Structured Copper-hydride Nanoclusters Provide Insight into the Surface-vacancy-defect to Non-defect Structural Evolution

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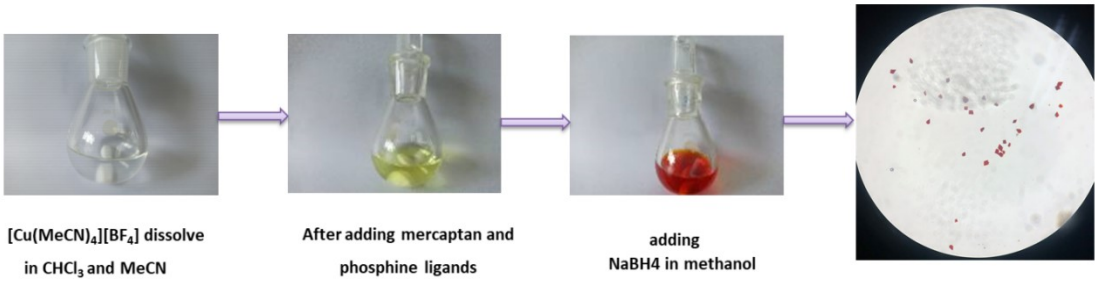

Figure S1. Scheme of the synthetic procedure for **$[Cu_{28}(C_6H_{11}S)_{18}(PPh_2Py)_3(H)_8][BF_4]_2$ nanoclusters (Cu_{28}-PPh_2Py)**

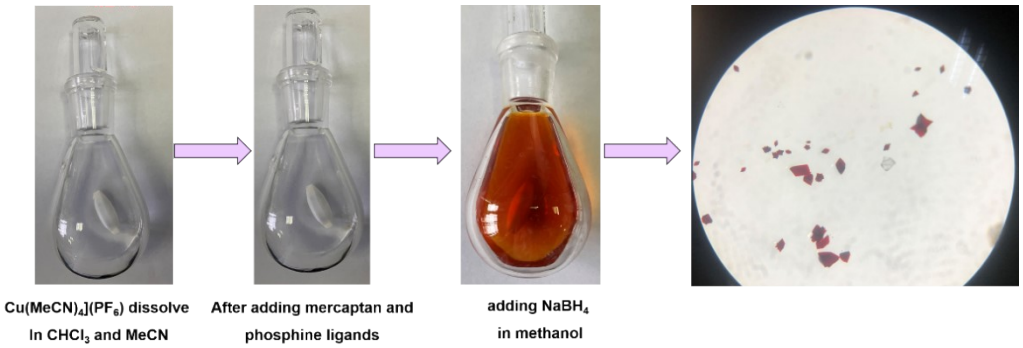

Figure S2. Scheme of the synthetic procedure for **$[Cu_{29}(SAdm)_{15}Cl_3(P(Ph\text{-}Cl)_3)_4H_{10}](PF_6)$(Cu_{29}-$P(Ph\text{-}Cl)_3$)**.

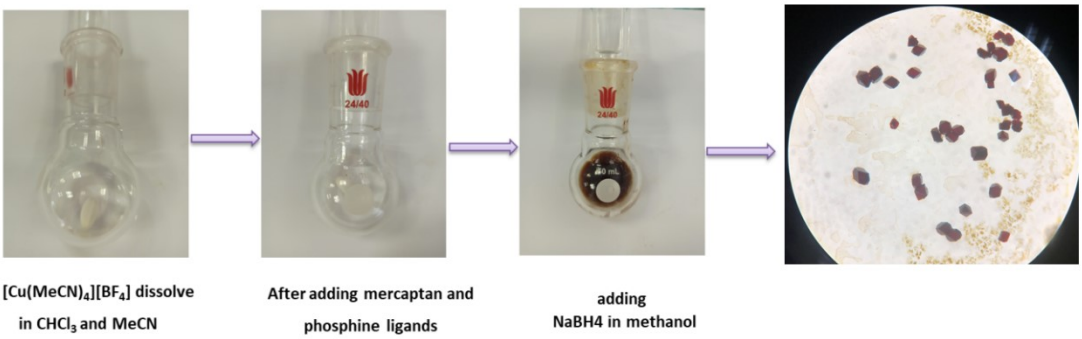

Figure S3. Scheme of the synthetic procedure for **$[Cu_{29}(C_6H_{11})_{18}((Ph\text{-}^pMe)_3P)_4H_{10}]^+$ (Cu_{29}-P(Ph-Me)$_3$)**.

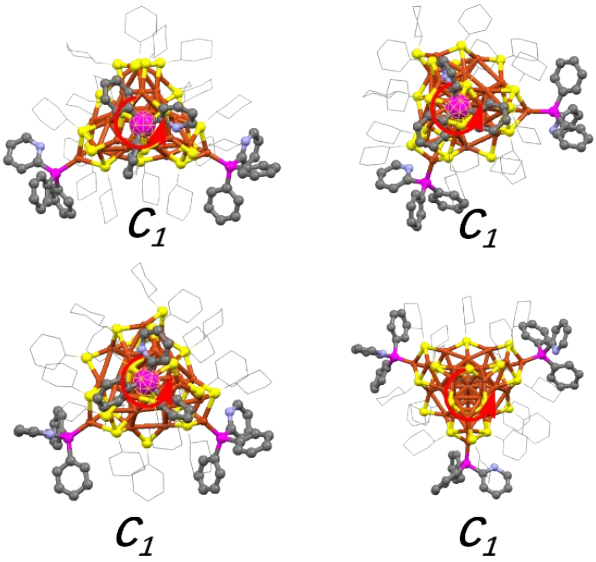

Figure S4. The overall structure of **Cu_{28}-PPh_2Py** exhibits four C_1 symmetry axes.

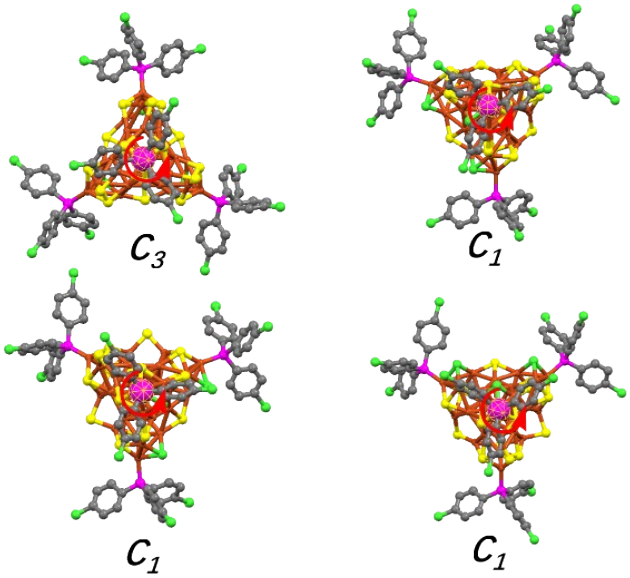

Figure S5. The overall structure of **Cu_{29}-P(Ph-Cl)$_3$** exhibits one C_3 and three C_1 symmetry axes.

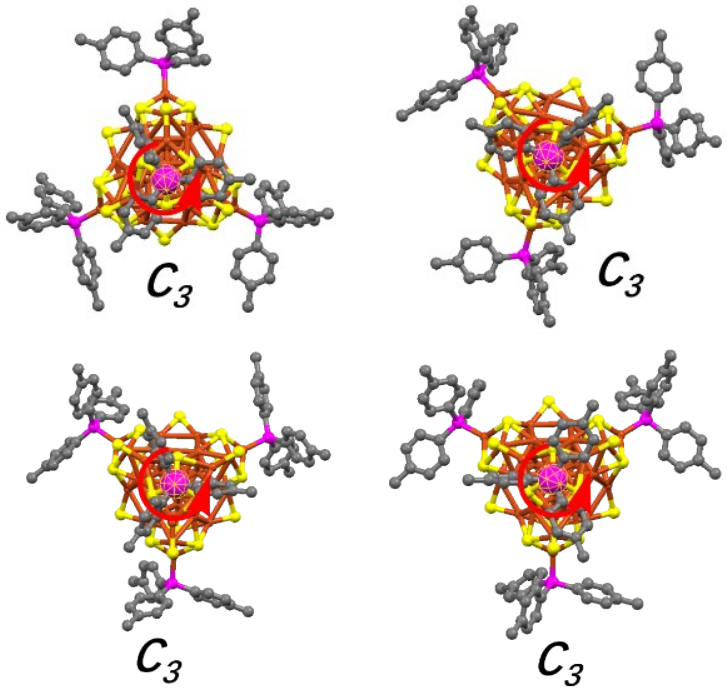

Figure S6. The overall structure of **Cu_{29}-P(Ph-Me)$_3$** exhibits four C_3 symmetry axes.

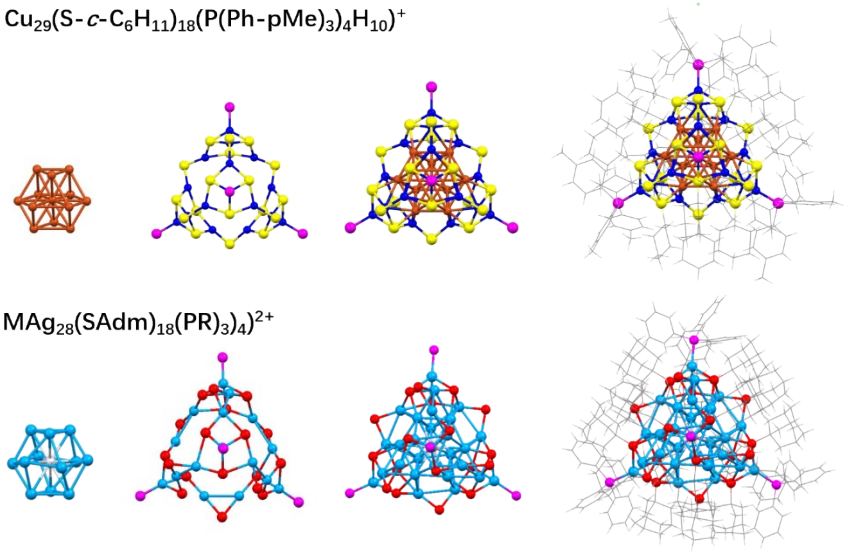

Figure S7. The structural anatomies of $Cu_{29}(S\text{-}c\text{-}C_6H_{11})_{18}(P(Ph\text{-}^pMe)_3)_4$ and $MAg_{28}(S\text{-}c\text{-}C_6H_{11})_{18}(PPh_3)_4$. The H^- in Cu_{29} is not shown. Color label: copper/blue = Cu, sky blue = Ag, yellow/red = S, purple = P, gray = C.

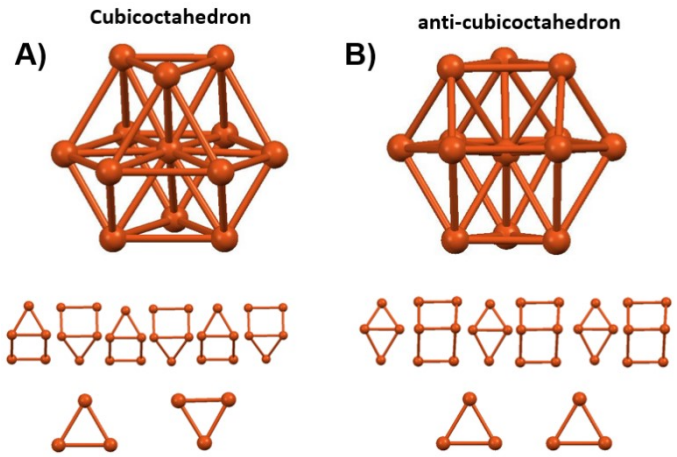

Figure S8. The difference between a cubic octahedron and an anti-cube octahedron Cu_{13}.

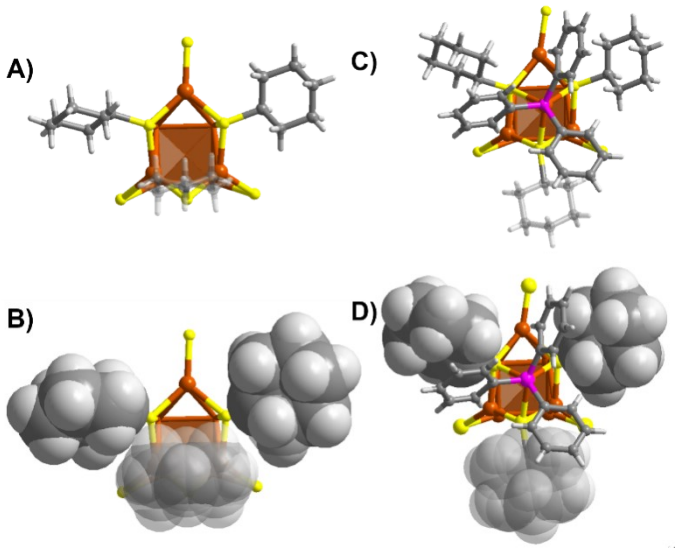

Figure S9. The spatial arrangement of thiol ligands in the Cu_3S_6 ring (Motif 1a in Figure 2), and $Cu_4S_6P_1$ (Motifs 3a/4a in Figure 2).

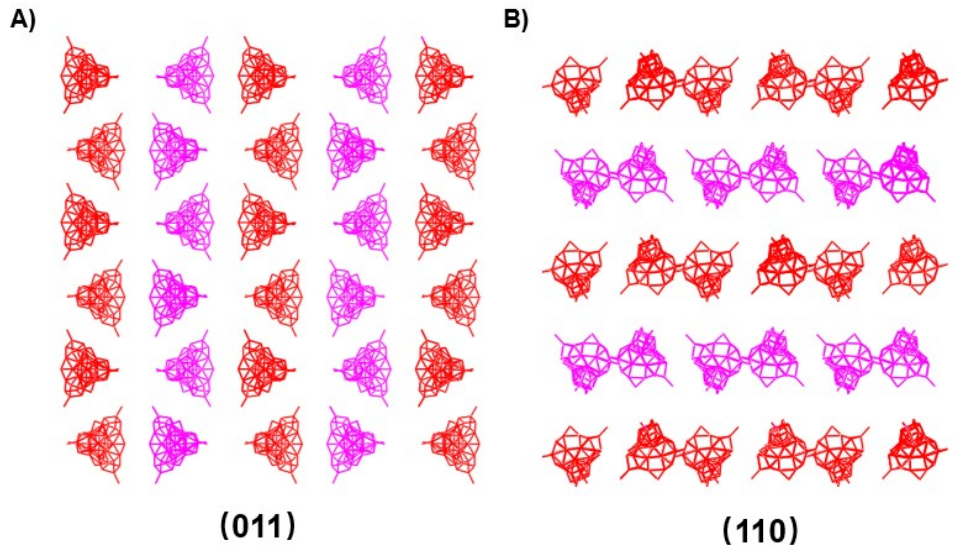

Figure S10. The crystallographic arrangement of $[Cu_{28}(S\text{-}c\text{-}C_6H_{11})_{18}(PPh_2Py)_3H_8]^{2+}$ nanoclusters.

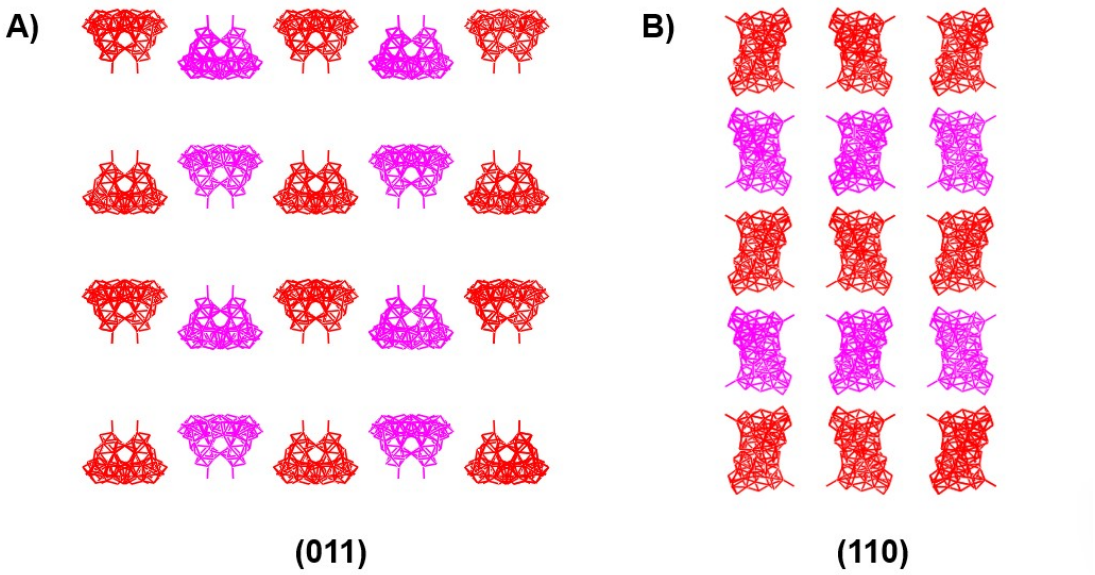

Figure S11. The crystallographic arrangement of $[Cu_{29}(SAdm)_{15}Cl_3(P(Ph\text{-}Cl)_3)_4H_{10}](PF_6)$ nanoclusters.

