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Supporting Information

Designing diphosphines toward photo- and electro-luminescent homoleptic Cu(I)/Ag(I) complexes

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Synthesis and characterization

Ligand **dppbz**, $AgPF_6$ and $[Cu(MeCN)_4]PF_6$ were purchased from TCI, **dpppyrz** and **dppquinox** were synthesized according to modified literature reports.[1] All chemicals were used without any further purification steps. If not otherwise indicated, all reactions were performed under inert atmosphere.

Synthesis of 2,3-bis(diphenylphosphino)pyrazine (dpppyrz)

1.61 mL (1.72 g, 9.26 mmol, 2.3 eq.) of diphenylphopshine were added to 50 mL of hexane at -78 °C, followed by the dropwise addition of 3.75 mL (9.38 mmol, 2. eq.) of 2.5 M butyllithium solution at -78 °C. The slightly yellow turbid solution was kept 1 h at this temperature and afterwards allowed to warm to room temperature within 1 h. Hexane and the unreacted BuLi were cannulated away from $LiPPh_2$, which remained as a yellow precipitate. The lithium phosphide was redissolved in 40 mL of THF, cooled to -78 °C, followed by the slow addition to 600 mg (4.03 mmol, 1.0 eq.) of 2,3-dichloropyrazine in 80 mL at the same temperature. The brownish solution was stirred for 3 h at this temperature and was then allowed to warm to room temperature overnight. The brown dispersion was filtered through celite to remove THF insoluble side products and evaporated to dryness. The resulting yellow powder was dissolved in CH_2Cl_2 and extracted with a degassed, aqueous solution of NH_4Cl (1 x 10 mL) and dried over $MgSO_4$. Evaporation to dryness gave **dpppyrz** as a yellow powder in 70% yield (1.29 g).

^{1}H-NMR (400 MHz, methylene chloride-*d_2,* δ): 8.51 (s, 2H, *pyrazine*$(PPh_2)_2$), 7.25 (m, 20H, pyrazine(P*Ph*$_2)_2$).
^{31}P{^{1}H}-NMR (162 MHz, methylene chloride-*d_2,* δ): -10.4 (s).

Synthesis of 2,3-bis(diphenylphosphino)quinoxaline (dppquinox)

Dppquinox was prepared using the same procedure as for **dpppyrz**, but using 2,3-dichloroquinoxaline instead of 2,3-dichloropyrazine as starting material. After monitoring the completeness of the reaction via ^{31}P{^{1}H}-NMR, the reaction mixture was first evaporated to dryness, redissolved in DCM and quenched with 5 ml of degassed EtOH, filtered through celite and evaporated to dryness. **Dppquinox** was obtained as orange powder in 75% yield (1.51 g).
^{1}H-NMR (400 MHz, methylene chloride-*d_2,* δ): 7.94 (dd, 2H, $^3J_{HH}$ = 6.4 Hz, *Quinox*$(PPh_2)_2$), 7.72 (dd, 2H, $^3J_{HH}$ = 6.4 Hz, *Quinox*$(PPh_2)_2$), 7.43-7.25 (m, 20H, Quinox(P*Ph*$_2)_2$).
^{31}P{^{1}H}-NMR (162 MHz, methylene chloride-*d_2,* δ): -9.08 (s).

Synthesis of Cu^{bz}, Cu^{pyrz}, Cu^{quinox}, Ag^{bz}, Ag^{pyrz}, Ag^{quinox}

$[Cu(dppbz)_2]PF_6$ (Cu^{bz}):

Bis(diphenylphosphino)benzene (119.8 mg, 268 µmol, 2.0 eq.) was added to $[Cu(MeCN)_4]PF_6$ (50.0 mg, 134 µmol, 1.0 eq.) in 50 mL of CH_2Cl_2, and stirred at room temperature for 2 h. The clear solution was concentrated under vacuum and layered with diethyl ether, which gave white crystals. Single crystals for X-ray diffraction were grown by slow diffusion of diethyl ether and pentane into a CH_2Cl_2 solution at room temperature. Yield: 103.4 mg (70 %).
^{1}H-NMR (400 MHz, chloroform-*d,* δ): 7.52-7.45 (m, 8H, *Ph*$(PPh_2)_2$), 7.31-7.25 (m, 8H, *Ph*$(PPh_2)_2$), 7.09-7.03 (m, 16H, Ph(P*Ph*$_2)_2$), 6.96-6.90 (m, 16H, Ph(P*Ph*$_2)_2$).
^{31}P{^{1}H}-NMR (162 MHz, chloroform-*d,* δ): 8.17 (bs), -144.3 (sept, *P*F_6).
^{13}C{^{1}H}-NMR (101 MHz, chloroform-*d*, δ): 142.17, 141.98, 141.80, 141.61, 141.46, 134.23, 134.21, 134.18, 134.15, 134.13, 132.66, 132.62, 132.58, 132.54, 132.51, 131.77, 131.56, 131.54, 131.46, 131.36, 131.26, 131.18, 131.16, 130.36, 129.17, 129.15, 129.12, 129.09, 129.07.
HRMS (ESI) *m/z*: $[M + H]^+$ calc. for $[C_{60}H_{48}CuP_4]^+$, 955.19997; found, 955.20192.

$[Cu(dpppyrz)_2]PF_6$ (Cu^{pyrz}):

2,3-bis(phenylphosphino)quinoxaline (101 mg, 225 µmol, 2.4 eq) was added to $[Cu(MeCN)_4]PF_6$ (35.0 mg, 93.9 µmol, 1.0 eq.) in 50 mL CH_2Cl_2, followed by a color change to yellow and stirred at room temperature for 2 h. The yellow, slightly turbid solution was filtered through celite and evaporated to dryness. The yellow powder

was washed with ethyl acetate, diethyl ether and pentane, dried under vacuum to give **Cu^{pyrz}** as a yellow powder. Single crystals for X-ray diffraction were grown by slow diffusion of diethyl ether and pentane into a CH_2Cl_2 solution at room temperature. Yield: 99.3 mg (67 %).

^{1}H-NMR (400 MHz, chloroform-*d,* δ): 8.84 (s, 4H, *Pyrz*(PPh$_2$)$_2$, 7.30-7.27 (m, 6H, Pyrz(P*Ph*$_2$)$_2$, 7.20-7.18 (m, 17H, Pyrz(P*Ph*$_2$)$_2$, 7.11-7.07 (m, 6H, Pyrz(P*Ph*$_2$)$_2$.

^{31}P{^{1}H}-NMR (162 MHz, chloroform-*d,* δ): 3.80 (bs), -144.3 (sept, *P*F$_6$).

^{13}C{^{1}H}-NMR (101 MHz, chloroform-*d*, δ): 146.94, 133.26, 130.91, 129.88, 129.14.

HRMS (ESI) *m/z*: [M + H]$^+$ calc. for [$C_{56}H_{44}N_4CuP_4$]$^+$, 959.18065; found, 959.18070.

[Cu(dppquinox)$_2$]PF$_6$ (Cu^{quinox}):

Cu^{quinox} was obtained by a similar method as described for **Cu^{bz}** using dppquinox instead of of dppbz. The obtained powder was washed with ethyl acetate and pentane to give **Cu^{quinox}** as a orange powder. Single crystals for X-ray diffraction were grown by slow diffusion of diethyl ether and pentane into a CH_2Cl_2 solution at room temperature. Yield: 161.2 mg, 84%.

^{1}H-NMR (400 MHz, chloroform-*d,* δ): 8.19 (m, 4H, *Quinox*(PPh$_2$)$_2$, 7.96 (m, 4H, *Quinox*(PPh$_2$)$_2$, 7.30-7.18 (m, 24H, Quinox(P*Ph*$_2$)$_2$, 7.05 (m, 16H, Quinox(P*Ph*$_2$)$_2$.

^{31}P{^{1}H}-NMR (162 MHz, chloroform-*d,* δ): 2.03 (bs), -144.3 (sept, *P*F$_6$).

^{13}C{^{1}H}-NMR (101 MHz, chloroform-*d,* δ): 129.1, 130.2, 130.32, 130.92, 133.16, 133.50, 142.55, 158.56.

HRMS (ESI) *m/z*: [M + H]$^+$ calcd for [$C_{64}H_{48}N_4CuP_4$]$^+$, 1059.21200; found, 1059.20842.

[Ag(dppbz)$_2$]PF$_6$ (Ag^{bz}):

Bis(diphenylphosphino)benzene (176.6 mg, 0.396, 2.0 eq.) was added to $AgPF_6$ (50.0 mg, 198 µmol, 1.0 eq.) in 50 mL of CH_2Cl_2, and stirred at room temperature for 2h. The clear solution was concentrated under vacuum and layered with diethyl ether, which gave white crystals. Single crystals for X-ray diffraction were grown by slow diffusion of diethyl ether and pentane into a CH_2Cl_2 solution at room temperature. Yield: 181.3 mg (80 %).

^{1}H-NMR (400 MHz, chloroform-*d,* δ): 7.55-7.48 (m, 8H, *Ph*(PPh$_2$)$_2$), 7.35-7.30 (m, 8H, *Ph*(PPh$_2$)$_2$), 7.12-7.05 (m, 34H, Ph(P*Ph*$_2$)$_2$).

^{31}P{^{1}H}-NMR (162 MHz, chloroform-*d,* δ): 0.11 (dd, $^1J(^{31}P\text{-}^{107}Ag)$ = 230 Hz, $^1J(^{31}P\text{-}^{109}Ag)$ = 265 Hz), -144.3 (sept, *P*F$_6$).

^{13}C{^{1}H}-NMR (101 MHz, chloroform-*d,* δ): 140.36, 134.46, 133.39, 133.35, 133.31, 133.26, 133.22, 131.47, 131.28, 131.14, 130.99, 130.55, 129.23, 129.19, 129.14.

HRMS (ESI) *m/z*: [M + H]$^+$ calc. for [$C_{60}H_{48}AgP_4$]$^+$: 999.17519; found: 999.17607.

[Ag(dpppyrz)$_2$]PF$_6$ (Ag^{pyrz}):

Ag^{pyrz} was obtained by a similar method as reported for **Ag^{bz}** using dpppyrz instead of of dppbz. Yield: 118.7 mg (58 %).

^{1}H-NMR (400 MHz, chloroform-*d,* δ): 8.78 (s, 4H, *Pyrz*(PPh$_2$)$_2$, 7.40-7.36 (m, 9H, Pyrz(P*Ph*$_2$)$_2$, 7.25-7.22 (m, 14 H, Pyrz(P*Ph*$_2$)$_2$, 7.18-7.14 (m, 17 H, Pyrz(P*Ph*$_2$)$_2$.

^{31}P{^{1}H}-NMR (162 MHz, chloroform-*d,* δ): 1.53 (dd, $^1J(^{31}P\text{-}^{107}Ag)$ = 225 Hz, $^1J(^{31}P\text{-}^{109}Ag)$ = 259 Hz), -144.3 (sept, *P*F$_6$).

^{13}C{^{1}H}-NMR (101 MHz, chloroform-*d,* δ): 160.31, 146.47, 133.66, 131.06, 130.16, 129.27.

HRMS (ESI) *m/z*: [M + H]$^+$ calc. for [$C_{56}H_{44}N_4AgP_4$]$^+$, 1003.1562; found, 1003.1535.

[Ag(dppquinox)$_2$]PF$_6$ (Ag^{quinox}):

Ag^{quinox} was obtained by a similar method as reported for **Ag^{bz}** using dpppyrz instead of of dppbz. Yield: 162.4 mg, 83%.

