Electronic Supporting Information

# Highly Soluble Fluorine Containing Cu(I) AlkylPyrPhos TADF Complexes

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# 1. General Information

**Column Chromatography.** The phosphine ligands described in this study were purified *via* column chromatography. For the stationary phase of the column silica gel 60 ($SiO_2$, 0.040 × 0.063 mm, 260 – 400 mesh ASTM) and sea sand (annealed and purified with hydrochloric acid), purchased from *Merck* respectively, were used. The solvents used for the column chromatography were purchased from *Fisher* in HPLC-grade and the described mixtures were prepared of the corresponding volumes of the solvents. Fractions were collected manually. Product control was performed *via* thin layer chromatography.

**Thin Layer Chromatography (TLC).** TLC aluminum plates with a fluorescence indicator, purchased from *Merck* (art. number 105554, silica gel 60 $F_{254}$, thickness 0.2 mm), were used for the analytical thin layer chromatography. The detection on the TLC plates was carried out *via* fluorescence quenching under UV light (λ = 254 nm) with a UV-lamp from *VWR*.

**Nuclear Magnetic Resonance Spectroscopy (NMR).** All NMR spectra of the AlkylPyrPhos ligands and corresponding copper complexes, described in this study, were recorded on a *Bruker* Avance 400 NMR instrument with 400 MHz for $^{1}$H NMR, 101 MHz for $^{13}$C NMR, 162 MHz for $^{31}$P NMR and 376 MHz for $^{19}$F NMR spectra. The NMR spectra were measured at room temperature in deuterated solvents commercially acquired from *Eurisotop*. The chemical shift δ is displayed in parts per million [ppm] and the $^{1}$H NMR and $^{13}$C NMR resonances of the solvents themselves were used as references: chloroform-$d_1$ ($CDCl_3$): 7.26 ppm for the $^{1}$H NMR and 77.2 ppm for the $^{13}$C NMR and dimethyl sulfoxide-$d_6$ (DMSO-$d_6$): 2.50 ppm for the $^{1}$H NMR and 39.5 ppm for the $^{13}$C NMR. Evaluation of the resonances was done according to first order spectra. For the characterization of centrosymmetrical signals, the signal's median point was chosen, for multiplets the signal range. For the description of couplings, the following abbreviations were used: d = doublet, t = triplet, dd = doublet of doublet and m = multiplet. Coupling constants '*J*' are given in Hertz [Hz], starting with the largest value. Coupling constants are given with their respective number of bindings and binding partners, as far as they could be determined, written as index of the coupling constants ($^{x}J_{HH}$ and $^{x}J_{CP}$). Resonances of the $^{1}$H NMR and $^{13}$C NMR spectra were assigned with *H-C-Heteronuclear Single Quantum Coherence* HSQC NMR spectra and *H-C-heteronuclear multiple bond correlation* NMR spectra HMBC and the help of *distortionless polarization by polarization transfer* NMR spectra DEPT90 and DEPT135.

**Mass Spectrometry (MS).** The mass spectrometrical identifications were performed either with the *electron ionization* (EI) or with the *fast atom bombardment* (FAB) mass spectrometry. An instrument by *Finnigan*, model MAT 95 (70 eV), was used. For FAB measurements 3-nitrobenzyl alcohol (3-NBA) served as internal standard. For the interpretation of the spectra the molecular peak $[M]^+$, the protonated molecular peak $[M+H]^+$ and characteristic fragment peaks are indicated with their mass to charge ratio (*m/z*) and their intensity in percent, relative to the base peak (100%). For the high resolution mass spectrometry the following abbreviation was used: calcd = calculated.

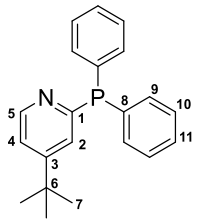
**Infrared Spectroscopy (IR).** Infrared spectra were recorded on a *Bruker*, model IFS 88. The powders were measured by the *attenuated total reflection* (ATR) method. The absorption is given in wave numbers $\bar{\upsilon}$ [$cm^{-1}$] and was measured in the range from 3600 $cm^{-1}$ to 400 $cm^{-1}$. The characterization of absorption bands was done according to the transmission strength T with the following abbreviations: vs = very strong (0−10% T), s = strong (11−40% T), m = medium (41−70% T), w = weak (71−90% T) and vw = very weak (91−100 % T).

**Elemental analysis.** The ratio of carbon (C), hydrogen (H) and nitrogen (N) in mass percentage of the synthesized compounds in this work were determined with an *Elementar*, model vario MICRO cube. The weight of the samples taken was measured with the balance Sartorius M2P. Acetanilide served as standard. The values for the elemental analysis were given with the following designations: Anal. calcd = calculated and found = actual values for the mass percentages of the CHN-analysis.

**Melting point (mp).** The melting curves of the compounds, synthesized in this study, were measured on a *Laboratory Devices Inc.*, model Mel-Temp II and were not corrected.

## 2. Experimental

### Ligands



***(2-(Diphenylphosphino)-4-tert-butylpyridine (3).***
The title ligand **3** was synthesized according to the same literature procedure as ligand **2**.[1] Colorless, microcrystalline solid (69% yield). The complete numeration for the exact NMR classification of ligand **3** is given on the left.
$\mathbf{R_f}$ (CH/EE 4/1) = 0.57; $\mathbf{R_f}$ (CH/EE 6/1) = 0.39; $\mathbf{R_f}$ (CH/EE 10/1) = 0.34. – **$^1$H NMR** (400 MHz, DMSO-$d_6$) δ [ppm] = 8.58 (d, $^3J_{HH}$ = 5.2 Hz, 1H, $H_5$), 7.42 – 7.39 (m, 6H, $H_{10}$, $H_{11}$), 7.36 – 7.30 (m, 5H, $H_4$, $H_9$), 7.08 – 7.07 (m, 1H, $H_2$), 1.13 (s, 9H, $H_7$). – **$^{13}$C NMR** (101 MHz, DMSO-$d_6$) δ [ppm] = 162.2 (d, $^1J_{CP}$ = 3.9 Hz, 1C, $C_{q1}$), 159.1 (d, $^3J_{CP}$ = 3.5 Hz, 1C, $C_{q3}$), 150.1 (d, $^3J_{CP}$ = 11.9 Hz, 1C, $C_5$), 136.2 (d, $^1J_{CP}$ = 10.9 Hz, 2C, $C_8$), 133.7 (d, $^2J_{CP}$ = 19.7 Hz, 4C, $C_9$), 129.1 (s, 2C, $C_{11}$), 128.6 (d, $^3J_{CP}$ = 7.1 Hz, 4C, $C_{10}$), 124.6 (d, $^2J_{CP}$ = 21.0 Hz, 1C, $C_2$), 119.7 (s, 1C, $C_4$), 34.4 (s, 1C, $C_{q6}$), 29.9 (s, 3C, $C_7$). – **$^{31}$P NMR** (162 MHz, DMSO-$d_6$) δ [ppm] = −4.61 (s, 1P). – **MS** (EI, 70 eV) *m/z* [%] = 320/319/318 (14/68/62) $[M]^+$, 211 (50), 196 (100). – **HRMS** ($C_{21}H_{22}NP$) calcd: 319.1490; found: 319.1491. – **IR** (ATR) $\tilde{\nu}$ [$cm^{-1}$] = 3065 (vw), 3044 (vw), 2964 (w), 2930 (w), 2866 (w), 1578 (m), 1530 (w), 1477 (w), 1454 (w), 1434 (m), 1377 (m), 1309 (w), 1266 (w), 1152 (w), 1092 (w), 1068 (w), 1028 (w), 988 (w), 846 (m), 743 (m), 696 (s), 633 (w), 495 (m), 469 (m), 429 (w), 401 (w). – Anal. calcd for **$C_{21}H_{22}NP$** (319.2): C 78.97, H 6.94, N 4.39; found: C 79.06, H 6.92, N 4.39. – **mp** = 111-113 °C. A molecular structure of the ligand was obtained.

### Cu(I) Complexes

***[(2-(Diphenylphosphino)pyridine)(tris(4-trifluoromethylphenyl)phosphine)$_2$Cu$_2$I$_2$]*** **(Cu-1c).**
The title compound was synthesized according to the general procedure. Complex **Cu-1c** could not be precipitated due to the high solubility in every kind of solvent. Therefore the solvent was removed completely and the obtained solid was washed with very small amounts of *n*-pentane and diethyl ether. Yellow powder (96% yield).
**$^1$H NMR** (400 MHz, DMSO-$d_6$) δ [ppm] = 8.73 (bs, 1H, $H_{Pyr}$), 7.96 (bs, 1H, $H_{Pyr}$), 7.84 – 7.27 (m, 36H). – **$^{13}$C NMR** (101 MHz, DMSO-$d_6$) δ [ppm] = 137.1 (d, *J* = 24.0 Hz), 134.5 (d, *J* = 14.0 Hz), 133.3 (d, *J* = 13.3 Hz), 131.8 (d, *J* = 26.1 Hz), 131.0 (s), 130.5 (d, *J* = 32.1 Hz), 130.1 (d, *J* = 7.4 Hz), 128.6 (d, *J* = 8.0 Hz), 127.9 (s), 125.5 (bd, *J* = 4.3 Hz), 125.1 (s), 122.4 (s), 119.7 (s). – **$^{31}$P NMR** (162 MHz, $CDCl_3$) δ [ppm] = −4.71 (bs, 1P, $P_{PyrPhos}$), −12.65 (bs, 2P, $P_{(CF3\text{-}Ph)3P}$). – **$^{19}$F NMR** (376 MHz, DMSO-$d_6$) δ [ppm] = −66.08 (s, 18F, $F_{(CF3\text{-}Ph)3P}$). – **MS** (FAB, 3-NBA) *m/z* [%] = 1637 (1) $[M+Cu]^+$, 1374 (1) $[Cu_3I_2P_2]^+$, 1184 (3) $[Cu_2IP_2]^+$, 792 (17) $[CuLP]^+$, 705 (75) $[Cu_3I_2L]^+$, 589 (21) $[CuL_2]^+$, 515 (80) $[Cu_2IL]^+$, 467 (16) $[P+H]^+$, 326 (100) $[CuL]^+$, 264 (19) $[L+H]^+$, 185 (14) $[PPh_2]^+$. – **IR** (ATR) $\tilde{\nu}$ [$cm^{-1}$] = 3055 (vw), 1607 (vw), 1436 (vw), 1397 (w), 1319 (m), 1166 (w), 1122 (m), 1059 (m), 1014 (w), 829 (w), 764 (vw), 742 (w), 702 (w), 693 (w), 634 (vw), 597 (w), 518 (w), 411 (w). – Anal. Calcd for **$C_{59}H_{38}Cu_2F_{18}I_2NP_3$** (1574.8): C 44.94, H 2.43, N 0.89; found: C 44.81, H 2.16, N 0.95.

***[(2-(Diphenylphosphino)pyridine)(tris(4-chlorophenyl)phosphine)$_2$Cu$_2$I$_2$]*** **(Cu-1d).**
Complex **Cu-1d** was synthesized according to the general procedure. Pale yellow powder (66% yield). **$^1$H NMR** (400 MHz, DMSO-$d_6$) δ [ppm] = 8.70 (bs, 1H, $H_{Pyr}$), 7.92 (t, $^3J_{HH}$ = 8.0 Hz, 1H, $H_{Pyr}$), 7.66 – 7.30 (m, 36H). – **$^{13}$C NMR** (101 MHz, DMSO-$d_6$) δ [ppm] = 135.3 (d, $J_{CP}$ = 16.8 Hz), 133.4 (d, $J_{CP}$ = 11.5 Hz), 131.4 (d, $J_{CP}$ = 27.3 Hz), 130.1 (s), 128.8 (d, $J_{CP}$ = 8.6 Hz), 128.6 (d, $J_{CP}$ = 7.5 Hz). – **$^{31}$P NMR** (162 MHz, DMSO-$d_6$) δ [ppm] = −5.06 (bs, 1P, $P_{PyrPhos}$), −13.06 (bs, 2P, $P_{(Cl\text{-}Ph)3P}$). – **MS** (FAB, 3-NBA) *m/z* [%] = 1433 (5) $[M+Cu]^+$, 1371 (4) $[M+H]^+$, 1243 (7) $[M\text{-}I]^+$, 1069 (16) $[Cu_3I_2LP]^+$, 980 (13) $[Cu_2IP_2]^+$, 968 (63) $[Cu_3I_2L_2]^+$,879 (43) $[Cu_2ILP]^+$, 806 (20) $[Cu_3I_2P]^+$, 790 (29) $[CuP_2]^+$. – **IR** (ATR) $\tilde{\nu}$ [$cm^{-1}$] = 1573 (vw), 1557 (vw), 1478 (w), 1454 (vw), 1433 (vw), 1384 (w), 1183 (vw), 1079 (w), 1012 (w), 817 (w), 767 (vw), 743 (m), 694 (w), 631 (vw), 554 (w), 541 (w), 519 (w), 494 (m), 438 (w), 425 (w), 384 (w). – Anal. calcd for **$C_{53}H_{38}Cl_6Cu_2I_2NP_3$** (1370.7): C 46.28, H 2.78, N 1.02; found: C 46.75, H 2.80 N 1.16. A molecular structure of the complex was obtained.

***[(4-Methyl-2-(diphenylphosphino)pyridine)(tris(4-chlorophenyl)phosphine)$_2$Cu$_2$I$_2$]*** **(Cu-2d).**
The complex was obtained according to the general procedure. Pale yellow powder (55% yield). **$^1$H NMR** (400 MHz, DMSO-$d_6$) δ [ppm] = 8.66 (bs, 1H, $H_{Pyr}$), 7.44 – 7.31 (m, 36H), 2.28 (s, 3H, $H_{Me}$). – **$^{13}$C NMR** (101 MHz, DMSO-$d_6$) δ [ppm] = 135.3 (d, $J_{CP}$ = 15.6 Hz), 133.3 (m), 131.4 (d, $J_{CP}$ = 27.6 Hz), 130.1 (s) 128.8 (d, $J_{CP}$ = 8.8 Hz), 128.6 (d, $J_{CP}$ = 7.8 Hz), 21.8 (s, 1C, $C_{Me}$). – **$^{31}$P NMR** (162 MHz, DMSO-$d_6$) δ [ppm] = −4.73 (bs, 1P, $P_{MePyrPhos}$), −12.98 (bs, 2P, $P_{(Cl\text{-}Ph)3P}$). – **MS** (FAB, 3-NBA) *m/z* [%] = 1447 (2) $[M+Cu]^+$, 1275 (1) $[M\text{-}I]^+$, 1083 (2) $[Cu_3I_2LP]^+$, 893 (8) $[Cu_2ILP]^+$, 790 (5) $[CuP_2]^+$, 719 (28) $[Cu_3I_2L]^+$, 704 (10) $[CuLP]^+$, 529 (56) $[Cu_2IL]^+$, 426 (7) $[CuP]^+$, 340 (66) $[CuL]^+$, 278 (21) $[L+H]^+$. – **IR** (ATR) $\tilde{\nu}$ [$cm^{-1}$] = 2950 (vw), 1573 (w), 1478 (m), 1436 (w), 1385 (w), 1183 (vw), 1097 (w), 1079 (m), 1013 (m), 816 (m), 743 (m), 692 (w), 631 (vw), 556 (w), 541 (m), 519 (m), 493 (m), 464 (w), 436 (w), 383 (w). – Anal. calcd for **$C_{54}H_{40}Cl_6Cu_2I_2NP_3$** (1384.7): C 46.68, H 2.90, N 1.01; found: C 46.78, H 3.09, N 1.12. A molecular structure of the complex with two molecules of dichloromethane was obtained.

***[(2-(Diphenylphosphino)-4-tert-butylpyridine)(triphenylphosphine)$_2$Cu$_2$I$_2$]*** **(Cu-3a).**
Compound **Cu-3a** was synthesized according to the general procedure. Pale yellow powder (83% yield). **$^1$H NMR** (400 MHz, DMSO-$d_6$) δ [ppm] = 8.53 (bs, 1H, $H_{Pyr}$), 7.62 (m, 1H, $H_{Pyr}$), 7.45 – 7.27 (m, 41H), 1.10 (s, 9H, $H_{tertBu}$). – **$^{13}$C-NMR** (101 MHz, DMSO-$d_6$) δ [ppm] = 133.7 (d, $J_{CP}$ = 13.8 Hz), 133.1 (d, $J_{CP}$ = 27.9 Hz), 129.8 (bs), 128.5 (d, $J_{CP}$ = 8.1 Hz), 34.8 (s, $C_{tertBu}$), 29.7 (s, $C_{tertBu}$). – **$^{31}$P NMR** (162 MHz, DMSO-$d_6$) δ [ppm] = −5.04 (bs, 1P, $P_{tertBuPyrPhos}$), −9.98 (bs, 2P, $P_{PPh3}$). – **MS** (FAB, 3-NBA) *m/z* [%] = 1285 (2) $[M+Cu]^+$, 1096 (2) $[M\text{-}I]^+$, 1023 (4) $[Cu_3I_2LP]^+$, 834 (15) $[Cu_2ILP]^+$, 761 (26) $[Cu_3I_2L]^+$, 644 (56) $[CuLP]^+$, 571 (72) $[Cu_2IL]^+$, 382 (100) $[CuL]^+$, 325 (28) $[CuP]^+$, 320 (22) $[L+H]^+$, 263 (16) $[P+H]^+$. – **IR** (ATR) $\tilde{\nu}$ [$cm^{-1}$] = 2961 (vw), 1585 (vw), 1479 (w), 1434 (w), 1382 (vw), 1156 (vw), 1093 (w), 1027 (vw), 998 (vw), 844 (vw), 741 (w), 692 (m), 518 (m), 504 (m), 427 (vw). – Anal. calcd for **$C_{57}H_{52}Cu_2I_2NP_3$** (1223.0): C 55.89, H 4.28, N 1.14; found: C 55.51, H 4.27, N 1.17.

***[(2-(Diphenylphosphino)-4-tert-butylpyridine)(tris(4-fluorophenyl)phosphine)$_2$Cu$_2$I$_2$]*** **(Cu-3b).**
The complex **Cu-3b** was synthesized according to the general procedure. Pale yellow, microcrystalline solid (57% yield).
**$^1$H NMR** (400 MHz, DMSO-d$_6$) δ [ppm] = 8.50 (bs, 1H, H$_{Pyr}$), 7.62 (bs, 1H, H$_{Pyr}$), 7.57 – 7.00 (m, 35H), 1.11 (s, 9H, H$_{tertBu}$). – **$^{13}$C-NMR** (101 MHz, DMSO-d$_6$) δ [ppm] = 164.4 (s), 162.0 (s), 136.0 (q, *J* = 15.5 Hz, *J* = 8.3 Hz), 133.3 (bd, *J* = 13.0 Hz), 130.0 (s), 129.0 (d, *J* = 27.9 Hz), 128.5 (d, *J* = 7.7 Hz), 115.9 (dd, *J* = 21.2 Hz, *J* = 9.3 Hz), 34.9 (s, C$_{tertBu}$), 29.7 (s, C$_{tertBu}$). – **$^{31}$P NMR** (162 MHz, DMSO-d$_6$) δ [ppm] = −4.76 (bs, 1P, P$_{tertBuPyrPhos}$), −14.47 (bs, 2P, P$_{(F-Ph)3P}$). – **$^{19}$F NMR** (376 MHz, DMSO-d$_6$) δ [ppm] = −114.82 (s, 6F, F$_{(F-Ph)3P}$). – **MS** (FAB, 3-NBA) *m/z* [%] = 1393 (1) [M+Cu]$^+$, 1077 (3) [Cu$_3$I$_2$LP]$^+$, 887 (7) [Cu$_2$ILP]$^+$, 884 (2) [Cu$_2$IP$_2$]$^+$, 761 (32) [Cu$_3$I$_2$L]$^+$, 698 (25) [CuLP]$^+$, 695 (6) [CuP$_2$]$^+$, 571 (74) [Cu$_2$IL]$^+$, 382 (100) [CuL]$^+$, 320 (22) [L+H]$^+$, 317 (14) [P+H]$^+$. – **IR** (ATR) $\tilde{\nu}$ [cm$^{-1}$] = 2962 (vw), 1586 (m), 1493 (m), 1434 (w), 1393 (w), 1225 (m), 1158 (m), 1092 (w), 1013 (w), 824 (m), 742 (w), 693 (w), 634 (w), 520 (m), 467 (w), 432 (m). – Anal. calcd for **C$_{57}$H$_{46}$Cu$_2$F$_6$I$_2$NP$_3$** (1330.9): C 51.37, H 3.48, N 1.05; found: C 51.26, H 3.48, N 1.13. A molecular structure of the complex was obtained.

***[(4-(Cyclopentylmethyl)-2-(diphenylphosphino)pyridine)(triphenylphosphine)$_2$Cu$_2$I$_2$]*** **(Cu-4a).**
Complex **Cu-4a** was obtained according to the general procedure. Pale yellow powder (99% yield).
**$^1$H NMR** (400 MHz, DMSO-d$_6$) δ [ppm] = 8.45 (bs, 1H, H$_{Pyr}$), 7.45 – 7.22 (m, 43H), 2.52 (bs, 1H, H$_{CH2}$), 1.88 (sept, $^3J_{HH}$ = 7.6 Hz, 1H, H$_{CH}$), 1.52 – 1.41 (m, 4H, H$_{Alkyl}$), 1.40 – 1.36 (m, 2H, H$_{Alkyl}$), 1.01 – 0.93 (m, 2H, H$_{Alkyl}$). – **$^{13}$C NMR** (101 MHz, DMSO-d$_6$) δ [ppm] = 133.7 (d, $J_{CP}$ = 13.8 Hz), 133.1 (d, $J_{CP}$ = 27.8 Hz), 129.8 (s), 128.4 (d, $J_{CP}$ = 8.4 Hz), 31.6 (s), 24.3 (s). – **$^{31}$P NMR** (162 MHz, DMSO-d$_6$) δ [ppm] = −5.35 (bs, 1P, P$_{CyclopentPyrPhos}$), −11.10 (bs, 2P, P$_{PPh3}$). – **MS** (FAB, 3-NBA) *m/z* [%] = 1311 (1) [M+Cu]$^+$, 1049 (3) [Cu$_3$I$_2$LP]$^+$, 860 (6) [Cu$_2$ILP]$^+$, 787 (21) [Cu$_3$I$_2$L]$^+$, 670 (49) [CuLP]$^+$, 597 (62) [Cu$_2$IL]$^+$, 587 (33) [CuP$_2$]$^+$, 408 (100) [CuL]$^+$, 346 (21) [L+H]$^+$, 325 (42) [CuP]$^+$, 263 (25) [P+H]$^+$. – **IR** (ATR) $\tilde{\nu}$ [cm$^{-1}$] = 3047 (vw), 2949 (w), 2860 (vw), 1812 (vw), 1586 (w), 1542 (vw), 1479 (w), 1433 (w), 1388 (w), 1308 (vw), 1182 (w), 1156 (vw), 1093 (w), 1068 (w), 1027 (w), 997 (w), 846 (vw), 740 (m), 691 (m), 618 (vw), 515 (m), 468 (w), 425 (w). – Anal. calcd for **C$_{59}$H$_{54}$Cu$_2$I$_2$NP$_3$** (1249.0): C 56.65, H 4.35, N 1.12; found: C 56.18, H 4.40, N 1.16. A molecular structure of the complex with two molecules of dichloromethane was obtained.

***[(4-(Cyclopentylmethyl)-2-(diphenylphosphino)pyridine)(tris(4-fluorophenyl)phosphin)$_2$Cu$_2$I$_2$]*** **(Cu-4b).**
The title complex was obtained via the general procedure. Pale yellow powder (91% yield).
**$^1$H NMR** (400 MHz, DMSO-d$_6$) δ [ppm] = 8.64 (bs, 1H, H$_{Pyr}$), 7.80 – 7.22 (m, 36H), 2.57 (d, $^3J_{HH}$ = 7.5 Hz, 2H, H$_{CH2}$), 1.91 (sept, $^3J_{HH}$ = 7.4 Hz, 1H, H$_{CH}$), 1.54 – 1.43 (m, 4H, H$_{Alkyl}$), 1.42 – 1.36 (m, 2H, H$_{Alkyl}$), 1.04 – 0.95 (m, 2H, H$_{Alkyl}$). – **$^{13}$C NMR** (101 MHz, DMSO-d$_6$) δ [ppm] = 164.5 (s), 162.0 (s), 136.0 (q, *J* = 15.8 Hz, *J* = 8.3 Hz), 133.3 (bs), 130.1 (s), 128.9 (d, *J* = 27.7 Hz), 128.6 (d, *J* = 6.8 Hz), 115.9 (dd, *J* = 21.3 Hz, *J* = 9.5 Hz), 31.6 (s), 24.3 (s). – **$^{31}$P NMR** (162 MHz, DMSO-d$_6$) δ [ppm] = −5.09 (bs, 1P, P$_{CyclopentPyrPhos}$), −12.90 (bs, 2P, P$_{(F-Ph)3P}$). – **$^{19}$F NMR** (376 MHz, DMSO-d$_6$) δ [ppm] = −114.79 (s, 6F, F$_{(F-Ph)3P}$). – **MS** (FAB, 3-NBA) *m/z* [%] = 1419 (1) [M+Cu]$^+$, 1103 (2) [Cu$_3$I$_2$LP]$^+$, 913 (6) [Cu$_2$ILP]$^+$, 884 (3) [Cu$_2$IP$_2$]$^+$, 787 (36) [Cu$_3$I$_2$L]$^+$, 724 (25) [CuLP]$^+$, 695 (9) [CuP$_2$]$^+$, 597 (72) [Cu$_2$IL]$^+$, 408 (100) [CuL]$^+$, 378 (24) [CuP]$^+$, 346 (21) [L+H]$^+$, 317 (14) [P+H]$^+$. – **IR** (ATR) $\tilde{\nu}$ [cm$^{-1}$] = 3053 (vw), 2949 (vw), 2860 (vw), 1586 (m), 1493 (m), 1434 (w), 1392 (w), 1300 (vw), 1223 (m), 1158 (m), 1092 (w), 1013 (w), 825 (m), 742 (w), 693 (m), 634 (w), 517 (m), 496 (w), 467 (m), 443 (m), 431 (m). – Anal. calcd for **C$_{59}$H$_{48}$Cu$_2$F$_6$I$_2$NP$_3$** (1356.9): C 52.15, H 3.56, N 1.03; found: C 51.14, H 3.50, N 1.10. A molecular structure of the complex with one molecule of dichloromethane was obtained.

# 3. Spectroscopic Data

## Ligands

*4-Methyl-2-(diphenylphosphino)pyridine* (**MePyrPhos**)