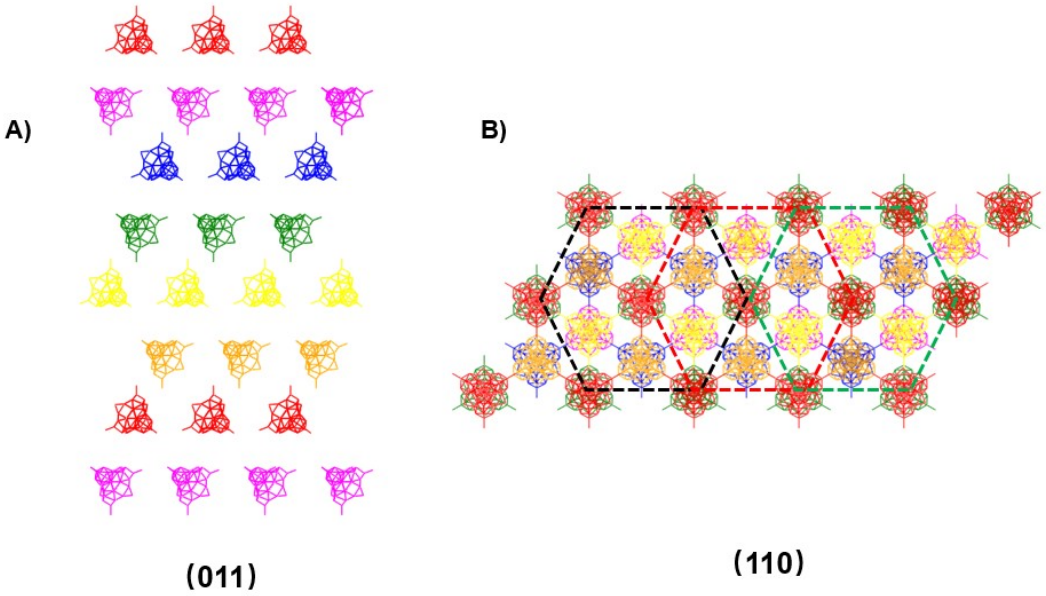

Figure S12. 6HLH crystallographic arrangement of $[Cu_{29}(S\text{-}c\text{-}C_6H_{11})_{18}(P(Ph\text{-}^pMe)_3)_4H_{10}]^+$ nanoclusters.

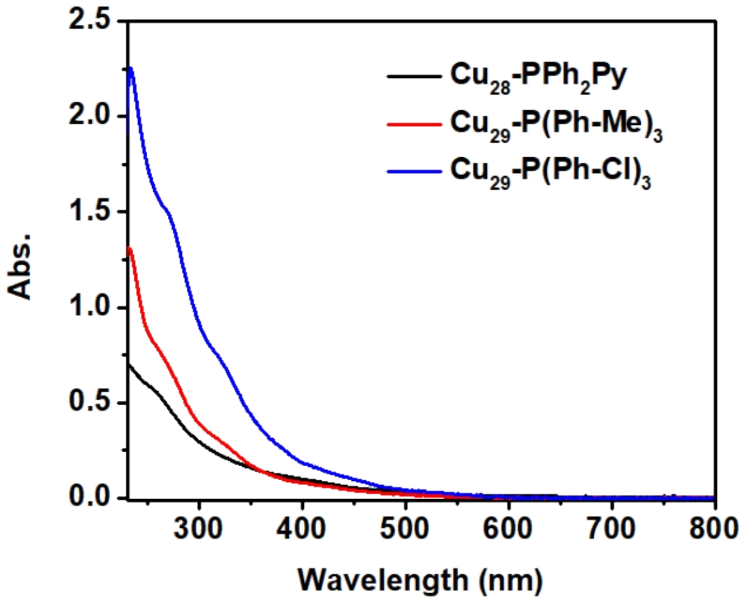

Figure S13. The UV-vis spectra of Cu_{28}-PPh_2Py, Cu_{29}-$P(Ph\text{-}Cl)_3$, and Cu_{29}-$P(Ph\text{-}Me)_3$.

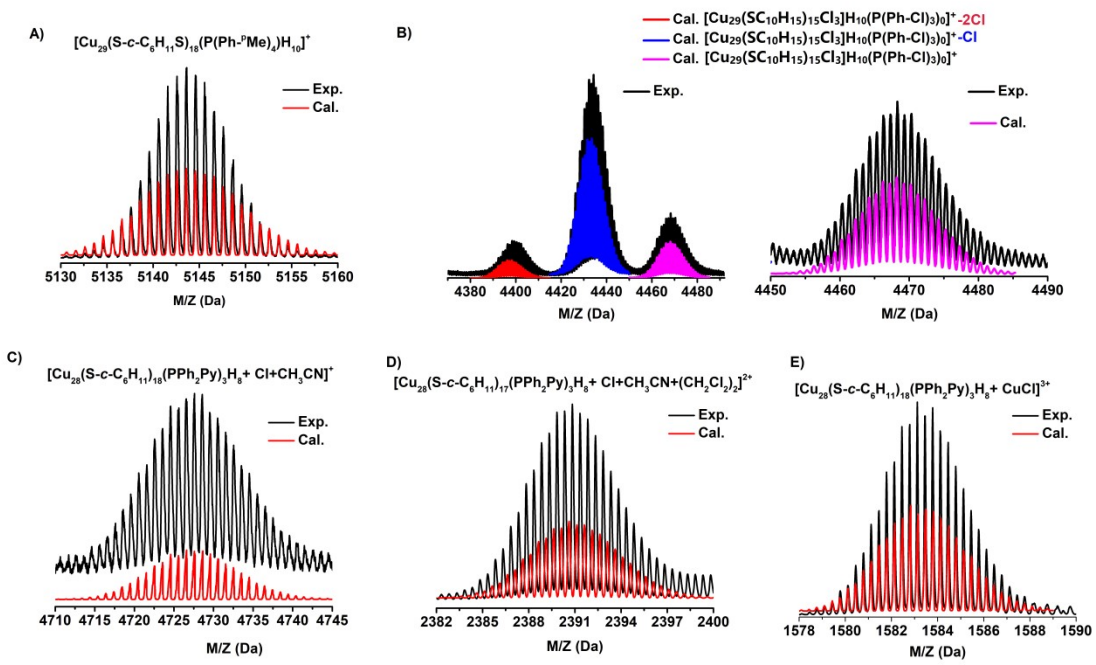

Figure S14. Experimental isotopic patterns with simulated ones.

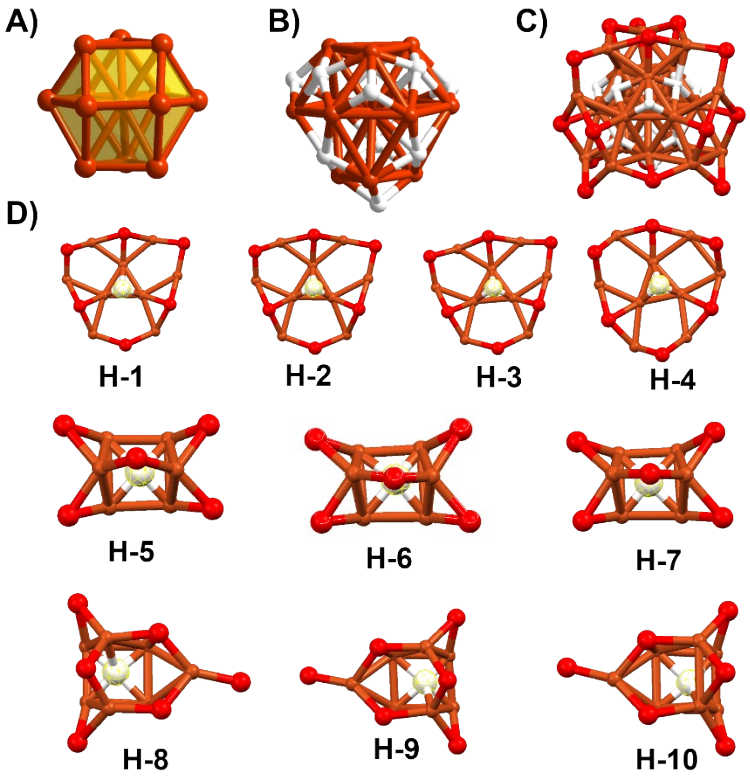

Figure S15. Structural anatomies of $[Cu_{25}(SPhCl_2)_{18}H_{10}]$ and bonding mode around H-.

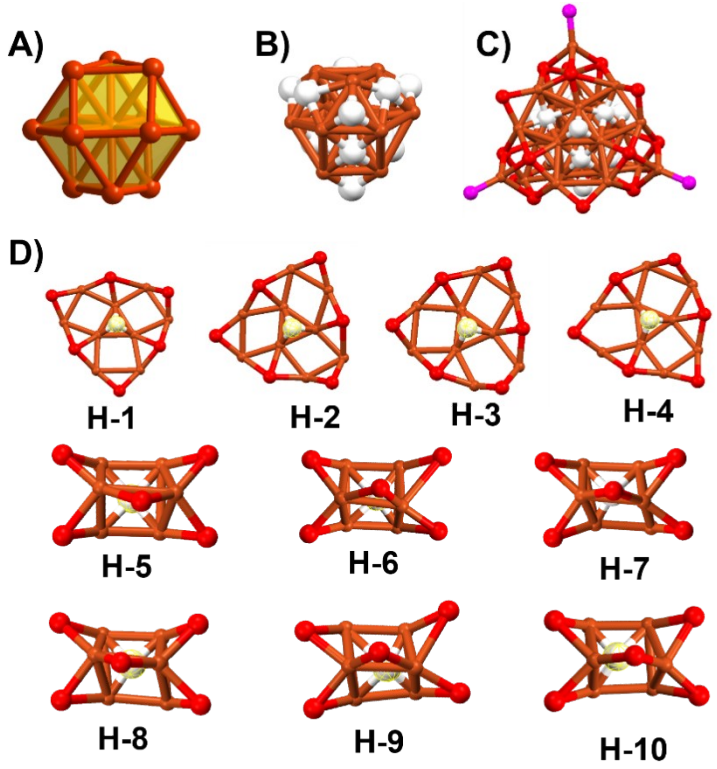

Figure S16. Structural anatomies of **Cu_{29}-P(Ph-Me)$_3$** and bonding mode around H-

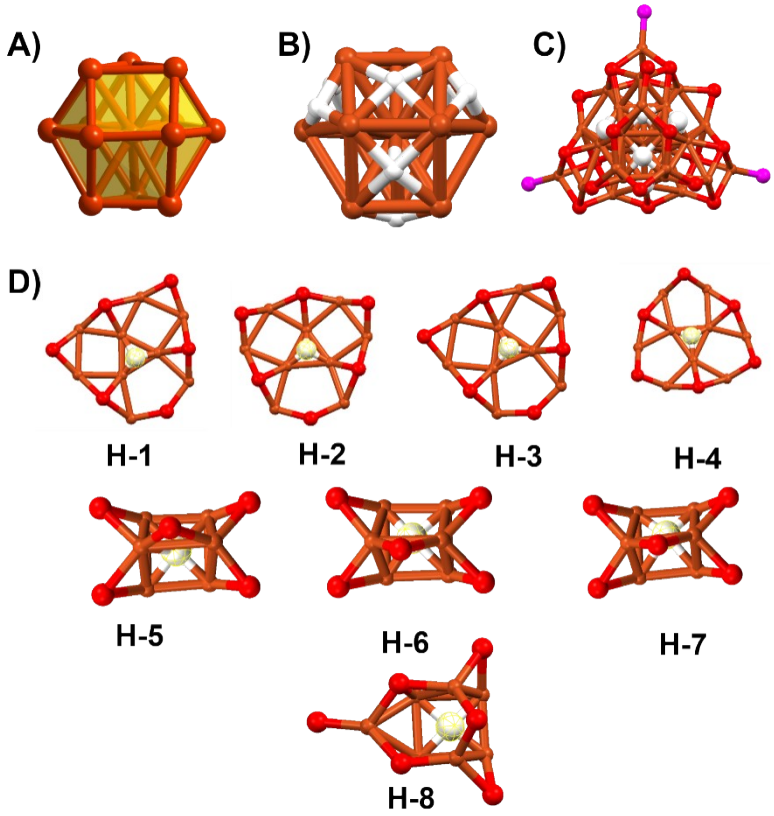

Figure S17. Structural anatomies of **Cu_{28}- PPh$_2$Py** and bonding mode around H-.

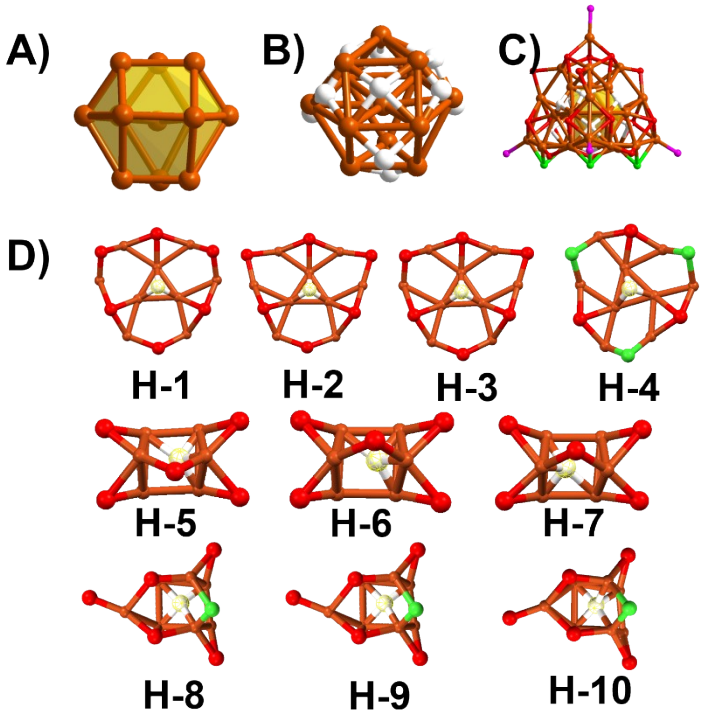

Figure S18. Structural anatomies of **Cu_{29}-P(Ph-Cl)$_3$** and bonding mode around H-.

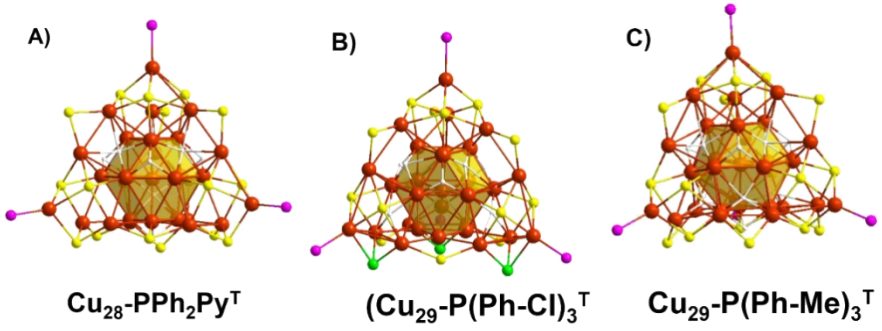

Figure S19. A) Optimized structure of **Cu_{28}-PPh_2Py^T**; B) optimized structure of **Cu_{29}-P(Ph-Cl)$_3^T$**; C) optimized structure of **Cu_{29}-P(Ph-Me)$_3$**. All carbon, hydrogen, and nitrogen atoms on the ligands are omitted. Color label: copper = Cu, yellow = S, purple = P, white = H.