^{1}H-NMR (400 MHz, chloroform-*d,* δ): 8.12-8.07 (m, 4H, *Quinox*(PPh$_2$)$_2$), 7.91-7.87 (m, 4H, $^3J_{HH}$ = 6.45 Hz, *Quinox*(PPh$_2$)$_2$), 7.40-7.34 (m, 8H, Quinox(P*Ph*$_2$)$_2$), 7.31-7.27 (m, 16H, Quinox(P*Ph*$_2$)$_2$), 7.16-7.12 (m, 16H, Quinox(P*Ph*$_2$)$_2$).

$^{31}P\{^{1}H\}$-NMR (162 MHz, chloroform-*d,* δ): 0.25 (dd, $^{1}J(^{31}P\text{-}^{107}Ag)$ = 221 Hz, $^{1}J(^{31}P\text{-}^{109}Ag)$ = 258 Hz), -144.3 (sept, PF_6).
$^{13}C\{^{1}H\}$-NMR (101 MHz, chloroform-*d,* δ): 158.83, 158.1, 157.7, 142.70, 133.99, 133.95, 133.90, 133.85, 133.81, 132.88, 131.01, 130.26, 130.15, 129.17.
HRMS (ESI) *m/z*: $[M + H]^+$ calc. for $[C_{64}H_{48}N_4AgP_4]^+$, 1103.18804; found, 1103.18776.

SC-XRD structure report for compounds **Cu^{bz}**, **Ag^{pyrz}**, and **Ag^{quinox}**: A colorless, block (**Cu^{bz}**), a yellow block (**Ag^{pyrz}**) or a yellow, needle (**Ag^{quinox}**) was selected, respectively, coated with perfluorinated ether and fixed on top of a Kapton micro sampler or on a MiTeGen MicroMesh sampler for X-ray crystallographic analysis. The X-ray intensity data were collected on a Bruker D8 VENTURE Duo three-angle or a Bruker APEX-II diffractometer with MoK_α radiation (λ=0.71073 Å) using APEX4.[2] The diffractometer was equipped with a Helios optic monochromator, a Bruker PHOTON II detector, and an Oxford Cryostream low temperature device.
A matrix scan was used to determine the initial lattice parameters. All data were integrated with SAINT package, using a narrow-frame algorithm and the reflections were corrected for Lorentz and polarisation effects, scan speed, and background.[3] The integration of the data for **Cu^{bz}** using a monoclinic unit cell yielded a total of 110611 reflections within a 2θ range [°] of 4.15 to 52.79 (0.80 Å), of which 5480 were independent. The integration of the data for **Ag^{pyrz}** using a monoclinic unit cell yielded a total of 11478 reflections within a 2θ range [°] of 4.60 to 51.73 (0.81 Å), of which 11478 were independent. The integration of the data for **Ag^{quinox}** using a monoclinic unit cell yielded a total of 278397 reflections within a 2θ range [°] of 4.09 to 50.79 (0.83 Å), of which 23592 were independent. All data were corrected for absorption effects including odd and even ordered spherical harmonics by the multi-scan method SADABS.[4] Space group assignment was based upon systematic absences, E statistics, and successful refinement of the structure.
The structures were solved by direct methods using SHELXT and refined by full-matrix least-squares methods against F^2 by minimizing $\Sigma w(F_o^2 - F_c^2)^2$ using SHELXL in conjunction with SHELXLE.[5-7] All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and a C–H distance of 0.99 Å. Non-methyl hydrogen atoms were refined using a riding model with methylene, aromatic, and other C–H distances of 0.99 Å, 0.95 Å, and 1.00 Å, respectively, and U_{iso} values constrained to 1.2 times the U_{eq} of their pivot atoms. The PF_6 counter ions and residual solvent ($CHCl_3$) in **Ag^{pyrz}** were heavily disordered and modelled using SADI, SIMU, RIGU and SAME restraints.[8,9] Furthermore, selected phenyl rings in all of the structures were disordered and modelled using SADI, FLAT, SIMU, RIGU, SAME commands. Residual solvent (CH_3Cl) in **Ag^{pyrz}** could not be modelled reasonably and the corresponding electron density was removed by the PLATON/SQUEEZE procedure.[10]
Neutral atom scattering factors for all atoms and anomalous dispersion corrections for the non-hydrogen atoms were taken from International Tables for Crystallography.[11] Supplementary crystallographic data reported in this paper have been deposited with the Cambridge Crystallographic Data Centre (**Cu^{bz}**: 2406496, **Ag^{pyrz}**: 2425241, **Ag^{quinox}**: 2406497) and can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.[12] This report and the CIF file were generated using FinalCif.[13]

High performance liquid-chromatography coupled with high-resolution mass spectrometry (HPLC-HRMS) was performed in positive mode using a Thermo Fisher Ultimate3000 with Scientific Vanquish Flex UHPLC and a Thermo Fisher Orbitrap (Exactive Plus with Extend Mass Range: Source HESI II). The detector was a Vanquish PDA Detector (VF-XX, detection ≤ 5 ppm). The reverse phase column was a Thermo Fisher Acclaim Phenyl1, (column size: 2.1 × 150 mm, particles size: 3 µm). ^{1}H-, $^{31}P\{^{1}H\}$,- and $^{13}C\{^{1}H\}$ NMR spectra were recorded on a JEOL JNM ECA 400 MHz or a Bruker AVANCE ARX 400 MHz spectrometer at 298 K. Chemical shifts are reported in ppm relative to tetramethylsilane and calibrated to the residual of the used deuterated solvents as internal standard for the ^{1}H NMR. MestReNova software by Mestrelab Research S.L. was used for data evaluation. Absorption spectra were measured with a Shimadzu UV-2600i UV-VIS Spectrophotmeter. Photoluminescence spectra were recorded with a FS5 Spectrofluorometer at 25 °C. PLQY values were measured with the FS5 Spectrofluorometer using the integrating sphere SC-30 (Edingburgh Instruments) and on a Quantaurus-QY Absolute PL quantum yield

spectrometer C11347-11 (Hamamatsu Photonics). Photoluminescence measurements of **M^{bz}**, **M^{pyrz}**, **M^{quinox}** at temperatures ranging from 77 to 400 K were conducted in powder and thin-film in Optistat-DN (Oxford Instruments) equipped with a temperature controller. Excited state decay lifetimes (τ) were measured with a microsecond flashlamp (λ_{exc} = 362-480 nm, 10 Hz). The photoluminescence spectra were recorded after 5 min of equilibrating the temperature of the sample to ensure complete sample thermalization. The following equation were applied to calculate the average lifetime:

$$< \tau > = \frac{\sum_i A_i \tau_i^2}{\sum_i A_i \tau_i}$$

where A_i and τ_i represent the preexponential factor and the excited state lifetime component obtained from the exponential fitting, respectively.

The energy splitting between S_1 and T_1 were estimated with the following Boltzmann-type equation (**Equation S1**):

$$< \tau > = \frac{3 + \exp\left(\frac{\Delta E_{S1-T1}}{k_B T}\right)}{\frac{3}{\tau(T_1)} + \frac{1}{\tau(S_1)} \exp\left(\frac{\Delta E_{S1-T1}}{k_B T}\right)}$$

while k_B is the Boltzmann constant and $\tau(S_1)$ and $\tau(T_1)$ correspond to the decay times of S_1 and T_1.[14]

PXRD measurements were performed on a Miniflex diffractometer (Rigaku, Tokyo, Japan) with a copper source (1.54 Å) and a silicon strip detector (D/teX Ultra, Rigaku), a goniometer radius of 150 mm; both Soller slits at 2.5°; a divergence slit fixed at 0.625°; an anti-scatter slit of 8 mm; and a kβ filter of 0.06 mm nickel foil. The powder was placed on a low background silicon wafer sample holder (cut 911).

Cyclic voltammetry measurements were carried out in a cylindrical one-compartment cell with a three-electrode set-up. A platinum disk working electrode with a diameter of 3.0 mm, a Pt wire as counter and Ag/Ag$^+$ wire as reference electrodes were used. Prior to every measurement, the working electrode was polished with Alumina slurry 0.04 mm from Schmitz Metallographie GmbH. The potential was controlled by a Metrohm μAutolabIII potentiostat. All measurements were conducted at 100 mV s^{-1} under inert nitrogen atmosphere with dry and degassed acetonitrile containing 0.1 M tetrabutylammonium hexafluorophosphate as supporting electrolyte. Ferrocene was added as internal standard to reference the acquired data to $Cp_2Fc^{+/0}$.

A filtered solution of **Cu^{bz}**, **Cu^{pyrz}**, **Cu^{quinox}** , **Ag^{bz}**, **Ag^{pyrz}** and **Ag^{quinox}** (20 mg mL^{-1} in CH_3CN) were spin-coated at 800 rpm for 30 s, 1500 rpm for 60 s and at 3000 rpm for 10 s to give thin films, whose topography images were then obtained with a MFP-3D Origin+ AFM (Asylum Research) and elaborated with Gwyddion evaluation software.

Theoretical Methods

The equilibrium structures of the ground state, S_1 and T_1 states were obtained using density functional theory (DFT) and time-dependent density functional theory (TDDFT), respectively.[15] The M06-2X exchange-correlation potential[16, 17] and the def2-TZVP basis set[18] where used. The core electrons of Ag were described using the def2-ECP pseudopotential. To assess the impact of solvent on the HOMO and LUMO levels the ground state equilibrium structures of the different complexes were relaxed accounting for the solvent effects using the polarizable continuum solvent model (PCM)[19] with acetonitrile as solvent using the same exchange-correlation functional and basis set. State characterization was carried out analyzing the largest single excitation contributions and constructing the natural transition orbitals for the different excited states when needed.[20] All these calculations were carried out using Gaussian 16.[21]

To analyze the impact of spin-orbit coupling, TDDFT calculations including 20 singlet and 20 triplet states were carried out at the ground state, S_1 and T_1 equilibrium structures of the different complexes, using the zero-order regular approximation (ZORA) Hamiltonian,[22, 23] the M06-2X exchange-correlation functional, and the ZORA recontracted def2-TZVP and SARC-ZORA-TZVP basis set[24] as implemented in ORCA 5.0.4.[25, 26] The corresponding Coulomb fitting auxiliary basis sets were used.[27] The results obtained (not reported here) showed no significant contribution of the spin-orbit coupling.