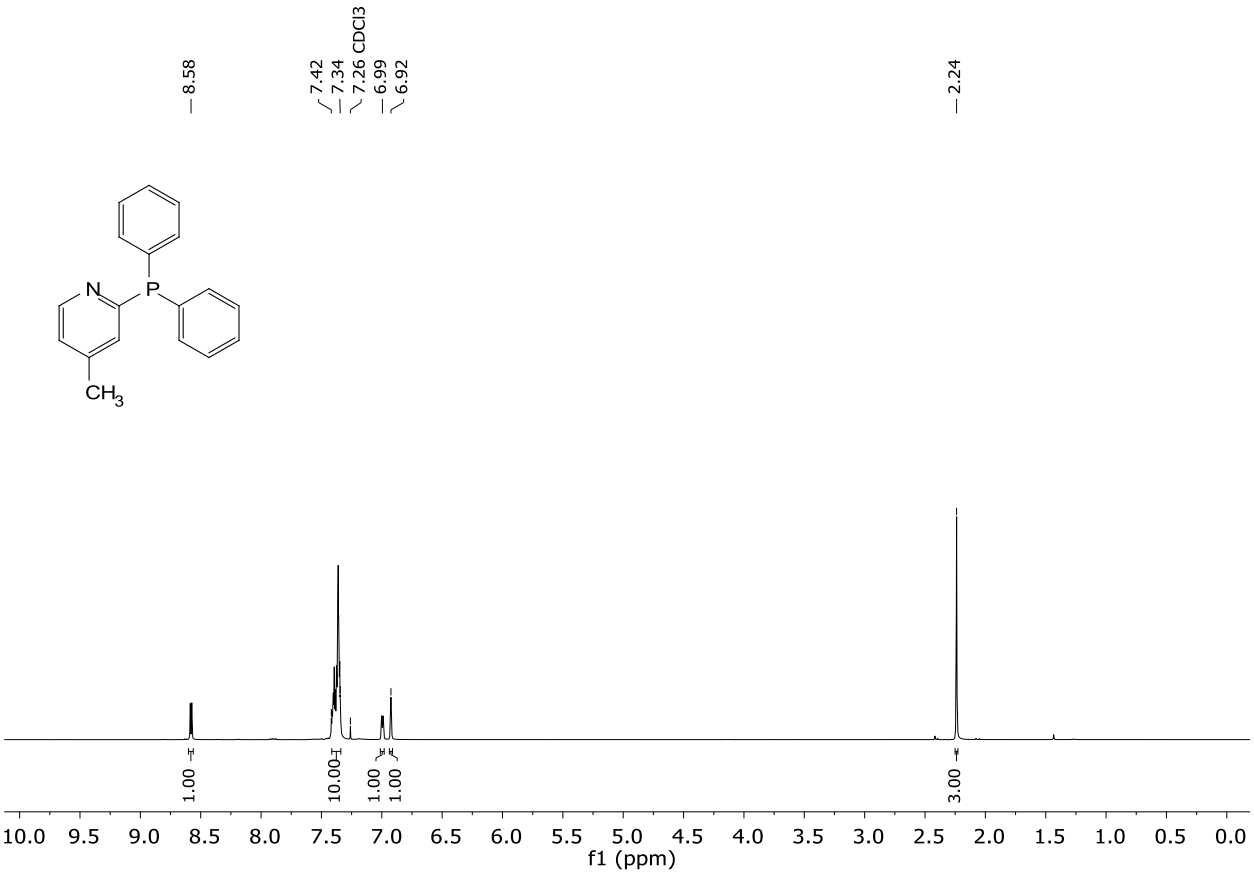



**Figure S1.** $^{1}$H NMR of **MePyrPhos** (**2**) in $CDCl_3$, 400 MHz.

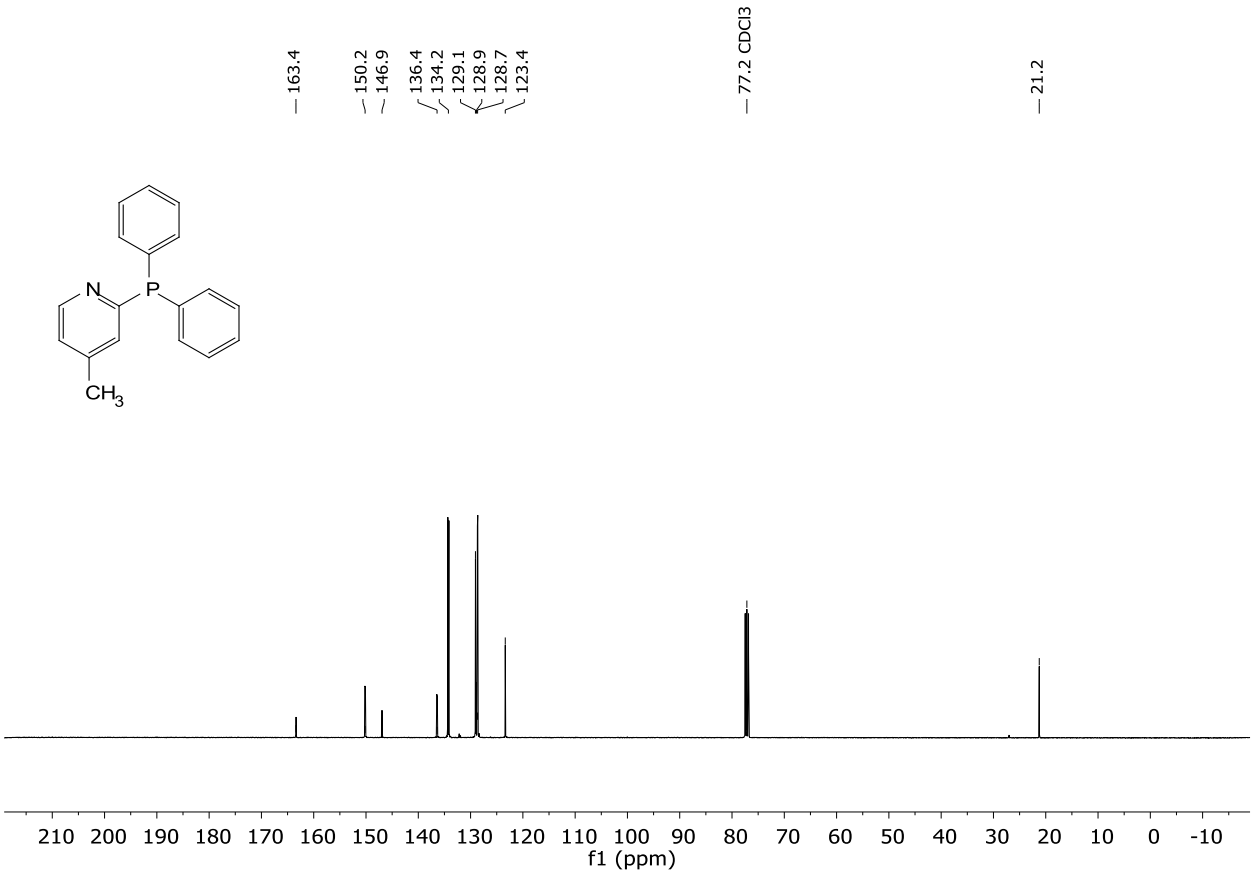



**Figure S2.** $^{13}C$ NMR of **MePyrPhos** (**2**) in $CDCl_3$, 400 MHz.

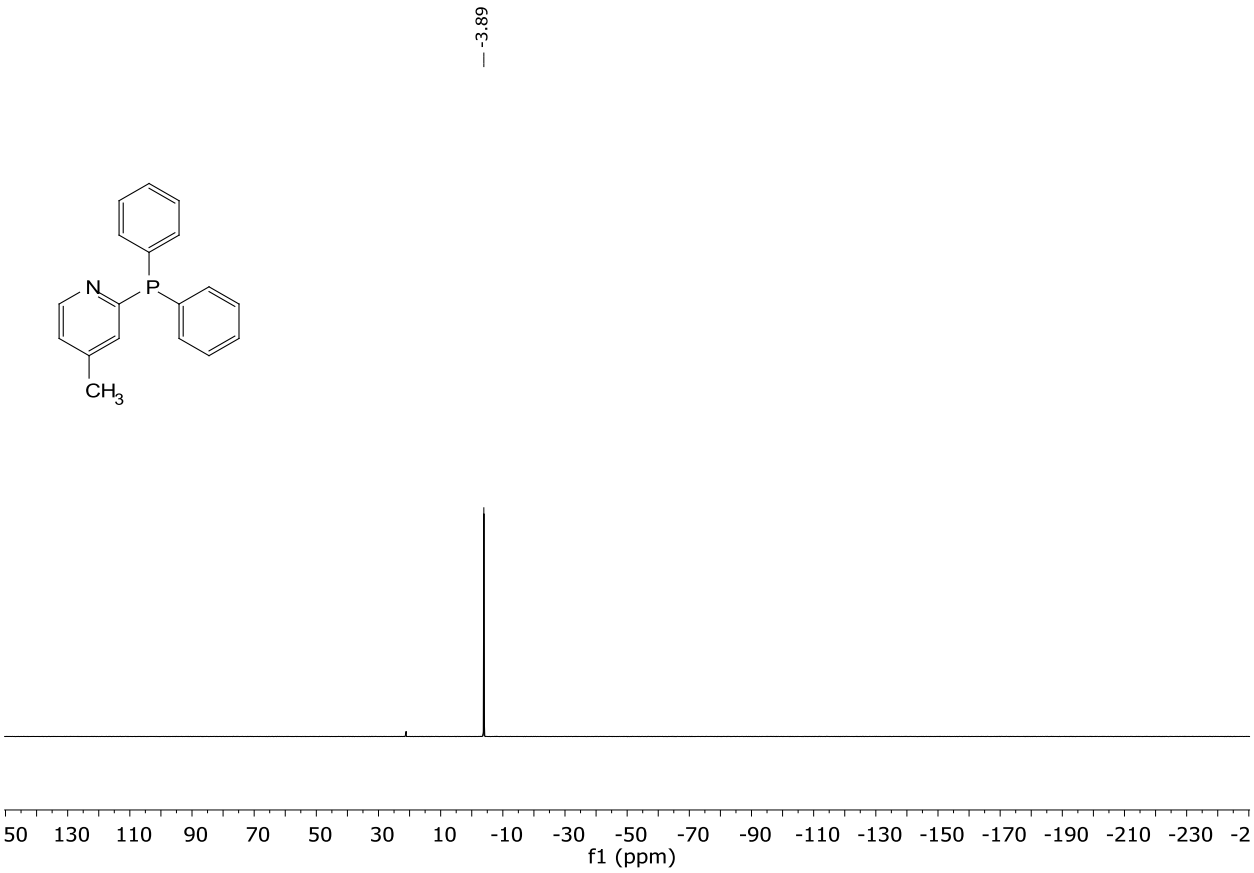



**Figure S3.** $^{31}P$ NMR of **MePyrPhos** (**2**) in $CDCl_3$, 400 MHz.

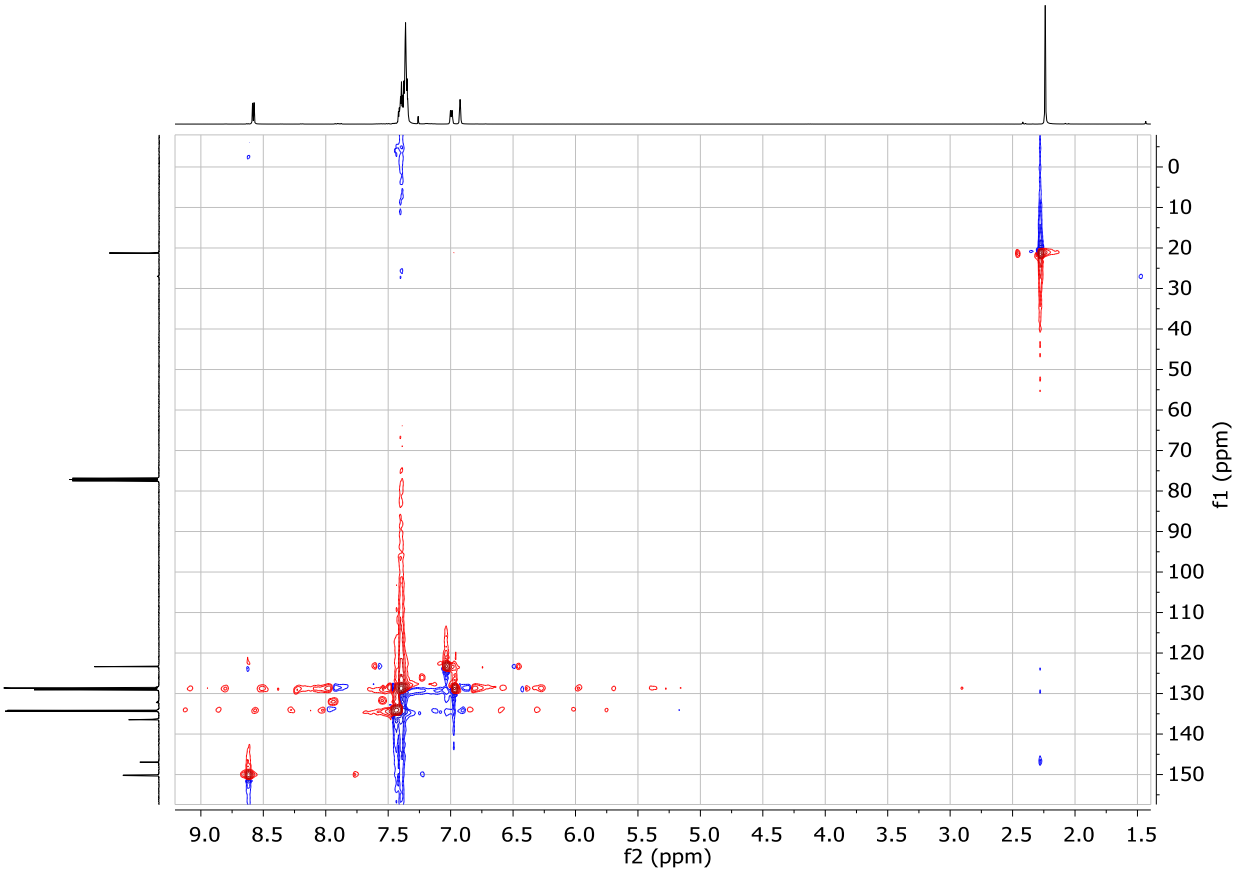



**Figure S4.** HSQC of **MePyrPhos** (**2**) in $CDCl_3$, 400 MHz.

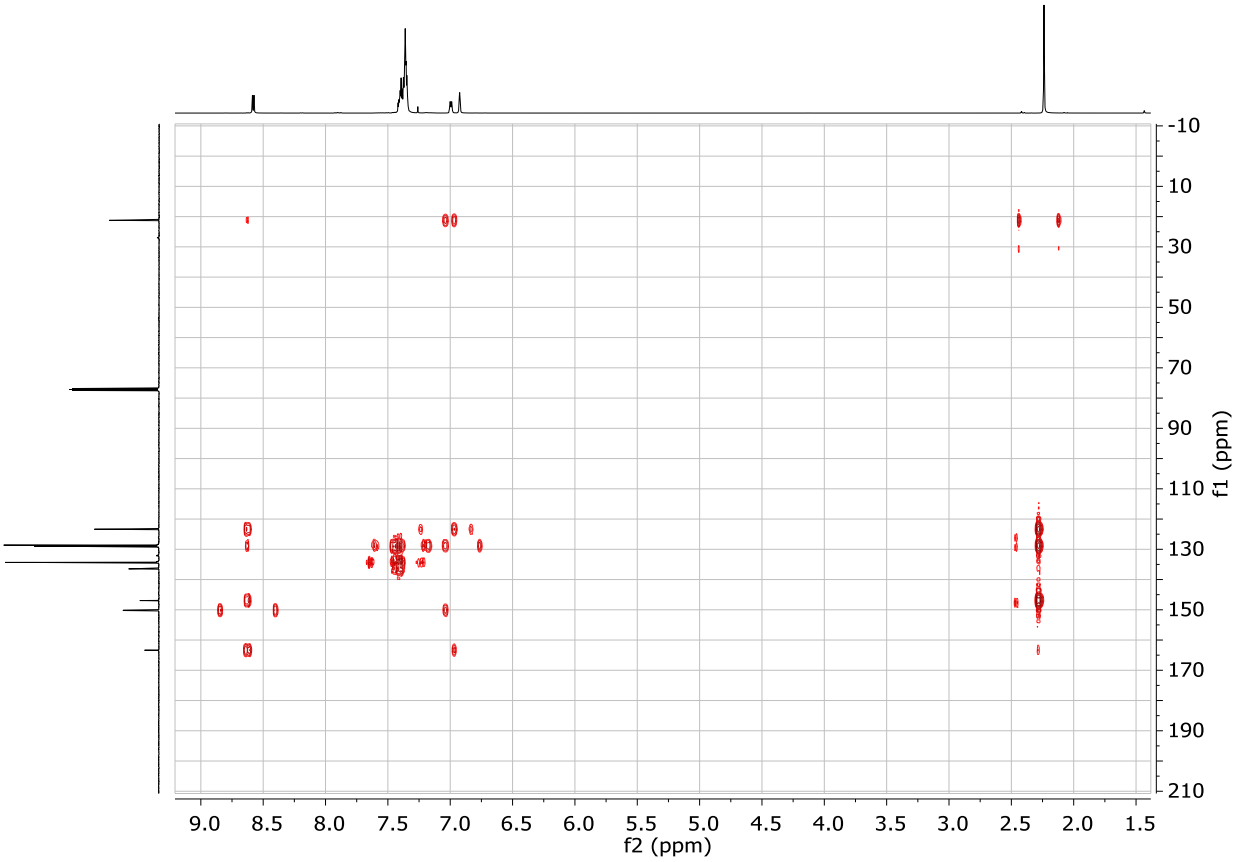



**Figure S5.** HMBC of **MePyrPhos** (**2**) in $CDCl_3$, 400 MHz.

*2-(Diphenylphosphino)-4-tertbutylpyridine* (***tert*BuPyrPhos**)

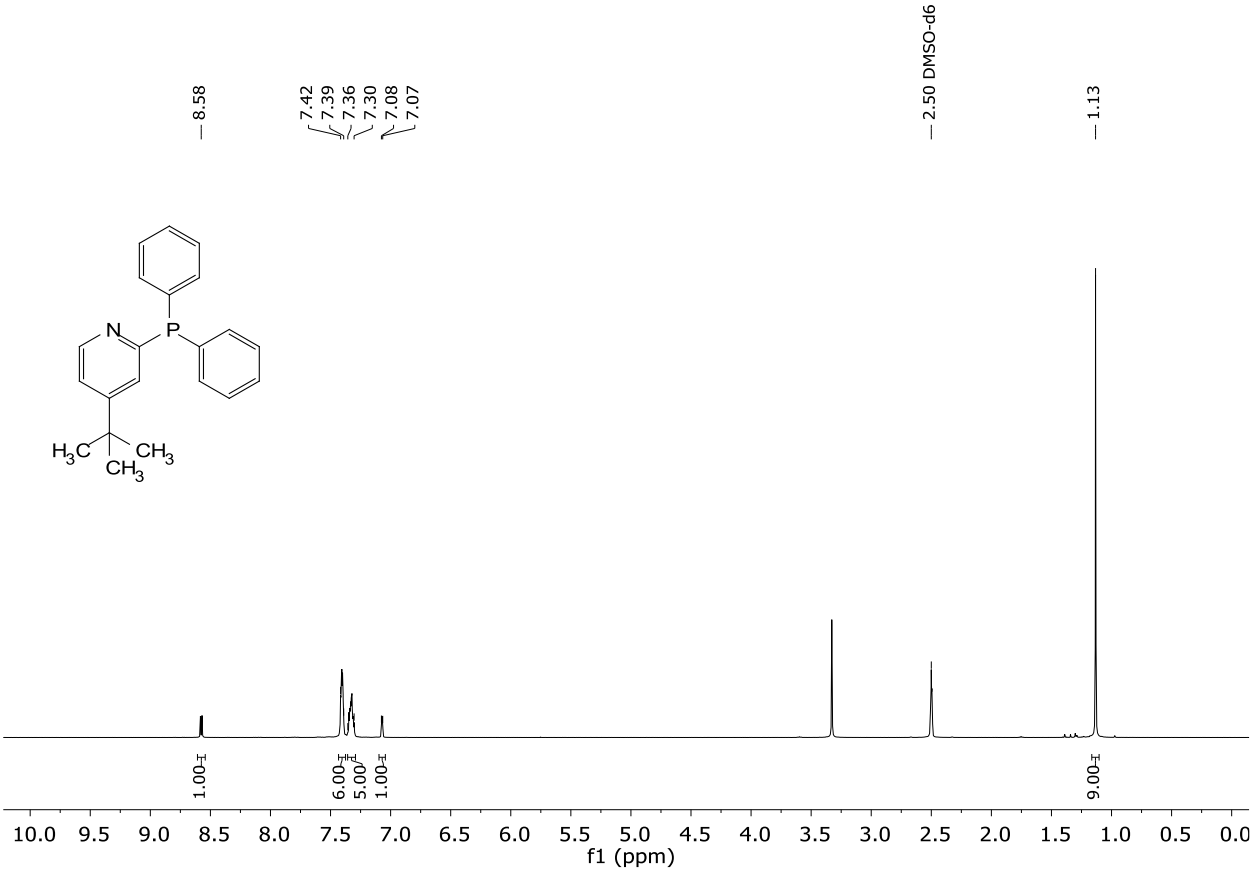



**Figure S6.** $^{1}$H NMR of ***tert*BuPyrPhos** (**3**) in DMSO-$d_6$, 400 MHz.

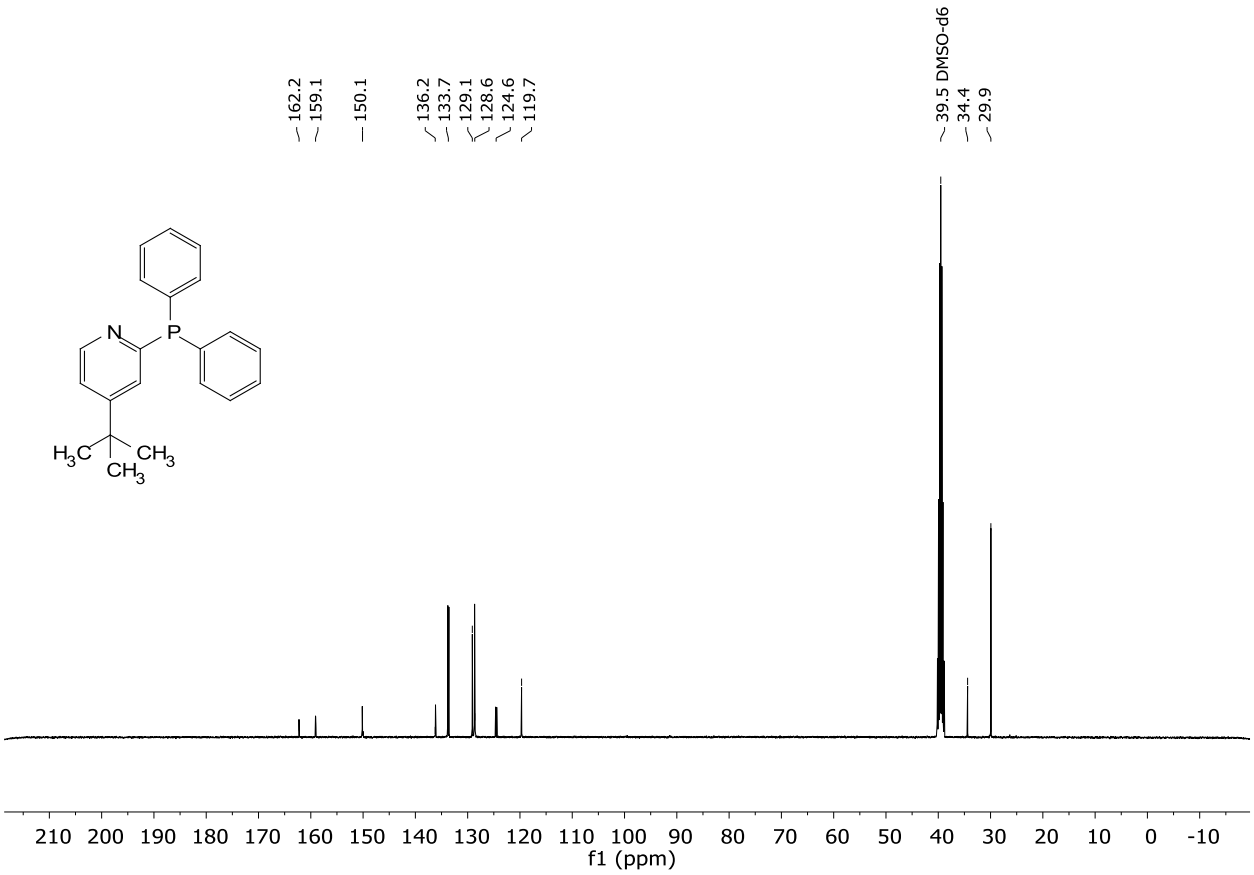



**Figure S7.** $^{13}$C NMR of ***tert*BuPyrPhos** (**3**) in DMSO-$d_6$, 400 MHz.

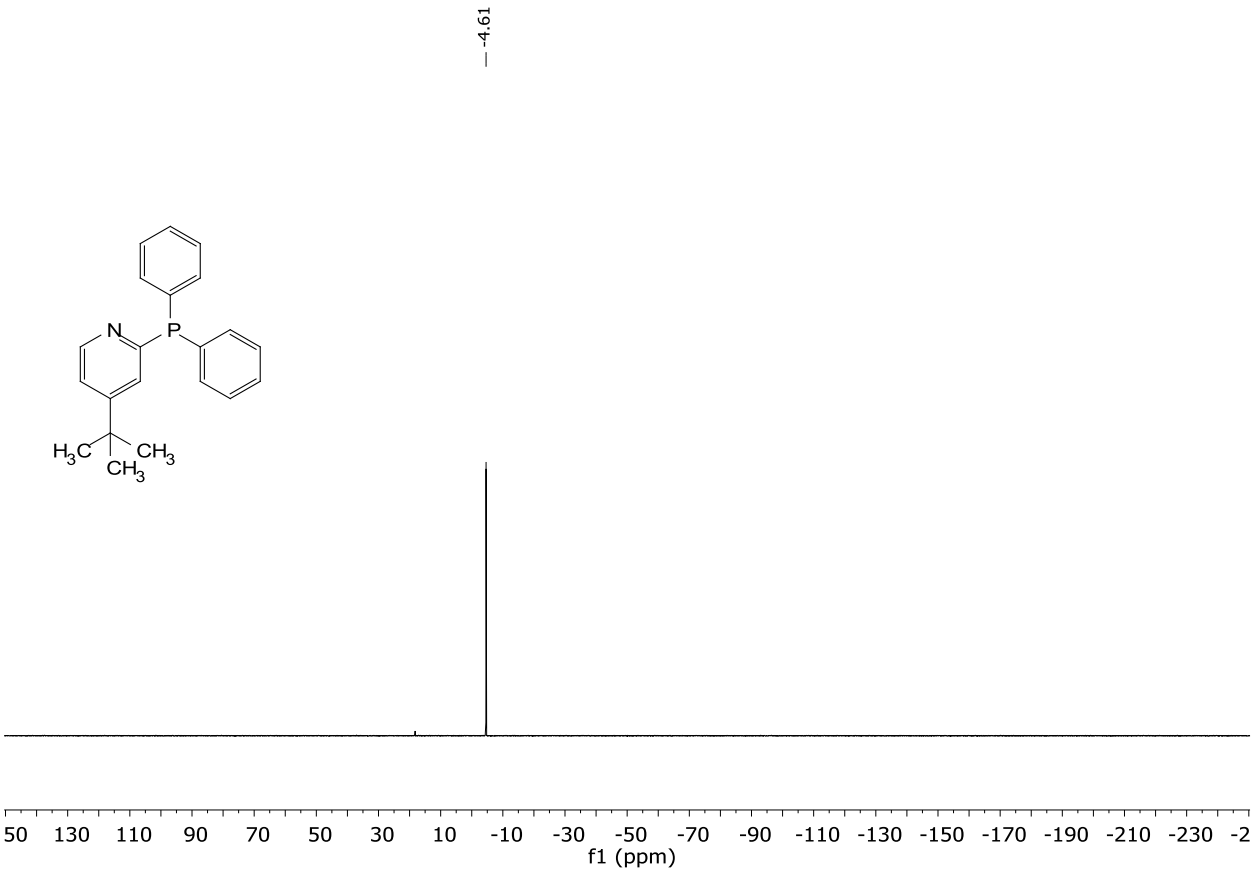



**Figure S8.** $^{31}$P NMR of ***tert*BuPyrPhos** (**3**) in DMSO-$d_6$, 400 MHz.

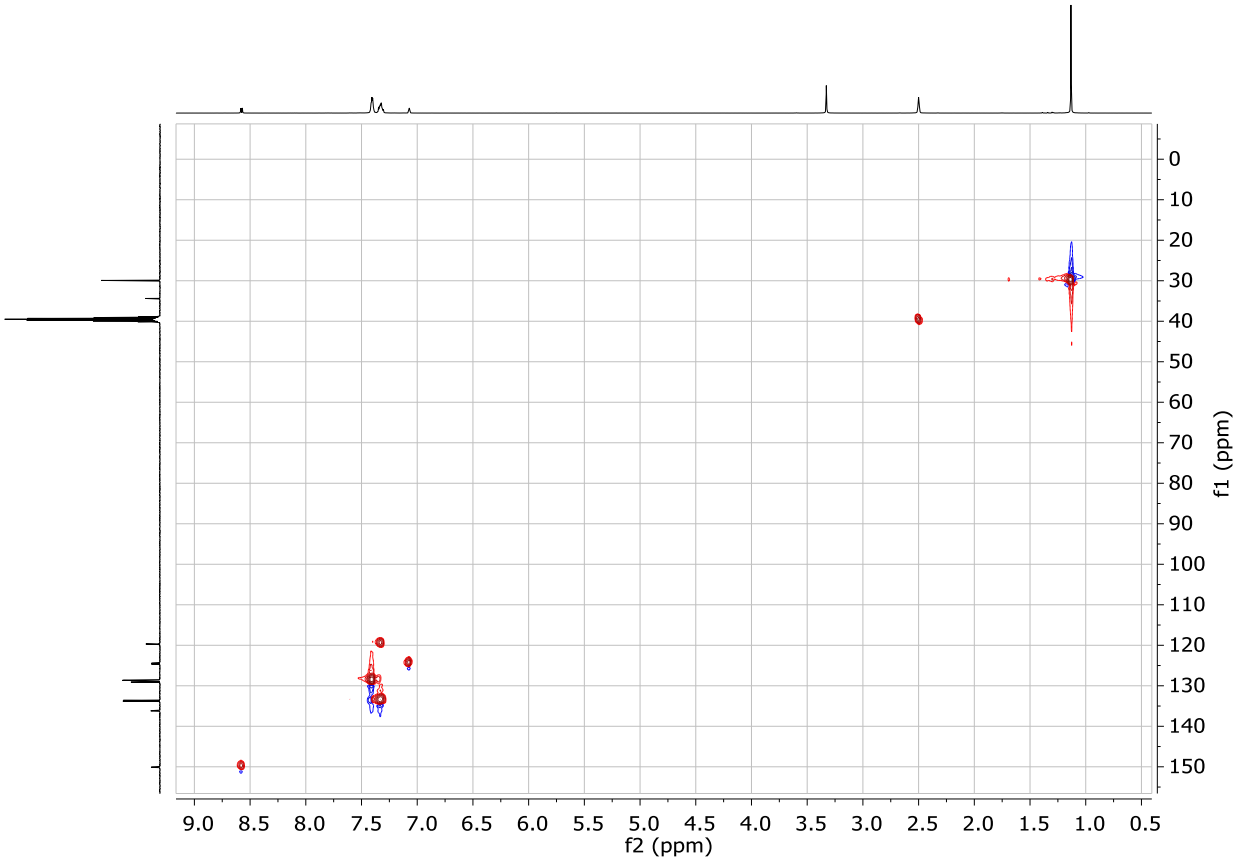



**Figure S9.** HSQC of ***tert*BuPyrPhos** (**3**) in DMSO-$d_6$, 400 MHz.

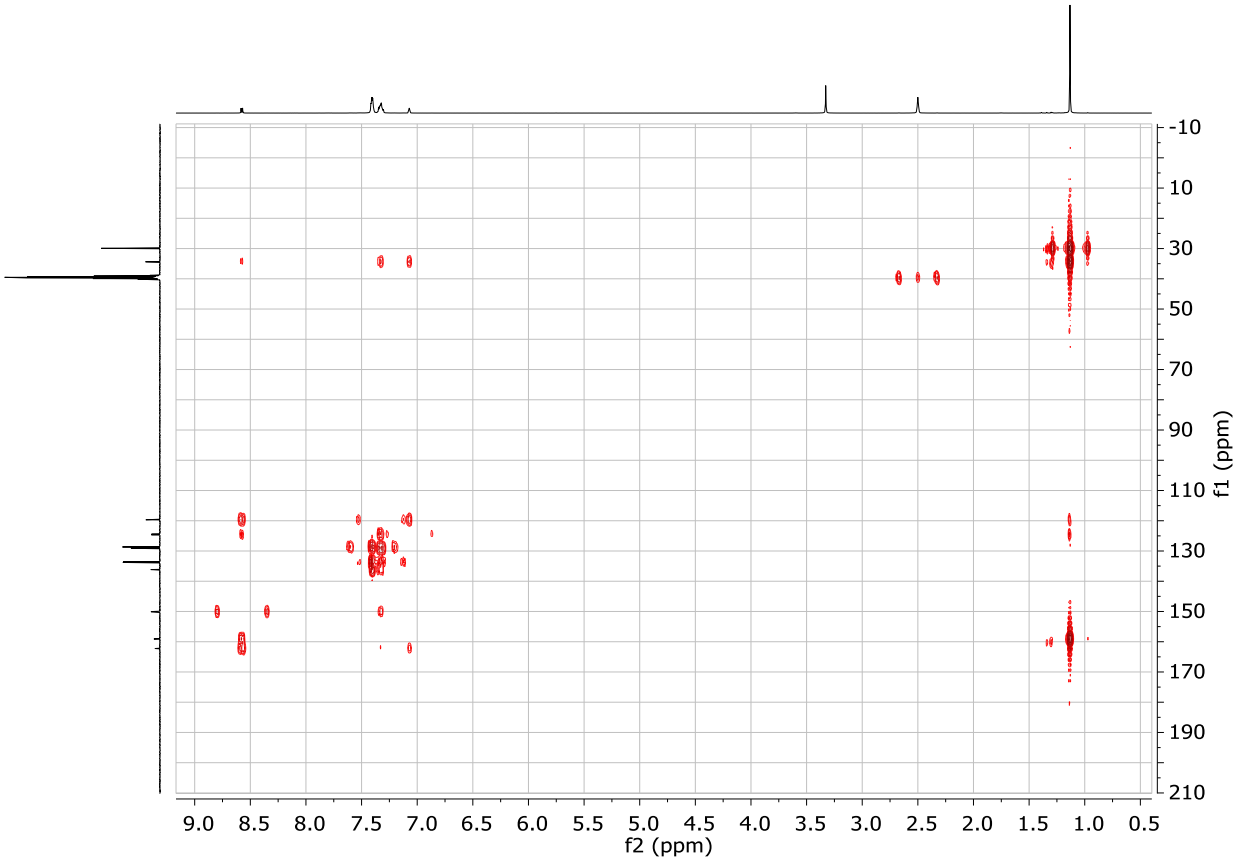



**Figure S10.** HMBC of ***tert*BuPyrPhos** (**3**) in DMSO-$d_6$, 400 MHz.

*(4-(Cyclopentylmethyl)-2-(diphenylphosphino)pyridine* (**CyclopentPyrPhos**)

