.2677452786	0.2642729269
O36	3.1849044000	4.3997920131	0.0601835604
O37	4.4339767850	2.3283482414	3.2988748222
O38	1.9045843793	3.1318646648	2.2578712906
H39	-1.4642299273	2.8204212265	-0.9027982221
H40	-3.3046698710	4.7566373210	2.4986155393
H41	-4.4235939170	2.5722318969	3.0315854052
H42	-3.9851512076	0.6015418507	1.5704615532
H43	1.2086356752	10.9632934557	-0.6790477223

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H44	2.4642367727	8.8011250417	-0.7589483365
H45	-2.3380944987	8.6869455857	0.3354237692
H46	-1.2496904048	10.9013253946	-0.1080197858
H47	1.2267593641	-8.4286330208	-0.2557390841
H48	-1.2497577499	-8.0574156269	0.0662295842
H49	-2.0463875148	-5.7123971054	0.4542195805
H50	2.7802426035	-6.4691569658	-0.1710417170
H51	6.0513113369	1.2371029980	0.0833187005
H52	6.7886226221	-0.9506934382	-0.8449481024
H53	5.2232969898	-2.9091309700	-0.7504891735
H54	2.3499753320	-0.3417644624	1.1971742933
H55	-4.0010582614	-1.9138277298	0.9424846996
H56	-5.0134161222	-1.2498367035	-0.1089319606
H57	6.0329045996	3.9007557521	0.1468444165
H58	6.4535163648	3.3034047606	1.5747638780
H59	-0.8887508048	-2.2363372517	0.3292774346
H60	-0.2406189503	-0.7976302778	0.6405240866
H61	4.6301342192	1.4478430691	3.6781215014
H62	4.6013357124	3.0276203347	3.9644280582
H63	-0.5753436012	-1.1435452897	-2.5317431824
H64	-1.5866676199	-0.2584894392	-3.4100196703
H65	1.2151544237	3.7167818874	1.8854703374
H66	1.8517623848	3.1276575111	3.2363118395
H67	-4.3150616433	-0.2207338872	-3.0171800102
H68	-4.2945229111	1.2635852419	-2.4147458919
H69	2.6482348796	5.2138483508	0.3060442446
H70	3.5619264152	4.5323158793	-0.8329984399

$\Delta r=2.9 \text{ \AA}$			
Atom	X	Y	Z
N1	4.1572173072	0.5943723495	0.6554360644
C2	5.3882753980	0.3958152232	0.0932515709
C3	5.7958118616	-0.8428021590	-0.4061078050
C4	4.9246975870	-1.9314720663	-0.3471780374
C5	3.6423068109	-1.7584352103	0.2284623028
C6	3.3089758543	-0.4746937271	0.7217673161
C7	2.7256336130	-2.8657785132	0.2665167650
C8	2.0158533605	-3.8635828465	0.2324052920
C9	1.1774412578	-5.0351900344	0.1832366759
N10	-0.1689196680	-4.8449934055	0.3473019274
C11	-0.9946539855	-5.9208278038	0.3061611441
C12	-0.5463999999	-7.2303999987	0.0930000000
C13	0.8357917139	-7.4246909825	-0.0794539651
C14	1.7081453512	-6.3240193037	-0.0336163235
Zn15	-2.5780846266	-0.1944118282	-0.9223170398
O16	-4.0305437799	0.4486562065	-2.3105310815
Zn17	3.7941270435	2.7850681625	1.2969615570
O18	5.7491189986	3.3819672067	0.8537644740
N19	-2.6860765168	1.7110164180	0.2333347719
C20	-2.0890435506	2.9002989832	-0.0595035600
C21	-2.2679190803	4.0553276717	0.7337374791
C22	-3.1274248352	3.9663832214	1.8553925524
C23	-3.7466574682	2.7491101260	2.1444246006
C24	-3.5053857469	1.6452050497	1.3249408965
C25	-1.6063810340	5.2923059259	0.4338650523
C26	-1.0842871426	6.3811388068	0.2419701221
C27	-0.4975870718	7.6741841916	0.0122295385
N28	0.8377913699	7.7123774890	-0.2842926559
C29	1.4128617573	8.9156658161	-0.5237767955
C30	0.7069999999	10.1249999987	-0.4789000000
C31	-0.6609918005	10.0848530504	-0.1662787286
C32	-1.2742948430	8.8480568356	0.0836795632
O33	-1.3069160826	-0.3629936248	-2.5754046195
O34	-4.0609297819	-1.1975743010	0.1286229067
O35	-1.0039535724	-1.1597599747	0.2009134091
O36	3.2094207991	4.4605542003	0.0046441066
O37	4.4310539545	2.3626921576	3.2439981257
O38	1.9251304483	3.2556697253	2.2044043451

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H39	-1.4576702518	2.9302304769	-0.9391359691
H40	-3.2940698396	4.8383563021	2.4807459720
H41	-4.4111991533	2.6487533117	2.9972120529
H42	-3.9734765275	0.6905752902	1.5189886232
H43	1.2150416537	11.0635988339	-0.6815294016
H44	2.4727535980	8.9008561176	-0.7572679910
H45	-2.3323268970	8.7855160623	0.3248186014
H46	-1.2434818323	11.0003570850	-0.1168361640
H47	1.2340314284	-8.4211721453	-0.2479791329
H48	-1.2477559567	-8.0591828832	0.0655165778
H49	-2.0510204426	-5.7165419647	0.4467186001
H50	2.7793349096	-6.4565909259	-0.1627676503
H51	6.0409686761	1.2556334765	0.0528814343
H52	6.7842320519	-0.9426289319	-0.8445298044
H53	5.2176539010	-2.9004246919	-0.7394883963
H54	2.3371328310	-0.3138967277	1.1661201180
H55	-3.9692101618	-1.8324561662	0.8676730672
H56	-4.9915920369	-1.1647281293	-0.1717010137
H57	6.0511237686	3.9150665373	0.0896392195
H58	6.4604289535	3.3249440285	1.5241801421
H59	-0.8763226439	-2.1281864732	0.2611017239
H60	-0.2346758720	-0.6885594806	0.5812900166
H61	4.6131477714	1.4781158190	3.6206871838
H62	4.6121524181	3.0576917833	3.9103905777
H63	-0.5706869060	-1.0045672560	-2.6162184087
H64	-1.5955510347	-0.1213361241	-3.4796532457
H65	1.2506948118	3.8513123884	1.8217706783
H66	1.8775101815	3.2737975126	3.1829112363
H67	-4.3169867813	-0.0997977259	-3.0699563260
H68	-4.2959517919	1.3805515702	-2.4577695568
H69	2.6797476802	5.2800222226	0.2475001964
H70	3.5919952014	4.5927309449	-0.8862305347

Δr=3.0 Å			
Atom	X	Y	Z
N1	3.9795354699	0.7086473770	0.3844485296
C2	5.2357870175	0.4912435608	-0.1125963514
C3	5.6814992592	-0.7684218007	-0.5151184443
C4	4.8227351446	-1.8632459767	-0.4243536126
C5	3.5146702903	-1.6731692439	0.0846150815
C6	3.1417050743	-0.3677158269	0.4840664870
C7	2.6225002042	-2.7969555001	0.1512961844
C8	1.9423883315	-3.8148089040	0.1445214079
C9	1.1323887512	-5.0053219688	0.1251398901
N10	-0.2171565381	-4.8352643224	0.2762717764
C11	-1.0223574221	-5.9255541862	0.2631036241
C12	-0.5463999996	-7.2303999951	0.0929999998
C13	0.8398208651	-7.4055705348	-0.0654387046
C14	1.6911058083	-6.2884286546	-0.0487772431
Zn15	-2.7392646766	-0.0230166079	-1.3042715391
O16	-4.2078642160	0.7016803809	-2.6369460125
Zn17	3.6161386750	2.9570522421	0.8568928159
O18	5.5881682615	3.5053758022	0.4237723216
N19	-2.8074582574	1.8531376274	-0.0957896980
C20	-2.1873424639	3.0397948554	-0.3432172060
C21	-2.3594157689	4.1690582352	0.4872811502
C22	-3.2403583868	4.0597626816	1.5902739841
C23	-3.8853958340	2.8455067679	1.8293690350
C24	-3.6461550586	1.7650936853	0.9792815345
C25	-1.6698583315	5.4011286679	0.2430691665
C26	-1.1244657405	6.4853564600	0.1014734165
C27	-0.5181647001	7.7758901438	-0.0743472532
N28	0.8267088361	7.8091334893	-0.3247165033
C29	1.4160768009	9.0132196180	-0.5213652328
C30	0.7141999996	10.2246999951	-0.4821999998
C31	-0.6630862349	10.1880600298	-0.2146463782
C32	-1.2909481428	8.9519342169	-0.0066288284
O33	-1.5214503994	-0.1680686100	-2.9966741948

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O34	-4.2171889054	-1.0280913823	-0.2465144364
O35	-1.1646239346	-0.9738274001	-0.1672271962
O36	3.0876676256	4.5754347846	-0.5452532040
O37	4.2135157959	2.6351446264	2.8387945988
O38	1.7683241450	3.5776179160	1.7219840799
H39	-1.5465907108	3.0896519898	-1.2156206591
H40	-3.4015812950	4.9137556121	2.2413206208
H41	-4.5668391945	2.7297826371	2.6666734614
H42	-4.1368693349	0.8142171602	1.1303996759
H43	1.2330459518	11.1643386330	-0.6494520099
H44	2.4831225657	8.9968482068	-0.7191847070
H45	-2.3577510490	8.8904705554	0.1920028382
H46	-1.2417195513	11.1063214084	-0.1721506820
H47	1.2563210594	-8.3996309079	-0.2005685416
H48	-1.2306723340	-8.0738008887	0.0864226496
H49	-2.0832914457	-5.7367205342	0.3916176011
H50	2.7656499748	-6.4032637219	-0.1669823685
H51	5.8786496338	1.3563134210	-0.1824528947
H52	6.6895616052	-0.8790005436	-0.9034481013
H53	5.1435849642	-2.8506454093	-0.7414028939
H54	2.1475790966	-0.1901882779	0.8788178275
H55	-4.1189048271	-1.6884376316	0.4690683900
H56	-5.1543693317	-0.9686930175	-0.5215229331
H57	5.9164345171	3.9831714979	-0.3657552519
H58	6.2820277157	3.4835699040	1.1142271149
H59	-1.0241052565	-1.9401635172	-0.1025827854
H60	-0.4003744957	-0.4992741565	0.2191380472
H61	4.3731629146	1.7695739795	3.2663975735
H62	4.4018595027	3.3601250555	3.4703333520
H63	-0.8051172474	-0.8262458994	-3.0914112585
H64	-1.8294442328	0.1185141136	-3.8811821719
H65	1.1094819357	4.1551998727	1.2880906511
H66	1.7223825818	3.6838918987	2.6949439118
H67	-4.5258385983	0.1872210733	-3.4074893815
H68	-4.4558339609	1.6437153487	-2.7451415536
H69	2.5561109277	5.4099667501	-0.3663601169
H70	3.5030491902	4.6599593431	-1.4271100889

Δr=3.1 Å			
Atom	X	Y	Z
N1	4.0619273808	0.6466652200	0.7969625884
C2	5.3668477807	0.3899836895	0.4851303575
C3	5.8224931887	-0.8935493287	0.1736050671
C4	4.9230570124	-1.9616115068	0.1627431470
C5	3.5615604385	-1.7223879790	0.4751434376
C6	3.1851166022	-0.3967958010	0.7911391738
C7	2.6208800869	-2.8072633095	0.4419654835
C8	1.9103507542	-3.8016020070	0.3647649809
C9	1.0989053527	-4.9877017279	0.2728548388
N10	-0.2586184478	-4.8192261873	0.1899742640
C11	-1.0469891746	-5.9209621230	0.1086995500
C12	-0.5463999964	-7.2303999495	0.0929999983
C13	0.8461016887	-7.3990591134	0.1737430082
C14	1.6790652028	-6.2729803687	0.2660760106
Zn15	-2.9279753590	0.1269762462	-0.9234383746
O16	-4.5302634310	0.9194622574	-2.0416153335
Zn17	3.7000524959	2.9918926467	1.1961759673
O18	5.7002090340	3.5133509257	0.9066600820
N19	-2.8438558159	1.9831406067	0.3203218605
C20	-2.2289501529	3.1548588973	0.0009336220
C21	-2.2968736159	4.2969514064	0.8282628013
C22	-3.0609021384	4.2141000968	2.0171746471
C23	-3.6944293950	3.0113871129	2.3376771050
C24	-3.5641693053	1.9182292122	1.4792546340
C25	-1.6179758895	5.5154463089	0.4922976459

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C26	-1.0837846331	6.5949884106	0.2782990768
C27	-0.4897577864	7.8810592997	0.0280923059
N28	0.8379951685	7.9073115782	-0.3028657764
C29	1.4157904366	9.1086186530	-0.5522565792
C30	0.7213999964	10.3243999495	-0.4854999983
C31	-0.6390307328	10.2929867658	-0.1406236324
C32	-1.2554493262	9.0603760155	0.1206370534
O33	-1.8861499024	0.0309653135	-2.7174989127
O34	-4.2659053420	-0.9190570804	0.2728348113
O35	-1.2494125245	-0.8948046884	0.0113768533
O36	3.2566947698	4.7877164869	-0.0912301230
O37	4.2479927223	2.4881111127	3.1771842563
O38	1.8974736826	3.6627388287	2.1287271362
H39	-1.6759042006	3.1817665629	-0.9302489606
H40	-3.1446419523	5.0784666042	2.6691043049
H41	-4.2850155520	2.9146851315	3.2436619894
H42	-4.0432572551	0.9737056198	1.6967699565
H43	1.2336430099	11.2585182255	-0.6982326263
H44	2.4692524633	9.0866457632	-0.8129857537
H45	-2.3069063543	9.0058610181	0.3903829104
H46	-1.2146318170	11.2118656086	-0.0755352010
H47	1.2820227735	-8.3938778575	0.1659520116
H48	-1.2217034375	-8.0780473750	0.0224994555
H49	-2.1153687314	-5.7419835836	0.0495040777
H50	2.7584715318	-6.3830122510	0.3319757664
H51	6.0350686431	1.2388229461	0.4855557361
H52	6.8710253475	-1.0462661774	-0.0645464759
H53	5.2546432539	-2.9653473601	-0.0845654778
H54	2.1620357181	-0.1703520863	1.0624887133
H55	-4.0788514521	-1.5915731530	0.9588431108
H56	-5.2261806456	-0.8894732767	0.0871109735
H57	6.0923183845	3.9930655073	0.1479767320
H58	6.3427945679	3.4637498298	1.6436196530
H59	-1.1364091987	-1.8667361555	0.0264954663
H60	-0.4436219247	-0.4566240734	0.3537961800
H61	4.3280988103	1.5769601769	3.5247804267
H62	4.5193900381	3.1302162800	3.8656290766
H63	-1.2097442102	-0.6376098185	-2.9431245396
H64	-2.2579617777	0.4195741757	-3.5360472041
H65	1.1967141182	4.2243874079	1.7422102236
H66	1.8596145072	3.6930639942	3.1072913841
H67	-4.9716046820	0.4341332212	-2.7691238570
H68	-4.7743619704	1.8677765860	-2.0821306128
H69	2.7053649881	5.6023735641	0.1174089399
H70	3.7503372865	4.9545951974	-0.9192826935

Δr=3.2 Å			
Atom	X	Y	Z
N1	4.0543179331	0.6292177318	0.7759661115
C2	5.3635884084	0.3950343940	0.4653229244
C3	5.8415984229	-0.8825572885	0.1619489745
C4	4.9612390686	-1.9667833323	0.1577873556
C5	3.5958777449	-1.7499558616	0.4688127545
C6	3.1970053137	-0.4299838967	0.7776464915
C7	2.6650606548	-2.8422988614	0.4378739922
C8	1.9519579575	-3.8339979022	0.3625982694
C9	1.1285600373	-5.0110002423	0.2720287636
N10	-0.2257891844	-4.8247014898	0.1833660923
C11	-1.0293864477	-5.9144221500	0.1021065666
C12	-0.5463999999	-7.2303999986	0.0930000000
C13	0.8435624817	-7.4172539732	0.1796933780
C14	1.6918903996	-6.3031672072	0.2715552488
Zn15	-2.8916445352	0.1461969558	-0.9424879801
O16	-4.4947752882	0.9346546359	-2.0622403403
Zn17	3.6545939319	2.9861048725	1.1359185329
O18	5.6465330078	3.5340729396	0.8416451407
N19	-2.7910128459	2.0246519412	0.2751438316
C20	-2.1717334999	3.1957685124	-0.0504903512

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C21	-2.2425157359	4.3465037604	0.7693728690
C22	-3.0142042903	4.2670795778	1.9546062720
C23	-3.6490999414	3.0670579614	2.2807402110
C24	-3.5162213098	1.9681062550	1.4309178995
C25	-1.5723527739	5.5754131577	0.4409042508
C26	-1.0495769617	6.6635046235	0.2370611897
C27	-0.4680330414	7.9612672072	0.0003676635
N28	0.8640300851	8.0059953420	-0.3123771065
C29	1.4338823630	9.2142867453	-0.5494072313
C30	0.7285999999	10.4240999986	-0.4888000000
C31	-0.6364793442	10.3762031901	-0.1620208009
C32	-1.2446545031	9.1350361769	0.0864837355
O33	-1.8606157494	0.0134071058	-2.7399658687
O34	-4.2289297435	-0.8785281039	0.2722336801
O35	-1.2276452302	-0.9014199907	-0.0076058247
O36	3.1567703969	4.7483401321	-0.1761407277
O37	4.2137250307	2.5407025311	3.1275206427
O38	1.8321164637	3.6295041852	2.0486282328
H39	-1.6154070013	3.2158293198	-0.9803208631
H40	-3.1029133156	5.1342172533	2.6021951482
H41	-4.2438944630	2.9775807000	3.1846823350
H42	-3.9987019417	1.0259786649	1.6517827044
H43	1.2346712865	11.3638130724	-0.6907501774
H44	2.4910071866	9.2027604510	-0.7955354414
H45	-2.2993195572	9.0710376640	0.3412117631
H46	-1.2228754861	11.2885272989	-0.1012689430
H47	1.2659633255	-8.4179671336	0.1770400521
H48	-1.2322727204	-8.0695328121	0.0223862981
H49	-2.0947820048	-5.7188693280	0.0381310278
H50	2.7695013677	-6.4272455286	0.3417645101
H51	6.0167841067	1.2567094355	0.4546297066
H52	6.8925263319	-1.0185374101	-0.0758386617
H53	5.3108859851	-2.9657849753	-0.0837638990
H54	2.1697707924	-0.2207765280	1.0453581634
H55	-4.0410258249	-1.5433879173	0.9653965729
H56	-5.1899475247	-0.8474484604	0.0904294727
H57	6.0323431021	4.0080968057	0.0761831001
H58	6.2885498376	3.5052208745	1.5801561281
H59	-1.1298794676	-1.8749326865	0.0146629153
H60	-0.4220704993	-0.4595027883	0.3303905489
H61	4.3110697382	1.6394427932	3.4957595227
H62	4.4747894011	3.2035861228	3.8000350800
H63	-1.1921129763	-0.6653268035	-2.9587447133
H64	-2.2313588290	0.3948808149	-3.5622886935
H65	1.1215667344	4.1706181875	1.6507281213
H66	1.7863581995	3.6684296696	3.0265901533
H67	-4.9443366002	0.4426757956	-2.7801327260
H68	-4.7330064331	1.8839073645	-2.1138458532
H69	2.5813325358	5.5487923611	0.0221752757
H70	3.6456438133	4.9165323246	-1.0067792466

$\Delta r=3.3 \text{ \AA}$			
Atom	X	Y	Z
N1	3.9971358707	0.6453818710	0.5172102153
C2	5.3092425797	0.4225482364	0.2059731251
C3	5.8072363414	-0.8536710206	-0.0660071365
C4	4.9437173180	-1.9497583321	-0.0376039523
C5	3.5773831364	-1.7430156945	0.2719325925
C6	3.1538948910	-0.4243832249	0.5483446307
C7	2.6635755392	-2.8462951286	0.2756937182
C8	1.9539721534	-3.8412267066	0.2362714207
C9	1.1288067756	-5.0159364796	0.1891699581
N10	-0.2245306739	-4.8265443523	0.0956430635
C11	-1.0297173000	-5.9162104041	0.0543820134
C12	-0.5463999998	-7.2303999974	0.0929999999
C13	0.8418828794	-7.4209297676	0.1848215113
C14	1.6919660002	-6.3069008637	0.2349527509
Zn15	-2.9224334687	0.1547024065	-1.1697518014