Device Fabrication and Characterization Methods

Indium-tin oxide (ITO) substrates were purchased from Naranjo with an ITO thickness of 130 nm. Prior to use, they were extensively cleaned using detergent, water, ethanol, and isopropanol as solvents in an ultrasonic bath (frequency 37–70 Hz) for 20 min each, followed by drying the slides with N_2 gas and then treated with an UV-ozone cleaner for 8 min. An aqueous solution of PEDOT:PSS was filtered and mixed with isopropanol in a ratio of 3:1. From this solution 50 µL were dropped onto the substrate at a rotation speed of 1200 rpm and spin for 60 s followed by 2500 rpm for 20 s. The resulting layers were dried on a hotplate at 120 °C giving a thickness of 80 nm. A solution of $\mathbf{M^{bz}}$ (20 mg mL^{-1}) in CH_3CN was filtered with a 0.2 µm PTFE syringe filter and was spin-coated on top of the PEDOT:PSS layer at 800 rpm for 30 s, 1500 rpm for 30 s and at 3000 rpm for an additional 10 s resulting in active layer thicknesses of 75-90 nm. In all cases, after the deposition of the active layer the devices were transferred to an inert atmosphere glovebox (< 0.1 ppm O_2 and H_2O, Angstrom Engineering). Onto all devices, an aluminum cathode electrode (100 nm) was thermally evaporated using a shadow mask under high vacuum (< 1×10^{-6} mbar) in an Angstrom Covap evaporator integrated into the inert atmosphere glovebox. One substrate consists of four pixels each with an area of 15 mm^2. The device statistics involved 3 different devices. The devices were driven at a pulsed current of 15 mA with a driving scheme based on a block wave at 1,000 Hz and a duty cycle of 50 % that corresponds to an average current density of 500 A/m^2. Time dependence of luminance, voltage, and current was measured by applying pulsed voltage and current by monitoring the desired parameters simultaneously using Avantes spectrophotometer (Avaspec-ULS2048L-USB2) in conjunction with a calibrated integrated sphere Avasphere 30-Irrad and Botest OLT OLED Lifetime-Test System. Electroluminescence spectra were recorded using the above-mentioned spectrophotometer.

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25 Neese, F. *The ORCA program system Wiley Interdiscip. Rev.: Comput. Mol. Sci.*, 2012, **2**, *1*, 73.

26 Neese, F. *Software update: the ORCA program system -- Version 5.0 Wiley Interdiscip. Rev.: Comput. Mol. Sci.*, 2022, **12**, e1606.

27 F. Weigend, *Phys. Chem. Chem. Phys.,* 2006, **8**, 1057.

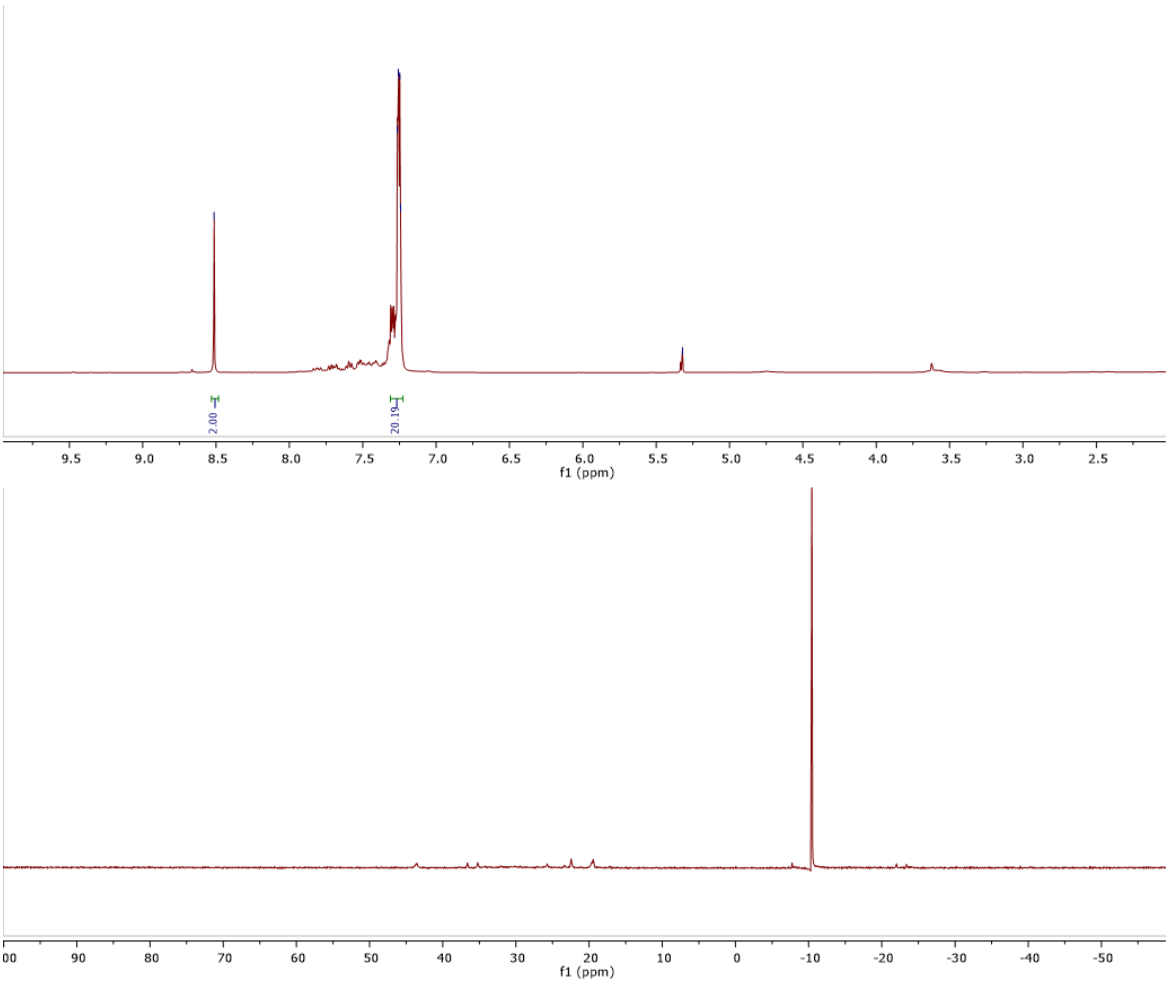


Figure S1 ^{1}H- and ^{31}P{^{1}H}-NMR of **dpppyrz**.