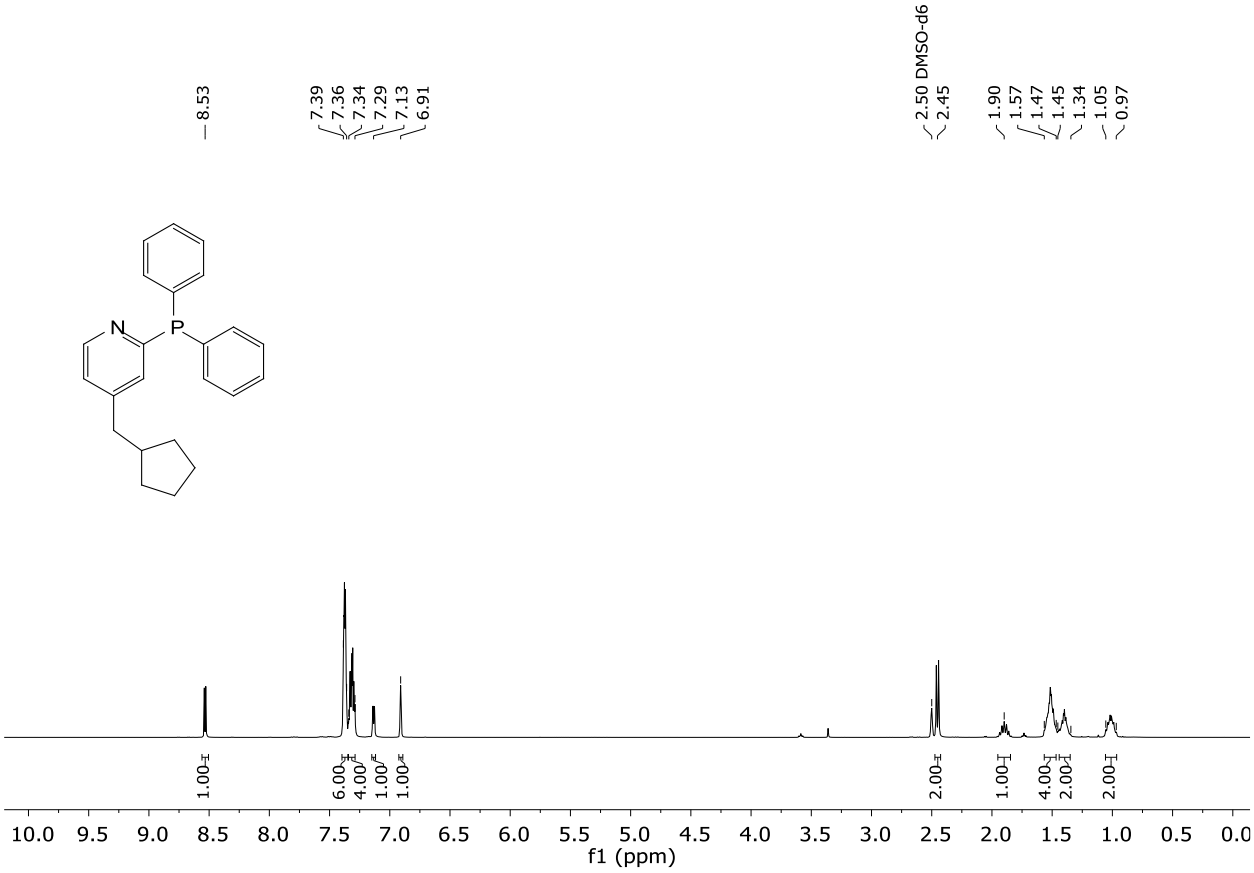



**Figure S11.** $^{1}$H NMR of ligand **CyclopentPyrPhos** (**4**) in DMSO-$d_6$, 400 MHz.

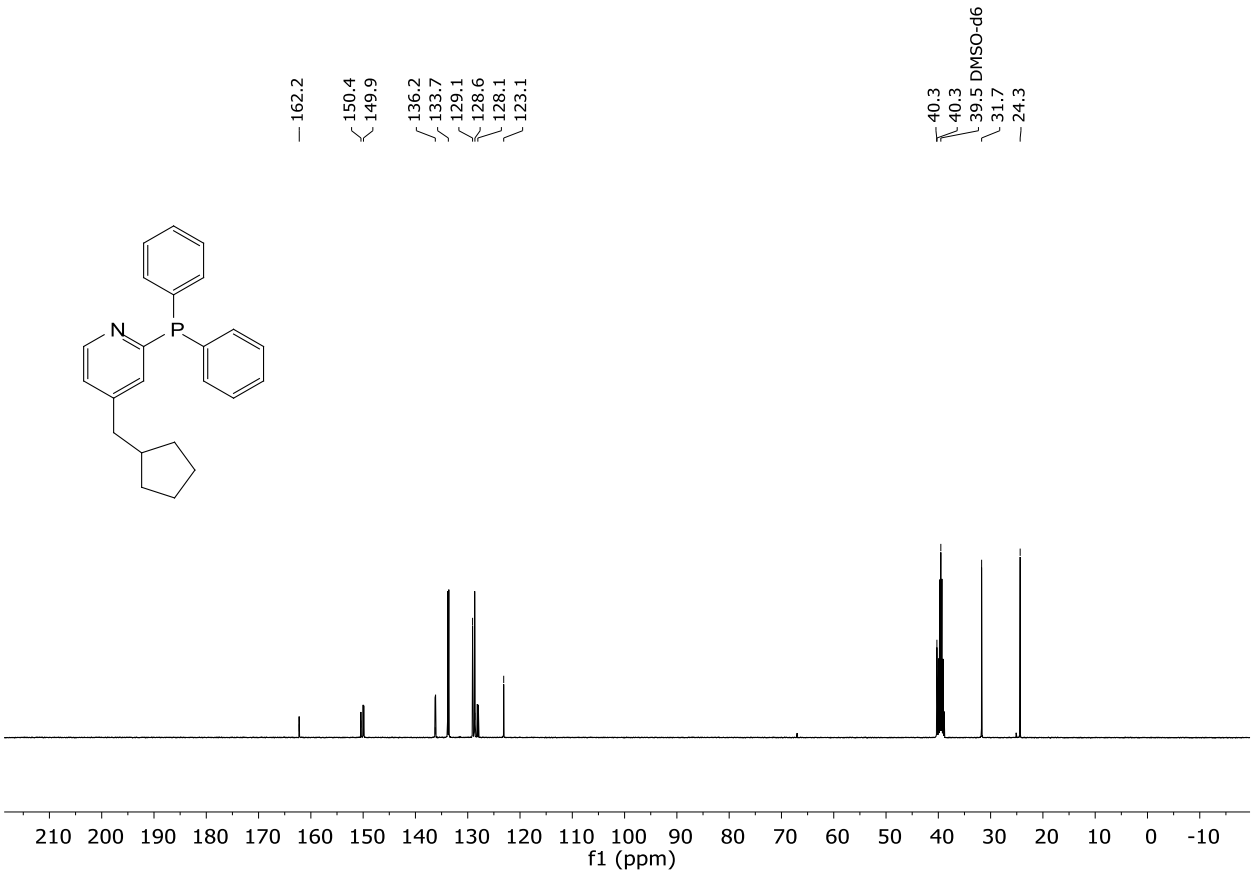



**Figure S12.** $^{13}C$ NMR of ligand **CyclopentPyrPhos** (**4**) in DMSO-$d_6$, 400 MHz.

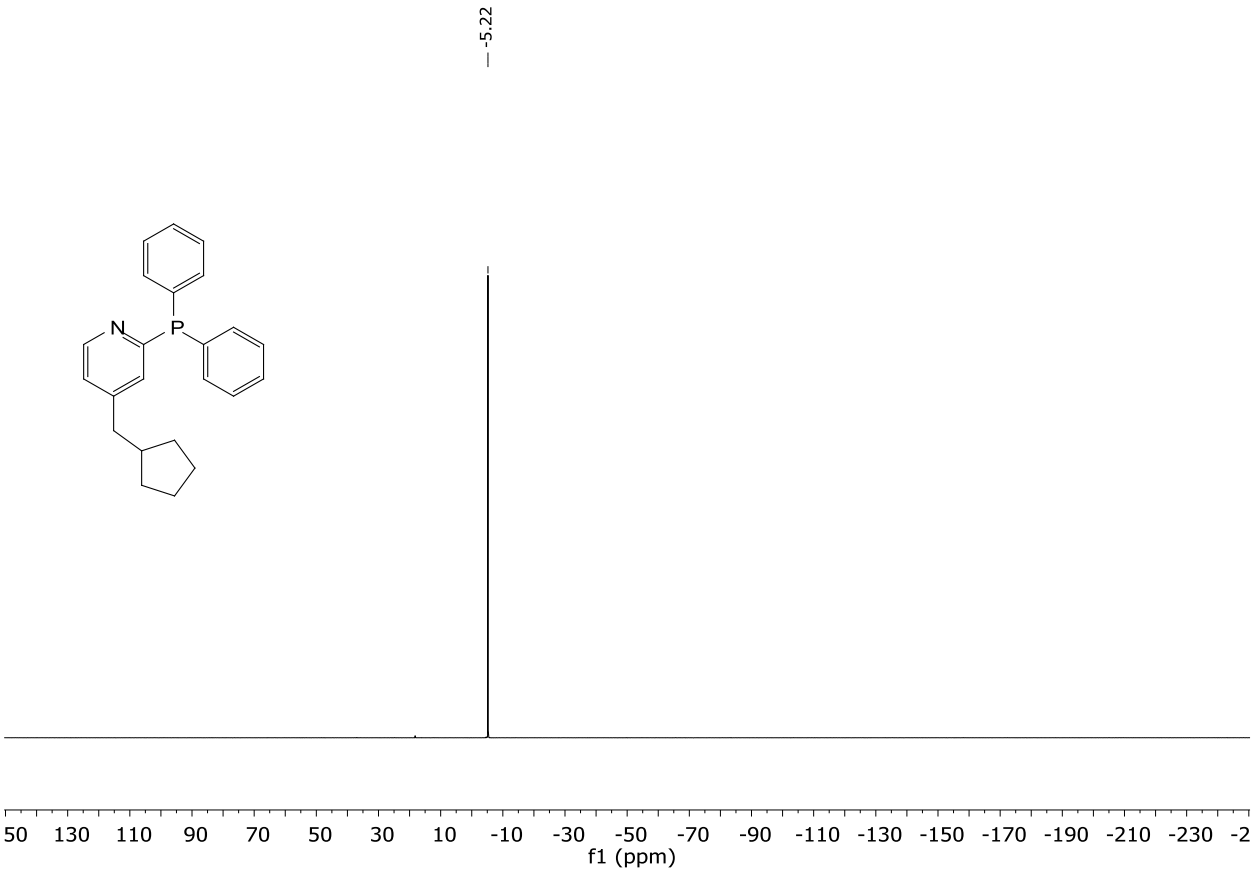



**Figure S13.** $^{31}P$ NMR of ligand **CyclopentPyrPhos** (**4**) in DMSO-$d_6$, 400 MHz.

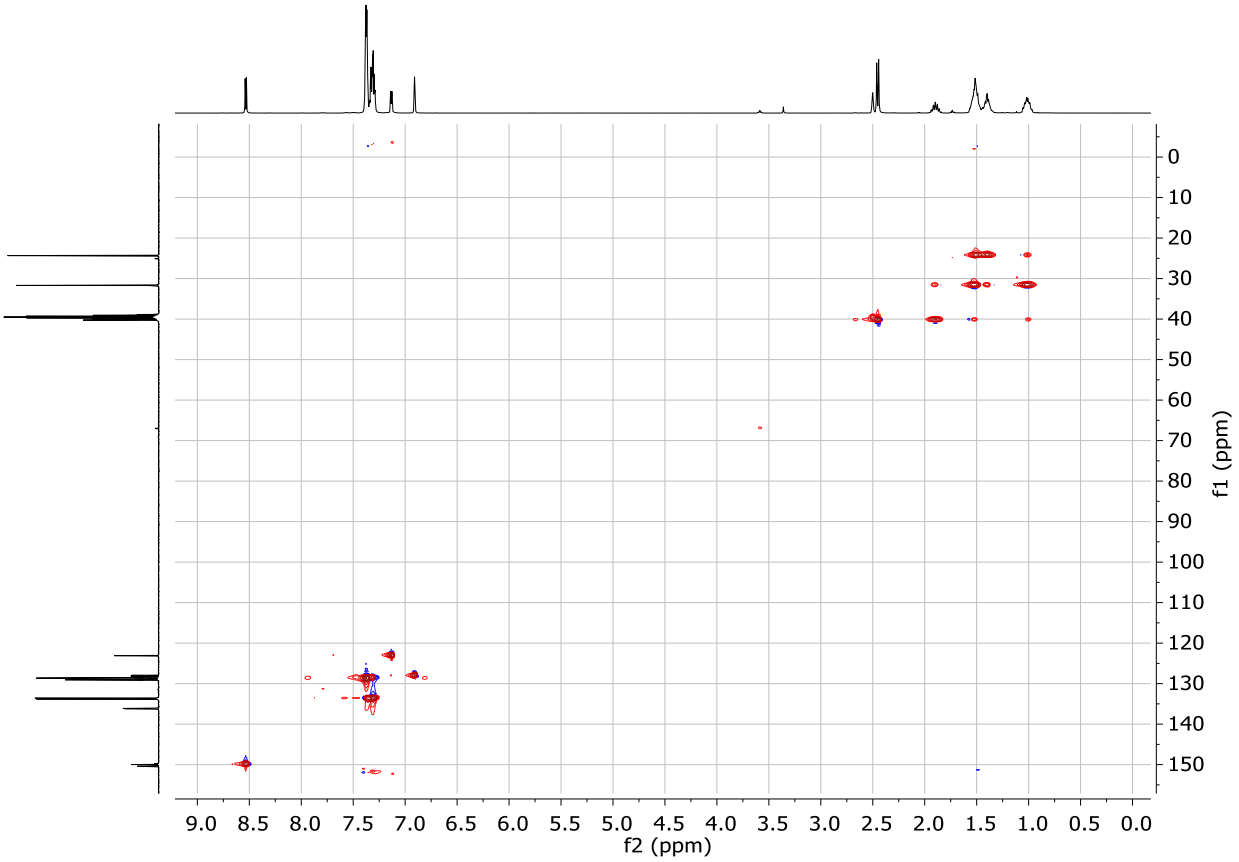



**Figure S14.** HSQC of ligand **CyclopentPyrPhos** (**4**) in DMSO-$d_6$, 400 MHz.

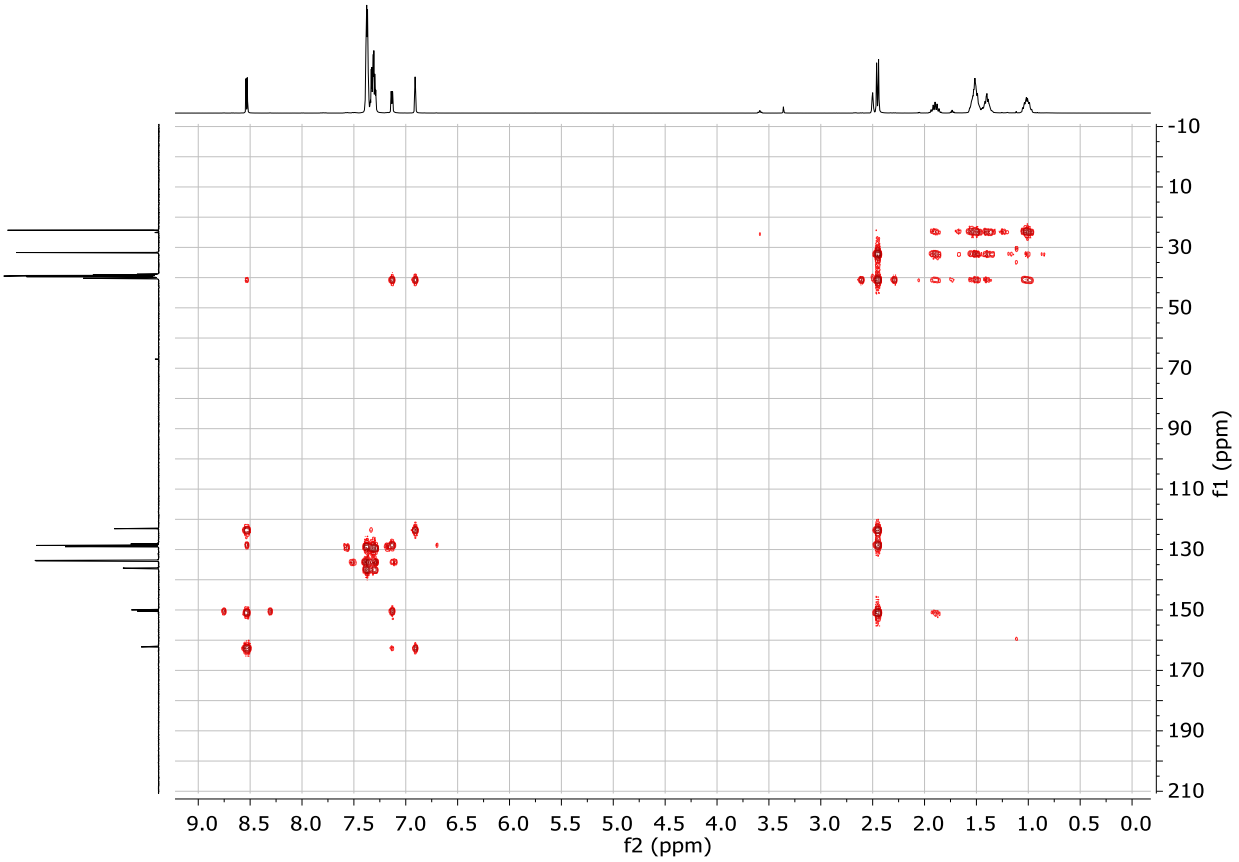



**Figure S15.** HMBC of ligand **CyclopentPyrPhos** (**4**) in DMSO-$d_6$, 400 MHz.

## 4. Crystallography

**General Information.** The molecular structures of the crystalline compounds **3**, **Cu-1b**, **Cu-1d**, **Cu-2b**, **Cu-2c**, **Cu-3b**, **Cu-4a** and **Cu-4b** were determined by single crystal X-ray analysis. Suitable crystals were selected and investigated on a *Stoe StadiVari* diffractometer using either Cu-Kα ($\lambda$ = 1.54186 Å) or Ga-Kα ($\lambda$ = 1.34143 Å) radiation. The crystals were kept at low temperature during data collection. Using Olex2[2], the structures were solved either with the ShelXS[3] structure solution program using Direct Methods and refined with the ShelXL[4] refinement package using Least Squares minimization. Non-hydrogen atoms were refined with anisotropic displacement parameters (disordered atoms and solvent molecules were refined isotropically); hydrogen atoms were modelled on idealized positions. Crystallographic and refinement data are summarized in **Table S1**.

**Crystal Structure Determination of Cu-2d.** The single-crystal X-ray diffraction study was carried out on a Bruker D8 Venture diffractometer with PhotonII CPAD detector at 123(2) K using Mo-Kα radiation ($\lambda$ = 0.71073 Å). Dual space methods (SHELXT)[5] were used for structure solution and refinement was carried out using SHELXL-2014 (full-matrix least-squares on $F^2$)[4]. Hydrogen atoms were localized by difference electron density determination and refined using a riding model. A semi-empirical absorption correction was applied.

CCDC-1918364 (**Cu-2d**) and CCDC-1919266–1919273 (**3**, **Cu-1b**, **Cu-1d**, **Cu-2b**, **Cu-2c**, **Cu-3b**, **Cu-4a** and **Cu-4b**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/structures/.

**Table S1.** Crystallographic and refinement data.

| Compound | **3** | **Cu-1b** | **Cu-1d** |
|---|---|---|---|
| Reaction code | JMB072_B | JMB049 | JMB176 |
| Emp. formula | $C_{21}H_{22}NP$ | $C_{53}H_{38}Cu_2F_6I_2NP_3$ | $C_{53}H_{38}Cl_6Cu_2I_2NP_3$ |
| Moiety formula | $C_{21}H_{22}NP$ | $C_{53}H_{38}Cu_2F_6I_2NP_3$ | $C_{53}H_{38}Cl_6Cu_2I_2NP_3$ |
| Molar mass | 319.36 | 1276.63 | 1375.33 |
| Temperature/K | 180.15 | 180.15 | 180.15 |
| Crystal system | monoclinic | monoclinic | monoclinic |
| Space group | $P2_1/c$ | $P2_1/c$ | $P2_1$ |
| a/Å | 10.9170(6) | 18.9070(5) | 10.61070(10) |
| b/Å | 14.2236(10) | 12.6700(2) | 13.40820(10) |
| c/Å | 11.8139(6) | 20.7952(5) | 18.7629(2) |
| α/° | 90 | 90 | 90 |
| β/° | 103.375(4) | 103.210(2) | 93.5340(10) |
| γ/° | 90 | 90 | 90 |
| Volume/Å$^3$ | 1784.69(19) | 4849.71(19) | 2664.33(4) |
| Z | 4 | 4 | 2 |
| $\rho_{calc}$g/cm$^3$ | 1.189 | 1.748 | 1.714 |
| μ/mm$^{-1}$ | 0.153 | 12.531 | 12.969 |
| F(000) | 680.0 | 2504.0 | 1348.0 |
| Radiation / Å | MoKα (λ = 0.71073) | CuKα (λ = 1.54186) | GaKα (λ = 1.34143) |
| 2Θ range /° | 3.8–66 | 4.8–126.0 | 4.1–124 |
| Refl. collected | 15137 | 16081 | 29745 |
| Independent refl. | 6095 [$R_{int}$ = 0.0279, $R_\sigma$ = 0.0485] | 7497 [$R_{int}$ = 0.0293, $R_\sigma$ = 0.0197] | 9041 [$R_{int}$ = 0.0410, $R_\sigma$ = 0.0268] |
| Ind. refl. I ≥ 2σ(I) | 3970 | 7328 | 8662 |
| Data/rest./param. | 6095/0/211 | 7497/0/604 | 9041/1/604 |
| Gof | 1.043 | 1.080 | 1.017 |
| R indexes [I ≥ 2σ(I)] | $R_1$ = 0.0456, $wR_2$ = 0.1142 | $R_1$ = 0.0264, $wR_2$ = 0.0710 | $R_1$ = 0.0748, $wR_2$ = 0.2003 |
| R indexes [all data] | $R_1$ = 0.0823, $wR_2$ = 0.1272 | $R_1$ = 0.0272, $wR_2$ = 0.0714 | $R_1$ = 0.0769, $wR_2$ = 0.2042 |
| Diff. peak/hole /eÅ$^{-3}$ | 0.39/–0.25 | 0.44/–0.55 | 3.46/–2.89 |
| Flack parameter | | | –0.013(8) |
| CCDC no. | 1919266 | 1919267 | 1919268 |

**Table S1.** (continued).

| Compound | **Cu-2b** | **Cu-2c** | **Cu-2d** |
|---|---|---|---|
| Reaction code | JMB057 | JMB053 | JMB181 |
| Emp. formula | $C_{59}H_{52}Cu_2F_6I_2NP_3$ | $C_{60.5}H_{40}ClCu_2F_{18}I_2NP_3$ | $C_{54}H_{40}Cl_6Cu_2I_2NP_3$ |
| Moiety formula | $C_{54}H_{40}Cu_2F_6I_2NP_3$ · $C_5H_{12}$ | $C_{60}H_{39}Cu_2F_{18}I_2NP_3$ · ½ $CH_2Cl_2$ | $C_{54}H_{40}Cl_6Cu_2I_2NP_3$ |
| Molar mass | 1362.80 | 1632.17 | 1389.36 |
| Temperature/K | 180.15 | 180.15 | 123 |
| Crystal system | monoclinic | triclinic | monoclinic |
| Space group | $P2_1/n$ | $P\bar{1}$ | $P2_1/n$ |
| a/Å | 18.9997(6) | 15.2045(10) | 12.3082(4) |
| b/Å | 12.9197(5) | 15.6811(6) | 24.7061(10) |
| c/Å | 23.7991(6) | 15.7442(10) | 18.5816(8) |
| α/° | 90 | 90.236(4) | 90 |
| β/° | 102.080(2) | 106.170(5) | 104.719(1) |
| γ/° | 90 | 116.415(4) | 90 |
| Volume/Å$^3$ | 5712.6(3) | 3192.9(3) | 5465.0(4) |
| Z | 4 | 2 | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.585 | 1.698 | 1.689 |
| μ/mm$^{-1}$ | 10.677 | 9.932 | 2.33 |
| F(000) | 2704.0 | 1596.0 | 2728 |
| Radiation / Å | CuKα (λ = 1.54186) | GaKα (λ = 1.34143) | MoKα (λ = 0.71073) |
| 2Θ range /° | 6.7–128.0 | 6.0–106.0 | 4.6 – 55 |
| Refl. collected | 22256 | 24934 | 286816 |
| Independent refl. | 9312 [$R_{int}$ = 0.1121, $R_\sigma$ = 0.0879] | 10843 [$R_{int}$ = 0.0150, $R_\sigma$ = 0.0186] | 12543 [$R_{int}$ = 0.043, $R_\sigma$ = 0.014] |
| Ind. refl. I ≥ 2σ(I) | 7879 | 9479 | 11785 |
| Data/rest./param. | 9312/7/635 | 10843/4/777 | 12543/0/614 |
| Gof | 1.266 | 1.079 | 1.16 |
| R indexes [I ≥ 2σ(I)] | $R_1$ = 0.1216, $wR_2$ = 0.2919 | $R_1$ = 0.0434, $wR_2$ = 0.1169 | $R_1$ = 0.026, $wR_2$ = 0.050 |
| R indexes [all data] | $R_1$ = 0.1290, $wR_2$ = 0.2999 | $R_1$ = 0.0493, $wR_2$ = 0.1198 | $R_1$ = 0.028, $wR_2$ = 0.051 |
| Diff. peak/hole /eÅ$^{-3}$ | 4.41/–4.41 | 1.67/–0.71 | 0.66/-0.49 |
| CCDC no. | 1919269 | 1919270 | 1918364 |

**Table S1.** (continued).

| Compound | **Cu-3b** | **Cu-4a** | **Cu-4b** |
|---|---|---|---|
| Reaction code | JMB080_ANW012 | JMB082-14 | JMB83-15 |
| Emp. formula | $C_{57}H_{46}Cu_2F_6I_2NP_3$ | $C_{61}H_{58}Cl_4Cu_2I_2NP_3$ | $C_{60}H_{50}Cl_2Cu_2F_6I_2NP_3$ |
| Moiety formula | $C_{57}H_{46}Cu_2F_6I_2NP_3$ | $C_{59}H_{54}Cu_2I_2NP_3$ $\cdot$ $2(CH_2Cl_2)$ | $C_{59}H_{48}Cu_2F_6I_2NP_3$ $\cdot$ $CH_2Cl_2$ |
| Molar mass | 1332.74 | 1420.67 | 1443.70 |
| Temperature/K | 150.15 | 160.15 | 180.15 |
| Crystal system | triclinic | triclinic | monoclinic |
| Space group | $P\bar{1}$ | $P\bar{1}$ | $P2_1/c$ |
| a/Å | 12.6116(7) | 11.2312(2) | 19.1297(5) |
| b/Å | 17.2115(8) | 14.2065(3) | 12.6256(2) |
| c/Å | 27.1045(9) | 21.3424(4) | 25.3784(6) |
| α/° | 103.391(3) | 72.1220(10) | 90 |
| β/° | 100.214(4) | 82.3480(10) | 111.373(2) |
| γ/° | 101.155(4) | 67.3660(10) | 90 |
| Volume/Å$^3$ | 5461.1(5) | 2990.83(10) | 5708.0(2) |
| Z | 4 | 2 | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.621 | 1.578 | 1.680 |
| μ/mm$^{-1}$ | 11.015 | 11.059 | 11.566 |
| F(000) | 2632.0 | 1416.0 | 2856.0 |
| Radiation / Å | GaKα (λ = 1.34143) | GaKα (λ = 1.34143) | CuKα (λ = 1.54186) |
| 2Θ range /° | 4.9–110.0 | 6.1–120.0 | 8.6–125.0 |
| Refl. collected | 47037 | 37037 | 38804 |
| Independent refl. | 20129 [$R_{int}$ = 0.0424, $R_\sigma$ = 0.0345] | 13129 [$R_{int}$ = 0.0253, $R_\sigma$ = 0.0194] | 9040 [$R_{int}$ = 0.0243, $R_\sigma$ = 0.0148] |
| Ind. refl. I ≥ 2σ(I) | 17952 | 11520 | 8926 |
| Data/rest./param. | 20129/0/1285 | 13129/0/658 | 9040/0/682 |
| Gof | 1.090 | 1.033 | 1.199 |
| R indexes [I ≥ 2σ(I)] | $R_1$ = 0.0466, $wR_2$ = 0.1309 | $R_1$ = 0.0316, $wR_2$ = 0.0861 | $R_1$ = 0.0569, $wR_2$ = 0.1359 |
| R indexes [all data] | $R_1$ = 0.0534, $wR_2$ = 0.1343 | $R_1$ = 0.0367, $wR_2$ = 0.0885 | $R_1$ = 0.0572, $wR_2$ = 0.1360 |
| Diff. peak/hole /eÅ$^{-3}$ | 1.68/–1.23 | 1.46/–0.94 | 1.13/–1.32 |
| CCDC no. | 1919271 | 1919272 | 1919273 |

**Ligand**

*2-(Diphenylphosphino)-4-tertbutylpyridine* (***tert*BuPyrPhos**)

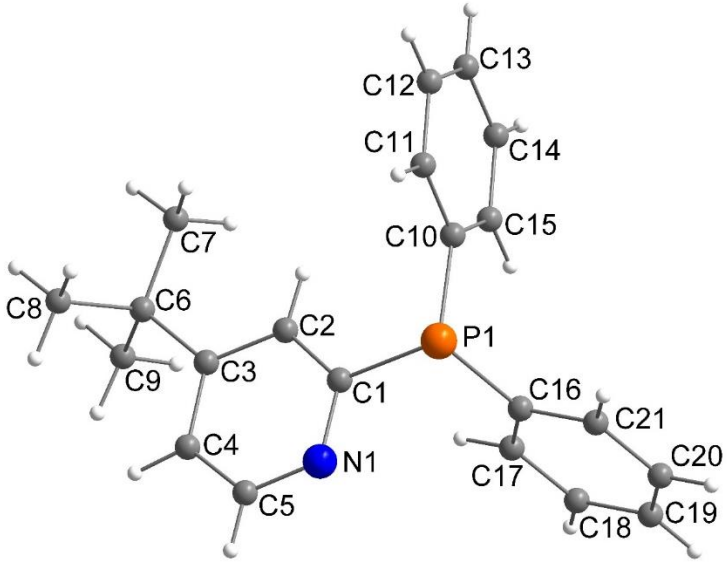



**Figure S16.** Molecular structure of ***tert*BuPyrPhos** (**3**).

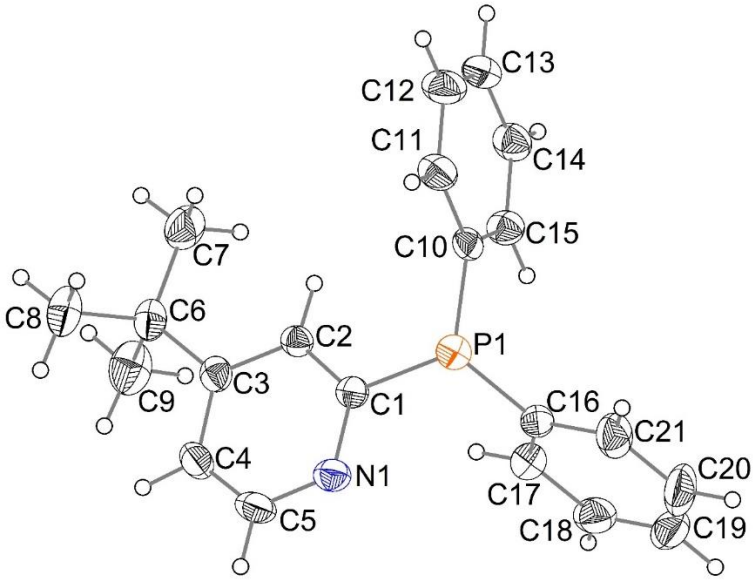



**Figure S17.** ORTEP plot of ***tert*BuPyrPhos** (**3**)
(displacement parameters are drawn at 50 % probability level).

## Cu(I) Complexes

Additionally the molecular structure of Cu(I) complex **Cu-4a** was obtained by X-Ray analysis.

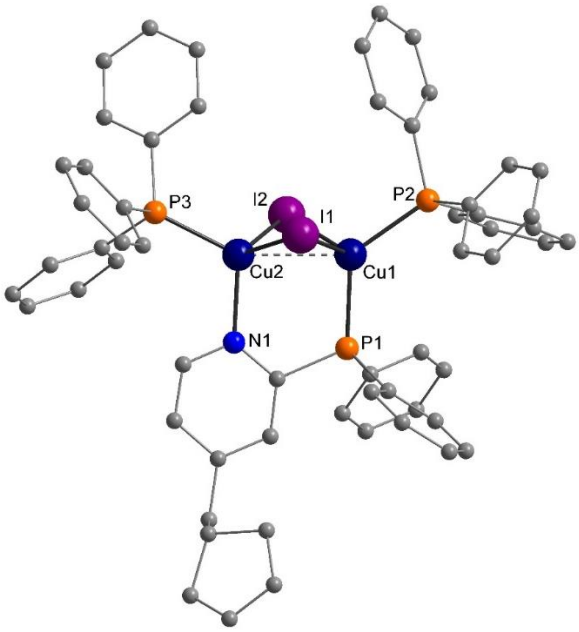



**Figure S18.** Molecular structure of Cu(I) complex **Cu-4a** bearing triphenylphosphine as ancillary ligands (hydrogen atoms and solvent were omitted for clarity).

**ORTEP plots**

In the following section the ORTEP plots of all obtained Cu(I) AlkylPyrPhos complexes **Cu-1b**, **Cu-1d**, **Cu-2b**, **Cu-2c**, **Cu-3b**, **Cu-4a** and **Cu-4b** are shown.

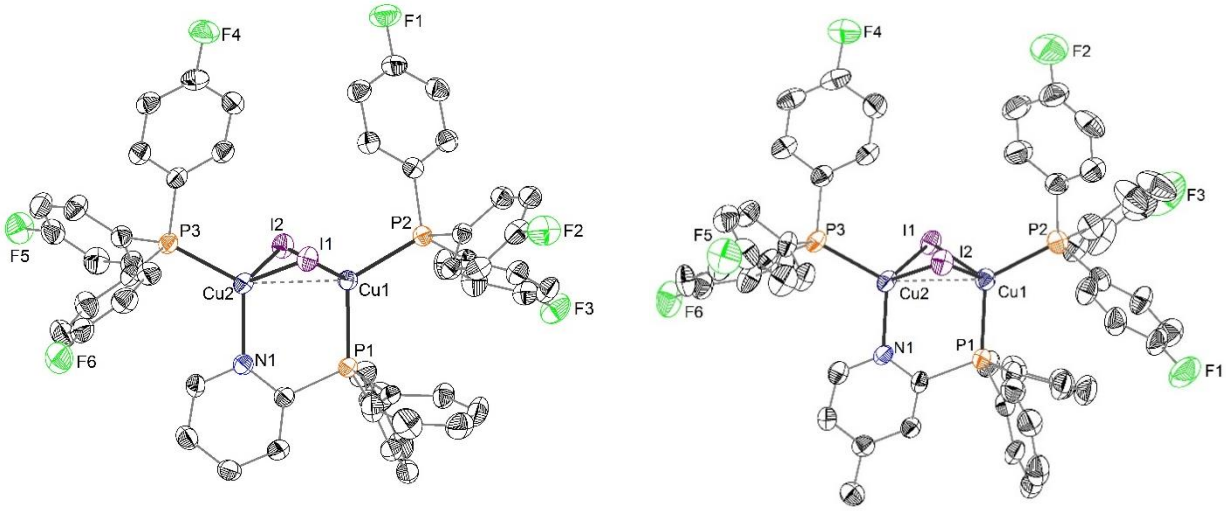



**Figure S19.** ORTEP plots of **Cu-1b** (left) and **Cu-2b** (right)
(displacement parameters are drawn at 50 % probability level,
hydrogen atoms and solvent (right) were omitted for clarity).

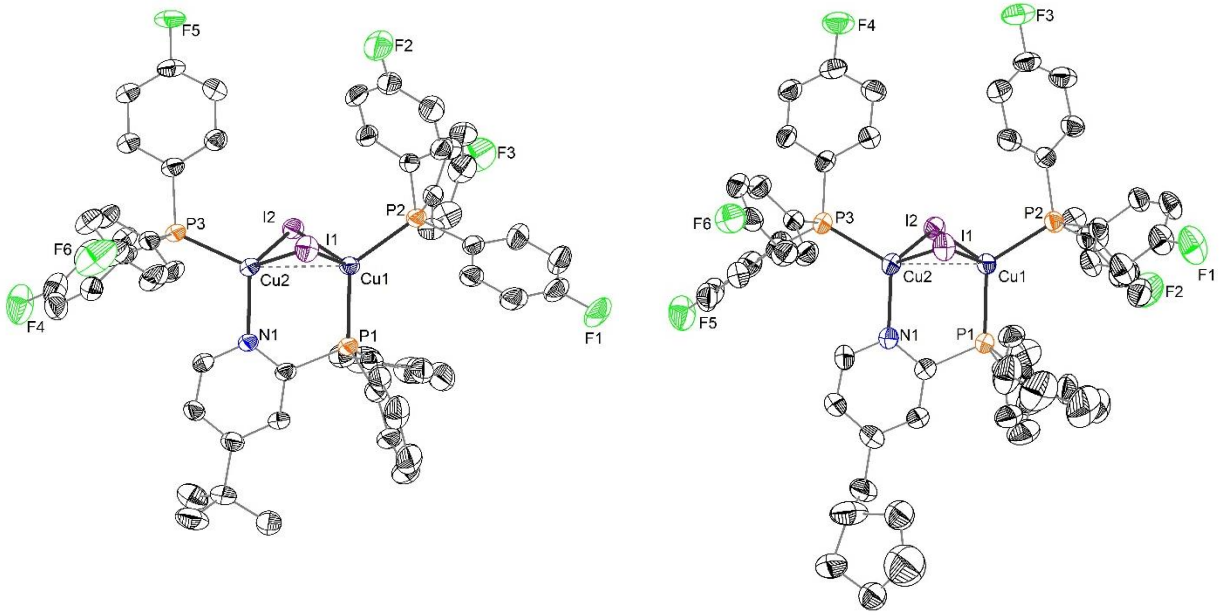



**Figure S20.** ORTEP plots of **Cu-3b** (left) and **Cu-4b** (right)
(displacement parameters are drawn at 50 % probability level,
hydrogen atoms and solvent and minor disordered parts (right) were omitted for clarity).

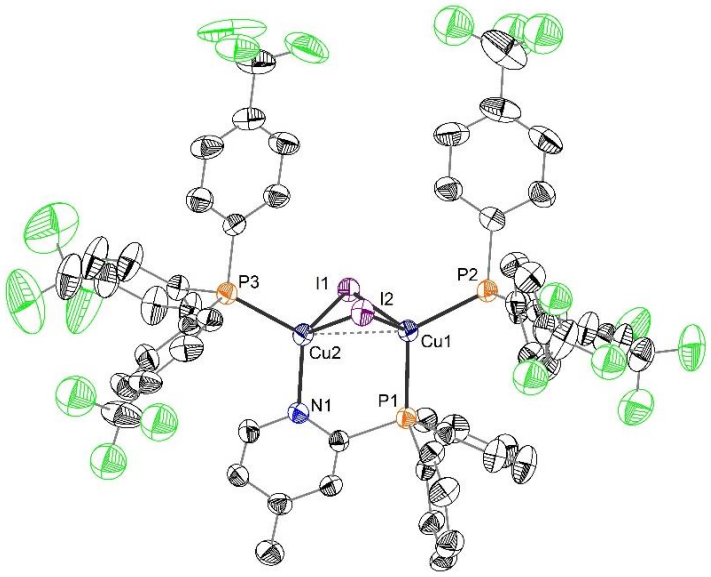



**Figure S21.** ORTEP plot of **Cu-2c**
(displacement parameters are drawn at 50 % probability level,
hydrogen atoms, solvent and minor disordered parts were omitted for clarity).

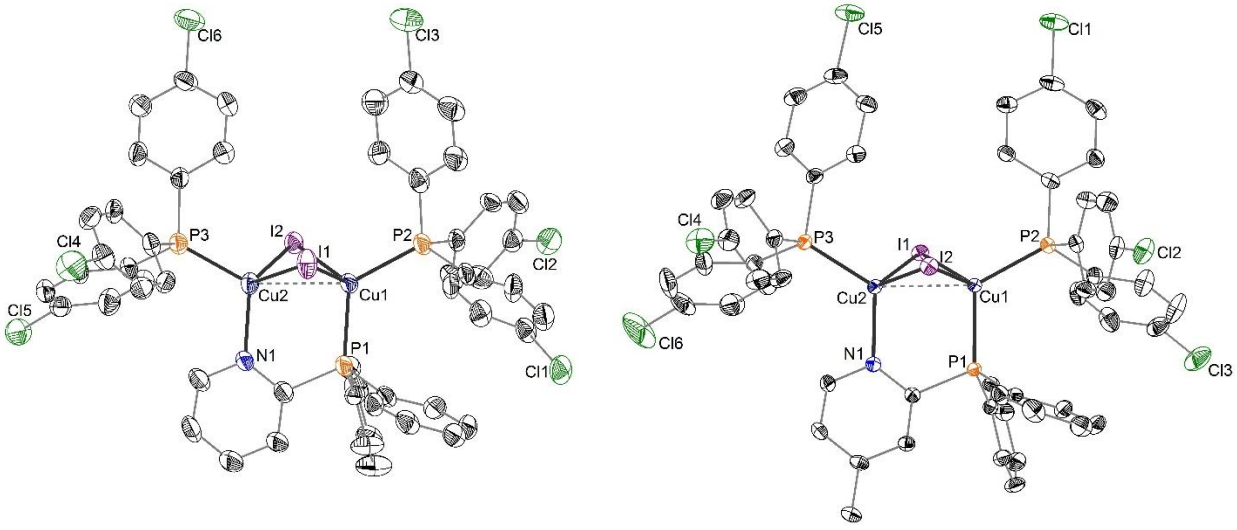



**Figure S22.** ORTEP plots of **Cu-1d** (left) and **Cu-2d** (right)
(displacement parameters are drawn at 50 % probability level,
hydrogen atoms were omitted for clarity).

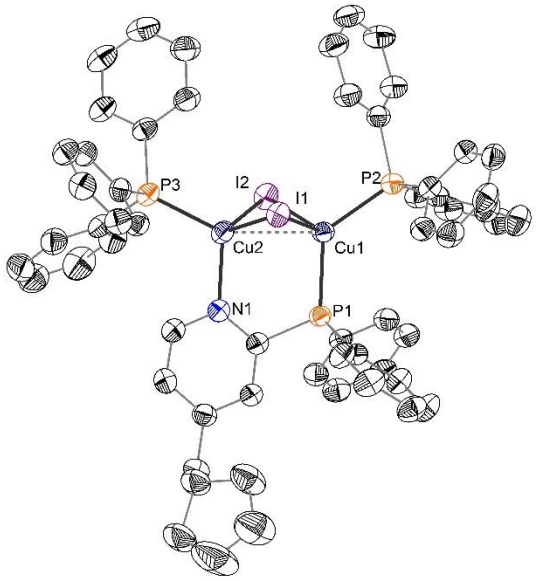



**Figure S23.** ORTEP plot of **Cu-4a**
(displacement parameters are drawn at 50 % probability level,
hydrogen atoms and solvent were omitted for clarity).

## 5. Theoretical Calculations

**Computational Details.** The different complexes were optimized using the `ridft` module within the standard jobex script. The energy threshold within a self-consistent (SCF) calculation was set to $10^{-10}\ E_h$ whereas convergence thresholds for the structure optimization were $10^{-8}\ E_h$ and $10^{-6}\ E_h/a_0$ for the total SCF energy and the Cartesian gradients, respectively. The structures used for the calculations are given in section **9. Structures in XYZ**.

For the calculation of IR absorption spectra of **Cu-1b** and **Cu-2b** the crystal structures were used as input structures. For geometry optimization and frequency calculation the DFT functional B3LYP with dispersion correction $(D_3)$[6], RI-approximation (resolution of identity) and the def2-TZVP basis set were used. The calculations of energies, gradients, force constants and frequencies were performed and taken from Turbomole 7.3[7]. Obtained vibrational frequencies were convolved with a Gaussian profile with a FWHM = 8 $cm^{-1}$. Triplet states were calculated as ground state using UDFT.
The $S_1$ and $T_1$ structures were optimized and the respective vertical transitions were calculated by TD-DFT (B3LYP-D3(BJ)/def2-TZVP) and considered for calculation of the singlet-triplet energy gaps of **Cu-1b** and **Cu-2b**.

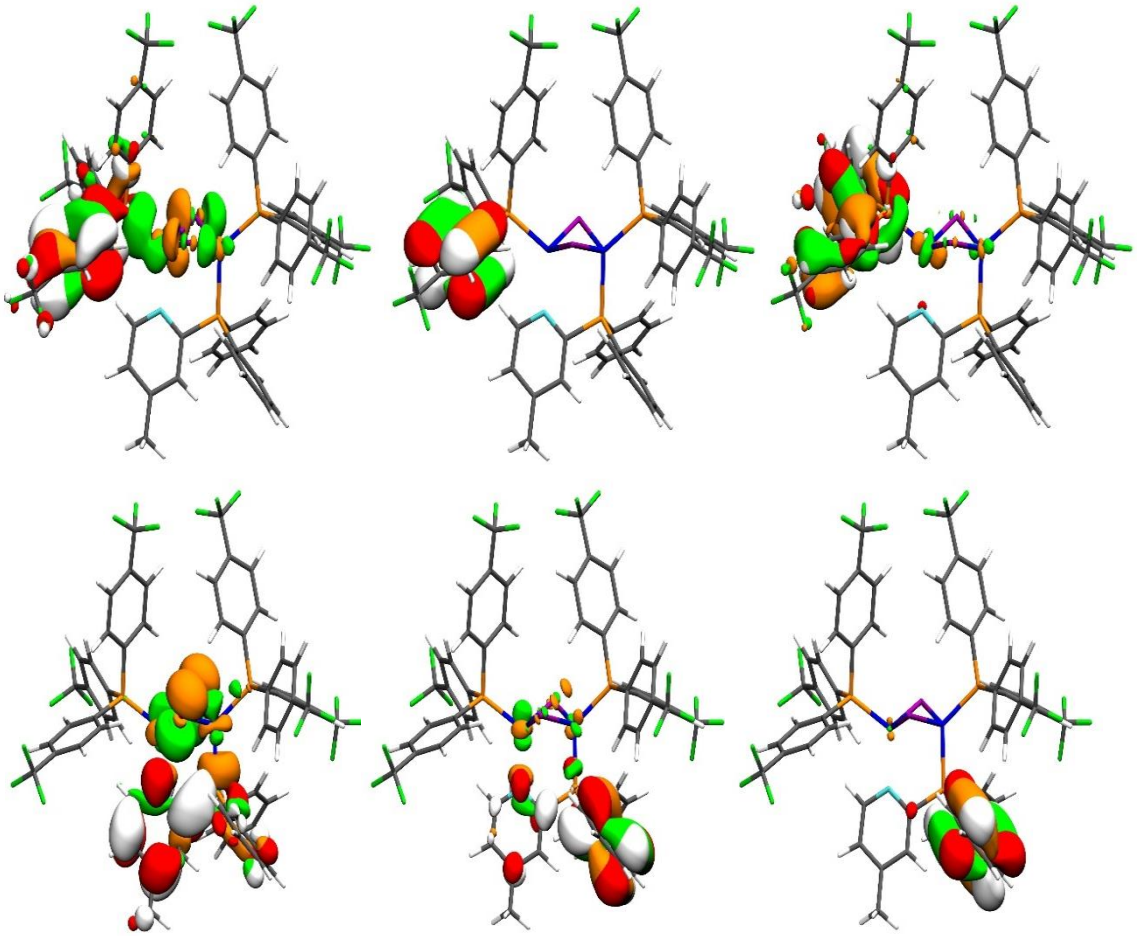


**Figure S24.** First three natural transition orbitals of **Cu-2c** for the first triplet excitation (top: 80%, 10%, 6%) and second triplet excitation (bottom: 79%, 12%, 5%) at the $S_0$ structure. The colours green/orange indicate the hole while red/white correspond to the electron. (isovalue: ±0.03 $a_0^{-3/2}$, Cu = blue, P = orange, I = purple, N = cyan, F = green, C = grey, H = white).

## 6. Absorption Spectra

**Absorption spectra measurements.** Absorption spectra were recorded on a *Thermo Scientific*, model Evolution 201. 10 mg of each sample were dissolved in 100 mL spectroscopical grade dichloromethane respectively. 1 mL of this stock solution was diluted 1:10 to give concentrations of 0.01 mg/mL.

