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Electronic Supplementary Information

The Rise and Fall of Copper Hydride Clusters. A Snapshot of Hexanuclear-to-Dodecanuclear Expansion

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General Methods. All copper complexes described in this paper were prepared and handled under an inert atmosphere using standard glovebox and Schlenk techniques. Toluene and pentane were deoxygenated and dried in a solvent purification system by passing through an activated alumina column and an oxygen-scavenging column under argon. Prior to distillation under argon, acetonitrile was dried over calcium hydride while benzene-d_6 (99.5% D) and benzene were dried over sodium-benzophenone. *N*-Methyl-2-pyrrolecarboxaldehyde, D_2O (99.9% D), and deuterium gas (99.8% D) were used as received from commercial sources without further purification. $HN(CH_2CH_2P^iPr_2)_2$ ($^{iPr}PN^HP$),[1] ($^{iPr}PN^HP$)CuBr,[2] $HN(CH_2CH_2PCy_2)_2$ ($^{Cy}PN^HP$),[3] and $HN(CH_2CH_2P^tBu_2)_2$ ($^{tBu}PN^HP$)[4] were prepared according to literature procedures. $HN(CH_2CH_2PPh_2)_2$ ($^{Ph}PN^HP$) was prepared from deprotonation of $^{Ph}PN^HP{\bullet}HCl$ with KO^{t}Bu following a reported procedure.[3] Unless otherwise noted, NMR spectra were recorded at ambient temperature on a Bruker AV400 MHz or NEO400 MHz spectrometer. Chemical shift values for ^1H, ^2H, and $^{13}C\{^1H\}$ NMR spectra were referenced internally to the residual solvent resonances. $^{31}P\{^1H\}$ NMR spectra were referenced externally to 85% H_3PO_4 (0 ppm). Infrared spectra were recorded on a PerkinElmer Spectrum Two FT-IR spectrometer equipped with a smart orbit diamond attenuated total reflectance (ATR) accessory. Electrospray ionization mass spectrum (ESI-MS) was recorded on a Thermo Scientific LTQ-FT hybrid mass spectrometer that combines a linear ion trap and Fourier transform ion cyclotron resonance technologies.

Synthesis of ($^{iPr}PN^HP$)$_4$Cu$_{12}$H$_{12}$. *Method A (based on a 1:2 ligand-to-copper ratio).* In a glovebox, an oven-dried pressure tube equipped with a stir bar was charged with $^{iPr}PN^HP$ (76 mg, 0.25 mmol), CuBr (72 mg, 0.50 mmol), and KO^{t}Bu (56 mg, 0.50 mmol), followed by the addition of 5 mL of toluene to ensure mixing of the reagents. The tube was subsequently connected to a PTFE male-threaded adapter in a standard Fischer-Porter setup and taken out of the glovebox. The system was purged with H_2 gas several times before being kept under 80 psig of H_2 pressure. The resulting mixture was stirred at room temperature for 1 h, during which time the solution color turned to bright orange/yellow. The remaining H_2 gas was carefully vented, and the apparatus was brought back to the glovebox. The reaction mixture was filtered through a short plug of Celite or a Titan3 PTFE syringe filter. The filtrate was concentrated under vacuum until ~1 mL of the solvent was left. Acetonitrile was added, resulting in the formation of an orange precipitate. The suspension was filtered through another short plug of Celite or a new Titan3 PTFE syringe filter, and the filtrate was discarded. The remaining solid material was dissolved in cold (−30 °C) pentane and passed through the same plug of Celite or syringe filter, which was repeatedly eluted with cold (−30 °C) pentane until the filtrate became very light colored. The combined pentane solutions were evaporated to dryness under vacuum to afford an

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[1] (a) Z. E. Clarke, P. T. Maragh, T. P. Dasgupta, D. G. Gusev, A. J. Lough and K. Abdur-Rashid, A Family of Active Iridium Catalysts for Transfer Hydrogenation of Ketones, *Organometallics,* 2006, **25***,* 4113-4117. (b) M. Bertoli, A. Choualeb, D. G. Gusev, A. J. Lough, Q. Major and B. Moore, PNP Pincer Osmium Polyhydrides for Catalytic Dehydrogenation of Primary Alcohols, *Dalton Trans*., 2011, **40**, 8941-8949.

[2] S. S. Rozenel, J. B. Kerr and J. Arnold, Metal Complexes of Co, Ni and Cu with the Pincer Ligand $HN(CH_2CH_2P^iPr_2)_2$: Preparation, Characterization and Electrochemistry, *Dalton Trans.*, 2011, **40**, 10397-10405.

[3] W. Ma, S. Cui, H. Sun, W. Tang, D. Xue, C. Li, J. Fan, J. Xiao and C. Wang, Iron-Catalyzed Alkylation of Nitriles with Alcohols, *Chem. Eur. J*., 2018, **24**, 13118-13123.

[4] (a) K. Abdur-Rashid, T. Graham, C.-W. Tsang, X. Chen, R. Guo, W. Jia, D. Amoroso and C. Sui-Seng, Method for the Production of Hydrogen from Ammonia Borane. WO 2008/141439. (b) J. Meiners, A. Friedrich, E. Herdtweck and S. Schneider, Facile Double C–H Activation of Tetrahydrofuran by an Iridium PNP Pincer Complex, *Organometallics*, 2009, **28**, 6331-6338.

orange solid consisting mainly of $(^{iPr}PN^{H}P)_{3}Cu_{6}H_{6}$, along with 0-20 mol% $(^{iPr}PN^{H}P)_{4}Cu_{12}H_{12}$. The yellow solid left on Celite or syringe filter was eluted with toluene. The filtrate was dried under vacuum to yield $(^{iPr}PN^{H}P)_{4}Cu_{12}H_{12}$ as a yellow powder (44 mg, 53% yield). To obtain the analytically pure form of $(^{iPr}PN^{H}P)_{3}Cu_{6}H_{6}$ and $(^{iPr}PN^{H}P)_{4}Cu_{12}H_{12}$, the isolated products were recrystallized multiple times with toluene layered with pentane.

Method B (based on a 1:3 ligand-to-copper ratio). In a glovebox, an oven-dried pressure tube equipped with a stir bar was charged with $^{iPr}PN^{H}P$ (76 mg, 0.25 mmol), CuBr (108 mg, 0.75 mmol), and KO^{t}Bu (84 mg, 0.75 mmol), followed by the addition of 10 mL of toluene to ensure mixing of the reagents. The rest of the procedure was similar to that described above for *Method A*. X-ray-quality, yellow crystals of $(^{iPr}PN^{H}P)_{4}Cu_{12}H_{12}$ were grown under the following conditions: a toluene solution of $(^{iPr}PN^{H}P)_{4}Cu_{12}H_{12}$ layered with acetonitrile was kept at −30 °C; after one week, pentane was added, and the mixture was kept at −30 °C again until crystals emerged from the solution.

^{1}H NMR (400 MHz, C_6D_6, δ): 3.73-3.46 (m, N*H*, 1H), 3.28-2.72 (m, NC*H*$_2$ + Cu*H*, 5H), 2.37 (br, Cu*H*, 1H), 1.98-1.83 (m, C*H*(CH$_3$)$_2$ + PC*H*$_2$, 3H), 1.81-1.66 (m, C*H*(CH$_3$)$_2$ + PC*H*$_2$, 3H), 1.65-1.55 (m, PC*H*$_2$, 2H), 1.54-1.46 (m, CH(C*H*$_3$)$_2$, 3H), 1.45-1.28 (m, CH(C*H*$_3$)$_2$, 12H), 1.28-1.16 (m, CH(C*H*$_3$)$_2$, 6H), 1.14-1.05 (m, CH(C*H*$_3$)$_2$, 3H), 0.87 (br, Cu*H*, 1H); integrations were normalized to only one $^{iPr}PN^{H}P$ ligand. In one sample, the two Cu*H* resonances in the 3.1-2.3 ppm region were observed as one broad resonance at 2.70 ppm. ^{13}C{^{1}H} NMR (101 MHz, C_6D_6, δ): 48.9 (d, $J_{C\text{-}P}$ = 11.1 Hz, N*C*H$_2$), 48.0 (br, N*C*H$_2$), 26.3 (d, $J_{C\text{-}P}$ = 12.1 Hz, P*C*H), 25.6 (d, $J_{C\text{-}P}$ = 11.5 Hz, P*C*H), 24.4 (d, $J_{C\text{-}P}$ = 13.4 Hz, P*C*H), 22.4 (s, P*C*H$_2$), 21.6 (s, P*C*H$_2$), 20.7-20.4 (m, *C*H$_3$), 19.7-19.5 (m, *C*H$_3$), 18.0 (s, *C*H$_3$), 17.9 (s, *C*H$_3$), 17.6 (s, *C*H$_3$). ^{31}P{^{1}H} NMR (162 MHz, C_6D_6, δ): 6.5 (br, 1P), 5.7 (br, 1P). Selected ATR-IR data (solid, cm^{-1}): 3234 (ν_{NH}), 3195 (ν_{NH}), 2945, 2904, 2902, 2864, 1462, 1381, 1361, 1334, 1236, 1120. ESI-MS of $(^{iPr}PN^{H}P)_{4}Cu_{12}H_{12}$ (*m*/*z*): calcd for $C_{16}H_{37}NP_{2}Cu$ ($[(^{iPr}PN^{H}P)Cu]^{+}$) 368.16918, found 368.16906. Anal. Cald for $C_{71}H_{168}N_{4}P_{8}Cu_{12}$ [$(^{iPr}PN^{H}P)_{4}Cu_{12}H_{12}\bullet C_{7}H_{8}$]: C, 40.83; H, 8.11; N, 2.68. Found: C, 40.39; H, 8.23; N, 2.71.

Synthesis of $(^{iPr}PN^{H}P)_{4}Cu_{12}D_{12}$. This deuterated compound was prepared from $^{iPr}PN^{H}P$, CuBr, and KO^{t}Bu under D_2 (20 psig) using *Method A* described above. The presence of copper deuteride was confirmed by ^{2}H NMR spectroscopy. ^{2}H NMR (61 MHz, C_6H_6, δ): 2.73 (br, CuD, 2D), 0.92 (br, CuD, 1D). Other $^{R}PN^{H}P$-ligated copper deuteride complexes were prepared similarly.

Reaction of Copper Hydride Clusters with D_2O. To a dry J. Young NMR tube were added $(^{iPr}PN^{H}P)_{3}Cu_{6}H_{6}$ (30 µmol Cu) or $(^{iPr}PN^{H}P)_{4}Cu_{12}H_{12}$ (60 µmol Cu), 400 µL of C_6D_6, and D_2O (50 µmol). The tube was secured to a rotation device (e.g., a rotovap) that allowed constant mixing of the reaction. The progress of the reaction (at 23 °C) was periodically monitored by NMR spectroscopy.

Attempted Reduction of (*N*-Methyl-2-pyrrolecarboxaldehyde with $(^{iPr}PN^{H}P)_{4}Cu_{12}H_{12}$. To a dry J. Young NMR tube were added $(^{iPr}PN^{H}P)_{4}Cu_{12}H_{12}$ (10.0 mg, 5 µmol), *N*-methyl-2-pyrrolecarboxaldehyde (5.4 µL, 50 µmol), and 400 µL of C_6D_6. The tube was secured to a rotation device (e.g., a rotovap) that allowed constant mixing of the reaction. The progress of the reaction (at 23 °C) was periodically monitored by NMR spectroscopy.

X-ray Structure Determination of (^{iPr}PN^{H}P)$_4$Cu$_{12}$H$_{12}$. Intensity data were collected at 150 K on a Bruker D8 Venture Mo-IµS Photon-II diffractometer, λ = 0.71073 Å. Data collection frames were measured in shutterless mode. Over the course of the data collection (~22 hours), the crystal changed color from yellow to dark red. A third data collection (completed ~3 days later) on the same dark red crystal showed the same overall structure as reported here. The data frames were processed using the program SAINT. The data were corrected for decay, Lorentz, and polarization effects as well as absorption and beam corrections. The structure was solved by a combination of direct methods and the difference Fourier technique as implemented in the SHELX suite of programs and refined by full-matrix least squares on F^2 for reflections out to 0.75Å resolution. Non-hydrogen atoms were refined with anisotropic displacement parameters. The hydride and N-bound H-atoms were located directly from the difference map. The hydride coordinates and isotropic displacement parameters were refined; for the N-H H-atoms only the coordinates were refined. All remaining H-atoms were calculated and treated with a riding model. The N- and C- bound H-atom isotropic displacement parameters were defined as a*U_{eq} of the adjacent atom (a = 1.5 for CH_3 and 1.2 for all others). A molecule of toluene resides in the lattice. The crystal structure has been deposited at the Cambridge Crystallographic Data Centre (CCDC) and allocated the deposition number CCDC 2401031.