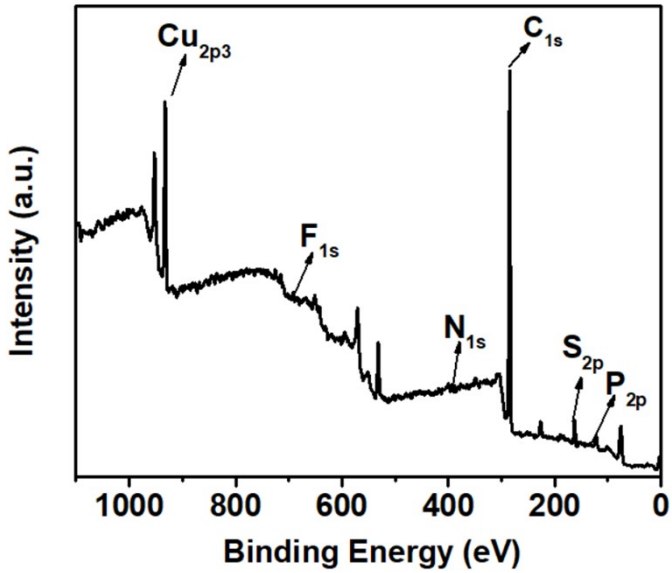

Figure S20. XPS spectra of $[Cu_{28}(S\text{-}c\text{-}C_6H_{11})_{18}(PPh_2Py)_3H_8]^{2+}$.

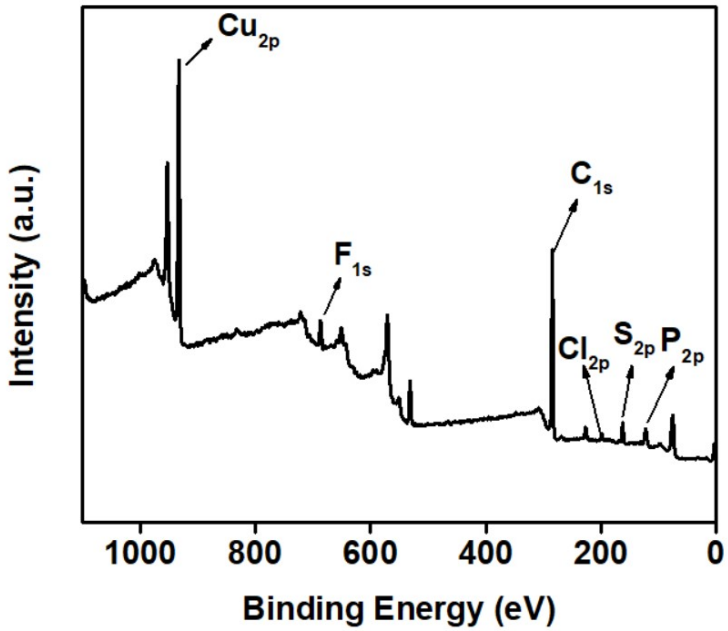

Figure S21. XPS spectra of $[Cu_{29}(SAdm)_{15}Cl_3(P(Ph\text{-}Cl)_3)_4H_{10}](PF_6)$.

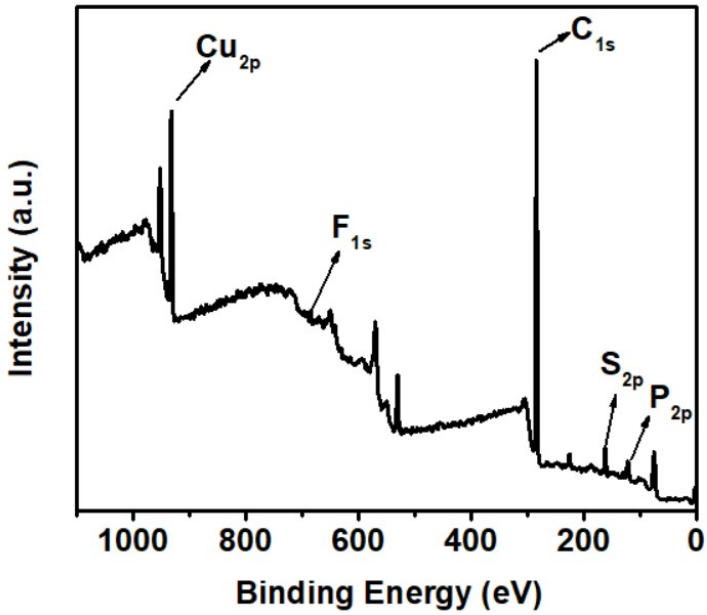

Figure S22. XPS spectra of $[Cu_{29}(S\text{-}c\text{-}C_6H_{11})_{18}(P(Ph\text{-}^pMe)_3)_4H_{10}]^+$.

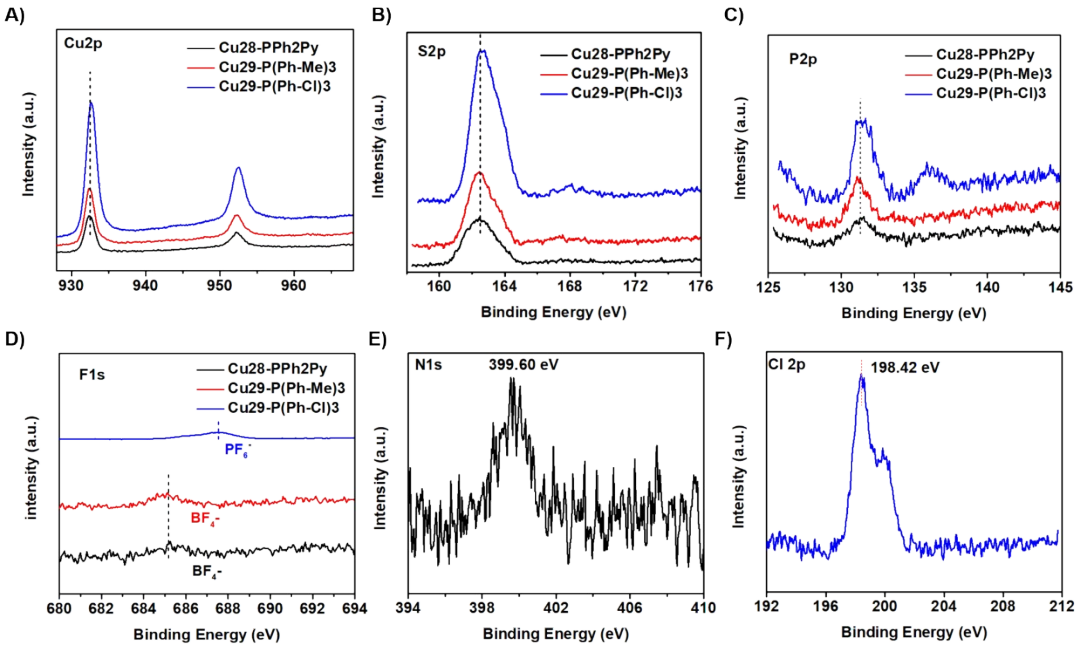

Figure S23. Survey spectrum of $[Cu_{29}(S\text{-}c\text{-}C_6H_{11})_{18}(P(Ph\text{-}^pMe)_3)_4H_{10}](BF_4)$, $[Cu_{29}(SAdm)_{15}Cl_3(P(Ph\text{-}Cl)_3)_4H_{10}](PF_6)$ and $[Cu_{28}(S\text{-}c\text{-}C_6H_{11})_{18}(PPh_2Py)_3H_8](BF_4)_2$. (A-F) High-resolution XPS spectra of Cu2p, S2p, P2p, F1s, N1s and Cl2p.

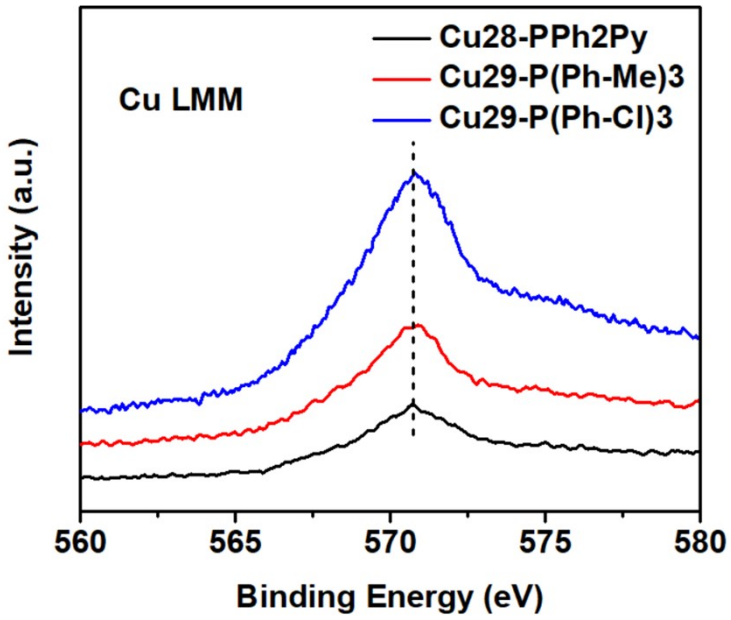

Figure S24. Cu LMM Auger spectrum of $[Cu_{29}(S\text{-}c\text{-}C_6H_{11})_{18}(P(Ph\text{-}^pMe)_3)_4H_{10}](BF_4)$, $[Cu_{29}(SAdm)_{15}Cl_3(P(Ph\text{-}Cl)_3)_4H_{10}](PF_6)$ and $[Cu_{28}(S\text{-}c\text{-}C_6H_{11})_{18}(PPh_2Py)_3H_8](BF_4)_2$.

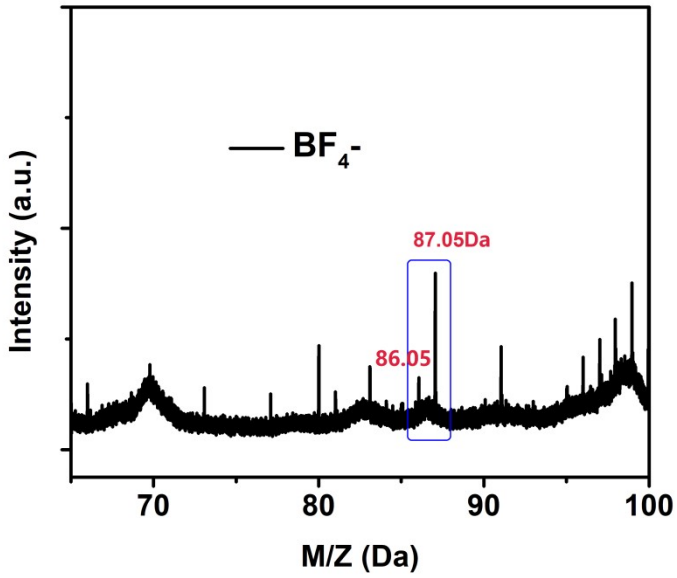

Figure S25. ESI-MS result of the BF_4- counterion in $[Cu_{28}(S\text{-}c\text{-}C_6H_{11})_{18}(PPh_2Py)_3H_8](BF_4)_2$. This suggests that the Cu_{28}- PPh_2py contains counter ions BF_4^-, although it was not observed in the crystal structure.

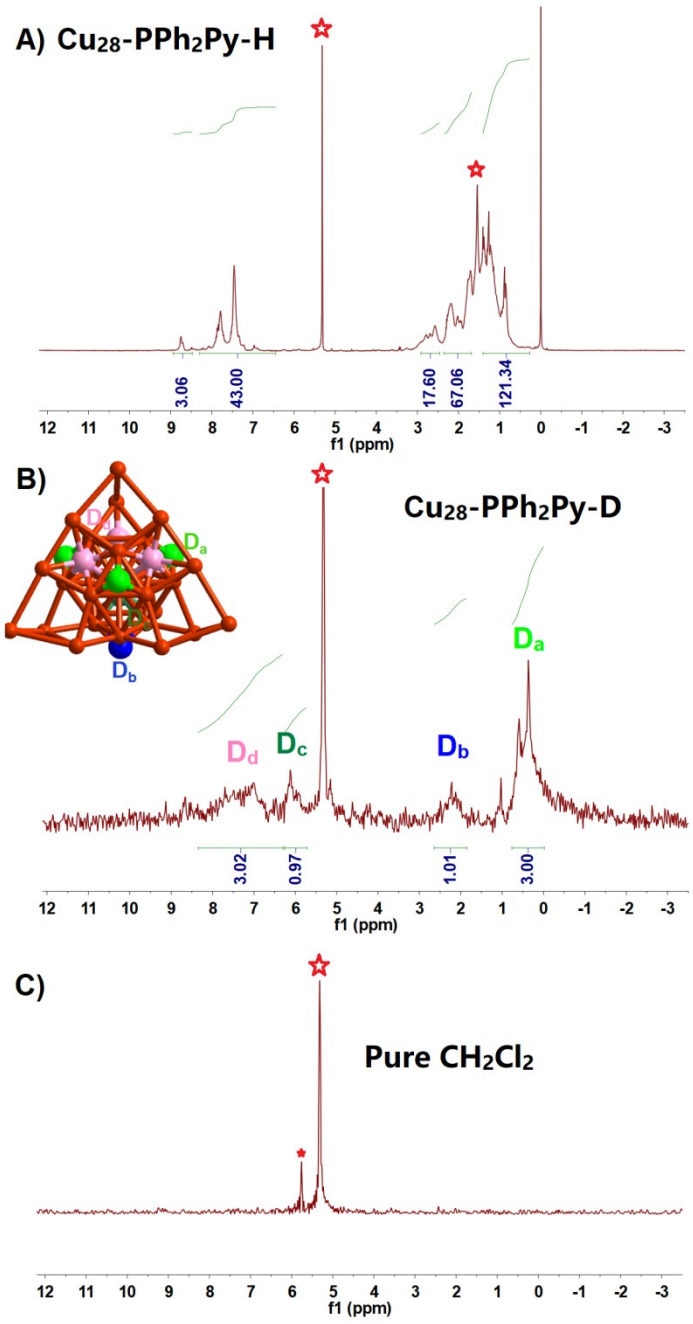

Figure S26. A) The ^{1}H-NMR of Cu_{28}-PPh_2Py-H dissolved in CD_2Cl_2. B) The ^{2}H-NMR of Cu_{28}-PPh_2Py-D dissolved in CH_2Cl_2. C) The ^{2}H-NMR of pure CH_2Cl_2, which is for calibration. Asterisked peaks are solvent peaks (5.32 ppm for CH_2Cl_2, and 1.54 ppm for H_2O). The inset in Figure S26B is optimized geometry of the Cu_{28}-PPh_2Py obtained from DFT (ligands not shown); the four different D (or H) atoms, viz., D_a, D_b, D_c, and D_d shown in pale green, blue, green and dark pink, respectively. Cu atoms are shown in brown. Three D_a (or H_a shown by the pale green sphere) cap the three Cu triangles on the top half of the core and one D_b (or H_b shown by the blue sphere)) caps the downward-facing Cu triangle (Cu_3) in the core. Three D_d (or H_d) covering the three Cu quadrilateral (Cu_4) on the top half of the core and one D_c (or H_c) are encapsulated in trigonal prismatic (tp) cages.