### Experimental Data

**Table S2.** Overview of the absorption maxima, concentration of the samples, extinction and molar extinction coefficient at the absorption maxima for all Cu(I) complexes and ligands investigated in this study respectively.

| compound | absorption maxima [nm] | c ($\times 10^{-6}$) [mol/L] | E(absorption maximum) | molar extinction coefficient at absorption maxima ($\times 10^{-4}$) [L/(mol × cm)] |
|---|---|---|---|---|
| **Cu-1b** | 250 | 7.96 | 0.283 | 3.55 |
| **Cu-1c** | 265 | 6.61 | 0.255 | 3.86 |
| **Cu-1d** | 250 | 7.44 | 0.371 | 4.99 |
| **Cu-2b** | 250 | 8.08 | 0.296 | 3.66 |
| **Cu-2c** | 266 | 6.34 | 0.233 | 3.67 |
| **Cu-2d** | 250 | 7.49 | 0.368 | 4.91 |
| **Cu-3a** | 250 | 8.28 | 0.335 | 4.05 |
| **Cu-3b** | 250 | 7.56 | 0.288 | 3.80 |
| **Cu-4a** | 250 | 8.17 | 0.302 | 3.70 |
| **Cu-4b** | 250 | 7.45 | 0.258 | 3.46 |

| compound | absorption maxima [nm] | c ($\times 10^{-5}$) [mol/L] | E(absorption maximum) | molar extinction coefficient at absorption maxima [L/(mol × cm)] |
|---|---|---|---|---|
| **ligand 1** | 258 | 3.81 | 0.372 | 9753 |
| **ligand 2** | 257 | 3.62 | 0.335 | 9250 |
| **ligand 3** | 257 | 3.18 | 0.287 | 9013 |
| **ligand 4** | 259 | 2.93 | 0.250 | 8529 |
| | | | | |
| **ligand a** | 263 | 3.84 | 0.360 | 9365 |
| **ligand b** | 257 | 3.23 | 0.348 | 10785 |
| **ligand c** | 270 | 2.19 | 0.244 | 11180 |
| **ligand d** | 266 | 2.83 | 0.389 | 13755 |

Comparison plots of the absorption spectra of the copper complexes **Cu-1b** – **Cu-4b** and their corresponding bridging and ancillary ligands, measured of the solution with the concentrations given in **Table S2** at room temperature.

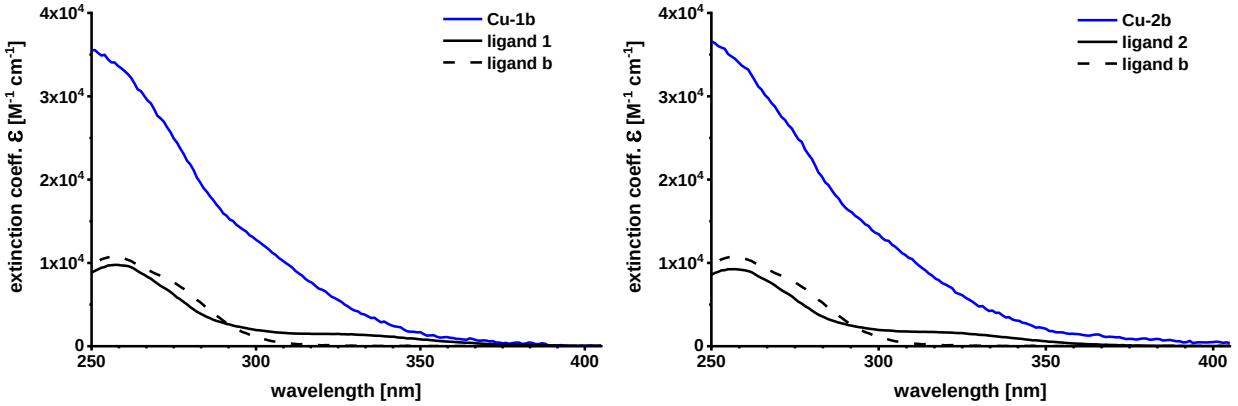



**Figure S25.** UV/Vis spectra of **Cu-1b**, **Cu-2b** and the corresponding ligands **1**, **2** and **b**.

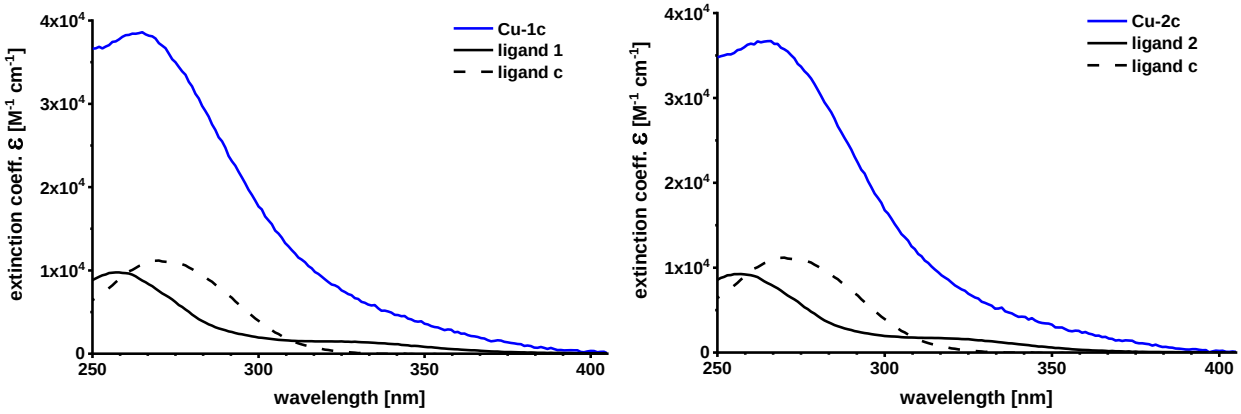



**Figure S26.** UV/Vis spectra of **Cu-1c**, **Cu-2c** and the corresponding ligands **1**, **2** and **c**.

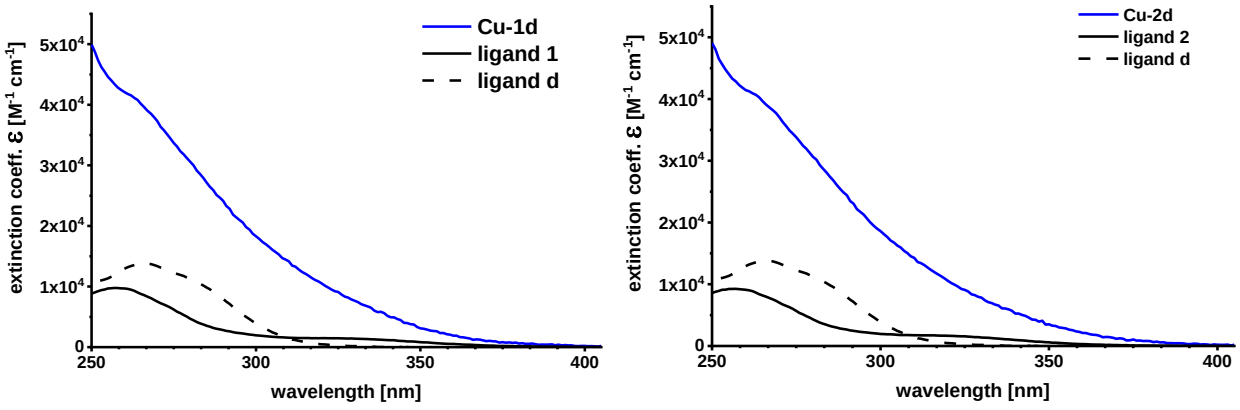



**Figure S27.** UV/Vis spectra of **Cu-1d**, **Cu-2d** and the corresponding ligands **1**, **2** and **d**.

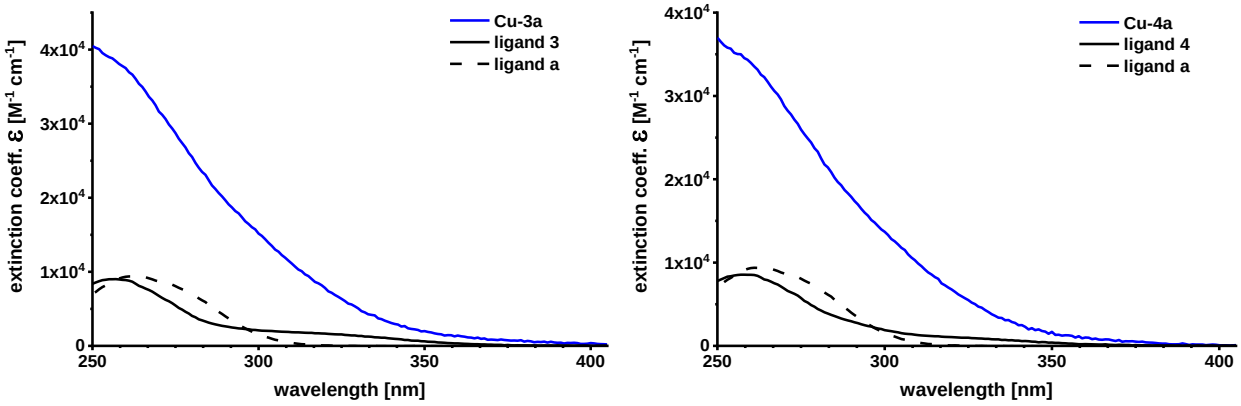



**Figure S28.** UV/Vis spectra of **Cu-3a**, **Cu-4a** and the corresponding ligands **3**, **4** and **a**.

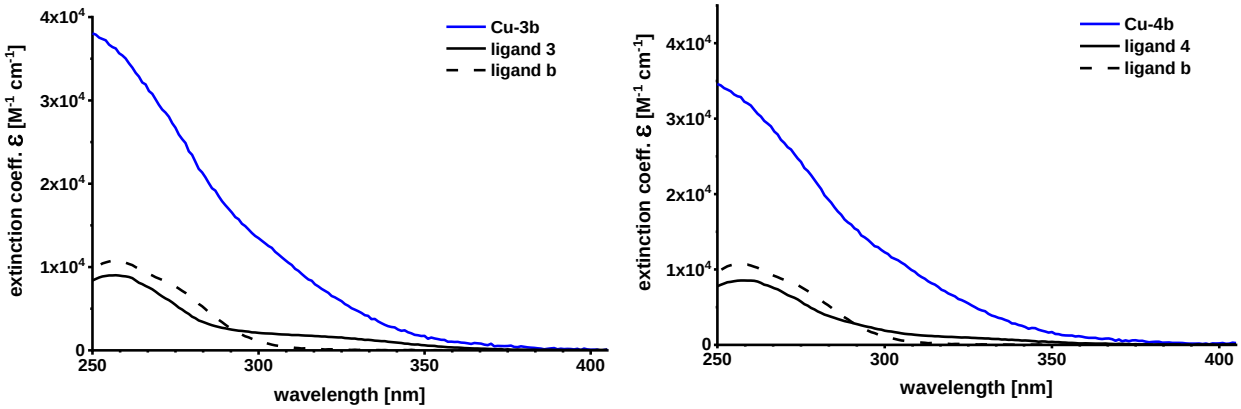



**Figure S29.** UV/Vis spectra of **Cu-3b**, **Cu-4b** and the corresponding ligands **3**, **4** and **b**.

Further absorption spectra were recorded using a *Perkin-Elmer* Lambda 900 double beam UV/VIS/NIR spectrophotometer with concentrations in the region of $2 \cdot 10^{-5}$ M.

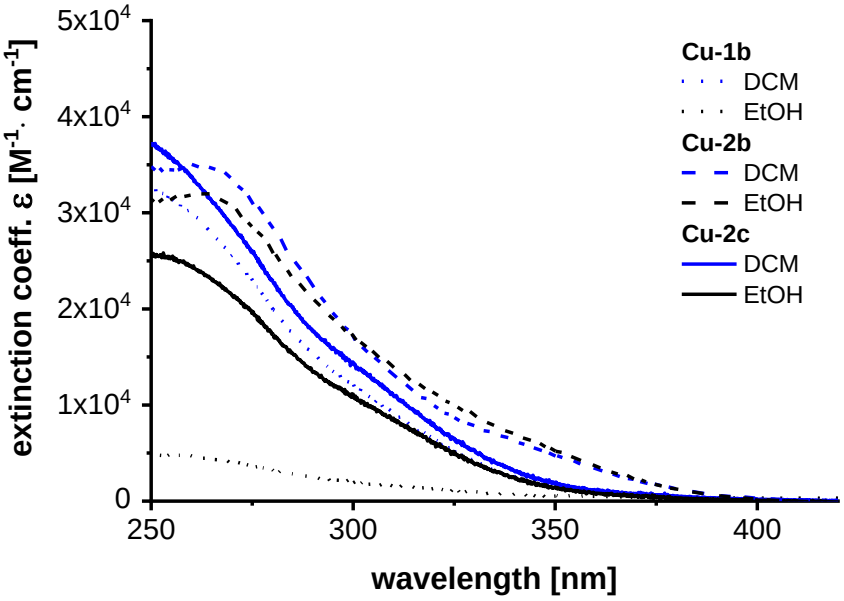



**Figure S30.** UV/Vis spectra of the complexes **Cu-1b**, **Cu-2b** and **Cu-2c**, measured in dichloromethane (blue) and ethanol (black).

**Absorption measurements of the Cu(I) complexes in neat films**

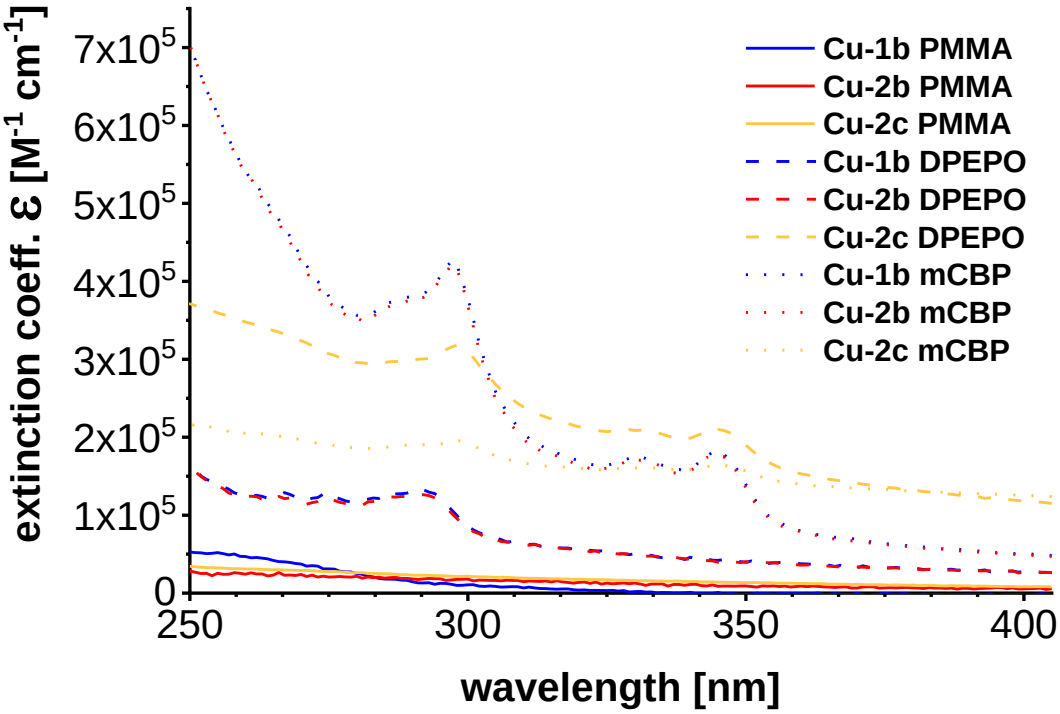



**Figure S31.** UV/Vis spectra of the complexes **Cu-1b**, **Cu-2b** and **Cu-2c**, measured of the PMMA, DPEPO and mCBP films respectively at room temperature.

**Computational Data**

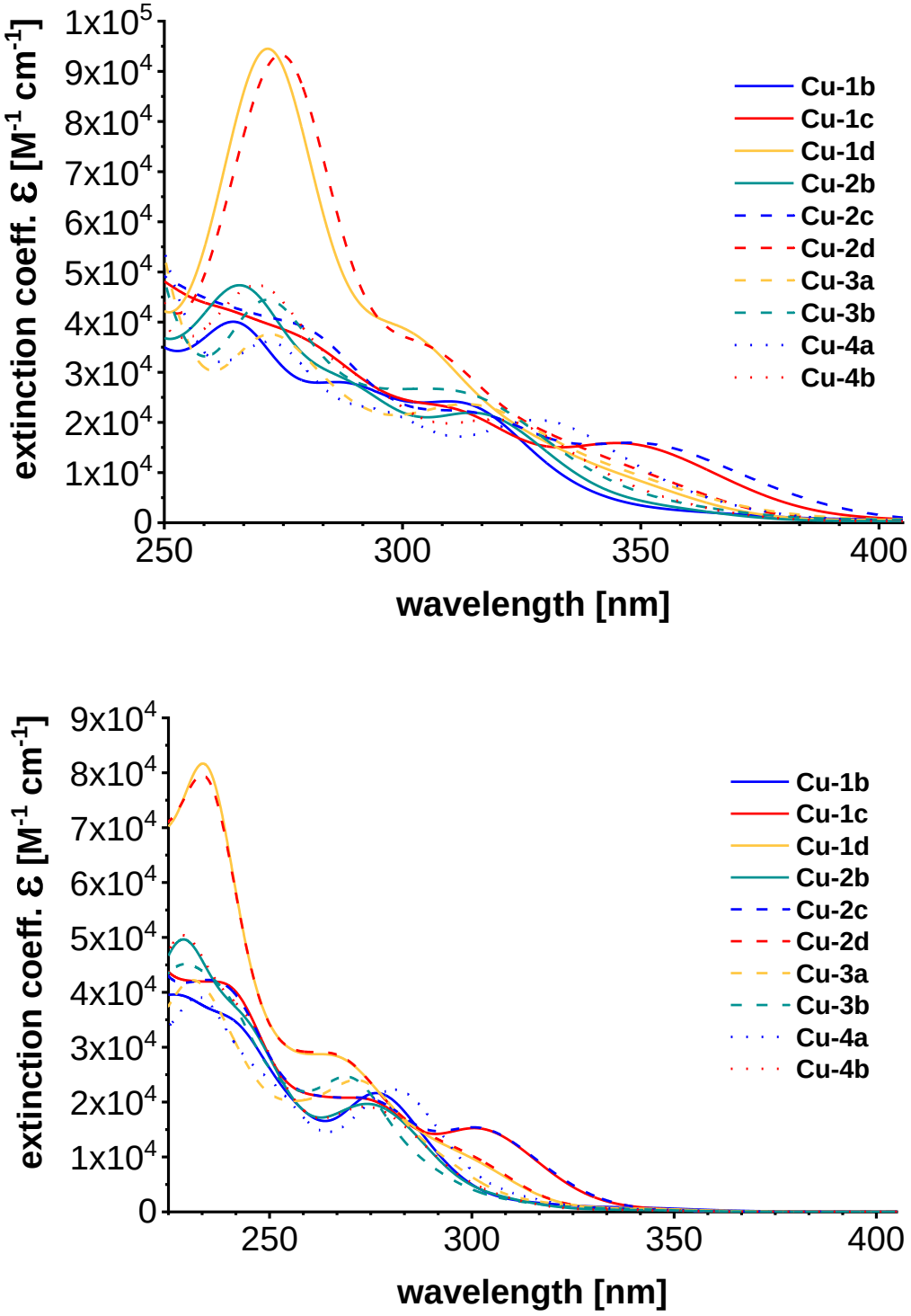



**Figure S32.** UV/Vis spectra computed using evGW/BSE[8, 9] with PBE0[10] (top) and CAM-B3LYP[11] (bottom) with the def2-TZVP basis (def2-SV(P) for hydrogen).

## 7. Photophysics

### Powder measurements

**Photophysical measurements.** Photoluminescence spectroscopy and TCSPC (*Time-correlated single-photon counting*). Steady-state emission spectra were measured by a *Horiba Scientific*, model FluoroMax-4 equipped with a 150 W Xenon-Arc lamp, excitation- and emissions monochromators and a Hamamatsu R928 photomultiplier and a time-correlated single-photon counting option. Emissions and excitation spectra were corrected using standard correction fits. Excited state lifetimes were determined employing the same system using the TCSPC method with FM-2013 equipment and a Horiba Yvon TCSPC hub. Excitation sources: NanoLED 370 (wavelength: 371 nm, pulse duration: 1.1 ns), NanoLED 290 (wavelength: 294 nm, pulse duration: <1 ns), SpectraLED 310 (wavelength: 314 nm), SpectraLED 355 (wavelength: 355 nm). Data analysis (exponential fit) was done using the software suite DataStation and DAS6 analysis software. The fit is specified using the chi-squared-test. For the photoluminescence quantum yield (PLQY) measurements an *Absolute PL Quantum Yield Measurement C9920-03G* system (*Hamamatsu Photonics*) was used. Quantum yields and CIE coordinates were determined using the software U6039-05 version 3.6.0. Emission maxima are given in nm, quantum yields **Φ** in % and CIE coordinates as x, y values. The PLQYs were measured with an integrating sphere set up of the powder of the Cu(I) complexes with an excitation wavelength of 350 nm. The yield was calculated using the following equation, wherein $n_{photon}$ denotes the photon count and *Int.* the intensity.

$$\Phi_{PL} = \frac{n_{photon}, emitted}{n_{photon}, absorbed} = \frac{\int \frac{\lambda}{hc}\left[Int_{emitted}^{sample}(\lambda) - Int_{absorbed}^{sample}(\lambda)\right]d\lambda}{\int \frac{\lambda}{hc}\left[Int_{emitted}^{reference}(\lambda) - Int_{absorbed}^{reference}(\lambda)\right]d\lambda}$$

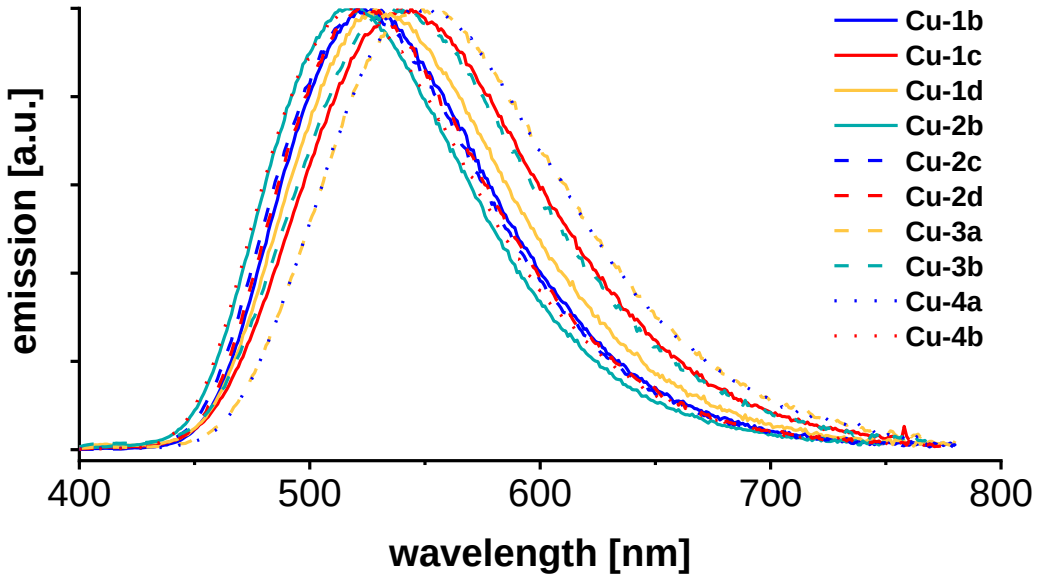



**Figure S33.** Overview of all emission spectra of the Cu(I) AlkylPyrPhos complexes, measured of the powder samples at room temperature with 350 nm excitation wavelength.

## Measurements of the Cu(I) complexes in neat films

The photophysical measurements were also performed of neat films of 10 wt% of the copper complex emitters **Cu-1b**, **Cu-2b** and **Cu-2c** in the corresponding host materials. Hereby, poly(methylmethacrylate) (PMMA), purchased from *Sigma-Aldrich* (art. number 182230-25G, used without further purification), bis(2-(diphenylphosphino)phenyl)ether oxide (DPEPO), purchased also from *Sigma-Aldrich* (98% purity, sublimed before usage) and 3,3-di(9H-carbazol-9-yl)biphenyl (mCBP) purchased from *Jilin OLED materials* in >98% purity (sublimed before usage) served as host materials (**Figure S34**).

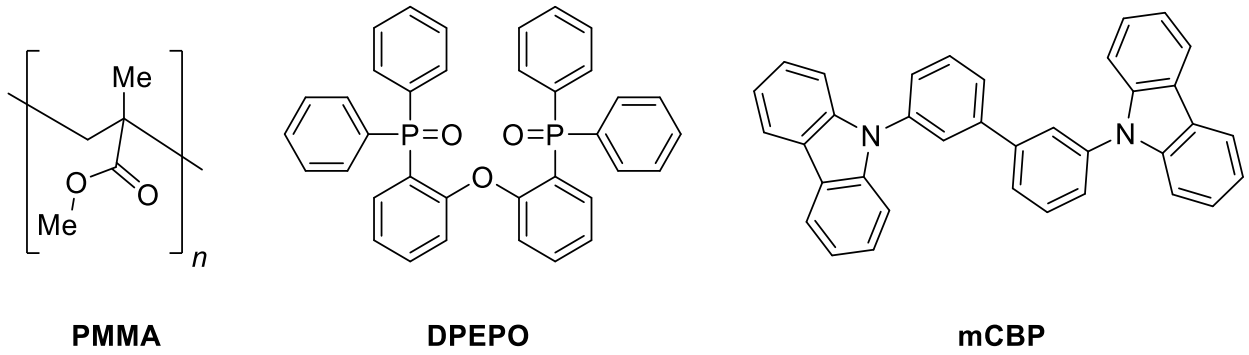



**Figure S34.** Host materials PMMA (left), DPEPO (center) and mCBP (right).

**Sample Preparation.** Stock solutions of the copper complexes and the host materials were prepared respectively. Dichloromethane was used as solvent.

Stock solution 1: 10 mg of the copper complex emitter was dissolved in 1 mL of DCM.
Stock solution 2: 10 mg of the host material was dissolved in 1 mL of DCM.

The stock solutions 1 and 2 were mixed by volume with an Eppendorf pipette in a ratio of 10/90 (stock solution 1/stock solution 2). In this case, the ratio by volume also corresponded to the ratio by weight, as both stock solutions had a concentration of 10 mg/mL.

**Film Preparation.** For the film preparation, 50 µL of the mixed solution (cf. section **sample preparation**) were applied on a commercially available fused quartz substrate with an Eppendorf pipette. Spin coating was performed with a Wafer Spinner Spin 150 (*APT GmbH*) with the following spin coating program:

Step 1: Speed 400 rpm, time 5 s, acceleration 1000
Step 2: Speed 1000 rpm, time 20 s, acceleration 1000
Step 3: Speed 4000 rpm, time 10 s, acceleration 1000

Subsequently, the spin-coated film was heated on a heating plate for 30 – 60 seconds at 70 °C. During the spin coating and due to the subsequent heating, the solvent was removed and a film with 10% by weight of copper complex emitter and 90% by weight PMMA (DPEPO, mCBP) was achieved. This film (nm scale thickness) was used to measure the PL, PLQY, lifetime and CIE coordinates were determined. For this the same equipment as described for the measurements in powder was used (see **photophysical measurements**). All emission spectra were plotted using the software ORIGIN®.

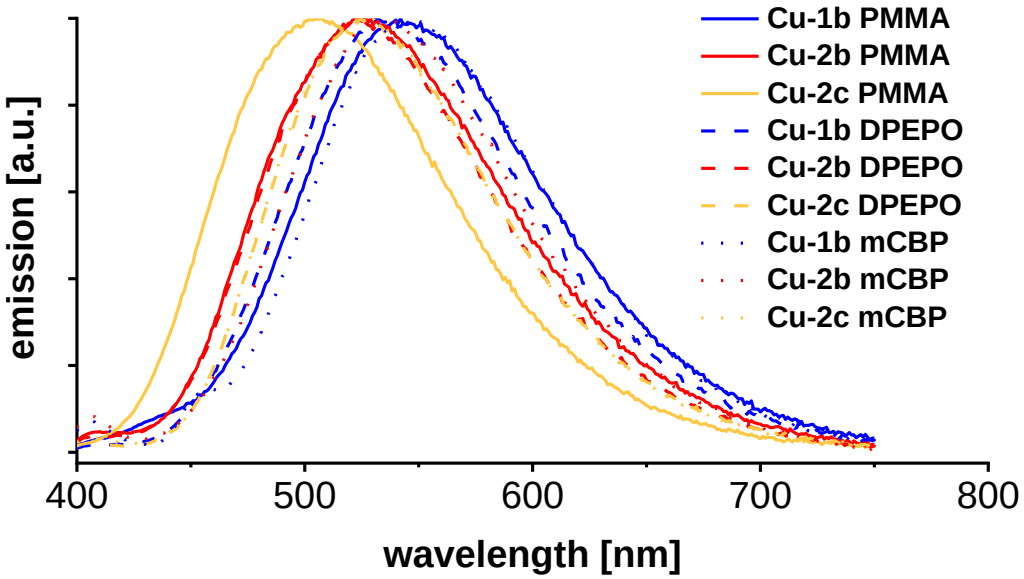



**Figure S35.** Overview of the emission spectra of the complexes **Cu-1b**, **Cu-2b** and **Cu-2c**, measured of the neat films (PMMA, DPEPO and mCBP as hosts) at room temperature with 350 nm excitation wavelength.

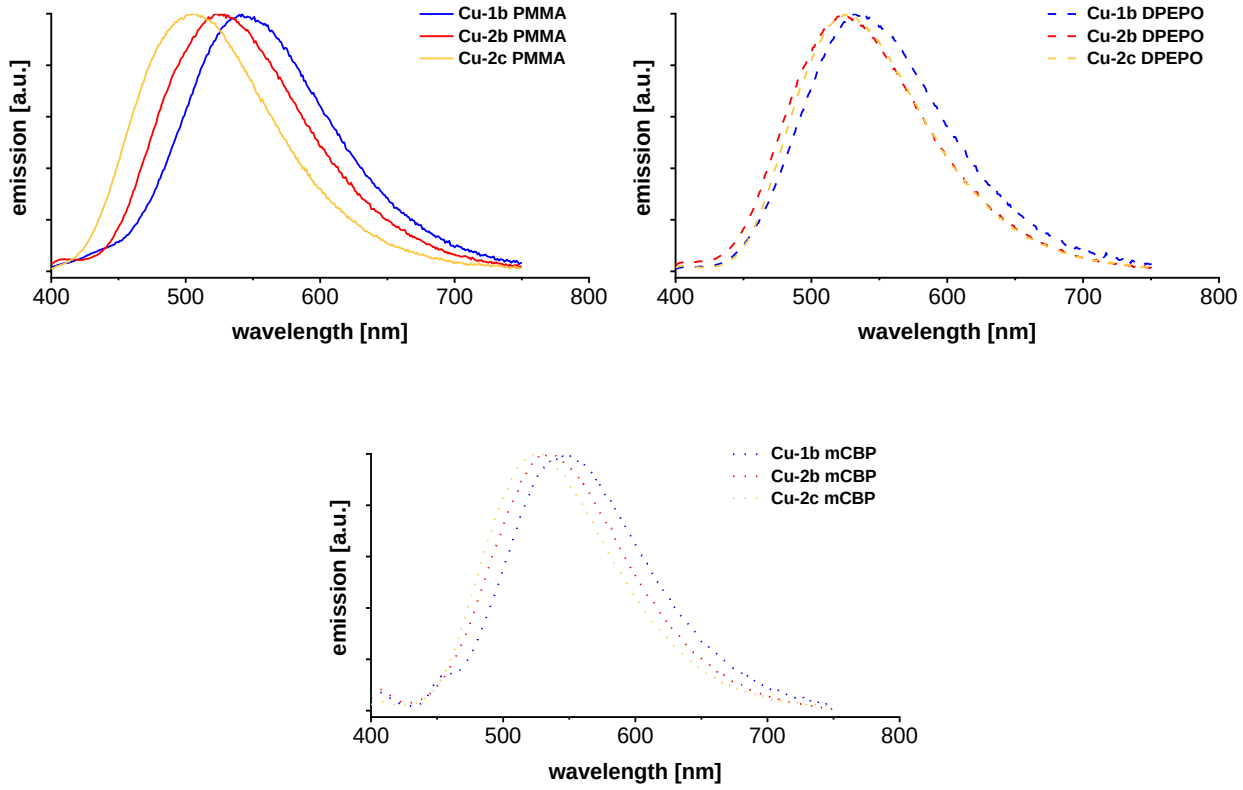



**Figure S36.** Comparison of the emission spectra of **Cu-1b**, **Cu-2b** and **Cu-2c** in PMMA (top, left), DPEPO (top, right) and mCBP (bottom) films, measured at rt with 350 nm excitation wavelength.

The photophysical properties of the complexes **Cu-1b**, **Cu-2b** and **Cu-2c**, measured of the neat films (PMMA, DPEPO and mCBP as hosts) at room temperature with 350 nm excitation wavelength, are given in **Table S3**.

**Table S3**. Photophysics and CIE-coordinates of 10wt% **Cu-1b**, **Cu-2b** and **Cu-2c** in PMMA, DPEPO and mCBP films, respectively, ordered according to the Cu(I) complex emitter (top) and host (bottom).

| Complex | Host | $\lambda_{PL}$ [nm] | $\Phi_{PL}$ [%] | τ [µs] | CIE X | CIE Y |
|---|---|---|---|---|---|---|
| **Cu-1b** | PMMA | 542 | 59 | 9.5 | 0.39 | 0.53 |
| | DPEPO | 532 | 64 | 7.2 | 0.36 | 0.51 |
| | mCBP | 544 | 54 | 7.3 | 0.38 | 0.52 |
| **Cu-2b** | PMMA | 529 | 78 | 7.8 | 0.35 | 0.52 |
| | DPEPO | 526 | 65 | 6.9 | 0.32 | 0.52 |
| | mCBP | 529 | 60 | 6.7 | 0.36 | 0.53 |
| **Cu-2c** | PMMA | 505 | 77 | 10.0 | 0.27 | 0.44 |
| | DPEPO | 526 | 69 | 8.3 | 0.32 | 0.52 |
| | mCBP | 526 | 60 | 8.4 | 0.32 | 0.52 |

| Complex | Host | $\lambda_{PL}$ [nm] | $\Phi_{PL}$ [%] | τ [µs] | CIE X | CIE Y |
|---|---|---|---|---|---|---|
| **Cu-1b** | PMMA | 542 | 59 | 9.5 | 0.39 | 0.53 |
| **Cu-2b** | | 529 | 78 | 7.8 | 0.35 | 0.52 |
| **Cu-2c** | | 505 | 77 | 10.0 | 0.27 | 0.44 |
| **Cu-1b** | DPEPO | 532 | 64 | 7.2 | 0.36 | 0.51 |
| **Cu-2b** | | 526 | 65 | 6.9 | 0.32 | 0.52 |
| **Cu-2c** | | 526 | 69 | 8.3 | 0.32 | 0.52 |
| **Cu-1b** | mCBP | 544 | 54 | 7.3 | 0.38 | 0.52 |
| **Cu-2b** | | 529 | 60 | 6.7 | 0.36 | 0.53 |
| **Cu-2c** | | 526 | 60 | 8.4 | 0.32 | 0.52 |

## Measurements of the Cu(I) complexes in the KBr matrix

**Pellet preparation.** For the preparation of KBr pellets the copper complexes (0.9 mg) were mixed with dry KBr, (200 mg, stored in a compartment dryer at 80 °C, purchased from Merck) and ground to a homogenous mixture. This mixture was filled in an evacuable pellet die with a diameter of 13 mm and sintered at a pressure of 0.75 GPa at room temperature.

**Photophysical measurements.** Temperature dependent emission spectra of KBr pellets were recorded using a Fluoromax-2 (*Jobin-Yvon*) fluorescence spectrometer. Luminescence lifetimes were determined by TCSPC using a DeltaFlex (*Horiba Scientific*) spectrometer with an analogous setup as applied for powder samples. Excitation sources: NanoLED 390 (wavelength: 389 nm, pulse duration: 1.3 ns), NanoLED 350 (wavelength: 345 nm, pulse duration: <1 ns). Long-wave pass filters (cutoff at 500/510 nm) were set between sample and emission monochromator to suppress the influence of scattered excitation light. Decay curves were analysed by multiexponential fits with the software ORIGIN®.