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O16	-4.5094489246	0.9073826249	-2.3345174597
Zn17	3.5900587484	2.9576702074	0.8460312933
O18	5.5527661719	3.5714483615	0.5119256903
N19	-2.8158425229	2.0861820871	-0.0125259732
C20	-2.1871106282	3.2591043055	-0.3245695164
C21	-2.2991956179	4.4189519176	0.4801065993
C22	-3.1277037730	4.3486353727	1.6278202244
C23	-3.7744998908	3.1517640929	1.9370869911
C24	-3.5957679122	2.0432006062	1.1087903319
C25	-1.6178311946	5.6516310712	0.1852250242
C26	-1.0886133298	6.7450964363	0.0314474746
C27	-0.4950858821	8.0495765303	-0.1368823578
N28	0.8543347917	8.1014511159	-0.3588848293
C29	1.4414333656	9.3122505243	-0.5294671730
C30	0.7357999998	10.5236999974	-0.4920999999
C31	-0.6479245336	10.4682377627	-0.2553781333
C32	-1.2731734840	9.2235209672	-0.0752260130
O33	-1.8941972592	-0.0580789833	-2.9620991700
O34	-4.2852080776	-0.8062593930	0.0691669293
O35	-1.2766684265	-0.9179611553	-0.2146943644
O36	2.9791523345	4.6889650169	-0.4582666894
O37	4.2118524094	2.5395902663	2.8278547069
O38	1.7687770526	3.5295087680	1.8022220381
H39	-1.5941173218	3.2738324307	-1.2317023233
H40	-3.2482909502	5.2230164123	2.2603692552
H41	-4.4121354853	3.0715047875	2.8122192556
H42	-4.0901787064	1.1046986352	1.3166209168
H43	1.2532929266	11.4674524475	-0.6377240545
H44	2.5127947910	9.3006014868	-0.7035398686
H45	-2.3423195668	9.1584267253	0.1084201864
H46	-1.2380890532	11.3792905033	-0.2145835106
H47	1.2590678607	-8.4232003283	0.2179807118
H48	-1.2328228107	-8.0711959903	0.0536735059
H49	-2.0950137515	-5.7226834010	-0.0165317950
H50	2.7693945813	-6.4289512623	0.3078505697
H51	5.9524333944	1.2908430880	0.1693272133
H52	6.8591922427	-0.9782987577	-0.3050332706
H53	5.3068335635	-2.9493691188	-0.2545860159
H54	2.1189548689	-0.2360127005	0.8116370287
H55	-4.1124761540	-1.4409348176	0.7937384227
H56	-5.2430762792	-0.7789257972	-0.1296028226
H57	5.9082576247	4.0528384825	-0.2634736792
H58	6.2075614455	3.5700009718	1.2397788542
H59	-1.1789897452	-1.8912155538	-0.1833961019
H60	-0.4671729261	-0.4686077927	0.1033440756
H61	4.3506038410	1.6432182172	3.1949221873
H62	4.4661139799	3.2126697798	3.4928215456
H63	-1.2328895069	-0.7514870198	-3.1553573702
H64	-2.2605322813	0.2968125414	-3.7981533241
H65	1.0312310295	4.0492215668	1.4255944436
H66	1.7404211674	3.5515919520	2.7814022983
H67	-4.9558359833	0.3899433454	-3.0362936686
H68	-4.7434639984	1.8547789971	-2.4253433896
H69	2.3680257950	5.4601948696	-0.2507762982
H70	3.4448700630	4.8786896106	-1.2975465889

$\Delta r=3.4 \text{ \AA}$			
Atom	X	Y	Z
N1	3.9823875289	0.6769242925	0.4046488611
C2	5.2919125898	0.4539371898	0.0811552593
C3	5.7879070890	-0.8177052247	-0.2162352819
C4	4.9271829720	-1.9159612334	-0.1961895057
C5	3.5639719571	-1.7142242892	0.1271538300
C6	3.1412703404	-0.3979842616	0.4220855645
C7	2.6541066835	-2.8240188958	0.1416075162
C8	1.9484035374	-3.8242202400	0.1245052558
C9	1.1274888071	-5.0059343596	0.1127170232
N10	-0.2284122963	-4.8241185710	0.0417704993

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C11	-1.0321209421	-5.9167317038	0.0372314274
C12	-0.5463999998	-7.2303999968	0.0929999999
C13	0.8447664663	-7.4139534423	0.1618664460
C14	1.6934353064	-6.2958422901	0.1731560342
Zn15	-2.9126179203	0.2421871543	-1.3015212533
O16	-4.5101320662	0.9770967151	-2.4632110122
Zn17	3.6189235562	2.9916134053	0.8075715656
O18	5.5862043263	3.5843101648	0.4643561608
N19	-2.8265975890	2.1756686598	-0.1304420979
C20	-2.2025924853	3.3555748195	-0.4282054990
C21	-2.3267546052	4.5117931514	0.3796064647
C22	-3.1661186402	4.4334218638	1.5187376841
C23	-3.8102851297	3.2314465552	1.8145335063
C24	-3.6175641557	2.1265143236	0.9834287410
C25	-1.6419353565	5.7474291600	0.0975990724
C26	-1.1098672171	6.8428552998	-0.0379138050
C27	-0.5094343171	8.1486616217	-0.1832910589
N28	0.8436757288	8.1979323915	-0.3838636439
C29	1.4408763605	9.4071474349	-0.5328666525
C30	0.7429999998	10.6233999968	-0.4953999999
C31	-0.6449316140	10.5702112818	-0.2796585539
C32	-1.2807449199	9.3270934796	-0.1214417033
O33	-1.8829039597	0.0545539574	-3.0969277183
O34	-4.2584512414	-0.7467375813	-0.0660421658
O35	-1.2719266402	-0.8519104944	-0.3577050798
O36	3.0256239326	4.7959110196	-0.4045825004
O37	4.2696594784	2.4986390515	2.7648039054
O38	1.8283532702	3.5787707573	1.8114707732
H39	-1.5988826037	3.3783013040	-1.3272903221
H40	-3.2965403845	5.3047026392	2.1535293848
H41	-4.4568558579	3.1430641558	2.6823343696
H42	-4.1076233408	1.1845090372	1.1849089877
H43	1.2678641235	11.5655762048	-0.6237351567
H44	2.5147611630	9.3903518840	-0.6899802132
H45	-2.3531587528	9.2674046187	0.0450249283
H46	-1.2322688169	11.4830939576	-0.2384463067
H47	1.2667735039	-8.4137383628	0.2072782637
H48	-1.2325976102	-8.0722957323	0.0833663394
H49	-2.0989271536	-5.7250650872	-0.0167714399
H50	2.7723483215	-6.4149173463	0.2303320964
H51	5.9369890108	1.3206045429	0.0553558966
H52	6.8384773108	-0.9379981365	-0.4635495748
H53	5.2894956094	-2.9117189755	-0.4323651036
H54	2.1071953583	-0.2253119283	0.6946037101
H55	-4.0720992032	-1.3812807825	0.6553054506
H56	-5.2168102420	-0.7370329716	-0.2642667520
H57	5.9393914243	4.0815166774	-0.3020744803
H58	6.2500684006	3.5530204916	1.1833198992
H59	-1.1702110268	-1.8250271068	-0.3345563738
H60	-0.4655854831	-0.4017917097	-0.0328122265
H61	4.3995644385	1.5882933509	3.0992512956
H62	4.5480915227	3.1444981866	3.4467971856
H63	-1.2115323730	-0.6279570710	-3.2944753551
H64	-2.2550627744	0.4087298078	-3.9306015235
H65	1.0960049982	4.1245774636	1.4625718510
H66	1.8164762451	3.5716952379	2.7912342565
H67	-4.9503568739	0.4555595186	-3.1658489213
H68	-4.7577706964	1.9213639406	-2.5506680050
H69	2.4342678740	5.5695937483	-0.1534168634
H70	3.4836086198	5.0155891666	-1.2407109343

$\Delta r=3.5 \text{ \AA}$			
Atom	X	Y	Z
N1	3.8967865651	0.7401526827	0.5561560904
C2	5.2108571012	0.5215895943	0.2478048390
C3	5.7213115588	-0.7523190480	-0.0135354728
C4	4.8711015849	-1.8589177720	0.0249635405
C5	3.5024774671	-1.6642113107	0.3319678941

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C6	3.0682940136	-0.3439567891	0.5936452218
C7	2.6023970367	-2.7845187165	0.3436397494
C8	1.9106517983	-3.7945469887	0.3032697703
C9	1.1047318303	-4.9873767858	0.2403480670
N10	-0.2495786799	-4.8185767847	0.1260272719
C11	-1.0415515308	-5.9183897735	0.0592956781
C12	-0.5463999995	-7.2303999929	0.0929999998
C13	0.8442380568	-7.3997490530	0.2069086168
C14	1.6806240685	-6.2737830827	0.2824592042
Zn15	-3.0080287972	0.3429498679	-1.0862623574
O16	-4.6239785688	1.0345596431	-2.2472406669
Zn17	3.5282003810	3.0777416198	0.8905354352
O18	5.4980255429	3.6512997500	0.5324081926
N19	-2.8993492074	2.3202690796	0.0221334441
C20	-2.2697077499	3.4860871798	-0.3135799371
C21	-2.3811122774	4.6649955183	0.4608918703
C22	-3.2138136890	4.6262315379	1.6068986992
C23	-3.8657855552	3.4385456234	1.9401960784
C24	-3.6849611940	2.3090097353	1.1408015456
C25	-1.6815695819	5.8824928236	0.1432299147
C26	-1.1356437004	6.9673002180	-0.0145961959
C27	-0.5195158322	8.2624903129	-0.1770330336
N28	0.8329560501	8.2970357820	-0.3838038153
C29	1.4382726548	9.5009658467	-0.5388718430
C30	0.7501999995	10.7230999929	-0.4986999998
C31	-0.6366748442	10.6832985510	-0.2770695402
C32	-1.2816956520	9.4466084042	-0.1143421620
O33	-2.0016687651	0.0978159915	-2.8883089701
O34	-4.3346185993	-0.6022074478	0.2022455372
O35	-1.3553529947	-0.7274851859	-0.1363113423
O36	2.9508160141	4.8555004459	-0.3753258906
O37	4.1755996708	2.6191441206	2.8595394618
O38	1.7336832975	3.6829246548	1.8824969548
H39	-1.6657213047	3.4767389282	-1.2127433663
H40	-3.3340067363	5.5160572515	2.2174348856
H41	-4.5081017874	3.3799772276	2.8137137980
H42	-4.1759770862	1.3748828205	1.3746126819
H43	1.2804097705	11.6615023272	-0.6319026225
H44	2.5112609450	9.4749118280	-0.7006471692
H45	-2.3530235189	9.3960310546	0.0622419680
H46	-1.2141581888	11.6024361796	-0.2333862687
H47	1.2771158300	-8.3954513484	0.2373460704
H48	-1.2234478597	-8.0776866943	0.0334067920
H49	-2.1073881238	-5.7332399823	-0.0276202742
H50	2.7587101571	-6.3853310108	0.3661204448
H51	5.8483037278	1.3929395717	0.2055815797
H52	6.7749530248	-0.8674216250	-0.2502831858
H53	5.2449444039	-2.8567781672	-0.1825146537
H54	2.0317281449	-0.1696237099	0.8533363798
H55	-4.1334017156	-1.2090843588	0.9431306301
H56	-5.2956060348	-0.6062195902	0.0166799378
H57	5.8551605542	4.1202155580	-0.2499298922
H58	6.1597785237	3.6433712672	1.2539206614
H59	-1.2476201020	-1.6984945405	-0.0785255544
H60	-0.5431354949	-0.2695103810	0.1617348239
H61	4.3037262535	1.7141115439	3.2086955372
H62	4.4548832412	3.2756350712	3.5309839422
H63	-1.3309064853	-0.5892361398	-3.0717954902
H64	-2.3847990416	0.4238657756	-3.7284744716
H65	0.9947588135	4.2119480234	1.5217151742
H66	1.7217071540	3.6999087482	2.8620745286
H67	-5.0753386113	0.4864410735	-2.9220096984
H68	-4.8746447701	1.9748756808	-2.3642288506
H69	2.3617290425	5.6404059990	-0.1556701750
H70	3.4177950441	5.0489280425	-1.2129485089

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[Cu₂(bPyeth)₂(H₂O)₆]⁴⁺

$\Delta r=0.00 \text{ \AA}$			
Atom	X	Y	Z
N1	2.9299027539	1.3178056243	-0.3685399899
C2	4.2788969634	1.1650202805	-0.4604315457
C3	4.8676900800	-0.1020645980	-0.4547503884
C4	4.0590052627	-1.2363986608	-0.3483583330
C5	2.6555839745	-1.0791864713	-0.2473264285
C6	2.1320688858	0.2273731867	-0.2671508518
C7	1.8092632520	-2.2234750000	-0.1296166136
C8	1.1579709378	-3.2531439142	-0.0309081750
C9	0.5908143167	-4.5598287324	0.0556879983
N10	-0.7633310222	-4.7256113839	0.2285203468
C11	-1.2753313128	-5.9818378041	0.3017412962
C12	-0.4757705107	-7.1229033774	0.2066225483
C13	0.9056944725	-6.9690674152	0.0307594732
C14	1.4408106303	-5.6792699712	-0.0438291567
Cu15	-2.1081508730	-3.1631828552	0.3880686117
O16	-2.2113467662	-3.0971815317	-1.6205407644
Cu17	2.0884640199	3.2023409802	-0.3755915933
O18	3.9595992041	4.3657079513	-0.6732696194
N19	-2.9366646498	-1.2750696872	0.4634620790
C20	-2.1441236040	-0.1873479114	0.3077411882
C21	-2.6609199292	1.1214986991	0.3427213060
C22	-4.0523084437	1.2840252180	0.5486945500
C23	-4.8555213726	0.1522157872	0.7094667218
C24	-4.2734697839	-1.1171275761	0.6622675446
C25	-1.8202218124	2.2629849555	0.1715567122
C26	-1.1747989751	3.2913683962	0.0304638067
C27	-0.6182684986	4.5964123971	-0.1217911151
N28	0.7342827732	4.7644322727	-0.3043663920
C29	1.2344927958	6.0195099764	-0.4481126441
C30	0.4238510423	7.1568380783	-0.4198630365
C31	-0.9563116496	6.9999182133	-0.2361745852
C32	-1.4789177758	5.7115337218	-0.0855504552
O33	-3.9908036746	-4.3254114114	0.5964530726
O34	-1.7846202931	-3.1026281576	2.3728721752
O35	1.7401609006	3.0149483468	-2.3488772643
O36	2.1993965778	3.2383610850	1.6334618562
H37	-1.0883964528	-0.3634402156	0.1509686187
H38	-4.4816609556	2.2826733723	0.5793325621
H39	-5.9255389472	0.2456824117	0.8697011307
H40	-4.8530681779	-2.0241458556	0.7774869398
H41	0.8723691548	8.1382031879	-0.5398839887
H42	2.3062643291	6.0879609796	-0.5880737290
H43	-2.5437003221	5.5497185947	0.0594123616
H44	-1.6158576231	7.8630823748	-0.2104136152
H45	1.5564312044	-7.8357518432	-0.0474870681
H46	-0.9337385480	-8.1053229985	0.2697589626
H47	-2.3478366982	-6.0481362468	0.4375923026
H48	2.5070796146	-5.5200030177	-0.1791404528
H49	4.8617470487	2.0737953361	-0.5402520883
H50	5.9470727116	-0.1924845497	-0.5326180313
H51	4.4937085167	-2.2328618969	-0.3435104039
H52	1.0660452462	0.3994863561	-0.2026584093
H53	-4.3701368280	-4.6301023157	1.4468838972
H54	-4.5567060041	-4.6399584139	-0.1389845536
H55	4.3309776656	4.6192666087	-1.5439614335
H56	4.5174669296	4.7473425441	0.0361631194
H57	-1.3552662312	-3.8230894668	2.8781248770
H58	-2.1490002456	-2.4200546723	2.9728409648
H59	2.6676968575	2.5697305756	2.1743167813
H60	1.8678660307	3.9735539815	2.1892313080
H61	-1.8390016757	-3.7820277649	-2.2127796897
H62	-2.7241807331	-2.4334667638	-2.1255018774
H63	1.2505808643	3.6719365325	-2.8849931200
H64	2.1606239969	2.3378745302	-2.9176809603

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$\Delta r=0.05 \text{ \AA}$			
Atom	X	Y	Z
N1	2.9079178988	1.2853503155	-0.4024865348
C2	4.2579079836	1.1336909732	-0.4879158782
C3	4.8472766129	-0.1334397889	-0.4855416378
C4	4.0390471855	-1.2693289541	-0.3879021769
C5	2.6342426429	-1.1146318444	-0.2956011685
C6	2.1105441736	0.1927313986	-0.3138204080
C7	1.7909354626	-2.2633125125	-0.1838152481
C8	1.1484648408	-3.2987347052	-0.0817902953
C9	0.5858871095	-4.6080171919	0.0166954637
N10	-0.7678449872	-4.7743718456	0.1907254829
C11	-1.2796118171	-6.0299365679	0.2835480916
C12	-0.4786999959	-7.1732999352	0.2087999972
C13	0.9025834337	-7.0178694498	0.0303468526
C14	1.4361717481	-5.7280317872	-0.0659494097
Cu15	-2.0931686780	-3.1953433733	0.3437419581
O16	-2.1820250970	-3.1025136648	-1.6647008434
Cu17	2.0800252660	3.1845835921	-0.3935983698
O18	3.9555700585	4.3363006874	-0.5960613942
N19	-2.9104103413	-1.3015056405	0.4411257798
C20	-2.1231398593	-0.2127972462	0.2633862165
C21	-2.6369760970	1.0970946747	0.3276606942
C22	-4.0215567410	1.2566145447	0.5802337888
C23	-4.8201066666	0.1237742024	0.7580643420
C24	-4.2404116574	-1.1454011306	0.6848450687
C25	-1.8035420320	2.2441953086	0.1466078168
C26	-1.1673770036	3.2794494222	0.0081302299
C27	-0.6158588250	4.5890815955	-0.1375935095
N28	0.7359366037	4.7610687996	-0.3227473746
C29	1.2349541382	6.0182699683	-0.4590043894
C30	0.4238999959	7.1567999352	-0.4198999972
C31	-0.9551149300	6.9945167117	-0.2313909728
C32	-1.4759656540	5.7036406372	-0.0894146349
O33	-3.9804110602	-4.3398454669	0.5570649023
O34	-1.7342694410	-3.1248300745	2.3232434192
O35	1.7858977749	3.0449643375	-2.3770504763
O36	2.1116196791	3.1586210898	1.6173491794
H37	-1.0738146770	-0.3892013541	0.0686604891
H38	-4.4501514758	2.2546062561	0.6328618429
H39	-5.8845948712	0.2170233868	0.9525225694
H40	-4.8158685348	-2.0532004644	0.8133603255
H41	0.8713006576	8.1393806663	-0.5344647976
H42	2.3064490594	6.0879367935	-0.6010661631
H43	-2.5398206357	5.5401767823	0.0594720887
H44	-1.6164914642	7.8559515005	-0.1952070843
H45	1.5557623953	-7.8840565332	-0.0331104269
H46	-0.9348904907	-8.1552355664	0.2885840811
H47	-2.3523219610	-6.0932271816	0.4188775878
H48	2.5022604818	-5.5692350877	-0.2031777351
H49	4.8410909175	2.0431591925	-0.5569018683
H50	5.9272789984	-0.2227846707	-0.5579930168
H51	4.4752029608	-2.2658406983	-0.3814962666
H52	1.0443252407	0.3649031036	-0.2546120597
H53	-4.3428475330	-4.6829254129	1.4005798306
H54	-4.5704720997	-4.6055094893	-0.1790280337
H55	4.3747900720	4.5846582937	-1.4465172500
H56	4.4774822978	4.7125143952	0.1433073884
H57	-1.3370384824	-3.8596143180	2.8343595016
H58	-2.0709130262	-2.4239881170	2.9183512661
H59	2.5445498998	2.4637641840	2.1533148163
H60	1.7949876847	3.8938402830	2.1808103351
H61	-1.8385496322	-3.7980871578	-2.2621334372
H62	-2.6865993321	-2.4268212716	-2.1624379136
H63	1.3320035270	3.7271400730	-2.9134183581
H64	2.2270863871	2.3824352067	-2.9476342015