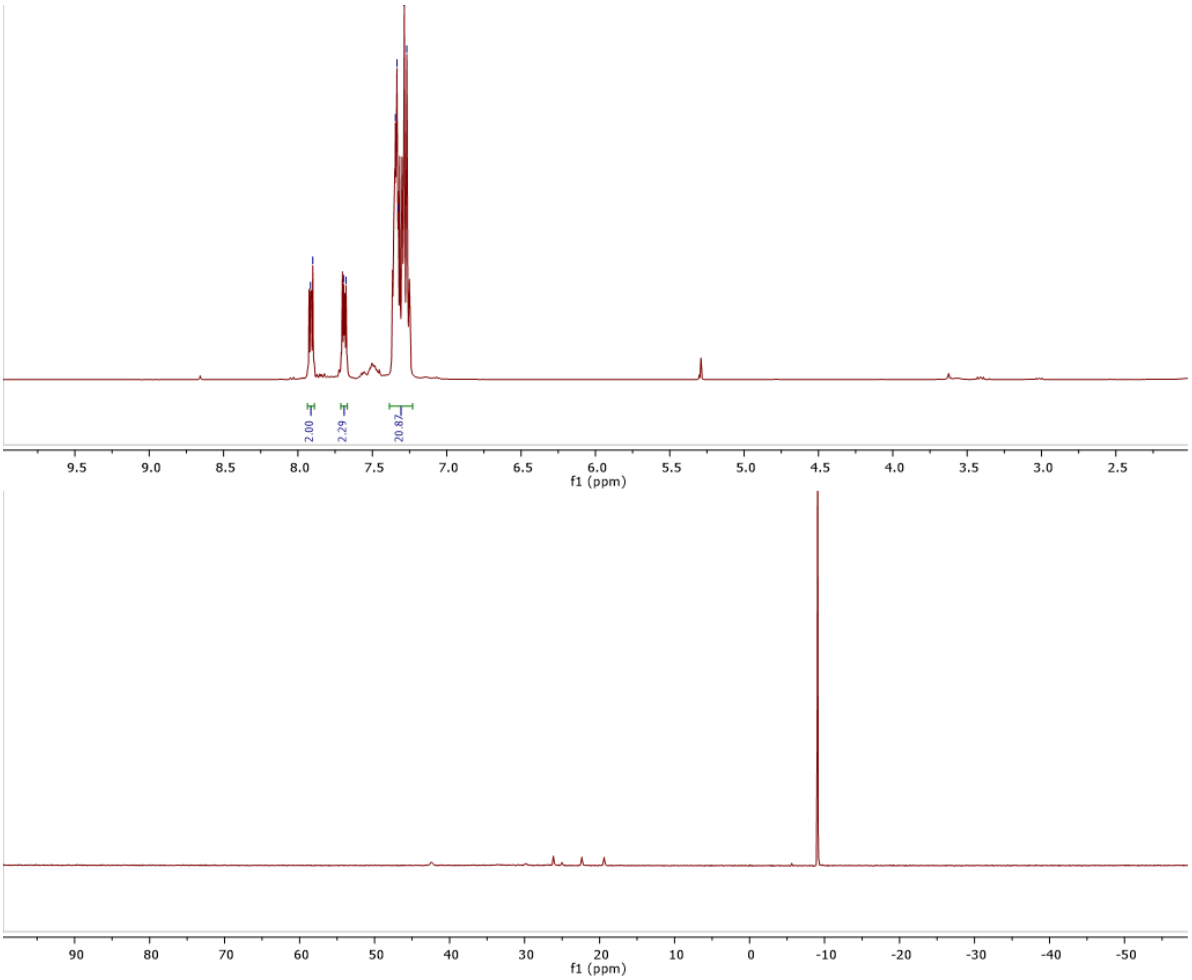
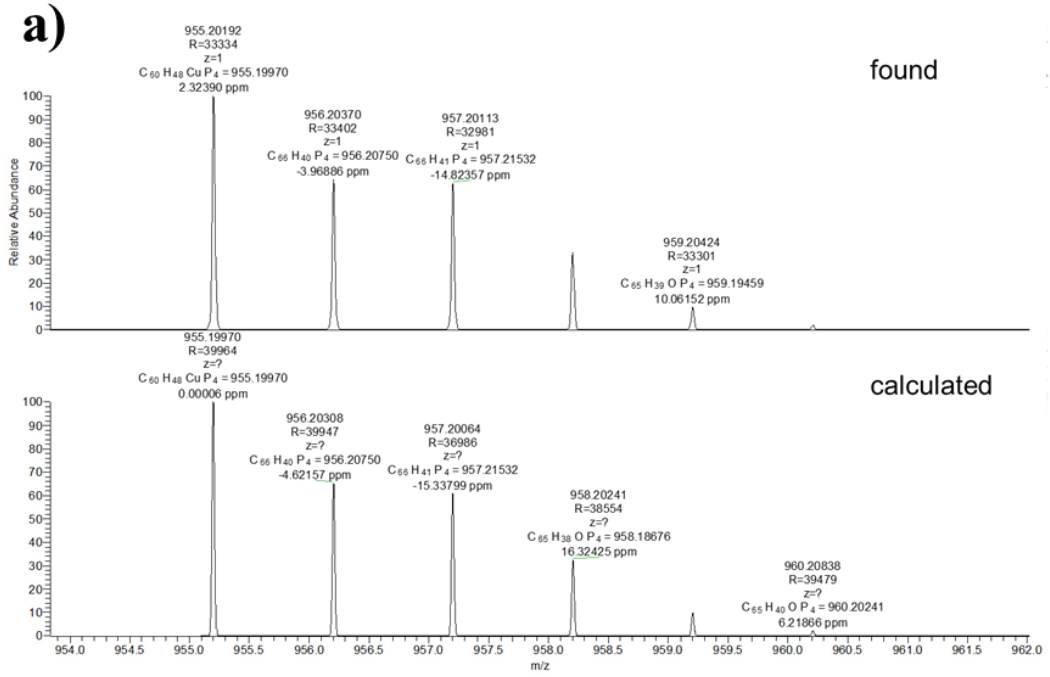
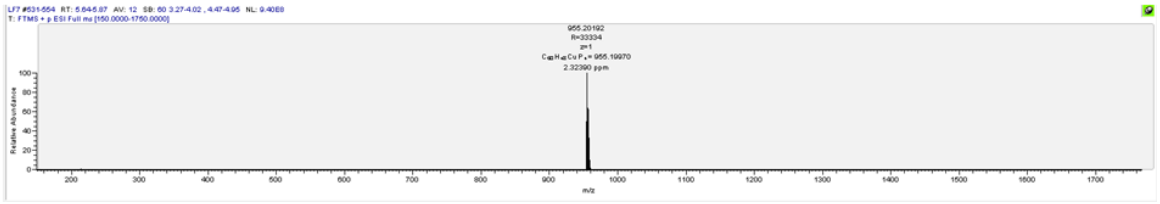
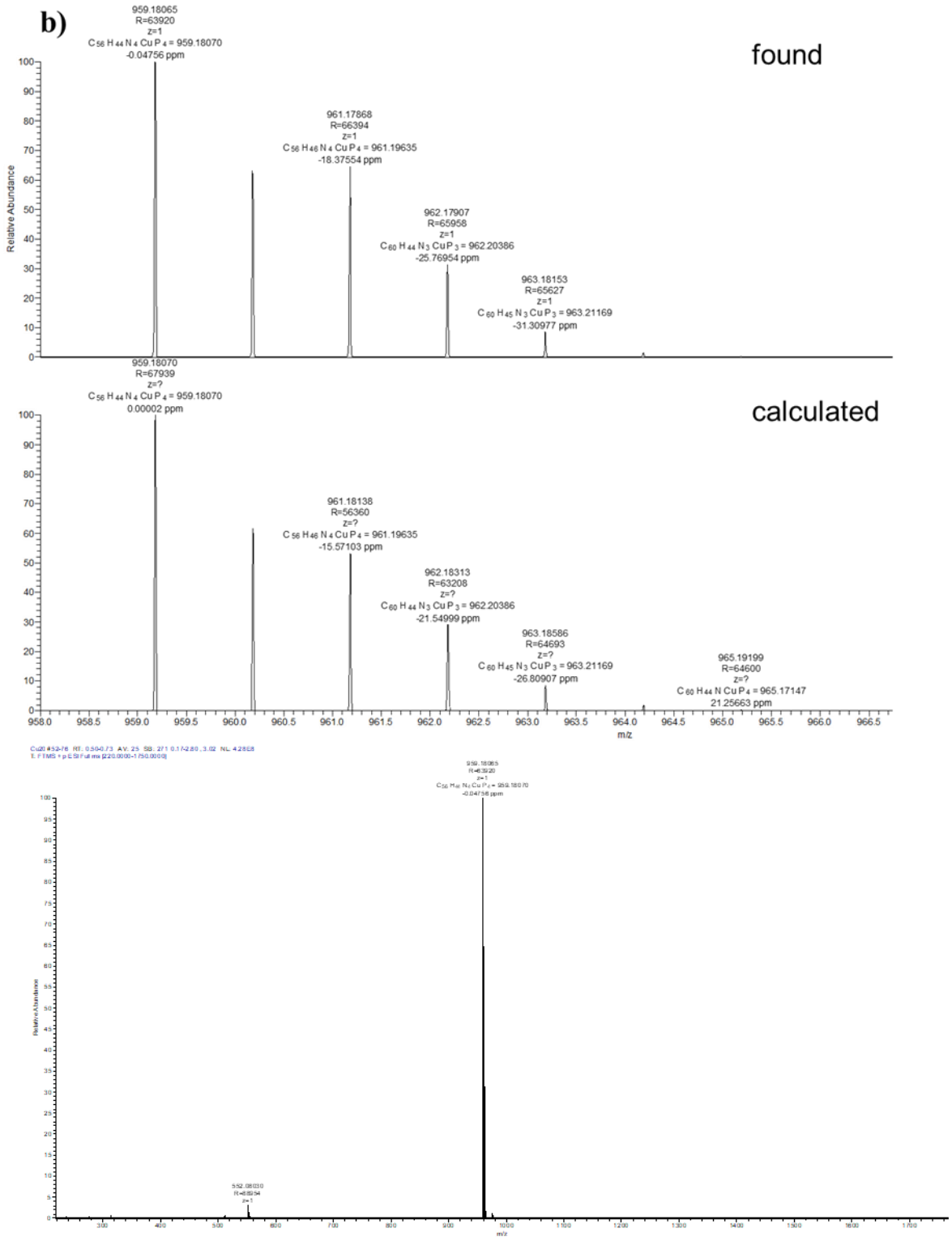
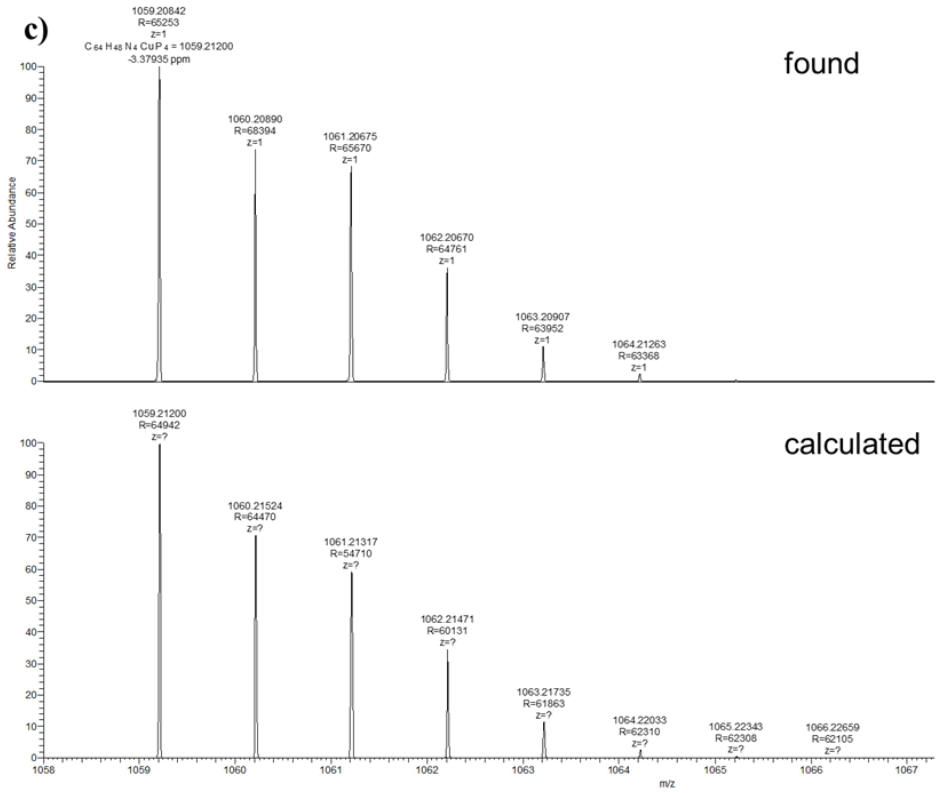


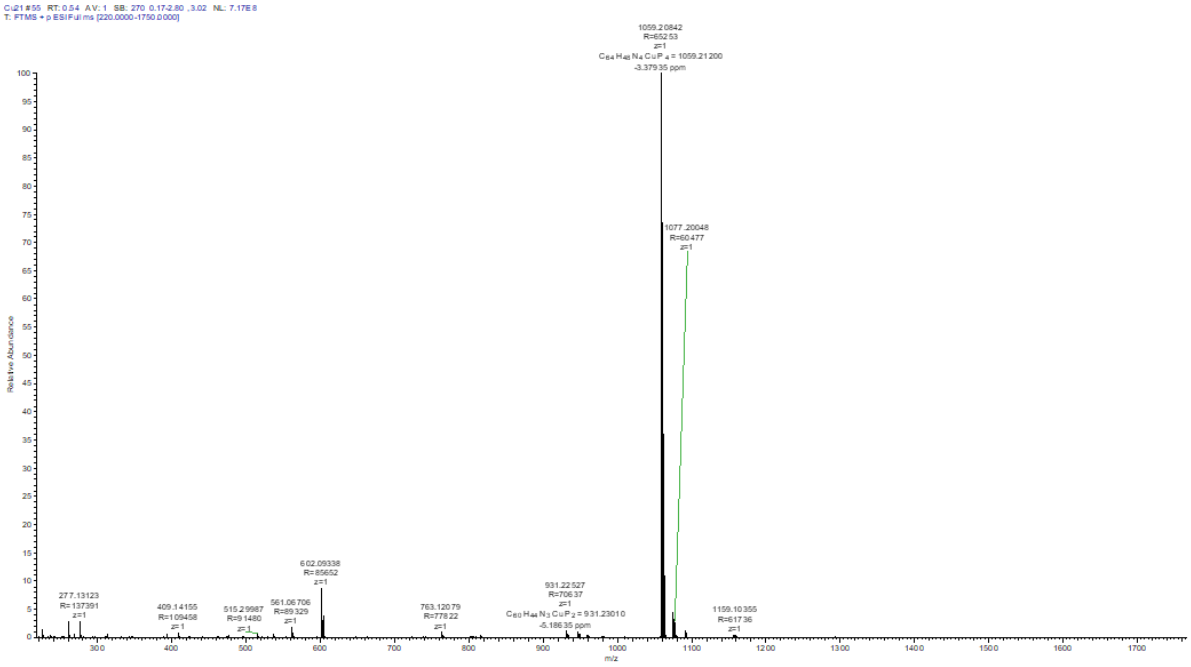
Figure S2 ^{1}H- and ^{31}P{^{1}H}-NMR of **dppquinox**.