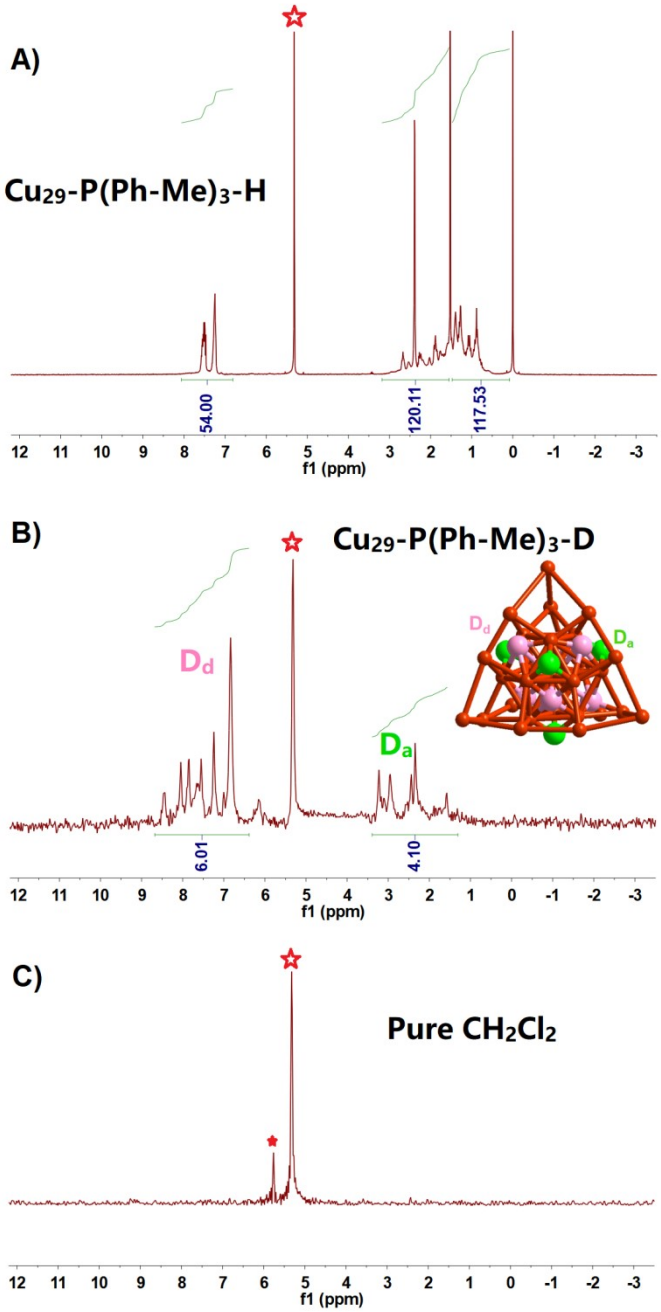

Figure S27. A) The ^{1}H-NMR of Cu_{29}-P(Ph-Me)-H dissolved in CD_2Cl_2. B) The ^{2}H-NMR of Cu_{28}-P(Ph-Me)-D dissolved in CH_2Cl_2. C) The ^{2}H-NMR of pure CH_2Cl_2, which is for calibration. Asterisked peaks are solvent peaks (5.32 ppm for CH_2Cl_2, and 1.54 ppm for H_2O). The inset in Figure S27B is optimized geometry of theCu_{29}-P(Ph-Me) obtained from DFT (ligands not shown); the two different D (or H) atoms, viz., D_a, D_d shown in pale green and dark pink, respectively. Cu atoms are shown in brown. Four D_a (or H_a shown by the pale green sphere) cap the four Cu triangles of the core. Six D_d (or H_d) covering the six Cu quadrilateral (Cu_4) of the core are encapsulated in trigonal prismatic (tp) cages.

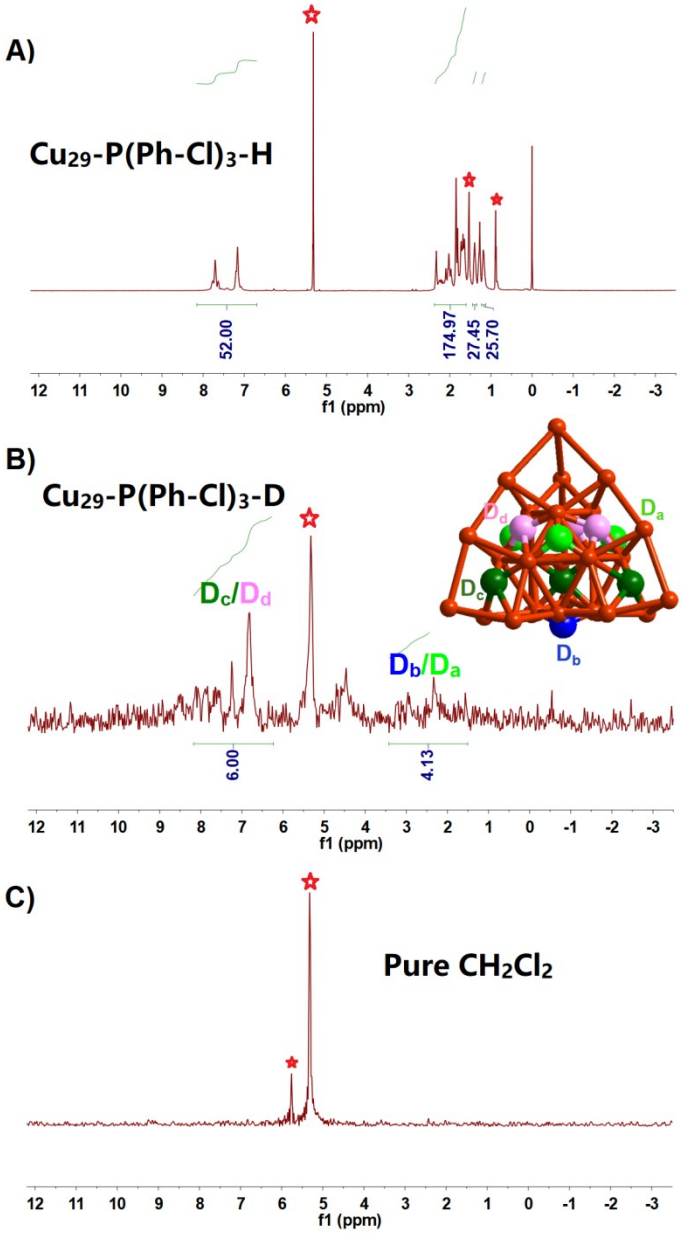

Figure S28. A) The ^{1}H-NMR of Cu_{29}-P(Ph-Cl)-H dissolved in CD_2Cl_2. B) The ^{2}H-NMR of Cu_{2P}-P(Ph-Cl)-D dissolved in CH_2Cl_2. C) The ^{2}H-NMR of pure CH_2Cl_2, which is for calibration. Asterisked peaks are solvent peaks (5.32 ppm for CH_2Cl_2, 0.89 and 1.27 ppm for n-hexane, which comes from the solvent in the crystal culture process).The inset in Figure S28B is optimized geometry of the Cu_{29}-P(Ph-Cl) obtained from DFT (ligands not shown); the four different D (or H) atoms, viz., D_a, D_b, D_c, and D_d shown in pale green, blue, green and dark pink, respectively. Cu atoms are shown in brown. Three D_a (or H_a shown by the pale green sphere) cap the three Cu triangles on the top half of the core and one D_b (or H_b shown by the blue sphere) caps the downward-facing Cu triangle (Cu_3) in the core. Three D_d (or H_d) covering the three Cu quadrilateral (Cu_4) on the top half of the core and three D_c (or H_c) are encapsulated in trigonal prismatic (tp) cages.

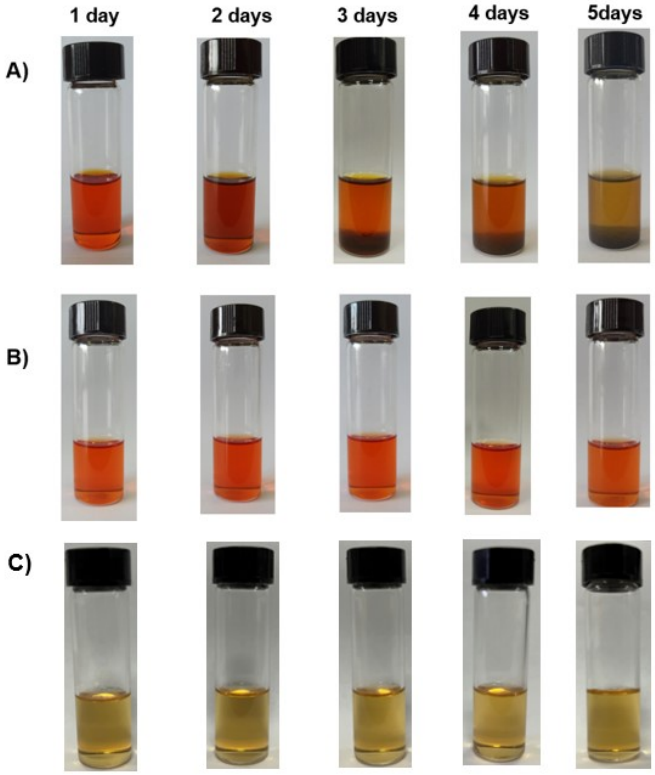

Figure S29. The stability of A) Cu_{28}-PPh_2Py, B) Cu_{29}-$P(Ph\text{-}Me)_3$, and C) Cu_{29}-$P(Ph\text{-}Cl)_3$ in the CH_2Cl_2 solution at room temperature.

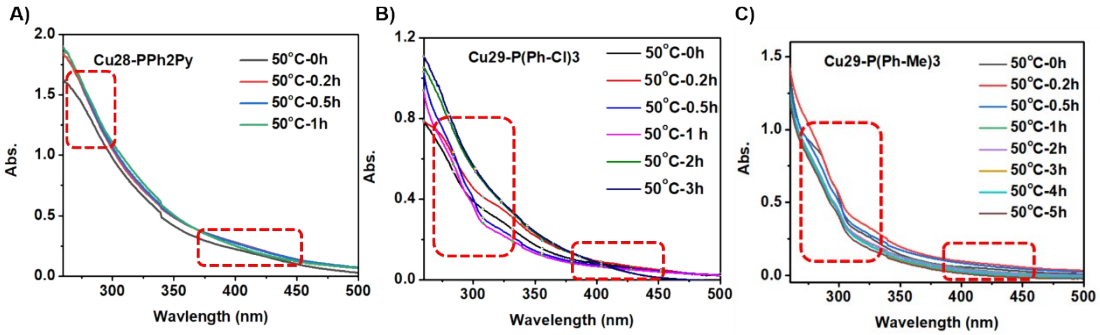

Figure S30. Time-dependent UV-vis spectra of A) Cu_{28}-PPh_2Py, B) Cu_{29}-$P(Ph\text{-}Cl)_3$, and C) Cu_{29}-$P(Ph\text{-}Me)_3$ in the $CHCl_3$ solution under a 50°C oil bath.

Table S1. Crystal data and structure refinement for Cu_{28}-PPh_2Py.

Empirical formula	$C_{159.5}H_{238.3}ClCu_{28}N_3P_3S_{18}$
Formula weight	4682.38
Temperature/K	150(2)
Crystal system	monoclinic
Space group	$P2_1/a$

a/Å	22.8639(13)
b/Å	32.229(2)
c/Å	26.6451(15)
α/°	90
β/°	90.576(5)
γ/°	90
Volume/Å^3	19633(2)
Z	4
Radiation	CuKα (λ = 1.54186)
Index ranges	-14 ≤ h ≤ 26, -37 ≤ k ≤ 31, -30 ≤ l ≤ 30
Reflections collected	110149
Independent reflections	31015 [R_{int} = 0.0269, R_{sigma} = 0.0322]
Final R indexes [I>=2σ (I)]	R_1 = 0.0846, wR_2 = 0.2320
Final R indexes [all data]	R_1 = 0.1018, wR_2 = 0.2434
Largest diff. peak/hole / e Å^{-3}	4.39/-2.71

Table S2. Crystal data and structure refinement for Cu_{29}-P(Ph-Cl)$_3$.

Empirical formula	$C_{226}H_{283}Cl_{15}Cu_{29}F_6OP_5S_{15}$
Formula weight	6139.67
Temperature/K	150(2)
Crystal system	monoclinic
Space group	I2/a
a/Å	36.1154(13)
b/Å	34.7927(17)
c/Å	50.324(2)
α /°	90
β /°	102.424(3)
γ /°	90
Volume/Å^3	61754(5)
Z	8
Radiation	CuKα (λ = 1.54186)
Index ranges	-41 ⩽ h ⩽ 17, -40 ⩽ k ⩽ 40, -56 ⩽ l ⩽ 59
Reflections collected	193152
Independent reflections	52172 [R_{int} = 0.1402, R_{sigma} = 0.0991]
Final R indexes [I>=2 σ (I)]	R_1 = 0.1162, wR_2 = 0.3023
Final R indexes [all data]	R_1 = 0.1599, wR_2 = 0.3282
Largest diff. peak/hole / e Å^{-3}	1.70/-1.78

Table S3. Crystal data and structure refinement for Cu_{29}-Ph-^{p}Me.

Empirical formula	$C_{192}H_{282}BCu_{29}F_4P_4S_{18}$
Formula weight	5220.59
Temperature/K	150(2)
Crystal system	trigonal
Space group	R-3
a/Å	21.191(2)
b/Å	21.191(2)
c/Å	90.410(6)
α /°	90
β /°	90
γ /°	120
Volume/Å^3	35160(7)
Z	6
Radiation	CuK α (λ = 1.54186)
Index ranges	-21 ⩽ h ⩽ 23, -24 ⩽ k ⩽ 25, -75 ⩽ l ⩽ 109
Reflections collected	34835
Independent reflections	14265 [R_{int} = 0.0046, R_{sigma} = 0.0618]
Final R indexes [I>=2 σ (I)]	R_1 = 0.0569, wR_2 = 0.1275
Final R indexes [all data]	R_1 = 0.0798, wR_2 = 0.1327
Largest diff. peak/hole / e Å^{-3}	1.05/-0.49

Table S4. The average value of Cu-H and Cu-Cu bond length in cuboctahedron core. Cu-H^{ave} represents the average value of Cu-H. The Cu-Cu^{ave} represents the average value of Cu-Cu.

	Cu-H^{ave}	**Cu-Cu^{ave}**
Cu_{25}	1.835	2.598
Cu_{29}-P(Ph-Me)$_3$	/	2.716
Cu_{29}-P(Ph-Me)$_3^T$	1.918	2.635
Cu_{28}-PPh_2Py	/	2.605
Cu_{28}-PPh_2Py ^{T}	1.848	2.641
Cu_{29}-P(Ph-Cl)$_3$	/	2.617
Cu_{29}-P(Ph-Cl)$_3^T$	1.928	2.659

Table S5. The coordinate of the optimized geometry of Cu_{28}-PPh_2Py^T

Cu	6.718000	1.178000	6.680000
Cu	8.737000	2.183000	7.938000
Cu	5.709000	-0.812000	8.079000
Cu	8.839000	2.082000	5.462000
Cu	5.116000	2.677000	5.217000
Cu	5.852000	-0.933000	5.407000
Cu	6.740000	0.964000	4.032000
Cu	8.202000	-0.448000	8.185000
Cu	4.944000	2.786000	7.832000
Cu	6.474000	1.187000	9.317000
Cu	8.333000	-0.552000	5.424000
Cu	4.163000	0.823000	6.559000
Cu	7.253000	3.747000	6.562000
Cu	10.696000	0.470000	8.250000
Cu	10.752000	0.289000	5.241000
Cu	4.030000	1.867000	10.172000
Cu	6.286000	4.957000	4.400000
Cu	8.813000	-2.734000	7.009000
Cu	3.407000	-0.628000	4.487000
Cu	3.216000	-0.378000	8.749000
Cu	8.068000	3.031000	10.320000
Cu	8.350000	2.937000	3.021000
Cu	4.431000	1.455000	2.827000
Cu	6.091000	5.009000	8.535000
S	6.108000	2.180000	11.356000
Cu	5.804000	3.913000	1.147000
Cu	5.474000	4.511000	11.764000
S	4.488000	3.821000	3.345000
S	10.042000	-1.715000	8.694000
S	4.183000	4.131000	9.571000
S	6.577000	1.759000	1.892000
S	6.344000	5.870000	6.455000
S	10.047000	2.075000	9.810000
Cu	6.069000	-3.111000	6.926000
S	12.357000	0.731000	6.758000
S	10.246000	1.900000	3.657000
S	2.555000	0.313000	10.776000
S	7.334000	5.192000	10.426000
S	10.160000	-1.935000	5.260000
P	5.133000	4.801000	-0.790000
S	4.241000	-2.568000	8.413000

S	2.253000	-0.459000	6.623000
P	4.856000	5.544000	13.639000
S	7.511000	4.991000	2.483000
S	2.535000	0.311000	2.654000
S	4.388000	-2.682000	5.038000
P	1.082000	-4.555000	6.641000
C	11.364000	4.274000	8.550000
H	10.371000	4.724000	8.379000
H	11.565000	3.603000	7.694000
C	9.563000	5.935000	0.835000
H	8.882000	5.748000	-0.016000
H	10.086000	4.985000	1.036000
C	4.233000	-3.478000	10.047000
H	4.609000	-4.478000	9.776000
C	4.389000	7.124000	0.592000
H	5.003000	6.708000	1.398000
C	8.018000	7.673000	1.823000
H	7.292000	7.550000	0.997000
H	7.437000	7.953000	2.721000
C	5.028000	7.372000	13.527000
C	11.338000	3.439000	9.824000
H	11.023000	4.073000	10.672000
C	3.184000	5.327000	14.375000
C	12.451000	5.356000	8.621000
H	12.195000	6.085000	9.416000
H	12.470000	5.922000	7.671000
C	14.175000	-1.038000	5.595000
H	14.817000	-0.149000	5.437000
H	13.494000	-1.101000	4.725000
C	4.062000	3.869000	-1.956000
C	6.596000	5.237000	-1.843000
C	9.874000	8.388000	0.247000
H	9.223000	8.322000	-0.647000
H	10.622000	9.174000	0.035000
C	4.235000	6.400000	-0.604000
C	13.793000	3.908000	10.196000
H	14.776000	3.433000	10.374000
H	13.605000	4.573000	11.064000
C	10.566000	-4.241000	3.796000
H	11.635000	-4.119000	4.064000
H	10.081000	-4.781000	4.627000
C	1.952000	4.400000	2.363000
H	2.458000	4.992000	1.576000