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$\Delta r=0.10 \text{ \AA}$			
Atom	X	Y	Z
N1	2.8845414876	1.2548275547	-0.3874743704
C2	4.2373337223	1.1130740347	-0.4404160043
C3	4.8359197420	-0.1494531438	-0.4306096959
C4	4.0346013596	-1.2919935384	-0.3581537835
C5	2.6269420654	-1.1496564178	-0.2956869269
C6	2.0940743506	0.1548877491	-0.3207796663
C7	1.7922828786	-2.3077569595	-0.1995568028
C8	1.1584005029	-3.3496016883	-0.1034473069
C9	0.5927806862	-4.6584191108	0.0009788477
N10	-0.7605692721	-4.8195908191	0.1886390859
C11	-1.2763762745	-6.0736797012	0.2887367433
C12	-0.4817999939	-7.2228999037	0.2109999958
C13	0.8985159618	-7.0714115485	0.0195593677
C14	1.4364490395	-5.7833607090	-0.0851643764
Cu15	-2.0733111640	-3.2212778451	0.3492223443
O16	-2.1853466499	-3.1430828080	-1.6563411750
Cu17	2.0581195010	3.1634645206	-0.3868169176
O18	3.9402605737	4.3135839217	-0.5691573797
N19	-2.8924651171	-1.3174991796	0.4424256880
C20	-2.1141381062	-0.2221168840	0.2620566725
C21	-2.6367172387	1.0852361385	0.3282669247
C22	-4.0215411194	1.2338897540	0.5847264318
C23	-4.8107522827	0.0952186518	0.7665955842
C24	-4.2223383169	-1.1698228963	0.6920253524
C25	-1.8132468975	2.2411592688	0.1483841439
C26	-1.1843978789	3.2818536371	0.0141034928
C27	-0.6286523752	4.5907745448	-0.1314704810
N28	0.7236479429	4.7568662342	-0.3222970533
C29	1.2282087890	6.0119103984	-0.4628465214
C30	0.4238999939	7.1567999037	-0.4198999958
C31	-0.9549131830	6.9994826811	-0.2223406517
C32	-1.4816224711	5.7107338730	-0.0772938873
O33	-3.9555211730	-4.3618704440	0.6061026667
O34	-1.6638598615	-3.1197936610	2.3164777113
O35	1.7775107218	3.0235792726	-2.3717407286
O36	2.0618181997	3.1349486727	1.6228167849
H37	-1.0648834380	-0.3914104745	0.0629771199
H38	-4.4580768651	2.2282427691	0.6370971608
H39	-5.8749377542	0.1807745158	0.9660068069
H40	-4.7907694824	-2.0813175400	0.8254454433
H41	0.8756570393	8.1368973994	-0.5375199337
H42	2.2997933082	6.0746698471	-0.6081008030
H43	-2.5454443775	5.5534761332	0.0790650592
H44	-1.6126564307	7.8636090488	-0.1814233915
H45	1.5486734454	-7.9396482016	-0.0473449739
H46	-0.9418267626	-8.2024084869	0.2973702027
H47	-2.3481656885	-6.1312970085	0.4342465120
H48	2.5023296706	-5.6306733606	-0.2301601212
H49	4.8154216398	2.0270140787	-0.4911333188
H50	5.9179603975	-0.2303393062	-0.4771388698
H51	4.4788927217	-2.2843514192	-0.3484989276
H52	1.0257993484	0.3189097105	-0.2832363229
H53	-4.3172891576	-4.6784334844	1.4598700510
H54	-4.5496254645	-4.6448643983	-0.1198448319
H55	4.3720266243	4.5619692518	-1.4131762634
H56	4.4608535283	4.6782304191	0.1765615876
H57	-1.2645675581	-3.8519992689	2.8291690772
H58	-2.0032699908	-2.4191707861	2.9104999677
H59	2.4971376168	2.4445234804	2.1638966866
H60	1.7599504632	3.8817865927	2.1796014641
H61	-1.8596687755	-3.8496312824	-2.2510183197
H62	-2.7155261339	-2.4840530838	-2.1495635213
H63	1.3406211326	3.7152359378	-2.9104212352
H64	2.2330452091	2.3689347700	-2.9403951756

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$\Delta r=0.15 \text{ \AA}$	X	Y	Z
N1	2.8759590222	1.2178557282	-0.4545191783
C2	4.2268189798	1.0686540324	-0.5372972851
C3	4.8201841216	-0.1964316702	-0.5351156504
C4	4.0165036211	-1.3358807513	-0.4411488853
C5	2.6106957966	-1.1884554496	-0.3518492798
C6	2.0830498516	0.1195028750	-0.3681354537
C7	1.7776018077	-2.3482020755	-0.2410567665
C8	1.1508278895	-3.3943680959	-0.1383766421
C9	0.5875968218	-4.7047172470	-0.0221180960
N10	-0.7675302765	-4.8670946524	0.1545288895
C11	-1.2815494240	-6.1216529456	0.2670484689
C12	-0.4848999930	-7.2727998896	0.2131999952
C13	0.8969108389	-7.1182992802	0.0328376321
C14	1.4330739685	-5.8300256359	-0.0853324158
Cu15	-2.0761655247	-3.2541789170	0.2826927077
O16	-2.1278611633	-3.1671031530	-1.7232796023
Cu17	2.0718227572	3.1502553220	-0.4478140301
O18	3.9505344455	4.2813166674	-0.7240386602
N19	-2.8847952492	-1.3347166795	0.3597639057
C20	-2.1013775092	-0.2385446595	0.2026503026
C21	-2.6236154466	1.0697885608	0.2556205669
C22	-4.0144403578	1.2199962951	0.4771855739
C23	-4.8089957972	0.0814634260	0.6364425977
C24	-4.2208719267	-1.1845228317	0.5743679592
C25	-1.7962348864	2.2259981590	0.0932583283
C26	-1.1686314786	3.2688185753	-0.0304052342
C27	-0.6161042116	4.5807864300	-0.1621872702
N28	0.7353919932	4.7539740175	-0.3563077684
C29	1.2328696068	6.0140704631	-0.4821107855
C30	0.4238999930	7.1567998896	-0.4198999952
C31	-0.9534226972	6.9897329481	-0.2203357151
C32	-1.4736255671	5.6965773169	-0.0917562856
O33	-3.9670313851	-4.3860582397	0.4809306104
O34	-1.7251400393	-3.1613163936	2.2601493243
O35	1.7168736355	2.9871304107	-2.4148562044
O36	2.1778930886	3.1654258015	1.5563202853
H37	-1.0475282618	-0.4086522944	0.0314328553
H38	-4.4507295210	2.2155366183	0.5206246245
H39	-5.8779594190	0.1678047903	0.8077067433
H40	-4.7951602415	-2.0949792324	0.6892254864
H41	0.8714068561	8.1401213244	-0.5258024217
H42	2.3031044085	6.0829488175	-0.6349203357
H43	-2.5368558035	5.5325751483	0.0632296705
H44	-1.6154226379	7.8498591726	-0.1655194914
H45	1.5508993546	-7.9849764599	-0.0154475818
H46	-0.9438823920	-8.2518049215	0.3093816745
H47	-2.3548693410	-6.1784761568	0.4014893495
H48	2.4999632543	-5.6782580283	-0.2245750867
H49	4.8084878128	1.9791144529	-0.6058555152
H50	5.9006799710	-0.2815355952	-0.6047486589
H51	4.4572632276	-2.3304474373	-0.4346404400
H52	1.0168682207	0.2882796575	-0.3088289583
H53	-4.3557277431	-4.7006934433	1.3233305100
H54	-4.5349261899	-4.6749240477	-0.2632824543
H55	4.3405261910	4.5243660264	-1.5894033240
H56	4.5107070316	4.6424726270	-0.0060068685
H57	-1.3551440469	-3.9014536227	2.7845497121
H58	-2.0828263480	-2.4612417817	2.8442148950
H59	2.6558337319	2.4939377004	2.0855424081
H60	1.9113674812	3.9284889544	2.1099810592
H61	-1.8118717358	-3.8853942877	-2.3088768919
H62	-2.6313420026	-2.4954573585	-2.2275020780
H63	1.3148844282	3.6996001048	-2.9532634773
H64	2.1156773107	2.2967409936	-2.9834103555

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$\Delta r=0.20 \text{ \AA}$	X	Y	Z
Atom			
N1	2.8506763968	1.1904384483	-0.3097227201
C2	4.2048622929	1.0550558581	-0.3561090548
C3	4.8115976844	-0.2034303033	-0.3370493224
C4	4.0181734730	-1.3512389090	-0.2638708306
C5	2.6090428092	-1.2192021196	-0.2088754587
C6	2.0682687944	0.0834193014	-0.2405964022
C7	1.7868786542	-2.3888132086	-0.1161604526
C8	1.1675415959	-3.4407593175	-0.0263005078
C9	0.6010786563	-4.7522295108	0.0633260105
N10	-0.7573645774	-4.9110458176	0.2188905465
C11	-1.2782115243	-6.1663078998	0.2892927738
C12	-0.4879999951	-7.3225999218	0.2153999966
C13	0.8978649922	-7.1691290040	0.0671562318
C14	1.4417904092	-5.8805041045	-0.0093324984
Cu15	-2.0527111954	-3.2779686515	0.3874048675
O16	-2.1540606165	-3.1786367198	-1.6117312024
Cu17	2.0388915336	3.1271852947	-0.3307776283
O18	3.9287841997	4.2553005049	-0.5394148852
N19	-2.8573158831	-1.3454264530	0.4989668305
C20	-2.0914836085	-0.2407407852	0.3101623735
C21	-2.6193738542	1.0647391538	0.3964071066
C22	-3.9990622979	1.2011741769	0.6864321860
C23	-4.7756108786	0.0555540542	0.8789140553
C24	-4.1821744399	-1.2055636777	0.7804186692
C25	-1.8100713175	2.2319623997	0.2067199101
C26	-1.1944699878	3.2808605530	0.0669058719
C27	-0.6375924070	4.5903901229	-0.0905836420
N28	0.7157188419	4.7507603569	-0.2855716167
C29	1.2224576063	6.0042432870	-0.4449613787
C30	0.4238999951	7.1567999218	-0.4198999966
C31	-0.9546778177	7.0020244657	-0.2145671701
C32	-1.4843287277	5.7157661085	-0.0482994028
O33	-3.9438745544	-4.4003251822	0.6319612539
O34	-1.6479264813	-3.1948541224	2.3516987745
O35	1.7392886879	2.9587539026	-2.3051125697
O36	2.0680672540	3.1325637551	1.6742994264
H37	-1.0448690724	-0.4035102740	0.0934417075
H38	-4.4412106785	2.1920242592	0.7566880400
H39	-5.8350552546	0.1325604928	1.1051359056
H40	-4.7435377489	-2.1206469806	0.9191722553
H41	0.8791244482	8.1329539560	-0.5548283662
H42	2.2942139788	6.0600564390	-0.5936013483
H43	-2.5480964539	5.5662814744	0.1145426273
H44	-1.6122389183	7.8667693286	-0.1838394471
H45	1.5499482648	-8.0368249626	0.0107882898
H46	-0.9543622311	-8.3008646852	0.2753568245
H47	-2.3535749645	-6.2198230385	0.4089568131
H48	2.5117868679	-5.7316954247	-0.1245995920
H49	4.7784089538	1.9716629952	-0.4089455508
H50	5.8944035257	-0.2769971552	-0.3775012759
H51	4.4692065344	-2.3406385969	-0.2483381052
H52	0.9994725999	0.2426286976	-0.2034134306
H53	-4.2993615336	-4.7357799170	1.4810808411
H54	-4.5431428192	-4.6675860472	-0.0955301661
H55	4.3652194378	4.4799982614	-1.3872598225
H56	4.4474332895	4.6354025433	0.1999494390
H57	-1.2613997947	-3.9364723005	2.8606427445
H58	-1.9845854115	-2.4968427589	2.9498283641
H59	2.5274849750	2.4597098069	2.2178329390
H60	1.7723396979	3.8885446769	2.2228376864
H61	-1.8604584893	-3.8977450274	-2.2081328344
H62	-2.6650684237	-2.5005173162	-2.0996513948
H63	1.3210634019	3.6543404939	-2.8536629989
H64	2.1724405029	2.2808948288	-2.8638618760

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$\Delta r=0.30 \text{ \AA}$			
Atom	X	Y	Z
N1	2.7925248009	1.1179248957	-0.4880946879
C2	4.1415562050	0.9749661279	-0.6092962512
C3	4.74447786208	-0.2854392589	-0.6227232414
C4	3.9530781546	-1.4306966201	-0.5045092994
C5	2.5490008672	-1.2942321050	-0.3751102710
C6	2.0120921472	0.0116738163	-0.3756864904
C7	1.7341030133	-2.4674329040	-0.2446774306
C8	1.1338882337	-3.5291535705	-0.1329119540
C9	0.5791454556	-4.8453567134	-0.0148028420
N10	-0.7772092984	-5.0095132946	0.1554405175
C11	-1.2898984360	-6.2661019024	0.2668106454
C12	-0.4942999899	-7.4222998393	0.2197999930
C13	0.8886878652	-7.2614880903	0.0473757811
C14	1.4246548477	-5.9712212979	-0.0712614472
Cu15	-2.0658828403	-3.3537360262	0.2646222997
O16	-2.1685767648	-3.3235881394	-1.7338633689
Cu17	2.0087740755	3.0856678762	-0.4653277296
O18	3.9045384489	4.1964746887	-0.6802447227
N19	-2.8472368505	-1.3918220833	0.3140382446
C20	-2.0728892088	-0.2839711676	0.1782712302
C21	-2.6092341973	1.0216710356	0.2179421216
C22	-4.0070217962	1.1523082194	0.4078213634
C23	-4.7924925783	0.0051659893	0.5449948812
C24	-4.1899008976	-1.2541729086	0.4947995019
C25	-1.7995974750	2.1979308015	0.0737092162
C26	-1.1983700114	3.2593404004	-0.0383627669
C27	-0.6434041108	4.5758324660	-0.1614706038
N28	0.7088389836	4.7409475547	-0.3661530347
C29	1.2169541342	5.9988305677	-0.4923516580
C30	0.4238999899	7.1567998393	-0.4198999930
C31	-0.9529812695	6.9938457002	-0.2032073522
C32	-1.4853414879	5.7028393137	-0.0750222284
O33	-3.9614112535	-4.4573238957	0.5160915042
O34	-1.6821507549	-3.2229029226	2.2253064407
O35	1.6950448236	2.9696608972	-2.4379497004
O36	2.0528195003	3.0452806917	1.5347083192
H37	-1.0142001635	-0.4449213134	0.0362767780
H38	-4.4573455019	2.1406430559	0.4443393108
H39	-5.8662538517	0.0800652889	0.6901734621
H40	-4.7575762876	-2.1704468148	0.5957179228
H41	0.8803096637	8.1355164781	-0.5276135711
H42	2.2874076066	6.0544001424	-0.6506761314
H43	-2.5489651357	5.5512026954	0.0917084485
H44	-1.6097328972	7.8572830645	-0.1345679520
H45	1.5464875005	-8.1257522896	0.0052078447
H46	-0.9536963757	-8.4010124536	0.3160848188
H47	-2.3640576850	-6.3216615785	0.3968593057
H48	2.4924879626	-5.8194312237	-0.2070390376
H49	4.7161088179	1.8888218212	-0.6929478605
H50	5.8232426901	-0.3614376358	-0.7232220375
H51	4.4011554485	-2.4219967774	-0.5095897299
H52	0.9479432088	0.1737173955	-0.2841705400
H53	-4.33667750599	-4.7564325640	1.3702617715
H54	-4.5316995943	-4.7738598209	-0.2149282599
H55	4.3086697285	4.4680919442	-1.5306571909
H56	4.4518946356	4.5336271110	0.0593891099
H57	-1.3256101380	-3.9626767726	2.7588475318
H58	-2.0083921326	-2.4995788855	2.7990395355
H59	2.4960644415	2.3485137578	2.0616746426
H60	1.7755064471	3.7953321690	2.1005274775
H61	-1.9198268803	-4.0823506652	-2.3010055472
H62	-2.6529605780	-2.6433807181	-2.2452626489
H63	1.3133969959	3.6977097824	-2.9709711854
H64	2.0863081393	2.2790963171	-3.0116192270

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$\Delta r=0.40 \text{ \AA}$			
Atom	X	Y	Z
N1	2.7656096818	1.0606768303	-0.3607507741
C2	4.1182663262	0.9308481699	-0.4575799211
C3	4.7327764904	-0.3238113535	-0.4600720985
C4	3.9505717969	-1.4770054188	-0.3585975367
C5	2.5425233181	-1.3583056828	-0.2536532701
C6	1.9947897501	-0.0551779960	-0.2621587493
C7	1.7407317724	-2.5462796031	-0.1419301176
C8	1.1542271527	-3.6187047312	-0.0479746400
C9	0.5956444880	-4.9386725897	0.0449653701
N10	-0.7618547993	-5.0987610971	0.2157584990
C11	-1.2835696782	-6.3553109169	0.3029879917
C12	-0.5005999915	-7.5219998657	0.2241999941
C13	0.8829699310	-7.3619405703	0.0494120029
C14	1.4290687161	-6.0718899412	-0.0384042156
Cu15	-2.0230977732	-3.4071375183	0.3435169280
O16	-2.1587008227	-3.3827077715	-1.6490732028
Cu17	1.9962963217	3.0558894734	-0.3719002944
O18	3.8997802340	4.1437686733	-0.6151314144
N19	-2.7942943295	-1.4201855257	0.4021420941
C20	-2.0341629798	-0.3059683798	0.2318399490
C21	-2.5762287847	0.9980652399	0.2859451890
C22	-3.9682975848	1.1198662600	0.5201454902
C23	-4.7396077131	-0.0321516265	0.6934855843
C24	-4.1305015257	-1.2879608476	0.6317524545
C25	-1.7817139480	2.1835039106	0.1173635560
C26	-1.1972301908	3.2535396176	-0.0077705592
C27	-0.6476187203	4.5726967930	-0.1461032132
N28	0.7094643912	4.7382927815	-0.3143362235
C29	1.2194985824	5.9960570006	-0.4439552470
C30	0.4238999915	7.1567998657	-0.4198999941
C31	-0.9592564435	6.9905334801	-0.2498527104
C32	-1.4924412516	5.6999971521	-0.1111782388
O33	-3.9243336725	-4.4959780450	0.6363071339
O34	-1.6042180693	-3.2734414685	2.2922024747
O35	1.6682935785	2.8945756632	-2.3340202072
O36	2.0563048123	3.0629331580	1.6235083607
H37	-0.9811408400	-0.4612537633	0.0504856107
H38	-4.4248696901	2.1056186133	0.5633520923
H39	-5.8080400744	0.0360596451	0.8768021037
H40	-4.6889532239	-2.2064214506	0.7609374613
H41	0.8824596691	8.1342288629	-0.5293225011
H42	2.2945055670	6.0498223445	-0.5696156340
H43	-2.5600569507	5.5514563325	0.0259170063
H44	-1.6221748645	7.8515859323	-0.2239912356
H45	1.5366937213	-8.2277456621	-0.0181879400
H46	-0.9679765533	-8.4985714347	0.2987347291
H47	-2.3575234289	-6.4025838234	0.4390884025
H48	2.4979932852	-5.9286566671	-0.1707165859
H49	4.6855260751	1.8499409336	-0.5331409440
H50	5.8139337819	-0.3903473052	-0.5405540229
H51	4.4110659983	-2.4614681973	-0.3588054951
H52	0.9285638824	0.0985193284	-0.1884695510
H53	-4.2737535806	-4.8031516812	1.4986373697
H54	-4.5176909904	-4.8049525620	-0.0796813750
H55	4.2993219496	4.3976593974	-1.4730055476
H56	4.4501202476	4.4978092813	0.1140862106
H57	-1.2466909069	-4.0165151691	2.8198386804
H58	-1.9001980851	-2.5389556256	2.8690130166
H59	2.4867532749	2.3694089136	2.1639982285
H60	1.7923407298	3.8295900678	2.1734841279
H61	-1.9126520216	-4.1392418382	-2.2206413876
H62	-2.6361094888	-2.6948487096	-2.1566590875
H63	1.2892469936	3.6106753909	-2.8832831891
H64	2.0282894632	2.1736179031	-2.8907046716

Error! Use the Home tab to apply Überschrift 1 to the text that you want to appear here.