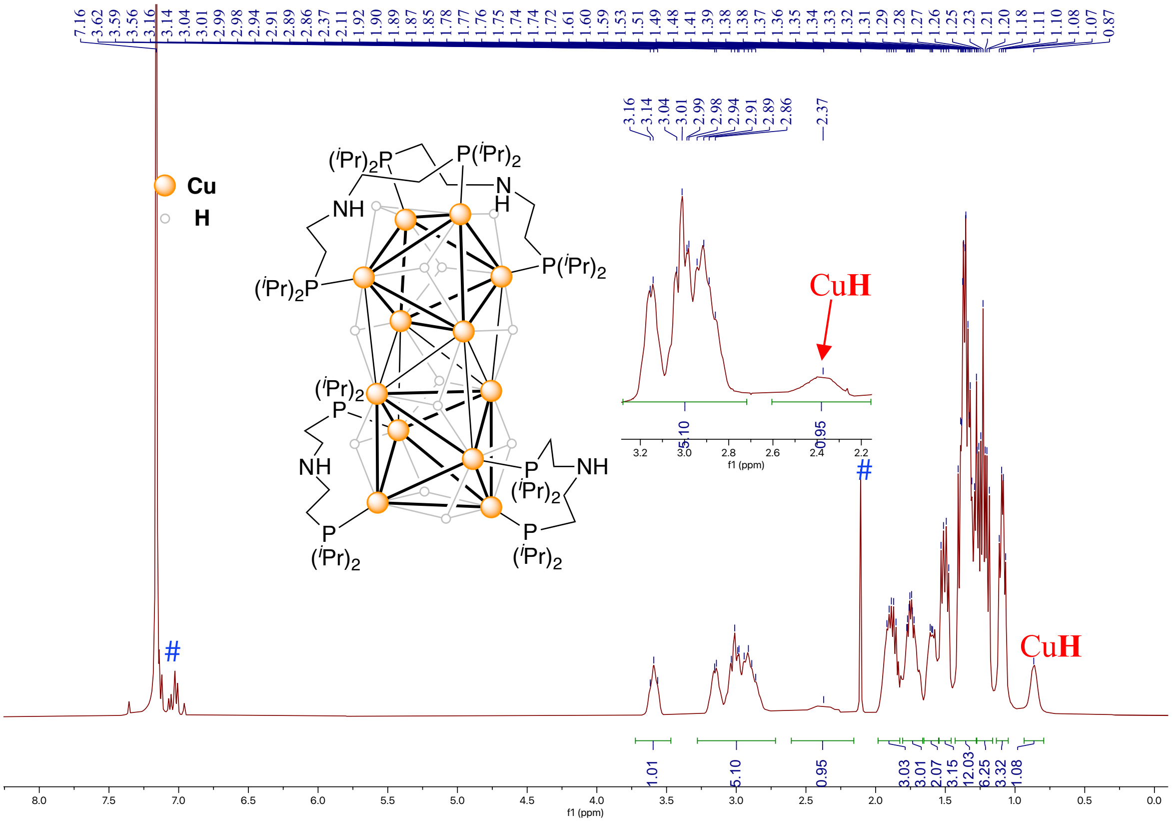

Figure S1. ^{1}H NMR (400 MHz, C_6D_6, 23 °C) spectrum of $(^{iPr}PN^HP)_4Cu_{12}H_{12}$ (# denotes residual toluene)

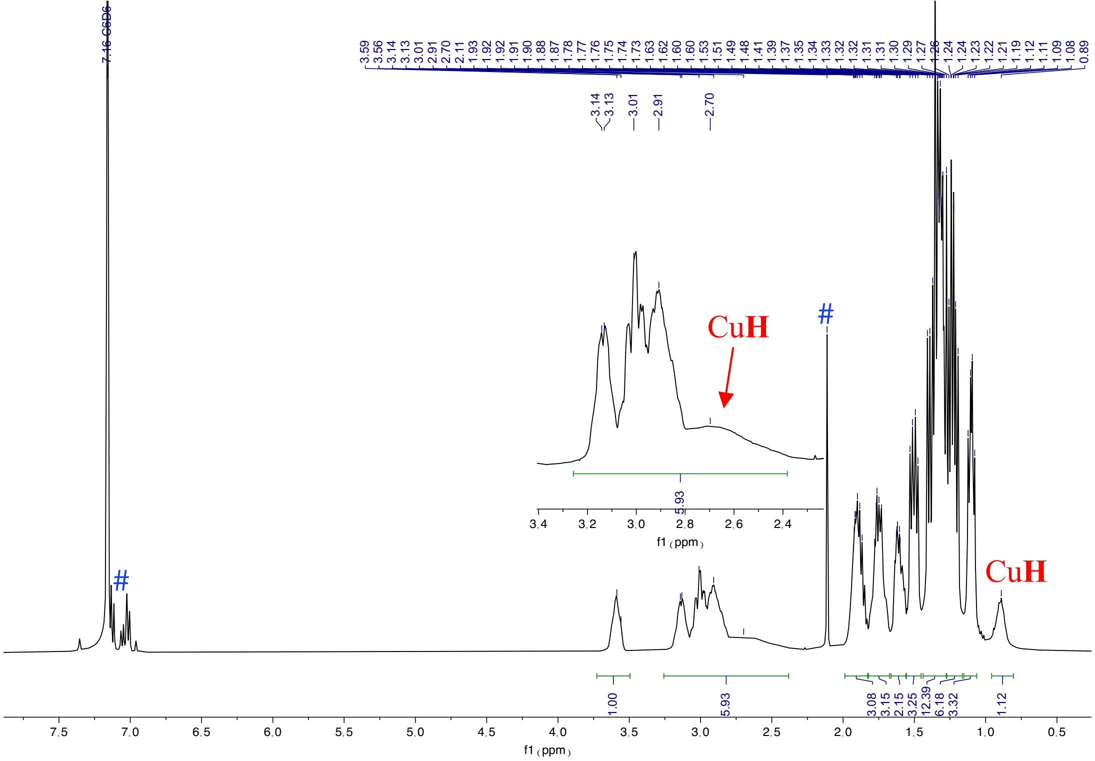

Figure S2. ^{1}H NMR (400 MHz, C_6D_6, 23 °C) spectrum of $(^{iPr}PN^HP)_4Cu_{12}H_{12}$ (a different sample, # denotes residual toluene)

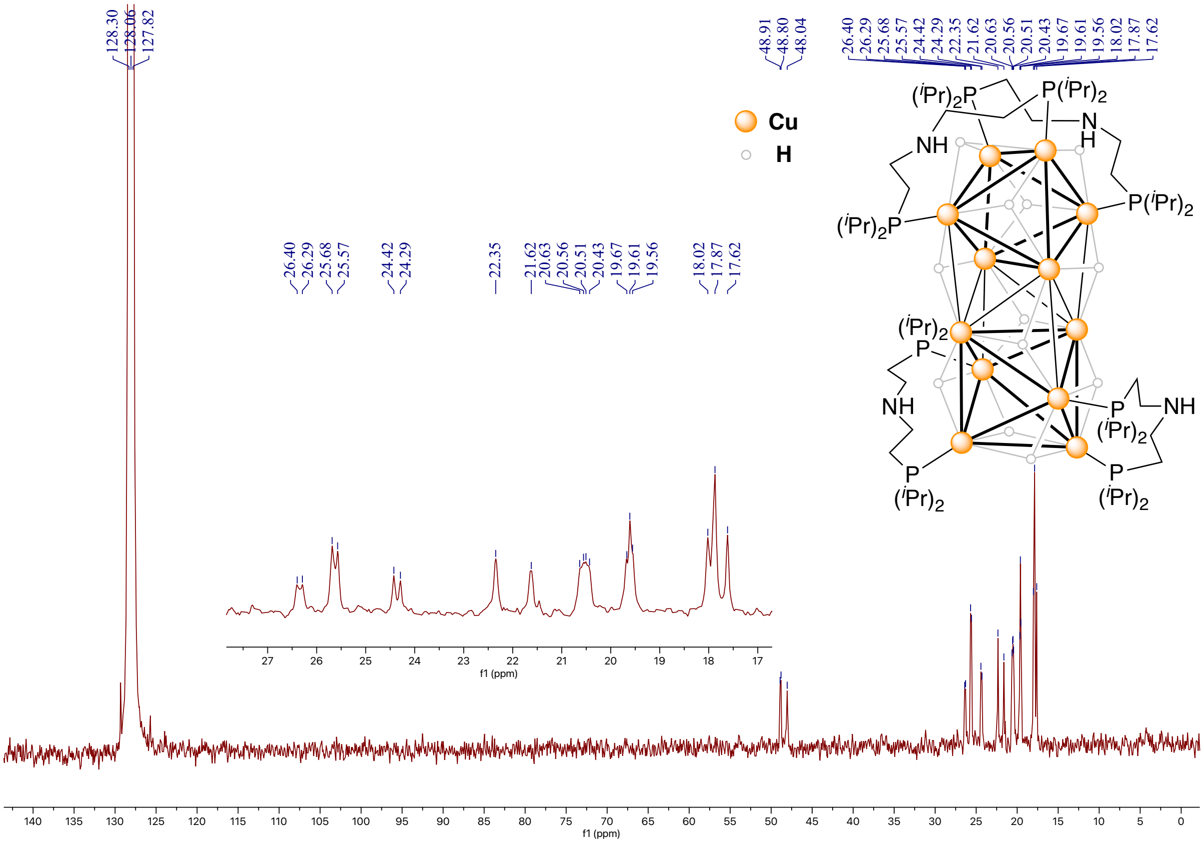

Figure S3. $^{13}C\{^1H\}$ NMR (101 MHz, C_6D_6, 23 °C) spectrum of $(^{iPr}PN^HP)_4Cu_{12}H_{12}$

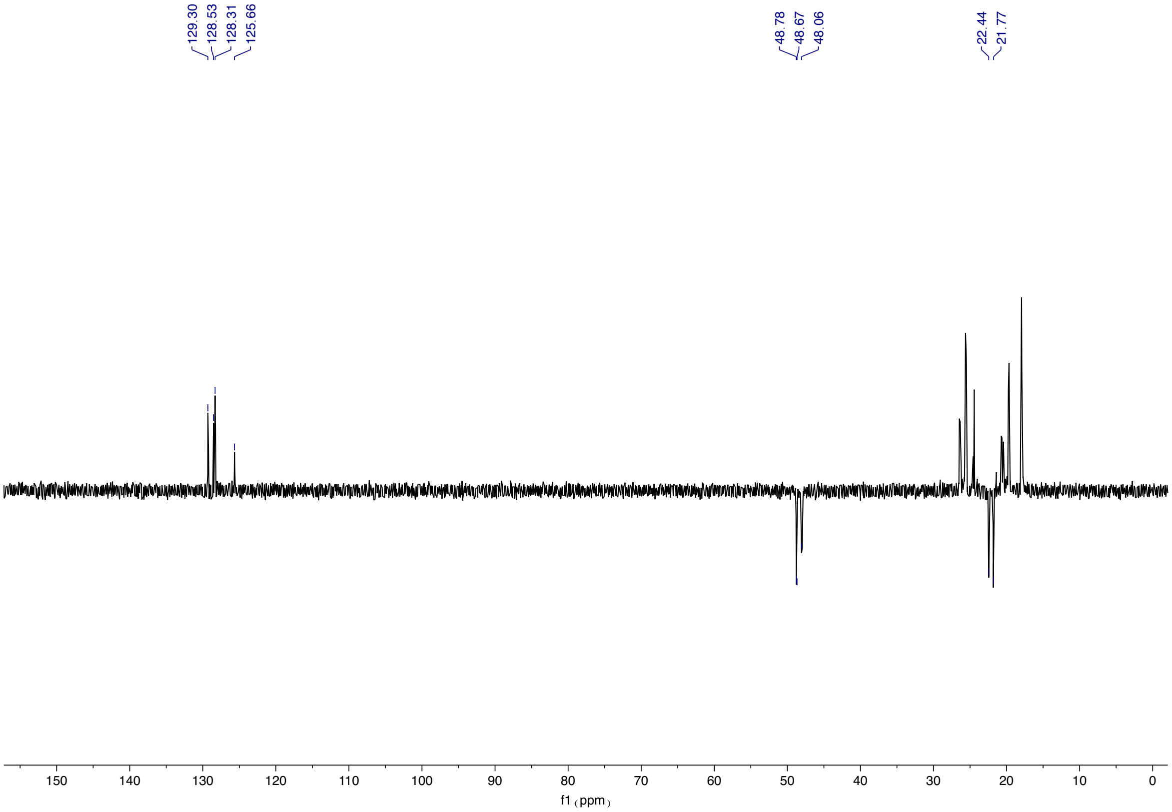

Figure S4. DEPT-135 NMR (101 MHz, C_6D_6, 23 °C) spectrum of $(^{iPr}PN^HP)_4Cu_{12}H_{12}$

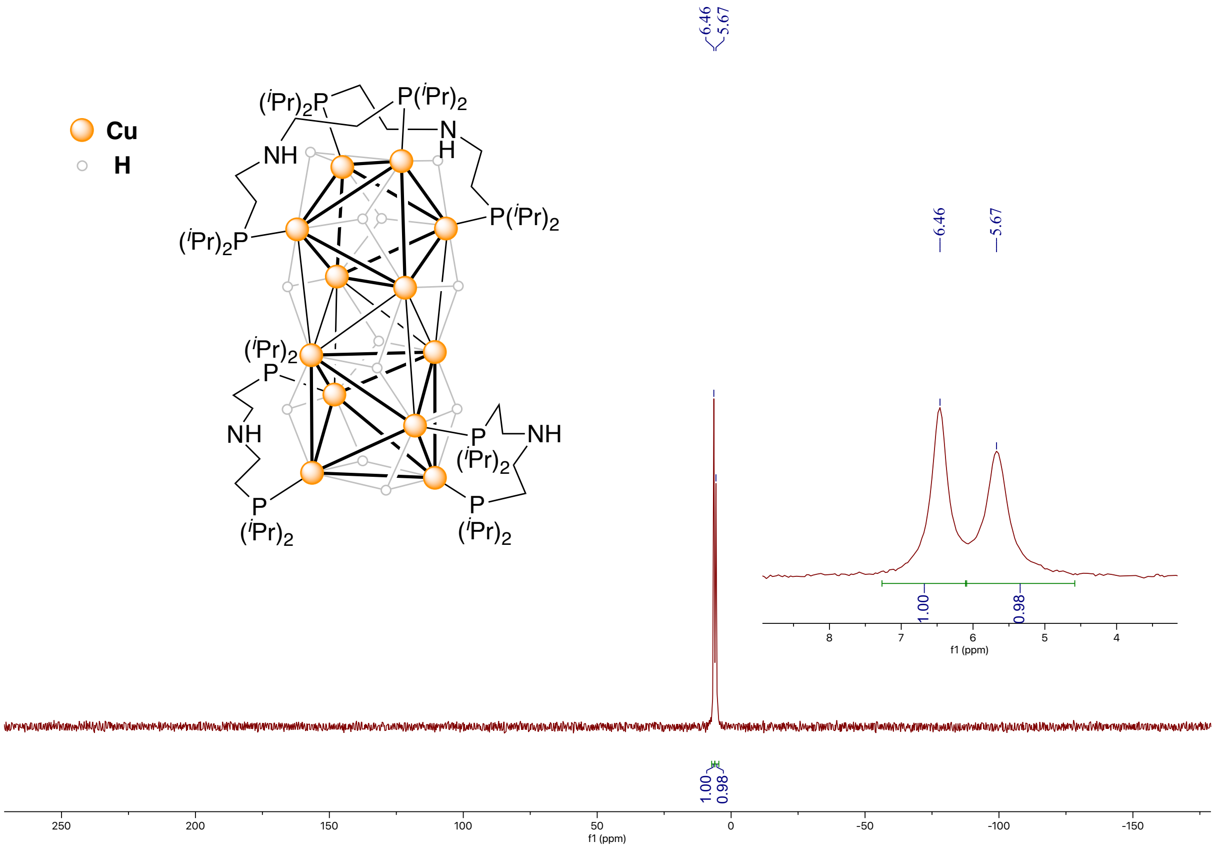

Figure S5. $^{31}P\{^{1}H\}$ NMR (162 MHz, C_6D_6, 23 ºC) spectrum of $(^{iPr}PN^{H}P)_4Cu_{12}H_{12}$