**Table S4.** Temperature dependent emission maxima and lifetimes in the KBr matrix determined by TCSPC of **Cu-1b** and **Cu-2b**. A is the contribution of the two lifetime components.

| Complex | T [K] | $\lambda_{EX}$ [nm] | $\lambda_{PL}$ [nm] | $\tau_1$ [µs] | $\tau_2$ [µs] | $A_1$ [%] | $A_2$ [%] |
|---|---|---|---|---|---|---|---|
| **Cu-1b** | 290 | 345 | 529 | / | 5.0 | / | 100 |
| | | 389 | 529 | / | 5.1 | / | 100 |
| | 20 | 345 | 533 | 0.4 | 35 | 1 | 99 |
| | | 389 | 533 | 0.4 | 38 | 1 | 99 |
| **Cu-2b** | 290 | 345 | 515 | / | 3.9 | / | 100 |
| | | 389 | 515 | / | 4.0 | / | 100 |
| | 20 | 345 | 519 | 0.8 | 33 | 1 | 99 |
| | | 389 | 519 | 0.4 | 31 | 1 | 99 |

**Table S5.** Measured temperature-dependent emission maxima and deduced singlet-triplet energy gaps $\Delta E_{ST}(\mathbf{exp})$.

| | $\lambda_{PL}$(290 K) [nm] | $\lambda_{PL}$(20 K) [nm] | $\Delta E_{ST}(\mathbf{exp})$ [$cm^{-1}$] | $\Delta E_{ST}(\mathbf{exp})$ [eV] |
|---|---|---|---|---|
| **Cu-1b** | 527 | 533 | 214 | 0.027 |
| **Cu-2b** | 514 | 518 | 150 | 0.019 |

## Measurements of the Cu(I) complexes in solution

Static emission spectra in solution were recorded using a Fluorolog 3-22 *τ* (*Horiba Jobin-Yvon*) fluorescence spectrometer. Spectroscopic grade solvents were purchased from *Merck*. The solutions were prepared using the common Schlenck technique with concentrations in the range of $2 \cdot 10^{-5}$ M and were measured in 1 cm x 1 cm quartz cuvettes. Lifetimes were determined by TCSPC using the same setup as used for KBr pellets. Excitation sources: NanoLED 350 (wavelength: 345 nm, pulse duration: <1 ns), NanoLED 320 (wavelength: 313 nm, pulse duration: <1 ns). The instrumental response function (IRF) of 125 ps (FWHM) was collected by use of LUDOX®. Decay curves were analysed by monoexponential fits with the software ORIGIN®.

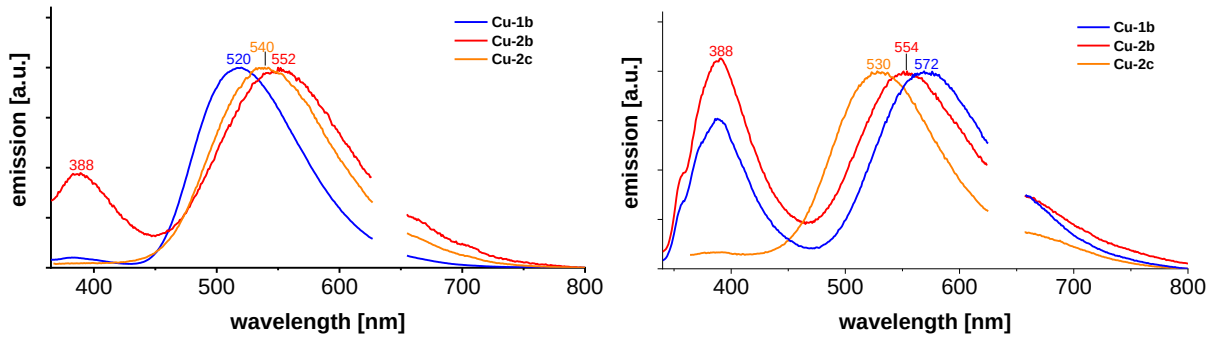



**Figure S37.** Emission spectra of **Cu-1b**, **Cu-2b** and **Cu-2c** in ethanol (left) and chlorobenzene (right) measured at room temperature with 320 nm excitation wavelength (second-order Rayleigh scattering cut out for clarity).

**Table S6.** Emission maxima and lifetimes of **Cu-1b**, **Cu-2b** and **Cu-2c** measured by TCSPC at room temperature.

| Complex | Solvent | $\lambda_{EX}$ [nm] | $\lambda_{PL}$ [nm] | τ [µs] |
|---|---|---|---|---|
| **Cu-1b** | chlorobenzene | 313 | 570 | 0.3 |
| | DCM | 345 | 578 | 0.3 |
| | EtOH | 345 | 518 | 4.9 |
| **Cu-2b** | chlorobenzene | 313 | 552 | 0.4 |
| | DCM | 345 | 558 | 0.2 |
| | EtOH | 313 | 550 | 0.2 |
| **Cu-2c** | chlorobenzene | 345 | 532 | 0.4 |
| | DCM | 345 | 538 | 0.3 |
| | EtOH | 345 | 532 | 0.1 |

## Step-scan FTIR spectroscopy on the Cu(I) complexes

**Step-scan FTIR measurements.** The experimental setup has been described in detail before, so that only a brief description of the general setup is given here.[12-14] All the time-resolved FTIR experiments were performed with the FTIR spectrometer Bruker Vertex 80v, operated in the step-scan mode. A liquid-nitrogen-cooled mercury cadmium telluride (MCT) detector (*Kolmar Tech.*, Model KV100-1-B-7/190) with a rise time of 25 ns, connected to a fast preamplifier and a 14-bit transient recorder board (Spectrum Germany, M3I4142, 400 MS/s), was used for signal detection and processing. The laser setup includes a Q-switched Nd:YAG laser (Innolas SpitLight Evo I) generating pulses with a band-width of 6 – 9 ns at a repetition rate of 100 Hz. The third harmonic (355 nm) of the Nd:YAG laser was used directly for sample excitation. The UV pump beam was attenuated to about 2.0 mJ per shot at a diameter of 9 mm. The beam was directed onto the sample and adjusted to have a maximal overlap with the IR beam of the spectrometer. The sample chamber was equipped with anti-reflection-coated germanium filters to prevent the entrance of laser radiation into the detector and interferometer compartments. The KBr pellets were prepared as described above (see **pellet preparation**) and cryogenically cooled (20 K or 290 K) with a closed cycle helium cryostat (ARS Model DE-202A). The cryo cooler was equipped with a homebuilt pellet holder and $CaF_2$ windows. The cryostat was hanging from a rack into the sample compartment without touching the spectrometer to prevent vibrations of the cooler to be transferred to the instrument. The temporal resolution of the 14-bit transient recorder board was set to 20 ns. The step-scan measurement was started 1.8 µs before the Q-Switch of the Nd:YAG laser was triggered, which means that the experiment was initiated 2.2 µs before the laser pulse reached the sample. Hence, this time was set as zero point in all spectra. The time delay between the start of the experiment and the laser pulse was controlled with a Stanford Research Systems DG535 delay generator. The spectral region was limited by undersampling to 988 – 1975 $cm^{-1}$ with a spectral resolution of 4 $cm^{-1}$ resulting in 555 interferogram points. An IR broad band filter (850 – 1750 $cm^{-1}$) and the $CaF_2$ windows (no IR transmission $<$ 1000 $cm^{-1}$) of the cryostat prevented problems when performing a Fourier transformation (*i.e.* no IR intensity outside the measured region should be observed).

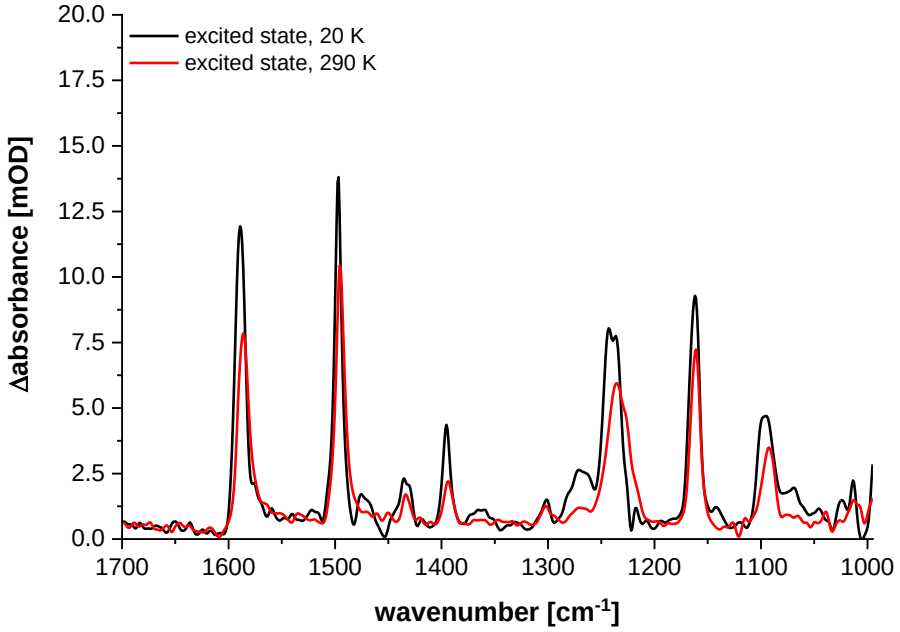



**Figure S38.** Excited state spectra at 20 K (black) and 290 K (red) of **Cu-2b**.

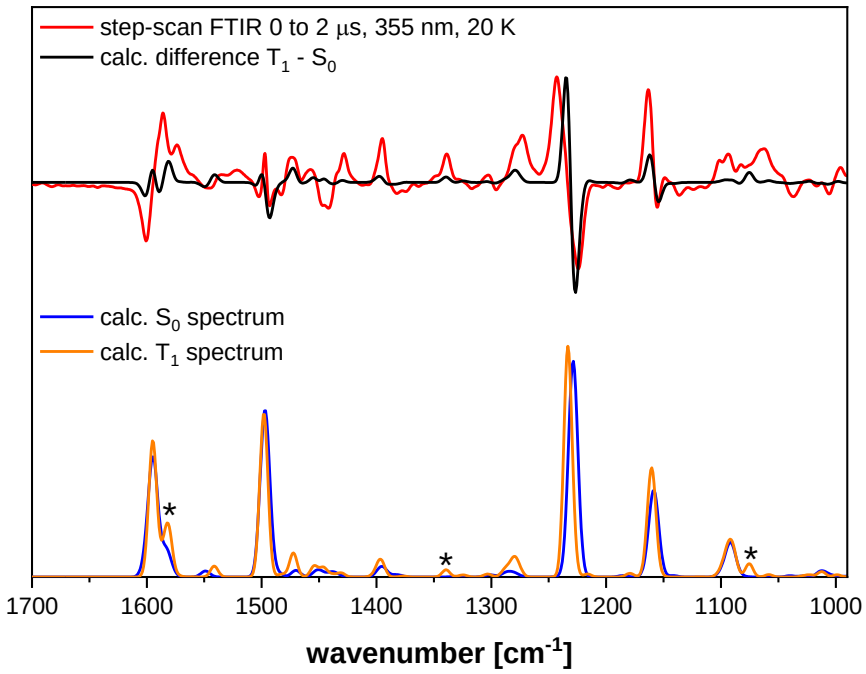



**Figure S39.** Step-scan difference spectrum 0 to 2 μs after excitation ($\lambda_{EX}$ = 355 nm) (red), calculated $S_0$ spectrum (blue), calculated $T_1$ spectrum (orange) (B3LYP/def2-TZVP, FWHM = 8 $cm^{-1}$, Gaussian profile, scaled by 0.975) and calculated difference spectrum $T_1 - S_0$ (black) of **Cu-2b**. The $T_1$ specific bands are marked with asterisks.

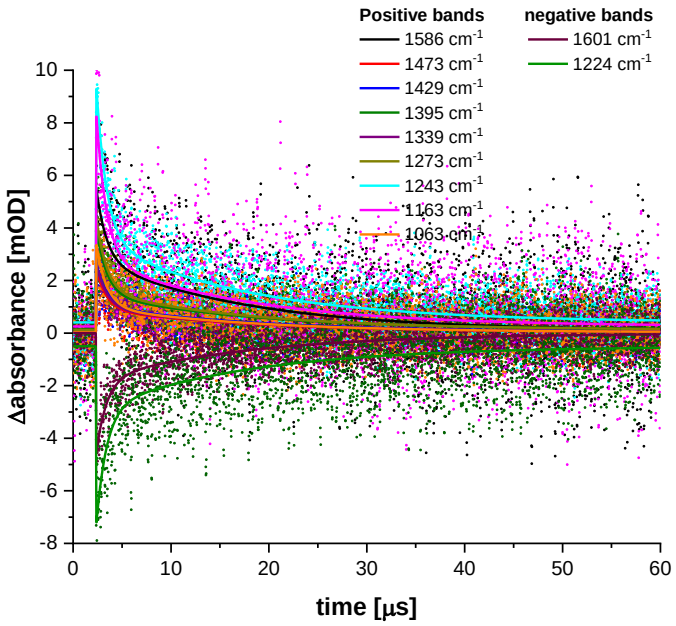



**Figure S40**. Time traces of the IR signal of nine positive and three negative bands (dots) in the step-scan spectrum of **Cu-2b** at 20 K with biexponential fits (convolution with Gaussian pulse), resulting in decay times of $\tau_1$ = 1053 ± 49 ns and $\tau_2$ = 15447 ± 494 ns.

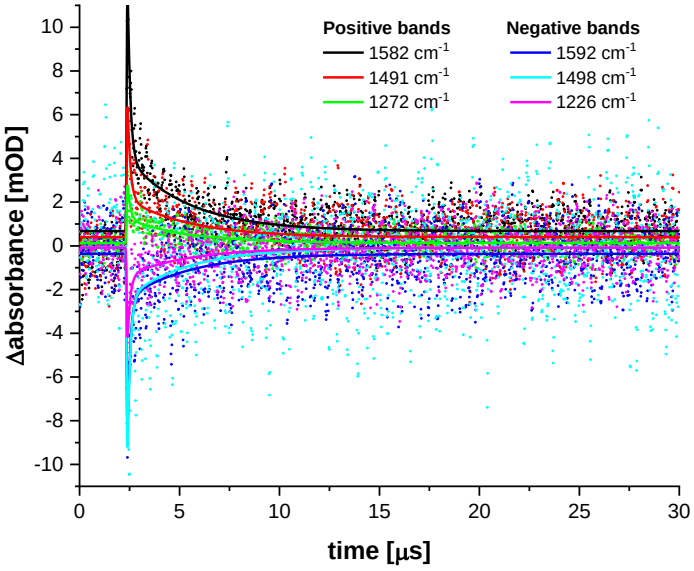



**Figure S41**. Time traces of the IR signal of nine positive and three negative bands (dots) in the step-scan spectrum of **Cu-2b** at 290 K with biexponential fits (convolution with Gaussian pulse), resulting in decay times of $\tau_1$ = 139 ± 16 ns and $\tau_2$ = 3083 ± 209 ns.

**optimized $S_0$ geometry** **optimized $T_1$ geometry**

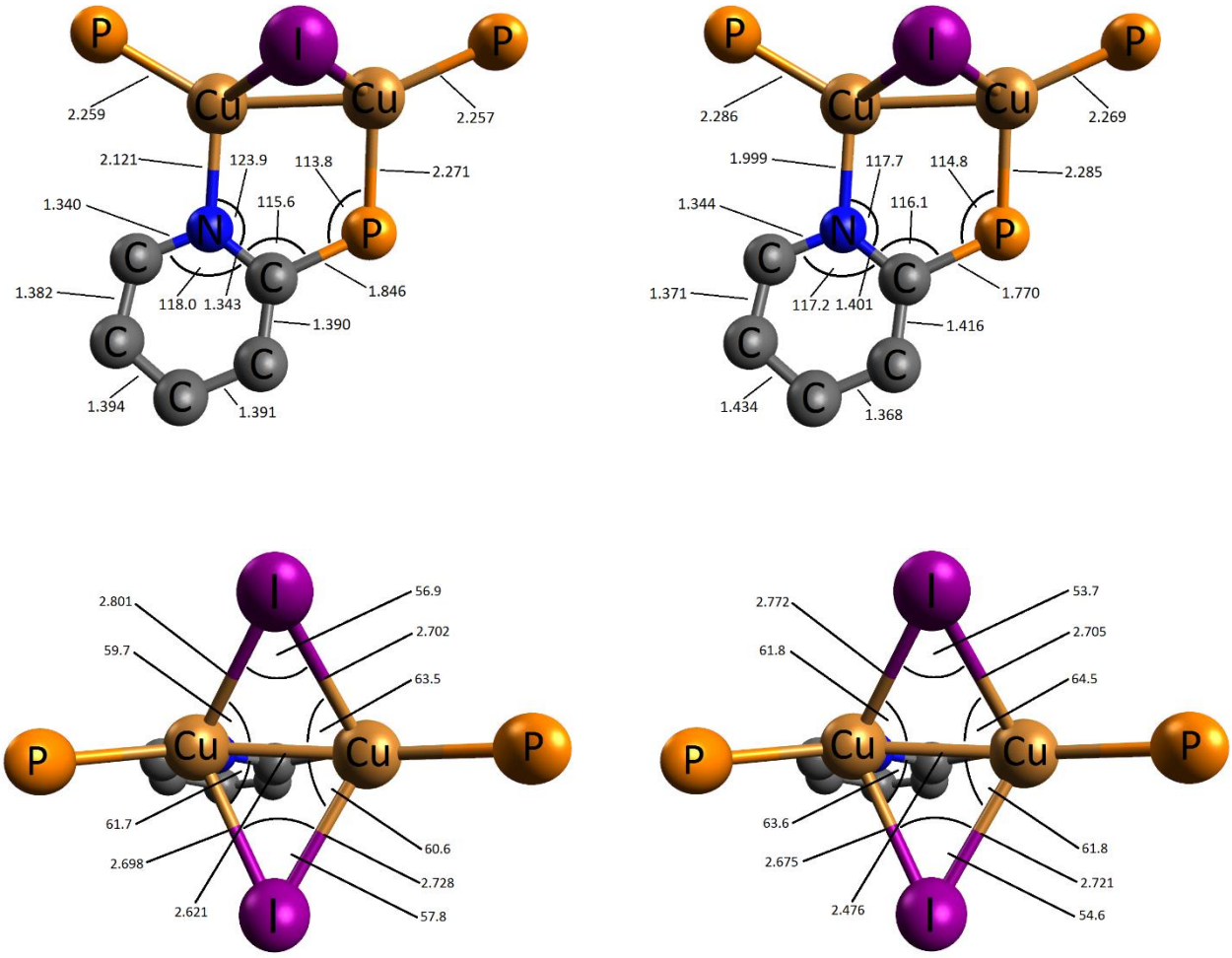



**Figure S42.** Bond lengths (Å) and angles (°) in the central $Cu_2I_2$ unit of **Cu-2b** in the $S_0$ and $T_1$ electronic state, calculated with B3LYP-D3(BJ)/def2-TZVP.

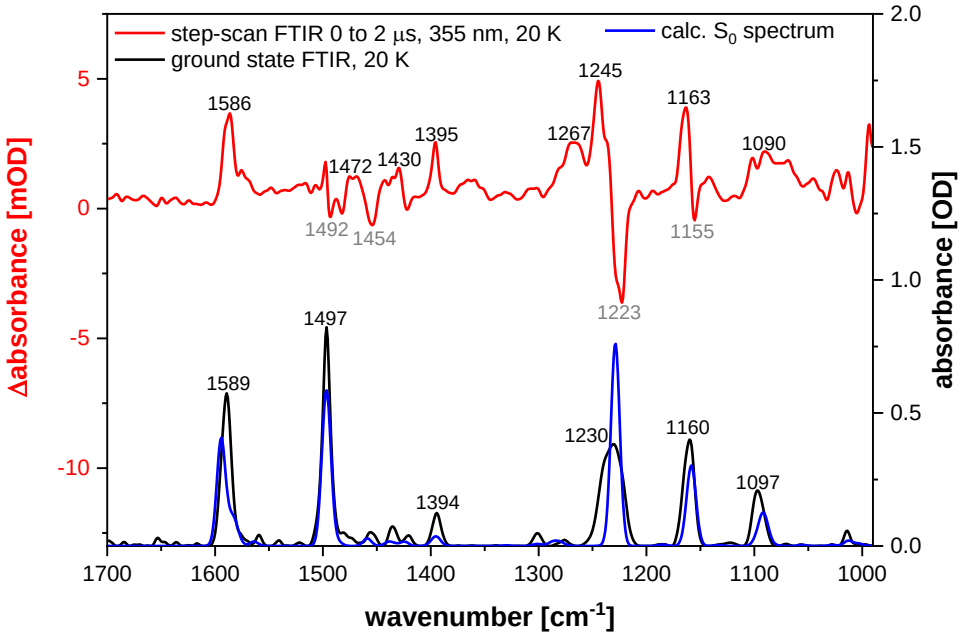



**Figure S43.** FTIR ground state spectrum at 20 K (black), calculated $S_0$ spectrum (B3LYP-D3(BJ)/def2-TZVP, FWHM = 8 $cm^{-1}$, Gaussian profile, scaled by 0.975) (blue) and step-scan difference spectrum 0 to 2 µs after excitation ($\lambda_{EX}$ = 355 nm) (red) of **Cu-1b**.

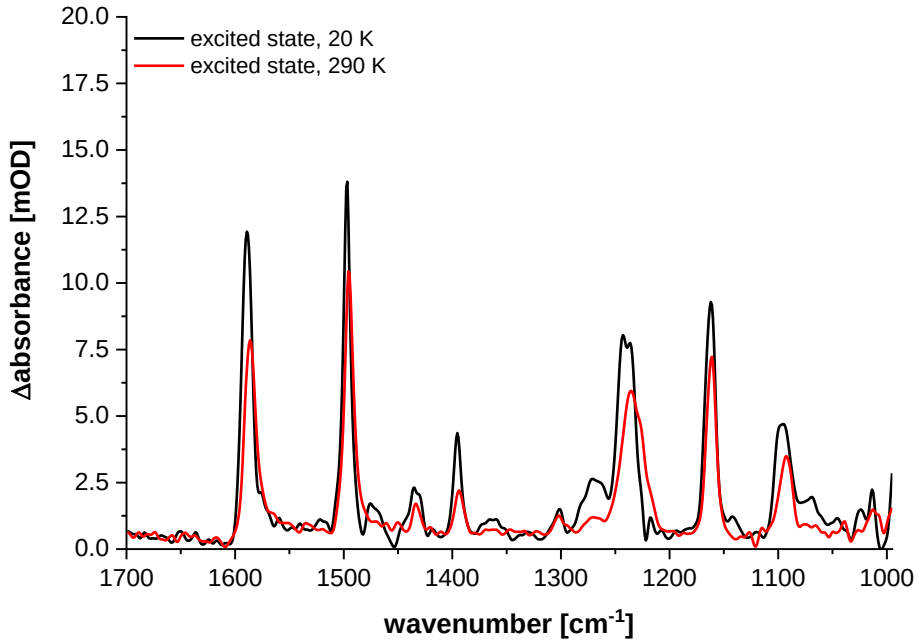



**Figure S44.** Excited state spectra at 20 K (black) and 290 K (red) of **Cu-1b**.

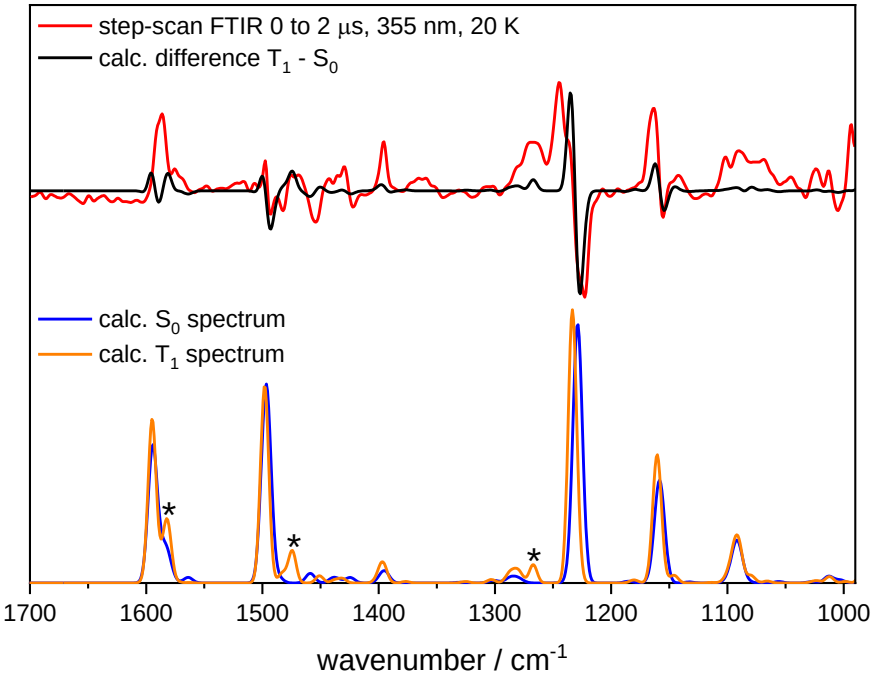



**Figure S45.** Step-scan difference spectrum 0 to 2 µs after excitation ($\lambda_{EX}$ = 355 nm) (red), calculated $S_0$ spectrum (blue), calculated $T_1$ spectrum (orange) (B3LYP-D3(BJ)/def2-TZVP, FWHM = 8 $cm^{-1}$, Gaussian profile, scaled by 0.975) and calculated difference spectrum $T_1 - S_0$ (black) of **Cu-1b**. The $T_1$ specific bands are marked with asterisks.

**optimized $S_0$ geometry** **optimized $T_1$ geometry**

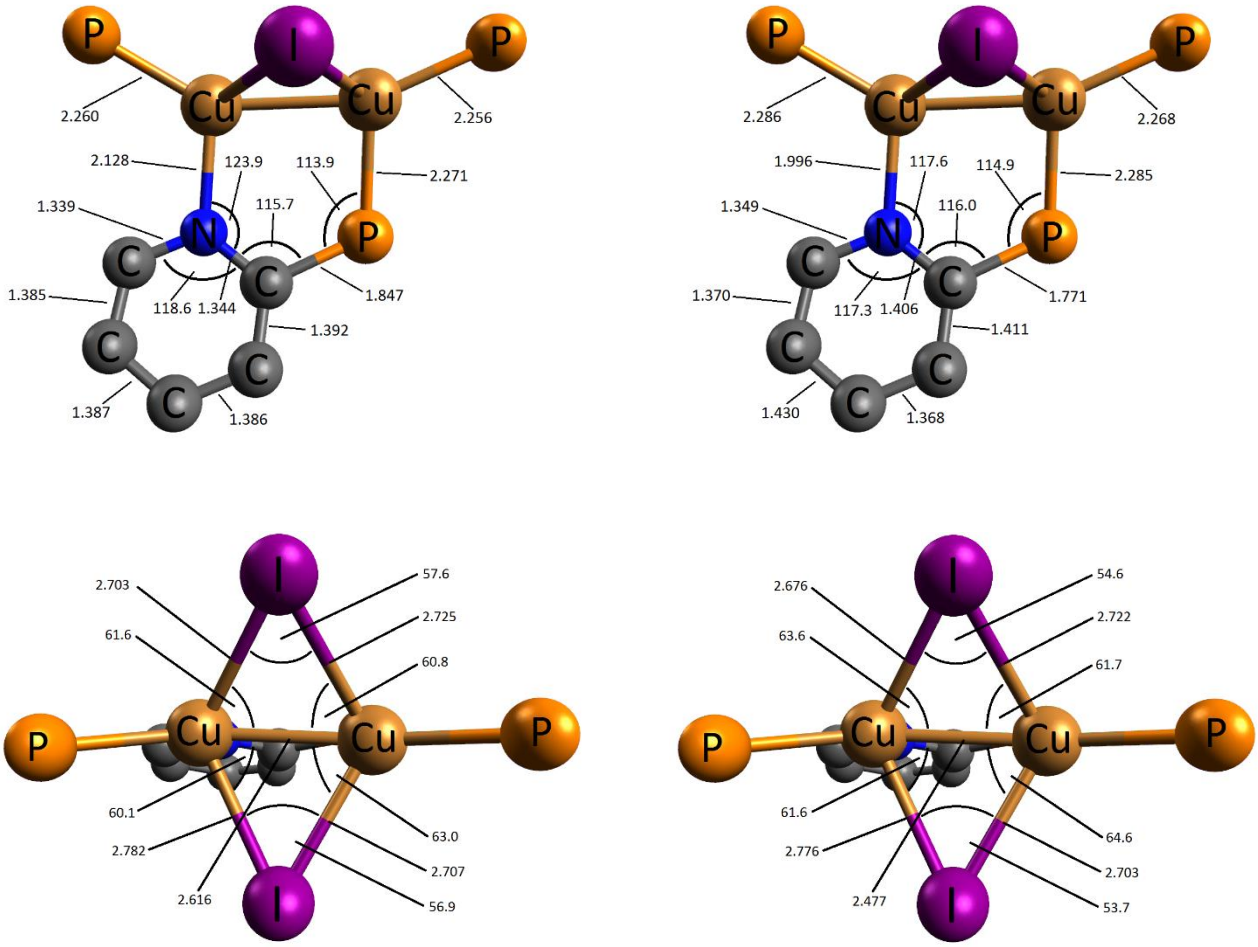



**Figure S46.** Bond lengths (Å) and angles (°) in the central $Cu_2I_2$ unit of **Cu-1b** in the $S_0$ and $T_1$ electronic state, calculated with B3LYP-D3(BJ)/def2-TZVP.

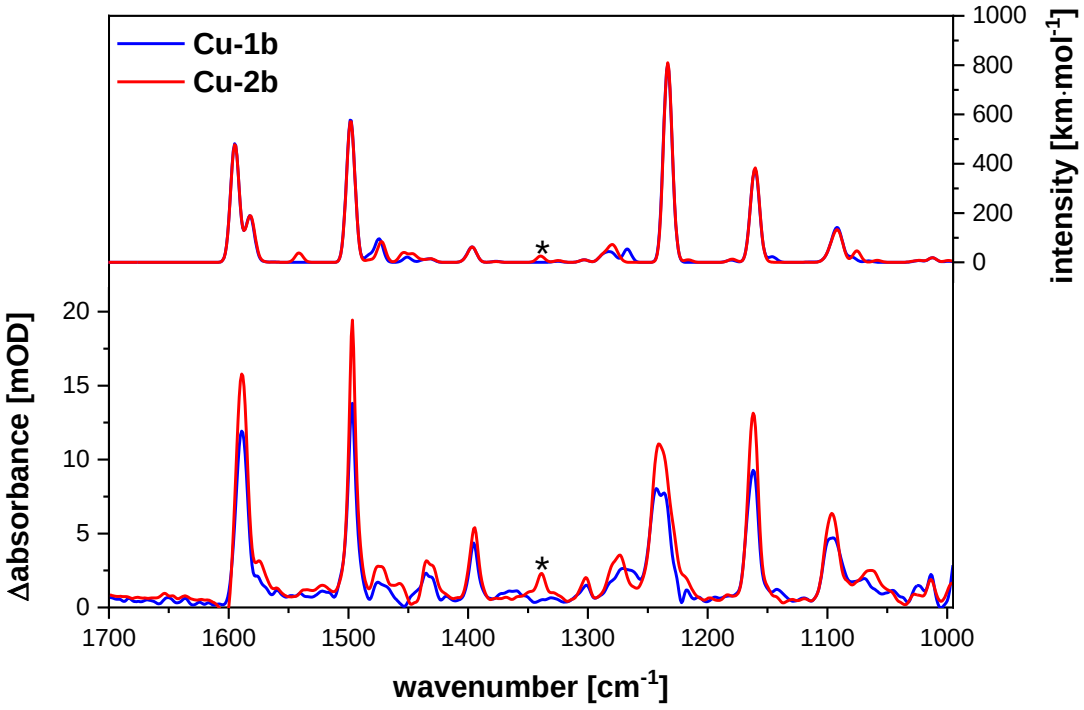
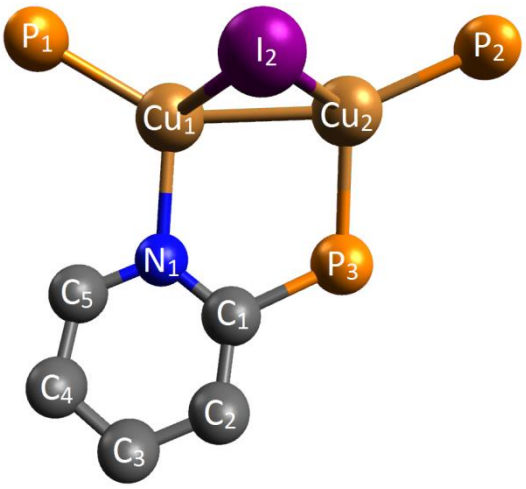


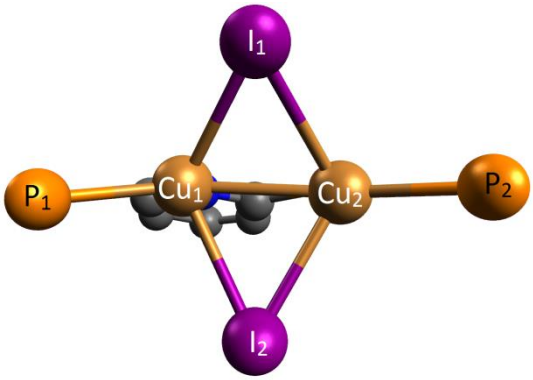

**Figure S47.** Excited state spectra at 20 K (bottom) and calculated $T_1$ spectra (top) (B3LYP-D3(BJ)/def2-TZVP, FWHM = 8 $cm^{-1}$, Gaussian profile, scaled by 0.975) of **Cu-1b** (blue) and **Cu-2b** (red). The band specific for **Cu-2b** is marked with an asterisk.