 $\Delta r=0.50 \text{ \AA}$

Atom	X	Y	Z
N1	2.7094908720	0.9913543629	-0.4237730911
C2	4.0610457927	0.8666642489	-0.5433666617
C3	4.6814332645	-0.3850516386	-0.5561222960
C4	3.9074133061	-1.5424764128	-0.4409813698
C5	2.5003556359	-1.4321832713	-0.3137097973
C6	1.9472630584	-0.1300234562	-0.3131510579
C7	1.7090546398	-2.6283359033	-0.1916966675
C8	1.1373319188	-3.7089148538	-0.0914628970
C9	0.5838419656	-5.0318954009	0.0152756377
N10	-0.7735528129	-5.1937491471	0.1905215575
C11	-1.2915913721	-6.4520245860	0.2930435250
C12	-0.5068999933	-7.6216998944	0.2285999954
C13	0.8757401986	-7.4566779782	0.0495280352
C14	1.4179103216	-6.1655604389	-0.0563745509
Cu15	-2.0210100616	-3.4737879887	0.2995889142
O16	-2.1157018244	-3.4422191895	-1.6916333681
Cu17	1.9515771600	3.0134580636	-0.4184244637
O18	3.8678097944	4.0754346056	-0.6517833252
N19	-2.7782403745	-1.4568747275	0.3465791343
C20	-2.0207733742	-0.3370486323	0.1924361847
C21	-2.5673080670	0.9671618942	0.2389473395
C22	-3.9636091344	1.0803540936	0.4528434513
C23	-4.7330428427	-0.0753529497	0.6086507201
C24	-4.1188771830	-1.3288554016	0.5526036655
C25	-1.7797551419	2.1625549996	0.0832951901
C26	-1.2103202016	3.2428967081	-0.0339941300
C27	-0.6607619635	4.5663151230	-0.1631416961
N28	0.6953937346	4.7297571017	-0.3452092976
C29	1.2107409582	5.9876071695	-0.4675688140
C30	0.4238999933	7.1567998944	-0.4198999954
C31	-0.9579065034	6.9902393875	-0.2335729623
C32	-1.4968690856	5.6993328575	-0.1052292640
O33	-3.9372863665	-4.5380486630	0.5588855519
O34	-1.6385744127	-3.3473228653	2.2520950691
O35	1.6121345777	2.8657749494	-2.3760375673
O36	1.9985494936	2.9938293778	1.5733088326
H37	-0.9651180860	-0.4896412183	0.0307658099
H38	-4.4259246395	2.0628172426	0.4946325642
H39	-5.8047083451	-0.0114863127	0.7739150865
H40	-4.6768277549	-2.2492707027	0.6690452651
H41	0.8870034676	8.1325673524	-0.5235815733
H42	2.2847486446	6.0346882645	-0.6050450728
H43	-2.5638292702	5.5570158442	0.0408912810
H44	-1.6182671938	7.8523943834	-0.1866408078
H45	1.5338539452	-8.3199130600	-0.0079459318
H46	-0.9726334391	-8.5977861345	0.3160988259
H47	-2.3656808277	-6.4988714044	0.4294487788
H48	2.4858292599	-6.0235471576	-0.1943525090
H49	4.6229870184	1.7882229102	-0.6278868324
H50	5.7614327476	-0.4459690782	-0.6551215103
H51	4.3738583713	-2.5241146236	-0.4480442848
H52	0.8824288160	0.0194699871	-0.2235402905
H53	-4.3043534929	-4.8396489527	1.4157662758
H54	-4.5219268242	-4.8411623830	-0.1665237386
H55	4.2712888215	4.3311682789	-1.5071727602
H56	4.4229151908	4.4159208735	0.0800328620
H57	-1.2870522139	-4.0895632008	2.7845432032
H58	-1.9560222893	-2.6196540271	2.8252333251
H59	2.3998772328	2.2771846745	2.1071840832
H60	1.7593558041	3.7617255477	2.1313652336
H61	-1.8664373168	-4.2008849734	-2.2579966309
H62	-2.5777545594	-2.7498792891	-2.2075961717
H63	1.2552483386	3.5952112888	-2.9229535679
H64	1.9442256764	2.1325192358	-2.9337297432

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$\Delta r=0.60 \text{ \AA}$	X	Y	Z
Atom			
N1	2.6882352885	0.9164128433	-0.4769680517
C2	4.0336899481	0.7775826628	-0.6409993137
C3	4.6404254777	-0.4805813776	-0.6729068425
C4	3.8593778752	-1.6306052826	-0.5341577661
C5	2.4579308639	-1.5082145908	-0.3632718695
C6	1.9196253171	-0.1990928846	-0.3419090858
C7	1.6637449294	-2.7028720768	-0.2215962911
C8	1.0991224484	-3.7873942264	-0.1134766570
C9	0.5546844621	-5.1157490339	0.0029593015
N10	-0.8028649776	-5.2891876896	0.1744022179
C11	-1.3079911840	-6.5538350730	0.2843631425
C12	-0.5131999878	-7.7213998068	0.2329999915
C13	0.8681447498	-7.5406622045	0.0570034629
C14	1.3981827856	-6.2441094983	-0.0573846235
Cu15	-2.0640701223	-3.5409462463	0.2604913933
O16	-2.1529918281	-3.5324995777	-1.7258591339
Cu17	1.9619576086	2.9731315009	-0.4547012424
O18	3.8856144460	4.0121594027	-0.6787145843
N19	-2.7842466046	-1.4832821467	0.2792771654
C20	-2.0152771215	-0.3687873822	0.1357036217
C21	-2.5505955147	0.9414655273	0.1720462895
C22	-3.9495610253	1.0647283179	0.3629894046
C23	-4.7311728184	-0.0841424550	0.5069821706
C24	-4.1270125568	-1.3429631791	0.4627104018
C25	-1.7569800584	2.1368051047	0.0282850267
C26	-1.1942599198	3.2227807255	-0.0771314947
C27	-0.6486005823	4.5515594686	-0.1892493322
N28	0.7081413376	4.7235044201	-0.3678737213
C29	1.2157610442	5.9872567260	-0.4780948280
C30	0.4238999878	7.1567998068	-0.4198999915
C31	-0.9566067278	6.9773866934	-0.2343258252
C32	-1.4890175144	5.6815413633	-0.1197575744
O33	-3.9817841966	-4.5806605603	0.5337596522
O34	-1.6869217670	-3.3943936655	2.2069654393
O35	1.6170457560	2.8482277125	-2.4079817185
O36	2.0024648585	2.9335367808	1.5301702980
H37	-0.9596501846	-0.5327246517	-0.0119438576
H38	-4.4051626492	2.0505739166	0.3965170548
H39	-5.8048419146	-0.0106802509	0.6538264439
H40	-4.6960301818	-2.2577300693	0.5707225891
H41	0.8827529688	8.1353229834	-0.5143148747
H42	2.2896083376	6.0403007263	-0.6163211511
H43	-2.5558998734	5.5346895179	0.0240606535
H44	-1.6233771806	7.8339795228	-0.1774659705
H45	1.5367779838	-8.3962773430	0.0078149697
H46	-0.9710630846	-8.7004977794	0.3269422929
H47	-2.3824683359	-6.6094660740	0.4168943435
H48	2.4655305128	-6.0952985321	-0.1942266452
H49	4.6029545390	1.6930176479	-0.7421771587
H50	5.7160048561	-0.5522763853	-0.8051597695
H51	4.3162852032	-2.6166174943	-0.5550454253
H52	0.8613601517	-0.0371983486	-0.2132053076
H53	-4.3574286965	-4.8585009842	1.3947447245
H54	-4.5616846563	-4.8983480741	-0.1888720055
H55	4.2765301367	4.3013501010	-1.5291558358
H56	4.4504634777	4.3226781833	0.0591127122
H57	-1.3502374313	-4.1370503338	2.7495457737
H58	-2.0218938858	-2.6674846451	2.7712818559
H59	2.4055095836	2.2113583731	2.0541514999
H60	1.7779776248	3.7012682704	2.0951316039
H61	-1.9358539834	-4.3116395902	-2.2781826936
H62	-2.6125693294	-2.8431207428	-2.2481486351
H63	1.2831501100	3.5943885794	-2.9474164490
H64	1.9466047154	2.1202858362	-2.9741887397

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$\Delta r=0.80 \text{ \AA}$			
Atom	X	Y	Z
N1	2.6455313275	0.7729750031	-0.4106312091
C2	3.9903763624	0.6330630757	-0.5822226724
C3	4.5983836416	-0.6248273677	-0.6222127220
C4	3.8213008778	-1.7778853558	-0.4847316440
C5	2.4197230001	-1.6606219102	-0.3043572765
C6	1.8829369977	-0.3489199631	-0.2734828712
C7	1.6329114970	-2.8667411305	-0.1669788646
C8	1.0867173018	-3.9639684238	-0.0696828657
C9	0.5473117024	-5.3001479654	0.0345725104
N10	-0.8126159113	-5.4786268892	0.1873645065
C11	-1.3187082717	-6.7462482011	0.2863552174
C12	-0.5257999862	-7.9207997813	0.2417999904
C13	0.8579669785	-7.7301053180	0.0848874134
C14	1.3893063613	-6.4306129458	-0.0177940525
Cu15	-2.0518492412	-3.6780128071	0.2674798381
O16	-2.1813680055	-3.6785456884	-1.7028101750
Cu17	1.9538496454	2.9208167412	-0.4010565403
O18	3.8970231098	3.8951854557	-0.5948523322
N19	-2.7418878355	-1.5288485156	0.2879689466
C20	-1.9874167238	-0.4095474678	0.0985789599
C21	-2.5138955976	0.9036922012	0.1843920846
C22	-3.8994276766	1.0269847088	0.4576335213
C23	-4.6701741916	-0.1239070089	0.6393373418
C24	-4.0701534438	-1.3833403536	0.5552457242
C25	-1.7297222950	2.1071371365	0.0204713042
C26	-1.1851110934	3.2043660814	-0.0812885622
C27	-0.6467309851	4.5397612585	-0.1898475210
N28	0.7128998027	4.7170692970	-0.3443772303
C29	1.2184488126	5.9836729307	-0.4531445834
C30	0.4238999862	7.1567997813	-0.4198999904
C31	-0.9593640835	6.9679073921	-0.2575772628
C32	-1.4900082649	5.6693906965	-0.1417730376
O33	-3.9777080067	-4.6581834338	0.5802225901
O34	-1.6245096135	-3.5059355887	2.1893729536
O35	1.6397868719	2.7927311687	-2.3471148346
O36	1.9641980092	2.8746281341	1.5725378298
H37	-0.9479205870	-0.5740773297	-0.1316677578
H38	-4.3518827270	2.0135198753	0.5229052719
H39	-5.7334382802	-0.0522102825	0.8493882563
H40	-4.6347185845	-2.2961380122	0.6983068227
H41	0.8817644501	8.1356077703	-0.5139980792
H42	2.2949977419	6.0381848822	-0.5696108589
H43	-2.5591773148	5.5220304154	-0.0137315475
H44	-1.6326421333	7.8205534152	-0.2196201967
H45	1.5317303259	-8.5821439692	0.0412728866
H46	-0.9846385382	-8.9000772578	0.3257297192
H47	-2.3951643651	-6.8005376341	0.4045295084
H48	2.4589005228	-6.2834661145	-0.1388742841
H49	4.5608949792	1.5476650498	-0.6840577902
H50	5.6735960806	-0.6940054535	-0.7605915295
H51	4.2817212137	-2.7617711024	-0.5145451999
H52	0.8269211591	-0.1860299253	-0.1337527634
H53	-4.3320330895	-4.9500213281	1.4457452198
H54	-4.5845623074	-4.9482913206	-0.1318479013
H55	4.3115961514	4.1739171467	-1.4372945159
H56	4.4538896420	4.1933149407	0.1538453998
H57	-1.3277444363	-4.2556454140	2.7451650668
H58	-1.8651274061	-2.7309415120	2.7374770555
H59	2.3364680023	2.1388481609	2.1001284072
H60	1.7478533259	3.6443965809	2.1372591248
H61	-2.0017479650	-4.4654353227	-2.2572360798
H62	-2.6150424670	-2.9690938030	-2.2203286695
H63	1.3347357185	3.5429180502	-2.8975690054
H64	1.9413238539	2.0436806933	-2.9011254148

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$\Delta r=1.00 \text{ \AA}$			
Atom	X	Y	Z
N1	2.4548370113	0.6447072080	-0.2938519006
C2	3.7389599454	0.5544592946	-0.7415782600
C3	4.3652515851	-0.6774899276	-0.9459987578
C4	3.6622743727	-1.8603323171	-0.710688653
C5	2.3256713867	-1.7995167897	-0.2424494684
C6	1.7750766094	-0.5101008470	-0.0253045443
C7	1.6099269174	-3.0431130276	-0.0483447001
C8	1.1278187996	-4.1720604387	0.0282243949
C9	0.5926459241	-5.5139861707	0.1006768592
N10	-0.7768116414	-5.6730378853	0.1393711843
C11	-1.3132414874	-6.9306351499	0.2093558672
C12	-0.5383999965	-8.1201999446	0.2505999976
C13	0.8568909485	-7.9471324656	0.2093026237
C14	1.4181524565	-6.6563039438	0.1339326967
Cu15	-1.8797647349	-3.8031333976	0.0927260045
O16	-1.8832080931	-3.8006534878	-1.8787375694
Cu17	1.7346820837	2.8320227994	-0.3055347600
O18	3.7107289920	3.7607410569	-0.5967153677
N19	-2.5949335725	-1.6007409403	0.1193878083
C20	-1.9229840816	-0.4433608815	-0.1587130106
C21	-2.4560830715	0.8431396320	0.1145700507
C22	-3.7707050110	0.8992738570	0.6414924893
C23	-4.4690541891	-0.2850743491	0.8815992957
C24	-3.8578787873	-1.5144425590	0.6250554192
C25	-1.7456231652	2.0885963558	-0.0887349242
C26	-1.2632980183	3.2168876071	-0.1699413500
C27	-0.7241823972	4.5570158923	-0.2535447714
N28	0.6451424107	4.7066999281	-0.3259111514
C29	1.1894572337	5.9605870653	-0.4054865235
C30	0.4238999965	7.1567999446	-0.4198999976
C31	-0.9714976556	6.9928054974	-0.3442296440
C32	-1.5410157261	5.7058277555	-0.2618605312
O33	-3.8634457030	-4.7428778384	0.2821143208
O34	-1.5820781894	-3.6164364721	2.0380124312
O35	1.3584899861	2.6119864531	-2.2353596471
O36	1.7982206639	2.8341817230	1.6670065672
H37	-0.9562061132	-0.5525733315	-0.6273900329
H38	-4.2267077998	1.8607791215	0.8569284858
H39	-5.4810880965	-0.2631472327	1.2754159045
H40	-4.3698486930	-2.4505581105	0.8056878293
H41	0.9075610812	8.1252090353	-0.4856053968
H42	2.2719440825	5.9837725114	-0.4583599379
H43	-2.6193448655	5.5892980189	-0.2048879417
H44	-1.6284517527	7.8589598137	-0.3495400151
H45	1.5195357719	-8.8084823457	0.2350188824
H46	-1.0168997544	-9.0915659094	0.3092823039
H47	-2.3963860851	-6.9641668094	0.2326422124
H48	2.4965992931	-6.5323327726	0.1037832368
H49	4.2518660531	1.4902329082	-0.9232501292
H50	5.3934857681	-0.7027197375	-1.2953791040
H51	4.1319430595	-2.8238983957	-0.8840320339
H52	0.7855119539	-0.3966428063	0.3912426600
H53	-4.2589171543	-5.0760723705	1.1142334287
H54	-4.4413984960	-4.9859501217	-0.4711014851
H55	4.0756583514	4.0671929447	-1.4526724471
H56	4.3204532176	4.0197221946	0.1253283873
H57	-1.2534489109	-4.3466408905	2.6012430686
H58	-1.7765680960	-2.8202500267	2.5725693774
H59	2.1905221643	2.1159273108	2.2044798062
H60	1.5004375710	3.5803030355	2.2268530828
H61	-1.6150870900	-4.5663326127	-2.4268999265
H62	-2.2395191065	-3.0736513460	-2.4293008554
H63	0.9695929692	3.3156222816	-2.7940209652
H64	1.5739297349	1.8183624773	-2.7663492965

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$\Delta r=1.20 \text{ \AA}$	X	Y	Z
N1	2.2043315741	0.5521648634	-0.2948452705
C2	3.4489626258	0.4829267598	-0.8474316002
C3	4.0656440843	-0.7369827966	-1.1342712873
C4	3.3939158111	-1.9315668857	-0.8724783753
C5	2.1036274871	-1.8969698980	-0.2861308843
C6	1.5615373543	-0.6179987416	0.0109556255
C7	1.4355865983	-3.1648118040	-0.0575161253
C8	1.0057094047	-4.3146898119	0.0342695815
C9	0.5175597303	-5.6766681756	0.1207509845
N10	-0.8475330410	-5.8726565625	0.1396611554
C11	-1.3531965162	-7.1448637307	0.2041146576
C12	-0.5509999981	-8.3196999706	0.2593999987
C13	0.8399090322	-8.1045699945	0.2439382129
C14	1.3694612334	-6.7984035003	0.1744724272
Cu15	-1.9481629966	-3.9465937769	0.0847802689
O16	-1.9232020496	-3.9212247544	-1.8689933120
Cu17	1.4960343643	2.7454534780	-0.2565811667
O18	3.5281023377	3.6188217759	-0.4299505145
N19	-2.6522846574	-1.5763273112	0.0782475813
C20	-2.0022078279	-0.4051532645	-0.1976491236
C21	-2.5498391090	0.8728104305	0.0910365882
C22	-3.8552764191	0.9059356421	0.6421064658
C23	-4.5339958558	-0.2907085189	0.8792812295
C24	-3.9096171235	-1.5094123936	0.5998256162
C25	-1.8620026045	2.1324139129	-0.1140135607
C26	-1.3978451806	3.2688794915	-0.1973940114
C27	-0.8309027833	4.5991857397	-0.2806266728
N28	0.5432668726	4.6999988460	-0.3000317900
C29	1.1405365994	5.9303701728	-0.3638689203
C30	0.4238999981	7.1567999706	-0.4198999987
C31	-0.9795131247	7.0413990517	-0.4038459567
C32	-1.6023603871	5.7769440789	-0.3338962966
O33	-3.9562038958	-4.7655486263	0.2555462481
O34	-1.6775961789	-3.7379160362	2.0144699553
O35	1.1770747396	2.5719758966	-2.2033968465
O36	1.4534075860	2.7047777318	1.7155367496
H37	-1.0396369796	-0.4988681589	-0.6789095543
H38	-4.3208011312	1.8590039052	0.8748016125
H39	-5.5407093908	-0.2868018118	1.2878770065
H40	-4.4080008699	-2.4538174208	0.7772274505
H41	0.9457253151	8.1059993788	-0.4706572229
H42	2.2241518019	5.9097766113	-0.3691710806
H43	-2.6858111473	5.7031994008	-0.3212542339
H44	-1.6044422229	7.9300960129	-0.4456329951
H45	1.5270600058	-8.9459763564	0.2854859355
H46	-1.0062475098	-9.3024852868	0.3106837374
H47	-2.4359629857	-7.2049514835	0.2111385384
H48	2.4449533981	-6.6475437768	0.1622595096
H49	3.9424917119	1.4263915714	-1.0407941364
H50	5.0611152503	-0.7429713449	-1.5689348322
H51	3.8531798974	-2.8855284965	-1.1131501990
H52	0.6095164125	-0.5211949996	0.5125272856
H53	-4.3546730102	-5.1202019952	1.0768800873
H54	-4.5448141191	-4.9595221574	-0.5031188639
H55	3.9165442497	4.0032996286	-1.2431270731
H56	4.1248166421	3.7962047499	0.3271290478
H57	-1.3872185045	-4.4640002703	2.6039552398
H58	-1.8287349204	-2.9125537165	2.5181486872
H59	1.7856222520	1.9601210124	2.2572491853
H60	1.2008468300	3.4680781426	2.2745354012
H61	-1.6555929976	-4.6810503893	-2.4260356244
H62	-2.2656242505	-3.1804860034	-2.4103578847
H63	0.8762627868	3.3119857515	-2.7691100611
H64	1.3052863773	1.7579672985	-2.7310025051

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 $\Delta r=1.40 \text{ \AA}$

Atom	X	Y	Z
N1	3.4549035086	-0.4137802380	0.0253700329
C2	4.7032101765	-0.4749103966	-0.5132755359
C3	5.2954050304	-1.6865892732	-0.8828458727
C4	4.5770358789	-2.8763185239	-0.7284753939
C5	3.2687907695	-2.8231195007	-0.1943248576
C6	2.7619478733	-1.5630791681	0.1909801411
C7	2.4729827042	-4.0037432211	-0.0646440919
C8	1.7950655349	-5.0187880713	0.0084534000
C9	1.0225490469	-6.2175186988	0.0960641105
N10	-0.3483456107	-6.0946680496	0.1347138550
C11	-1.1125036077	-7.2210323530	0.2131853564
C12	-0.5635999758	-8.5190996163	0.2681999831
C13	0.8331632211	-8.6406214348	0.2265327774
C14	1.6273657326	-7.4875395196	0.1381368357
Cu15	-1.1682817614	-4.0839171253	0.0959125519
O16	-1.2085361522	-4.0701808447	-1.8764874289
Cu17	2.7187240734	3.6096232730	-0.6808019808
O18	4.6822827814	3.4975763602	-0.4105344616
N19	-1.7666908961	-1.8597105823	0.1494674095
C20	-1.0924912590	-0.7035087093	-0.1424314570
C21	-1.6603645394	0.5826727025	0.0585485150
C22	-2.9913698087	0.6422507424	0.5436289258
C23	-3.6801316512	-0.5394252141	0.8124435530
C24	-3.0464374409	-1.7674577253	0.6128962893
C25	-0.9866249636	1.8430577734	-0.1610834728
C26	-0.5744909155	2.9976235400	-0.2491432582
C27	-0.2318963208	4.3963336688	-0.3149450159
N28	1.0760407112	4.8009960557	-0.4707622871
C29	1.3841715234	6.1359546021	-0.5169254131
C30	0.4238999758	7.1567996163	-0.4198999831
C31	-0.9137248927	6.7495069693	-0.2634802388
C32	-1.2364007465	5.3830685524	-0.2083525241
O33	-3.2519765036	-4.8541313327	0.3228702175
O34	-0.8025959966	-3.9223620030	2.0319433711
O35	2.9532051931	4.1929238698	-2.5578760457
O36	2.4814810564	2.1400536301	0.6037380000
H37	-0.0889292106	-0.8076644505	-0.5340867802
H38	-3.4639115088	1.6081685907	0.7016395608
H39	-4.7018449415	-0.5194025599	1.1810220249
H40	-3.5516709934	-2.7025462767	0.8133932908
H41	0.7204783073	8.1991634807	-0.4643068670
H42	2.4338903121	6.3810685575	-0.6379938711
H43	-2.2685964929	5.0667207012	-0.0831893977
H44	-1.7080210402	7.4868646476	-0.1838612433
H45	1.3057929180	-9.6186241256	0.2620713645
H46	-1.2196856959	-9.3809516475	0.3354316892
H47	-2.1824819365	-7.0562747697	0.2347449817
H48	2.7103439409	-7.5586254801	0.1032017658
H49	5.2202382487	0.4682524862	-0.6462687141
H50	6.3009110305	-1.6931084333	-1.2944899347
H51	5.0077592887	-3.8289670404	-1.0220996351
H52	1.7852076734	-1.4816385699	0.6519759027
H53	-3.6356154139	-5.2133911967	1.1493053095
H54	-3.8814178728	-4.9998751795	-0.4134728911
H55	5.3790585829	3.8849671883	-0.9799712471
H56	5.0358132113	3.2898850085	0.4797478569
H57	-0.4917670428	-4.6646340710	2.5898906996
H58	-0.8675445291	-3.0945369498	2.5497096407
H59	2.7736850797	1.2252370344	0.4141270699
H60	2.0496380446	2.2349017441	1.4774828751
H61	-0.9874846357	-4.8464219773	-2.4313682749
H62	-1.4826866455	-3.3063151048	-2.4245817307
H63	2.2961154068	4.7066445099	-3.0701467297
H64	3.7278662227	3.9705113408	-3.1127198185