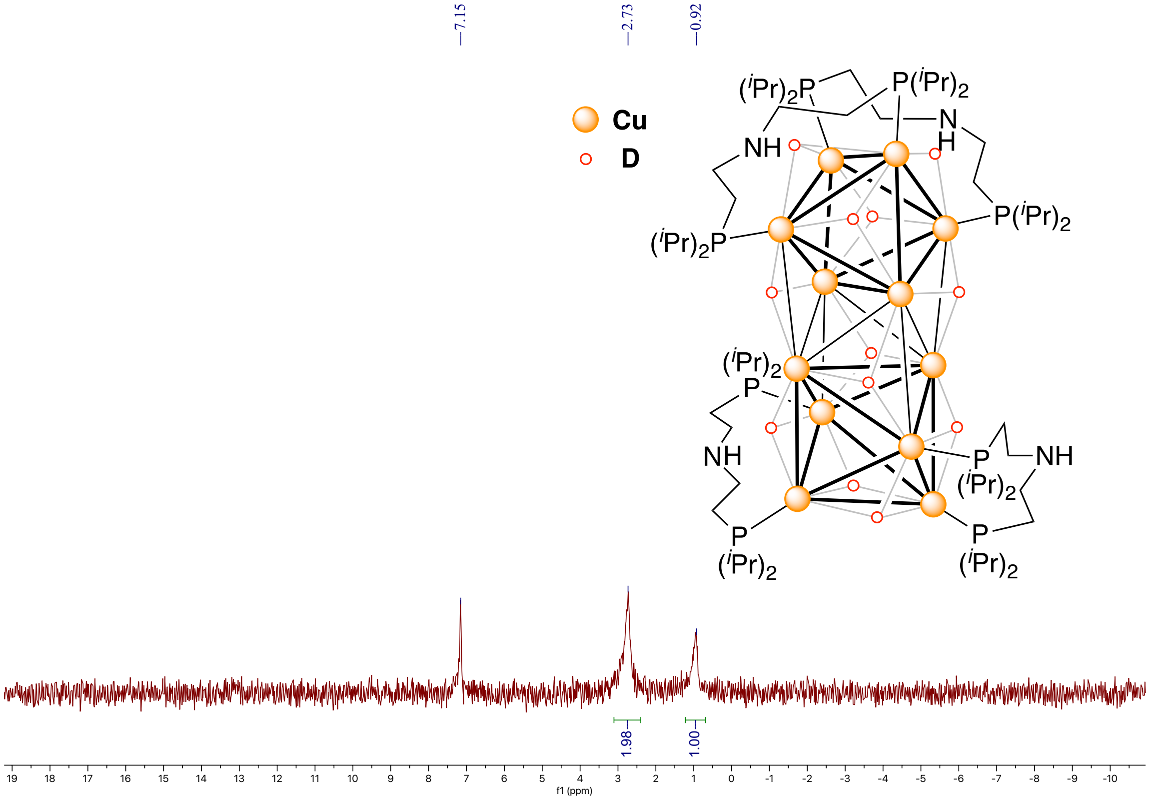

Figure S6. ^{2}H NMR (61 MHz, C_6H_6, 23 ºC) spectrum of $(^{iPr}PN^{H}P)_4Cu_{12}D_{12}$

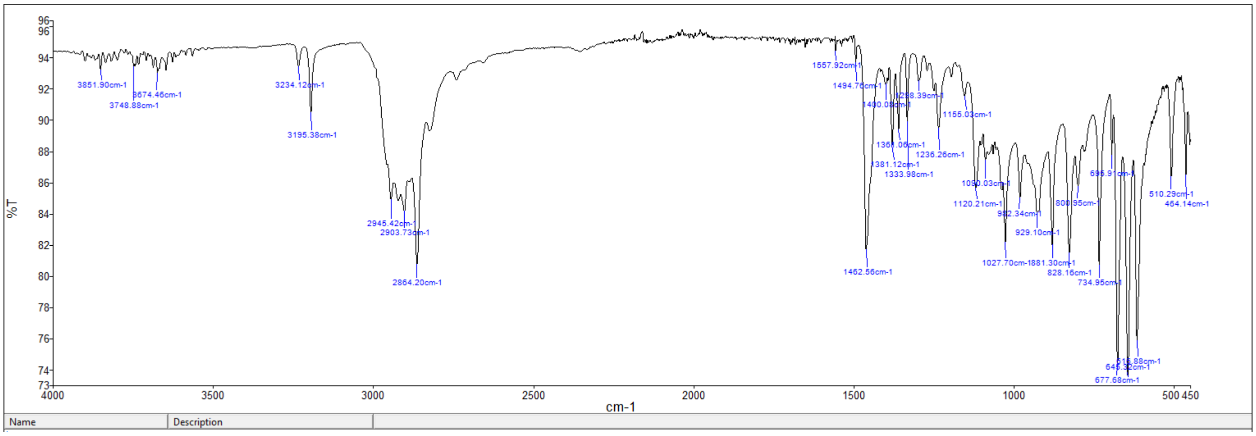

Figure S7. ATR-IR spectrum of $(^{iPr}PN^{H}P)_4Cu_{12}H_{12}$ (solid sample)

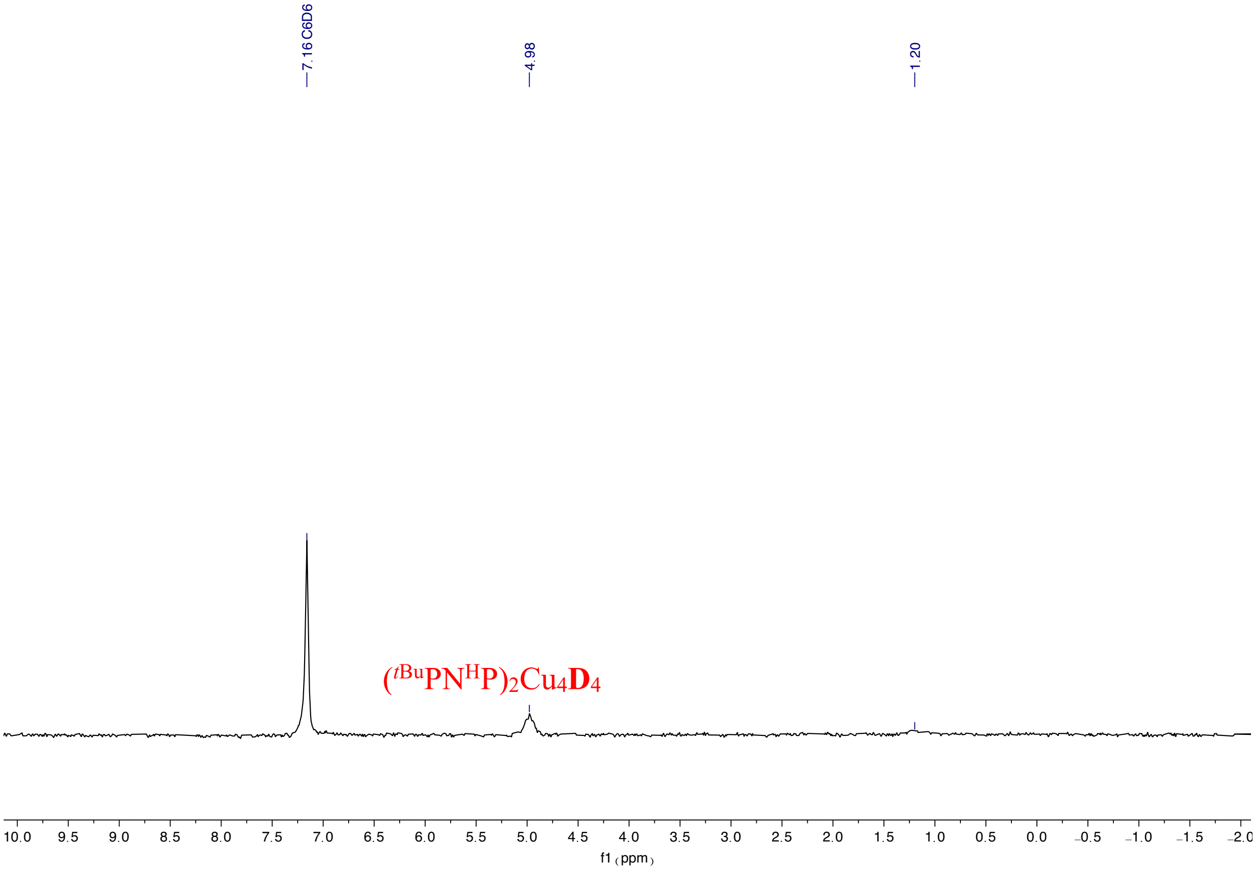

Figure S8. ^{2}H NMR (61 MHz, C_6H_6, 23 °C) spectrum of the crude product from the reaction of CuBr with $^{tBu}PN^{H}P$ and $KO^{t}Bu$ performed under D_2 gas (from MeCN wash*)

*The remaining solid after MeCN wash was pure $(^{tBu}PN^{H}P)_2Cu_4D_4$

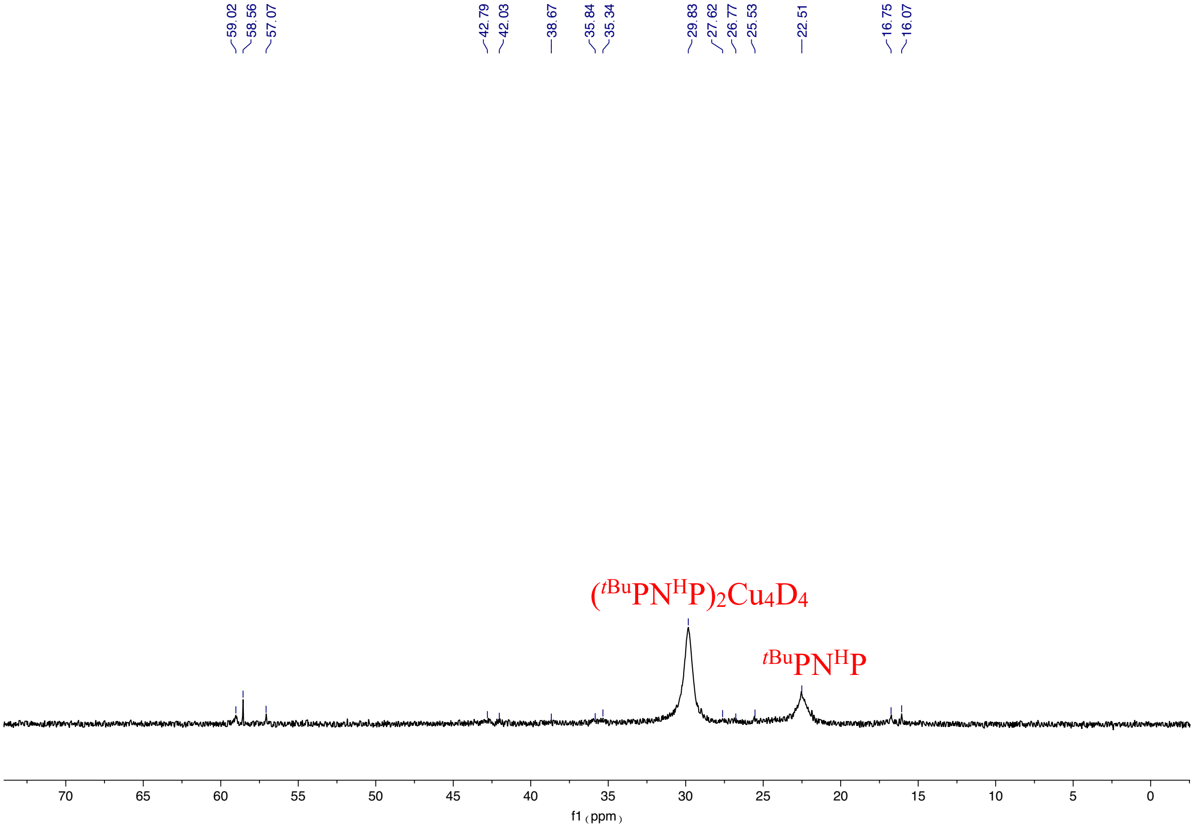

Figure S9. $^{31}P\{^1H\}$ NMR (162 MHz, C_6H_6, 23 °C) spectrum of the crude product from the reaction of CuBr with $^{tBu}PN^HP$ and KO^tBu performed under D_2 gas for 1 h