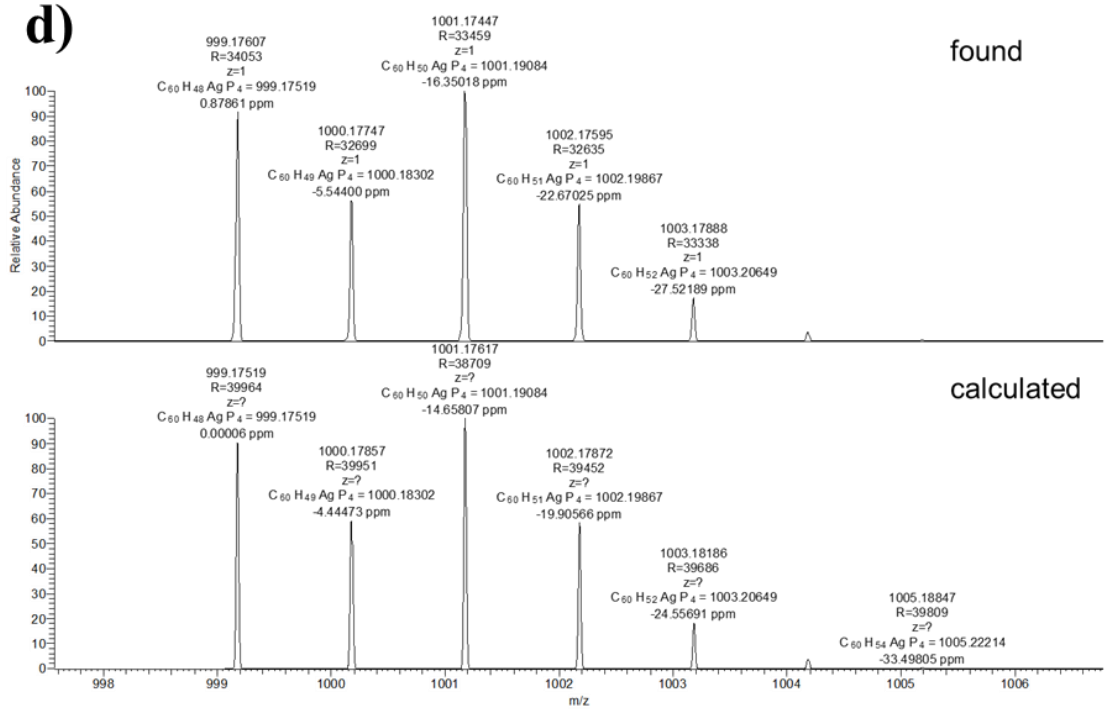

a)
found
955.20192
R=33334
z=1
C 60 H 48 Cu P 4 = 955.19970
2.32390 ppm
956.20370
R=33402
z=1
C 66 H 40 P 4 = 956.20750
-3.96886 ppm
957.20113
R=32981
z=1
C 66 H 41 P 4 = 957.21532
-14.82357 ppm
959.20424
R=33301
z=1
C 65 H 39 O P 4 = 959.19459
10.06152 ppm
Relative Abundance
calculated
955.19970
R=39964
z=?
C 60 H 48 Cu P 4 = 955.19970
0.00006 ppm
956.20308
R=39947
z=?
C 66 H 40 P 4 = 956.20750
-4.62157 ppm
957.20064
R=36986
z=?
C 66 H 41 P 4 = 957.21532
-15.33799 ppm
958.20241
R=38554
z=?
C 65 H 38 O P 4 = 958.18676
16.32425 ppm
960.20838
R=39479
z=?
C 65 H 40 O P 4 = 960.20241
6.21866 ppm
m/z

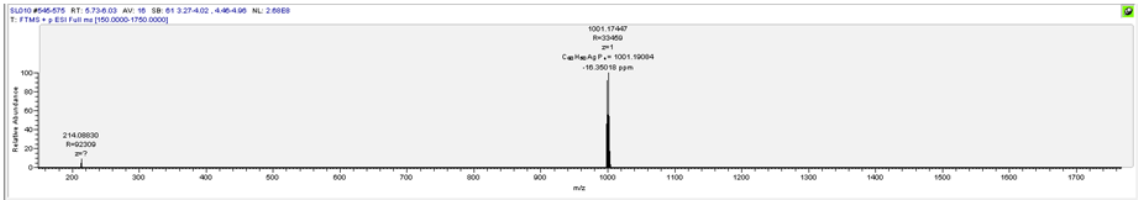


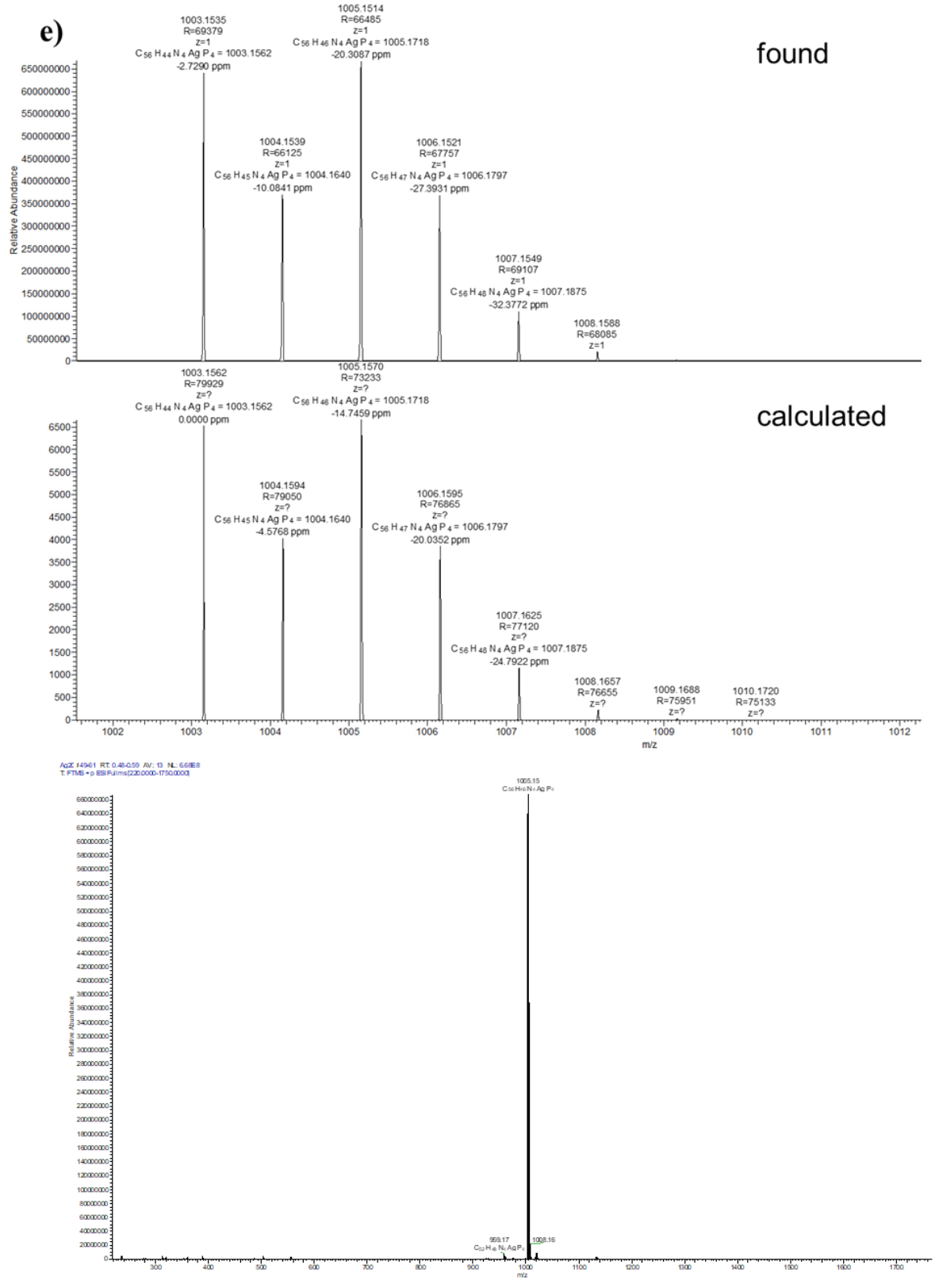

b)
found
959.18065
R=63920
z=1
C 56 H 44 N 4 Cu P 4 = 959.18070
-0.04756 ppm
961.17868
R=66394
z=1
C 56 H 46 N 4 Cu P 4 = 961.19635
-18.37554 ppm
962.17907
R=65958
z=1
C 60 H 44 N 3 Cu P 3 = 962.20386
-25.76954 ppm
963.18153
R=65627
z=1
C 60 H 45 N 3 Cu P 3 = 963.21169
-31.30977 ppm
Relative Abundance
959.18070
R=67939
z=?
C 56 H 44 N 4 Cu P 4 = 959.18070
0.00002 ppm
calculated
961.18138
R=56360
z=?
C 56 H 46 N 4 Cu P 4 = 961.19635
-15.57103 ppm
962.18313
R=63208
z=?
C 60 H 44 N 3 Cu P 3 = 962.20386
-21.54999 ppm
963.18586
R=64693
z=?
C 60 H 45 N 3 Cu P 3 = 963.21169
-26.80907 ppm
965.19199
R=64600
z=?
C 60 H 44 N Cu P 4 = 965.17147
21.25663 ppm
m/z


c)
found
calculated
Relative Abundance
m/z
1059.20842
R=65253
z=1
C64 H48 N4 Cu P4 = 1059.21200
-3.37935 ppm
1060.20890
R=68394
z=1
1061.20675
R=65670
z=1
1062.20670
R=64761
z=1
1063.20907
R=63952
z=1
1064.21263
R=63368
z=1
1059.21200
R=64942
z=?
1060.21524
R=64470
z=?
1061.21317
R=54710
z=?
1062.21471
R=60131
z=?
1063.21735
R=61863
z=?
1064.22033
R=62310
z=?
1065.22343
R=62308
z=?
1066.22659
R=62105
z=?


C:\21 #55 RT: 0.54 AV: 1 SB: 270 0.17-2.80 , 3.02 NL: 7.17E8
T: FTMS + p ESI Full ms [220.0000-1750.0000]
Relative Abundance
m/z
1059.20842
R=65253
z=1
C64 H48 N4 Cu P4 = 1059.21200
-3.37935 ppm
1077.20048
R=60477
z=1
602.09338
R=85652
z=1
277.13123
R=137391
z=1
409.14155
R=109458
z=1
515.29987
R=91480
z=1
561.06706
R=89329
z=1
763.12079
R=77822
z=1
931.22527
R=70637
z=1
C60 H44 N3 Cu P2 = 931.23010
-5.18635 ppm
1159.10355
R=61736
z=1


d)
found
999.17607
R=34053
z=1
C 60 H 48 Ag P 4 = 999.17519
0.87861 ppm
1000.17747
R=32699
z=1
C 60 H 49 Ag P 4 = 1000.18302
-5.54400 ppm
1001.17447
R=33459
z=1
C 60 H 50 Ag P 4 = 1001.19084
-16.35018 ppm
1002.17595
R=32635
z=1
C 60 H 51 Ag P 4 = 1002.19867
-22.67025 ppm
1003.17888
R=33338
z=1
C 60 H 52 Ag P 4 = 1003.20649
-27.52189 ppm
Relative Abundance
calculated
999.17519
R=39964
z=?
C 60 H 48 Ag P 4 = 999.17519
0.00006 ppm
1000.17857
R=39951
z=?
C 60 H 49 Ag P 4 = 1000.18302
-4.44473 ppm
1001.17617
R=38709
z=?
C 60 H 50 Ag P 4 = 1001.19084
-14.65807 ppm
1002.17872
R=39452
z=?
C 60 H 51 Ag P 4 = 1002.19867
-19.90566 ppm
1003.18186
R=39686
z=?
C 60 H 52 Ag P 4 = 1003.20649
-24.55691 ppm
1005.18847
R=39809
z=?
C 60 H 54 Ag P 4 = 1005.22214
-33.49805 ppm
m/z




e)
found
1003.1535
R=69379
z=1
C56 H44 N4 Ag P4 = 1003.1562
-2.7290 ppm
1005.1514
R=66485
z=1
C56 H46 N4 Ag P4 = 1005.1718
-20.3087 ppm
1004.1539
R=66125
z=1
C56 H45 N4 Ag P4 = 1004.1640
-10.0841 ppm
1006.1521
R=67757
z=1
C56 H47 N4 Ag P4 = 1006.1797
-27.3931 ppm
1007.1549
R=69107
z=1
C56 H48 N4 Ag P4 = 1007.1875
-32.3772 ppm
1008.1588
R=68085
z=1
Relative Abundance
calculated
1003.1562
R=79929
z=?
C56 H44 N4 Ag P4 = 1003.1562
0.0000 ppm
1005.1570
R=73233
z=?
C56 H46 N4 Ag P4 = 1005.1718
-14.7459 ppm
1004.1594
R=79050
z=?
C56 H45 N4 Ag P4 = 1004.1640
-4.5768 ppm
1006.1595
R=76865
z=?
C56 H47 N4 Ag P4 = 1006.1797
-20.0352 ppm
1007.1625
R=77120
z=?
C56 H48 N4 Ag P4 = 1007.1875
-24.7922 ppm
1008.1657
R=76655
z=?
1009.1688
R=75951
z=?
1010.1720
R=75133
z=?
m/z