**Table S7.** Lifetimes of **Cu-1b** and **Cu-2b** determined by transient FTIR spectroscopy at 20 K and 290 K ($\lambda_{EX}$ = 355 nm).

| Complex | T [K] | $\tau_1$ [µs] | $\tau_2$ [µs] | $A_1$ [%] | $A_2$ [%] |
|---|---|---|---|---|---|
| **Cu-1b** | 20 | 1.1 | 16 | 14 | 86 |
| | 290 | 0.1 | 2.4 | 19 | 81 |
| **Cu-2b** | 20 | 1.1 | 15 | 11 | 89 |
| | 290 | 0.1 | 3.1 | 13 | 87 |

**Table S8.** Change of geometrical parameters of **Cu-2b** and **Cu-1b** concerning the copper – iodide core with transition from the $S_0$ structure to the $T_1$ structure, calculated with B3LYP-D3(BJ)/def2-TZVP. The numbers of the atoms are shown in the figures above.




| | Differences | |
|---|---|---|
| **parameter** | **Cu-2b** | **Cu-1b** |
| d(N1-C1) | +0.06 Å | +0.06 Å |
| d(Cu1-Cu2) | -0.15 Å | -0.14 Å |
| d(Cu1-N1) | -0.12 Å | -0.13 Å |
| ∠(Cu1-I1-Cu2) | -3.2° | -3.0° |
| ∠(C19-I2-Cu2) | -3.2° | -3.2° |

**Table S9**. Characterization of vibrational modes of a) **Cu-2b** and b) **Cu-1b**. The calculated frequencies are indicated in brackets.

a)

| $\tilde{\nu}$ / cm$^{-1}$ ground state | $\tilde{\nu}$ / cm$^{-1}$ excited state | Character of the vibration |
|---|---|---|
| 1589 (1596) | 1589 (1595) | Aromatic C–C stretching |
| | 1575 (1580) | Aromatic C–C stretching |
| 1497 (1498) | 1497 (1498) | C–H scissoring in the fluorinated phenyl moieties |
| 1394 (1396) | 1394 (1396) | C–H scissoring, combined with aromatic C–C stretching in the fluorinated phenyl moieties |
| | 1338 (1340) | C–H scissoring in the pyridine ring, combined with aliphatic C–H of the methyl group |
| 1276 (1278) | 1274 (1284) | C–C stretching in the phenyl rings |
| 1231 (1229) | 1241 (1234) | C–F stretching vibration |
| 1160 (1156) | 1162 (1162) | C–H scissoring |
| 1097 (1092) | 1096 (1091) | C–P stretching vibration |
| | 1065 (1075) | C–H scissoring in the bridging ligand, combined with aliphatic C–H of the methyl group |

b)

| $\tilde{\nu}$ / cm$^{-1}$ ground state | $\tilde{\nu}$ / cm$^{-1}$ excited state | Character of the vibration |
|---|---|---|
| 1589 (1593) | 1589 (1594) | C–C stretching in the phenyl rings |
| | 1578 (1581) | C–C stretching in the phenyl moieties |
| 1497 (1497) | 1497 (1498) | C–C stretching in the pyridine ring, combined with C–H scissoring |
| | 1475 (1474) | C–H scissoring, combined with C–C stretching in the pyridine moiety |
| 1394 (1396) | 1395 (1397) | C–H scissoring in the fluorinated phenyl rings |
| 1276 (1279) | 1280 (1284) | Asymmetric C–C stretching in the phenyl moieties |
| | 1271 (1268) | C–H scissoring, combined with C–C stretching in the pyridine moiety |
| 1230 (1229) | 1243 (1233) | C–F stretching vibration |
| 1160 (1159) | 1162 (1159) | C–H scissoring |
| 1097 (1092) | 1095 (1095) | C–P stretching vibration |

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## 9. Structures in XYZ

The following structures were used for calculating electronic excitations for either the UV/Vis Spectra or vertical singlet-triplet gap.

```
#Cu-1b singlet ground state
105

Cu   -1.1896460   -0.1358123   -0.0909001
Cu    1.4350184   -0.6022229   -0.0380301
I     0.2413979    0.0689196   -2.3795012
I     0.2570360    0.4598836    2.1180214
P    -1.4734687   -2.4026332    0.1445288
P    -2.8919959    1.4080169   -0.1447875
P     3.5884645    0.1807497   -0.0717902
F    -1.0947189    7.1258365   -0.0875361
F    -6.4807942    1.0864121   -4.9384822
F    -6.4693627    0.4726187    4.5754754
F     4.0745615    6.0073546   -1.3976299
F     6.4428511   -0.2870627    5.1809878
F     7.0031641   -2.7718233   -4.0309759
N     1.2627750   -2.7168160   -0.1179244
C     0.0814966   -3.3793210   -0.2142976
C     0.0225085   -4.7417664   -0.5672997
H    -0.9560619   -5.2395301   -0.6542665
C     1.2095016   -5.4494673   -0.8037901
H     1.1805861   -6.5164396   -1.0801449
C     2.4277655   -4.7677085   -0.6778883
H     3.3928014   -5.2694306   -0.8512261
C     2.4029503   -3.4101587   -0.3352118
H     3.3412510   -2.8383907   -0.2463996
C    -1.9554458   -2.9893891    1.8329263
C    -1.3858431   -4.1045797    2.4818715
H    -0.5930796   -4.6909519    1.9909501
C    -1.8163627   -4.4744155    3.7669338
H    -1.3554987   -5.3431868    4.2659589
C    -2.8253387   -3.7432496    4.4140263
H    -3.1611261   -4.0361454    5.4226276
C    -3.3957138   -2.6293063    3.7758796
H    -4.1786882   -2.0380236    4.2789901
C    -2.9544939   -2.2462476    2.5000486
H    -3.3842889   -1.3500658    2.0224930
C    -2.6755728   -3.2660522   -0.9730917
C    -3.8147121   -3.9524757   -0.5027729
H    -3.9935880   -4.0466669    0.5805664
C    -4.7250319   -4.5207000   -1.4109908
H    -5.6114294   -5.0545572   -1.0294100
C    -4.5066422   -4.4167542   -2.7939747
H    -5.2202174   -4.8679336   -3.5032553
C    -3.3728268   -3.7333614   -3.2695206
H    -3.1920076   -3.6459565   -4.3540576
C    -2.4663396   -3.1542308   -2.3687502
H    -1.5896160   -2.6008126   -2.7504929
```

| | | | |
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| C | -1.1859344 | 3.5452735 | -0.7438152 |
| H | -0.5917365 | 2.7757297 | -1.2677082 |
| C | -0.7579609 | 4.8798771 | -0.7648330 |
| H | 0.1566625 | 5.1790077 | -1.3001179 |
| C | -1.5075638 | 5.8455617 | -0.0801255 |
| C | -2.6740378 | 5.5082244 | 0.6185278 |
| H | -3.2329908 | 6.2937838 | 1.1508068 |
| C | -3.1007154 | 4.1712439 | 0.6220918 |
| H | -4.0168772 | 3.9032698 | 1.1732125 |
| C | -4.0000584 | 1.3648271 | -1.6248293 |
| C | -4.7646065 | 2.4755737 | -2.0439495 |
| H | -4.7009133 | 3.4300397 | -1.4962505 |
| C | -5.6038861 | 2.3865204 | -3.1634148 |
| H | -6.2016204 | 3.2456012 | -3.5063369 |
| C | -5.6762560 | 1.1740974 | -3.8642900 |
| C | -4.9262392 | 0.0573546 | -3.4761416 |
| H | -4.9965294 | -0.8776338 | -4.0536171 |
| C | -4.0835551 | 0.1637710 | -2.3600133 |
| H | -3.4733991 | -0.7043890 | -2.0610021 |
| C | -4.0671443 | 1.2340872 | 1.2726228 |
| C | -5.3857469 | 0.7582589 | 1.1071733 |
| H | -5.7836935 | 0.5759403 | 0.0960027 |
| C | -6.2041157 | 0.5025759 | 2.2195499 |
| H | -7.2325649 | 0.1263851 | 2.1026544 |
| C | -5.6961554 | 0.7327365 | 3.5037216 |
| C | -4.3957274 | 1.2180648 | 3.7002930 |
| H | -4.0272856 | 1.3872148 | 4.7242362 |
| C | -3.5835648 | 1.4593256 | 2.5841135 |
| H | -2.5487418 | 1.8086255 | 2.7376739 |
| C | 3.7770138 | 1.9602674 | -0.5354548 |
| C | 4.7462179 | 2.4277150 | -1.4476223 |
| H | 5.4312782 | 1.7188845 | -1.9401960 |
| C | 4.8489370 | 3.7958083 | -1.7463713 |
| H | 5.5962767 | 4.1751554 | -2.4608060 |
| C | 3.9787983 | 4.6947089 | -1.1176453 |
| C | 3.0060313 | 4.2578564 | -0.2075282 |
| H | 2.3356825 | 4.9920602 | 0.2661017 |
| C | 2.9013179 | 2.8888535 | 0.0722235 |
| H | 2.1229155 | 2.5346060 | 0.7713394 |
| C | 4.4948292 | 0.0802273 | 1.5370606 |
| C | 4.0537446 | -0.8577151 | 2.4955025 |
| H | 3.1633769 | -1.4738970 | 2.2836661 |
| C | 4.7120200 | -0.9936605 | 3.7266213 |
| H | 4.3726558 | -1.7149193 | 4.4862062 |
| C | 5.8107162 | -0.1692793 | 4.0001411 |
| C | 6.2621459 | 0.7841965 | 3.0764837 |
| H | 7.1212116 | 1.4230375 | 3.3349654 |
| C | 5.5984236 | 0.9051564 | 1.8472028 |
| H | 5.9428998 | 1.6607413 | 1.1217122 |
| C | 4.7151646 | -0.6921063 | -1.2561018 |
| C | 4.2528639 | -0.8743306 | -2.5822778 |
| H | 3.2652547 | -0.4772748 | -2.8773587 |
| C | 5.0250022 | -1.5660462 | -3.5247519 |

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H     4.6757325   -1.7091924   -4.5593769
C     6.2621646   -2.0976985   -3.1327810
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H     7.7155482   -2.3800602   -1.5525994
C     5.9642464   -1.2401252   -0.8918666
H     6.3434845   -1.1169140    0.1352926

#Cu-1c singlet ground state
123

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I     0.2390519   -0.3089439   -2.3365621
Cu   -1.2681004   -0.6083938   -0.1085904
Cu    1.3607625   -0.8599582    0.0686122
P    -1.4013540   -2.8862264    0.1533075
P    -3.0520904    0.8219991   -0.2891237
P     3.3990375    0.1753100    0.0980102
F    -6.8539121   -1.6703014    4.6389428
F    -6.9060427    0.3968000    5.3302823
F    -8.3755919   -0.3074672    3.8737031
F    -5.8806398   -0.6181812   -6.3141026
F    -6.4728385    1.4810989   -6.1659632
F    -7.6426997   -0.0580693   -5.1591880
F     6.8735260   -3.5441590   -4.3867456
F     8.5443759   -3.0485186   -3.0674007
F     7.9212823   -1.6490650   -4.6218702
F    -2.1125447    7.5340967    0.6968866
F    -0.0614571    6.8048428    0.5298752
F    -1.1931656    7.2905894   -1.2690537
F     3.8193253    6.4883111   -2.5199616
F     2.9341683    6.9295253   -0.5724642
F     1.6697075    6.2601487   -2.2174795
F     5.5151895   -0.2589427    6.5609946
F     7.4172121   -0.3409629    5.4977809
F     6.5377766    1.5894192    5.9984725
N     1.3710361   -2.9711633    0.0470815
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C     0.3252261   -5.1233982   -0.2870564
H    -0.6041127   -5.7089357   -0.3687239
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C    -4.2336643   -5.4086160   -1.6161987
H    -5.0492208   -6.0781620   -1.2957010
C    -3.4697273   -4.7350064   -0.6470429
H    -3.6918493   -4.8837024    0.4219534
C    -1.9747889   -3.4615655    1.8135943
```

| | | | |
|---|---|---|---|
| C | -3.2079416 | -2.9479251 | 2.2759603 |
| H | -3.7811525 | -2.2437563 | 1.6493457 |
| C | -3.7090848 | -3.3166492 | 3.5333586 |
| H | -4.6736973 | -2.9080464 | 3.8762396 |
| C | -2.9712227 | -4.1833691 | 4.3577870 |
| H | -3.3578770 | -4.4632940 | 5.3515812 |
| C | -1.7355169 | -4.6806967 | 3.9158605 |
| H | -1.1455154 | -5.3516666 | 4.5621150 |
| C | -1.2395487 | -4.3268369 | 2.6497594 |
| H | -0.2669697 | -4.7267086 | 2.3224230 |
| C | -4.3308858 | 0.5802741 | 1.0254385 |
| C | -5.6535633 | 0.1811683 | 0.7387730 |
| H | -5.9914535 | 0.0909108 | -0.3056611 |
| C | -6.5518111 | -0.1096449 | 1.7771573 |
| H | -7.5814443 | -0.4214096 | 1.5423992 |
| C | -6.1423075 | 0.0041958 | 3.1167297 |
| C | -4.8293325 | 0.4179900 | 3.4131468 |
| H | -4.5038171 | 0.5127078 | 4.4611041 |
| C | -3.9288252 | 0.6940138 | 2.3777380 |
| H | -2.8918877 | 0.9798413 | 2.6230803 |
| C | -7.0760040 | -0.3834754 | 4.2385604 |
| C | -4.0325562 | 0.7319096 | -1.8557837 |
| C | -4.7603634 | 1.8291005 | -2.3631513 |
| H | -4.7438033 | 2.7964904 | -1.8352019 |
| C | -5.5017394 | 1.7017512 | -3.5458569 |
| H | -6.0596513 | 2.5644212 | -3.9425951 |
| C | -5.5274330 | 0.4738233 | -4.2329914 |
| C | -4.7970466 | -0.6209336 | -3.7391372 |
| H | -4.7973417 | -1.5778497 | -4.2841212 |
| C | -4.0483007 | -0.4884198 | -2.5613067 |
| H | -3.4584698 | -1.3441276 | -2.1931387 |
| C | -6.3774806 | 0.3210622 | -5.4750123 |
| C | -2.6135641 | 2.6164809 | -0.1806449 |
| C | -1.5615354 | 3.0686954 | -1.0093936 |
| H | -1.0377447 | 2.3594808 | -1.6738876 |
| C | -1.1632750 | 4.4097727 | -0.9812900 |
| H | -0.3440106 | 4.7534817 | -1.6321411 |
| C | -1.7932681 | 5.3140518 | -0.1037593 |
| C | -2.8392165 | 4.8727564 | 0.7224518 |
| H | -3.3367206 | 5.5806942 | 1.4028189 |
| C | -3.2526896 | 3.5313139 | 0.6791447 |
| H | -4.0779887 | 3.2024191 | 1.3302874 |
| C | -1.2990566 | 6.7413575 | -0.0382589 |
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| C | 4.3014938 | -0.9172883 | -2.3203823 |
| H | 3.2783609 | -0.6880686 | -2.6677953 |
| C | 5.2020434 | -1.5478579 | -3.1864308 |
| H | 4.8904578 | -1.7987012 | -4.2131013 |
| C | 6.4972953 | -1.8791749 | -2.7416776 |
| C | 6.8809569 | -1.5728369 | -1.4260317 |
| H | 7.8900146 | -1.8373080 | -1.0740887 |
| C | 5.9821457 | -0.9289106 | -0.5602394 |
| H | 6.3017813 | -0.6921710 | 0.4669597 |
| C | 7.4647940 | -2.5341671 | -3.7011911 |

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C     3.3420266    1.9433559   -0.4431002
C     4.0860414    2.4543187   -1.5243943
H     4.7765028    1.8032045   -2.0833870
C     3.9520969    3.7992682   -1.9054576
H     4.5327548    4.1911987   -2.7544844
C     3.0820618    4.6474068   -1.2019846
C     2.3449488    4.1467362   -0.1101970
H     1.6601310    4.8097943    0.4416913
C     2.4645025    2.8023830    0.2583892
H     1.8561940    2.4105561    1.0920838
C     2.8866866    6.0846374   -1.6269266
C     4.2490221    0.2833606    1.7391006
C     3.9267677   -0.6752228    2.7218072
H     3.1510326   -1.4313021    2.5136556
C     4.5603745   -0.6542990    3.9729530
H     4.2954245   -1.3995512    4.7387288
C     5.5150621    0.3365098    4.2592434
C     5.8266684    1.3115580    3.2931723
H     6.5598171    2.1000130    3.5254129
C     5.1972455    1.2843456    2.0413274
H     5.4425758    2.0564526    1.2937302
C     6.2421539    0.3343583    5.5861389
H     3.4560211   -2.9200725    0.0028948
H     3.7364824   -5.3773175   -0.4086357
H     1.6484216   -6.8252885   -0.6111411

#Cu-1d singlet ground state
105

I     7.8510738    2.4160014    4.6575193
I    10.4026676   -0.8613287    6.4073086
Cu    7.9823723   -0.1928451    5.3729919
Cu   10.1512276    1.0270518    4.4956613
Cl    0.4096269   -0.5691754    5.0711256
Cl    7.1800052   -5.6566139   10.7540636
Cl    7.1175263    4.5464725   11.0600436
Cl   11.2574339    8.0307833    1.5317757
Cl   11.8847830    4.3375803   11.0060815
Cl   17.6187570    0.2900491    3.4047613
P     7.9817791   -1.4485054    3.4603701
P     6.4913985   -0.4424726    7.0980012
P    11.8005350    2.5766893    4.8495815
N    10.3174077   -0.1287693    2.7318207
C     9.5158973   -1.1750265    2.4114373
C     9.7834462   -2.0010023    1.3028479
H     9.1084336   -2.8399621    1.0724417
C    10.9035823   -1.7473249    0.5010927
C    11.7250431   -0.6592369    0.8306811
H    12.6180314   -0.4078797    0.2370181
C    11.3920097    0.1166712    1.9465266
H    12.0188909    0.9740802    2.2417348
C     6.6761582   -1.2558597    2.1502749
C     6.1166909    0.0299329    1.9858260
H     6.4453960    0.8562816    2.6417813
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| | | | |
|---|---|---|---|
| C | 5.1550462 | 0.2638225 | 0.9896311 |
| H | 4.7303867 | 1.2747091 | 0.8717550 |
| C | 4.7335019 | -0.7822293 | 0.1530800 |
| H | 3.9732885 | -0.5994986 | -0.6245260 |
| C | 5.2834194 | -2.0652912 | 0.3128547 |
| H | 4.9562083 | -2.8930452 | -0.3383942 |
| C | 6.2515601 | -2.3023993 | 1.3016401 |
| H | 6.6670715 | -3.3168815 | 1.4167858 |
| C | 8.0276941 | -3.2641786 | 3.7889396 |
| C | 6.8165183 | -3.9542711 | 4.0327023 |
| H | 5.8510379 | -3.4333995 | 3.9190258 |
| C | 6.8301427 | -5.3003754 | 4.4285839 |
| H | 5.8763910 | -5.8241399 | 4.6069539 |
| C | 8.0510738 | -5.9747831 | 4.6044523 |
| H | 8.0605898 | -7.0325046 | 4.9156696 |
| C | 9.2581841 | -5.2901697 | 4.3887314 |
| H | 10.2216709 | -5.8047818 | 4.5389595 |
| C | 9.2501670 | -3.9442018 | 3.9867718 |
| H | 10.2066409 | -3.4169430 | 3.8425266 |
| C | 4.7150132 | -0.5023861 | 6.5815870 |
| C | 4.3144648 | 0.3255777 | 5.5082003 |
| H | 5.0538386 | 0.9878004 | 5.0238285 |
| C | 2.9914665 | 0.3168868 | 5.0456483 |
| H | 2.6842350 | 0.9634325 | 4.2094523 |
| C | 2.0560092 | -0.5413178 | 5.6495360 |
| C | 2.4344519 | -1.3815923 | 6.7096950 |
| H | 1.6916696 | -2.0517646 | 7.1692249 |
| C | 3.7593833 | -1.3557827 | 7.1719606 |
| H | 4.0476612 | -2.0193061 | 8.0031199 |
| C | 6.6865989 | -1.9178228 | 8.1915235 |
| C | 7.2701400 | -3.0840024 | 7.6542559 |
| H | 7.6270092 | -3.0899775 | 6.6115068 |
| C | 7.4182574 | -4.2400585 | 8.4342956 |
| H | 7.8759609 | -5.1463442 | 8.0095702 |
| C | 6.9918869 | -4.2259103 | 9.7724373 |
| C | 6.4232887 | -3.0694379 | 10.3349483 |
| H | 6.1042105 | -3.0725419 | 11.3885342 |
| C | 6.2744277 | -1.9222982 | 9.5421419 |
| H | 5.8360779 | -1.0147775 | 9.9892531 |
| C | 6.5737428 | 0.9636915 | 8.2932203 |
| C | 7.8043505 | 1.1828163 | 8.9536051 |
| H | 8.6585636 | 0.5075204 | 8.7724927 |
| C | 7.9668791 | 2.2670489 | 9.8245417 |
| H | 8.9249366 | 2.4355034 | 10.3396866 |
| C | 6.8981973 | 3.1600625 | 10.0185593 |
| C | 5.6688118 | 2.9626935 | 9.3710982 |
| H | 4.8422800 | 3.6712101 | 9.5341257 |
| C | 5.5106658 | 1.8611409 | 8.5141989 |
| H | 4.5434478 | 1.7127444 | 8.0075498 |
| C | 11.6579852 | 4.1766408 | 3.9347760 |
| C | 10.9223988 | 4.1997612 | 2.7311648 |
| H | 10.4141180 | 3.2836613 | 2.3850402 |
| C | 10.8006651 | 5.3795045 | 1.9822248 |
| H | 10.2209561 | 5.3966540 | 1.0468017 |

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C    11.4100335    6.5556486    2.4500233
C    12.1326347    6.5614418    3.6565672
H    12.5935321    7.4951559    4.0138759
C    12.2514454    5.3735125    4.3918472
H    12.8115064    5.3834425    5.3416763
C    11.9204150    3.1258673    6.6101106
C    13.0567859    2.9176643    7.4171030
H    13.9600806    2.4476392    6.9963144
C    13.0547076    3.2949053    8.7697817
H    13.9384161    3.1211188    9.4027216
C    11.9095130    3.8950450    9.3161117
C    10.7709636    4.1271965    8.5242947
H     9.8795650    4.5974006    8.9673057
C    10.7773457    3.7306046    7.1813185
H     9.8671780    3.8781565    6.5745219
C    13.5128846    1.9970483    4.4412861
C    14.4463722    2.7606262    3.7080462
H    14.1912477    3.7806934    3.3786590
C    15.7085840    2.2386424    3.3833854
H    16.4329955    2.8368438    2.8093391
C    16.0493869    0.9419195    3.8019947
C    15.1353731    0.1619459    4.5327085
H    15.4117221   -0.8554000    4.8498258
C    13.8725118    0.6871340    4.8385329
H    13.1459118    0.0635173    5.3905239
H    11.1279812   -2.3865596   -0.3686418

#Cu-2b singlet ground state
108

N    -1.3480693   -2.5623783    0.1128592
C    -2.5405055   -3.1977642    0.1834321
C    -2.6742905   -4.5659581    0.4355873
C    -1.5245412   -5.3568119    0.6319942
C    -1.6150663   -6.8277818    0.9431436
C    -0.2880234   -4.6909786    0.5406579
C    -0.2292329   -3.3105639    0.2759718
P     1.4280902   -2.4443167    0.1417762
C     2.3472199   -3.2872564    1.5196073
C     3.3029407   -4.3079479    1.3273712
C     3.9659227   -4.8757301    2.4291513
C     3.6789285   -4.4387474    3.7323795
C     2.7249976   -3.4252014    3.9312438
C     2.0668511   -2.8474342    2.8345949
C     2.1527493   -3.1789078   -1.3904657
C     3.5044763   -2.8797988   -1.6784849
C     4.1016032   -3.3433042   -2.8597776
C     3.3518524   -4.0912123   -3.7841884
C     2.0025741   -4.3704503   -3.5179588
C     1.4048508   -3.9201433   -2.3288066
H     0.6505823   -5.2533796    0.6754679
H     3.5359996   -4.6636369    0.3107878
H     4.7129357   -5.6701241    2.2636425
H     2.4913215   -3.0748785    4.9506240
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| | | | |
|---|---|---|---|
| H | 4.0962821 | -2.2698465 | -0.9750224 |
| H | 5.1584296 | -3.1044222 | -3.0642991 |
| H | 3.8185155 | -4.4476411 | -4.7173766 |
| H | 1.4020101 | -4.9429518 | -4.2442452 |
| H | 0.3427939 | -4.1430025 | -2.1414510 |
| Cu | 1.2545904 | -0.1652858 | 0.1006742 |
| Cu | -1.3861414 | -0.4497552 | -0.0629380 |
| I | -0.0176323 | 0.1833673 | -2.2796651 |
| I | -0.2966855 | 0.4347254 | 2.2372000 |
| P | 2.9709761 | 1.3544921 | 0.1389489 |
| P | -3.4586005 | 0.4898846 | -0.3104195 |
| C | 4.3304392 | 1.1318382 | -1.1005293 |
| C | 3.8710104 | 1.5244779 | 1.7418039 |
| C | 2.3469711 | 3.0610203 | -0.1946225 |
| C | -3.5029531 | 2.1410193 | -1.1380635 |
| C | -4.4509221 | 0.7557375 | 1.2286943 |
| C | -4.5870767 | -0.5335395 | -1.3671493 |
| C | 5.6764632 | 1.4677473 | -0.8371176 |
| C | 2.5847491 | 3.7315524 | -1.4120519 |
| C | 4.4365376 | 2.7400109 | 2.1858956 |
| C | 5.1316896 | 2.8056156 | 3.4027096 |
| C | -2.4649115 | 3.0576572 | -0.8561083 |
| C | -5.4309729 | 1.7648610 | 1.3503597 |
| C | -5.8781871 | -0.9422976 | -0.9696392 |
| C | -6.1640497 | 1.9160307 | 2.5366487 |
| C | -2.4655509 | 4.3367585 | -1.4301991 |
| C | -6.6566560 | -1.7718421 | -1.7946060 |
| C | 1.9707853 | 4.9645297 | -1.6847425 |
| C | 6.6686216 | 1.2764062 | -1.8104340 |
| C | 3.9975070 | 0.5907515 | -2.3632514 |
| C | 4.9789142 | 0.4073296 | -3.3485483 |
| C | 6.3052820 | 0.7519425 | -3.0579966 |
| H | 2.9519792 | 0.3058784 | -2.5782717 |
| H | 4.7278333 | -0.0112624 | -4.3357016 |
| H | 7.7227821 | 1.5290224 | -1.6156948 |
| H | 5.9629432 | 1.8794923 | 0.1438997 |
| C | -4.0850368 | -0.9783506 | -2.6143147 |
| C | -4.8580669 | -1.7945646 | -3.4500946 |
| C | -6.1374081 | -2.1847023 | -3.0272660 |
| H | -3.0678855 | -0.6856391 | -2.9304330 |
| H | -4.4795517 | -2.1418797 | -4.4242872 |
| H | -7.6655003 | -2.0975550 | -1.4956999 |
| H | 1.3289071 | -2.0405795 | 2.9966957 |
| H | -3.4323987 | -2.5701665 | 0.0216818 |
| H | -3.6823470 | -5.0103135 | 0.4774335 |
| H | -1.6377826 | 2.7635786 | -0.1876776 |
| C | -3.5031596 | 4.6883699 | -2.3037922 |
| H | -1.6639740 | 5.0638245 | -1.2276105 |
| C | -4.5361517 | 3.7952944 | -2.6157082 |
| C | -4.5305589 | 2.5211970 | -2.0278340 |
| H | -5.3280526 | 4.1051518 | -3.3155213 |
| H | -5.3382349 | 1.8129240 | -2.2749805 |
| H | -6.2882279 | -0.6100166 | -0.0022367 |
| C | -4.2055795 | -0.0907549 | 2.3323060 |

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C    -4.9374636    0.0431513    3.5210852
C    -5.9097014    1.0478087    3.6071438
H    -3.4099554   -0.8521409    2.2690486
H    -4.7494540   -0.6056193    4.3906737
H    -5.6229148    2.4511811    0.5093968
H     3.2480328    3.2852922   -2.1698505
C     1.1196211    5.5229780   -0.7256428
H     2.1359344    5.4914431   -2.6373557
C     0.8761053    4.8892891    0.5002371
C     1.4850298    3.6542613    0.7573110
H     0.2015629    5.3598797    1.2327564
H     1.2676776    3.1364287    1.7062812
C     4.0058801    0.3751252    2.5499038
C     4.7056592    0.4243043    3.7634957
C     5.2602939    1.6430472    4.1750473
H     3.5449992   -0.5749240    2.2315355
H     4.8122700   -0.4671229    4.4011935
H     5.5738736    3.7470236    3.7648398
H     4.3275369    3.6536035    1.5787357
H     4.2000138   -4.8874485    4.5944324
F     7.2541846    0.5688430   -3.9943197
F     5.9252044    1.7024470    5.3424805
H    -6.9275641    2.7020069    2.6472493
F    -6.6090945    1.1898089    4.7471601
F    -3.5038960    5.9113465   -2.8639606
F    -6.8793208   -2.9774771   -3.8224685
F     0.4953029    6.6891187   -0.9933860
H    -0.6596651   -7.3520728    0.7301601
H    -2.4254425   -7.3182814    0.3613163
H    -1.8477225   -6.9854055    2.0218155

#Cu-2c singlet ground state
126

I     0.0020425    0.1481756    2.1991697
I     0.2370401   -0.3400653   -2.2954575
Cu   -1.2763591   -0.6047638   -0.0674294
Cu    1.3521163   -0.8580487    0.1241688
P    -1.4136814   -2.8790306    0.2279467
P    -3.0573065    0.8251711   -0.2774804
P     3.3899391    0.1740361    0.1424265
F    -6.8699454   -1.5813821    4.6856201
F    -6.9367274    0.5000228    5.3310885
F    -8.3949393   -0.2439951    3.8829216
F    -5.8696324   -0.7047871   -6.2882552
F    -6.4573244    1.3979137   -6.1751284
F    -7.6342516   -0.1224195   -5.1482602
F     6.8556456   -3.6311663   -4.2741685
F     8.5297470   -3.1123710   -2.9680056
F     7.9061008   -1.7429751   -4.5488739
F    -2.1127867    7.5515659    0.6030136
F    -0.0620795    6.8166024    0.4583619
F    -1.1839189    7.2745036   -1.3540111
F     3.8385069    6.4498277   -2.5600476
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| | | | |
|---|---|---|---|
| F | 2.9438814 | 6.9194647 | -0.6235796 |
| F | 1.6868603 | 6.2297029 | -2.2658440 |
| F | 5.4927815 | -0.1889348 | 6.6142291 |
| F | 7.3968756 | -0.2836245 | 5.5557901 |
| F | 6.5174070 | 1.6525808 | 6.0332841 |
| N | 1.3564049 | -2.9657431 | 0.1334205 |
| C | 0.2414541 | -3.7341911 | 0.0458349 |
| C | 0.3102875 | -5.1210990 | -0.1775778 |
| H | -0.6244374 | -5.7008905 | -0.2500356 |
| C | 1.5527304 | -5.7714919 | -0.3060586 |
| C | 2.6977435 | -4.9585689 | -0.1907670 |
| H | 3.7092728 | -5.3885478 | -0.2745897 |
| C | 2.5538383 | -3.5850309 | 0.0243175 |
| C | 1.6509550 | -7.2494265 | -0.5775863 |
| H | 2.5141846 | -7.7057371 | -0.0466187 |
| H | 1.8029631 | -7.4353931 | -1.6661068 |
| H | 0.7258511 | -7.7848603 | -0.2767344 |
| C | -2.4381551 | -3.8799270 | -0.9520980 |
| C | -2.1660558 | -3.7275241 | -2.3326885 |
| H | -1.3549533 | -3.0530033 | -2.6615819 |
| C | -2.9271021 | -4.4214656 | -3.2856201 |
| H | -2.6989737 | -4.2986240 | -4.3576920 |
| C | -3.9763549 | -5.2645784 | -2.8775439 |
| H | -4.5770205 | -5.8050961 | -3.6277211 |
| C | -4.2553981 | -5.4135283 | -1.5097041 |
| H | -5.0760189 | -6.0728413 | -1.1809366 |
| C | -3.4901493 | -4.7290467 | -0.5491663 |
| H | -3.7162084 | -4.8593179 | 0.5214097 |
| C | -1.9924043 | -3.4268533 | 1.8956676 |
| C | -3.2256632 | -2.9044448 | 2.3477571 |
| H | -3.7973256 | -2.2103552 | 1.7086085 |
| C | -3.7288406 | -3.2513440 | 3.6105522 |
| H | -4.6933612 | -2.8357784 | 3.9452231 |
| C | -2.9928279 | -4.1046718 | 4.4504734 |
| H | -3.3808733 | -4.3672125 | 5.4484771 |
| C | -1.7569934 | -4.6104773 | 4.0185300 |
| H | -1.1683589 | -5.2706806 | 4.6770612 |
| C | -1.2590561 | -4.2785567 | 2.7472537 |
| H | -0.2862962 | -4.6839573 | 2.4272203 |
| C | -4.3408401 | 0.6057607 | 1.0363304 |
| C | -5.6619942 | 0.2001181 | 0.7518080 |
| H | -5.9960153 | 0.0915952 | -0.2921339 |
| C | -6.5637261 | -0.0739734 | 1.7917289 |
| H | -7.5921291 | -0.3909241 | 1.5585658 |
| C | -6.1593878 | 0.0634429 | 3.1306374 |
| C | -4.8478782 | 0.4837141 | 3.4246713 |
| H | -4.5262385 | 0.5967075 | 4.4720298 |
| C | -3.9438793 | 0.7430047 | 2.3880071 |
| H | -2.9080803 | 1.0340329 | 2.6320825 |
| C | -7.0967829 | -0.3049095 | 4.2557985 |
| C | -4.0330225 | 0.7121052 | -1.8457101 |
| C | -4.7618267 | 1.8008758 | -2.3695854 |
| H | -4.7488529 | 2.7751772 | -1.8543819 |
| C | -5.4996197 | 1.6562581 | -3.5524943 |

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H    -6.0582942    2.5123784   -3.9621740
C    -5.5207411    0.4192137   -4.2233656
C    -4.7893383   -0.6672316   -3.7130518
H    -4.7860985   -1.6313507   -4.2451578
C    -4.0440488   -0.5174241   -2.5350579
H    -3.4531509   -1.3667200   -2.1539791
C    -6.3669802    0.2486595   -5.4655953
C    -2.6170488    2.6208139   -0.1963082
C    -1.5619269    3.0584473   -1.0289649
H    -1.0371520    2.3380934   -1.6806125
C    -1.1617446    4.3992358   -1.0207495
H    -0.3398658    4.7314572   -1.6742837
C    -1.7930877    5.3181984   -0.1595836
C    -2.8422229    4.8914863    0.6702488
H    -3.3408506    5.6107901    1.3377589
C    -3.2574353    3.5500932    0.6469163
H    -4.0852126    3.2326739    1.3005988
C    -1.2968816    6.7455612   -0.1149341
C     4.6752681   -0.6090957   -0.9393994
C     4.2948115   -0.9502068   -2.2604252
H     3.2746274   -0.7178486   -2.6143207
C     5.1939861   -1.5972082   -3.1155583
H     4.8844983   -1.8572608   -4.1405988
C     6.4849552   -1.9333276   -2.6618403
C     6.8658428   -1.6145018   -1.3483930
H     7.8716103   -1.8821361   -0.9895176
C     5.9684558   -0.9539268   -0.4936714
H     6.2859785   -0.7075707    0.5319296
C     7.4498246   -2.6084966   -3.6096487
C     3.3407967    1.9347722   -0.4228705
C     4.0956822    2.4305785   -1.5037201
H     4.7906437    1.7712332   -2.0472962
C     3.9666226    3.7703558   -1.9042610
H     4.5555396    4.1502582   -2.7530726
C     3.0907002    4.6285994   -1.2206292
C     2.3429544    4.1433590   -0.1290919
H     1.6535401    4.8143877    0.4072405
C     2.4575873    2.8039919    0.2586380
H     1.8405831    2.4237071    1.0913343
C     2.9003172    6.0600717   -1.6665316
C     4.2371518    0.3006358    1.7836961
C     3.9093406   -0.6444917    2.7775500
H     3.1315242   -1.4004522    2.5767488
C     4.5401632   -0.6100487    4.0298055
H     4.2709603   -1.3447840    4.8042108
C     5.4975428    0.3810565    4.3059108
C     5.8146190    1.3429474    3.3284539
H     6.5498786    2.1317989    3.5525763
C     5.1880041    1.3021585    2.0755722
H     5.4376578    2.0640167    1.3189271
C     6.2218442    0.3931877    5.6341763
H     3.4425029   -2.9371503    0.1020992

#Cu-2d singlet ground state
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108

| | | | |
|---|---|---|---|
| I | 7.8432185 | 2.4229043 | 4.6675738 |
| I | 10.3958736 | -0.8587753 | 6.4084593 |
| Cu | 7.9760066 | -0.1882464 | 5.3751648 |
| Cu | 10.1448068 | 1.0330692 | 4.4974844 |
| Cl | 0.4022371 | -0.5604486 | 5.0857008 |
| Cl | 7.1800706 | -5.6602555 | 10.7492464 |
| Cl | 7.1228700 | 4.5409602 | 11.0733710 |
| Cl | 11.2522501 | 8.0372698 | 1.5398634 |
| Cl | 11.8966977 | 4.3388402 | 11.0094699 |
| Cl | 17.6054441 | 0.2842198 | 3.3922234 |
| P | 7.9695735 | -1.4378209 | 3.4579145 |
| P | 6.4877371 | -0.4399256 | 7.1023839 |
| P | 11.7942198 | 2.5795860 | 4.8525467 |
| N | 10.3011072 | -0.1145561 | 2.7313827 |
| C | 9.4980441 | -1.1556474 | 2.4034437 |
| C | 9.7558390 | -1.9709875 | 1.2864234 |
| H | 9.0707975 | -2.8029875 | 1.0559503 |
| C | 10.8696380 | -1.7349002 | 0.4607726 |
| C | 11.6868726 | -0.6411728 | 0.8133986 |
| H | 12.5766557 | -0.3819152 | 0.2163909 |
| C | 11.3691958 | 0.1272657 | 1.9352801 |
| H | 12.0046314 | 0.9797719 | 2.2265409 |
| C | 11.1816599 | -2.6046337 | -0.7286831 |
| H | 10.3452588 | -3.2959399 | -0.9630372 |
| H | 12.0893695 | -3.2222328 | -0.5387844 |
| H | 11.3927881 | -1.9914519 | -1.6324615 |
| C | 6.6545281 | -1.2442370 | 2.1575055 |
| C | 6.0971145 | 0.0427844 | 1.9953862 |
| H | 6.4329128 | 0.8691080 | 2.6478245 |
| C | 5.1283709 | 0.2778128 | 1.0063915 |
| H | 4.7054733 | 1.2896734 | 0.8903996 |
| C | 4.6972369 | -0.7683645 | 0.1748203 |
| H | 3.9311401 | -0.5847951 | -0.5968111 |
| C | 5.2449674 | -2.0526154 | 0.3323239 |
| H | 4.9100918 | -2.8805695 | -0.3148251 |
| C | 6.2203839 | -2.2907636 | 1.3137844 |
| H | 6.6344266 | -3.3060167 | 1.4272989 |
| C | 8.0204099 | -3.2541459 | 3.7824475 |
| C | 6.8124809 | -3.9461469 | 4.0367085 |
| H | 5.8454021 | -3.4259344 | 3.9339742 |
| C | 6.8312579 | -5.2931165 | 4.4295175 |
| H | 5.8797978 | -5.8182063 | 4.6161229 |
| C | 8.0545292 | -5.9665338 | 4.5924299 |
| H | 8.0682067 | -7.0247815 | 4.9017421 |
| C | 9.2587275 | -5.2800105 | 4.3665670 |
| H | 10.2241559 | -5.7937840 | 4.5071030 |
| C | 9.2453628 | -3.9333832 | 3.9669969 |
| H | 10.1995110 | -3.4044511 | 3.8138949 |
| C | 4.7102221 | -0.4981570 | 6.5893497 |
| C | 4.3079947 | 0.3326965 | 5.5188091 |
| H | 5.0467377 | 0.9960082 | 5.0349302 |
| C | 2.9842386 | 0.3253910 | 5.0584054 |

| | | | |
|---|---|---|---|
| H | 2.6757718 | 0.9741429 | 4.2243748 |
| C | 2.0496856 | -0.5343175 | 5.6615182 |
| C | 2.4297305 | -1.3774886 | 6.7187677 |
| H | 1.6876191 | -2.0488123 | 7.1777106 |
| C | 3.7554332 | -1.3530377 | 7.1789463 |
| H | 4.0449835 | -2.0187943 | 8.0078723 |
| C | 6.6838208 | -1.9171069 | 8.1934512 |
| C | 7.2676770 | -3.0820537 | 7.6538988 |
| H | 7.6242000 | -3.0858612 | 6.6110223 |
| C | 7.4166591 | -4.2394451 | 8.4318189 |
| H | 7.8746165 | -5.1447596 | 8.0052907 |
| C | 6.9909121 | -4.2278057 | 9.7701586 |
| C | 6.4221468 | -3.0725755 | 10.3350277 |
| H | 6.1036497 | -3.0776667 | 11.3887841 |
| C | 6.2724203 | -1.9241098 | 9.5442867 |
| H | 5.8339979 | -1.0175100 | 9.9932078 |
| C | 6.5725664 | 0.9639522 | 8.3002078 |
| C | 7.8047440 | 1.1817517 | 8.9580969 |
| H | 8.6585910 | 0.5069688 | 8.7732805 |
| C | 7.9693364 | 2.2641781 | 9.8308881 |
| H | 8.9286812 | 2.4315993 | 10.3439711 |
| C | 6.9010985 | 3.1567152 | 10.0293722 |
| C | 5.6701852 | 2.9607059 | 9.3844303 |
| H | 4.8440515 | 3.6688985 | 9.5508656 |
| C | 5.5100279 | 1.8609406 | 8.5255929 |
| H | 4.5416355 | 1.7136574 | 8.0208622 |
| C | 11.6526662 | 4.1806788 | 3.9392109 |
| C | 10.9143412 | 4.2057379 | 2.7373151 |
| H | 10.4040025 | 3.2905193 | 2.3918725 |
| C | 10.7926105 | 5.3862433 | 1.9895510 |
| H | 10.2106898 | 5.4049795 | 1.0555262 |
| C | 11.4047881 | 6.5611222 | 2.4568026 |
| C | 12.1301311 | 6.5650370 | 3.6616757 |
| H | 12.5931606 | 7.4978373 | 4.0186289 |
| C | 12.2488513 | 5.3763553 | 4.3958026 |
| H | 12.8110340 | 5.3847457 | 5.3444004 |
| C | 11.9194905 | 3.1280206 | 6.6130251 |
| C | 13.0588493 | 2.9214460 | 7.4162204 |
| H | 13.9614449 | 2.4529115 | 6.9922590 |
| C | 13.0606872 | 3.2983037 | 8.7690232 |
| H | 13.9467482 | 3.1257383 | 9.3990096 |
| C | 11.9163818 | 3.8965179 | 9.3192889 |
| C | 10.7747799 | 4.1269229 | 8.5313676 |
| H | 9.8840627 | 4.5954746 | 8.9775026 |
| C | 10.7773155 | 3.7306376 | 7.1882803 |
| H | 9.8648268 | 3.8765969 | 6.5845384 |
| C | 13.5049807 | 1.9978532 | 4.4401133 |
| C | 14.4380585 | 2.7602943 | 3.7052028 |
| H | 14.1838959 | 3.7810384 | 3.3771613 |
| C | 15.6985863 | 2.2363489 | 3.3770462 |
| H | 16.4226591 | 2.8336781 | 2.8016543 |
| C | 16.0380364 | 0.9387787 | 3.7939595 |
| C | 15.1245413 | 0.1599542 | 4.5264823 |
| H | 15.3999118 | -0.8580469 | 4.8423701 |

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C    13.8633128    0.6870959    4.8356476
H    13.1367692    0.0643413    5.3887006

#Cu-3a singlet ground state
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I     0.3562667   10.2178972   10.3005664
I    -3.0663185    7.6387532    9.0637494
Cu   -2.2493751    9.6374711   10.7011044
Cu   -1.2257319    9.4338771    8.2579912
P    -3.5047336   11.3995129    9.9554830
P    -2.4442928    8.9149607   12.8724126
P     0.1506132    8.3916565    6.7494322
N    -2.3932867   10.9980201    7.4463483
C    -3.3608538   11.6780975    8.1046660
C    -4.2043455   12.5995918    7.4553977
H    -4.9684669   13.1156660    8.0532520
C    -4.0789093   12.8601490    6.0787208
C    -3.0567847   12.1452425    5.4161420
H    -2.8699875   12.2735076    4.3381543
C    -2.2557521   11.2466279    6.1224978
H    -1.4653822   10.6809376    5.6029369
C    -4.9765078   13.8503645    5.3202008
C    -6.0061734   14.5265686    6.2462401
H    -6.6916573   13.7871559    6.7158258
H    -6.6311297   15.2336370    5.6577599
H    -5.5150024   15.1093305    7.0563743
C    -5.7375184   13.0870181    4.2078657
H    -5.0441559   12.6042948    3.4850393
H    -6.3856834   13.7891741    3.6369762
H    -6.3861158   12.2928982    4.6393918
C    -4.0904300   14.9488205    4.6822984
H    -3.5283517   15.5114056    5.4600977
H    -4.7237235   15.6731471    4.1226211
H    -3.3518379   14.5255767    3.9670807
C    -5.3187945   11.1527098   10.1896779
C    -6.0929705   10.4662215    9.2273420
H    -5.6397514   10.1582572    8.2714500
C    -7.4374002   10.1530792    9.4875616
H    -8.0260419    9.6162280    8.7251015
C    -8.0270636   10.5131061   10.7103995
H    -9.0836219   10.2692388   10.9106899
C    -7.2579921   11.1770957   11.6818128
H    -7.7057895   11.4507434   12.6516316
C    -5.9130360   11.4870679   11.4294852
H    -5.3168111   11.9877543   12.2107349
C    -3.2057082   13.1338110   10.5576620
C    -4.2071155   14.1283807   10.6225057
H    -5.2485953   13.8881491   10.3525319
C    -3.8908132   15.4278343   11.0496469
H    -4.6839757   16.1926428   11.1017519
C    -2.5721142   15.7527104   11.4108144
H    -2.3263415   16.7744050   11.7456036
C    -1.5721420   14.7691813   11.3482025
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| | | | |
|---|---|---|---|
| H | -0.5349191 | 15.0127159 | 11.6328691 |
| C | -1.8853662 | 13.4656978 | 10.9297033 |
| H | -1.0959610 | 12.6938020 | 10.8850219 |
| C | -2.4719724 | 10.3059286 | 14.0927156 |
| C | -1.4081652 | 11.2376833 | 14.0543128 |
| H | -0.5799870 | 11.0928406 | 13.3385813 |
| C | -1.4042599 | 12.3462411 | 14.9132992 |
| H | -0.5661358 | 13.0619347 | 14.8739851 |
| C | -2.4675596 | 12.5522967 | 15.8100229 |
| C | -3.5324544 | 11.6384378 | 15.8451370 |
| H | -4.3709954 | 11.7922811 | 16.5451473 |
| C | -3.5355244 | 10.5186959 | 14.9949316 |
| H | -4.3733612 | 9.8041395 | 15.0356709 |
| C | -1.0545576 | 7.8390186 | 13.4487919 |
| C | -0.4262366 | 7.9815328 | 14.7028210 |
| H | -0.7418485 | 8.7831607 | 15.3904367 |
| C | 0.6078545 | 7.1073133 | 15.0793737 |
| H | 1.0956805 | 7.2302474 | 16.0609566 |
| C | 1.0168703 | 6.0816994 | 14.2121439 |
| C | 0.3944424 | 5.9377511 | 12.9600972 |
| H | 0.7117980 | 5.1374737 | 12.2706229 |
| C | -0.6281625 | 6.8164321 | 12.5727336 |
| H | -1.1002282 | 6.7127981 | 11.5798573 |
| C | -3.9369271 | 7.9135146 | 13.3144578 |
| C | -5.0866332 | 8.0200628 | 12.5048729 |
| H | -5.0683149 | 8.6651625 | 11.6115622 |
| C | -6.2469340 | 7.2936226 | 12.8206486 |
| H | -7.1366815 | 7.3870795 | 12.1763325 |
| C | -6.2649673 | 6.4445549 | 13.9384274 |
| C | -5.1179578 | 6.3226324 | 14.7423160 |
| H | -5.1230634 | 5.6497357 | 15.6162255 |
| C | -3.9592581 | 7.0515910 | 14.4327877 |
| H | -3.0612134 | 6.9441190 | 15.0635186 |
| C | -0.6217376 | 8.1312127 | 5.0838825 |
| C | -1.8998876 | 7.5239798 | 5.0475662 |
| H | -2.3773119 | 7.1992509 | 5.9891819 |
| C | -2.5667051 | 7.3457821 | 3.8266332 |
| H | -3.5591425 | 6.8648646 | 3.8147752 |
| C | -1.9802496 | 7.7864170 | 2.6265059 |
| C | -0.7190258 | 8.4023564 | 2.6559460 |
| H | -0.2510093 | 8.7509394 | 1.7198074 |
| C | -0.0398392 | 8.5715179 | 3.8756146 |
| H | 0.9534589 | 9.0487523 | 3.8849043 |
| C | 0.7145300 | 6.6960510 | 7.2299494 |
| C | 1.1435398 | 6.5062239 | 8.5622144 |
| H | 1.1017772 | 7.3469264 | 9.2770040 |
| C | 1.6163105 | 5.2526820 | 8.9785025 |
| H | 1.9569911 | 5.1205025 | 10.0192112 |
| C | 1.6470191 | 4.1714690 | 8.0809629 |
| C | 1.2061252 | 4.3510382 | 6.7601384 |
| H | 1.2209890 | 3.5061219 | 6.0512853 |
| C | 0.7448375 | 5.6079894 | 6.3330959 |
| H | 0.4019507 | 5.7391748 | 5.2938416 |
| C | 1.7400767 | 9.2547404 | 6.3498907 |

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C     1.8072006   10.6501164    6.5481671
H     0.9383151   11.1801775    6.9744980
C     2.9799232   11.3577389    6.2373604
H     3.0207835   12.4471923    6.4025584
C     4.1024573   10.6759987    5.7402420
C     4.0495663    9.2835016    5.5559030
H     4.9323090    8.7417789    5.1766799
C     2.8759878    8.5752844    5.8595053
H     2.8444148    7.4818450    5.7199970
H     2.0101843    3.1846950    8.4136639
H     5.0272563   11.2295591    5.5063739
H     1.8273735    5.3957535   14.5102655
H    -7.1727583    5.8667107   14.1805889
H    -2.4661826   13.4283793   16.4798113
H    -2.5087517    7.6504225    1.6681076

#Cu-3b singlet ground state
117

I     0.3607996   10.2107089   10.3048163
I    -3.0481729    7.6230527    9.0701871
Cu   -2.2481739    9.6375740   10.6980741
Cu   -1.2257097    9.4361091    8.2584329
P    -3.5068911   11.3971740    9.9529719
P    -2.4448024    8.9141621   12.8675665
P     0.1517085    8.3955100    6.7517435
F    -2.4188007   13.5967497   16.6182516
F     1.9689296    5.2323204   14.5640393
F    -7.3799851    5.7793022   14.1982367
F    -2.6316625    7.5712920    1.4955124
F     2.1237575    3.0097189    8.4968297
F     5.1899427   11.3785278    5.4517046
N    -2.3919195   10.9987212    7.4457209
C    -3.3606110   11.6781383    8.1033434
C    -4.2023850   12.6012593    7.4543851
H    -4.9677726   13.1162757    8.0515618
C    -4.0735890   12.8656107    6.0786451
C    -3.0498213   12.1520933    5.4168708
H    -2.8602385   12.2843020    4.3398752
C    -2.2513034   11.2510148    6.1227611
H    -1.4595774   10.6863741    5.6040099
C    -4.9687530   13.8580270    5.3205775
C    -5.9992221   14.5334422    6.2462698
H    -6.6868925   13.7940684    6.7127335
H    -6.6221094   15.2424273    5.6580811
H    -5.5089606   15.1142462    7.0583823
C    -5.7283782   13.0970863    4.2055292
H    -5.0345245   12.6155531    3.4823843
H    -6.3749073   13.8010009    3.6351636
H    -6.3786446   12.3027955    4.6341795
C    -4.0801951   14.9566780    4.6862720
H    -3.5185636   15.5172980    5.4657979
H    -4.7121533   15.6826703    4.1274618
H    -3.3414779   14.5344679    3.9705867
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| | | | |
|---|---|---|---|
| C | -5.3201220 | 11.1424757 | 10.1839985 |
| C | -6.0862451 | 10.4467989 | 9.2217330 |
| H | -5.6278645 | 10.1383531 | 8.2684145 |
| C | -7.4295430 | 10.1258629 | 9.4784003 |
| H | -8.0121165 | 9.5824568 | 8.7159982 |
| C | -8.0260720 | 10.4875027 | 10.6975067 |
| H | -9.0818436 | 10.2381222 | 10.8947859 |
| C | -7.2652733 | 11.1615571 | 11.6685095 |
| H | -7.7193170 | 11.4381457 | 12.6345487 |
| C | -5.9213335 | 11.4791960 | 11.4197980 |
| H | -5.3319399 | 11.9890632 | 12.2002218 |
| C | -3.2104253 | 13.1288490 | 10.5613035 |
| C | -4.2130788 | 14.1221013 | 10.6278170 |
| H | -5.2538009 | 13.8823291 | 10.3546202 |
| C | -3.8987760 | 15.4200445 | 11.0609766 |
| H | -4.6927598 | 16.1837207 | 11.1152384 |
| C | -2.5810799 | 15.7448772 | 11.4257469 |
| H | -2.3371925 | 16.7651289 | 11.7658915 |
| C | -1.5795448 | 14.7631368 | 11.3598842 |
| H | -0.5430139 | 15.0074611 | 11.6462704 |
| C | -1.8907286 | 13.4609698 | 10.9357638 |
| H | -1.1000727 | 12.6906587 | 10.8881257 |
| C | -2.4576270 | 10.3009069 | 14.0911216 |
| C | -1.3962428 | 11.2359201 | 14.0411059 |
| H | -0.5769484 | 11.0968071 | 13.3141237 |
| C | -1.3735690 | 12.3439703 | 14.8978146 |
| H | -0.5518043 | 13.0764751 | 14.8690054 |
| C | -2.4314888 | 12.5288104 | 15.7993858 |
| C | -3.5011036 | 11.6283016 | 15.8640453 |
| H | -4.3148945 | 11.8055367 | 16.5847521 |
| C | -3.5072893 | 10.5131566 | 15.0098051 |
| H | -4.3459550 | 9.8006707 | 15.0633969 |
| C | -1.0644221 | 7.8291776 | 13.4431004 |
| C | -0.4434242 | 7.9572012 | 14.7027794 |
| H | -0.7600723 | 8.7519463 | 15.3976729 |
| C | 0.5866310 | 7.0836074 | 15.0864766 |
| H | 1.0850159 | 7.1734992 | 16.0644232 |
| C | 0.9854909 | 6.0754600 | 14.2004475 |
| C | 0.3869743 | 5.9268750 | 12.9415837 |
| H | 0.7303643 | 5.1247642 | 12.2694941 |
| C | -0.6298692 | 6.8128747 | 12.5622565 |
| H | -1.0931052 | 6.7154851 | 11.5646019 |
| C | -3.9445586 | 7.9259972 | 13.3041366 |
| C | -5.0875881 | 8.0285340 | 12.4830117 |
| H | -5.0622307 | 8.6674389 | 11.5855914 |
| C | -6.2554048 | 7.3114172 | 12.7833804 |
| H | -7.1507555 | 7.3833505 | 12.1467996 |
| C | -6.2668227 | 6.4764343 | 13.9068868 |
| C | -5.1423614 | 6.3417563 | 14.7339559 |
| H | -5.1868527 | 5.6657363 | 15.6022397 |
| C | -3.9836384 | 7.0683276 | 14.4260791 |
| H | -3.0943651 | 6.9574906 | 15.0683543 |
| C | -0.6251522 | 8.1172485 | 5.0922364 |
| C | -1.9147856 | 7.5325890 | 5.0662718 |

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H    -2.4006656    7.2361595    6.0130414
C    -2.5910868    7.3368627    3.8550659
H    -3.5921615    6.8787818    3.8237858
C    -1.9812355    7.7469951    2.6605171
C    -0.7133138    8.3403845    2.6544357
H    -0.2653296    8.6506305    1.6972262
C    -0.0376775    8.5193414    3.8732558
H     0.9630865    8.9804233    3.8680253
C     0.7292826    6.7078573    7.2366194
C     1.1627003    6.5215800    8.5690031
H     1.1199567    7.3625856    9.2834920
C     1.6438090    5.2766878    8.9953919
H     1.9931074    5.1192587   10.0280187
C     1.6700630    4.2084674    8.0880872
C     1.2312237    4.3597555    6.7671422
H     1.2596174    3.4959265    6.0846203
C     0.7642799    5.6148661    6.3454201
H     0.4184349    5.7365104    5.3061328
C     1.7307684    9.2688164    6.3444663
C     1.7977590   10.6625769    6.5592965
H     0.9323787   11.1875795    6.9983440
C     2.9606145   11.3843451    6.2521029
H     3.0282791   12.4700608    6.4225383
C     4.0681491   10.6959376    5.7412397
C     4.0397579    9.3095682    5.5338240
H     4.9362848    8.8027676    5.1435209
C     2.8683696    8.6016909    5.8391003
H     2.8447770    7.5097828    5.6873179

#Cu-4a singlet ground state
121

I     3.6051093   11.1169097    6.8998190
I     4.8763476   10.4106122    2.6053267
Cu    4.1818184   12.2229816    4.4943445
Cu    5.3271831    9.9164518    5.2020057
P     6.2129595   13.2282316    4.8481537
P     2.2865208   13.2833916    3.7408091
P     5.1935351    7.6450344    5.4630393
N     7.1881932   10.7812403    5.7250214
C     7.4563302   12.1104528    5.6931100
C     8.6194085   12.6488585    6.2725894
H     8.7877449   13.7373610    6.2302817
C     9.5650091   11.8164664    6.9014992
C     9.2820236   10.4365227    6.8961209
H     9.9785741    9.7136997    7.3524014
C     8.1038069    9.9713231    6.3036094
H     7.8754483    8.8928076    6.2849852
C    10.7901485   12.3762836    7.5834734
H    11.0968474   13.3246230    7.0857402
H    11.6343459   11.6592366    7.4684798
C    10.5777659   12.6534031    9.0871129
H    10.2367835   11.7041779    9.5675462
C     9.5573179   13.7542393    9.4330540
```