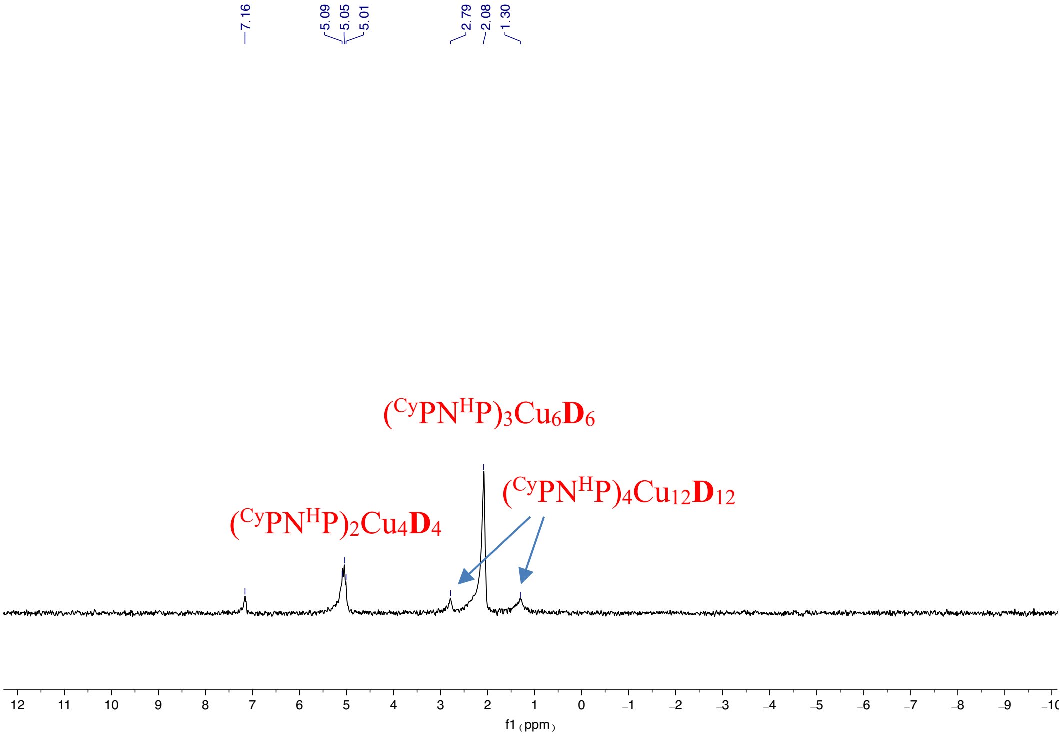

Figure S10. ^2H NMR (61 MHz, C_6H_6, 23 °C) spectrum of the crude product from the reaction of CuBr with $^{Cy}PN^HP$ and KO^tBu performed under D_2 gas for 1 h

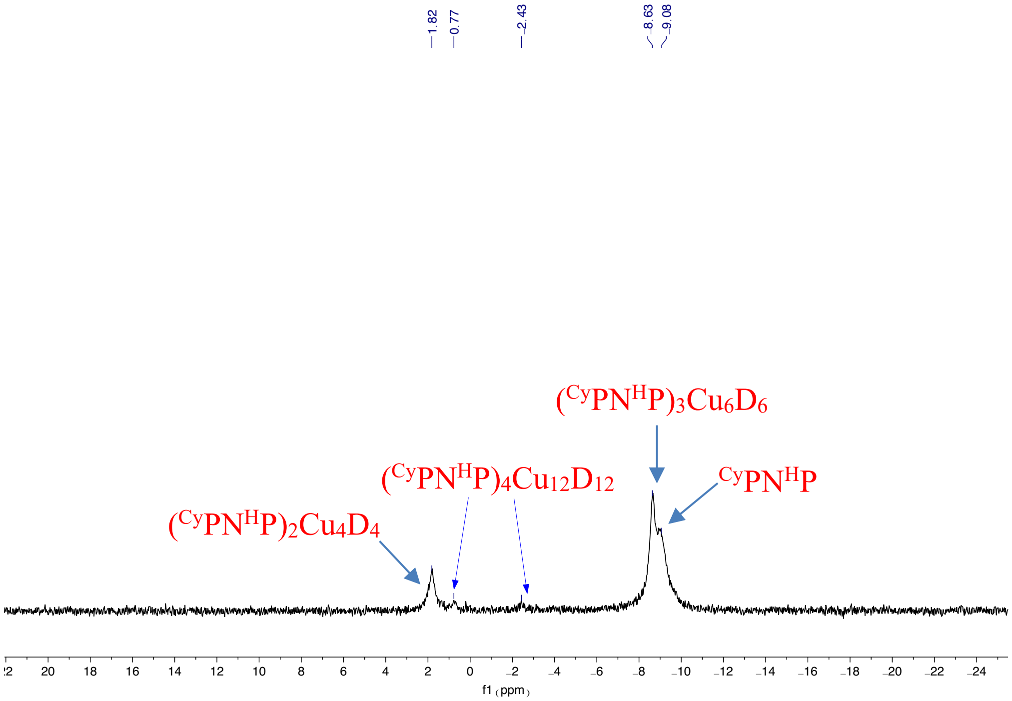

Figure S11. ^{31}P{^{1}H} NMR (162 MHz, C_6H_6, 23 °C) spectrum of the crude product from the reaction of CuBr with ^{Cy}PN^{H}P and KO^{t}Bu performed under D_2 gas for 1 h

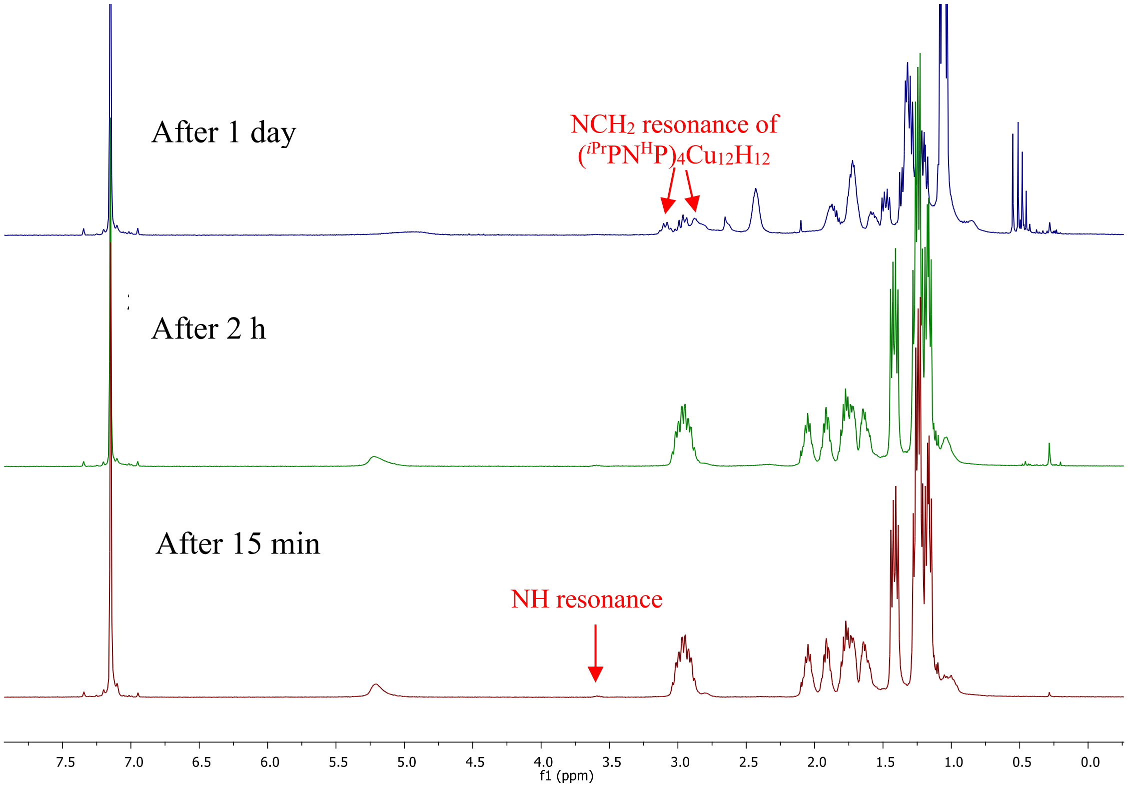

Figure S12. ^{1}H NMR (400 MHz, C_6D_6, 23 °C) spectrum of (^{iPr}PN^{H}P)$_3$Cu$_6$H$_6$ mixed with 10 equiv of D_2O

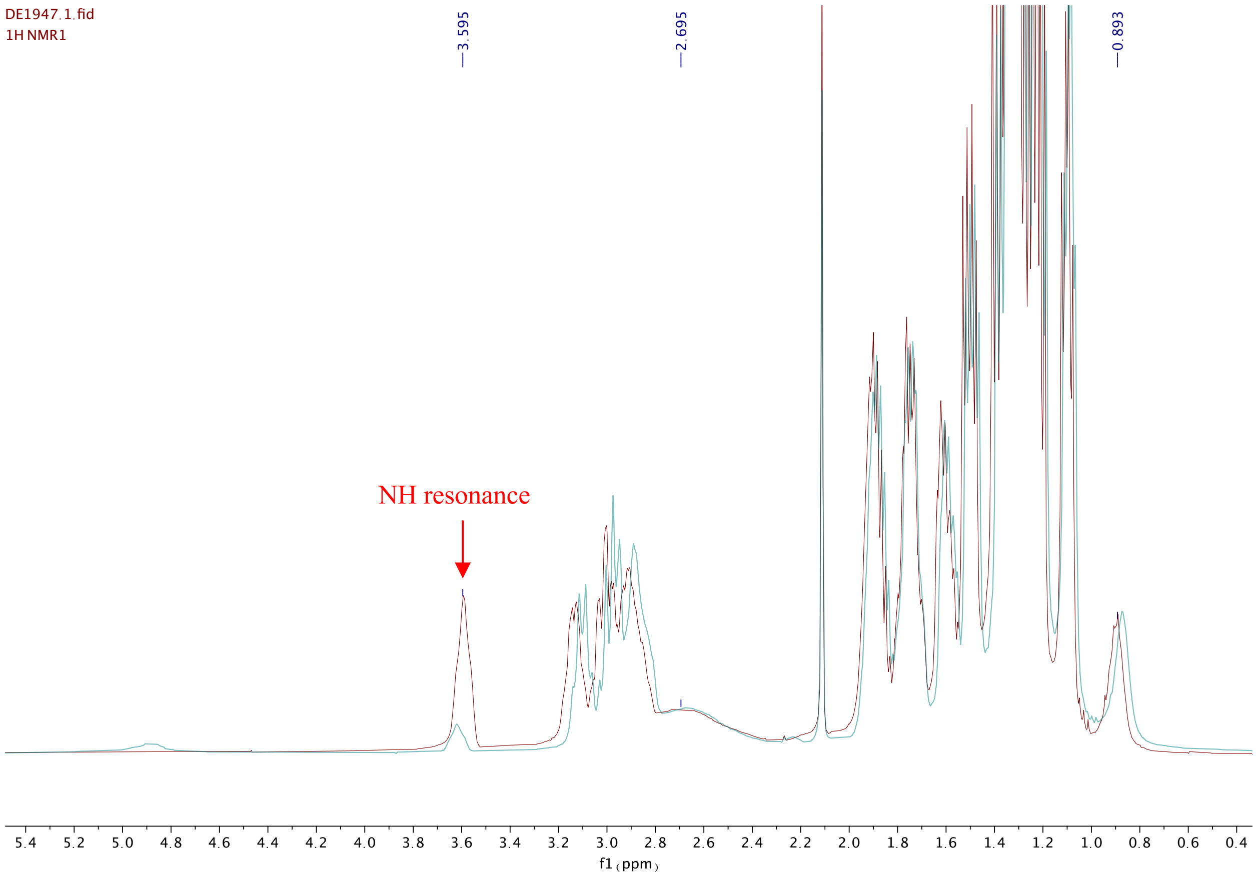

Figure S13. ^{1}H NMR (400 MHz, C_6D_6, 23 °C) spectrum of (^{iPr}PN^{H}P)$_4$Cu$_{12}$H$_{12}$ mixed with 10 equiv of D_2O for 15 min (red line: before adding D_2O; cyan line: after adding D_2O)
*The ^{31}P{^{1}H} NMR spectrum is identical to that of (^{iPr}PN^{H}P)$_4$Cu$_{12}$H$_{12}$ without adding D_2O

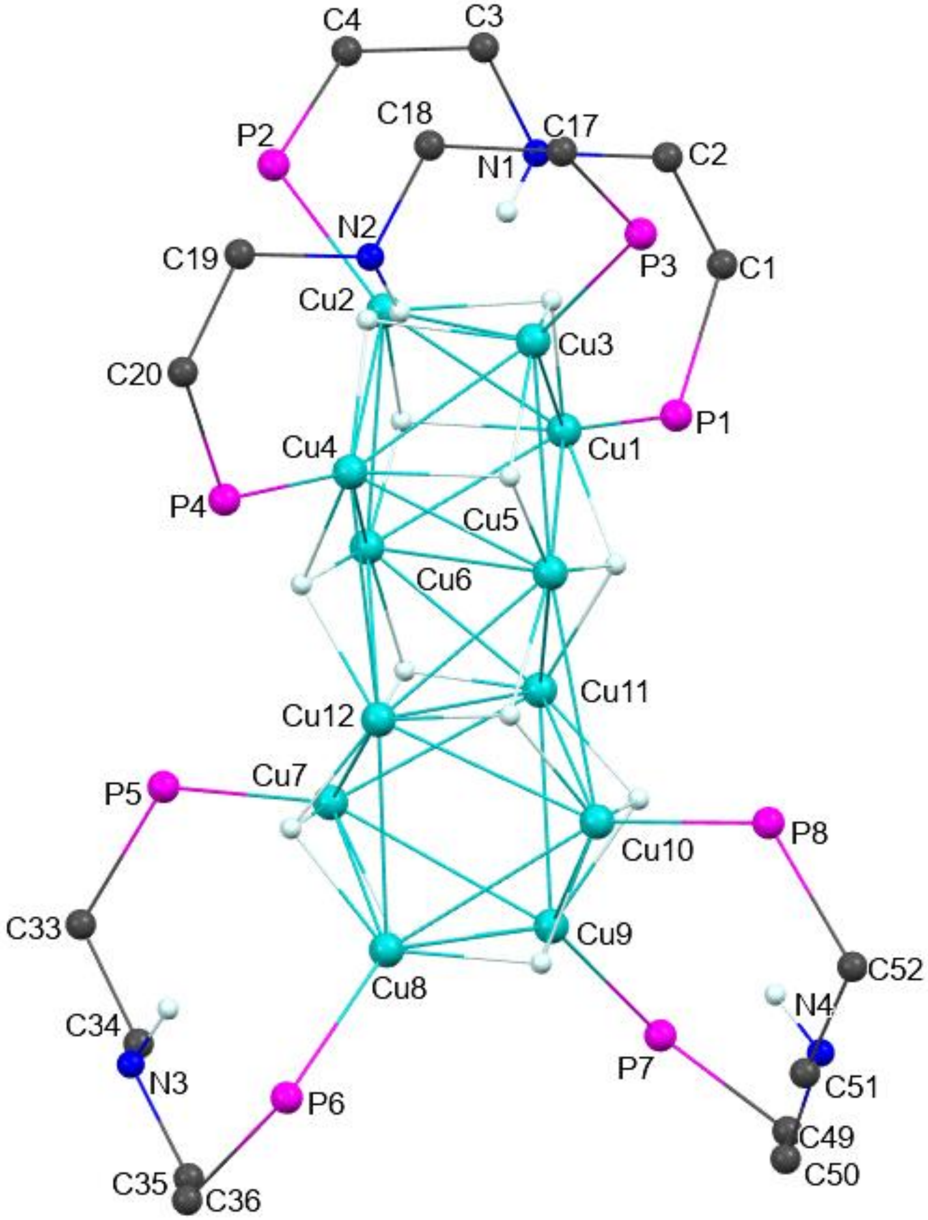

Figure S14. Structure of (^{iPr}PN^{H}P)$_4$Cu$_{12}$H$_{12}$ showing the atomic numbering scheme of the ligand backbone, ^{i}Pr groups and C–H hydrogen atoms omitted for clarity.