1005.15
959.17
1008.16
Relative Abundance
m/z

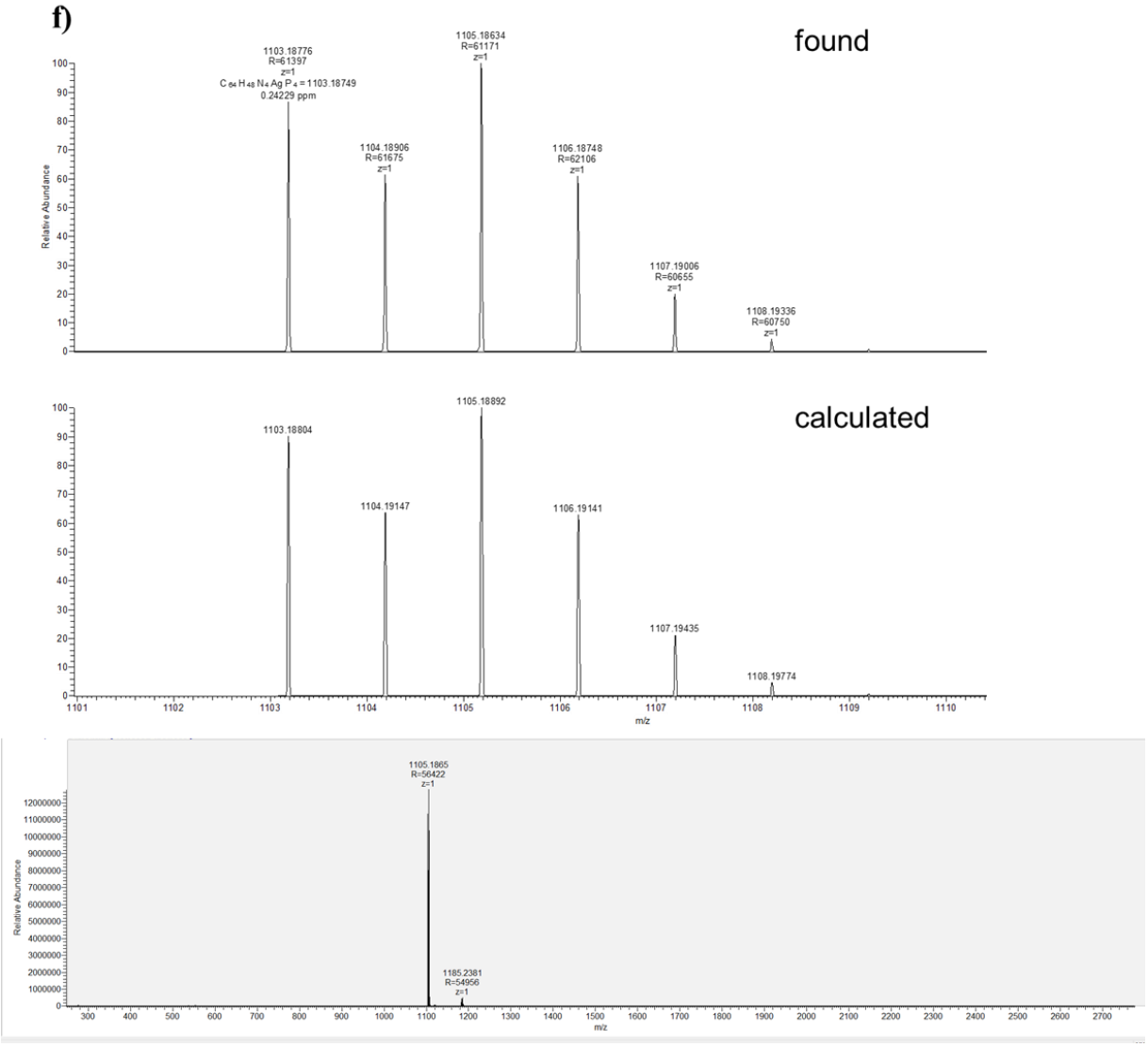
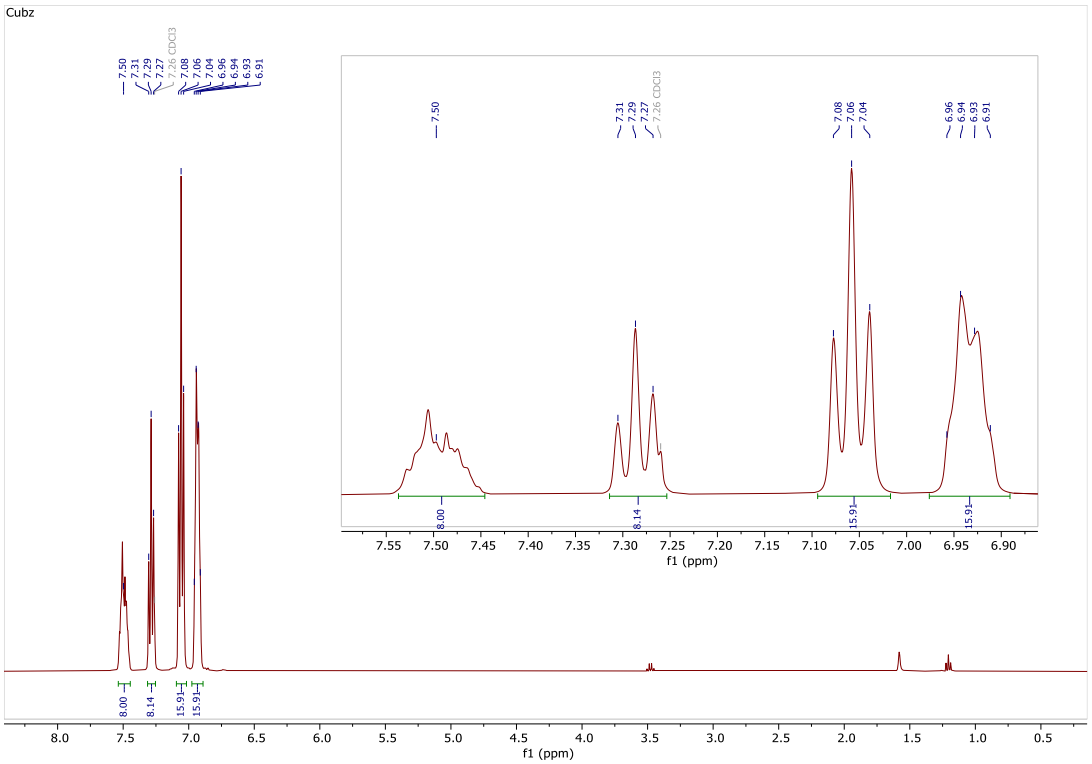
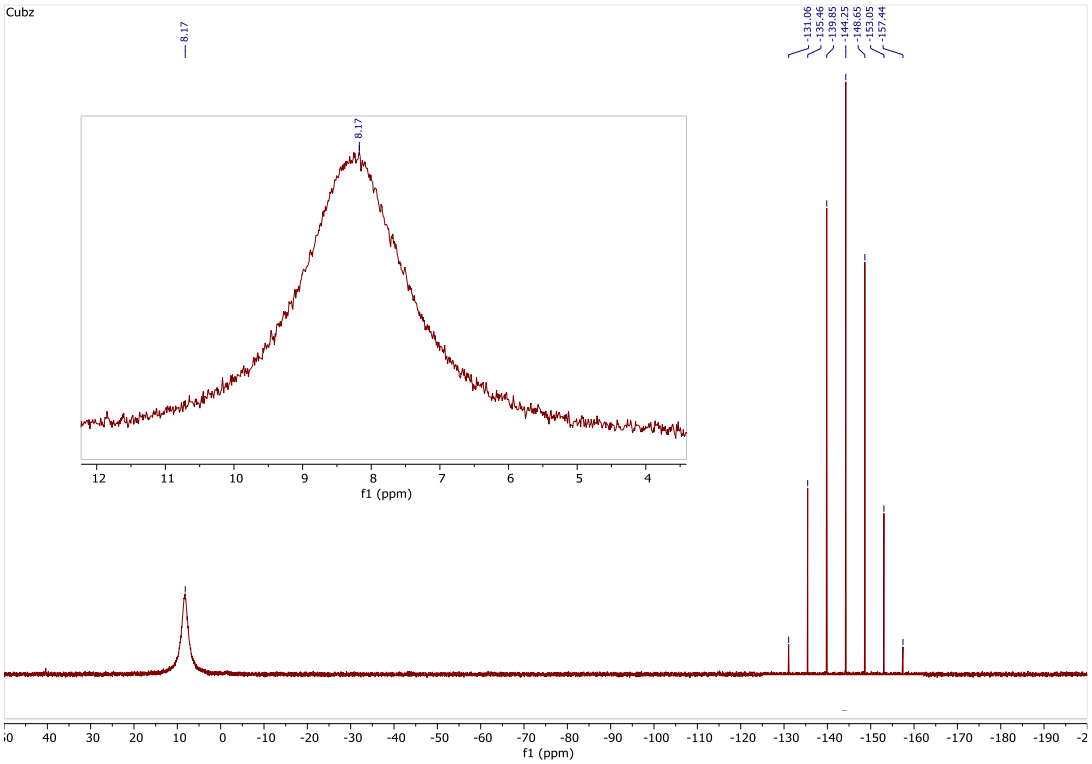


Figure S3. Full and zoom-in (found and calculated) ESI HR-MS spectra of **Cu**^{bz} (a), **Cu**^{pyrz} (b), **Cu**^{quinox} (c), **Ag**^{bz} (d), **Ag**^{pyrz} (e) and **Ag**^{quinox} (f).