| | | | |
|---|---|---|---|
| H | 9.7810450 | 14.6630825 | 8.8247948 |
| H | 8.5040896 | 13.4713710 | 9.2182296 |
| C | 9.8189080 | 14.0292649 | 10.9267431 |
| H | 9.4921279 | 15.0456536 | 11.2339924 |
| H | 9.2372419 | 13.3090607 | 11.5437263 |
| C | 11.3471580 | 13.7967583 | 11.1281868 |
| H | 11.5353239 | 13.1398546 | 12.0045241 |
| H | 11.8862822 | 14.7470966 | 11.3302914 |
| C | 11.8504301 | 13.1403187 | 9.8139720 |
| H | 12.5822768 | 12.3211767 | 9.9862358 |
| H | 12.3596217 | 13.8969247 | 9.1731618 |
| C | 6.3289175 | 14.7178443 | 5.9527014 |
| C | 6.9030510 | 15.9457682 | 5.5615922 |
| H | 7.3430751 | 16.0541346 | 4.5571274 |
| C | 6.9190816 | 17.0362390 | 6.4489330 |
| H | 7.3703062 | 17.9904770 | 6.1288701 |
| C | 6.3696793 | 16.9131518 | 7.7351920 |
| H | 6.3866055 | 17.7697189 | 8.4295505 |
| C | 5.7943295 | 15.6921720 | 8.1309349 |
| H | 5.3561121 | 15.5853420 | 9.1374818 |
| C | 5.7664406 | 14.6032147 | 7.2463387 |
| H | 5.2937048 | 13.6534071 | 7.5561102 |
| C | 7.0984612 | 13.7572057 | 3.3136690 |
| C | 6.3964259 | 14.6191713 | 2.4406606 |
| H | 5.3752866 | 14.9505097 | 2.6946721 |
| C | 6.9798129 | 15.0464807 | 1.2389880 |
| H | 6.4142973 | 15.7187006 | 0.5728357 |
| C | 8.2623091 | 14.5990211 | 0.8783930 |
| H | 8.7160015 | 14.9237246 | -0.0727677 |
| C | 8.9563907 | 13.7241240 | 1.7284275 |
| H | 9.9568875 | 13.3555924 | 1.4465963 |
| C | 8.3816543 | 13.3069071 | 2.9408518 |
| H | 8.9398500 | 12.6156128 | 3.5915484 |
| C | 0.8898004 | 12.1561267 | 3.2831929 |
| C | 0.5940335 | 11.0964321 | 4.1690260 |
| H | 1.2089811 | 10.9532871 | 5.0753739 |
| C | -0.4744813 | 10.2272229 | 3.9008468 |
| H | -0.6995198 | 9.4096782 | 4.6063205 |
| C | -1.2481682 | 10.3927078 | 2.7387444 |
| H | -2.0836870 | 9.7049869 | 2.5255764 |
| C | -0.9504013 | 11.4365690 | 1.8482306 |
| H | -1.5499795 | 11.5713300 | 0.9323456 |
| C | 0.1103383 | 12.3179778 | 2.1190448 |
| H | 0.3323047 | 13.1355378 | 1.4142463 |
| C | 1.4923150 | 14.4575206 | 4.9311819 |
| C | 0.1069972 | 14.7266665 | 4.9281510 |
| H | -0.5521321 | 14.2129646 | 4.2090530 |
| C | -0.4381282 | 15.6418999 | 5.8429205 |
| H | -1.5229105 | 15.8410574 | 5.8349218 |
| C | 0.3923723 | 16.2987725 | 6.7670986 |
| H | -0.0394838 | 17.0145601 | 7.4865292 |
| C | 1.7712311 | 16.0321284 | 6.7783405 |
| H | 2.4312881 | 16.5327147 | 7.5063073 |
| C | 2.3169457 | 15.1102967 | 5.8708650 |

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H     3.3962556   14.8861237    5.8994823
C     2.5230644   14.3166725    2.2217283
C     3.0766103   13.6968886    1.0766813
H     3.3345500   12.6239114    1.1042674
C     3.3162131   14.4422177   -0.0873831
H     3.7442619   13.9424583   -0.9723137
C     3.0255730   15.8177652   -0.1219969
H     3.2171442   16.4028835   -1.0371515
C     2.4900833   16.4425310    1.0160073
H     2.2597980   17.5211114    0.9992666
C     2.2350888   15.6976133    2.1807294
H     1.8066931   16.1976050    3.0641948
C     4.8273154    6.9996262    7.1601304
C     5.2455229    7.7720054    8.2652892
H     5.7320032    8.7473809    8.0947828
C     5.0179629    7.3223874    9.5758335
H     5.3456468    7.9389475   10.4293032
C     4.3537838    6.1048833    9.7976801
H     4.1642091    5.7571796   10.8270100
C     3.9179078    5.3387049    8.7034006
H     3.3857863    4.3872399    8.8709922
C     4.1526660    5.7819174    7.3916945
H     3.8012599    5.1771483    6.5396134
C     3.9334297    6.8064581    4.4017204
C     4.1352015    5.5315815    3.8318061
H     5.0856561    4.9977933    3.9969830
C     3.1326253    4.9421658    3.0437844
H     3.3015880    3.9467795    2.5996418
C     1.9233937    5.6201522    2.8172623
H     1.1404674    5.1591194    2.1920408
C     1.7204059    6.8930152    3.3763172
H     0.7840302    7.4432450    3.1853144
C     2.7211293    7.4873842    4.1600272
H     2.5703089    8.4980895    4.5751816
C     6.7665501    6.7716339    5.0116304
C     7.4341641    5.8695852    5.8672704
H     6.9954556    5.6118438    6.8450012
C     8.6562101    5.2928676    5.4774311
H     9.1665695    4.5884367    6.1558236
C     9.2204023    5.6036024    4.2300528
H    10.1767533    5.1468588    3.9250023
C     8.5605272    6.5023921    3.3724324
H     8.9978713    6.7555975    2.3921844
C     7.3480821    7.0901965    3.7611654
H     6.8451363    7.8119917    3.0932201

#Cu-4b singlet ground state
121

I     3.3153208    7.8722438    5.7173849
I     0.2167261    4.8003445    4.4882249
Cu    2.8587063    5.3940527    4.7205252
Cu    1.0903113    6.5007622    6.3710697
P     3.4427097    3.9699439    6.4094712
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| | | | |
|---|---|---|---|
| P | 3.7034952 | 5.4374717 | 2.5895215 |
| P | -0.6219001 | 7.9784984 | 6.7193585 |
| F | 9.3871003 | 7.2949878 | 2.1723291 |
| F | 3.5787297 | 0.2247778 | -0.3864010 |
| F | 0.2224318 | 9.2069208 | -0.4988465 |
| F | -3.6120297 | 9.6165562 | 1.7910200 |
| F | -4.7222757 | 5.5388193 | 10.3656669 |
| F | 0.9023796 | 13.1625758 | 9.3267490 |
| N | 1.6611126 | 5.3397319 | 8.0487597 |
| C | 2.6353802 | 4.3962126 | 8.0470132 |
| C | 3.0591646 | 3.7609447 | 9.2275081 |
| H | 3.8584069 | 3.0037371 | 9.1748296 |
| C | 2.4810655 | 4.0835079 | 10.4698952 |
| C | 1.4592544 | 5.0531100 | 10.4476517 |
| H | 0.9451037 | 5.3546868 | 11.3752733 |
| C | 1.0850127 | 5.6406291 | 9.2352030 |
| H | 0.2777855 | 6.3909335 | 9.2036143 |
| C | 2.9656545 | 3.4622682 | 11.7574643 |
| H | 2.1113734 | 3.3699571 | 12.4655021 |
| H | 3.3384008 | 2.4312461 | 11.5592250 |
| C | 4.0902413 | 4.2703286 | 12.4402325 |
| H | 3.7171105 | 5.3104495 | 12.6043946 |
| C | 4.5303589 | 3.6872715 | 13.8009476 |
| H | 3.7897216 | 3.8814571 | 14.6071421 |
| H | 4.6162730 | 2.5802305 | 13.7035448 |
| C | 5.9219217 | 4.3141997 | 14.0858309 |
| H | 5.8533399 | 5.1133225 | 14.8548921 |
| H | 6.6260899 | 3.5547478 | 14.4882080 |
| C | 6.4110721 | 4.8953817 | 12.7245690 |
| H | 7.4635130 | 4.6259787 | 12.4923350 |
| H | 6.3654498 | 6.0067540 | 12.7437999 |
| C | 5.4222058 | 4.3586333 | 11.6710974 |
| H | 5.7218284 | 3.3348785 | 11.3420050 |
| H | 5.3715077 | 4.9913303 | 10.7586179 |
| C | 5.2144877 | 3.8430576 | 6.9591214 |
| C | 5.9093170 | 5.0604138 | 7.1509747 |
| H | 5.3938556 | 6.0205004 | 6.9647601 |
| C | 7.2493632 | 5.0545130 | 7.5688583 |
| H | 7.7756477 | 6.0122457 | 7.7180299 |
| C | 7.9180922 | 3.8374582 | 7.7893683 |
| H | 8.9726863 | 3.8339851 | 8.1115817 |
| C | 7.2360386 | 2.6256465 | 7.5938170 |
| H | 7.7529503 | 1.6660742 | 7.7627595 |
| C | 5.8912290 | 2.6252061 | 7.1844726 |
| H | 5.3681763 | 1.6661792 | 7.0397223 |
| C | 2.9342759 | 2.2152093 | 6.1397897 |
| C | 1.8853261 | 1.5925547 | 6.8478847 |
| H | 1.3616431 | 2.1317382 | 7.6528145 |
| C | 1.4888832 | 0.2837865 | 6.5252962 |
| H | 0.6627791 | -0.1862082 | 7.0843570 |
| C | 2.1341271 | -0.4204481 | 5.4970196 |
| H | 1.8219432 | -1.4481043 | 5.2477654 |
| C | 3.1726166 | 0.1967976 | 4.7782841 |
| H | 3.6774338 | -0.3405469 | 3.9583870 |

| | | | |
|---|---|---|---|
| C | 3.5617508 | 1.5081046 | 5.0880944 |
| H | 4.3591020 | 1.9907106 | 4.4978091 |
| C | 5.4355001 | 6.0526983 | 2.4156500 |
| C | 6.3402207 | 5.7818936 | 3.4646682 |
| H | 5.9895744 | 5.2523616 | 4.3663545 |
| C | 7.6788530 | 6.1901320 | 3.3867205 |
| H | 8.3898481 | 5.9858981 | 4.2024920 |
| C | 8.1069027 | 6.8906467 | 2.2515901 |
| C | 7.2301947 | 7.1882715 | 1.1993739 |
| H | 7.6022159 | 7.7494300 | 0.3278153 |
| C | 5.8951656 | 6.7656305 | 1.2865578 |
| H | 5.2007136 | 7.0043168 | 0.4644010 |
| C | 3.7126296 | 3.8422468 | 1.6464040 |
| C | 4.6865751 | 3.5283090 | 0.6732468 |
| H | 5.4953939 | 4.2420826 | 0.4486029 |
| C | 4.6475445 | 2.3061856 | -0.0143409 |
| H | 5.4041248 | 2.0466167 | -0.7714446 |
| C | 3.6199503 | 1.3974145 | 0.2722374 |
| C | 2.6407813 | 1.6792530 | 1.2334366 |
| H | 1.8517864 | 0.9397196 | 1.4415258 |
| C | 2.6971990 | 2.8992525 | 1.9236707 |
| H | 1.9376164 | 3.1237777 | 2.6937229 |
| C | 2.7228319 | 6.5753315 | 1.5145103 |
| C | 1.8395993 | 6.1035772 | 0.5214604 |
| H | 1.7918981 | 5.0280519 | 0.2883436 |
| C | 0.9989499 | 6.9892022 | -0.1714981 |
| H | 0.2942726 | 6.6324313 | -0.9386509 |
| C | 1.0528159 | 8.3527102 | 0.1354791 |
| C | 1.9307193 | 8.8545164 | 1.1055458 |
| H | 1.9470175 | 9.9347776 | 1.3195495 |
| C | 2.7574486 | 7.9607331 | 1.7983713 |
| H | 3.4240703 | 8.3479653 | 2.5866643 |
| C | -1.5898440 | 8.4610794 | 5.2216793 |
| C | -0.8919292 | 8.6429150 | 4.0062672 |
| H | 0.1949669 | 8.4580680 | 3.9628554 |
| C | -1.5696918 | 9.0424852 | 2.8458545 |
| H | -1.0456299 | 9.1859166 | 1.8882471 |
| C | -2.9554795 | 9.2417666 | 2.9037263 |
| C | -3.6767694 | 9.0523740 | 4.0893778 |
| H | -4.7669557 | 9.2084136 | 4.0916915 |
| C | -2.9865683 | 8.6623391 | 5.2472001 |
| H | -3.5508987 | 8.5065184 | 6.1811946 |
| C | -1.9232313 | 7.3067957 | 7.8566328 |
| C | -2.4212593 | 6.0099027 | 7.5822148 |
| H | -2.0506786 | 5.4567151 | 6.7008107 |
| C | -3.3723688 | 5.4134541 | 8.4200823 |
| H | -3.7704676 | 4.4076511 | 8.2131352 |
| C | -3.8158819 | 6.1121670 | 9.5526270 |
| C | -3.3328994 | 7.3900717 | 9.8578899 |
| H | -3.7041376 | 7.9088796 | 10.7557874 |
| C | -2.3889270 | 7.9848106 | 9.0035765 |
| H | -2.0133594 | 8.9939164 | 9.2382589 |
| C | -0.1900099 | 9.6044416 | 7.4900221 |
| C | -0.9430240 | 10.7807354 | 7.2825480 |

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H    -1.8249212   10.7615851    6.6214489
C    -0.5792711   11.9859878    7.9010778
H    -1.1543452   12.9120238    7.7439052
C     0.5487672   12.0088603    8.7326174
C     1.3219115   10.8614397    8.9507353
H     2.2146558   10.9229191    9.5923622
C     0.9519719    9.6653205    8.3187900
H     1.5777733    8.7667456    8.4519066

#Cu-1b first triplet exctied state
105

Cu   -1.0399834   -0.1743719   -0.0317738
Cu    1.4727399   -0.7439028   -0.0551604
I     0.3247855    0.2044831   -2.2936110
I     0.4755508    0.4580353    2.0828468
P    -1.4235968   -2.4959667    0.2302449
P    -2.7289980    1.3938506   -0.0967787
P     3.5890906    0.1091971   -0.1348915
F    -1.0076321    7.1159217    0.3487123
F    -5.9686773    1.2132790   -5.1308761
F    -6.6546527    0.5043374    4.3412177
F     3.1345044    5.9210884   -1.4602872
F     6.6563111   -0.5311175    4.9659196
F     7.0242096   -2.3536557   -4.3843761
N     1.3178074   -2.8493783   -0.0387032
C     0.0675363   -3.4993995    0.0277310
C    -0.0138908   -4.9146946   -0.0439104
H    -1.0090242   -5.3904170   -0.0143124
C     1.1277943   -5.6981668   -0.1589110
H     1.0565107   -6.7947186   -0.2276586
C     2.4023140   -5.0260154   -0.2047614
H     3.3485563   -5.5781401   -0.2997372
C     2.4103069   -3.6322429   -0.1497629
H     3.3748355   -3.0970786   -0.2089455
C    -2.1447002   -2.9217154    1.8875858
C    -1.4369359   -3.7265161    2.8036697
H    -0.4601582   -4.1469215    2.5150885
C    -1.9680977   -3.9929393    4.0768669
H    -1.4012068   -4.6242031    4.7815136
C    -3.2122991   -3.4618172    4.4515590
H    -3.6291068   -3.6744483    5.4501442
C    -3.9201640   -2.6491546    3.5496197
H    -4.8923703   -2.2161894    3.8389734
C    -3.3854358   -2.3719495    2.2816490
H    -3.9440501   -1.7157050    1.5929375
C    -2.6168585   -3.2482718   -0.9818612
C    -3.7860629   -3.9494569   -0.6217878
H    -4.0461864   -4.0818281    0.4404119
C    -4.6223722   -4.4967761   -1.6117603
H    -5.5292611   -5.0483532   -1.3117421
C    -4.3032753   -4.3534661   -2.9704644
H    -4.9583222   -4.7880257   -3.7438491
C    -3.1351612   -3.6602146   -3.3381992
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| | | | |
|---|---|---|---|
| H | -2.8672842 | -3.5498057 | -4.4024869 |
| C | -2.2993340 | -3.1127322 | -2.3538929 |
| H | -1.3806960 | -2.5775668 | -2.6507992 |
| C | -2.2039697 | 3.1544780 | 0.0949968 |
| C | -0.9763680 | 3.5687793 | -0.4681139 |
| H | -0.3251986 | 2.8342685 | -0.9723064 |
| C | -0.5715823 | 4.9090445 | -0.3923841 |
| H | 0.3817452 | 5.2490362 | -0.8260395 |
| C | -1.3953989 | 5.8319043 | 0.2655047 |
| C | -2.6115177 | 5.4476410 | 0.8455928 |
| H | -3.2286057 | 6.2003752 | 1.3606100 |
| C | -3.0118133 | 4.1063514 | 0.7558886 |
| H | -3.9670075 | 3.8009760 | 1.2127327 |
| C | -3.7207414 | 1.3891596 | -1.6524321 |
| C | -4.3139841 | 2.5562651 | -2.1804217 |
| H | -4.1766426 | 3.5258906 | -1.6751667 |
| C | -5.0745691 | 2.5009825 | -3.3573295 |
| H | -5.5375352 | 3.4031320 | -3.7868002 |
| C | -5.2410256 | 1.2677761 | -4.0027802 |
| C | -4.6611253 | 0.0943814 | -3.5034221 |
| H | -4.7986619 | -0.8583534 | -4.0379733 |
| C | -3.8953388 | 0.1640907 | -2.3316358 |
| H | -3.4210395 | -0.7552624 | -1.9502644 |
| C | -3.9888734 | 1.1808998 | 1.2373372 |
| C | -5.3459001 | 0.9078184 | 0.9662252 |
| H | -5.7045739 | 0.8640874 | -0.0744691 |
| C | -6.2538611 | 0.6816593 | 2.0135921 |
| H | -7.3144075 | 0.4593043 | 1.8175725 |
| C | -5.7944392 | 0.7404315 | 3.3346698 |
| C | -4.4541582 | 1.0229216 | 3.6341834 |
| H | -4.1263082 | 1.0513877 | 4.6847793 |
| C | -3.5543417 | 1.2306203 | 2.5821490 |
| H | -2.4922588 | 1.4197001 | 2.8132251 |
| C | 3.6037541 | 1.9083635 | -0.5272761 |
| C | 3.8943730 | 2.3772408 | -1.8258504 |
| H | 4.2247955 | 1.6746537 | -2.6073869 |
| C | 3.7510269 | 3.7359717 | -2.1451643 |
| H | 3.9611512 | 4.1142788 | -3.1575521 |
| C | 3.3156226 | 4.6220448 | -1.1527856 |
| C | 3.0395754 | 4.1889416 | 0.1509285 |
| H | 2.7033267 | 4.9152798 | 0.9069887 |
| C | 3.1748526 | 2.8287901 | 0.4560904 |
| H | 2.9230896 | 2.4800558 | 1.4707229 |
| C | 4.5438150 | -0.0321371 | 1.4350808 |
| C | 4.2476751 | -1.1077672 | 2.3013116 |
| H | 3.4355736 | -1.8095572 | 2.0480697 |
| C | 4.9631430 | -1.2861478 | 3.4931310 |
| H | 4.7394911 | -2.1174933 | 4.1792643 |
| C | 5.9725565 | -0.3713881 | 3.8214082 |
| C | 6.2796301 | 0.7138068 | 2.9891661 |
| H | 7.0717317 | 1.4179364 | 3.2881331 |
| C | 5.5614515 | 0.8788697 | 1.7959519 |
| H | 5.7902596 | 1.7399795 | 1.1469356 |
| C | 4.6799581 | -0.6536120 | -1.4181486 |