Table S1. Crystal data and structure refinement for $(^{iPr}PN^{H}P)_4Cu_{12}H_{12}{\bullet}C_7H_8$.

CCDC deposition number	**CCDC-2401031**	
Formula	$C_{64}H_{160}N_4P_8Cu_{12}.C_7H_8$	
Formula weight	2088.32	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 30.2346(13) Å	$\alpha = 90°$
	b = 20.7857(10) Å	$\beta = 90°$
	c = 30.2931(13) Å	$\gamma = 90°$
Volume	19037.6(15) Å^3	
Z	8	
Density (calculated)	1.457 Mg/m^3	
Absorption coefficient	2.792 mm^{-1}	
F(000)	8720	
Crystal size	0.153 x 0.101 x 0.065 mm^3	
θ range for data collection	1.903 to 28.305°	
Index ranges	$-40 \leq h \leq 40$, $-27 \leq k \leq 27$, $-40 \leq l \leq 40$	
Reflections collected	863719	
Independent reflections	23644 [$R_{int} = 0.0576$]	
Completeness to $\theta = 25.242°$	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.862 and 0.763	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	23644 / 0 / 949	
Goodness-of-fit on F^2	1.032	
Final R indices [$I>2\sigma(I)$]	R1 = 0.0251, wR2 = 0.0605	
R indices (all data)	R1 = 0.0326, wR2 = 0.0646	
Largest diff. peak and hole	1.702 and -0.793 eÅ^{-3}	

Table S2. Bond lengths [Å] and angles [°] for $(^{iPr}PN^{H}P)_4Cu_{12}H_{12}$•$C_7H_8$.

Cu(1)-P(1)	2.2531(6)	Cu(1)-Cu(2)	2.5011(3)
Cu(1)-Cu(6)	2.5562(3)	Cu(1)-Cu(5)	2.6604(3)
Cu(1)-Cu(3)	2.7835(3)	Cu(1)-Cu(11)	2.8867(3)
Cu(2)-P(2)	2.2535(5)	Cu(2)-Cu(3)	2.5074(4)
Cu(2)-Cu(6)	2.6499(3)	Cu(2)-Cu(4)	2.7892(3)
Cu(3)-P(3)	2.2539(6)	Cu(3)-Cu(4)	2.5071(3)
Cu(3)-Cu(5)	2.6112(3)	Cu(4)-P(4)	2.2475(5)
Cu(4)-Cu(5)	2.5742(3)	Cu(4)-Cu(6)	2.6256(3)
Cu(4)-Cu(12)	2.8817(3)	Cu(5)-Cu(12)	2.5035(3)
Cu(5)-Cu(11)	2.5301(3)	Cu(5)-Cu(6)	2.7181(3)
Cu(5)-Cu(10)	2.8086(3)	Cu(6)-Cu(11)	2.5105(3)
Cu(6)-Cu(12)	2.5202(3)	Cu(6)-Cu(7)	2.9389(3)
Cu(7)-P(5)	2.2521(5)	Cu(7)-Cu(8)	2.5072(3)
Cu(7)-Cu(12)	2.5624(3)	Cu(7)-Cu(11)	2.6459(3)
Cu(7)-Cu(9)	2.8015(3)	Cu(8)-P(6)	2.2397(5)
Cu(8)-Cu(9)	2.4823(3)	Cu(8)-Cu(12)	2.6073(3)
Cu(8)-Cu(10)	2.7751(3)	Cu(9)-P(7)	2.2479(5)
Cu(9)-Cu(10)	2.5212(3)	Cu(9)-Cu(11)	2.6222(3)
Cu(10)-P(8)	2.2557(5)	Cu(10)-Cu(11)	2.5588(3)
Cu(10)-Cu(12)	2.6699(3)	Cu(11)-Cu(12)	2.7153(3)
Cu(1)-H(123)	1.74(3)	Cu(1)-H(126)	1.86(3)
Cu(1)-H(151)	1.72(3)	Cu(2)-H(123)	1.88(3)
Cu(2)-H(126)	1.70(3)	Cu(2)-H(234)	1.70(3)
Cu(3)-H(123)	1.69(3)	Cu(3)-H(234)	1.86(3)
Cu(3)-H(345)	1.71(3)	Cu(4)-H(234)	1.75(3)
Cu(4)-H(345)	1.85(3)	Cu(4)-H(461)	1.72(3)
Cu(5)-H(151)	1.65(3)	Cu(5)-H(345)	1.69(3)
Cu(5)-H(511)	1.76(3)	Cu(6)-H(126)	1.65(3)
Cu(6)-H(461)	1.65(3)	Cu(6)-H(671)	1.78(3)
Cu(7)-H(671)	1.72(3)	Cu(7)-H(781)	1.92(3)
Cu(7)-H(789)	1.75(3)	Cu(8)-H(781)	1.71(3)
Cu(8)-H(789)	1.79(3)	Cu(8)-H(891)	1.72(3)
Cu(9)-H(789)	1.71(3)	Cu(9)-H(891)	1.80(3)
Cu(9)-H(911)	1.74(3)	Cu(10)-H(511)	1.72(3)
Cu(10)-H(891)	1.74(3)	Cu(10)-H(911)	1.93(3)
Cu(11)-H(151)	1.77(3)	Cu(11)-H(671)	1.66(3)
Cu(11)-H(911)	1.64(3)	Cu(12)-H(461)	1.73(3)
Cu(12)-H(511)	1.65(3)	Cu(12)-H(781)	1.62(3)
P(1)-C(8)	1.851(3)	P(1)-C(5)	1.859(3)
P(1)-C(1)	1.864(2)	P(2)-C(14)	1.848(2)
P(2)-C(11)	1.862(2)	P(2)-C(4)	1.864(2)
P(3)-C(25)	1.847(3)	P(3)-C(17)	1.855(3)

P(3)-C(21)	1.858(2)	P(4)-C(30)	1.854(2)
P(4)-C(20)	1.855(2)	P(4)-C(24)	1.859(2)
P(5)-C(37)	1.855(2)	P(5)-C(40)	1.856(2)
P(5)-C(33)	1.862(2)	P(6)-C(36)	1.851(2)
P(6)-C(43)	1.853(2)	P(6)-C(46)	1.856(2)
P(7)-C(56)	1.848(2)	P(7)-C(49)	1.851(2)
P(7)-C(53)	1.861(2)	P(8)-C(62)	1.851(2)
P(8)-C(59)	1.856(2)	P(8)-C(52)	1.857(2)

N(1)-C(2)	1.456(3)	N(1)-C(3)	1.458(3)
N(2)-C(18)	1.417(4)	N(2)-C(19)	1.460(4)
N(3)-C(35)	1.461(3)	N(3)-C(34)	1.462(3)
N(4)-C(50)	1.456(3)	N(4)-C(51)	1.461(3)
N(1)-H(1)	0.83(3)	N(2)-H(2)	0.91(3)
N(3)-H(3)	0.83(3)	N(4)-H(4)	0.85(3)

C(1)-C(2)	1.525(3)	C(3)-C(4)	1.520(3)
C(5)-C(6)	1.511(4)	C(5)-C(7)	1.525(4)
C(8)-C(9)	1.504(5)	C(8)-C(10)	1.535(4)
C(11)-C(12)	1.524(3)	C(11)-C(13)	1.531(3)
C(14)-C(16)	1.527(3)	C(14)-C(15)	1.529(3)
C(17)-C(18)	1.470(4)	C(19)-C(20)	1.483(4)
C(21)-C(22)	1.522(4)	C(21)-C(23)	1.534(3)
C(24)-C(28)	1.521(3)	C(24)-C(27)	1.527(3)
C(25)-C(26)	1.508(5)	C(25)-C(29)	1.527(4)
C(30)-C(31)	1.528(3)	C(30)-C(32)	1.529(3)
C(33)-C(34)	1.522(3)	C(35)-C(36)	1.525(3)
C(37)-C(39)	1.526(3)	C(37)-C(38)	1.527(3)
C(40)-C(42)	1.528(3)	C(40)-C(41)	1.532(3)
C(43)-C(44)	1.533(3)	C(43)-C(45)	1.538(3)
C(46)-C(47)	1.519(4)	C(46)-C(48)	1.527(4)
C(49)-C(50)	1.524(3)	C(51)-C(52)	1.523(3)
C(53)-C(54)	1.522(4)	C(53)-C(55)	1.531(3)
C(56)-C(57)	1.522(4)	C(56)-C(58)	1.531(4)
C(59)-C(60)	1.529(3)	C(59)-C(61)	1.530(3)
C(62)-C(63)	1.531(4)	C(62)-C(64)	1.533(3)
C(71)-C(72)	1.414(5)	C(72)-C(77)	1.377(5)
C(72)-C(73)	1.381(4)	C(73)-C(74)	1.413(5)
C(74)-C(75)	1.303(6)	C(75)-C(76)	1.462(6)
C(76)-C(77)	1.327(6)		

P(1)-Cu(1)-Cu(2)	129.899(19)	P(1)-Cu(1)-Cu(6)	128.38(2)
Cu(2)-Cu(1)-Cu(6)	63.187(9)	P(1)-Cu(1)-Cu(5)	137.967(19)
Cu(2)-Cu(1)-Cu(5)	92.037(10)	Cu(6)-Cu(1)-Cu(5)	62.768(9)
P(1)-Cu(1)-Cu(3)	144.16(2)	Cu(2)-Cu(1)-Cu(3)	56.345(9)
Cu(6)-Cu(1)-Cu(3)	87.109(10)	Cu(5)-Cu(1)-Cu(3)	57.273(8)