H	1.923000	3.350000	2.024000
C	8.730000	6.338000	2.053000
H	9.390000	6.423000	2.935000
C	6.439000	0.918000	12.701000
H	6.381000	-0.055000	12.183000
C	6.890000	6.540000	-2.270000
H	6.237000	7.376000	-2.005000
C	12.706000	2.823000	10.136000
H	12.664000	2.264000	11.090000
H	12.955000	2.095000	9.342000
C	2.766000	4.498000	3.655000
H	2.337000	3.821000	4.411000
N	7.369000	4.174000	-2.144000
C	5.177000	-2.833000	11.059000
H	6.195000	-2.760000	10.638000
H	4.836000	-1.798000	11.251000
C	8.570000	6.567000	10.670000
H	9.245000	6.502000	9.796000
C	8.033000	6.741000	-3.052000
H	8.289000	7.746000	-3.404000
C	13.826000	4.747000	8.914000
H	14.126000	4.104000	8.063000
H	14.589000	5.542000	8.996000
C	7.830000	1.100000	13.306000
H	8.600000	1.001000	12.520000
H	7.912000	2.125000	13.714000
C	3.073000	6.573000	8.744000
H	3.826000	6.619000	7.939000
H	3.548000	6.991000	9.652000
C	11.753000	3.013000	3.792000
H	12.419000	2.432000	4.454000
C	10.567000	7.039000	0.465000
H	11.314000	7.139000	1.276000
H	11.128000	6.739000	-0.440000
C	9.024000	8.778000	1.460000
H	8.485000	9.724000	1.271000
H	9.688000	8.965000	2.327000
C	2.950000	8.878000	-0.263000
H	2.447000	9.841000	-0.129000
C	0.529000	4.945000	2.569000
H	-0.019000	4.905000	1.609000
H	-0.018000	4.287000	3.271000
C	2.813000	-3.614000	10.595000

H	2.398000	-2.605000	10.777000
H	2.168000	-4.112000	9.850000
C	11.493000	4.374000	4.421000
H	10.755000	4.922000	3.806000
H	11.044000	4.247000	5.420000
C	-0.214000	-0.055000	10.609000
H	-0.053000	-0.620000	9.676000
H	-0.072000	-0.771000	11.442000
C	1.592000	5.003000	10.072000
H	1.995000	5.349000	11.044000
H	1.312000	3.946000	10.207000
C	3.773000	-3.797000	12.939000
H	3.800000	-4.415000	13.856000
H	3.385000	-2.803000	13.239000
C	9.875000	-2.040000	10.530000
H	9.153000	-1.300000	10.918000
C	11.054000	-4.279000	1.305000
H	10.915000	-4.848000	0.368000
H	12.148000	-4.184000	1.456000
C	13.353000	-0.839000	6.872000
H	12.624000	-1.661000	6.972000
C	2.803000	5.924000	4.207000
H	3.340000	6.573000	3.489000
H	3.369000	5.950000	5.155000
C	5.339000	1.005000	13.759000
H	5.342000	2.025000	14.191000
H	4.351000	0.846000	13.291000
C	9.368000	6.337000	11.957000
H	8.662000	6.289000	12.806000
H	9.872000	5.355000	11.915000
C	7.359000	0.576000	0.665000
H	7.753000	-0.249000	1.286000
C	5.183000	10.167000	13.240000
H	5.241000	11.256000	13.136000
C	8.831000	5.645000	-3.380000
H	9.730000	5.759000	-3.993000
C	-0.242000	-0.107000	5.392000
H	-0.356000	-1.202000	5.474000
H	0.288000	0.090000	4.442000
C	0.841000	1.049000	10.727000
H	0.784000	1.705000	9.841000
C	3.753000	8.359000	0.758000
H	3.884000	8.915000	1.692000

C	5.774000	-3.287000	2.669000
H	5.650000	-2.226000	2.386000
H	6.689000	-3.346000	3.286000
C	6.974000	0.141000	15.498000
H	7.144000	-0.634000	16.269000
H	7.031000	1.119000	16.017000
C	1.590000	-1.994000	1.396000
H	0.594000	-1.509000	1.418000
H	1.703000	-2.515000	2.363000
C	2.828000	-4.418000	11.906000
H	3.145000	-5.458000	11.691000
H	1.801000	-4.483000	12.309000
C	5.895000	8.121000	14.338000
H	6.512000	7.624000	15.094000
C	5.187000	-3.632000	12.371000
H	5.844000	-3.130000	13.105000
H	5.632000	-4.631000	12.188000
C	9.352000	-3.452000	10.783000
H	10.022000	-4.178000	10.283000
H	8.357000	-3.570000	10.321000
C	2.688000	5.117000	9.014000
H	2.359000	4.637000	8.075000
C	8.065000	0.072000	14.425000
H	9.063000	0.234000	14.873000
H	8.083000	-0.944000	13.987000
C	9.938000	-2.852000	3.646000
H	8.851000	-2.950000	3.494000
C	4.285000	3.832000	-3.345000
H	5.171000	4.304000	-3.777000
C	3.420000	6.926000	-1.624000
H	3.272000	6.365000	-2.552000
C	9.029000	6.793000	6.097000
H	8.921000	6.590000	5.017000
H	9.371000	5.853000	6.560000
C	0.756000	1.942000	6.504000
H	1.323000	2.209000	5.594000
H	1.355000	2.290000	7.365000
C	5.582000	-0.020000	14.879000
H	4.797000	0.086000	15.651000
H	5.475000	-1.042000	14.467000
C	8.455000	4.383000	-2.901000
H	9.056000	3.494000	-3.132000
C	1.374000	6.457000	4.409000

H	0.873000	5.863000	5.199000
H	1.416000	7.497000	4.780000
C	7.668000	7.184000	6.659000
H	7.744000	7.288000	7.754000
C	12.397000	3.132000	2.409000
H	11.694000	3.639000	1.722000
H	12.588000	2.127000	1.988000
C	-0.620000	2.628000	6.478000
H	-0.484000	3.723000	6.401000
H	-1.138000	2.447000	7.441000
C	2.920000	3.241000	-1.429000
H	2.745000	3.246000	-0.347000
C	12.803000	5.174000	4.514000
H	12.601000	6.174000	4.942000
H	13.485000	4.666000	5.223000
C	10.448000	-5.040000	2.488000
H	10.939000	-6.023000	2.612000
H	9.379000	-5.249000	2.286000
C	2.512000	-0.184000	-0.090000
H	3.291000	0.589000	-0.191000
H	1.537000	0.343000	-0.093000
C	14.245000	-0.798000	8.117000
H	13.616000	-0.695000	9.020000
H	14.892000	0.100000	8.069000
C	1.656000	-2.985000	0.222000
H	0.866000	-3.751000	0.329000
H	2.622000	-3.529000	0.259000
N	7.277000	4.968000	14.667000
H	6.941000	-0.487000	9.340000
C	8.498000	1.283000	-0.070000
H	9.263000	1.615000	0.655000
H	8.094000	2.186000	-0.564000
C	2.660000	-0.909000	1.250000
H	3.659000	-1.372000	1.307000
C	13.489000	5.305000	3.149000
H	12.861000	5.928000	2.484000
H	14.454000	5.834000	3.255000
C	9.295000	-3.762000	12.287000
H	8.944000	-4.800000	12.437000
H	8.542000	-3.106000	12.767000
C	13.706000	3.934000	2.500000
H	14.440000	3.358000	3.098000
H	14.145000	4.048000	1.491000

C	5.988000	5.088000	15.038000
C	10.438000	-2.882000	1.172000
H	9.368000	-2.980000	0.897000
H	10.921000	-2.321000	0.351000
C	10.552000	-2.078000	2.478000
H	11.620000	-1.885000	2.702000
H	10.066000	-1.091000	2.376000
C	9.124000	0.356000	-1.125000
H	9.917000	0.905000	-1.668000
H	9.623000	-0.494000	-0.622000
C	7.158000	8.500000	6.067000
H	6.183000	8.769000	6.513000
H	6.987000	8.365000	4.982000
C	0.363000	5.843000	9.692000
H	-0.394000	5.766000	10.495000
H	-0.104000	5.417000	8.781000
C	15.118000	-2.059000	8.209000
H	15.780000	-1.992000	9.093000
H	14.465000	-2.940000	8.372000
C	7.878000	7.934000	10.685000
H	7.319000	8.091000	9.746000
H	7.136000	7.951000	11.503000
C	11.241000	-1.817000	11.187000
H	11.569000	-0.775000	11.023000
H	11.986000	-2.469000	10.691000
C	15.943000	-2.269000	6.934000
H	16.531000	-3.201000	7.006000
H	16.675000	-1.442000	6.833000
C	8.184000	9.623000	6.297000
H	7.822000	10.560000	5.833000
H	8.264000	9.823000	7.384000
C	-1.638000	0.524000	10.657000
H	-1.809000	1.150000	9.758000
H	-2.377000	-0.295000	10.611000
C	-1.869000	1.366000	11.915000
H	-2.882000	1.809000	11.902000
H	-1.825000	0.708000	12.806000
C	15.046000	-2.298000	5.691000
H	15.657000	-2.401000	4.775000
H	14.389000	-3.190000	5.733000
C	2.782000	8.157000	-1.452000
H	2.146000	8.552000	-2.250000
C	2.224000	2.585000	-3.657000

H	1.505000	2.091000	-4.320000
C	2.001000	2.614000	-2.275000
H	1.111000	2.139000	-1.849000
C	2.503000	6.373000	15.027000
H	2.934000	7.378000	15.050000
C	0.600000	0.424000	6.553000
H	0.126000	0.137000	7.509000
C	0.714000	4.848000	15.626000
H	-0.249000	4.663000	16.114000
C	8.071000	-0.178000	-2.102000
H	8.536000	-0.869000	-2.829000
H	7.654000	0.666000	-2.686000
C	8.905000	9.058000	10.894000
H	8.385000	10.033000	10.929000
H	9.588000	9.097000	10.021000
C	1.838000	7.411000	8.376000
H	2.139000	8.466000	8.229000
H	1.439000	7.065000	7.403000
C	11.192000	-2.137000	12.689000
H	12.201000	-2.016000	13.125000
H	10.542000	-1.397000	13.198000
C	-1.618000	0.581000	5.378000
H	-2.204000	0.212000	4.516000
H	-2.183000	0.291000	6.286000
C	0.611000	1.877000	11.996000
H	1.365000	2.678000	12.064000
H	0.772000	1.218000	12.873000
C	3.371000	3.187000	-4.186000
H	3.556000	3.161000	-5.265000
C	10.658000	-3.549000	12.954000
H	10.588000	-3.734000	14.041000
H	11.378000	-4.292000	12.555000
C	-1.763000	-4.771000	6.599000
H	-1.647000	-5.538000	5.827000
C	0.740000	7.305000	9.438000
H	-0.150000	7.884000	9.129000
H	1.095000	7.759000	10.385000
N	0.323000	-4.548000	4.071000
H	7.155000	-0.724000	4.205000
Cu	2.608000	-2.914000	6.616000
C	2.570000	-1.165000	-1.271000
H	2.430000	-0.614000	-2.219000
H	3.580000	-1.617000	-1.318000

H	6.295000	-6.962000	10.739000
C	7.456000	-8.299000	9.459000
H	6.541000	-8.695000	8.974000
C	4.588000	-3.744000	3.514000
H	3.650000	-3.590000	2.953000
C	-0.809000	2.462000	12.044000
H	-0.947000	3.033000	12.981000
H	-0.933000	3.191000	11.218000
C	10.052000	7.916000	6.324000
H	10.235000	8.028000	7.410000
H	11.020000	7.627000	5.875000
C	1.384000	3.805000	14.978000
H	0.950000	2.801000	14.958000
C	8.586000	-8.232000	8.426000
H	9.129000	-7.146000	6.609000
C	4.245000	8.039000	12.565000
H	3.571000	7.464000	11.922000
C	0.550000	6.376000	3.119000
H	-0.480000	6.735000	3.298000
H	0.994000	7.051000	2.360000
C	5.971000	9.511000	14.191000
H	6.647000	10.086000	14.833000
H	8.758000	-9.227000	7.975000
H	6.728000	-4.880000	9.381000
H	7.402000	-7.528000	6.737000
C	4.860000	-6.100000	2.665000
H	4.984000	-7.156000	2.973000
H	3.928000	-6.056000	2.066000
C	4.708000	-5.216000	3.913000
H	3.819000	-5.522000	4.493000
H	5.587000	-5.339000	4.571000
C	9.567000	9.250000	5.748000
H	10.294000	10.053000	5.968000
H	9.510000	9.173000	4.645000
C	5.549000	4.883000	16.355000
H	4.493000	4.998000	16.617000
H	9.530000	-7.952000	8.935000
H	7.712000	-9.011000	10.265000
H	5.942000	-6.140000	8.417000
C	-0.813000	-3.141000	8.121000
H	0.060000	-2.631000	8.541000
C	1.270000	6.132000	15.640000
H	0.743000	6.953000	16.138000

C	6.301000	0.046000	-0.300000
H	5.817000	0.903000	-0.806000
H	5.514000	-0.485000	0.261000
C	6.935000	-0.880000	-1.352000
H	7.326000	-1.789000	-0.854000
H	6.154000	-1.220000	-2.056000
C	1.525000	-2.276000	-1.130000
H	1.623000	-3.005000	-1.957000
H	0.510000	-1.839000	-1.214000
C	8.173000	4.645000	15.610000
H	9.215000	4.565000	15.272000
C	10.393000	7.460000	12.174000
H	10.932000	7.292000	13.125000
H	11.156000	7.421000	11.371000
C	7.836000	4.413000	16.949000
H	8.608000	4.141000	17.675000
C	9.725000	8.840000	12.172000
H	10.484000	9.636000	12.282000
H	9.052000	8.919000	13.049000
C	2.608000	4.044000	14.346000
H	3.123000	3.229000	13.826000
C	4.315000	9.426000	12.429000
H	3.690000	9.932000	11.684000
C	5.931000	-4.173000	1.423000
H	5.057000	-4.026000	0.758000
H	6.818000	-3.848000	0.848000
C	6.044000	-5.655000	1.799000
H	6.108000	-6.278000	0.888000
H	6.986000	-5.815000	2.359000
C	-1.487000	2.107000	5.326000
H	-2.486000	2.582000	5.352000
H	-1.024000	2.402000	4.364000
C	-3.047000	-4.436000	7.043000
H	-3.917000	-4.941000	6.612000
C	-2.098000	-2.817000	8.570000
H	-2.225000	-2.054000	9.343000
C	1.522000	-5.955000	7.754000
C	0.575000	-6.604000	8.567000
H	-0.465000	-6.264000	8.574000
C	0.954000	-7.684000	9.370000
H	0.205000	-8.175000	10.001000
C	2.276000	-8.138000	9.364000
H	2.571000	-8.988000	9.989000

C	3.224000	-7.496000	8.558000
H	4.262000	-7.842000	8.554000
C	2.857000	-6.404000	7.768000
H	3.613000	-5.891000	7.160000
C	6.496000	4.534000	17.325000
H	6.189000	4.366000	18.364000
C	1.002000	-6.758000	4.779000
H	1.374000	-7.411000	5.574000
C	0.701000	-7.270000	3.511000
H	0.851000	-8.334000	3.295000
C	0.793000	-5.391000	5.010000
C	-0.635000	-4.124000	7.134000
C	0.191000	-6.410000	2.539000
H	-0.073000	-6.769000	1.540000
C	0.016000	-5.060000	2.873000
H	-0.389000	-4.352000	2.141000
C	-3.217000	-3.461000	8.030000
H	-4.222000	-3.200000	8.376000
C	7.158000	-6.915000	10.047000
S	7.679000	-4.622000	6.532000
H	8.023000	-6.578000	10.652000
C	8.010000	-5.822000	7.922000
C	8.287000	-7.205000	7.322000
C	6.879000	-5.881000	8.945000
H	8.928000	-5.461000	8.417000
H	8.928000	3.365000	6.647000
H	6.815000	-1.446000	6.813000
H	8.447000	0.691000	6.789000
H	4.925000	0.914000	8.292000
H	5.095000	0.714000	4.973000
H	3.908000	2.615000	6.459000