Cubz
7.50
7.31
7.29
7.27
7.26 CDCl3
7.08
7.06
7.04
6.96
6.94
6.93
6.91
8.00
8.14
15.91
15.91
f1 (ppm)


Cubz
8.17
-131.06
-135.46
-139.85
-144.25
-148.65
-153.05
-157.44
f1 (ppm)

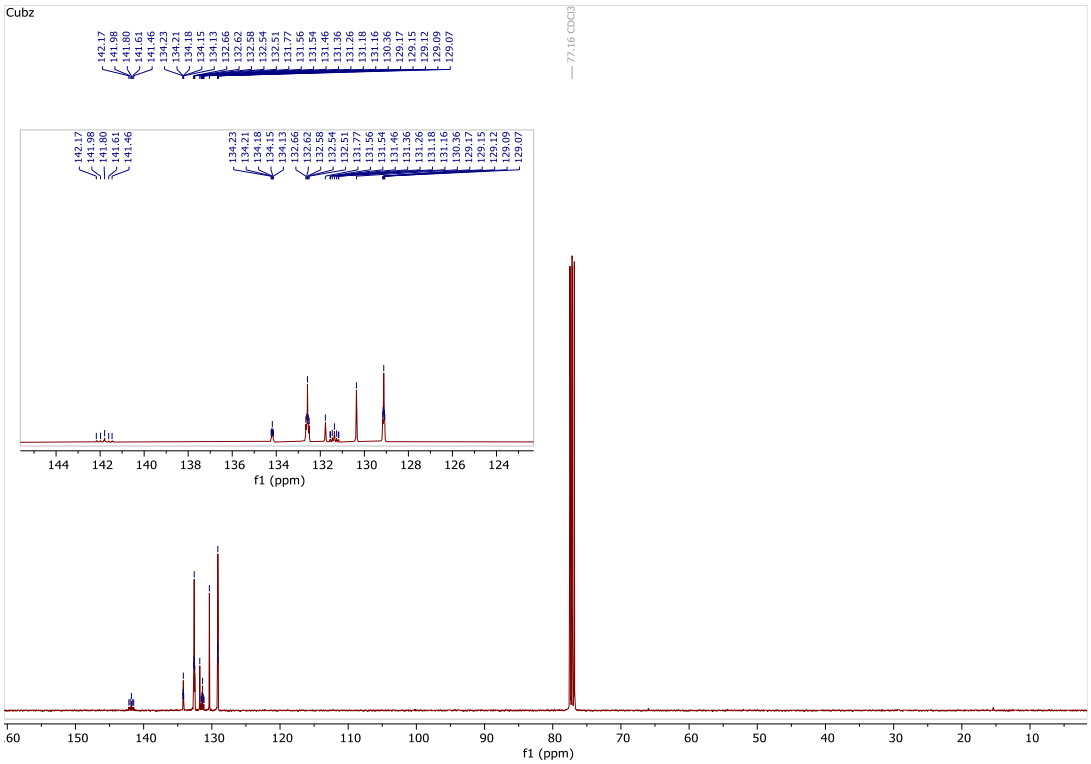
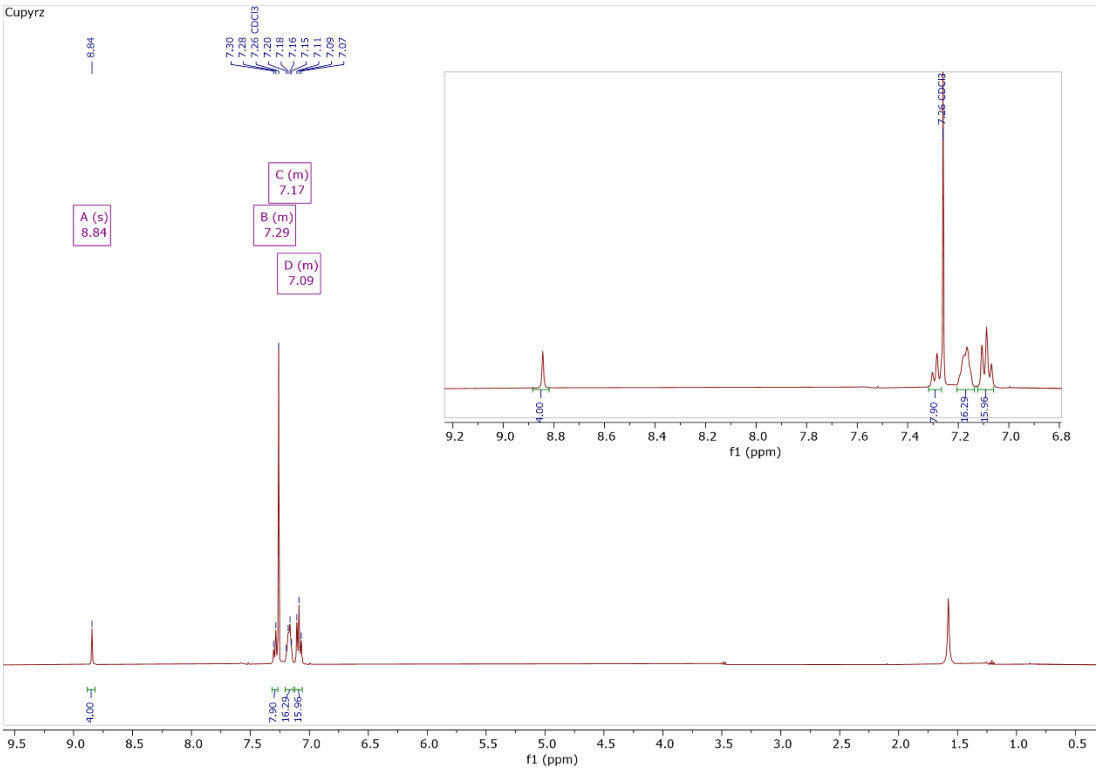
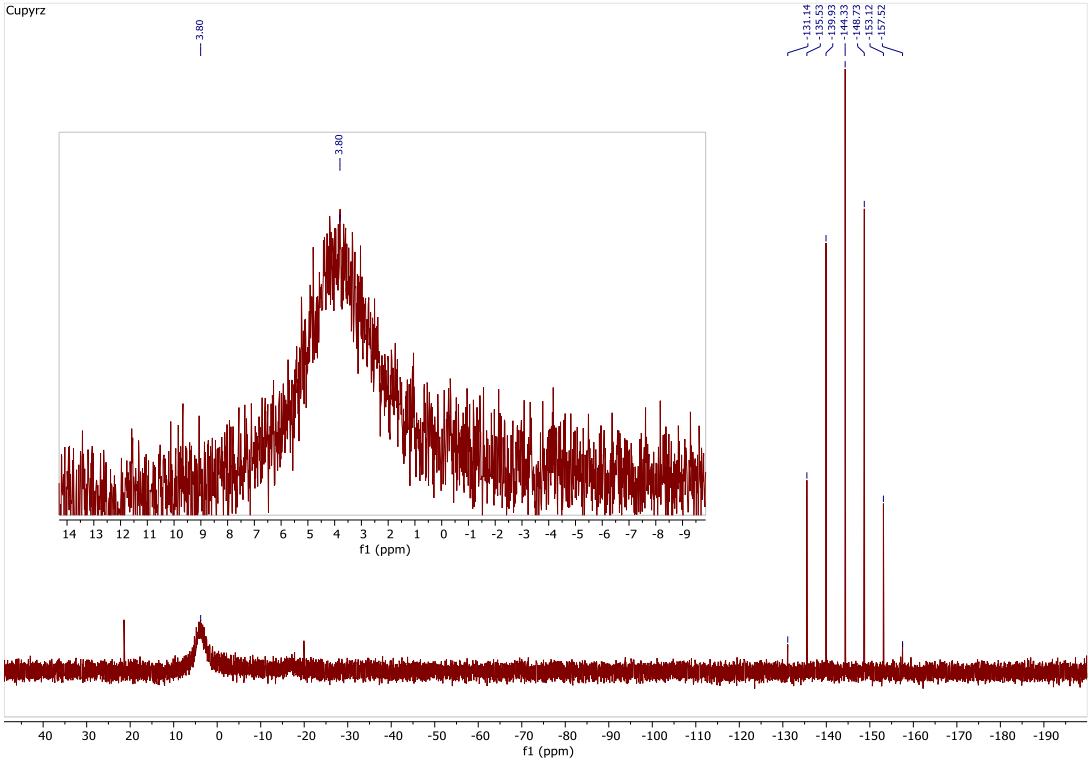


Figure S4. ^{1}H-, ^{31}P{^{1}H}- and ^{13}C{^{1}H}-NMR of **Cu^{bz}**.


Cupyrz
8.84
7.30
7.28
7.26 CDCl3
7.20
7.18
7.16
7.15
7.11
7.09
7.07
A (s)
8.84
B (m)
7.29
C (m)
7.17
D (m)
7.09
4.00
7.90
16.29
15.96
f1 (ppm)


Cupyrz
3.80
-131.14
-135.53
-139.93
-144.33
-148.73
-153.12
-157.52
f1 (ppm)

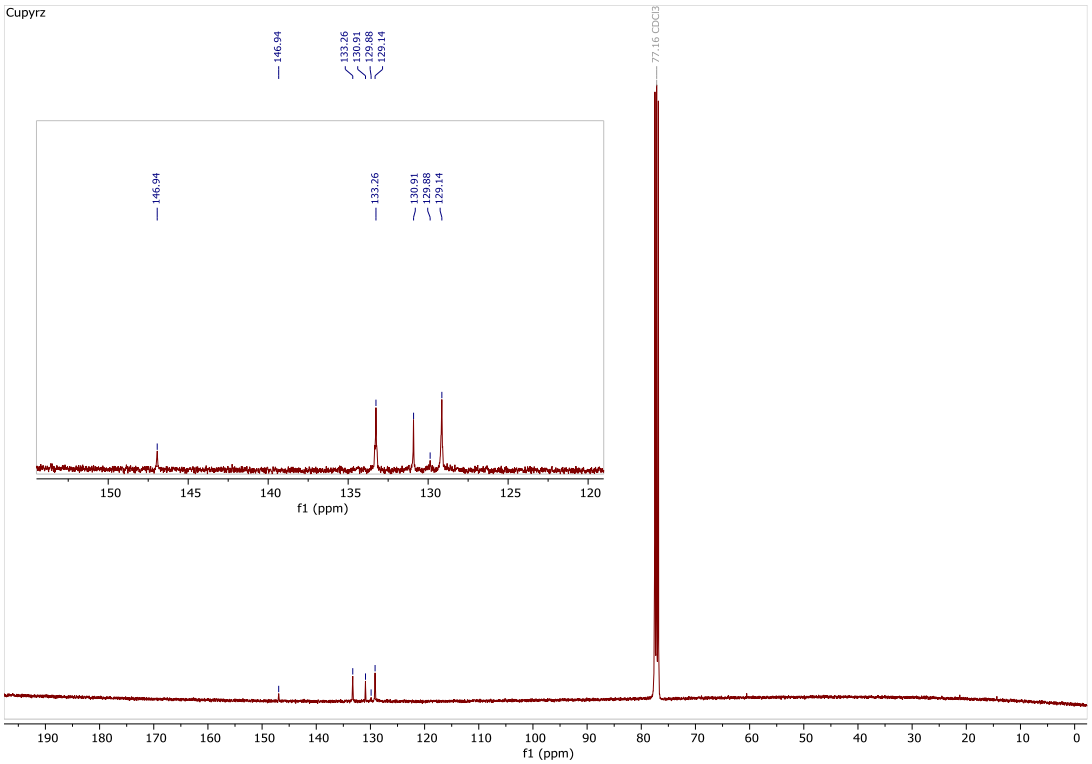
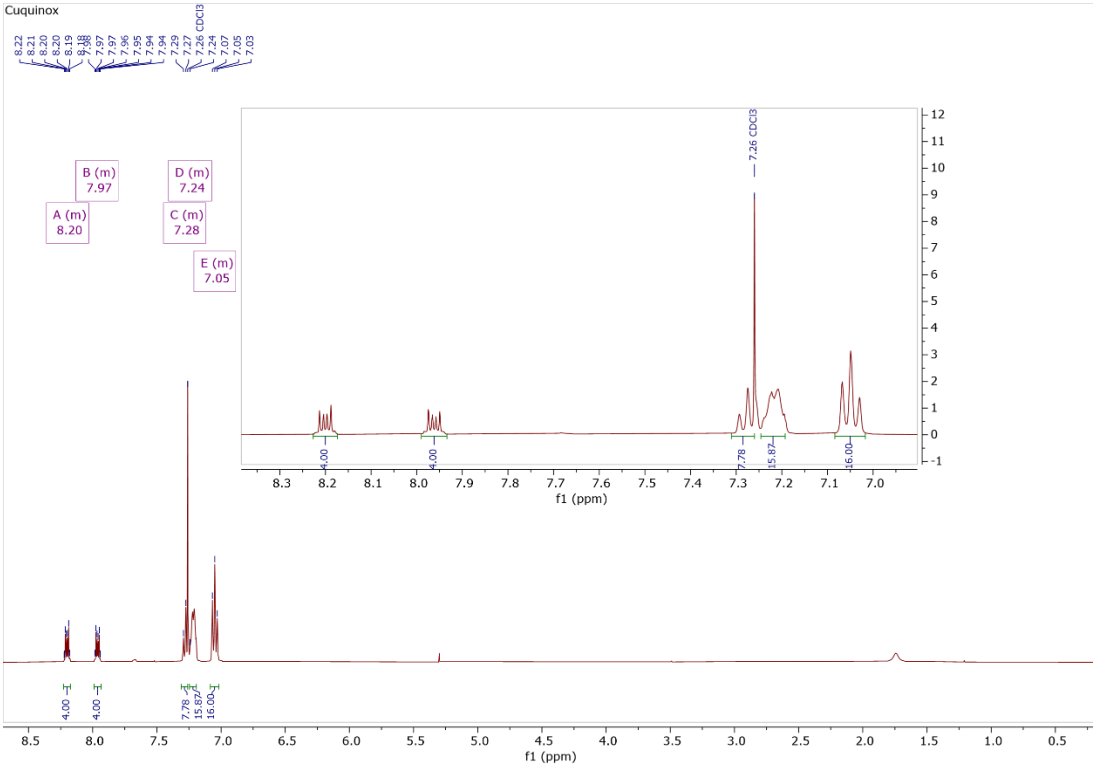