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C     4.0813862   -1.3019649   -2.5208714
H     2.9818603   -1.3642724   -2.5894599
C     4.8683175   -1.8739889   -3.5311898
H     4.4131171   -2.3843777   -4.3939213
C     6.2628318   -1.8029694   -3.4253919
C     6.8856896   -1.1763912   -2.3361596
H     7.9852908   -1.1492953   -2.2838386
C     6.0892422   -0.6039351   -1.3354863
H     6.5791943   -0.1206352   -0.4749891

#Cu-2b first triplet exctied state
108

N    -1.4300264   -2.5833798    0.0799744
C    -2.5874324   -3.2653536    0.0881261
C    -2.7105822   -4.6500736    0.2346080
C    -1.5109422   -5.4389558    0.4063520
C    -1.5947235   -6.9279771    0.5934090
C    -0.3069780   -4.7474317    0.3940077
C    -0.2474841   -3.3326396    0.2188673
P     1.3369012   -2.4723573    0.2279423
C     2.2140287   -3.1359124    1.7276260
C     3.1167846   -4.2215397    1.6937714
C     3.6756938   -4.7228044    2.8823067
C     3.3427912   -4.1509163    4.1202191
C     2.4386756   -3.0736458    4.1646894
C     1.8783224   -2.5719682    2.9805167
C     2.3321882   -3.1560773   -1.1821008
C     3.7231544   -2.9188055   -1.2546692
C     4.4698540   -3.3768049   -2.3509494
C     3.8337553   -4.0604816   -3.4019460
C     2.4480256   -4.2809141   -3.3479964
C     1.7009388   -3.8339899   -2.2448524
H     0.6368091   -5.3043397    0.5284423
H     3.3892656   -4.6834498    0.7311694
H     4.3767663   -5.5732377    2.8365486
H     2.1633189   -2.6202038    5.1316970
H     4.2328257   -2.3721094   -0.4427684
H     5.5565111   -3.1920132   -2.3871647
H     4.4200556   -4.4193843   -4.2643329
H     1.9399238   -4.8112144   -4.1707800
H     0.6143505   -4.0141023   -2.2009540
Cu    1.1546211   -0.1362231    0.0556699
Cu   -1.3974096   -0.4740225   -0.1033754
I    -0.1110092    0.3259367   -2.2786278
I    -0.4084078    0.7581053    2.0425884
P     2.9323957    1.3308344    0.0185125
P    -3.4655126    0.4853401   -0.3137827
C     4.2100336    1.0744395   -1.2944731
C     3.9060812    1.4487479    1.5798072
C     2.3344340    3.0509137   -0.2823205
C    -3.5131209    2.1840910   -1.0289756
C    -4.3913359    0.6225019    1.2753046
C    -4.5896097   -0.4850477   -1.4120557
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| | | | |
|---|---|---|---|
| C | 5.5105655 | 1.6170377 | -1.1897681 |
| C | 2.4053687 | 3.6378018 | -1.5634596 |
| C | 4.5342696 | 2.6384379 | 2.0114551 |
| C | 5.2923971 | 2.6597518 | 3.1912867 |
| C | -2.4841926 | 3.0965339 | -0.7029729 |
| C | -5.2702029 | 1.6919032 | 1.5495755 |
| C | -5.9332455 | -0.7597662 | -1.0792656 |
| C | -5.9641850 | 1.7527648 | 2.7674035 |
| C | -2.5020633 | 4.4017686 | -1.2134875 |
| C | -6.7486023 | -1.4988445 | -1.9501479 |
| C | 1.8060847 | 4.8807771 | -1.8178634 |
| C | 6.4474876 | 1.4357380 | -2.2155645 |
| C | 3.8703704 | 0.3330213 | -2.4463609 |
| C | 4.7973523 | 0.1511693 | -3.4837788 |
| C | 6.0756814 | 0.7063196 | -3.3545738 |
| H | 2.8661793 | -0.1140213 | -2.5368290 |
| H | 4.5421005 | -0.4301722 | -4.3830245 |
| H | 7.4657227 | 1.8493207 | -2.1461573 |
| H | 5.8056361 | 2.1848269 | -0.2928236 |
| C | -4.0686051 | -0.9760911 | -2.6310157 |
| C | -4.8762115 | -1.7078264 | -3.5106897 |
| C | -6.2093167 | -1.9606816 | -3.1576968 |
| H | -3.0120998 | -0.7919446 | -2.8917829 |
| H | -4.4832655 | -2.0984429 | -4.4620805 |
| H | -7.7980407 | -1.7243839 | -1.7044700 |
| H | 1.1621360 | -1.7333424 | 3.0262130 |
| H | -3.5007548 | -2.6581078 | -0.0399941 |
| H | -3.7066258 | -5.1172650 | 0.2236663 |
| H | -1.6525025 | 2.7812388 | -0.0501988 |
| C | -3.5496532 | 4.7863110 | -2.0614496 |
| H | -1.7050213 | 5.1253515 | -0.9827702 |
| C | -4.5763674 | 3.8996147 | -2.4104882 |
| C | -4.5519426 | 2.5967065 | -1.8916484 |
| H | -5.3771798 | 4.2358385 | -3.0873642 |
| H | -5.3525624 | 1.8930454 | -2.1712334 |
| H | -6.3532821 | -0.3967830 | -0.1273827 |
| C | -4.2078869 | -0.3841910 | 2.2498952 |
| C | -4.9020616 | -0.3375862 | 3.4660051 |
| C | -5.7726442 | 0.7337441 | 3.7095405 |
| H | -3.5034069 | -1.2120441 | 2.0646823 |
| H | -4.7660547 | -1.1128922 | 4.2356648 |
| H | -5.4120284 | 2.4959225 | 0.8092990 |
| H | 2.9240834 | 3.1160967 | -2.3833708 |
| C | 1.1351215 | 5.5335609 | -0.7777482 |
| H | 1.8429317 | 5.3436782 | -2.8160890 |
| C | 1.0610344 | 4.9847159 | 0.5090970 |
| C | 1.6554150 | 3.7388655 | 0.7492910 |
| H | 0.5286998 | 5.5297297 | 1.3042640 |
| H | 1.5756754 | 3.2942413 | 1.7540765 |
| C | 4.0437967 | 0.2816040 | 2.3617029 |
| C | 4.8026738 | 0.2884891 | 3.5399118 |
| C | 5.4197626 | 1.4809638 | 3.9393923 |
| H | 3.5388778 | -0.6503078 | 2.0574863 |
| H | 4.9064526 | -0.6174772 | 4.1570317 |

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H     5.7842130    3.5797764    3.5439605
H     4.4236710    3.5674707    1.4286894
H     3.7819185   -4.5469080    5.0510174
F     6.9731624    0.5310223   -4.3390401
F     6.1436834    1.5003734    5.0706469
H    -6.6482082    2.5837589    3.0000290
F    -6.4336615    0.7892296    4.8773513
F    -3.5660038    6.0341394   -2.5588737
F    -6.9860287   -2.6683676   -3.9938819
F     0.5226631    6.7094817   -1.0213737
H    -0.5894421   -7.3883560    0.7049688
H    -2.1038803   -7.4190210   -0.2702844
H    -2.1939780   -7.1915442    1.4976470

#Cu-2c first triplet exctied state
126

I     0.1524143    0.2485098    2.1169989
I     0.2409663   -0.1123686   -2.2470870
Cu   -1.1930323   -0.6128960   -0.0417684
Cu    1.3556367   -0.9047793    0.0555911
P    -1.3499931   -2.9477886    0.2426990
P    -3.0075081    0.7976378   -0.2050330
P     3.3731639    0.1718258    0.0282100
F    -7.3063034   -1.6169241    4.3584833
F    -6.9117112    0.2796412    5.3609101
F    -8.4835647    0.1469476    3.8480625
F    -5.6723700   -0.6657376   -6.2913183
F    -6.2025668    1.4530915   -6.1991785
F    -7.4529831   -0.0306334   -5.2052313
F     7.7551331   -3.6950807   -3.3806433
F     8.6235147   -1.7571178   -3.8719020
F     6.9749799   -2.5530545   -5.0668713
F    -1.9733803    7.4285604    1.1474460
F     0.0468806    6.7327000    0.6999076
F    -1.2770144    7.3431253   -0.9209133
F     3.6210902    6.3753715   -2.8315431
F     2.9742539    6.9125197   -0.8156206
F     1.5154578    6.2176136   -2.2790680
F     5.5550947   -0.4173949    6.4444021
F     7.4498911   -0.4215656    5.3662863
F     6.5322842    1.4716727    5.9387640
N     1.4237377   -2.9985909    0.1656682
C     0.2494718   -3.7774017    0.1998062
C     0.3282270   -5.2009300    0.1977929
H    -0.6111824   -5.7812527    0.1947659
C     1.5432918   -5.8738818    0.1909028
C     2.7354838   -5.0516511    0.1829255
H     3.7396611   -5.5010239    0.1723172
C     2.5935407   -3.6633311    0.1593261
C     1.6481659   -7.3728383    0.1767758
H     2.2222058   -7.7499503    1.0568705
H     2.1937525   -7.7348168   -0.7274178
H     0.6482610   -7.8575542    0.1876296
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| | | | |
|---|---|---|---|
| C | -2.3627009 | -3.8410195 | -1.0369389 |
| C | -2.0090297 | -3.6323686 | -2.3906865 |
| H | -1.1760475 | -2.9517295 | -2.6382456 |
| C | -2.6976296 | -4.2916322 | -3.4196618 |
| H | -2.4039974 | -4.1197014 | -4.4688544 |
| C | -3.7506171 | -5.1740198 | -3.1151958 |
| H | -4.2901234 | -5.6950284 | -3.9234826 |
| C | -4.1013518 | -5.3943413 | -1.7746374 |
| H | -4.9165986 | -6.0936592 | -1.5238931 |
| C | -3.4132625 | -4.7343774 | -0.7404578 |
| H | -3.6966090 | -4.9273505 | 0.3064029 |
| C | -2.1657597 | -3.3989676 | 1.8477957 |
| C | -3.5101976 | -3.0383217 | 2.0908882 |
| H | -4.0950228 | -2.5263167 | 1.3076150 |
| C | -4.1170242 | -3.3260305 | 3.3237593 |
| H | -5.1664731 | -3.0374430 | 3.4995398 |
| C | -3.3813217 | -3.9621802 | 4.3386635 |
| H | -3.8561533 | -4.1843001 | 5.3088123 |
| C | -2.0390593 | -4.3060937 | 4.1129275 |
| H | -1.4532609 | -4.7992152 | 4.9066184 |
| C | -1.4336869 | -4.0271269 | 2.8760422 |
| H | -0.3802147 | -4.2996892 | 2.7017692 |
| C | -4.3178912 | 0.5425724 | 1.0755434 |
| C | -5.6855730 | 0.4275365 | 0.7507139 |
| H | -6.0184413 | 0.5195608 | -0.2949626 |
| C | -6.6355196 | 0.1891325 | 1.7551888 |
| H | -7.7010287 | 0.0962373 | 1.4935188 |
| C | -6.2296744 | 0.0739401 | 3.0957877 |
| C | -4.8692003 | 0.2018545 | 3.4298962 |
| H | -4.5469018 | 0.1086668 | 4.4784754 |
| C | -3.9188847 | 0.4211500 | 2.4251291 |
| H | -2.8504775 | 0.4812424 | 2.6937814 |
| C | -7.2379891 | -0.2693855 | 4.1691105 |
| C | -3.9280736 | 0.7069386 | -1.8027553 |
| C | -4.5905392 | 1.8217252 | -2.3591222 |
| H | -4.5492743 | 2.8010475 | -1.8555445 |
| C | -5.2978804 | 1.6944716 | -3.5629137 |
| H | -5.8039038 | 2.5695395 | -3.9997815 |
| C | -5.3544523 | 0.4513634 | -4.2190818 |
| C | -4.6903561 | -0.6612410 | -3.6735454 |
| H | -4.7132969 | -1.6321893 | -4.1924653 |
| C | -3.9763293 | -0.5318235 | -2.4744519 |
| H | -3.4415833 | -1.4069182 | -2.0690939 |
| C | -6.1680131 | 0.3025578 | -5.4870092 |
| C | -2.5714776 | 2.5896436 | -0.0505503 |
| C | -1.6215320 | 3.1162978 | -0.9551867 |
| H | -1.1765433 | 2.4709751 | -1.7310215 |
| C | -1.2189534 | 4.4529351 | -0.8637874 |
| H | -0.4766247 | 4.8521749 | -1.5724828 |
| C | -1.7445992 | 5.2795724 | 0.1483963 |
| C | -2.6911332 | 4.7656377 | 1.0485839 |
| H | -3.1098388 | 5.4130525 | 1.8340566 |
| C | -3.1068304 | 3.4280377 | 0.9470540 |
| H | -3.8528260 | 3.0427218 | 1.6595061 |

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C    -1.2467672    6.7024894    0.2686906
C     4.6279126   -0.5993906   -1.0943204
C     4.1733877   -1.2624616   -2.2539671
H     3.0916664   -1.3332733   -2.4596081
C     5.0886511   -1.8389367   -3.1464397
H     4.7259757   -2.3492724   -4.0518544
C     6.4670134   -1.7705660   -2.8816709
C     6.9274592   -1.1189567   -1.7229902
H     8.0078116   -1.0619978   -1.5168776
C     6.0134915   -0.5373054   -0.8339435
H     6.3880928   -0.0334600    0.0713713
C     7.4577432   -2.4439481   -3.8080840
C     3.2919404    1.9308090   -0.5269850
C     3.9166033    2.3791818   -1.7074607
H     4.5228319    1.6888334   -2.3147045
C     3.7676443    3.7110345   -2.1257854
H     4.2561738    4.0547837   -3.0501881
C     2.9984143    4.6063399   -1.3656142
C     2.3794931    4.1677116   -0.1785716
H     1.7723438    4.8668544    0.4175700
C     2.5171888    2.8373152    0.2322068
H     2.0008409    2.4964178    1.1452102
C     2.7880037    6.0322484   -1.8239265
C     4.2264723    0.2518183    1.6644086
C     4.0290942   -0.8122226    2.5701899
H     3.3488285   -1.6404316    2.3108462
C     4.6781178   -0.8142500    3.8120210
H     4.5120843   -1.6430220    4.5174901
C     5.5230903    0.2527488    4.1664500
C     5.7107626    1.3248374    3.2767268
H     6.3571359    2.1691609    3.5626501
C     5.0668130    1.3241839    2.0307772
H     5.2133658    2.1747704    1.3455759
C     6.2631385    0.2245516    5.4870527
H     3.5005236   -3.0336544    0.1245832

#Cu-2d first triplet exctied state
108

I     8.0312492    2.4471819    4.7914637
I    10.4401338   -0.7310891    6.5457738
Cu    8.1019184   -0.1685614    5.3797020
Cu   10.2194138    0.9648607    4.4927776
Cl    0.5589169   -1.1343214    5.0521993
Cl    7.6038168   -5.4712371   10.9553131
Cl    6.8279463    4.7970242   10.7100085
Cl   11.3951588    7.7787025    1.2937318
Cl   11.5677727    4.2052914   11.0733849
Cl   17.7781336    0.3182758    3.9372654
P     8.0304969   -1.3815203    3.3648817
P     6.5919544   -0.4706908    7.0902337
P    11.8428722    2.5208720    4.9118494
N    10.4039988   -0.1209225    2.6889729
C     9.4710228   -1.1058992    2.3161116
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| | | | |
|---|---|---|---|
| C | 9.6115703 | -1.7967489 | 1.0751289 |
| H | 8.8481755 | -2.5437559 | 0.7953923 |
| C | 10.6735160 | -1.5565064 | 0.2138322 |
| C | 11.6306926 | -0.5558629 | 0.6300039 |
| H | 12.5034645 | -0.3047897 | 0.0090230 |
| C | 11.4248570 | 0.1038003 | 1.8452656 |
| H | 12.1493203 | 0.8736023 | 2.1661658 |
| C | 10.8426429 | -2.2784384 | -1.0936754 |
| H | 10.0288205 | -3.0146848 | -1.2684397 |
| H | 11.8152675 | -2.8248206 | -1.1341216 |
| H | 10.8505231 | -1.5661866 | -1.9530301 |
| C | 6.5709808 | -1.1479001 | 2.2367664 |
| C | 6.1172566 | 0.1735141 | 2.0187245 |
| H | 6.5931977 | 1.0094225 | 2.5601505 |
| C | 5.0810875 | 0.4346048 | 1.1097094 |
| H | 4.7422685 | 1.4726756 | 0.9538651 |
| C | 4.4809518 | -0.6195258 | 0.3970646 |
| H | 3.6669226 | -0.4149516 | -0.3180546 |
| C | 4.9331249 | -1.9333783 | 0.5969146 |
| H | 4.4767543 | -2.7665263 | 0.0361886 |
| C | 5.9700012 | -2.1980135 | 1.5079518 |
| H | 6.3103896 | -3.2363403 | 1.6509516 |
| C | 7.9793449 | -3.1929829 | 3.7592093 |
| C | 6.7854542 | -3.7878813 | 4.2287983 |
| H | 5.8585790 | -3.1917887 | 4.2870640 |
| C | 6.7658576 | -5.1352482 | 4.6218282 |
| H | 5.8241906 | -5.5871331 | 4.9760042 |
| C | 7.9423055 | -5.9037921 | 4.5692712 |
| H | 7.9267532 | -6.9625576 | 4.8774734 |
| C | 9.1361768 | -5.3148630 | 4.1215010 |
| H | 10.0644754 | -5.9089121 | 4.0809229 |
| C | 9.1559288 | -3.9690733 | 3.7171501 |
| H | 10.0928589 | -3.5099552 | 3.3614283 |
| C | 4.8381230 | -0.6825688 | 6.5527201 |
| C | 4.4629580 | -0.1760829 | 5.2902275 |
| H | 5.2125420 | 0.3200361 | 4.6514724 |
| C | 3.1475505 | -0.3064504 | 4.8219832 |
| H | 2.8669240 | 0.0797874 | 3.8302679 |
| C | 2.1953350 | -0.9562656 | 5.6248916 |
| C | 2.5489644 | -1.4746868 | 6.8838442 |
| H | 1.7917658 | -1.9880629 | 7.4961147 |
| C | 3.8670550 | -1.3368684 | 7.3409230 |
| H | 4.1386495 | -1.7567845 | 8.3231063 |
| C | 6.8914973 | -1.8807475 | 8.2414282 |
| C | 7.4800801 | -3.0576342 | 7.7329320 |
| H | 7.7821835 | -3.1138577 | 6.6746737 |
| C | 7.6950788 | -4.1682332 | 8.5606591 |
| H | 8.1547614 | -5.0834175 | 8.1579669 |
| C | 7.3305167 | -4.0985617 | 9.9158855 |
| C | 6.7553052 | -2.9308848 | 10.4467199 |
| H | 6.4843467 | -2.8892437 | 11.5128048 |
| C | 6.5382339 | -1.8282852 | 9.6075508 |
| H | 6.0972754 | -0.9115393 | 10.0321397 |
| C | 6.5688343 | 0.9998770 | 8.2038826 |

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C     7.7458821    1.3079595    8.9231256
H     8.6285289    0.6497055    8.8529461
C     7.8203536    2.4603681    9.7147393
H     8.7362455    2.6983674   10.2770545
C     6.7171497    3.3305096    9.7686296
C     5.5387222    3.0434194    9.0616242
H     4.6834372    3.7341012    9.1162477
C     5.4683047    1.8761347    8.2846258
H     4.5423961    1.6584466    7.7282639
C    11.7101865    4.0678395    3.9177326
C    11.1296253    3.9904368    2.6333743
H    10.7307966    3.0303577    2.2650836
C    11.0358551    5.1269882    1.8186803
H    10.5803567    5.0650138    0.8188480
C    11.5159882    6.3587740    2.2960389
C    12.0843433    6.4610823    3.5776297
H    12.4454396    7.4356060    3.9403651
C    12.1791531    5.3160077    4.3818274
H    12.6142018    5.4054144    5.3907787
C    11.8629815    3.0968117    6.6624366
C    12.8413764    2.6551780    7.5768411
H    13.6745701    2.0199503    7.2361947
C    12.7639872    3.0052095    8.9332371
H    13.5227523    2.6523092    9.6481299
C    11.6987100    3.8040970    9.3790127
C    10.7212129    4.2681677    8.4818258
H     9.8891347    4.8898745    8.8467323
C    10.8036353    3.9060425    7.1312528
H    10.0152647    4.2453614    6.4397179
C    13.5657290    1.9216479    4.6060870
C    14.6304452    2.8009933    4.3127494
H    14.4515546    3.8855219    4.2340459
C    15.9276043    2.3123086    4.1067612
H    16.7571007    2.9978562    3.8752592
C    16.1668721    0.9290403    4.1939728
C    15.1201828    0.0360938    4.4772674
H    15.3185477   -1.0450141    4.5314586
C    13.8247838    0.5358020    4.6760468
H    13.0004920   -0.1674983    4.8855244

#Cu-4a first triplet exctied state
121

I     3.2020313   10.9096827    6.6734429
I     4.8202180   10.2715853    2.6809603
Cu    4.1241883   12.1403571    4.4790649
Cu    5.2735192    9.9685554    5.2778284
P     6.1268408   13.2567900    5.0290148
P     2.3167004   13.2223781    3.5327285
P     5.1185572    7.7052515    5.6001241
N     7.1277761   10.8058279    5.8603553
C     7.4041304   12.1757875    5.7025765
C     8.6493156   12.7143208    6.1442118
H     8.8270681   13.7983051    6.0328826
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| | | | |
|---|---|---|---|
| C | 9.6357840 | 11.9211291 | 6.7151123 |
| C | 9.3385106 | 10.5119369 | 6.8408974 |
| H | 10.0705218 | 9.8056351 | 7.2607507 |
| C | 8.0934607 | 10.0474361 | 6.4050092 |
| H | 7.8620794 | 8.9716070 | 6.4959028 |
| C | 10.9388804 | 12.4859290 | 7.2229143 |
| H | 11.0834342 | 13.5170271 | 6.8237193 |
| H | 11.7859599 | 11.8703363 | 6.8328344 |
| C | 11.0494265 | 12.5351428 | 8.7599436 |
| H | 10.8889355 | 11.5021026 | 9.1545379 |
| C | 10.0514913 | 13.4699768 | 9.4674349 |
| H | 10.0695541 | 14.4664953 | 8.9643106 |
| H | 9.0026614 | 13.1060180 | 9.4243097 |
| C | 10.6047677 | 13.5795461 | 10.9021419 |
| H | 10.2913441 | 14.5174826 | 11.4096126 |
| H | 10.2115815 | 12.7402634 | 11.5180938 |
| C | 12.1534497 | 13.4581614 | 10.7590188 |
| H | 12.5555573 | 12.6958432 | 11.4612956 |
| H | 12.6688222 | 14.4112569 | 11.0074400 |
| C | 12.4072912 | 13.0500752 | 9.2829983 |
| H | 13.2226535 | 12.3020094 | 9.1710111 |
| H | 12.7044661 | 13.9408131 | 8.6814911 |
| C | 6.0249732 | 14.6454919 | 6.2625579 |
| C | 6.7464622 | 15.8544656 | 6.1472929 |
| H | 7.3521706 | 16.0521801 | 5.2482725 |
| C | 6.7010050 | 16.8143563 | 7.1733901 |
| H | 7.2736959 | 17.7511894 | 7.0664731 |
| C | 5.9372599 | 16.5844346 | 8.3283749 |
| H | 5.9044443 | 17.3386694 | 9.1322144 |
| C | 5.2199005 | 15.3803332 | 8.4551524 |
| H | 4.6211718 | 15.1839832 | 9.3604965 |
| C | 5.2647522 | 14.4196761 | 7.4339772 |
| H | 4.7085172 | 13.4732211 | 7.5488146 |
| C | 6.8558707 | 14.0715950 | 3.5295764 |
| C | 6.2450155 | 15.2148659 | 2.9679187 |
| H | 5.3579317 | 15.6607075 | 3.4492462 |
| C | 6.7591142 | 15.7974916 | 1.7995056 |
| H | 6.2738088 | 16.6939399 | 1.3789427 |
| C | 7.8784185 | 15.2338131 | 1.1628508 |
| H | 8.2814322 | 15.6906561 | 0.2434029 |
| C | 8.4770467 | 14.0836349 | 1.7016248 |
| H | 9.3515510 | 13.6305876 | 1.2051183 |
| C | 7.9710718 | 13.5060341 | 2.8782405 |
| H | 8.4461302 | 12.6071834 | 3.3040105 |
| C | 0.9944890 | 12.0745466 | 2.9294024 |
| C | 0.3925530 | 11.1996506 | 3.8617295 |
| H | 0.7143261 | 11.2117083 | 4.9168342 |
| C | -0.6111506 | 10.3096627 | 3.4515352 |
| H | -1.0797501 | 9.6410461 | 4.1931665 |
| C | -1.0144555 | 10.2674555 | 2.1052570 |
| H | -1.8004060 | 9.5641694 | 1.7831284 |
| C | -0.4106150 | 11.1251526 | 1.1729413 |
| H | -0.7185435 | 11.0981859 | 0.1144674 |
| C | 0.5863157 | 12.0278475 | 1.5807208 |

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|---|---|---|---|
| H | 1.0468148 | 12.7001028 | 0.8396681 |
| C | 1.4111980 | 14.3581702 | 4.6732965 |
| C | 0.0175464 | 14.5667751 | 4.5902531 |
| H | -0.5790491 | 14.0208991 | 3.8413234 |
| C | -0.6143756 | 15.4646390 | 5.4659813 |
| H | -1.7042732 | 15.6178522 | 5.3965119 |
| C | 0.1358044 | 16.1615363 | 6.4283067 |
| H | -0.3648924 | 16.8622456 | 7.1170589 |
| C | 1.5224872 | 15.9558144 | 6.5165294 |
| H | 2.1212168 | 16.4871607 | 7.2746489 |
| C | 2.1566801 | 15.0551346 | 5.6468487 |
| H | 3.2423757 | 14.8850494 | 5.7378163 |
| C | 2.6817791 | 14.2740391 | 2.0540267 |
| C | 3.6041495 | 13.7945498 | 1.0984109 |
| H | 4.1210675 | 12.8341029 | 1.2659093 |
| C | 3.8763660 | 14.5390691 | -0.0596390 |
| H | 4.5994850 | 14.1515526 | -0.7957659 |
| C | 3.2488339 | 15.7785947 | -0.2666318 |
| H | 3.4697593 | 16.3669665 | -1.1728417 |
| C | 2.3458874 | 16.2710391 | 0.6902634 |
| H | 1.8551378 | 17.2469406 | 0.5387228 |
| C | 2.0588718 | 15.5230169 | 1.8439373 |
| H | 1.3446012 | 15.9164649 | 2.5848536 |
| C | 4.7704283 | 7.2117570 | 7.3456546 |
| C | 5.3265006 | 7.9899911 | 8.3843432 |
| H | 5.9234666 | 8.8856034 | 8.1439665 |
| C | 5.1085418 | 7.6378928 | 9.7249619 |
| H | 5.5460166 | 8.2541253 | 10.5274652 |
| C | 4.3229533 | 6.5167769 | 10.0418966 |
| H | 4.1442393 | 6.2474038 | 11.0961432 |
| C | 3.7567674 | 5.7468340 | 9.0130201 |
| H | 3.1314459 | 4.8715954 | 9.2558133 |
| C | 3.9786005 | 6.0901975 | 7.6689964 |
| H | 3.5254090 | 5.4849487 | 6.8670273 |
| C | 3.8230063 | 6.8439038 | 4.6074614 |
| C | 4.0232137 | 5.5514020 | 4.0777259 |
| H | 4.9818883 | 5.0311668 | 4.2360324 |
| C | 3.0050873 | 4.9269368 | 3.3385252 |
| H | 3.1716827 | 3.9180305 | 2.9257252 |
| C | 1.7849270 | 5.5871324 | 3.1199011 |
| H | 0.9901584 | 5.0979261 | 2.5324091 |
| C | 1.5848440 | 6.8768490 | 3.6400057 |
| H | 0.6384511 | 7.4116744 | 3.4557539 |
| C | 2.5984986 | 7.5069697 | 4.3773547 |
| H | 2.4440762 | 8.5272517 | 4.7672778 |
| C | 6.6739177 | 6.7998860 | 5.1749943 |
| C | 7.2135947 | 5.7873044 | 5.9955279 |
| H | 6.7101734 | 5.5122623 | 6.9364694 |
| C | 8.3962265 | 5.1290917 | 5.6179287 |
| H | 8.8119506 | 4.3406581 | 6.2671869 |
| C | 9.0464566 | 5.4740638 | 4.4222336 |
| H | 9.9764458 | 4.9585455 | 4.1302756 |
| C | 8.5149300 | 6.4855833 | 3.6040495 |
| H | 9.0263485 | 6.7692465 | 2.6695598 |

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C     7.3390575    7.1517646    3.9795086
H     6.9372178    7.9603290    3.3446496

#Cu-4b first triplet exctied state
121

I     3.0639271    8.0548637    5.3415549
I     0.1685860    4.9357863    4.4599416
Cu    2.7999923    5.4705405    4.6715604
Cu    1.1532988    6.5048595    6.3604909
P     3.5871067    4.1251708    6.4272119
P     3.5500402    5.3449650    2.4956678
P    -0.5295941    8.0126510    6.7445514
F     9.3079029    6.8004529    1.7126072
F     2.9643988    0.0289254   -0.2113883
F     0.0553494    9.1111450   -0.5716517
F    -3.5231581    9.8862374    1.9107689
F    -4.7526278    5.7337387   10.3294466
F     1.3875577   12.9786751    9.4842002
N     1.7322278    5.3845546    8.0599091
C     2.7085738    4.3755534    7.9821445
C     3.0797356    3.6436761    9.1505476
H     3.8630386    2.8706927    9.0657579
C     2.4903958    3.8768524   10.3856140
C     1.4776813    4.9057337   10.4347350
H     0.9442823    5.1422970   11.3676752
C     1.1660428    5.5965349    9.2591921
H     0.3855803    6.3771389    9.2886475
C     2.8984668    3.1334599   11.6332679
H     1.9840923    2.7646159   12.1584864
H     3.4939242    2.2323045   11.3567679
C     3.7179690    3.9778995   12.6292715
H     3.1240923    4.8890578   12.8859134
C     4.0748109    3.2464405   13.9400237
H     3.2019896    3.1274996   14.6190350
H     4.4287879    2.2191769   13.6885246
C     5.2265910    4.0736581   14.5681012
H     4.8479814    4.7257099   15.3851139
H     5.9947575    3.4145990   15.0274709
C     5.8113395    4.9334357   13.4041310
H     6.9175501    4.8577506   13.3277935
H     5.5799098    6.0090647   13.5695750
C     5.0991644    4.4385053   12.1283363
H     5.6369725    3.5605864   11.6966712
H     5.0422615    5.2068270   11.3278368
C     5.3865665    4.2660953    6.8705964
C     5.9724945    5.5535400    6.8516947
H     5.3802481    6.4165531    6.5020831
C     7.2930830    5.7467199    7.2843194
H     7.7307152    6.7588573    7.2602122
C     8.0537442    4.6580360    7.7489100
H     9.0910020    4.8098229    8.0908898
C     7.4793111    3.3769249    7.7790236
H     8.0647789    2.5169917    8.1460188
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| | | | |
|---|---|---|---|
| C | 6.1580080 | 3.1795605 | 7.3442104 |
| H | 5.7270133 | 2.1654824 | 7.3697016 |
| C | 3.3989749 | 2.3293988 | 5.9993546 |
| C | 2.2959543 | 1.5945240 | 6.4809342 |
| H | 1.5872899 | 2.0764386 | 7.1744274 |
| C | 2.1039034 | 0.2590371 | 6.0881096 |
| H | 1.2383173 | -0.3034350 | 6.4763965 |
| C | 3.0116828 | -0.3602593 | 5.2134354 |
| H | 2.8654334 | -1.4116144 | 4.9141246 |
| C | 4.1084884 | 0.3683022 | 4.7208021 |
| H | 4.8233479 | -0.1069142 | 4.0284360 |
| C | 4.2954044 | 1.7054727 | 5.1029077 |
| H | 5.1549805 | 2.2688379 | 4.7014046 |
| C | 5.3031724 | 5.8447700 | 2.2122483 |
| C | 6.2429602 | 5.5547949 | 3.2249739 |
| H | 5.9130806 | 5.0873048 | 4.1675682 |
| C | 7.5989790 | 5.8691385 | 3.0625811 |
| H | 8.3340586 | 5.6529054 | 3.8533263 |
| C | 8.0117455 | 6.4880221 | 1.8755179 |
| C | 7.1018240 | 6.7991039 | 0.8555753 |
| H | 7.4633343 | 7.2949345 | -0.0588437 |
| C | 5.7481437 | 6.4752483 | 1.0288410 |
| H | 5.0303613 | 6.7317194 | 0.2326480 |
| C | 3.4076234 | 3.7046611 | 1.6547967 |
| C | 4.0807916 | 3.4284480 | 0.4431868 |
| H | 4.7369365 | 4.1866102 | -0.0139978 |
| C | 3.9337137 | 2.1884335 | -0.1912559 |
| H | 4.4537834 | 1.9571071 | -1.1339507 |
| C | 3.1054336 | 1.2195450 | 0.3952518 |
| C | 2.4315679 | 1.4617322 | 1.5974764 |
| H | 1.8017719 | 0.6748445 | 2.0398900 |
| C | 2.5910332 | 2.7061378 | 2.2260588 |
| H | 2.0710920 | 2.8992760 | 3.1790055 |
| C | 2.5668048 | 6.4772125 | 1.4208628 |
| C | 1.5061410 | 5.9916402 | 0.6267984 |
| H | 1.3239322 | 4.9079766 | 0.5498072 |
| C | 0.6605700 | 6.8757682 | -0.0601610 |
| H | -0.1782665 | 6.5105797 | -0.6725947 |
| C | 0.8854822 | 8.2522647 | 0.0533497 |
| C | 1.9386824 | 8.7651794 | 0.8216374 |
| H | 2.0874218 | 9.8544928 | 0.8843009 |
| C | 2.7711831 | 7.8731651 | 1.5105722 |
| H | 3.5835838 | 8.2764579 | 2.1358681 |
| C | -1.4774563 | 8.5764523 | 5.2671530 |
| C | -0.7938918 | 8.7751123 | 4.0461408 |
| H | 0.2875342 | 8.5675310 | 3.9783400 |
| C | -1.4813627 | 9.2240609 | 2.9102395 |
| H | -0.9717885 | 9.3743677 | 1.9459388 |
| C | -2.8595463 | 9.4629365 | 2.9993836 |
| C | -3.5646186 | 9.2637356 | 4.1932910 |
| H | -4.6489964 | 9.4530236 | 4.2213361 |
| C | -2.8673507 | 8.8179323 | 5.3257732 |
| H | -3.4201453 | 8.6508991 | 6.2643115 |
| C | -1.8301273 | 7.3540278 | 7.8783561 |

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|---|---|---|---|
| C | -2.2916957 | 6.0345695 | 7.6675799 |
| H | -1.8607162 | 5.4241440 | 6.8553362 |
| C | -3.2847137 | 5.4849084 | 8.4881411 |
| H | -3.6519130 | 4.4579794 | 8.3374686 |
| C | -3.8060456 | 6.2586092 | 9.5347143 |
| C | -3.3579634 | 7.5637739 | 9.7757858 |
| H | -3.7862914 | 8.1374730 | 10.6124126 |
| C | -2.3682784 | 8.1080964 | 8.9429506 |
| H | -2.0116570 | 9.1336331 | 9.1309991 |
| C | 0.0360744 | 9.5677633 | 7.5579733 |
| C | -0.5550588 | 10.8207926 | 7.2905537 |
| H | -1.3755316 | 10.9005848 | 6.5591403 |
| C | -0.1013151 | 11.9785798 | 7.9401951 |
| H | -0.5467299 | 12.9650999 | 7.7378877 |
| C | 0.9489665 | 11.8726842 | 8.8613005 |
| C | 1.5582823 | 10.6418699 | 9.1423955 |
| H | 2.3907882 | 10.5995892 | 9.8615037 |
| C | 1.1027319 | 9.4934735 | 8.4817247 |
| H | 1.5958240 | 8.5273036 | 8.6804172 |