Table S6. The coordinate of the optimized geometry of Cu_{29}-P(Ph-Me)$_3^T$

P	-6.548000	15.946000	40.726000
S	-1.810000	11.251000	33.289000
S	-3.742000	14.971000	34.478000
S	-4.692000	13.043000	38.356000
S	-2.855000	14.173000	40.992000
S	-4.002000	10.204000	41.475000
S	-1.953000	7.856000	38.389000
C	3.228000	10.442000	32.646000
H	2.875000	9.503000	32.186000

C	4.192000	10.125000	33.786000
H	3.693000	9.482000	34.529000
H	4.455000	11.067000	34.300000
C	5.469000	9.456000	33.252000
H	6.166000	9.274000	34.092000
H	5.217000	8.461000	32.833000
C	6.139000	10.312000	32.171000
H	6.487000	11.260000	32.628000
H	7.036000	9.801000	31.773000
C	5.158000	10.631000	31.037000
H	4.881000	9.694000	30.513000
H	5.634000	11.283000	30.281000
C	3.880000	11.308000	31.566000
H	4.132000	12.292000	32.004000
H	3.170000	11.478000	30.738000
C	0.445000	6.385000	33.449000
H	-0.050000	6.360000	32.457000
C	1.909000	6.772000	33.247000
H	2.381000	6.904000	34.239000
H	1.957000	7.752000	32.744000
C	2.667000	5.708000	32.439000
H	2.259000	5.675000	31.408000
H	3.731000	5.999000	32.344000
C	2.540000	4.320000	33.074000
H	3.056000	4.322000	34.055000
H	3.052000	3.563000	32.450000
C	1.069000	3.935000	33.279000
H	0.998000	2.955000	33.790000
H	0.584000	3.807000	32.290000
C	0.310000	4.999000	34.088000
H	-0.759000	4.728000	34.176000
H	0.711000	5.042000	35.118000
C	3.197000	7.050000	37.990000
H	3.592000	6.923000	39.014000
C	3.033000	5.682000	37.332000
H	2.373000	5.044000	37.938000
H	2.536000	5.821000	36.354000
C	4.396000	5.003000	37.127000
H	4.247000	4.032000	36.619000
H	4.841000	4.772000	38.116000
C	5.356000	5.892000	36.331000
H	6.345000	5.407000	36.236000
H	4.967000	6.018000	35.301000

C	5.500000	7.271000	36.983000
H	6.145000	7.923000	36.368000
H	6.010000	7.162000	37.962000
C	4.137000	7.948000	37.193000
H	4.253000	8.921000	37.699000
H	3.675000	8.160000	36.212000
C	-0.570000	9.175000	42.860000
H	-1.238000	10.053000	42.884000
C	-1.309000	7.976000	43.459000
H	-0.696000	7.066000	43.322000
H	-2.258000	7.822000	42.917000
C	-1.580000	8.194000	44.956000
H	-2.295000	9.033000	45.075000
H	-2.071000	7.298000	45.378000
C	-0.291000	8.511000	45.724000
H	0.376000	7.625000	45.694000
H	-0.517000	8.701000	46.791000
C	0.439000	9.710000	45.108000
H	1.392000	9.901000	45.637000
H	-0.179000	10.620000	45.238000
C	0.719000	9.493000	43.612000
H	1.201000	10.382000	43.173000
H	1.434000	8.660000	43.483000
C	5.217000	8.814000	41.107000
H	5.355000	8.679000	40.021000
C	5.007000	7.444000	41.759000
H	4.130000	6.945000	41.311000
H	4.769000	7.599000	42.831000
C	6.255000	6.558000	41.630000
H	6.426000	6.321000	40.561000
H	6.083000	5.590000	42.138000
C	7.499000	7.250000	42.202000
H	7.378000	7.367000	43.297000
H	8.394000	6.616000	42.052000
C	7.707000	8.629000	41.566000
H	7.958000	8.503000	40.494000
H	8.572000	9.139000	42.032000
C	6.453000	9.505000	41.694000
H	6.256000	9.724000	42.762000
H	6.603000	10.476000	41.194000
C	6.110000	11.985000	37.319000
H	5.649000	11.516000	36.433000
C	7.119000	13.046000	36.874000

H	7.495000	13.559000	37.779000
H	6.619000	13.797000	36.238000
C	8.303000	12.407000	36.130000
H	9.028000	13.191000	35.841000
H	7.939000	11.953000	35.185000
C	8.988000	11.331000	36.982000
H	9.452000	11.808000	37.868000
H	9.806000	10.849000	36.415000
C	7.975000	10.280000	37.448000
H	8.457000	9.535000	38.109000
H	7.601000	9.720000	36.569000
C	6.787000	10.921000	38.181000
H	6.051000	10.156000	38.477000
H	7.143000	11.396000	39.114000
C	0.937000	10.858000	28.952000
C	1.775000	11.045000	27.840000
H	1.818000	12.022000	27.345000
C	2.567000	9.995000	27.366000
H	3.218000	10.163000	26.499000
C	2.553000	8.733000	27.983000
C	1.704000	8.552000	29.088000
H	1.674000	7.576000	29.589000
C	0.914000	9.597000	29.575000
H	0.286000	9.437000	30.458000
C	3.447000	7.624000	27.498000
H	-1.977000	11.193000	39.240000
H	0.261000	14.290000	39.125000
H	1.686000	11.051000	39.379000
H	3.080000	6.637000	27.823000
H	4.471000	7.743000	27.898000
H	3.526000	7.618000	26.398000
C	0.697000	3.499000	39.365000
C	1.897000	2.876000	39.741000
H	2.327000	3.066000	40.731000
C	2.558000	2.012000	38.858000
H	3.497000	1.541000	39.176000
C	2.048000	1.735000	37.583000
C	0.840000	2.357000	37.215000
H	0.414000	2.166000	36.222000
C	0.182000	3.231000	38.080000
H	-0.743000	3.715000	37.751000
H	3.088000	1.358000	35.723000
C	-7.333000	15.058000	42.126000

C	-8.619000	15.369000	42.611000
H	-9.230000	16.126000	42.106000
C	-5.756000	2.399000	41.585000
H	-6.403000	2.489000	40.692000
H	-5.724000	1.331000	41.858000
C	-1.807000	3.994000	40.718000
C	-2.087000	2.629000	40.525000
H	-1.313000	1.957000	40.142000
C	-3.358000	2.121000	40.813000
H	-3.558000	1.054000	40.655000
C	-4.382000	2.945000	41.307000
C	-4.092000	4.307000	41.499000
H	-4.872000	4.976000	41.880000
C	-2.831000	4.828000	41.202000
H	-2.637000	5.897000	41.340000
H	-6.251000	2.948000	42.402000
C	-9.129000	14.710000	43.733000
H	-10.130000	14.967000	44.097000
C	-8.383000	13.725000	44.403000
C	2.817000	4.257000	45.824000
H	2.995000	5.246000	46.279000
H	2.273000	3.634000	46.553000
C	0.690000	4.572000	42.050000
C	0.471000	3.478000	42.907000
H	-0.246000	2.699000	42.629000
C	1.153000	3.384000	44.123000
H	0.965000	2.527000	44.780000
C	2.066000	4.374000	44.525000
C	2.272000	5.467000	43.667000
H	2.965000	6.262000	43.963000
C	1.592000	5.572000	42.450000
H	1.750000	6.448000	41.812000
H	3.806000	3.787000	45.665000
C	-7.110000	13.410000	43.905000
H	-6.510000	12.635000	44.395000
C	-6.596000	14.057000	42.777000
C	-5.074000	21.629000	42.691000
H	-5.504000	22.384000	42.006000
H	-5.449000	21.850000	43.704000
Cu	-0.062000	12.271000	37.578000
Cu	1.277000	11.205000	35.532000
Cu	2.617000	12.376000	37.308000
Cu	-0.254000	10.873000	39.835000

Cu	-0.091000	12.182000	31.902000
Cu	-0.033000	9.759000	33.895000
Cu	0.321000	8.322000	36.344000
Cu	1.388000	10.212000	37.822000
Cu	3.533000	11.535000	39.816000
Cu	1.890000	9.360000	40.190000
Cu	-0.196000	6.800000	39.584000
P	-0.080000	12.201000	29.686000
P	-0.152000	4.742000	40.423000
S	1.660000	11.257000	33.273000
S	-0.558000	7.636000	34.391000
S	1.535000	7.861000	38.267000
S	-0.278000	8.883000	41.032000
S	3.730000	9.894000	41.376000
S	4.685000	12.786000	38.228000
C	0.621000	13.740000	28.968000
C	0.102000	14.376000	27.826000
H	-0.769000	13.953000	27.316000
C	0.687000	15.549000	27.341000
H	0.263000	16.031000	26.452000
C	1.802000	16.124000	27.974000
C	2.315000	15.483000	29.113000
H	3.180000	15.914000	29.629000
C	1.733000	14.315000	29.611000
H	2.137000	13.849000	30.517000
H	2.560000	17.365000	26.367000
H	-0.017000	12.312000	40.812000
H	2.567000	10.779000	36.642000
H	-2.646000	10.724000	36.635000
H	-0.003000	10.182000	36.465000
H	-1.403000	13.014000	36.537000
H	1.910000	13.622000	36.213000
C	-1.729000	12.023000	28.898000
C	-1.938000	11.300000	27.711000
H	-1.092000	10.821000	27.207000
C	-3.225000	11.163000	27.183000
H	-3.370000	10.586000	26.262000
C	-4.338000	11.742000	27.814000
C	-4.121000	12.464000	29.000000
H	-4.975000	12.916000	29.519000
C	-2.840000	12.601000	29.539000
H	-2.699000	13.143000	30.481000
H	-6.500000	11.795000	27.976000

C	-10.944000	16.752000	36.456000
H	-11.350000	17.777000	36.422000
H	-10.488000	16.552000	35.467000
C	2.761000	0.815000	36.629000
H	3.653000	0.363000	37.092000
H	2.102000	-0.005000	36.291000
C	-0.061000	15.886000	32.635000
H	0.888000	16.015000	32.086000
C	-0.138000	16.911000	33.762000
H	0.716000	16.783000	34.447000
H	-1.051000	16.720000	34.353000
C	-0.176000	18.339000	33.194000
H	-0.269000	19.063000	34.025000
H	0.786000	18.560000	32.691000
C	-1.328000	18.513000	32.198000
H	-2.290000	18.405000	32.738000
H	-1.318000	19.532000	31.767000
C	-1.257000	17.464000	31.082000
H	-0.349000	17.635000	30.470000
H	-2.119000	17.568000	30.396000
C	-1.221000	16.034000	31.648000
H	-2.166000	15.815000	32.177000
H	-1.115000	15.301000	30.829000
C	4.809000	15.580000	33.320000
H	4.974000	15.147000	32.313000
C	3.737000	16.661000	33.216000
H	3.480000	17.002000	34.236000
H	2.818000	16.223000	32.794000
C	4.208000	17.854000	32.370000
H	4.342000	17.529000	31.318000
H	3.424000	18.634000	32.357000
C	5.530000	18.429000	32.892000
H	5.363000	18.865000	33.897000
H	5.872000	19.257000	32.243000
C	6.607000	17.342000	32.984000
H	7.539000	17.760000	33.413000
H	6.862000	16.993000	31.964000
C	6.137000	16.150000	33.831000
H	6.904000	15.354000	33.842000
H	5.998000	16.469000	34.882000
C	3.098000	17.768000	37.922000
H	3.080000	18.203000	38.938000
C	4.368000	18.214000	37.201000

H	5.259000	17.921000	37.775000
H	4.424000	17.683000	36.232000
C	4.364000	19.734000	36.961000
H	5.271000	20.016000	36.396000
H	4.431000	20.256000	37.937000
C	3.102000	20.192000	36.222000
H	3.096000	21.294000	36.114000
H	3.109000	19.775000	35.195000
C	1.835000	19.719000	36.944000
H	0.933000	20.004000	36.373000
H	1.759000	20.230000	37.925000
C	1.847000	18.198000	37.164000
H	0.946000	17.865000	37.705000
H	1.832000	17.681000	36.186000
C	2.899000	13.358000	42.705000
H	2.443000	12.354000	42.709000
C	4.306000	13.266000	43.297000
H	4.810000	14.246000	43.190000
H	4.893000	12.523000	42.731000
C	4.245000	12.874000	44.782000
H	3.847000	11.843000	44.865000
H	5.268000	12.852000	45.202000
C	3.358000	13.833000	45.584000
H	3.822000	14.839000	45.588000
H	3.297000	13.507000	46.639000
C	1.957000	13.928000	44.971000
H	1.335000	14.658000	45.525000
H	1.448000	12.948000	45.068000
C	2.014000	14.326000	43.487000
H	1.002000	14.347000	43.051000
H	2.416000	15.351000	43.390000
C	0.266000	18.581000	40.938000
H	0.294000	18.765000	39.850000
C	1.559000	19.102000	41.573000
H	2.432000	18.614000	41.106000
H	1.565000	18.807000	42.641000
C	1.673000	20.629000	41.456000
H	1.774000	20.906000	40.387000
H	2.599000	20.974000	41.955000
C	0.448000	21.336000	42.048000
H	0.416000	21.157000	43.142000
H	0.529000	22.431000	41.911000
C	-0.847000	20.812000	41.418000

H	-0.873000	21.097000	40.346000
H	-1.727000	21.287000	41.890000
C	-0.952000	19.286000	41.543000
H	-1.023000	19.004000	42.612000
H	-1.871000	18.910000	41.063000
C	-2.969000	17.556000	37.102000
H	-2.451000	17.226000	36.187000
C	-4.393000	17.984000	36.737000
H	-4.950000	18.230000	37.661000
H	-4.920000	17.148000	36.251000
C	-4.362000	19.212000	35.814000
H	-5.396000	19.523000	35.573000
H	-3.888000	18.926000	34.854000
C	-3.583000	20.371000	36.445000
H	-4.122000	20.722000	37.349000
H	-3.540000	21.233000	35.752000
C	-2.168000	19.934000	36.842000
H	-1.632000	20.759000	37.348000
H	-1.588000	19.700000	35.928000
C	-2.191000	18.697000	37.753000
H	-1.168000	18.365000	37.992000
H	-2.669000	18.960000	38.715000
C	7.310000	17.120000	39.255000
C	7.425000	18.462000	39.651000
H	7.129000	18.762000	40.661000
C	7.906000	19.428000	38.759000
H	7.971000	20.472000	39.089000
C	8.299000	19.091000	37.456000
C	8.183000	17.745000	37.068000
H	8.462000	17.451000	36.049000
C	7.690000	16.777000	37.943000
H	7.580000	15.747000	37.594000
C	8.832000	20.126000	36.502000
C	2.403000	17.404000	27.459000
H	1.738000	18.264000	27.659000
H	3.374000	17.616000	27.935000
H	8.570000	19.882000	35.458000
H	9.935000	20.188000	36.557000
H	8.436000	21.130000	36.729000
C	8.087000	14.752000	40.702000
C	9.404000	15.139000	40.402000
H	9.596000	16.100000	39.913000
C	10.477000	14.304000	40.727000