P(1)-Cu(1)-Cu(11)	96.642(18)	Cu(2)-Cu(1)-Cu(11)	117.189(11)
Cu(6)-Cu(1)-Cu(11)	54.525(8)	Cu(5)-Cu(1)-Cu(11)	54.086(8)
Cu(3)-Cu(1)-Cu(11)	110.672(10)	P(2)-Cu(2)-Cu(1)	133.065(17)
P(2)-Cu(2)-Cu(3)	141.165(17)	Cu(1)-Cu(2)-Cu(3)	67.526(10)
P(2)-Cu(2)-Cu(6)	127.326(17)	Cu(1)-Cu(2)-Cu(6)	59.422(9)
Cu(3)-Cu(2)-Cu(6)	91.101(10)	P(2)-Cu(2)-Cu(4)	136.048(17)
Cu(1)-Cu(2)-Cu(4)	89.194(10)	Cu(3)-Cu(2)-Cu(4)	56.199(8)
Cu(6)-Cu(2)-Cu(4)	57.659(8)	P(3)-Cu(3)-Cu(4)	131.52(2)
P(3)-Cu(3)-Cu(2)	140.579(18)	Cu(4)-Cu(3)-Cu(2)	67.591(9)
P(3)-Cu(3)-Cu(5)	126.187(18)	Cu(4)-Cu(3)-Cu(5)	60.350(9)
Cu(2)-Cu(3)-Cu(5)	93.066(10)	P(3)-Cu(3)-Cu(1)	137.865(19)
Cu(4)-Cu(3)-Cu(1)	89.201(10)	Cu(2)-Cu(3)-Cu(1)	56.129(9)
Cu(5)-Cu(3)-Cu(1)	58.991(8)	P(4)-Cu(4)-Cu(3)	131.095(18)
P(4)-Cu(4)-Cu(5)	133.018(17)	Cu(3)-Cu(4)-Cu(5)	61.830(9)
P(4)-Cu(4)-Cu(6)	137.188(17)	Cu(3)-Cu(4)-Cu(6)	91.678(10)
Cu(5)-Cu(4)-Cu(6)	63.022(9)	P(4)-Cu(4)-Cu(2)	139.005(17)
Cu(3)-Cu(4)-Cu(2)	56.211(9)	Cu(5)-Cu(4)-Cu(2)	87.605(10)
Cu(6)-Cu(4)-Cu(2)	58.507(8)	P(4)-Cu(4)-Cu(12)	99.490(16)
Cu(3)-Cu(4)-Cu(12)	115.639(10)	Cu(5)-Cu(4)-Cu(12)	54.272(8)
Cu(6)-Cu(4)-Cu(12)	54.225(8)	Cu(2)-Cu(4)-Cu(12)	111.906(10)
Cu(12)-Cu(5)-Cu(11)	65.290(9)	Cu(12)-Cu(5)-Cu(4)	69.139(9)
Cu(11)-Cu(5)-Cu(4)	114.475(11)	Cu(12)-Cu(5)-Cu(3)	126.385(11)
Cu(11)-Cu(5)-Cu(3)	130.233(11)	Cu(4)-Cu(5)-Cu(3)	57.820(8)
Cu(12)-Cu(5)-Cu(1)	112.337(11)	Cu(11)-Cu(5)-Cu(1)	67.527(9)
Cu(4)-Cu(5)-Cu(1)	90.562(10)	Cu(3)-Cu(5)-Cu(1)	63.735(9)
Cu(12)-Cu(5)-Cu(6)	57.542(8)	Cu(11)-Cu(5)-Cu(6)	57.020(8)
Cu(4)-Cu(5)-Cu(6)	59.412(8)	Cu(3)-Cu(5)-Cu(6)	87.407(9)
Cu(1)-Cu(5)-Cu(6)	56.741(8)	Cu(12)-Cu(5)-Cu(10)	60.019(8)
Cu(11)-Cu(5)-Cu(10)	56.993(8)	Cu(4)-Cu(5)-Cu(10)	126.794(11)
Cu(3)-Cu(5)-Cu(10)	170.923(11)	Cu(1)-Cu(5)-Cu(10)	121.602(10)
Cu(6)-Cu(5)-Cu(10)	101.666(9)	Cu(11)-Cu(6)-Cu(12)	65.333(9)
Cu(11)-Cu(6)-Cu(1)	69.458(9)	Cu(12)-Cu(6)-Cu(1)	115.376(11)
Cu(11)-Cu(6)-Cu(4)	113.365(11)	Cu(12)-Cu(6)-Cu(4)	68.077(9)
Cu(1)-Cu(6)-Cu(4)	91.753(10)	Cu(11)-Cu(6)-Cu(2)	126.222(11)
Cu(12)-Cu(6)-Cu(2)	130.686(11)	Cu(1)-Cu(6)-Cu(2)	57.391(8)
Cu(4)-Cu(6)-Cu(2)	63.834(8)	Cu(11)-Cu(6)-Cu(5)	57.716(8)
Cu(12)-Cu(6)-Cu(5)	56.948(8)	Cu(1)-Cu(6)-Cu(5)	60.491(9)
Cu(4)-Cu(6)-Cu(5)	57.566(8)	Cu(2)-Cu(6)-Cu(5)	87.597(9)
Cu(11)-Cu(6)-Cu(7)	57.452(8)	Cu(12)-Cu(6)-Cu(7)	55.347(8)
Cu(1)-Cu(6)-Cu(7)	124.796(10)	Cu(4)-Cu(6)-Cu(7)	121.107(10)
Cu(2)-Cu(6)-Cu(7)	173.246(11)	Cu(5)-Cu(6)-Cu(7)	98.984(9)
P(1)-Cu(1)-H(123)	116.3(10)	Cu(2)-Cu(1)-H(123)	48.5(9)
Cu(6)-Cu(1)-H(123)	106.0(10)	Cu(5)-Cu(1)-H(123)	92.4(10)
Cu(3)-Cu(1)-H(123)	35.1(10)	Cu(11)-Cu(1)-H(123)	145.5(10)
P(1)-Cu(1)-H(126)	109.2(9)	Cu(2)-Cu(1)-H(126)	42.9(8)

Cu(6)-Cu(1)-H(126)	40.2(8)	Cu(5)-Cu(1)-H(126)	99.9(9)
Cu(3)-Cu(1)-H(126)	94.9(8)	Cu(11)-Cu(1)-H(126)	88.0(8)
H(123)-Cu(1)-H(126)	90.6(12)	P(1)-Cu(1)-H(151)	101.4(10)
Cu(2)-Cu(1)-H(151)	127.7(9)	Cu(6)-Cu(1)-H(151)	78.3(10)
Cu(5)-Cu(1)-H(151)	37.0(10)	Cu(3)-Cu(1)-H(151)	89.6(10)
Cu(11)-Cu(1)-H(151)	34.6(10)	H(123)-Cu(1)-H(151)	121.9(13)
H(126)-Cu(1)-H(151)	117.7(13)	P(2)-Cu(2)-H(123)	123.3(9)
Cu(1)-Cu(2)-H(123)	43.9(9)	Cu(3)-Cu(2)-H(123)	42.4(9)
Cu(6)-Cu(2)-H(123)	98.4(9)	Cu(4)-Cu(2)-H(123)	94.3(9)
P(2)-Cu(2)-H(126)	105.7(9)	Cu(1)-Cu(2)-H(126)	47.9(9)
Cu(3)-Cu(2)-H(126)	109.7(9)	Cu(6)-Cu(2)-H(126)	37.2(9)
Cu(4)-Cu(2)-H(126)	94.4(9)	H(123)-Cu(2)-H(126)	91.0(13)
P(2)-Cu(2)-H(234)	115.0(9)	Cu(1)-Cu(2)-H(234)	110.0(9)
Cu(3)-Cu(2)-H(234)	47.9(9)	Cu(6)-Cu(2)-H(234)	94.2(9)
Cu(4)-Cu(2)-H(234)	36.5(9)	H(123)-Cu(2)-H(234)	89.2(13)
H(126)-Cu(2)-H(234)	130.7(13)	P(3)-Cu(3)-H(123)	115.9(10)
Cu(4)-Cu(3)-H(123)	110.3(10)	Cu(2)-Cu(3)-H(123)	48.4(10)
Cu(5)-Cu(3)-H(123)	95.2(10)	Cu(1)-Cu(3)-H(123)	36.2(10)
P(3)-Cu(3)-H(234)	121.0(8)	Cu(4)-Cu(3)-H(234)	44.1(8)
Cu(2)-Cu(3)-H(234)	42.8(8)	Cu(5)-Cu(3)-H(234)	100.3(8)
Cu(1)-Cu(3)-H(234)	94.8(8)	H(123)-Cu(3)-H(234)	90.1(13)
P(3)-Cu(3)-H(345)	103.5(9)	Cu(4)-Cu(3)-H(345)	47.4(9)
Cu(2)-Cu(3)-H(345)	110.8(9)	Cu(5)-Cu(3)-H(345)	39.4(9)
Cu(1)-Cu(3)-H(345)	97.6(9)	H(123)-Cu(3)-H(345)	133.6(13)
H(234)-Cu(3)-H(345)	89.9(12)	P(4)-Cu(4)-H(234)	112.5(9)
Cu(3)-Cu(4)-H(234)	47.9(9)	Cu(5)-Cu(4)-H(234)	105.1(9)
Cu(6)-Cu(4)-H(234)	94.1(9)	Cu(2)-Cu(4)-H(234)	35.6(9)
Cu(12)-Cu(4)-H(234)	146.6(9)	P(4)-Cu(4)-H(345)	111.5(8)
Cu(3)-Cu(4)-H(345)	43.0(8)	Cu(5)-Cu(4)-H(345)	40.8(8)
Cu(6)-Cu(4)-H(345)	101.3(8)	Cu(2)-Cu(4)-H(345)	96.0(8)
Cu(12)-Cu(4)-H(345)	87.5(8)	H(234)-Cu(4)-H(345)	89.4(12)
P(4)-Cu(4)-H(461)	100.7(9)	Cu(3)-Cu(4)-H(461)	127.5(9)
Cu(5)-Cu(4)-H(461)	77.9(9)	Cu(6)-Cu(4)-H(461)	37.9(9)
Cu(2)-Cu(4)-H(461)	92.2(9)	Cu(12)-Cu(4)-H(461)	33.6(9)
H(234)-Cu(4)-H(461)	125.7(12)	H(345)-Cu(4)-H(461)	117.3(12)
Cu(12)-Cu(5)-H(151)	108.5(10)	Cu(11)-Cu(5)-H(151)	44.0(10)
Cu(4)-Cu(5)-H(151)	126.6(10)	Cu(3)-Cu(5)-H(151)	97.3(10)
Cu(1)-Cu(5)-H(151)	38.8(10)	Cu(6)-Cu(5)-H(151)	74.4(10)
Cu(10)-Cu(5)-H(151)	85.6(10)	Cu(12)-Cu(5)-H(345)	104.6(9)
Cu(11)-Cu(5)-H(345)	159.4(9)	Cu(4)-Cu(5)-H(345)	45.7(9)
Cu(3)-Cu(5)-H(345)	40.1(9)	Cu(1)-Cu(5)-H(345)	102.9(9)
Cu(6)-Cu(5)-H(345)	102.4(9)	Cu(10)-Cu(5)-H(345)	135.5(9)
H(151)-Cu(5)-H(345)	137.1(14)	Cu(12)-Cu(5)-H(511)	41.1(9)
Cu(11)-Cu(5)-H(511)	80.6(9)	Cu(4)-Cu(5)-H(511)	94.2(9)
Cu(3)-Cu(5)-H(511)	143.5(9)	Cu(1)-Cu(5)-H(511)	146.7(9)
Cu(6)-Cu(5)-H(511)	98.2(9)	Cu(10)-Cu(5)-H(511)	35.6(9)

H(151)-Cu(5)-H(511)	119.0(13)	H(345)-Cu(5)-H(511)	103.9(13)
Cu(11)-Cu(6)-H(126)	106.5(10)	Cu(12)-Cu(6)-H(126)	160.5(10)
Cu(1)-Cu(6)-H(126)	46.4(10)	Cu(4)-Cu(6)-H(126)	101.9(9)
Cu(2)-Cu(6)-H(126)	38.6(9)	Cu(5)-Cu(6)-H(126)	103.6(10)
Cu(7)-Cu(6)-H(126)	137.0(9)	Cu(11)-Cu(6)-H(461)	107.9(9)
Cu(12)-Cu(6)-H(461)	43.2(9)	Cu(1)-Cu(6)-H(461)	128.2(9)
Cu(4)-Cu(6)-H(461)	39.8(9)	Cu(2)-Cu(6)-H(461)	98.9(9)
Cu(5)-Cu(6)-H(461)	74.6(9)	Cu(7)-Cu(6)-H(461)	84.4(9)
H(126)-Cu(6)-H(461)	136.8(13)	Cu(11)-Cu(6)-H(671)	41.3(8)
Cu(12)-Cu(6)-H(671)	78.3(8)	Cu(1)-Cu(6)-H(671)	96.1(8)
Cu(4)-Cu(6)-H(671)	145.6(8)	Cu(2)-Cu(6)-H(671)	145.6(8)
Cu(5)-Cu(6)-H(671)	98.0(8)	Cu(7)-Cu(6)-H(671)	32.2(8)
H(126)-Cu(6)-H(671)	107.7(13)	H(461)-Cu(6)-H(671)	115.3(12)
P(5)-Cu(7)-H(671)	101.7(9)	Cu(8)-Cu(7)-H(671)	126.4(9)
Cu(12)-Cu(7)-H(671)	78.2(9)	Cu(11)-Cu(7)-H(671)	37.6(9)
Cu(9)-Cu(7)-H(671)	90.6(9)	Cu(6)-Cu(7)-H(671)	33.6(9)
P(5)-Cu(7)-H(781)	111.5(8)	Cu(8)-Cu(7)-H(781)	43.1(8)
Cu(12)-Cu(7)-H(781)	39.2(8)	Cu(11)-Cu(7)-H(781)	99.0(8)
Cu(9)-Cu(7)-H(781)	94.7(8)	Cu(6)-Cu(7)-H(781)	87.0(7)
H(671)-Cu(7)-H(781)	116.5(11)	P(5)-Cu(7)-H(789)	115.3(9)
Cu(8)-Cu(7)-H(789)	45.7(9)	Cu(12)-Cu(7)-H(789)	103.2(9)
Cu(11)-Cu(7)-H(789)	92.8(9)	Cu(9)-Cu(7)-H(789)	35.4(9)
Cu(6)-Cu(7)-H(789)	143.9(9)	H(671)-Cu(7)-H(789)	124.4(13)
H(781)-Cu(7)-H(789)	87.5(12)	P(6)-Cu(8)-H(781)	104.8(8)
Cu(9)-Cu(8)-H(781)	112.9(9)	Cu(7)-Cu(8)-H(781)	49.9(9)
Cu(12)-Cu(8)-H(781)	37.3(9)	Cu(10)-Cu(8)-H(781)	96.4(9)
P(6)-Cu(8)-H(789)	122.0(9)	Cu(9)-Cu(8)-H(789)	43.5(9)
Cu(7)-Cu(8)-H(789)	44.1(9)	Cu(12)-Cu(8)-H(789)	100.1(9)
Cu(10)-Cu(8)-H(789)	96.3(9)	H(781)-Cu(8)-H(789)	92.8(12)
P(6)-Cu(8)-H(891)	113.9(9)	Cu(9)-Cu(8)-H(891)	46.5(9)
Cu(7)-Cu(8)-H(891)	109.6(9)	Cu(12)-Cu(8)-H(891)	96.2(9)
Cu(10)-Cu(8)-H(891)	36.8(9)	H(781)-Cu(8)-H(891)	132.9(12)
H(789)-Cu(8)-H(891)	88.8(13)	P(7)-Cu(9)-H(789)	114.8(9)
Cu(8)-Cu(9)-H(789)	46.2(9)	Cu(10)-Cu(9)-H(789)	108.5(9)
Cu(11)-Cu(9)-H(789)	94.5(9)	Cu(7)-Cu(9)-H(789)	36.3(9)
P(7)-Cu(9)-H(891)	122.8(8)	Cu(8)-Cu(9)-H(891)	43.8(8)
Cu(10)-Cu(9)-H(891)	43.6(8)	Cu(11)-Cu(9)-H(891)	99.1(8)
Cu(7)-Cu(9)-H(891)	96.0(8)	H(789)-Cu(9)-H(891)	88.9(13)
P(7)-Cu(9)-H(911)	105.1(9)	Cu(8)-Cu(9)-H(911)	111.5(9)
Cu(10)-Cu(9)-H(911)	49.7(9)	Cu(11)-Cu(9)-H(911)	37.6(9)
Cu(7)-Cu(9)-H(911)	95.6(9)	H(789)-Cu(9)-H(911)	131.5(13)
H(891)-Cu(9)-H(911)	92.0(12)	P(8)-Cu(10)-H(511)	103.0(9)
Cu(9)-Cu(10)-H(511)	127.1(9)	Cu(11)-Cu(10)-H(511)	80.4(9)
Cu(12)-Cu(10)-H(511)	36.7(9)	Cu(8)-Cu(10)-H(511)	88.1(9)
Cu(5)-Cu(10)-H(511)	36.5(9)	P(8)-Cu(10)-H(891)	115.4(9)
Cu(9)-Cu(10)-H(891)	45.5(9)	Cu(11)-Cu(10)-H(891)	103.2(9)