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$\Delta r=1.50 \text{ \AA}$			
Atom	X	Y	Z
N1	3.4666117113	-0.3872875890	0.1879590860
C2	4.7118000988	-0.4519045133	-0.3517754924
C3	5.2935609371	-1.6628753992	-0.7395866965
C4	4.5696721461	-2.8485129062	-0.5953350502
C5	3.2685856903	-2.7971248184	-0.0466160412
C6	2.7704242650	-1.5359072894	0.3512317857
C7	2.4773074106	-3.9844930921	0.0753855940
C8	1.8177489217	-5.0138548820	0.1304421429
C9	1.0459650727	-6.2178223714	0.1837351177
N10	-0.3268006860	-6.0877060708	0.2176456266
C11	-1.1009922421	-7.2115548697	0.2538294259
C12	-0.5635999933	-8.5190998932	0.2681999953
C13	0.8343732539	-8.6450796489	0.2398590094
C14	1.6386697206	-7.4953091798	0.1955874139
Cu15	-1.0740309208	-4.0576613438	0.2360956135
O16	-1.1106629292	-3.9820383473	-1.7321475601
Cu17	2.7509282590	3.6969809664	-0.5691367218
O18	4.7256447755	3.5501103472	-0.3352597008
N19	-1.6630219714	-1.7941299465	0.3402456323
C20	-0.9952004587	-0.6280378338	0.0672321588
C21	-1.5587478843	0.6539091962	0.3092506521
C22	-2.87583838402	0.6972658165	0.8358709749
C23	-3.5557808690	-0.4920430913	1.0958048068
C24	-2.9297920401	-1.7147750887	0.8417382325
C25	-0.9022660116	1.9238229581	0.0751705059
C26	-0.5114533606	3.0843056553	-0.0397438231
C27	-0.1856899485	4.4870504445	-0.1556919017
N28	1.1140598806	4.9026774956	-0.3657392200
C29	1.4013528298	6.2393491044	-0.4918341410
C30	0.4301999933	7.2564998932	-0.4242999953
C31	-0.8946608341	6.8400072539	-0.1991835095
C32	-1.1962269882	5.4720092487	-0.0632540573
O33	-3.1984244125	-4.7773706249	0.4561203239
O34	-0.7219358100	-3.9611988722	2.1808575732
O35	2.9620934795	4.2372079995	-2.4673173487
O36	2.5460959138	2.2167187406	0.7306987641
H37	-0.0080377884	-0.7238699005	-0.3663929985
H38	-3.3464138552	1.6566382897	1.0307030772
H39	-4.5667547343	-0.4815009278	1.4940488305
H40	-3.4353577063	-2.6550607287	1.0146907376
H41	0.7109252675	8.2990426600	-0.5346545349
H42	2.4447911507	6.4888412696	-0.6535058576
H43	-2.2195956146	5.1539424229	0.1105213294
H44	-1.6972573757	7.5713606847	-0.1295361011
H45	1.3025600003	-9.6265754092	0.2511161372
H46	-1.2253738858	-9.3776008549	0.2984170964
H47	-2.1701544666	-7.0376944524	0.2693240625
H48	2.7211049096	-7.5782984587	0.1700591427
H49	5.2378874393	0.4876512905	-0.4705463725
H50	6.2951690591	-1.6723008712	-1.1554707169
H51	4.9936898021	-3.7985754312	-0.9042482297
H52	1.8003019405	-1.4517152869	0.8219201348
H53	-3.5836143395	-5.1679910655	1.2675339616
H54	-3.8229430497	-4.8980820357	-0.2888259273
H55	5.4181364784	3.9744123708	-0.8830817925
H56	5.0884536839	3.2373904027	0.5198835810
H57	-0.4590865073	-4.7424837527	2.7093702595
H58	-0.7457386191	-3.1516057854	2.7300152464
H59	2.8241018479	1.2915231772	0.5728571527
H60	2.1079135707	2.3363764539	1.5982087501
H61	-0.9200632037	-4.7536267145	-2.3044801436
H62	-1.3592593118	-3.1946039899	-2.2587303469
H63	2.2826826862	4.7207232664	-2.9797926170
H64	3.7193745725	3.9943269303	-3.0372332130

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$\Delta r=1.60 \text{ \AA}$

Atom	X	Y	Z
N1	3.2535333261	-0.3084529381	0.0841834682
C2	4.4548992500	-0.3180995457	-0.5557996067
C3	5.0249667708	-1.4937639815	-1.0546883106
C4	4.3367999749	-2.7018828978	-0.9120725499
C5	3.0853330409	-2.7063120181	-0.2526835133
C6	2.5931862964	-1.4789962222	0.2445393317
C7	2.3294537527	-3.9122118188	-0.1136972040
C8	1.6864360599	-4.9490233626	-0.0302054552
C9	0.9524368547	-6.1710879930	0.0648364303
N10	-0.4190440216	-6.0873818723	0.1495122305
C11	-1.1490024754	-7.2345868287	0.2489000385
C12	-0.5635999818	-8.5190997118	0.2681999874
C13	0.8335330287	-8.6001293179	0.1738092387
C14	1.5925187733	-7.4245059948	0.0715789274
Cu15	-1.2866075123	-4.0665984638	0.1200534974
O16	-1.2756246527	-4.0165556458	-1.8302325905
Cu17	2.6597059914	3.7528417292	-0.5872275177
O18	4.6022830163	3.3946316339	-0.3623146909
N19	-1.8589764391	-1.6268746507	0.1066755447
C20	-1.1768241476	-0.4627963193	-0.1194238058
C21	-1.7574840440	0.8180757005	0.0764334698
C22	-3.1083582646	0.8654667478	0.5027021448
C23	-3.8047200255	-0.3239216103	0.7139184219
C24	-3.1582881480	-1.5456812093	0.5114840653
C25	-1.0744776695	2.0766913343	-0.1119065525
C26	-0.6446202890	3.2238875406	-0.1982888742
C27	-0.2721650330	4.6129032478	-0.2717098554
N28	1.0470428511	4.9898846347	-0.4060205069
C29	1.3808097419	6.3170397914	-0.4754350818
C30	0.4364999818	7.3561997118	-0.4286999873
C31	-0.9112168707	6.9783126054	-0.2892011668
C32	-1.2596562325	5.6200229681	-0.2069556717
O33	-3.3437817539	-4.7227018121	0.3289313637
O34	-0.9468187325	-3.8681426870	2.0338134163
O35	2.9414607150	4.3795613046	-2.4458950995
O36	2.3229067975	2.2907953512	0.6934675896
H37	-0.1574482720	-0.5554006357	-0.4704337502
H38	-3.5908214594	1.8264347500	0.6598697110
H39	-4.8418350152	-0.3141013259	1.0367358562
H40	-3.6716962746	-2.4862660472	0.6612934906
H41	0.7537623709	8.3913490460	-0.4931488571
H42	2.4373899034	6.5390884124	-0.5788742795
H43	-2.2995283682	5.3250656651	-0.0941037254
H44	-1.6931073661	7.7317077599	-0.2447306693
H45	1.3336611330	-9.5650198123	0.1803473879
H46	-1.1930176632	-9.3991951024	0.3513422669
H47	-2.2224776919	-7.1005939798	0.3105634443
H48	2.6752258468	-7.4648511350	-0.0025608751
H49	4.9520886857	0.6383080803	-0.6642299208
H50	5.9891738874	-1.4577938205	-1.5548697012
H51	4.7501701550	-3.6264884419	-1.3045626060
H52	1.6567667172	-1.4447197046	0.7904537222
H53	-3.7550277683	-5.0350269654	1.1611856026
H54	-3.9597376389	-4.8774035896	-0.4169804324
H55	5.3290746009	3.6640990657	-0.9614327683
H56	4.9473624768	3.1328832035	0.5168946977
H57	-0.6058070835	-4.5861345199	2.6057025395
H58	-1.1053354183	-3.0509693211	2.5483417634
H59	2.6192139362	1.3727944920	0.5271652535
H60	1.8640376673	2.3974322296	1.5519240072
H61	-1.1099689850	-4.7941406748	-2.4021958456
H62	-1.4889124506	-3.2188355191	-2.3567866947
H63	2.2401344301	4.7779006526	-3.0004040167
H64	3.7571493765	4.2442790129	-2.9690016540

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 $\Delta r=1.70 \text{ \AA}$

Atom	X	Y	Z
N1	3.0718237802	-0.2155958083	0.0078216770
C2	4.3374504272	-0.2589828529	-0.4891964552
C3	4.9528966080	-1.4600616112	-0.8546696073
C4	4.2465087646	-2.6584424152	-0.7213620431
C5	2.9268683017	-2.6244241110	-0.2135919894
C6	2.3860888521	-1.3723728874	0.1494408676
C7	2.1612024214	-3.8223233676	-0.0822975360
C8	1.5278956595	-4.8640540006	0.0040435945
C9	0.8453038892	-6.1114501265	0.0960795208
N10	-0.5278146922	-6.1033384778	0.1716666291
C11	-1.2112590815	-7.2771955673	0.2536529033
C12	-0.5635999946	-8.5190999148	0.2681999963
C13	0.8373356062	-8.5397038257	0.1956482541
C14	1.5439127258	-7.3335928723	0.1079054346
Cu15	-1.6413878215	-4.3546065536	0.1537016167
O16	-1.5274620778	-4.1229090955	-1.7771772707
Cu17	2.3274755546	3.7152240834	-0.8353822911
O18	4.2811413313	3.3294487302	-0.7690792000
N19	-2.3508185103	-1.2373796339	0.0465938215
C20	-1.6709733916	-0.0724573380	-0.0815980048
C21	-2.2918465337	1.1924609846	0.0251674148
C22	-3.6853599064	1.2311950629	0.2681441233
C23	-4.3845938036	0.0291756195	0.3916828311
C24	-3.6904318231	-1.1798623965	0.2774614013
C25	-1.5567135053	2.4110215606	-0.0978841759
C26	-0.9922909449	3.4924747815	-0.1807014931
C27	-0.4947989122	4.8254674844	-0.2550018810
N28	0.8370526607	5.0654356778	-0.4985429048
C29	1.2870113892	6.3519182437	-0.5784225134
C30	0.4427999946	7.4558999148	-0.4330999963
C31	-0.9180899491	7.2233027772	-0.1810134253
C32	-1.3843323781	5.9078724140	-0.0895616250
O33	-3.6942154105	-4.5546073244	0.2135262770
O34	-1.4348229178	-4.0182163335	2.0639768248
O35	2.4290146741	4.2676813959	-2.7363270107
O36	2.0458188532	2.3184352309	0.5120992440
H37	-0.6076522758	-0.1399360697	-0.2749083906
H38	-4.1939851307	2.1870030286	0.3560445178
H39	-5.4557732784	0.0210092992	0.5761881683
H40	-4.1974473856	-2.1314427916	0.3673455789
H41	0.8493816505	8.4593149256	-0.5096496346
H42	2.3460905529	6.4877526708	-0.7678074418
H43	-2.4332508856	5.6964086908	0.1021707359
H44	-1.6074804002	8.0541603155	-0.0592505261
H45	1.3769822425	-9.4827497165	0.2070324354
H46	-1.1480110866	-9.4314276576	0.3348685485
H47	-2.2919196378	-7.2032732662	0.3036389696
H48	2.6280775302	-7.3226743413	0.0499069992
H49	4.8476154436	0.6905120198	-0.5940673130
H50	5.9677841089	-1.4516803079	-1.2420128163
H51	4.6971993360	-3.6044875030	-1.0060141246
H52	1.3869224553	-1.3051505849	0.5648697203
H53	-4.2146622759	-4.7156869960	1.0274847820
H54	-4.2603988013	-4.6685175821	-0.5777338309
H55	4.9433742218	3.5498559775	-1.4565801451
H56	4.7137070005	3.1886798944	0.0990081332
H57	-1.0649240973	-4.6632713287	2.7011216760
H58	-1.7610954412	-3.2157428464	2.5190235104
H59	2.3901889031	1.4114242059	0.3820462095
H60	1.6253138469	2.4533902990	1.3860363173
H61	-1.2555873880	-4.8192027070	-2.4099276202
H62	-1.7677614372	-3.2913710576	-2.2355330643
H63	1.7200693729	4.7536551082	-3.2045583890
H64	3.1410551955	4.0147130904	-3.3578448994

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$\Delta r=1.80 \text{ \AA}$			
Atom	X	Y	Z
N1	2.7690133235	-0.0815293353	0.6510798871
C2	3.9892977329	-0.0705732042	1.2541846010
C3	4.6220046809	-1.2436150990	1.6759902425
C4	3.9815336945	-2.4719529072	1.4885625091
C5	2.7087822580	-2.4981155222	0.8730280399
C6	2.1469164617	-1.2701839302	0.4610861417
C7	2.0104537529	-3.7347358223	0.6886281021
C8	1.4370740789	-4.8079906733	0.5690994842
C9	0.7884876609	-6.0748733411	0.4358594811
N10	-0.5202101398	-6.1723695811	0.8469132019
C11	-1.1803203966	-7.3594108313	0.7579549016
C12	-0.5635999845	-8.5190997545	0.2681999892
C13	0.7719114877	-8.4317278867	-0.1537501179
C14	1.4486710522	-7.2060675445	-0.0743761530
Cu15	-1.3940321447	-4.5783361456	1.7444557958
O16	-1.6724793194	-3.5444799100	0.0927116199
Cu17	1.7397549347	3.6053848138	-1.4333319526
O18	3.3731665375	2.7383674706	-2.1709909798
N19	-2.6416547233	-1.0062440729	-0.2969395644
C20	-1.9988090041	0.1827916692	-0.2222681395
C21	-2.5896374683	1.3920794576	-0.6476421001
C22	-3.9076537104	1.3440449349	-1.1590924345
C23	-4.5647513617	0.1125799829	-1.2337654826
C24	-3.9047502527	-1.0416474853	-0.8014808454
C25	-1.8828879910	2.6338033536	-0.5693521450
C26	-1.3109558740	3.7137110017	-0.5286494160
C27	-0.7281811638	5.0160494744	-0.4723049406
N28	0.6081105735	5.1602228217	-0.7667650253
C29	1.1798136362	6.3984035309	-0.7438136300
C30	0.4490999845	7.5555997545	-0.4374999892
C31	-0.9119351883	7.4170471177	-0.1273879140
C32	-1.4996631161	6.1453934846	-0.1414079714
O33	-2.6302351641	-3.3974806335	2.7558039995
O34	-0.6716835187	-5.1581761016	3.4967217253
O35	1.0903613295	3.9025878285	-3.2844081617
O36	1.9369632906	2.5563155344	0.2268923290
H37	-0.9948547366	0.1769982664	0.1865723679
H38	-4.3952766891	2.2552163121	-1.4925344854
H39	-5.5753229652	0.0436458224	-1.6260387541
H40	-4.3782320351	-2.0155725962	-0.8562156880
H41	0.9446806073	8.5210893265	-0.4385679548
H42	2.2371148608	6.4493536662	-0.9782281429
H43	-2.5508924389	6.0134513516	0.0952661137
H44	-1.5125844832	8.2868312227	0.1225719477
H45	1.2860147577	-9.3070259565	-0.5408465948
H46	-1.1218613162	-9.4484705370	0.2206126019
H47	-2.2125174412	-7.3663873424	1.0895702144
H48	2.4810274103	-7.1147568197	-0.3978804594
H49	4.4508737159	0.8994965471	1.4011796831
H50	5.5983440539	-1.1911924652	2.1494316561
H51	4.4468484150	-3.3966884806	1.8153175788
H52	1.1802637219	-1.2474178664	-0.0279513999
H53	-3.0866173425	-3.7220338644	3.5593713762
H54	-3.0403541572	-2.5656477070	2.4403866465
H55	3.7017522137	2.9170812289	-3.0764644176
H56	4.0828012084	2.3468849207	-1.6198706772
H57	-0.1943890550	-5.9968609305	3.6630718552
H58	-0.5838746878	-4.5437835524	4.2532244139
H59	2.1620829358	1.6060936104	0.2945174852
H60	1.6920182545	2.9378679486	1.0948754539
H61	-1.4878737294	-3.9510402586	-0.7789207979
H62	-1.9626550126	-2.6125686105	0.0112943638
H63	0.5437908014	4.6623964044	-3.5708989938
H64	1.1346366527	3.2225874507	-3.9865640938

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$\Delta r=1.90 \text{ \AA}$			
Atom	X	Y	Z
N1	2.7960678596	-0.0861628120	0.3764579680
C2	4.0484781278	-0.0719802427	0.9082465520
C3	4.7163216783	-1.2448038666	1.2728003417
C4	4.0774352179	-2.4770048834	1.1048667151
C5	2.7701054109	-2.5068900636	0.5670976795
C6	2.1754660350	-1.2782221427	0.2039130567
C7	2.0674848386	-3.7461634837	0.4216586164
C8	1.4854823625	-4.8194459895	0.3422763027
C9	0.8195683998	-6.0825910861	0.2786334436
N10	-0.5029162867	-6.1316476582	0.6549531390
C11	-1.1773558208	-7.3152594367	0.6420668044
C12	-0.5635999786	-8.5190996609	0.2681999851
C13	0.7829610233	-8.4792803727	-0.1267003827
C14	1.4742289127	-7.2588748760	-0.1261224312
Cu15	-1.3908774111	-4.4759887425	1.4077330296
O16	-1.7091971535	-3.5001293189	-0.2787642308
Cu17	1.7181788859	3.7341962194	-1.5619622388
O18	3.3858473982	2.9565439209	-2.3085185640
N19	-2.5974215246	-0.9069843972	-0.7011817763
C20	-1.9721694764	0.2863249496	-0.5660289273
C21	-2.5707802273	1.5043612403	-0.9547269377
C22	-3.8777861753	1.4608158684	-1.4940280387
C23	-4.5158102200	0.2255755824	-1.6335163141
C24	-3.8486466978	-0.9366163634	-1.2351906029
C25	-1.8849208628	2.7505042170	-0.8079086575
C26	-1.3295302103	3.8344113655	-0.7067713871
C27	-0.7436283305	5.1302587294	-0.5904324909
N28	0.5999324615	5.2719097268	-0.8481278779
C29	1.1825228150	6.5019365527	-0.7662091375
C30	0.4553999786	7.6552996609	-0.4418999851
C31	-0.9153180351	7.5204026549	-0.1759698257
C32	-1.5132946062	6.2554293301	-0.2449079790
O33	-2.7190636679	-3.3500614715	2.3506356061
O34	-0.5135862332	-4.8052265360	3.1675466429
O35	0.9732858785	3.9825563761	-3.3839753211
O36	1.9207867044	2.6161909719	0.0625721611
H37	-0.9770016158	0.2758610077	-0.1364069706
H38	-4.3713522040	2.3789219684	-1.7978831346
H39	-5.5178913071	0.1595596049	-2.0478454424
H40	-4.3098230314	-1.9125217956	-1.3384386132
H41	0.9592460679	8.6153886874	-0.3982517672
H42	2.2465656553	6.5487646796	-0.9707211150
H43	-2.5717497274	6.1256023183	-0.0404924398
H44	-1.5155370179	8.3881899146	0.0825017896
H45	1.2946425396	-9.3878971776	-0.4322403560
H46	-1.1336858230	-9.4424863795	0.2802009386
H47	-2.2196366210	-7.2821587139	0.9415514059
H48	2.5157333750	-7.2062345197	-0.4283598661
H49	4.5078015793	0.9011660964	1.0445126175
H50	5.7183882116	-1.1894574108	1.6887314986
H51	4.5697210523	-3.4018319609	1.3896668883
H52	1.1815379347	-1.2567913631	-0.2275309404
H53	-2.9735868007	-3.5411961603	3.2769507121
H54	-3.3933551842	-2.7883779263	1.9151572987
H55	3.6996507445	3.1620257022	-3.2134856946
H56	4.1220127063	2.6301056526	-1.7497104786
H57	-0.0681144680	-5.6421820145	3.4124596345
H58	-0.2398833686	-4.0763865447	3.7603092083
H59	2.1351702008	1.6611783139	0.0750507818
H60	1.6699555065	2.9451095624	0.9502178343
H61	-1.5254228193	-3.9268826905	-1.1408051370
H62	-1.9494881188	-2.5560250395	-0.3797952630
H63	0.4635860097	4.7662808004	-3.6738418600
H64	0.8789969640	3.2485944408	-4.0240662351