H	11.498000	14.623000	40.485000
C	10.277000	13.069000	41.363000
C	8.957000	12.692000	41.663000
H	8.771000	11.734000	42.161000
C	7.877000	13.510000	41.327000
H	6.857000	13.185000	41.556000
C	11.435000	12.166000	41.689000
Cu	-2.186000	13.437000	34.017000
Cu	-3.834000	14.243000	36.587000
Cu	-2.634000	12.113000	37.724000
H	11.230000	11.548000	42.579000
H	12.358000	12.740000	41.873000
H	11.642000	11.473000	40.852000
C	6.325000	16.677000	41.936000
C	7.362000	16.977000	42.839000
H	8.386000	16.654000	42.621000
C	7.095000	17.678000	44.016000
H	7.918000	17.895000	44.710000
C	5.793000	18.101000	44.336000
C	4.763000	17.788000	43.434000
H	3.736000	18.091000	43.664000
C	5.019000	17.083000	42.254000
H	4.192000	16.828000	41.582000
C	5.518000	18.869000	45.600000
H	4.436000	18.944000	45.799000
H	5.918000	19.897000	45.535000
H	5.995000	18.392000	46.474000
Cu	-2.472000	9.449000	39.996000
Cu	-3.475000	11.954000	40.160000
Cu	-4.806000	14.884000	39.832000
Cu	-0.064000	13.845000	35.544000
Cu	-1.350000	14.592000	37.548000
Cu	1.277000	12.846000	39.692000
Cu	2.158000	13.454000	34.279000
Cu	3.473000	14.638000	36.360000
Cu	1.192000	14.591000	37.601000
Cu	-1.440000	15.847000	39.866000
Cu	1.469000	15.459000	39.978000
Cu	4.835000	14.750000	39.537000
P	6.619000	15.804000	40.345000
S	0.051000	14.136000	33.285000
S	4.328000	14.120000	34.362000
S	3.108000	15.925000	38.238000

S	3.002000	13.799000	40.887000
S	0.101000	16.752000	41.217000
S	-3.022000	16.031000	38.192000
C	-3.286000	10.261000	32.680000
H	-3.923000	11.021000	32.194000
C	-4.047000	9.619000	33.835000
H	-4.365000	10.394000	34.550000
H	-3.364000	8.942000	34.379000
C	-5.259000	8.827000	33.318000
H	-5.766000	8.337000	34.171000
H	-5.997000	9.525000	32.873000
C	-4.843000	7.789000	32.270000
H	-4.201000	7.026000	32.754000
H	-5.731000	7.256000	31.881000
C	-4.070000	8.446000	31.122000
H	-4.742000	9.132000	30.569000
H	-3.735000	7.685000	30.392000
C	-2.852000	9.235000	31.632000
H	-2.122000	8.545000	32.093000
H	-2.350000	9.745000	30.792000
C	-5.295000	14.732000	33.479000
H	-5.024000	15.154000	32.490000
C	-5.707000	13.274000	33.283000
H	-5.874000	12.813000	34.274000
H	-4.874000	12.722000	32.819000
C	-6.977000	13.156000	32.429000
H	-6.759000	13.511000	31.401000
H	-7.270000	12.093000	32.336000
C	-8.130000	13.985000	33.010000
H	-8.434000	13.553000	33.984000
H	-9.017000	13.925000	32.350000
C	-7.715000	15.448000	33.210000
H	-8.535000	16.020000	33.685000
H	-7.541000	15.915000	32.219000
C	-6.441000	15.570000	34.061000
H	-6.129000	16.628000	34.137000
H	-6.646000	15.226000	35.093000
C	-6.239000	12.061000	37.993000
H	-6.646000	11.853000	38.999000
C	-7.233000	12.905000	37.199000
H	-7.448000	13.847000	37.728000
H	-6.761000	13.184000	36.240000
C	-8.528000	12.122000	36.933000

H	-9.211000	12.740000	36.321000
H	-9.048000	11.940000	37.894000
C	-8.248000	10.783000	36.241000
H	-9.186000	10.213000	36.110000
H	-7.852000	10.975000	35.224000
C	-7.223000	9.955000	37.026000
H	-6.983000	9.023000	36.484000
H	-7.664000	9.646000	37.995000
C	-5.932000	10.747000	37.284000
H	-5.214000	10.153000	37.875000
H	-5.434000	10.970000	36.324000
C	-2.364000	14.351000	42.796000
H	-1.270000	14.481000	42.745000
C	-2.981000	15.619000	43.387000
H	-4.085000	15.552000	43.339000
H	-2.680000	16.493000	42.784000
C	-2.536000	15.794000	44.849000
H	-1.443000	15.977000	44.870000
H	-3.015000	16.694000	45.277000
C	-2.863000	14.556000	45.692000
H	-3.964000	14.438000	45.754000
H	-2.501000	14.691000	46.729000
C	-2.253000	13.291000	45.077000
H	-2.534000	12.396000	45.663000
H	-1.149000	13.359000	45.123000
C	-2.690000	13.104000	43.613000
H	-2.202000	12.221000	43.168000
H	-3.777000	12.907000	43.575000
C	-5.675000	9.475000	41.123000
H	-5.814000	9.441000	40.030000
C	-6.769000	10.346000	41.746000
H	-6.735000	11.361000	41.314000
H	-6.552000	10.462000	42.826000
C	-8.163000	9.728000	41.566000
H	-8.423000	9.715000	40.488000
H	-8.921000	10.365000	42.062000
C	-8.220000	8.298000	42.118000
H	-8.076000	8.329000	43.217000
H	-9.218000	7.853000	41.942000
C	-7.125000	7.423000	41.495000
H	-7.330000	7.292000	40.414000
H	-7.141000	6.409000	41.940000
C	-5.733000	8.047000	41.677000

H	-5.475000	8.077000	42.754000
H	-4.960000	7.434000	41.183000
C	-3.264000	7.002000	37.371000
H	-3.372000	7.628000	36.470000
C	-2.784000	5.608000	36.962000
H	-2.593000	5.025000	37.883000
H	-1.832000	5.691000	36.412000
C	-3.844000	4.888000	36.114000
H	-3.490000	3.872000	35.858000
H	-3.969000	5.428000	35.154000
C	-5.193000	4.816000	36.840000
H	-5.089000	4.176000	37.739000
H	-5.954000	4.337000	36.195000
C	-5.662000	6.211000	37.271000
H	-6.608000	6.148000	37.841000
H	-5.878000	6.818000	36.370000
C	-4.596000	6.926000	38.117000
H	-4.929000	7.939000	38.396000
H	-4.441000	6.370000	39.060000
C	-7.947000	16.262000	39.569000
C	-8.915000	15.269000	39.339000
H	-8.913000	14.349000	39.935000
C	-9.892000	15.442000	38.354000
H	-10.635000	14.650000	38.192000
C	-9.927000	16.594000	37.554000
C	-8.966000	17.588000	37.800000
H	-8.978000	18.509000	37.203000
C	-7.991000	17.430000	38.787000
H	-7.259000	18.228000	38.954000
H	-11.788000	16.053000	36.580000
H	-0.065000	15.282000	36.583000
Cu	-1.466000	11.405000	35.557000
Cu	-1.396000	9.914000	37.589000
C	-8.950000	13.001000	45.595000
H	-9.662000	13.631000	46.153000
H	-9.494000	12.091000	45.279000
C	-6.137000	17.616000	41.392000
C	-5.100000	18.330000	40.768000
H	-4.527000	17.855000	39.965000
C	-4.775000	19.624000	41.181000
H	-3.968000	20.162000	40.672000
C	-5.439000	20.236000	42.254000
C	-6.450000	19.505000	42.897000

H	-6.973000	19.950000	43.751000
C	-6.803000	18.221000	42.470000
H	-7.597000	17.686000	43.000000
H	-3.981000	21.778000	42.689000
H	-5.613000	13.771000	42.388000
H	-8.155000	12.679000	46.288000
Cu	-1.173000	13.187000	39.820000
C	-5.716000	11.604000	27.225000
H	-5.865000	12.326000	26.400000
H	-5.879000	10.596000	26.806000

Table S7. The coordinate of the optimized geometry of Cu_{29}-P(Ph-Cl)$_3^T$

Cu	0.830000	1.469000	-1.925000
Cu	1.156000	3.877000	-1.225000
Cu	4.296000	3.911000	-2.094000
Cu	-3.352000	2.316000	1.452000
Cu	-5.587000	2.487000	-1.025000
Cu	3.606000	3.130000	0.680000
Cu	-1.257000	0.874000	4.630000
Cu	0.803000	-0.446000	6.193000
Cu	-1.057000	-1.927000	0.275000
Cu	-0.264000	-0.768000	-2.010000
Cu	2.623000	0.817000	-0.103000
Cu	1.548000	-1.498000	-0.192000
Cu	-1.804000	1.210000	-1.708000
Cu	0.751000	-3.741000	0.987000
Cu	1.938000	-1.893000	-2.795000
Cu	-2.575000	0.061000	0.536000
Cu	-0.944000	-0.751000	2.539000
Cu	1.632000	-0.396000	2.055000
Cu	3.225000	0.804000	-2.920000
Cu	1.514000	1.494000	3.755000
Cu	-2.958000	3.512000	-1.172000
Cu	-0.851000	2.983000	0.078000
Cu	0.308000	-4.842000	-2.229000
Cu	-0.992000	1.921000	2.366000
Cu	-2.245000	-2.471000	-2.088000
Cu	1.257000	2.541000	1.406000
Cu	-4.237000	-0.170000	-1.777000
Cu	1.069000	-2.537000	3.615000
S	-1.276000	-4.152000	-0.508000
S	2.072000	-3.703000	-0.982000
Cl	0.474000	2.176000	5.752000

S	2.380000	2.899000	-3.138000
S	0.469000	-4.604000	3.073000
S	-0.894000	-1.352000	4.864000
S	2.306000	-0.772000	4.352000
S	-3.903000	1.965000	-2.611000
S	4.593000	1.904000	-0.929000
S	4.020000	-1.204000	-3.409000
S	-0.213000	-2.722000	-3.433000
S	-0.998000	4.667000	-1.600000
S	3.101000	2.948000	2.858000
S	-4.828000	0.732000	0.356000
S	-2.960000	2.096000	3.735000
S	-4.520000	-2.340000	-2.119000
Cl	2.838000	5.265000	-0.350000
Cl	-4.301000	4.342000	0.583000
P	0.486000	-6.846000	-3.250000
P	5.713000	5.512000	-2.750000
P	-7.532000	3.585000	-1.184000
P	1.133000	-0.388000	8.409000
Cl	-11.594000	1.145000	-5.471000
Cl	-11.006000	3.739000	4.174000
Cl	-2.549000	3.687000	11.680000
C	4.719000	-1.292000	-5.150000
C	4.120000	-1.119000	4.756000
C	4.728000	-3.314000	-0.152000
H	4.317000	-2.988000	0.819000
H	4.754000	-2.433000	-0.815000
C	-4.201000	2.459000	-4.428000
C	1.964000	3.498000	-4.881000
C	1.471000	-7.221000	3.010000
H	0.416000	-7.515000	2.849000
H	1.911000	-7.019000	2.018000
C	-1.096000	6.447000	-0.969000
C	1.570000	-8.093000	-2.425000
C	4.878000	-2.769000	-5.557000
H	5.503000	-3.292000	-4.809000
H	3.888000	-3.259000	-5.558000
C	8.471000	0.512000	-1.601000
H	8.915000	0.178000	-2.559000
C	2.112000	6.329000	5.955000
H	1.347000	5.676000	6.419000
H	2.125000	7.274000	6.534000
C	-2.526000	-5.336000	0.282000

C	8.654000	1.038000	1.291000
H	8.219000	1.375000	2.252000
H	9.702000	0.746000	1.498000
C	3.817000	-4.386000	-0.763000
C	4.833000	0.197000	5.103000
H	4.309000	0.699000	5.935000
H	4.804000	0.882000	4.237000
C	6.281000	-2.102000	3.955000
H	6.779000	-2.583000	3.092000
C	6.294000	-0.114000	5.498000
H	6.803000	0.837000	5.748000
C	3.269000	3.511000	-5.694000
H	3.995000	4.181000	-5.201000
H	3.711000	2.499000	-5.713000
C	4.550000	6.587000	5.396000
H	5.554000	6.121000	5.457000
H	4.600000	7.538000	5.961000
C	-1.954000	-3.315000	-7.210000
H	-2.834000	-3.930000	-7.479000
C	6.388000	6.154000	-0.096000
H	5.952000	5.183000	0.150000
C	1.579000	-8.652000	5.080000
H	0.528000	-8.971000	4.937000
H	2.105000	-9.485000	5.586000
C	7.149000	2.592000	0.009000
H	6.679000	2.953000	0.945000
H	7.117000	3.414000	-0.727000
C	6.308000	-3.048000	5.168000
H	7.354000	-3.293000	5.436000
H	5.806000	-4.003000	4.920000
C	2.204000	-9.234000	-0.364000
H	2.107000	-9.365000	0.716000
C	-5.343000	-4.295000	-3.930000
H	-4.289000	-4.418000	-4.236000
H	-5.496000	-4.924000	-3.034000
C	7.422000	8.210000	0.625000
C	-1.710000	-3.431000	-5.688000
H	-2.596000	-3.104000	-5.120000
H	-1.517000	-4.486000	-5.420000
C	-5.606000	-2.821000	-3.572000
C	1.154000	-6.853000	-4.974000
C	7.004000	0.918000	-1.851000
H	6.427000	0.068000	-2.254000

H	6.958000	1.733000	-2.595000
C	-0.761000	-1.110000	-5.662000
H	-1.636000	-0.740000	-5.100000
H	0.103000	-0.494000	-5.354000
C	7.418000	8.688000	-0.690000
H	7.810000	9.686000	-0.908000
C	8.617000	2.184000	0.265000
H	9.167000	3.060000	0.659000
C	2.235000	-8.362000	3.718000
H	2.196000	-9.272000	3.087000
C	-0.501000	-2.574000	-5.294000
C	-3.588000	3.831000	-4.733000
H	-2.496000	3.805000	-4.565000
H	-3.995000	4.596000	-4.047000
C	6.398000	0.250000	0.492000
H	5.926000	0.587000	1.434000
H	5.810000	-0.606000	0.120000
C	-8.580000	3.599000	0.333000
C	4.148000	-2.047000	5.980000
H	3.591000	-2.973000	5.757000
H	3.644000	-1.548000	6.826000
C	-2.215000	-1.845000	-7.581000
H	-2.400000	-1.758000	-8.670000
H	-3.124000	-1.477000	-7.071000
C	-6.164000	-0.220000	1.287000
C	-2.477000	7.021000	-1.338000
H	-3.271000	6.435000	-0.846000
H	-2.630000	6.944000	-2.432000
C	9.255000	1.719000	-1.056000
H	10.314000	1.442000	-0.887000
H	9.250000	2.543000	-1.795000
C	-8.030000	-3.126000	-4.237000
H	-9.075000	-3.018000	-3.886000
C	3.495000	5.655000	6.018000
H	3.760000	5.441000	7.073000
C	-0.997000	-0.994000	-7.183000
H	-1.179000	0.068000	-7.438000
C	8.509000	-0.634000	-0.577000
H	9.556000	-0.949000	-0.396000
H	7.969000	-1.514000	-0.973000
C	5.607000	-2.369000	6.358000
H	5.607000	-3.048000	7.234000
C	4.183000	6.862000	3.928000

H	4.944000	7.521000	3.466000
C	-1.800000	-6.632000	0.673000
H	-1.365000	-7.092000	-0.234000
H	-0.977000	-6.402000	1.369000
C	1.412000	4.928000	-4.800000
H	2.143000	5.580000	-4.290000
H	0.484000	4.942000	-4.201000
C	6.371000	1.387000	-0.533000
C	7.202000	4.852000	-3.614000
C	5.059000	6.784000	-3.913000
C	6.390000	6.602000	-1.426000
C	4.363000	-4.821000	-2.130000
H	4.366000	-3.961000	-2.820000
H	3.700000	-5.598000	-2.548000
C	2.483000	-8.902000	-3.127000
H	2.596000	-8.795000	-4.209000
C	-0.887000	6.535000	0.547000
H	0.092000	6.103000	0.814000
H	-1.660000	5.936000	1.058000
C	1.452000	-8.268000	-1.035000
H	0.767000	-7.637000	-0.460000
C	3.760000	-5.608000	0.158000
H	3.330000	-5.308000	1.128000
H	3.089000	-6.368000	-0.277000
C	-0.013000	7.258000	-1.702000
H	-0.171000	7.185000	-2.795000
H	0.983000	6.835000	-1.484000
C	0.939000	2.576000	-5.547000
H	0.010000	2.555000	-4.949000
H	1.325000	1.542000	-5.582000
C	-4.715000	4.152000	4.332000
H	-5.378000	3.363000	4.738000
H	-4.906000	4.219000	3.248000
C	6.910000	6.946000	0.931000
H	6.901000	6.597000	1.966000
C	6.147000	-3.896000	0.027000
H	6.798000	-3.122000	0.475000
C	-3.927000	1.773000	-6.825000
H	-3.487000	1.006000	-7.490000
C	4.816000	-1.796000	3.571000
H	4.778000	-1.134000	2.688000
H	4.284000	-2.726000	3.303000
C	6.899000	7.885000	-1.708000