Cu(12)-Cu(10)-H(891)	93.5(9)	Cu(8)-Cu(10)-H(891)	36.3(9)
Cu(5)-Cu(10)-H(891)	146.4(9)	H(511)-Cu(10)-H(891)	122.3(13)
P(8)-Cu(10)-H(911)	108.7(8)	Cu(9)-Cu(10)-H(911)	43.4(8)
Cu(11)-Cu(10)-H(911)	39.7(8)	Cu(12)-Cu(10)-H(911)	99.6(8)
Cu(8)-Cu(10)-H(911)	95.0(8)	Cu(5)-Cu(10)-H(911)	88.4(8)
H(511)-Cu(10)-H(911)	119.4(12)	H(891)-Cu(10)-H(911)	87.8(12)
Cu(6)-Cu(11)-H(151)	78.9(9)	Cu(5)-Cu(11)-H(151)	40.5(9)
Cu(10)-Cu(11)-H(151)	91.5(9)	Cu(9)-Cu(11)-H(151)	142.1(9)
Cu(7)-Cu(11)-H(151)	146.4(9)	Cu(12)-Cu(11)-H(151)	96.8(9)
Cu(1)-Cu(11)-H(151)	33.6(9)	Cu(6)-Cu(11)-H(671)	45.1(9)
Cu(5)-Cu(11)-H(671)	109.2(9)	Cu(10)-Cu(11)-H(671)	128.5(9)
Cu(9)-Cu(11)-H(671)	98.4(9)	Cu(7)-Cu(11)-H(671)	39.2(9)
Cu(12)-Cu(11)-H(671)	74.5(9)	Cu(1)-Cu(11)-H(671)	87.6(9)
H(151)-Cu(11)-H(671)	119.2(13)	Cu(6)-Cu(11)-H(911)	163.8(9)
Cu(5)-Cu(11)-H(911)	105.6(9)	Cu(10)-Cu(11)-H(911)	48.8(9)
Cu(9)-Cu(11)-H(911)	40.3(9)	Cu(7)-Cu(11)-H(911)	104.3(9)
Cu(12)-Cu(11)-H(911)	106.4(9)	Cu(1)-Cu(11)-H(911)	132.3(9)
H(151)-Cu(11)-H(911)	103.2(13)	H(671)-Cu(11)-H(911)	137.4(13)
Cu(5)-Cu(12)-H(461)	79.7(9)	Cu(6)-Cu(12)-H(461)	40.6(8)
Cu(7)-Cu(12)-H(461)	95.4(9)	Cu(8)-Cu(12)-H(461)	146.6(9)
Cu(10)-Cu(12)-H(461)	144.0(9)	Cu(11)-Cu(12)-H(461)	97.2(8)
Cu(4)-Cu(12)-H(461)	33.3(9)	Cu(5)-Cu(12)-H(511)	44.4(9)
Cu(6)-Cu(12)-H(511)	109.3(9)	Cu(7)-Cu(12)-H(511)	128.5(9)
Cu(8)-Cu(12)-H(511)	95.4(9)	Cu(10)-Cu(12)-H(511)	38.5(9)
Cu(11)-Cu(12)-H(511)	76.7(9)	Cu(4)-Cu(12)-H(511)	86.0(9)
H(461)-Cu(12)-H(511)	117.8(12)	Cu(5)-Cu(12)-H(781)	162.5(9)
Cu(6)-Cu(12)-H(781)	109.8(9)	Cu(7)-Cu(12)-H(781)	48.5(9)
Cu(8)-Cu(12)-H(781)	39.9(9)	Cu(10)-Cu(12)-H(781)	103.0(9)
Cu(11)-Cu(12)-H(781)	105.1(9)	Cu(4)-Cu(12)-H(781)	136.7(9)
H(461)-Cu(12)-H(781)	108.0(12)	H(511)-Cu(12)-H(781)	133.6(13)

P(5)-Cu(7)-Cu(8)	131.215(18)	P(5)-Cu(7)-Cu(12)	131.016(17)
Cu(8)-Cu(7)-Cu(12)	61.890(9)	P(5)-Cu(7)-Cu(11)	138.469(17)
Cu(8)-Cu(7)-Cu(11)	90.315(10)	Cu(12)-Cu(7)-Cu(11)	62.823(9)
P(5)-Cu(7)-Cu(9)	141.321(17)	Cu(8)-Cu(7)-Cu(9)	55.420(9)
Cu(12)-Cu(7)-Cu(9)	87.218(10)	Cu(11)-Cu(7)-Cu(9)	57.464(8)
P(5)-Cu(7)-Cu(6)	99.852(15)	Cu(8)-Cu(7)-Cu(6)	115.048(10)
Cu(12)-Cu(7)-Cu(6)	54.007(8)	Cu(11)-Cu(7)-Cu(6)	53.111(7)
Cu(9)-Cu(7)-Cu(6)	109.831(10)	P(6)-Cu(8)-Cu(9)	139.184(18)
P(6)-Cu(8)-Cu(7)	133.847(18)	Cu(9)-Cu(8)-Cu(7)	68.315(9)
P(6)-Cu(8)-Cu(12)	126.914(18)	Cu(9)-Cu(8)-Cu(12)	93.356(10)
Cu(7)-Cu(8)-Cu(12)	60.094(9)	P(6)-Cu(8)-Cu(10)	134.351(18)
Cu(9)-Cu(8)-Cu(10)	56.987(8)	Cu(7)-Cu(8)-Cu(10)	90.476(10)
Cu(12)-Cu(8)-Cu(10)	59.379(8)	P(7)-Cu(9)-Cu(8)	140.595(18)
P(7)-Cu(9)-Cu(10)	134.488(17)	Cu(8)-Cu(9)-Cu(10)	67.364(9)
P(7)-Cu(9)-Cu(11)	127.347(18)	Cu(8)-Cu(9)-Cu(11)	91.419(10)

Cu(10)-Cu(9)-Cu(11)	59.630(8)	P(7)-Cu(9)-Cu(7)	134.435(17)
Cu(8)-Cu(9)-Cu(7)	56.265(8)	Cu(10)-Cu(9)-Cu(7)	89.584(10)
Cu(11)-Cu(9)-Cu(7)	58.284(8)	P(8)-Cu(10)-Cu(9)	129.378(17)
P(8)-Cu(10)-Cu(11)	129.456(18)	Cu(9)-Cu(10)-Cu(11)	62.146(9)
P(8)-Cu(10)-Cu(12)	139.575(17)	Cu(9)-Cu(10)-Cu(12)	90.990(10)
Cu(11)-Cu(10)-Cu(12)	62.530(9)	P(8)-Cu(10)-Cu(8)	143.459(18)
Cu(9)-Cu(10)-Cu(8)	55.649(9)	Cu(11)-Cu(10)-Cu(8)	86.412(10)
Cu(12)-Cu(10)-Cu(8)	57.181(8)	P(8)-Cu(10)-Cu(5)	97.447(16)
Cu(9)-Cu(10)-Cu(5)	117.576(11)	Cu(11)-Cu(10)-Cu(5)	56.015(8)
Cu(12)-Cu(10)-Cu(5)	54.312(8)	Cu(8)-Cu(10)-Cu(5)	110.958(10)
Cu(6)-Cu(11)-Cu(5)	65.264(9)	Cu(6)-Cu(11)-Cu(10)	115.412(11)
Cu(5)-Cu(11)-Cu(10)	66.992(9)	Cu(6)-Cu(11)-Cu(9)	132.494(11)
Cu(5)-Cu(11)-Cu(9)	124.543(11)	Cu(10)-Cu(11)-Cu(9)	58.224(8)
Cu(6)-Cu(11)-Cu(7)	69.437(9)	Cu(5)-Cu(11)-Cu(7)	112.475(11)
Cu(10)-Cu(11)-Cu(7)	92.348(10)	Cu(9)-Cu(11)-Cu(7)	64.252(8)
Cu(6)-Cu(11)-Cu(12)	57.507(8)	Cu(5)-Cu(11)-Cu(12)	56.883(8)
Cu(10)-Cu(11)-Cu(12)	60.738(8)	Cu(9)-Cu(11)-Cu(12)	87.862(9)
Cu(7)-Cu(11)-Cu(12)	57.085(8)	Cu(6)-Cu(11)-Cu(1)	56.017(8)
Cu(5)-Cu(11)-Cu(1)	58.387(9)	Cu(10)-Cu(11)-Cu(1)	122.399(11)
Cu(9)-Cu(11)-Cu(1)	171.274(11)	Cu(7)-Cu(11)-Cu(1)	123.412(10)
Cu(12)-Cu(11)-Cu(1)	99.922(9)	Cu(5)-Cu(12)-Cu(6)	65.510(9)
Cu(5)-Cu(12)-Cu(7)	116.312(11)	Cu(6)-Cu(12)-Cu(7)	70.646(9)
Cu(5)-Cu(12)-Cu(8)	128.345(11)	Cu(6)-Cu(12)-Cu(8)	127.568(11)
Cu(7)-Cu(12)-Cu(8)	58.016(9)	Cu(5)-Cu(12)-Cu(10)	65.669(9)
Cu(6)-Cu(12)-Cu(10)	111.278(11)	Cu(7)-Cu(12)-Cu(10)	91.713(10)
Cu(8)-Cu(12)-Cu(10)	63.440(9)	Cu(5)-Cu(12)-Cu(11)	57.827(8)
Cu(6)-Cu(12)-Cu(11)	57.160(8)	Cu(7)-Cu(12)-Cu(11)	60.093(8)
Cu(8)-Cu(12)-Cu(11)	86.715(9)	Cu(10)-Cu(12)-Cu(11)	56.732(8)
Cu(5)-Cu(12)-Cu(4)	56.589(8)	Cu(6)-Cu(12)-Cu(4)	57.697(8)
Cu(7)-Cu(12)-Cu(4)	125.776(10)	Cu(8)-Cu(12)-Cu(4)	173.171(11)
Cu(10)-Cu(12)-Cu(4)	120.211(10)	Cu(11)-Cu(12)-Cu(4)	100.110(9)

C(8)-P(1)-C(5)	104.04(14)	C(8)-P(1)-C(1)	103.04(12)
C(5)-P(1)-C(1)	100.84(13)	C(8)-P(1)-Cu(1)	109.82(10)
C(5)-P(1)-Cu(1)	116.63(9)	C(1)-P(1)-Cu(1)	120.49(8)
C(14)-P(2)-C(11)	103.51(10)	C(14)-P(2)-C(4)	100.55(10)
C(11)-P(2)-C(4)	102.06(10)	C(14)-P(2)-Cu(2)	114.41(7)
C(11)-P(2)-Cu(2)	113.26(7)	C(4)-P(2)-Cu(2)	120.78(7)
C(25)-P(3)-C(17)	101.71(15)	C(25)-P(3)-C(21)	103.67(12)
C(17)-P(3)-C(21)	100.32(13)	C(25)-P(3)-Cu(3)	112.52(11)
C(17)-P(3)-Cu(3)	119.90(9)	C(21)-P(3)-Cu(3)	116.42(7)
C(30)-P(4)-C(20)	102.21(12)	C(30)-P(4)-C(24)	104.25(10)
C(20)-P(4)-C(24)	101.38(11)	C(30)-P(4)-Cu(4)	108.71(8)
C(20)-P(4)-Cu(4)	120.98(8)	C(24)-P(4)-Cu(4)	117.20(7)
C(37)-P(5)-C(40)	103.93(10)	C(37)-P(5)-C(33)	100.70(11)
C(40)-P(5)-C(33)	103.20(11)	C(37)-P(5)-Cu(7)	116.54(7)

C(40)-P(5)-Cu(7)	109.96(7)	C(33)-P(5)-Cu(7)	120.51(8)
C(36)-P(6)-C(43)	102.36(11)	C(36)-P(6)-C(46)	102.02(11)
C(43)-P(6)-C(46)	103.75(11)	C(36)-P(6)-Cu(8)	119.66(8)
C(43)-P(6)-Cu(8)	114.10(7)	C(46)-P(6)-Cu(8)	113.01(7)
C(56)-P(7)-C(49)	100.64(11)	C(56)-P(7)-C(53)	103.37(12)
C(49)-P(7)-C(53)	102.71(10)	C(56)-P(7)-Cu(9)	114.61(8)
C(49)-P(7)-Cu(9)	121.22(7)	C(53)-P(7)-Cu(9)	112.10(7)
C(62)-P(8)-C(59)	103.80(11)	C(62)-P(8)-C(52)	102.44(11)
C(59)-P(8)-C(52)	100.84(11)	C(62)-P(8)-Cu(10)	110.82(8)
C(59)-P(8)-Cu(10)	117.52(8)	C(52)-P(8)-Cu(10)	119.31(8)

C(2)-N(1)-C(3)	112.12(19)	C(18)-N(2)-C(19)	114.6(2)
C(35)-N(3)-C(34)	110.69(18)	C(50)-N(4)-C(51)	111.38(18)
C(2)-N(1)-H(1)	108.8(19)	C(3)-N(1)-H(1)	104.9(18)
C(18)-N(2)-H(2)	108(2)	C(19)-N(2)-H(2)	106(2)
C(35)-N(3)-H(3)	107.7(18)	C(34)-N(3)-H(3)	108.0(18)
C(50)-N(4)-H(4)	108.3(17)	C(51)-N(4)-H(4)	107.7(17)