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$\Delta r=2.00 \text{ \AA}$	X	Y	Z
Atom			
N1	2.7126916098	-0.0366425126	0.4266662402
C2	3.9493141268	-0.0245647860	0.9957223307
C3	4.6023663092	-1.1981798960	1.3853480149
C4	3.9637654116	-2.4291035809	1.2052572706
C5	2.6722496159	-2.4568707870	0.6294763167
C6	2.0922815799	-1.2278875632	0.2445119204
C7	1.9734107954	-3.6964495704	0.4626210121
C8	1.4021037109	-4.7734453049	0.3666069584
C9	0.7574265360	-6.0469182472	0.2858688348
N10	-0.5445313962	-6.1396954313	0.7205787295
C11	-1.1881049315	-7.3410139773	0.7064023725
C12	-0.5635999750	-8.5190996031	0.2681999826
C13	0.7591443230	-8.4319146658	-0.1931799354
C14	1.4197052553	-7.1943333150	-0.1860528022
Cu15	-1.4595147555	-4.5235228619	1.5305135809
O16	-1.7667061656	-3.4759761920	-0.1132558291
Cu17	1.7040620682	3.7848407360	-1.5365024081
O18	3.2731812921	2.8336544648	-2.3050636930
N19	-2.5827059062	-0.8320144373	-0.5182452045
C20	-1.9606186205	0.3624208545	-0.3712345195
C21	-2.5212555984	1.5729468555	-0.8317931750
C22	-3.7903152931	1.5225750557	-1.4550818002
C23	-4.4293999363	0.2878447484	-1.5999526886
C24	-3.7988550125	-0.8674279761	-1.1281029624
C25	-1.8343161205	2.8195417773	-0.6814420589
C26	-1.2848976573	3.9083688403	-0.5947649646
C27	-0.7077366564	5.2117213188	-0.5073706083
N28	0.6235769079	5.3632214572	-0.8213000013
C29	1.1910290096	6.6031932289	-0.7845593868
C30	0.4616999750	7.7549996031	-0.4462999826
C31	-0.8935624013	7.6055551835	-0.1160110197
C32	-1.4762639607	6.3313428460	-0.1411475001
O33	-2.8347407603	3.4616585908	2.4785273714
O34	-0.5945254643	-4.9174124892	3.2778149457
O35	1.0331332413	4.1393628889	-3.3664419881
O36	1.8769715664	2.6718297895	0.0910344974
H37	-0.9983277149	0.3587980901	0.1275004928
H38	-4.2537266226	2.4350931522	-1.8176909743
H39	-5.4035001745	0.2161555231	-2.0759651239
H40	-4.2620983895	-1.8420625313	-1.2320597639
H41	0.9538396375	8.7219999563	-0.4427386761
H42	2.2456753379	6.6588626666	-1.0316349121
H43	-2.5221815609	6.1903781754	0.1141230886
H44	-1.4946389758	8.4688317491	0.1566961364
H45	1.2764226763	-9.3167209452	-0.5540637074
H46	-1.1089696914	-9.4573502474	0.2789922448
H47	-2.2149326442	-7.3447801398	1.0565682872
H48	2.4452065567	-7.1067997356	-0.5317133505
H49	4.4080400650	0.9471853908	1.1407046958
H50	5.5926733692	-1.1440210072	1.8294231752
H51	4.4445507879	-3.3545923351	1.5077754440
H52	1.1108642480	-1.2064764319	-0.2143667549
H53	-3.1119473820	-3.6972804326	3.3880026358
H54	-3.4977467836	-2.8821737117	2.0491314841
H55	3.6505699928	3.0674617014	-3.1783549587
H56	3.9007902122	2.2810741412	-1.7936471607
H57	-0.1003484273	-5.7377011063	3.4827048935
H58	-0.4150175632	-4.2242841602	3.9447654710
H59	2.0661532856	1.7117310193	0.1149005597
H60	1.6735049039	3.0284622469	0.9800645237
H61	-1.6113075161	-3.8698045847	-0.9962819537
H62	-1.9693020355	-2.5189069052	-0.1606224276
H63	0.5278119931	4.9329842655	-3.6365088627
H64	1.0171700682	3.4570874068	-4.0674035017

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$\Delta r=2.10 \text{ \AA}$			
Atom	X	Y	Z
N1	2.6682634648	-0.0029734037	0.3007376519
C2	3.9433554463	-0.0093972583	0.7781997335
C3	4.6090474736	-1.1926284796	1.1129746881
C4	3.9442917301	-2.4143494556	0.9744290123
C5	2.6135512564	-2.4236494174	0.4947157451
C6	2.0235273541	-1.1861816922	0.1565556123
C7	1.8915261621	-3.6534982694	0.3711075694
C8	1.3132788979	-4.7290014809	0.3066259195
C9	0.6899127953	-6.0127198734	0.2492521218
N10	-0.6311116371	-6.1199345900	0.6199526475
C11	-1.2396262183	-7.3409785090	0.6220474162
C12	-0.5635999831	-8.5190997314	0.2681999882
C13	0.7783673599	-8.4153367221	-0.1279745742
C14	1.4030387755	-7.1603631464	-0.1416105635
Cu15	-1.6310664984	-4.5076914650	1.3552877073
O16	-1.8311078890	-3.4127014998	-0.2795936097
Cu17	1.6738235331	3.8851574614	-1.5546848382
O18	3.2581383974	2.9612418591	-2.3277809570
N19	-2.6280152805	-0.7187377245	-0.6057631360
C20	-2.0005916688	0.4702964916	-0.4320787234
C21	-2.5771705328	1.6989046372	-0.8212528140
C22	-3.8731184884	1.6743548851	-1.3877320215
C23	-4.5192999649	0.4469610346	-1.5563392638
C24	-3.8680264290	-0.7269176153	-1.1668884293
C25	-1.8775480750	2.9383433664	-0.6678877188
C26	-1.3190558082	4.0226370071	-0.5833563659
C27	-0.7284639697	5.3202550057	-0.5001309019
N28	0.6007304518	5.4601233534	-0.8271852799
C29	1.1812540746	6.6947556115	-0.7941636240
C30	0.4679999831	7.8546997314	-0.45066999882
C31	-0.8845893886	7.7167842970	-0.1055509407
C32	-1.4802898957	6.4484209890	-0.1259049100
O33	-3.1099836152	-3.4715203419	2.1779086761
O34	-0.9326070984	-4.9056187325	3.1672260087
O35	1.0129078449	4.2813132615	-3.3867740244
O36	1.8464980948	2.7333294361	0.0475675165
H37	-1.0193638710	0.4482216519	0.0263753611
H38	-4.3513517522	2.6007844795	-1.6905601864
H39	-5.5139959163	0.3956415742	-1.9901191188
H40	-4.3338419480	-1.6965651088	-1.3018606370
H41	0.9696845499	8.8168530654	-0.4494828505
H42	2.2329134687	6.7407733409	-1.0551586194
H43	-2.5257381862	6.3198122219	0.1357456870
H44	-1.4740746138	8.5850689310	0.1756675959
H45	1.3370498067	-9.2993557529	-0.4216663230
H46	-1.0855504958	-9.4700174680	0.2969536605
H47	-2.2825658798	-7.3605373267	0.9189253005
H48	2.4408981572	-7.0565365635	-0.4422807540
H49	4.4238306288	0.9555483891	0.8947962907
H50	5.6303993074	-1.1532350243	1.4822732810
H51	4.4355927305	-3.3468384613	1.2357252998
H52	1.0135776934	-1.1519133955	-0.2344577959
H53	-3.4656452928	-3.6927003665	3.0634150950
H54	-3.7399126086	-2.9118473592	1.6781795237
H55	3.6197489416	3.1896892274	-3.2091676339
H56	3.9165738704	2.4667469995	-1.7961743996
H57	-0.4678633174	-5.7297843243	3.4199591392
H58	-0.8205240826	-4.2173929132	3.8537239907
H59	2.0271552246	1.7713240140	0.0424621610
H60	1.6446804406	3.0666539191	0.9459730838
H61	-1.6493346799	-3.7801086207	-1.1689119486
H62	-2.0139542890	-2.4509052347	-0.3085742476
H63	0.5121694954	5.0846915185	-3.6356264737
H64	0.9890420406	3.6177837006	-4.1053462512

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$\Delta r=2.20 \text{ \AA}$	X	Y	Z
Atom			
N1	2.8747676615	-0.0932703018	-0.1129145927
C2	4.1986394458	-0.1278230759	0.2031164444
C3	4.8715406073	-1.3216020899	0.4807811025
C4	4.1672935468	-2.5284807609	0.4468223211
C5	2.7885593573	-2.5112649836	0.1311570798
C6	2.1903176380	-1.2626331865	-0.1496616159
C7	2.0333947523	-3.7267880329	0.1087524732
C8	1.4280531038	-4.7892781194	0.1202659855
C9	0.7744583243	-6.0582056678	0.1424548366
N10	-0.5686486740	-6.1009382379	0.4394969194
C11	-1.2184188066	-7.2992998646	0.4932287890
C12	-0.5635999787	-8.5190996616	0.2681999851
C13	0.8055909363	-8.4848928200	-0.0400601712
C14	1.4729244747	-7.2541151828	-0.1074730609
Cu15	-1.5778107128	-4.4358884886	1.0115524860
O16	-1.6157906409	-3.3895560762	-0.6741477111
Cu17	1.6987938518	4.0834279807	-1.8002841849
O18	3.3323682906	3.4464530373	-2.7314968136
N19	-2.4542837273	-0.6448669063	-1.0609769857
C20	-1.8756333576	0.5517691307	-0.7963226104
C21	-2.4728988997	1.7813031313	-1.1509205267
C22	-3.7375052848	1.7484865865	-1.7828959308
C23	-4.3304187668	0.5123238308	-2.0525383880
C24	-3.6600201496	-0.6605795827	-1.6918123662
C25	-1.8138588460	3.0286264882	-0.9106496300
C26	-1.2757236788	4.1155774537	-0.7572732393
C27	-0.6982690598	5.4133649164	-0.6103694100
N28	0.6234110599	5.5847385586	-0.9510785920
C29	1.1927718513	6.8221773951	-0.8684158898
C30	0.4742999787	7.9543996616	-0.4550999851
C31	-0.8697644920	7.7844569259	-0.0898018782
C32	-1.4539139458	6.5122168250	-0.1639885258
O33	-3.1271461369	-3.3817577714	1.6530202937
O34	-0.9899702534	-4.6881665837	2.8919389877
O35	0.7539792724	4.3432268962	-3.5371483595
O36	2.0433703515	2.8400478202	-0.2752828937
H37	-0.9160745244	0.5340157586	-0.2924773222
H38	-4.2312798448	2.6752198268	-2.0597164666
H39	-5.2975000170	0.4534611329	-2.5437901491
H40	-4.0818967597	-1.6351981123	-1.9082235380
H41	0.9668997635	8.9205107287	-0.4142116570
H42	2.2389502078	6.8933363192	-1.1451318551
H43	-2.4928372599	6.3573171125	0.1101482422
H44	-1.4613200729	8.6311100995	0.2473293215
H45	1.3528225545	-9.4051939984	-0.2252865249
H46	-1.1186130217	-9.4496099490	0.3299128802
H47	-2.2776963384	-7.2651308782	0.7247509859
H48	2.5314143888	-7.2051727311	-0.3442885594
H49	4.7150796029	0.8247212882	0.2346109254
H50	5.9304781559	-1.3011996664	0.7236810867
H51	4.6641615448	-3.4692304384	0.6635797485
H52	1.1405476613	-1.2079478895	-0.4099925754
H53	-3.5395766440	-3.5423707026	2.5268598746
H54	-3.7386968145	-2.9024116372	1.0563870375
H55	3.5110070987	3.6955864419	-3.6619145815
H56	4.1657022894	3.2397398259	-2.2586594688
H57	-0.5253895703	-5.4798906031	3.2332561949
H58	-0.9119700303	-3.9407382058	3.5186244631
H59	2.2040523378	1.8768522063	-0.3425300060
H60	1.8677711148	3.1058279444	0.6507447483
H61	-1.3556155982	-3.7723497248	-1.5370882999
H62	-1.7880466705	-2.4272365182	-0.7343302013
H63	0.2356554212	5.1397455565	-3.7715665734
H64	0.5366003430	3.5982765113	-4.1328337086

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 $\Delta r=2.30 \text{ \AA}$

Atom	X	Y	Z
N1	2.7098684876	-0.0036374005	0.0308752312
C2	3.9713591256	-0.0148352951	0.5419372257
C3	4.6013412330	-1.1921895135	0.9569791781
C4	3.9152771282	-2.4056023264	0.8585497576
C5	2.6015000517	-2.4125143343	0.3351699016
C6	2.0448133479	-1.1802252717	-0.0737647848
C7	1.8665579584	-3.6378235458	0.2446163461
C8	1.2795480379	-4.7098929873	0.2103983179
C9	0.6653328343	-5.9988758513	0.1864838232
N10	-0.6626962153	-6.1066207261	0.5313210317
C11	-1.2579230721	-7.3353201369	0.5655260485
C12	-0.5635999961	-8.5190999389	0.2681999973
C13	0.7858896712	-8.4138035435	-0.1015660614
C14	1.3976187207	-7.1536993263	-0.1453555912
Cu15	-1.7380131830	-4.4910818961	1.1667424814
O16	-1.7768828590	-3.3253483669	-0.4426084124
Cu17	1.6823263253	4.1711219907	-1.8102195939
O18	3.2945180009	3.4395777955	-2.7153455524
N19	-2.5094863090	-0.5640073433	-0.7568868539
C20	-1.8946366533	0.6274210448	-0.5532311361
C21	-2.4782155677	1.8593097575	-0.9238932762
C22	-3.7687017291	1.8346690422	-1.5028169662
C23	-4.4012432633	0.6049894874	-1.7036568779
C24	-3.7431774122	-0.5709566060	-1.3314450727
C25	-1.7930807940	3.1040820388	-0.7417511292
C26	-1.2505273741	4.1951216299	-0.6388905783
C27	-0.6777019954	5.5005994804	-0.5372652927
N28	0.6224444037	5.6812110345	-0.9497686314
C29	1.1849785639	6.9241804790	-0.9037816881
C30	0.4805999962	8.0540999389	-0.4594999973
C31	-0.8429248830	7.8755191760	-0.0279580568
C32	-1.4191950745	6.5978222424	-0.0631245471
O33	-3.3506851780	-3.5184475488	1.8038938359
O34	-1.2216383545	-4.8761067278	3.0420693089
O35	0.8422314526	4.5537002920	-3.5683209471
O36	1.9624893807	2.9458113099	-0.2605469748
H37	-0.9167617827	0.6019783062	-0.0867334084
H38	-4.2531750446	2.7627964044	-1.7905513210
H39	-5.3907608568	0.5532810358	-2.1492069253
H40	-4.1978277672	-1.5415427635	-1.4942426948
H41	0.9668049856	9.0241227815	-0.4490006633
H42	2.2140429546	7.0024819088	-1.2366623773
H43	-2.4422702326	6.4378862591	0.2627086322
H44	-1.4247177260	8.7195788425	0.3319766188
H45	1.3611458528	-9.3007867921	-0.3520115367
H46	-1.0773773925	-9.4734312533	0.3191332262
H47	-2.3069623445	-7.3560960298	0.8417034281
H48	2.4411378581	-7.0506861101	-0.4263815851
H49	4.4723830079	0.9432735573	0.6183627468
H50	5.6116861590	-1.1538412379	1.3547963637
H51	4.3774476891	-3.3336562019	1.1806466626
H52	1.0458543355	-1.1448671323	-0.4914718084
H53	-3.8240781973	-3.7533564779	2.6287372701
H54	-3.9147796018	-2.9714696238	1.2187245094
H55	3.5501429404	3.7146708482	-3.6201153852
H56	4.0570669734	3.0459453792	-2.2415007909
H57	-0.7238866159	-5.6671151706	3.3348949713
H58	-1.2897309067	-4.2195800198	3.7645160144
H59	2.0751119892	1.9739215646	-0.2889898508
H60	1.8400916309	3.2655578660	0.6569899959
H61	-1.5450582505	-3.6622329412	-1.3323828116
H62	-1.9062273408	-2.3543904510	-0.4413854882
H63	0.2686929557	5.3249845153	-3.7534384581
H64	0.8134640556	3.9137874998	-4.3077000196

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 $\Delta r=2.40 \text{ \AA}$

Atom	X	Y	Z
N1	2.9647470925	-0.1306379227	0.3340346595
C2	4.2539289078	-0.2051274248	0.7666473161
C3	4.8865334853	-1.4228908578	1.0378810920
C4	4.1731018101	-2.6142412957	0.8782853902
C5	2.8306366214	-2.5540229712	0.4380450897
C6	2.2752043316	-1.2844664167	0.1684866284
C7	2.0528287357	-3.7456440866	0.2995665184
C8	1.4208905471	-4.7895144635	0.2341286553
C9	0.7536919110	-6.0490194060	0.1867321742
N10	-0.5436717189	-6.1212269798	0.6389389424
C11	-1.1832269155	-7.3268057113	0.6743027886
C12	-0.5635999972	-8.5190999554	0.2681999980
C13	0.7522627970	-8.4490531308	-0.2139350229
C14	1.4089459001	-7.2121458371	-0.2570311496
Cu15	-1.5029913403	-4.4935035522	1.4128780059
O16	-1.6598153166	-3.2994449588	-0.1732814314
Cu17	1.9241584016	4.2253381023	-1.3843889261
O18	3.6658521821	3.4382433701	-1.9329295032
N19	-2.3814059981	-0.5246801647	-0.4863006493
C20	-1.7629499522	0.6713328022	-0.3268969095
C21	-2.3605896849	1.8962736775	-0.6985316074
C22	-3.6684611664	1.8588805174	-1.2370431137
C23	-4.3050617578	0.6247302852	-1.3931915167
C24	-3.6339143678	-0.5432584472	-1.0189384695
C25	-1.6765816311	3.1469281762	-0.5571551795
C26	-1.1409950948	4.2448999965	-0.4877935916
C27	-0.5975251017	5.5651454024	-0.4318597068
N28	0.7246573920	5.7539488836	-0.7635570422
C29	1.2493972124	7.0154290985	-0.7715183489
C30	0.4868999972	8.1537999554	-0.4638999980
C31	-0.8579860713	7.9657865166	-0.1092498715
C32	-1.3965658556	6.6719254419	-0.0892263799
O33	-3.0018926797	-3.4689090411	2.2246052577
O34	-0.8431830272	-4.9358872684	3.2287098792
O35	1.4669186102	4.6195838465	-3.2705037745
O36	1.9737930432	3.0080405477	0.1977750681
H37	-0.7690953611	0.6541865789	0.1040484012
H38	-4.1633203197	2.7807730733	-1.5269168101
H39	-5.3085924685	0.5631012762	-1.8050904708
H40	-4.0935825557	-1.5167973501	-1.1463658948
H41	0.9471487506	9.1359625313	-0.4945416748
H42	2.2987508755	7.1017382760	-1.0321479698
H43	-2.4351786370	6.5053202890	0.1790709315
H44	-1.4856765216	8.8145266011	0.1479378615
H45	1.2668616480	-9.3456291223	-0.5484308977
H46	-1.1088686124	-9.4561491252	0.3246850425
H47	-2.2057320409	-7.3218949582	1.0374783861
H48	2.4284892683	-7.1333376990	-0.6211950324
H49	4.7775351961	0.7349088628	0.8985011980
H50	5.9194100366	-1.4327760967	1.3755440012
H51	4.6361614198	-3.5732400263	1.0912369746
H52	1.2544580440	-1.2003499264	-0.1843995616
H53	-3.3976439213	-3.6896079878	3.0931100329
H54	-3.5884287759	-2.8717588872	1.7155329823
H55	4.1623963073	3.7314231815	-2.7248663722
H56	4.2445902585	2.9386061322	-1.3195466071
H57	-0.3400968155	-5.7441354466	3.4583994329
H58	-0.8472082801	-4.3023499993	3.9744350031
H59	2.1103336341	2.0392226418	0.1689786319
H60	1.7210430776	3.3042256596	1.0963583798
H61	-1.5351134452	-3.6383563565	-1.0835371164
H62	-1.780970961	-2.3276138895	-0.1582420696
H63	0.9070045929	5.3676233205	-3.5620535241
H64	1.6483641699	4.0091159623	-4.0130806147