H	6.882000	8.274000	-2.730000
C	-6.627000	0.608000	2.494000
H	-6.986000	1.596000	2.156000
H	-5.778000	0.783000	3.179000
C	-2.384000	6.064000	6.216000
H	-2.574000	7.030000	6.721000
H	-1.327000	5.798000	6.412000
C	6.701000	-4.314000	-1.348000
H	6.748000	-3.434000	-2.018000
H	7.732000	-4.703000	-1.242000
C	2.293000	-6.849000	-7.540000
C	-0.962000	8.011000	0.992000
H	-0.808000	8.061000	2.087000
C	1.700000	5.284000	3.703000
H	1.424000	5.464000	2.650000
H	0.939000	4.612000	4.134000
C	-5.265000	-5.995000	1.150000
H	-5.802000	-5.072000	0.862000
H	-6.009000	-6.675000	1.609000
C	7.867000	-0.165000	0.741000
H	7.883000	-0.992000	1.474000
C	0.732000	-3.091000	-6.043000
H	1.619000	-2.517000	-5.728000
H	0.914000	-4.144000	-5.772000
C	-4.086000	6.588000	4.435000
H	-4.258000	6.694000	3.347000
H	-4.310000	7.569000	4.898000
C	1.631000	-7.384000	5.949000
H	1.148000	-7.579000	6.927000
C	6.114000	-0.634000	-5.119000
H	6.746000	-1.135000	-4.363000
H	6.012000	0.421000	-4.804000
C	1.522000	-5.945000	3.868000
C	3.074000	4.608000	3.769000
C	-3.243000	3.769000	4.578000
C	-2.253000	-7.073000	-3.794000
H	-2.213000	-5.984000	-3.897000
C	6.328000	-1.056000	6.713000
H	7.378000	-1.263000	6.998000
H	5.843000	-0.580000	7.585000
C	-2.620000	6.199000	4.701000
H	-1.946000	6.970000	4.280000
C	1.746000	6.613000	4.487000

H	0.749000	7.092000	4.438000
C	1.140000	5.448000	-6.230000
H	0.744000	6.479000	-6.162000
C	6.773000	-0.722000	-6.510000
H	7.772000	-0.246000	-6.468000
C	7.026000	3.749000	-4.472000
H	6.033000	3.303000	-4.590000
C	2.369000	-6.188000	-5.223000
H	2.870000	-5.645000	-4.417000
C	0.874000	-6.245000	5.237000
H	-0.187000	-6.523000	5.090000
H	0.883000	-5.328000	5.855000
C	-7.343000	-0.436000	0.326000
H	-7.719000	0.547000	-0.012000
H	-6.997000	-0.997000	-0.560000
C	2.802000	7.539000	3.857000
H	2.536000	7.753000	2.803000
H	2.828000	8.510000	4.389000
C	3.855000	-0.564000	-6.187000
H	2.844000	-1.000000	-6.200000
H	3.739000	0.491000	-5.883000
C	-8.468000	-1.203000	1.051000
H	-9.308000	-1.355000	0.344000
C	-1.092000	-7.783000	-3.445000
C	-8.691000	1.566000	-2.729000
H	-7.981000	0.914000	-2.210000
C	-5.406000	-1.940000	-4.810000
H	-5.617000	-0.890000	-4.535000
H	-4.354000	-1.981000	-5.135000
C	2.949000	-6.196000	-6.492000
H	3.895000	-5.680000	-6.676000
C	-7.072000	-2.680000	-3.111000
H	-7.239000	-3.284000	-2.200000
H	-7.265000	-1.625000	-2.839000
C	1.074000	-7.498000	-7.326000
H	0.571000	-8.001000	-8.156000
C	4.139000	5.529000	3.148000
H	3.898000	5.716000	2.089000
H	5.127000	5.029000	3.186000
C	-3.141000	-4.687000	1.528000
H	-3.639000	-3.744000	1.244000
H	-2.341000	-4.440000	2.248000
C	5.787000	-5.392000	-1.959000

H	6.176000	-5.692000	-2.952000
C	-4.781000	5.379000	6.529000
H	-5.466000	4.624000	6.963000
H	-5.003000	6.341000	7.031000
C	8.497000	5.373000	-3.450000
H	8.669000	6.218000	-2.775000
C	1.955000	3.084000	-7.797000
H	1.754000	3.428000	-8.830000
H	2.353000	2.053000	-7.873000
C	-2.317000	4.851000	4.015000
H	-2.464000	4.932000	2.926000
H	-1.266000	4.559000	4.184000
C	0.245000	-1.500000	-7.939000
H	0.087000	-1.410000	-9.032000
H	1.124000	-0.877000	-7.689000
C	-2.805000	-7.610000	1.321000
H	-2.268000	-8.536000	1.611000
C	2.805000	0.154000	8.970000
C	6.093000	-5.121000	0.957000
H	7.111000	-5.532000	1.107000
H	5.715000	-4.822000	1.954000
C	7.005000	-0.791000	4.315000
H	8.061000	-1.000000	4.577000
H	7.016000	-0.111000	3.447000
C	-8.684000	2.950000	-2.477000
C	-6.248000	5.860000	-2.209000
H	-5.442000	5.164000	-2.457000
C	-7.930000	-2.563000	1.524000
H	-8.732000	-3.136000	2.029000
H	-7.597000	-3.166000	0.657000
C	-0.713000	-3.822000	-7.966000
H	-0.527000	-4.886000	-7.727000
H	-0.880000	-3.758000	-9.059000
C	0.654000	3.095000	-6.975000
H	-0.092000	2.429000	-7.452000
C	-2.268000	-2.274000	5.784000
C	2.982000	-5.536000	4.098000
H	3.004000	-4.621000	4.715000
H	3.463000	-5.284000	3.139000
C	-3.468000	-7.733000	-3.993000
H	-4.368000	-7.175000	-4.261000
C	3.901000	7.480000	-3.516000
H	3.403000	7.222000	-2.575000

C	3.097000	-6.969000	6.164000
H	3.151000	-6.071000	6.813000
H	3.651000	-7.775000	6.685000
C	-5.626000	-1.576000	1.752000
H	-4.760000	-1.427000	2.418000
H	-5.279000	-2.158000	0.880000
C	-5.453000	1.823000	-7.021000
H	-5.904000	0.833000	-6.815000
H	-5.686000	2.069000	-8.075000
C	-2.759000	-4.388000	7.049000
H	-2.325000	-5.350000	7.385000
C	0.516000	-7.505000	-6.042000
H	-0.431000	-8.030000	-5.882000
C	-5.015000	5.505000	5.014000
H	-6.072000	5.777000	4.820000
C	1.427000	-3.158000	8.578000
H	1.945000	-3.046000	7.620000
C	0.505000	-2.970000	-7.566000
H	1.407000	-3.338000	-8.091000
C	0.137000	8.813000	0.273000
H	0.117000	9.871000	0.601000
H	1.133000	8.409000	0.537000
C	-3.529000	-9.119000	-3.819000
C	3.257000	-9.858000	-2.461000
H	3.968000	-10.481000	-3.012000
C	-1.684000	-3.612000	6.258000
H	-0.803000	-3.427000	6.898000
H	-1.341000	-4.199000	5.389000
C	5.176000	-6.191000	0.339000
H	5.121000	-7.071000	1.010000
C	-7.392000	5.385000	-1.545000
C	-5.724000	2.506000	-4.627000
H	-6.169000	3.243000	-3.936000
H	-6.164000	1.524000	-4.379000
C	3.379000	8.509000	-4.302000
H	2.484000	9.053000	-3.987000
C	3.749000	-6.675000	4.801000
H	4.802000	-6.363000	4.950000
C	5.154000	8.152000	-5.928000
H	5.635000	8.423000	-6.873000
C	-3.916000	-7.947000	0.311000
H	-4.635000	-8.662000	0.757000
H	-3.482000	-8.435000	-0.583000

C	-7.805000	-2.253000	-5.485000
H	-8.028000	-1.192000	-5.260000
H	-8.496000	-2.562000	-6.294000
C	-4.639000	-6.650000	-0.095000
H	-5.430000	-6.877000	-0.837000
C	3.454000	4.325000	5.234000
H	4.440000	3.823000	5.272000
H	2.715000	3.642000	5.686000
C	4.014000	8.840000	-5.505000
C	-6.752000	-2.335000	2.489000
H	-6.355000	-3.310000	2.828000
C	-3.469000	-2.520000	4.868000
H	-3.154000	-3.082000	3.973000
H	-3.875000	-1.551000	4.525000
C	6.923000	-2.202000	-6.909000
H	7.571000	-2.727000	-6.181000
H	7.415000	-2.283000	-7.898000
C	-4.154000	-5.665000	2.163000
H	-4.599000	-5.188000	3.056000
C	-7.118000	8.107000	-2.164000
C	9.382000	3.731000	-4.985000
C	-3.317000	4.980000	6.784000
H	-3.141000	4.873000	7.872000
C	-3.632000	-5.667000	-0.728000
H	-4.140000	-4.740000	-1.039000
H	-3.182000	-6.120000	-1.627000
C	-2.554000	8.498000	-0.892000
H	-3.553000	8.899000	-1.154000
C	-1.462000	9.312000	-1.607000
H	-1.618000	9.279000	-2.704000
H	-1.518000	10.375000	-1.304000
C	-7.752000	-4.598000	-4.589000
H	-7.929000	-5.241000	-3.706000
H	-8.445000	-4.939000	-5.382000
C	-6.345000	-2.392000	-5.950000
H	-6.171000	-1.752000	-6.836000
C	-3.017000	3.627000	6.094000
H	-1.974000	3.325000	6.292000
H	-3.681000	2.837000	6.499000
C	-6.106000	7.212000	-2.527000
H	-5.209000	7.577000	-3.035000
C	5.736000	-6.617000	-1.030000
H	5.097000	-7.405000	-1.475000

H	6.748000	-7.049000	-0.908000
C	-3.584000	1.413000	-5.360000
H	-3.961000	0.410000	-5.107000
H	-2.489000	1.395000	-5.219000
C	9.587000	4.816000	-4.125000
H	10.595000	5.218000	-3.987000
C	-6.061000	-3.862000	-6.304000
H	-5.021000	-3.976000	-6.663000
H	-6.723000	-4.188000	-7.129000
C	-1.178000	-9.177000	-3.280000
H	-0.291000	-9.756000	-3.004000
C	-6.293000	-4.741000	-5.062000
H	-6.090000	-5.801000	-5.313000
C	-8.391000	6.307000	-1.180000
H	-9.278000	5.972000	-0.631000
C	3.269000	1.398000	8.500000
H	2.661000	1.978000	7.797000
C	-7.760000	-0.152000	3.219000
H	-8.094000	0.451000	4.086000
C	8.103000	3.194000	-5.164000
H	7.957000	2.337000	-5.826000
C	-2.705000	-1.446000	6.998000
H	-1.834000	-1.259000	7.649000
H	-3.096000	-0.466000	6.663000
C	-10.475000	1.837000	-4.329000
C	3.107000	-10.024000	-1.083000
C	-8.008000	4.089000	1.523000
H	-6.967000	4.428000	1.530000
C	3.701000	-7.945000	3.933000
H	4.193000	-7.762000	2.960000
H	4.260000	-8.764000	4.427000
C	2.988000	4.008000	-7.127000
H	3.935000	3.994000	-7.701000
C	-9.587000	1.005000	-3.640000
H	-9.597000	-0.073000	-3.822000
C	-3.329000	3.149000	-7.152000
H	-3.552000	3.426000	-8.202000
H	-2.232000	3.109000	-7.060000
C	5.532000	-2.861000	-6.952000
H	5.637000	-3.928000	-7.235000
C	-3.785000	-2.219000	7.786000
H	-4.095000	-1.608000	8.656000
C	-6.049000	2.886000	-6.084000

H	-7.148000	2.926000	-6.205000
C	-5.440000	4.266000	-6.391000
H	-5.678000	4.565000	-7.431000
H	-5.884000	5.032000	-5.726000
C	3.604000	-0.571000	9.868000
H	3.267000	-1.540000	10.248000
C	5.674000	7.127000	-5.128000
H	6.575000	6.599000	-5.459000
C	-10.466000	3.221000	-4.121000
H	-11.155000	3.860000	-4.680000
C	-2.346000	8.584000	0.632000
H	-3.140000	8.018000	1.155000
H	-2.421000	9.637000	0.964000
C	-3.913000	4.206000	-6.199000
H	-3.466000	5.196000	-6.416000
C	-2.391000	-9.846000	-3.461000
H	-2.458000	-10.929000	-3.324000
C	-0.081000	8.732000	-1.251000
H	0.713000	9.304000	-1.771000
C	5.892000	0.005000	-7.544000
H	5.794000	1.076000	-7.275000
H	6.365000	-0.033000	-8.544000
C	-3.422000	-6.956000	2.572000
H	-4.128000	-7.658000	3.057000
H	-2.630000	-6.725000	3.309000
C	-8.942000	-0.376000	2.258000
H	-9.761000	-0.904000	2.784000
H	-9.348000	0.596000	1.920000
C	-3.965000	-4.649000	6.131000
H	-3.655000	-5.262000	5.264000
H	-4.742000	-5.225000	6.672000
C	0.904000	-2.022000	9.226000
C	0.106000	4.533000	-6.906000
H	-0.122000	4.900000	-7.925000
H	-0.839000	4.559000	-6.333000
C	2.438000	5.443000	-7.055000
H	3.187000	6.113000	-6.595000
H	2.240000	5.829000	-8.074000
C	-7.230000	-1.513000	3.699000
H	-6.399000	-1.362000	4.411000
H	-8.025000	-2.062000	4.240000
C	-8.260000	7.664000	-1.488000
H	-9.032000	8.380000	-1.196000

C	4.649000	-2.136000	-7.985000
H	3.654000	-2.617000	-8.039000
H	5.101000	-2.215000	-8.993000
C	-3.203000	-3.560000	8.266000
H	-3.964000	-4.115000	8.850000
H	-2.343000	-3.385000	8.941000
C	4.503000	-0.656000	-7.583000
H	3.859000	-0.131000	-8.317000
C	-9.910000	3.149000	0.353000
H	-10.378000	2.763000	-0.558000
C	-4.994000	-2.478000	6.870000
H	-5.431000	-1.516000	6.536000
H	-5.787000	-3.014000	7.428000
C	-1.093000	1.288000	8.804000
H	-1.367000	1.012000	7.784000
C	4.494000	1.910000	8.925000
H	4.847000	2.880000	8.564000
C	-9.576000	3.768000	-3.193000
H	-9.579000	4.851000	-3.034000
C	1.281000	-4.433000	9.125000
H	1.692000	-5.309000	8.617000
C	4.840000	-0.071000	10.292000
H	5.463000	-0.638000	10.989000
C	-1.543000	2.567000	10.800000
C	0.432000	1.189000	10.678000
H	1.359000	0.832000	11.138000
C	0.079000	0.773000	9.379000
C	-4.545000	-3.306000	5.654000
H	-5.407000	-3.490000	4.987000
C	-1.906000	2.182000	9.507000
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H	-8.305000	4.522000	3.626000
C	-10.075000	3.688000	2.700000
C	5.275000	1.171000	9.822000
C	-0.374000	2.077000	11.393000
H	-0.097000	2.397000	12.401000
C	0.200000	-2.201000	10.430000
H	-0.239000	-1.342000	10.946000
C	-10.660000	3.190000	1.534000
H	-11.697000	2.842000	1.548000
C	0.581000	-4.584000	10.327000
C	0.035000	-3.475000	10.980000

H	-0.517000	-3.614000	11.913000
Cl	8.058000	9.212000	1.903000
Cl	4.063000	-11.217000	-0.246000
Cl	2.998000	-6.838000	-9.136000
Cl	10.734000	3.027000	-5.827000
Cl	-5.048000	-9.944000	-4.041000
Cl	6.810000	1.805000	10.353000
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Cl	3.368000	10.125000	-6.493000
Cl	0.376000	-6.176000	11.008000
Cu	-0.063000	0.505000	0.317000
H	-1.802000	-0.971000	-1.108000
H	1.506000	-0.479000	-1.694000
H	0.495000	-1.932000	1.268000
H	0.221000	0.617000	2.807000
H	-2.231000	1.834000	-0.045000
H	1.523000	2.224000	-0.380000
H	2.789000	-0.632000	0.787000
H	-2.199000	-1.314000	1.522000
H	-0.533000	0.838000	-2.785000
H	-0.269000	3.346000	1.664000