C(2)-C(1)-P(1)	114.76(16)	N(1)-C(2)-C(1)	111.4(2)
N(1)-C(3)-C(4)	110.94(19)	C(3)-C(4)-P(2)	114.80(15)
C(6)-C(5)-C(7)	110.5(3)	C(6)-C(5)-P(1)	110.17(18)
C(7)-C(5)-P(1)	112.69(19)	C(9)-C(8)-C(10)	112.3(3)
C(9)-C(8)-P(1)	108.80(19)	C(10)-C(8)-P(1)	115.5(2)
C(12)-C(11)-C(13)	110.6(2)	C(12)-C(11)-P(2)	110.14(16)
C(13)-C(11)-P(2)	115.27(17)	C(16)-C(14)-C(15)	110.7(2)
C(16)-C(14)-P(2)	108.74(15)	C(15)-C(14)-P(2)	110.85(15)
C(18)-C(17)-P(3)	115.85(19)	N(2)-C(18)-C(17)	114.1(3)
N(2)-C(19)-C(20)	111.8(2)	C(19)-C(20)-P(4)	115.84(17)
C(22)-C(21)-C(23)	111.1(2)	C(22)-C(21)-P(3)	110.78(17)
C(23)-C(21)-P(3)	114.24(18)	C(28)-C(24)-C(27)	110.2(2)
C(28)-C(24)-P(4)	112.64(15)	C(27)-C(24)-P(4)	108.71(16)
C(26)-C(25)-C(29)	111.6(3)	C(26)-C(25)-P(3)	110.7(2)
C(29)-C(25)-P(3)	107.7(2)	C(31)-C(30)-C(32)	110.7(2)
C(31)-C(30)-P(4)	109.36(16)	C(32)-C(30)-P(4)	115.9(2)
C(34)-C(33)-P(5)	115.03(15)	N(3)-C(34)-C(33)	112.1(2)
N(3)-C(35)-C(36)	112.07(19)	C(35)-C(36)-P(6)	114.25(15)
C(39)-C(37)-C(38)	110.66(19)	C(39)-C(37)-P(5)	109.00(15)
C(38)-C(37)-P(5)	111.87(14)	C(42)-C(40)-C(41)	111.7(2)
C(42)-C(40)-P(5)	116.11(18)	C(41)-C(40)-P(5)	108.97(17)
C(44)-C(43)-C(45)	111.0(2)	C(44)-C(43)-P(6)	109.77(16)
C(45)-C(43)-P(6)	115.44(17)	C(47)-C(46)-C(48)	111.2(2)
C(47)-C(46)-P(6)	109.91(17)	C(48)-C(46)-P(6)	109.09(18)
C(50)-C(49)-P(7)	113.83(14)	N(4)-C(50)-C(49)	110.79(18)
N(4)-C(51)-C(52)	111.35(19)	C(51)-C(52)-P(8)	115.26(15)
C(54)-C(53)-C(55)	110.7(2)	C(54)-C(53)-P(7)	109.97(16)
C(55)-C(53)-P(7)	116.00(18)	C(57)-C(56)-C(58)	112.2(3)

C(57)-C(56)-P(7)	109.63(19)	C(58)-C(56)-P(7)	109.00(18)
C(60)-C(59)-C(61)	110.9(2)	C(60)-C(59)-P(8)	111.81(16)
C(61)-C(59)-P(8)	109.17(15)	C(63)-C(62)-C(64)	111.9(2)
C(63)-C(62)-P(8)	109.66(16)	C(64)-C(62)-P(8)	114.74(18)
C(77)-C(72)-C(73)	118.8(4)	C(77)-C(72)-C(71)	118.7(4)
C(73)-C(72)-C(71)	122.5(4)	C(72)-C(73)-C(74)	117.3(3)
C(75)-C(74)-C(73)	126.5(4)	C(74)-C(75)-C(76)	113.5(4)
C(77)-C(76)-C(75)	122.3(4)	C(76)-C(77)-C(72)	121.4(4)

Table S3. Torsion angles [°] for (^{iPr}PN^{H}P)$_4$Cu$_{12}$H$_{12}$•C$_7$H$_8$.

C(8)-P(1)-C(1)-C(2)	-128.7(2)	C(5)-P(1)-C(1)-C(2)	124.0(2)
Cu(1)-P(1)-C(1)-C(2)	-6.0(3)	C(3)-N(1)-C(2)-C(1)	-177.03(19)
P(1)-C(1)-C(2)-N(1)	-65.1(3)	C(2)-N(1)-C(3)-C(4)	-175.01(18)
N(1)-C(3)-C(4)-P(2)	72.7(2)	C(14)-P(2)-C(4)-C(3)	113.63(18)
C(11)-P(2)-C(4)-C(3)	-139.94(17)	Cu(2)-P(2)-C(4)-C(3)	-13.3(2)
C(8)-P(1)-C(5)-C(6)	179.1(2)	C(1)-P(1)-C(5)-C(6)	-74.4(2)
Cu(1)-P(1)-C(5)-C(6)	58.0(2)	C(8)-P(1)-C(5)-C(7)	55.1(2)
C(1)-P(1)-C(5)-C(7)	161.7(2)	Cu(1)-P(1)-C(5)-C(7)	-66.0(2)
C(5)-P(1)-C(8)-C(9)	171.1(2)	C(1)-P(1)-C(8)-C(9)	66.2(2)
Cu(1)-P(1)-C(8)-C(9)	-63.4(2)	C(5)-P(1)-C(8)-C(10)	43.8(2)
C(1)-P(1)-C(8)-C(10)	-61.1(3)	Cu(1)-P(1)-C(8)-C(10)	169.3(2)
C(14)-P(2)-C(11)-C(12)	174.03(15)	C(4)-P(2)-C(11)-C(12)	69.92(17)
Cu(2)-P(2)-C(11)-C(12)	-61.50(16)	C(14)-P(2)-C(11)-C(13)	48.0(2)
C(4)-P(2)-C(11)-C(13)	-56.1(2)	Cu(2)-P(2)-C(11)-C(13)	172.49(16)
C(11)-P(2)-C(14)-C(16)	-176.14(16)	C(4)-P(2)-C(14)-C(16)	-70.88(18)
Cu(2)-P(2)-C(14)-C(16)	60.14(17)	C(11)-P(2)-C(14)-C(15)	61.93(19)
C(4)-P(2)-C(14)-C(15)	167.20(17)	Cu(2)-P(2)-C(14)-C(15)	-61.79(18)
C(25)-P(3)-C(17)-C(18)	115.6(3)	C(21)-P(3)-C(17)-C(18)	-137.9(3)
Cu(3)-P(3)-C(17)-C(18)	-9.2(3)	C(19)-N(2)-C(18)-C(17)	-175.9(2)
P(3)-C(17)-C(18)-N(2)	71.0(3)	C(18)-N(2)-C(19)-C(20)	-177.7(2)
N(2)-C(19)-C(20)-P(4)	-65.7(3)	C(30)-P(4)-C(20)-C(19)	-122.3(2)
C(24)-P(4)-C(20)-C(19)	130.2(2)	Cu(4)-P(4)-C(20)-C(19)	-1.5(3)
C(25)-P(3)-C(21)-C(22)	178.44(19)	C(17)-P(3)-C(21)-C(22)	73.57(19)
Cu(3)-P(3)-C(21)-C(22)	-57.45(19)	C(25)-P(3)-C(21)-C(23)	52.1(2)
C(17)-P(3)-C(21)-C(23)	-52.7(2)	Cu(3)-P(3)-C(21)-C(23)	176.24(19)
C(30)-P(4)-C(24)-C(28)	52.28(19)	C(20)-P(4)-C(24)-C(28)	158.16(18)
Cu(4)-P(4)-C(24)-C(28)	-67.90(18)	C(30)-P(4)-C(24)-C(27)	174.73(16)
C(20)-P(4)-C(24)-C(27)	-79.38(18)	Cu(4)-P(4)-C(24)-C(27)	54.56(17)
C(17)-P(3)-C(25)-C(26)	169.1(2)	C(21)-P(3)-C(25)-C(26)	65.3(2)
Cu(3)-P(3)-C(25)-C(26)	-61.3(2)	C(17)-P(3)-C(25)-C(29)	-68.6(3)
C(21)-P(3)-C(25)-C(29)	-172.5(2)	Cu(3)-P(3)-C(25)-C(29)	60.9(3)
C(20)-P(4)-C(30)-C(31)	74.56(19)	C(24)-P(4)-C(30)-C(31)	179.83(17)
Cu(4)-P(4)-C(30)-C(31)	-54.44(18)	C(20)-P(4)-C(30)-C(32)	-51.4(2)
C(24)-P(4)-C(30)-C(32)	53.9(2)	Cu(4)-P(4)-C(30)-C(32)	179.61(19)

C(37)-P(5)-C(33)-C(34)	-132.94(19)	C(40)-P(5)-C(33)-C(34)	119.8(2)
Cu(7)-P(5)-C(33)-C(34)	-3.2(2)	C(35)-N(3)-C(34)-C(33)	-179.12(18)
P(5)-C(33)-C(34)-N(3)	69.6(2)	C(34)-N(3)-C(35)-C(36)	177.41(18)
N(3)-C(35)-C(36)-P(6)	-69.7(2)	C(43)-P(6)-C(36)-C(35)	131.15(17)
C(46)-P(6)-C(36)-C(35)	-121.67(17)	Cu(8)-P(6)-C(36)-C(35)	3.9(2)
C(40)-P(5)-C(37)-C(39)	-177.14(16)	C(33)-P(5)-C(37)-C(39)	76.23(17)
Cu(7)-P(5)-C(37)-C(39)	-56.00(17)	C(40)-P(5)-C(37)-C(38)	-54.43(17)
C(33)-P(5)-C(37)-C(38)	-161.06(16)	Cu(7)-P(5)-C(37)-C(38)	66.71(16)
C(37)-P(5)-C(40)-C(42)	-50.4(2)	C(33)-P(5)-C(40)-C(42)	54.4(2)
Cu(7)-P(5)-C(40)-C(42)	-175.81(17)	C(37)-P(5)-C(40)-C(41)	-177.46(16)
C(33)-P(5)-C(40)-C(41)	-72.71(18)	Cu(7)-P(5)-C(40)-C(41)	57.09(17)
C(36)-P(6)-C(43)-C(44)	-67.92(18)	C(46)-P(6)-C(43)-C(44)	-173.77(16)
Cu(8)-P(6)-C(43)-C(44)	62.85(18)	C(36)-P(6)-C(43)-C(45)	58.5(2)
C(46)-P(6)-C(43)-C(45)	-47.4(2)	Cu(8)-P(6)-C(43)-C(45)	-170.78(18)
C(36)-P(6)-C(46)-C(47)	-170.23(18)	C(43)-P(6)-C(46)-C(47)	-64.12(19)
Cu(8)-P(6)-C(46)-C(47)	59.98(19)	C(36)-P(6)-C(46)-C(48)	67.60(19)
C(43)-P(6)-C(46)-C(48)	173.71(17)	Cu(8)-P(6)-C(46)-C(48)	-62.19(19)
C(56)-P(7)-C(49)-C(50)	-109.81(18)	C(53)-P(7)-C(49)-C(50)	143.72(16)
Cu(9)-P(7)-C(49)-C(50)	17.73(19)	C(51)-N(4)-C(50)-C(49)	172.91(17)
P(7)-C(49)-C(50)-N(4)	-73.7(2)	C(50)-N(4)-C(51)-C(52)	174.73(17)
N(4)-C(51)-C(52)-P(8)	66.1(2)	C(62)-P(8)-C(52)-C(51)	129.35(19)
C(59)-P(8)-C(52)-C(51)	-123.73(19)	Cu(10)-P(8)-C(52)-C(51)	6.6(2)
C(56)-P(7)-C(53)-C(54)	-170.32(16)	C(49)-P(7)-C(53)-C(54)	-65.95(17)
Cu(9)-P(7)-C(53)-C(54)	65.73(16)	C(56)-P(7)-C(53)-C(55)	-43.8(2)
C(49)-P(7)-C(53)-C(55)	60.6(2)	Cu(9)-P(7)-C(53)-C(55)	-167.77(17)
C(49)-P(7)-C(56)-C(57)	66.9(2)	C(53)-P(7)-C(56)-C(57)	172.87(19)
Cu(9)-P(7)-C(56)-C(57)	-64.8(2)	C(49)-P(7)-C(56)-C(58)	-169.9(2)
C(53)-P(7)-C(56)-C(58)	-63.9(2)	Cu(9)-P(7)-C(56)-C(58)	58.4(2)
C(62)-P(8)-C(59)-C(60)	-54.15(19)	C(52)-P(8)-C(59)-C(60)	-159.99(17)
Cu(10)-P(8)-C(59)-C(60)	68.58(18)	C(62)-P(8)-C(59)-C(61)	-177.28(17)
C(52)-P(8)-C(59)-C(61)	76.88(18)	Cu(10)-P(8)-C(59)-C(61)	-54.55(18)
C(59)-P(8)-C(62)-C(63)	-176.78(18)	C(52)-P(8)-C(62)-C(63)	-72.2(2)
Cu(10)-P(8)-C(62)-C(63)	56.18(19)	C(59)-P(8)-C(62)-C(64)	-49.9(2)
C(52)-P(8)-C(62)-C(64)	54.7(2)	Cu(10)-P(8)-C(62)-C(64)	-176.92(18)
C(77)-C(72)-C(73)-C(74)	-1.0(4)	C(71)-C(72)-C(73)-C(74)	-178.5(3)
C(72)-C(73)-C(74)-C(75)	-1.9(5)	C(73)-C(74)-C(75)-C(76)	2.5(5)
C(74)-C(75)-C(76)-C(77)	-0.3(6)	C(75)-C(76)-C(77)-C(72)	-2.5(6)
C(73)-C(72)-C(77)-C(76)	3.1(6)	C(71)-C(72)-C(77)-C(76)	-179.3(4)