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$\Delta r=2.50 \text{ \AA}$			
Atom	X	Y	Z
N1	2.6621002057	0.0206952618	0.0943101950
C2	3.9420187483	0.0026777949	0.5577623406
C3	4.6037564141	-1.1831076169	0.8899230714
C4	3.9296037329	-2.4005800530	0.7613294919
C5	2.5945649306	-2.4027224280	0.2943090235
C6	2.0089493759	-1.1601661320	-0.0403049648
C7	1.8719461042	-3.6355407900	0.1859638329
C8	1.2999614082	-4.7161096598	0.1433602139
C9	0.6781714899	-6.0034583828	0.1296319345
N10	-0.6287486963	-6.1038156479	0.5521325824
C11	-1.2299024347	-7.3293520747	0.6134075864
C12	-0.5635999980	-8.5190999679	0.2681999986
C13	0.7611444215	-8.4173249058	-0.1840536773
C14	1.3792372070	-7.1604934307	-0.2563371328
Cu15	-1.6129289038	-4.4475252354	1.2436640175
O16	-1.7291480684	-3.3025982084	-0.3891975458
Cu17	1.8428779702	4.3390835815	-1.5509595515
O18	3.5772003078	3.6101206640	-2.1939675621
N19	-2.5052251342	-0.3760232285	-0.6599496302
C20	-1.8708630537	0.8096104810	-0.4848862117
C21	-2.4671630529	2.0510980645	-0.7997282201
C22	-3.7927987476	2.0426967288	-1.2940828736
C23	-4.4450077940	0.8195111188	-1.4697803260
C24	-3.7727961608	-0.3656788825	-1.1556492367
C25	-1.7624264711	3.2883897409	-0.6472288544
C26	-1.2069959276	4.3750516301	-0.5649629974
C27	-0.6385144139	5.6831195398	-0.4870656771
N28	0.6795625685	5.8591948228	-0.8415133140
C29	1.2272125526	7.1108279515	-0.8239197441
C30	0.4931999980	8.2534999679	-0.4682999986
C31	-0.8474108145	8.0781784957	-0.0915221251
C32	-1.4090310537	6.7941306098	-0.0968001231
O33	-3.0705079055	-3.3313071060	1.9931654239
O34	-0.9857813618	-4.8572439072	3.0777161105
O35	1.2931228035	4.7514558014	-3.4092306142
O36	1.9434362677	3.0159102105	-0.0491242682
H37	-0.8636932690	0.7720558047	-0.0878699635
H38	-4.2885123881	2.9772837624	-1.5383168389
H39	-5.4613446479	0.7794951040	-1.8519379509
H40	-4.2437674454	-1.3302068210	-1.3041154786
H41	0.9703384051	9.2278928149	-0.4813771492
H42	2.2715615973	7.1855512394	-1.1067894819
H43	-2.4442925657	6.6386607126	0.1894877730
H44	-1.4547576385	8.9299644543	0.2018668938
H45	1.3143371188	-9.3058659784	-0.4755718916
H46	-1.0799185500	-9.4702599392	0.3447258765
H47	-2.2607743952	-7.3435496950	0.9504405956
H48	2.4046086533	-7.0634514545	-0.5986527698
H49	4.4327409318	0.9633624392	0.6654029264
H50	5.6284510393	-1.1490379572	1.2497039716
H51	4.4169892057	-3.3354190638	1.0209166861
H52	0.9942015051	-1.1189411884	-0.4167661022
H53	-3.4972849152	-3.5065031114	2.8573106721
H54	-3.5894565670	-2.6887563501	1.4663691365
H55	4.0184710479	3.9167269614	-3.0130509001
H56	4.2040175637	3.1316747526	-1.6115941746
H57	-0.4878108977	-5.6613043731	3.3318246932
H58	-1.0013779539	-4.2078503187	3.8095482080
H59	2.0251210858	2.0450815939	-0.1442468996
H60	1.7541520601	3.2703376064	0.8774302252
H61	-1.5900164342	-3.6679426095	-1.2870288436
H62	-1.8348220123	-2.3290096495	-0.4056633392
H63	0.6992954876	5.4858355593	-3.6661737494
H64	1.4640050611	4.1596148151	-4.1692269956

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$\Delta r=2.55 \text{ \AA}$			
Atom	X	Y	Z
N1	2.7213056073	-0.0181361047	-0.1527501173
C2	4.0266402608	-0.0364599828	0.2342743512
C3	4.7002343496	-1.2198946156	0.5513261629
C4	4.0139975974	-2.4356643561	0.4886868530
C5	2.6527553244	-2.4374309509	0.1048164846
C6	2.0545300969	-1.1980025681	-0.2167037010
C7	1.9144130167	-3.6629520924	0.0629750554
C8	1.3252160235	-4.7347102858	0.0678406573
C9	0.6990710982	-6.0173947269	0.0987361908
N10	-0.6518076431	-6.0890197210	0.3571645885
C11	-1.2621645705	-7.3095551085	0.4310210002
C12	-0.5635999791	-8.5190996676	0.2681999854
C13	0.8106017679	-8.4490019453	-0.0084230621
C14	1.4386474737	-7.1987922119	-0.0971245847
Cu15	-1.7336004551	-4.4190715394	0.8449321844
O16	-1.6823522154	-3.2442230631	-0.7714637748
Cu17	1.6899803064	4.4204063966	-1.8352658744
O18	3.3374428243	3.7545708591	-2.7208956363
N19	-2.5029971915	-0.2918534700	-1.0248115107
C20	-1.8766214585	0.8932672010	-0.8243118664
C21	-2.5045344997	2.1384879182	-1.0486648792
C22	-3.8506038606	2.1342245911	-1.4821051916
C23	-4.4928296320	0.9108471215	-1.6898868490
C24	-3.7917529793	-0.2768664654	-1.4618471881
C25	-1.8105762745	3.3753228939	-0.8555947859
C26	-1.2632581930	4.4610062367	-0.7239273788
C27	-0.6803204722	5.7581247051	-0.5945888640
N28	0.6305992827	5.9316053357	-0.9768881075
C29	1.2014362871	7.1705882407	-0.9088622766
C30	0.4962999791	8.3033996676	-0.4704999854
C31	-0.8373521694	8.1312091608	-0.0684356720
C32	-1.4221737667	6.8582364085	-0.1256911705
O33	-3.3715181401	-3.4124294593	1.3574953458
O34	-1.2494705213	-4.6536571274	2.7542561088
O35	0.8336835103	4.7684041491	-3.5914362172
O36	1.9142021775	3.0760961285	-0.3533505570
H37	-0.8512624509	0.8546020185	-0.4765613597
H38	-4.3695924869	3.0715332005	-1.6557688663
H39	-5.5241280391	0.8728628309	-2.0290978692
H40	-4.2574323852	-1.2403430947	-1.6345387709
H41	0.9894375745	9.2696053295	-0.4443945939
H42	2.2391818523	7.2425793552	-1.2150662717
H43	-2.4520383951	6.7035033002	0.1802900969
H44	-1.4207732237	8.9771724519	0.2844083244
H45	1.3922462608	-9.3554754864	-0.1521520365
H46	-1.0930501791	-9.4630654063	0.3464743953
H47	-2.3283696253	-7.3037440672	0.6301111387
H48	2.5010439640	-7.1229199963	-0.3071819485
H49	4.5294759513	0.9219885994	0.2895106185
H50	5.7448883436	-1.1844854185	0.8477952948
H51	4.5113323148	-3.3684525436	0.7360238729
H52	1.0183920244	-1.1608535285	-0.5298767152
H53	-3.8420545952	-3.5598258363	2.2038946857
H54	-3.9400154495	-2.9406810188	0.7141061156
H55	3.6103302880	4.0762440602	-3.6049595671
H56	4.0939081082	3.3474400990	-2.2484970350
H57	-0.7498347294	-5.4139090681	3.1169249415
H58	-1.2882685831	-3.9214285847	3.4021998035
H59	2.0292752506	2.1080980141	-0.4433718072
H60	1.7608186942	3.3225846331	0.5818889975
H61	-1.4203519207	-3.5431261102	-1.6663663137
H62	-1.8464905639	-2.2790702595	-0.7417866719
H63	0.2241261093	5.5112944083	-3.7776173322
H64	0.8210761747	4.1176385872	-4.3217410292

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$\Delta r=2.55 \text{ \AA} (\text{truncated complex})$			
Atom	X	Y	Z
C 1	2.2326971818	-5.6118051011	-1.3222185704
C2	1.2758167936	-6.6310412371	-0.7715448582
N3	0.1342279992	-6.1945320016	-0.1566827548
C4	-0.7655099232	-7.0891314343	0.3498637967
C5	-0.5604999874	-8.4692998000	0.2659999912
C6	0.6049154478	-8.9334072900	-0.3604578414
C7	1.5185631114	-8.0082699827	-0.8762155967
Cu8	-0.2206491712	-4.2026984995	0.0593709161
O9	-0.8762302418	-4.0484648584	-1.8066700224
N10	-2.2288033773	-0.1793926172	-0.3123385382
C11	-1.7234283904	1.0775868037	-0.3485849558
C12	-2.5162861055	2.2047119092	-0.6665621915
C13	-3.8830209119	1.9901063405	-0.9599736281
C14	-4.3964133414	0.6900548245	-0.9176861750
C15	-3.5465751763	-0.3699464050	-0.5886423532
C16	-1.9553849399	3.5212392216	-0.6794137025
C17	-1.4946714782	4.6548905567	-0.6837296129
C18	-0.8681225419	5.9454005672	-0.6412256988
N19	0.4166472916	5.9639551513	-0.1743092653
C20	1.0769712827	7.1405648446	-0.0948214418
C21	0.4994999874	8.3531998000	-0.4726999912
C22	-0.8193617982	8.3429982160	-0.9570354249
C23	-1.5153133599	7.1284924095	-1.0442816468
O24	-0.9433539114	-2.4428083364	0.6233632201
O25	1.0354610903	-4.1125473423	1.5953405057
H26	-0.6694528019	1.1896607921	-0.1184522616
H27	-4.5222493063	2.8313868552	-1.2111169505
H28	-5.4432967909	0.4971130722	-1.1343994072
H29	-3.9089694443	-1.3914304012	-0.5405804352
H30	1.0640134568	9.2785990017	-0.3923915900
H31	2.0936968311	7.0970048689	0.2831171446
H32	-2.5362433566	7.0915494331	-1.4154867940
H33	-1.3012997982	9.2674358748	-1.2625013835
H34	0.7996857188	-9.9991310091	-0.4459204777
H35	-1.2982592477	-9.1496961934	0.6798535126
H36	-1.6496812571	-6.6766062181	0.8230919966
H37	2.4289868017	-8.3418886224	-1.3646847405
H38	-1.0096669395	-2.3386945279	1.5951055838
H39	-1.3364086057	-1.6658907510	0.1741337690
H40	1.3937318949	-4.8901854589	2.0711091287
H41	1.5131441534	-3.2936248319	1.8380206816
H42	-1.1377023674	-4.8179396274	-2.3528068688
H43	-0.8151436855	-3.2375992000	-2.3529728757
H44	3.1226842737	-6.0991883396	-1.7298980218
H45	1.7629917376	-5.0297472214	-2.1259738656
H46	2.5519432693	-4.9089166990	-0.5423329775

$\Delta r=2.70 \text{ \AA} (\text{truncated complex})$			
Atom	X	Y	Z
C 1	2.3256747266	-6.0671118187	-1.7648638271
C2	1.3331929742	-6.9441633028	-1.0551618509
N3	0.2912086606	-6.3559858545	-0.3906812182
C4	-0.6392157359	-7.1223733403	0.2530133119
C5	-0.5635999746	-8.5190995971	0.2681999823
C6	0.5020498901	-9.1363603925	-0.4020346891
C7	1.4459628366	-8.3422034231	-1.0616368028
Cu8	0.1334992264	-4.3257023511	-0.3094983093
O9	-0.6215157699	-4.2029363129	-2.1346364685
N10	-1.8018406982	-0.2212799743	-0.7633815355
C11	-1.3400345581	1.0536100685	-0.7349641394
C12	-2.1642368856	2.1659525066	-1.0253215607
C13	-3.5143196496	1.9181603432	-1.3662277830
C14	-3.9821227847	0.6011771171	-1.3959970822
C15	-3.1048475293	-0.4419433924	-1.0867119976
C16	-1.6573878941	3.5029501138	-0.9651514335

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C17	-1.2548528013	4.6567877531	-0.9075916285
C18	-0.7061286386	5.9777051742	-0.7909606100
N19	0.5460893720	6.0555376561	-0.2480851926
C20	1.1306755511	7.2649718913	-0.0982289751
C21	0.5057999746	8.4528995971	-0.4770999823
C22	-0.7806636618	8.3821415998	-1.0382257836
C23	-1.3980947357	7.1332074352	-1.1988229491
O24	-0.4270347717	-2.4850320663	0.1936675252
O25	1.5481530335	-4.2264222327	1.0858216545
H26	-0.2963705197	1.1925321897	-0.4737375249
H27	-4.1763031356	2.7472813208	-1.5981232940
H28	-5.0146751429	0.3816928014	-1.6525072119
H29	-3.4364445344	-1.4741483792	-1.0927054348
H30	1.0099758061	9.4059300319	-0.3401023144
H31	2.1242937557	7.2684410225	0.3383758195
H32	-2.3923873823	7.0479519550	-1.6295934815
H33	-1.2972731151	9.2869057494	-1.3462983759
H34	0.5966013097	10.2190058897	-0.4114944538
H35	-1.3224019269	-9.0930249016	0.7910880956
H36	-1.4417820293	-6.5939309507	0.7559367604
H37	2.2801044188	-8.7954295562	-1.5885547011
H38	-0.3138921639	-2.2682327530	1.1422930533
H39	-0.8600648998	-1.7408249388	-0.2737122247
H40	1.9193130788	-5.0028331600	1.5533023014
H41	2.1225912071	-3.4414622680	1.1927031645
H42	-1.0462057431	-4.9516991684	-2.6012381525
H43	-0.4669658166	-3.4501384575	-2.7420059840
H44	3.1268104130	-6.6693752863	-2.2030622143
H45	1.8388807013	-5.5027984493	-2.5713115032
H46	2.7776685400	-5.3414127423	-1.0754044401

Δr=2.80 Å (truncated complex)			
Atom	X	Y	Z
C 1	2.2895997073	-5.9579390425	-1.6893760669
C2	1.3085800742	-6.8716427117	-1.0076083313
N3	0.2355259883	-6.3220627706	-0.3584416575
C4	-0.6825120040	-7.1241330217	0.2618738423
C5	-0.5635999810	-8.5190996990	0.2681999868
C6	0.5325582894	-9.0957392798	-0.3893969063
C7	1.4633411048	-8.2658207407	-1.0246927740
Cu8	0.0332582921	-4.2935693806	-0.2472174814
O9	-0.6605563403	-4.1379089449	-2.1013894031
N10	-1.9182767788	-0.0940150041	-0.4289295727
C11	-1.4482982730	1.1780435779	-0.4564847477
C12	-2.2972434509	2.2991129271	-0.6127557005
C13	-3.6847410491	2.0630121442	-0.7532270099
C14	-4.1617919038	0.7490793425	-0.7243026285
C15	-3.2564416760	-0.3030650956	-0.5577885933
C16	-1.7747602169	3.6320875706	-0.6201879810
C17	-1.3556408650	4.7820918627	-0.6190938628
C18	-0.7765294393	6.0955977843	-0.5888655966
N19	0.5579247314	6.1494147742	-0.2968702684
C20	1.1792103305	7.3492523819	-0.2463066007
C21	0.5120999810	8.5525996990	-0.4814999868
C22	-0.8596738552	8.5065496895	-0.7831484535
C23	-1.5158787860	7.2676784840	-0.8383974053
O24	-0.5638549463	-2.4739592424	0.3115271854
O25	1.4111323752	-4.2005135408	1.1835576870
H26	-0.3768038819	1.3076232742	-0.3482933212
H27	-4.3670739092	2.8987098263	-0.8781043589
H28	-5.2228101912	0.5388045503	-0.8264185759
H29	-3.5912645840	-1.3341372676	-0.5229112127
H30	1.0480432814	9.4969580349	-0.4314540858
H31	2.2384533524	7.3320746084	-0.0090143379
H32	-2.5761055740	7.2035094939	-1.0698468284
H33	-1.4127704754	9.4223335081	-0.9732981216
H34	0.6611915106	10.1749484993	-0.4079057331
H35	-1.3133570966	-9.1218510789	0.7720950223

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H36	-1.5106060064	-6.6253545249	0.7542122144
H37	2.3206850840	-8.6880980479	-1.5405413261
H38	-0.4788295428	-2.3206457289	1.2753225600
H39	-0.9557660805	-1.6823148938	-0.1122385491
H40	1.7801146177	-4.9779854340	1.6509526913
H41	1.9672010992	-3.4076301603	1.3233957790
H42	-0.9778060710	-4.9057671070	-2.6195917965
H43	-0.5334004358	-3.3552189336	-2.6764900217
H44	3.1170326760	-6.5316009920	-2.1161506051
H45	1.8072177560	-5.4001229034	-2.5012736180
H46	2.7055017584	-5.2265707209	-0.9850106249

Δr=2.90 Å (truncated complex)

Atom	X	Y	Z
C 1	1.9752492634	-5.8839557470	-1.9964424429
C2	1.0974933267	-6.8253601156	-1.2192610349
N3	0.1240020269	-6.3017481296	-0.4114457526
C4	-0.6894285367	-7.1262333753	0.3155302588
C5	-0.5635999787	-8.5190996627	0.2681999852
C6	0.4243098197	-9.0701945219	-0.5605004646
C7	1.2510319649	-8.2170847999	-1.3000535878
Cu8	-0.0871502185	-4.2753949449	-0.2588016671
O9	-1.0253710503	-4.1564758657	-2.0055915257
N10	-1.9355115190	-0.0081330091	-0.3860145510
C11	-1.4419101981	1.2551544433	-0.4339262460
C12	-2.2693232180	2.3886679788	-0.6141200798
C13	-3.6604614333	2.1754287868	-0.7565973920
C14	-4.1621621054	0.8716822062	-0.7037867764
C15	-3.2772603228	-0.1932196796	-0.5142675431
C16	-1.7273679529	3.7140847899	-0.6408222878
C17	-1.3029513524	4.8624139830	-0.6541694453
C18	-0.7330907992	6.1798943130	-0.6247586519
N19	0.5510165914	6.2635528506	-0.1667921669
C20	1.1543840523	7.4714320538	-0.1020186732
C21	0.5183999788	8.6522996627	-0.4858999852
C22	-0.8011630439	8.5745382201	-0.9606345831
C23	-1.4384318448	7.3274830124	-1.0326342830
O24	-0.6147160250	-2.4412170120	0.3366063147
O25	1.4225923325	-4.1885550393	1.0231971138
H26	-0.3683674020	1.3667679862	-0.3246828965
H27	-4.3267040713	3.0208764987	-0.9005628012
H28	-5.2266687110	0.6790736452	-0.8050398393
H29	-3.6330915655	-1.2160482744	-0.4610097363
H30	1.0383061357	9.6044288776	-0.4185112888
H31	2.1737467750	7.4797184149	0.2694645851
H32	-2.4588967447	7.2376230070	-1.3952424526
H33	-1.3288388528	9.4720227468	-1.2702270950
H34	0.5501204482	10.1476835365	-0.6296303257
H35	-1.2289862351	-9.1399673880	0.8602746959
H36	-1.4402553243	-6.6476780149	0.9348070363
H37	2.0250324321	-8.6187085477	-1.9472952435
H38	-0.4724811522	-2.2853468988	1.2932451135
H39	-1.0063352237	-1.6407239696	-0.0705079673
H40	1.8430329835	-4.9705443615	1.4365400975
H41	1.9821592686	-3.3913641649	1.1172890869
H42	-1.4249029200	-4.9325397713	-2.4493444367
H43	-0.9480806573	-3.4010931555	-2.6244310433
H44	2.7119180617	-6.4407997325	-2.5827773324
H45	1.3811991058	-5.2698653091	-2.6863145554
H46	2.5152668915	-5.2029493803	-1.3245129228

Δr=3.00 Å (truncated complex)

Atom	X	Y	Z
C 1	2.1310654943	-5.7460477095	-1.6199966276
C2	1.2014323388	-6.7337189867	-0.9728141267

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N3	0.1455274029	-6.2614365888	-0.2410471418
C4	-0.7196730789	-7.1307005198	0.3639647682
C5	-0.5635999822	-8.5190997183	0.2681999876
C6	0.5128225427	-9.0165034423	-0.4796713831
C7	1.3898808333	-8.1179871081	-1.0969794550
Cu8	-0.0897347508	-4.2410161674	-0.0149876641
O9	-0.8926423175	-4.0421677868	-1.8128452639
N10	-1.9382405888	0.1025103056	-0.0542446796
C11	-1.4499813822	1.3660196032	-0.1365070354
C12	-2.2879932514	2.5016551363	-0.2378578368
C13	-3.6867067291	2.2918387931	-0.2617811961
C14	-4.1837379753	0.9881644587	-0.1774111699
C15	-3.2869027874	-0.0791661301	-0.0712107727
C16	-1.7471522269	3.8254703408	-0.3071727487
C17	-1.3231639378	4.9723494221	-0.3602228676
C18	-0.7496398938	6.2872345666	-0.4113351462
N19	0.6122839938	6.3499524400	-0.3124389078
C20	1.2260536815	7.5537823750	-0.3516888560
C21	0.5246999822	8.7519997183	-0.4902999876
C22	-0.8759201357	8.6963147471	-0.5923354239
C23	-1.5247228759	7.4537052437	-0.5527118939
O24	-0.6366793815	-2.4132027844	0.6030976432
O25	1.3112015328	-4.2131872137	1.3882314399
H26	-0.3711185404	1.4770458525	-0.1187440835
H27	-4.3608238821	3.1396044554	-0.3427465077
H28	-5.2532580539	0.7968108450	-0.1905234217
H29	-3.6384340862	-1.1019158535	0.0056322291
H30	1.0552457726	9.7000619998	-0.5178661513
H31	2.3083416956	7.5437468338	-0.2682372051
H32	-2.6067646627	7.3812670317	-0.6290618731
H33	-1.4570433557	9.6076965510	-0.7013228987
H34	0.6678155310	10.0875143513	-0.5810756427
H35	-1.2710068549	-9.1764746539	0.7641872165
H36	-1.5365870576	-6.6921570222	0.9260882610
H37	2.2314313306	-8.4782074466	-1.6807782234
H38	-0.5458726640	-2.2856114967	1.5700949681
H39	-0.9910803850	-1.5947376087	0.1976394123
H40	1.6768082749	-5.0095754920	1.8252876097
H41	1.8624183938	-3.4246944518	1.5670441067
H42	-1.2340638419	-4.7926272866	-2.3409435866
H43	-0.8475271308	-3.2259444461	-2.3525322015
H44	2.9222903095	-6.2649655310	-2.1680637862
H45	1.5920997177	-5.1002599937	-2.3246133002
H46	2.6017166383	-5.0995972597	-0.8683862610

Δr=3.10 Å (truncated complex)			
Atom	X	Y	Z
C 1	2.0629656445	-5.7602531179	-1.7329747713
C2	1.1598025313	-6.7432605962	-1.0426856185
N3	0.1172865529	-6.2655457451	-0.2953184623
C4	-0.7275514977	-7.1304364624	0.3438049324
C5	-0.5635999806	-8.5190996923	0.2681999865
C6	0.5019541606	-9.0219201358	-0.4921922551
C7	1.3580385689	-8.1280419046	-1.1445069401
Cu8	-0.1264281934	-4.2400198679	-0.0992387119
O9	-0.9957660392	-4.0894855427	-1.8691677770
N10	-1.9832004930	0.2169980751	-0.0995698799
C11	-1.4919160101	1.4798003236	-0.1804581068
C12	-2.3260105364	2.6216579374	-0.2333364403
C13	-3.7257130159	2.4200270168	-0.2050532902
C14	-4.2266005069	1.1178692887	-0.1199085173
C15	-3.3327285985	0.0439112947	-0.0665757340
C16	-1.7794395534	3.9429676418	-0.3087823316
C17	-1.3482067062	5.0867161068	-0.3677395355
C18	-0.7646342372	6.3971453107	-0.4211362269
N19	0.5945175990	6.4513566562	-0.2858583608
C20	1.2189643753	7.6501239616	-0.3224418907
C21	0.5309999806	8.8516996924	-0.4946999865

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C22	-0.8667657700	8.8049795789	-0.6355062898
C23	-1.5263382330	7.5676688369	-0.5985150698
O24	-0.6594875921	-2.3932436777	0.4971749079
O25	1.2992206710	-4.1773895117	1.2759535593
H26	-0.4126482440	1.5854534507	-0.2025599026
H27	-4.3975568549	3.2722773712	-0.2471833718
H28	-5.2969434721	0.9321000750	-0.0938516589
H29	-3.6875699713	-0.9781919870	0.0051559719
H30	1.0692325809	9.7954549208	-0.5189938994
H31	2.2983585190	7.6328124451	-0.2093531840
H32	-2.6063032594	7.5024730200	-0.7040003262
H33	-1.4373430640	9.7192946805	-0.7721335470
H34	0.6642198794	-10.0933655671	-0.5764335276
H35	-1.2554020618	-9.1722410515	0.7909749736
H36	-1.5335098526	-6.6882209508	0.9185728222
H37	2.1901544197	-8.4922894390	-1.7394139489
H38	-0.5394036304	-2.2453429236	1.4580706687
H39	-1.0097150738	-1.5752071359	0.0871391651
H40	1.6729327663	-4.9624866770	1.7264360395
H41	1.8579280399	-3.3865968339	1.4174322484
H42	-1.3653842989	-4.8557674767	-2.3537360737
H43	-0.9557805518	-3.2963950879	-2.4428092539
H44	2.8480957710	-6.2828582064	-2.2865497600
H45	1.4999876127	-5.1382030529	-2.4408429954
H46	2.5424254039	-5.0898127161	-1.0076493375

Δr=3.30 Å (truncated complex)			
Atom	X	Y	Z
C 1	-0.5851832265	-6.2709597287	-3.3158964770
C2	-0.5720498208	-7.0741296831	-2.0681888568
N3	-0.4509737805	-6.4156497163	-0.8857731610
C4	-0.4602853747	-7.1180890621	0.2563362261
C5	-0.5635999705	-8.5190995323	0.2681999795
C6	-0.6647606216	-9.2074908564	-0.9375442619
C7	-0.6699583035	-8.4787795797	-2.0947908287
Cu8	-0.2627981313	-4.3686145798	-0.8045279258
O9	-2.0531609177	-4.2113182903	-0.0219840345
N10	-1.3388361264	0.2850831634	-1.5613031517
C11	-0.9042455734	1.5641712236	-1.4294452395
C12	-1.6825912457	2.6877202980	-1.8041348017
C13	-2.9436844917	2.4422077530	-2.3864515200
C14	-3.3761149783	1.1255906136	-2.5449749404
C15	-2.5574040316	0.0766153643	-2.1153863782
C16	-1.2314158703	4.0339621882	-1.5914378135
C17	-0.8934903269	5.1932973521	-1.4011868602
C18	-0.4444949783	6.5328977206	-1.1298474948
N19	0.7369849580	6.6530638618	-0.4440762707
C20	1.2082665605	7.8798376056	-0.1454840885
C21	0.5435999705	9.0510995323	-0.5034999795
C22	-0.6655215749	8.9392374225	-1.2114209048
C23	-1.1692435870	7.6694284159	-1.5311985142
O24	-0.0344726362	-2.3580284086	-0.5636026480
O25	1.5286581303	-4.4687482813	-1.6113099979
H26	0.0761420948	1.7013871283	-0.9871633838
H27	-3.5680936813	3.2733609546	-2.6975085674
H28	-4.3394905870	0.9109610348	-2.9918962104
H29	-2.8693979194	-0.9518094143	-2.2110292757
H30	0.9578814963	10.0184854359	-0.2415504560
H31	2.1474012768	7.9106649615	0.3965654096
H32	-2.1020843120	7.5553014614	-2.0783388144
H33	-1.2126863549	9.8299673234	-1.5135506403
H34	-0.7432488066	10.2953983126	-0.9684144529
H35	-0.5690454421	-9.0426775166	1.2000492147
H36	-0.3702180249	-6.5356751107	1.1570725553
H37	-0.7476314311	-8.9905000424	-3.0400398687
H38	0.8073011875	-2.1512262577	-0.1072289743
H39	-0.3354700110	-1.5627997865	-1.0503868576
H40	2.0823359648	-5.2761963643	-1.6303444107

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H41	1.8648643218	-3.7863765506	-2.2268085827
H42	-2.6739753892	-4.9596839596	0.0924638446
H43	-2.2969566101	-3.4456013153	0.5382531872
H44	-0.7459384609	-6.9283880713	-4.1743800329
H45	-1.3767782938	-5.5156947453	-3.2960086488
H46	0.3562838435	-5.7405005363	-3.4545948009

$\Delta r=3.40 \text{ \AA} (\text{truncated complex})$			
Atom	X	Y	Z
C 1	-1.4811414597	-5.6004330838	-2.7488935785
C2	-1.1693689466	-6.6290521886	-1.6982268249
N3	-0.6600182649	-6.2198183269	-0.4924454878
C4	-0.3677929335	-7.1457305002	0.4701680797
C5	-0.5635999813	-8.5190997031	0.2681999869
C6	-1.0741861440	-8.9465075120	-0.9638972087
C7	-1.3739253463	-7.9939647637	-1.9426023667
Cu8	-0.3980609078	-4.2007137797	-0.1252612047
O9	-1.9783275481	-4.1525645192	1.0380771641
N10	-0.9937385045	0.2127707151	-1.2613126792
C11	-0.6057617796	1.4977030986	-1.0285233638
C12	-1.1285243418	2.5987516221	-1.7534793589
C13	-2.0786325627	2.3305339698	-2.7666856996
C14	-2.4674447195	1.0124745983	-3.0091858349
C15	-1.9135021576	-0.0134902667	-2.2406773361
C16	-0.7455213370	3.9579026658	-1.4977491120
C17	-0.4897421079	5.1447993214	-1.3387042918
C18	-0.1652611476	6.5265202243	-1.1015362548
N19	0.6869930752	6.7809396898	-0.0638503719
C20	1.0301334858	8.0586281453	0.2186900435
C21	0.5498999813	9.1508997031	-0.5078999870
C22	-0.3255245452	8.8964746000	-1.5778459724
C23	-0.6895072273	7.5755037844	-1.8814322242
O24	-0.2712504043	-2.1705860778	0.1259249534
O25	1.2815621901	-4.1704616060	-1.1472620664
H26	0.1296469234	1.6521737448	-0.2462097462
H27	-2.4990610455	3.1482137955	-3.3449305765
H28	-3.1949782347	0.7789427301	-3.7816289048
H29	-2.2114535779	-1.0399312665	-2.4078994707
H30	0.8492579949	10.1627816649	-0.2481582000
H31	1.7092105067	8.1965787613	1.0541983711
H32	-1.3655043286	7.3551488770	-2.7037584529
H33	-0.7225133451	9.7157783114	-2.1713613663
H34	-1.2377432463	-10.0033568442	-1.1595806400
H35	-0.3182049222	-9.2185533814	1.0614565020
H36	0.0288275303	-6.7663577239	1.4054224575
H37	-1.7639688416	-8.2973013147	-2.9095940116
H38	0.2492346851	-1.9069929734	0.9128864508
H39	-0.4934643331	-1.3786195904	-0.4063614518
H40	1.7532468652	-4.9447369941	-1.5172639686
H41	1.7387348050	-3.3293208318	-1.3494486337
H42	-2.5110718994	-4.9209353985	1.3285855537
H43	-2.2428503073	-3.3248897548	1.4904633013
H44	-1.8494909604	-6.0807426399	-3.6603522260
H45	-2.2539661763	-4.9009406674	-2.4045927758
H46	-0.5864168741	-5.0230802388	-3.0131575253

$\Delta r=3.60 \text{ \AA} (\text{truncated complex})$			
Atom	X	Y	Z
C 1	-2.0981399555	-5.7772599907	-2.6612106587
C2	-1.5679369298	-6.7465222874	-1.6488889043
N3	-0.8439594821	-6.2677062491	-0.5930289051
C4	-0.3536091295	-7.1362003596	0.3446990995
C5	-0.5635999738	-8.5190995837	0.2681999817
C6	-1.3044577470	-9.0146830611	-0.8108910931
C7	-1.8027890252	-8.1214011909	-1.7654266235

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Cu8	-0.5565209087	-4.2117680939	-0.4617959292
O9	-2.0325388669	-4.0045948907	0.7945812152
N10	-1.0606947778	0.5337655965	-1.9015183992
C11	-0.7306050139	1.8162557859	-1.5827478700
C12	-1.1433399052	2.9354700670	-2.3474790964
C13	-1.9276353603	2.6867347681	-3.4982047957
C14	-2.2667869247	1.3688350715	-3.8235356027
C15	-1.8230259725	0.3217433391	-3.0086149173
C16	-0.7863864497	4.2830816653	-1.9953935794
C17	-0.5198548061	5.4555233315	-1.7403164219
C18	-0.1746915787	6.8070104745	-1.3718512334
N19	0.4310917300	6.9685062294	-0.1580122126
C20	0.7862591904	8.2072543860	0.2504200006
C21	0.5624999738	9.3502995837	-0.5166999817
C22	-0.0605583211	9.1914825008	-1.7618630844
C23	-0.4344105111	7.9121100072	-2.1984234046
O24	-0.3317438784	-2.1609434921	-0.3871024867
O25	0.9710408533	-4.3105287233	-1.6620803001
H26	-0.1235602618	1.9579919125	-0.6971396517
H27	-2.2627505558	3.5136261881	-4.1148536946
H28	-2.8682781245	1.1470839510	-4.6994592230
H29	-2.0709000155	-0.7103725771	-3.2358239799
H30	0.8647907550	10.3289660643	-0.1535902327
H31	1.2612209135	8.2696003246	1.2208923516
H32	-0.9217817282	7.7675618745	-3.1551965701
H33	-0.2542559598	10.0528872200	-2.3902577554
H34	-1.4930945122	-10.0785294053	-0.9109629372
H35	-0.1538403801	-9.1665158060	1.0346302157
H36	0.2133167391	-6.7022886220	1.1573380085
H37	-2.3823726061	-8.4763823248	-2.6081258591
H38	0.2437352795	-1.8419209150	0.3386512278
H39	-0.5997799289	-1.3989582148	-0.9416837444
H40	1.3897213811	-5.1238348139	-2.0112679554
H41	1.4098080224	-3.4982270526	-1.9861969878
H42	-2.5358083329	-4.7289188540	1.2195819455
H43	-2.3189152857	-3.1197929903	1.1025218651
H44	-2.6410936154	-6.3055880614	-3.4452077552
H45	-2.7874476183	-5.0574089595	-2.1974758378
H46	-1.2842152811	-5.2154494625	-3.1316388532

Δr=3.70 Å (truncated complex)			
Atom	X	Y	Z
C 1	-1.9702271603	-5.4617440250	-2.4132490907
C2	-1.4891661863	-6.5466631303	-1.4906996535
N3	-0.7312345844	-6.1933525962	-0.4058662009
C4	-0.2775182045	-7.1565093956	0.4545160230
C5	-0.5635999768	-8.5190996314	0.2681999838
C6	-1.3387068386	-8.8880655224	-0.8393578995
C7	-1.7968928551	-7.8960398430	-1.7137957246
Cu8	-0.3379660163	-4.1612732615	-0.1473981034
O9	-1.8578758211	-3.9531137177	1.0564538403
N10	-0.7024607935	0.4688161057	-1.4559526268
C11	-0.4112137641	1.7660512302	-1.1528917002
C12	-0.8198388015	2.8558536559	-1.9628553282
C13	-1.5591086220	2.5625229593	-3.1339036516
C14	-1.8548001749	1.2327013463	-3.4431685469
C15	-1.4160402201	0.2169772671	-2.5887797146
C16	-0.5163776250	4.2252371307	-1.6454163000
C17	-0.3074825799	5.4187571957	-1.4571768627
C18	-0.0365635935	6.8090360234	-1.1874291955
N19	0.6400820453	7.0836118982	-0.0314275047
C20	0.9302545131	8.3673188597	0.2853013901
C21	0.5687999768	9.4499996314	-0.5210999838
C22	-0.1285322566	9.1745644986	-1.7111700189
C23	-0.4356646475	7.8472783561	-2.0516063113
O24	-0.0604081941	-2.1088553435	-0.0165526897
O25	1.2857533375	-4.2718746158	-1.2228796267
H26	0.1586779522	1.9379514218	-0.2459614948

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H27	-1.8895601302	3.3693026151	-3.7815632632
H28	-2.4199076141	0.9807427429	-4.336579894
H29	-1.6338877834	-0.8226709285	-2.8072411596
H30	0.8206425622	10.4664452459	-0.2306413755
H31	1.4686950837	8.5183197526	1.2157748187
H32	-0.9727271684	7.6151775885	-2.9678440875
H33	-0.4315172423	9.9830669832	-2.3707730463
H34	-1.5836114217	-9.9312108173	-1.0210733266
H35	-0.1830136847	-9.2487238218	0.9759601954
H36	0.3168106127	-6.8155100973	1.2949370806
H37	-2.3982191117	-8.1563128541	-2.5793537198
H38	0.4635500892	-1.8412358482	0.7666965191
H39	-0.2924297708	-1.3137868560	-0.5399866089
H40	1.6916331166	-5.0914861663	-1.5724589899
H41	1.8101175137	-3.4762341733	-1.4451768085
H42	-2.3996978517	-4.6714496691	1.4424185123
H43	-2.1255857748	-3.0684734030	1.3811711086
H44	-2.5463999458	-5.8857516256	-3.2404292995
H45	-2.6205684699	-4.7538950859	-1.8821348247
H46	-1.1273928915	-4.9047378180	-2.8447710705

<i>Δr=3.80 Å (truncated complex)</i>			
Atom	X	Y	Z
C 1	-2.0027708370	-5.7750230688	-2.7228003527
C 2	-1.5078296514	-6.7517981249	-1.6931650557
N3	-0.8931128978	-6.2622695819	-0.5721497568
C4	-0.4324288419	-7.1257243631	0.3864743867
C5	-0.5635999776	-8.5190996438	0.2681999844
C6	-1.1893565396	-9.0262248140	-0.8787270390
C7	-1.6581935739	-8.1368165293	-1.8526256132
Cu8	-0.7098104384	-4.1822244377	-0.4193488778
O9	-2.3391974427	-4.0648853513	0.6422772978
N10	-1.2825144772	0.7238202067	-1.7223352772
C11	-0.8634511620	1.9898861716	-1.4400747619
C12	-1.3117423228	3.1299426461	-2.1529173819
C13	-2.2313095906	2.9229230313	-3.2093073498
C14	-2.6592564142	1.6247558014	-3.4991822034
C15	-2.1721471703	0.5552844234	-2.7403928350
C16	-0.8827875118	4.4639264523	-1.8322476682
C17	-0.5810250087	5.6319043049	-1.6126965632
C18	-0.2101240704	6.9868410760	-1.2931637853
N19	0.5755393375	7.1578371871	-0.1872258027
C20	0.9532901012	8.4050232297	0.1788000071
C21	0.5750999776	9.5496996438	-0.5254999844
C22	-0.2312995326	9.3818403821	-1.6655253112
C23	-0.6289944232	8.0935917966	-2.0563342614
O24	-0.5665147386	-2.1229241418	-0.2879920976
O25	0.9501144980	-4.1887608361	-1.4460759978
H26	-0.1588494346	2.0987340178	-0.6221064818
H27	-2.5990321963	3.7690164010	-3.7822879451
H28	-3.3663194314	1.4367752036	-4.3035109539
H29	-2.4942510769	-0.4603350608	-2.9410761011
H30	0.8973928686	10.5336879774	-0.1960458374
H31	1.5752302300	8.4757480526	1.0660431653
H32	-1.2513638189	7.9422262085	-2.9349250866
H33	-0.5498436260	10.2429094081	-2.2460947538
H34	-1.3123684669	-10.0974166633	-1.0149672293
H35	-0.1833302203	-9.1641159504	1.0541455007
H36	0.0429835547	-6.6788132497	1.2521704639
H37	-2.1492712867	-8.5060106976	-2.7476554375
H38	-0.0992918832	-1.8193803533	0.5178380035
H39	-0.8233404114	-1.3423831118	-0.8216140893
H40	1.4391103036	-4.9811774944	-1.7487257984
H41	1.3892511425	-3.3574724467	-1.7173044829
H42	-2.8497318983	-4.8175355945	1.0048194210
H43	-2.7160102710	-3.1989922096	0.9027608857
H44	-2.4823148576	-6.2994389914	-3.5541312698
H45	-2.7385032876	-5.0829999467	-2.2909731088

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H46	-1.1757950543	-5.1803271076	-3.1329288857
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