Figure S5. ^{1}H-, ^{31}P{^{1}H}- and ^{13}C{^{1}H}-NMR of **Cu^{pyrz}**.



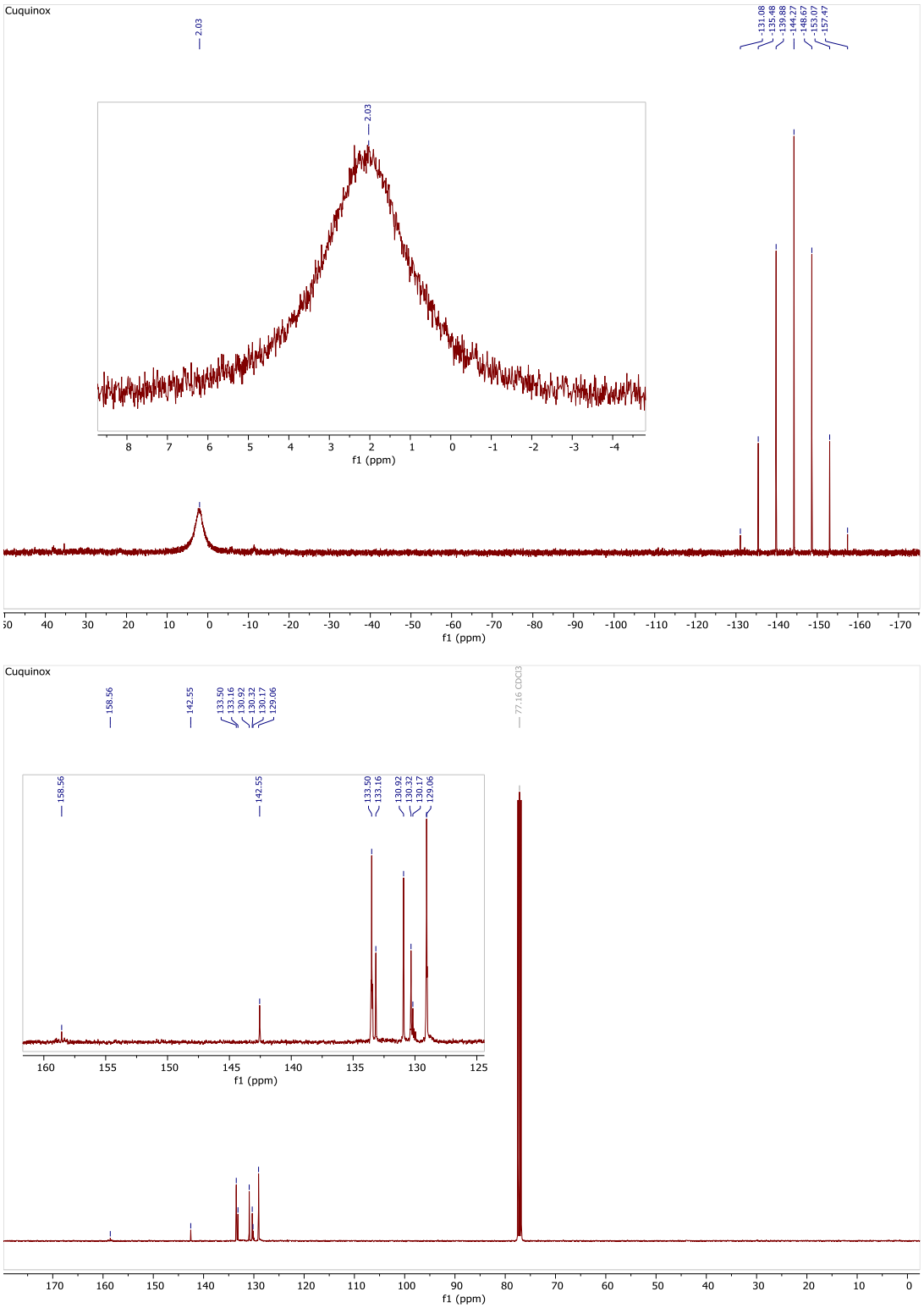
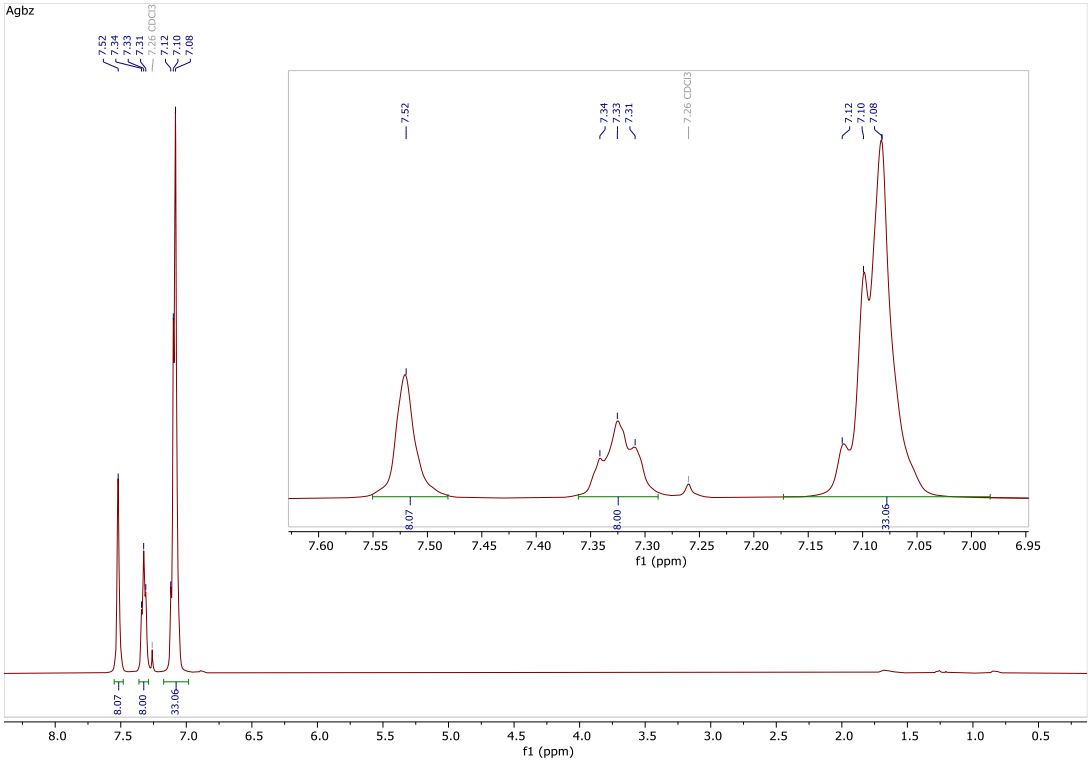
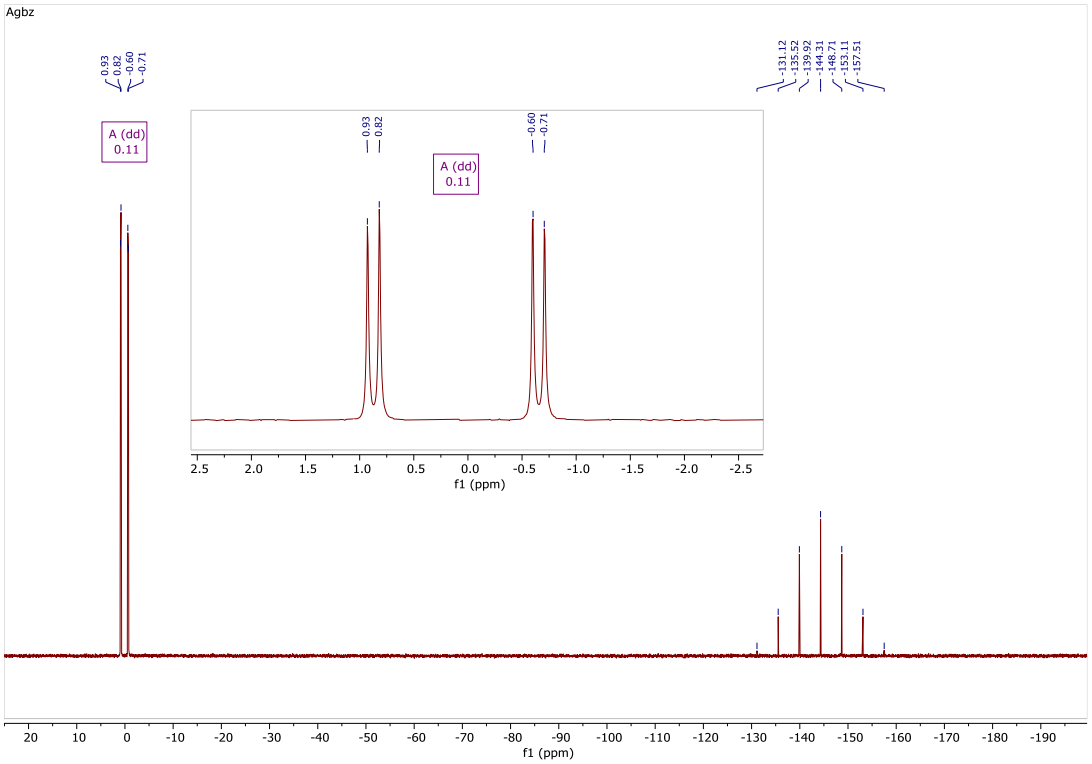


Figure S6. ^{1}H-, ^{31}P{^{1}H}- and ^{13}C{^{1}H}-NMR of **Cu^{quinox}**.


Agbz
7.52
7.34
7.33
7.31
7.26 CDCl3
7.12
7.10
7.08
8.07
8.00
33.06
f1 (ppm)


Agbz
0.93
0.82
-0.60
-0.71
A (dd)
0.11
-131.12
-135.52
-139.92
-144.31
-148.71
-153.11
-157.51
f1 (ppm)

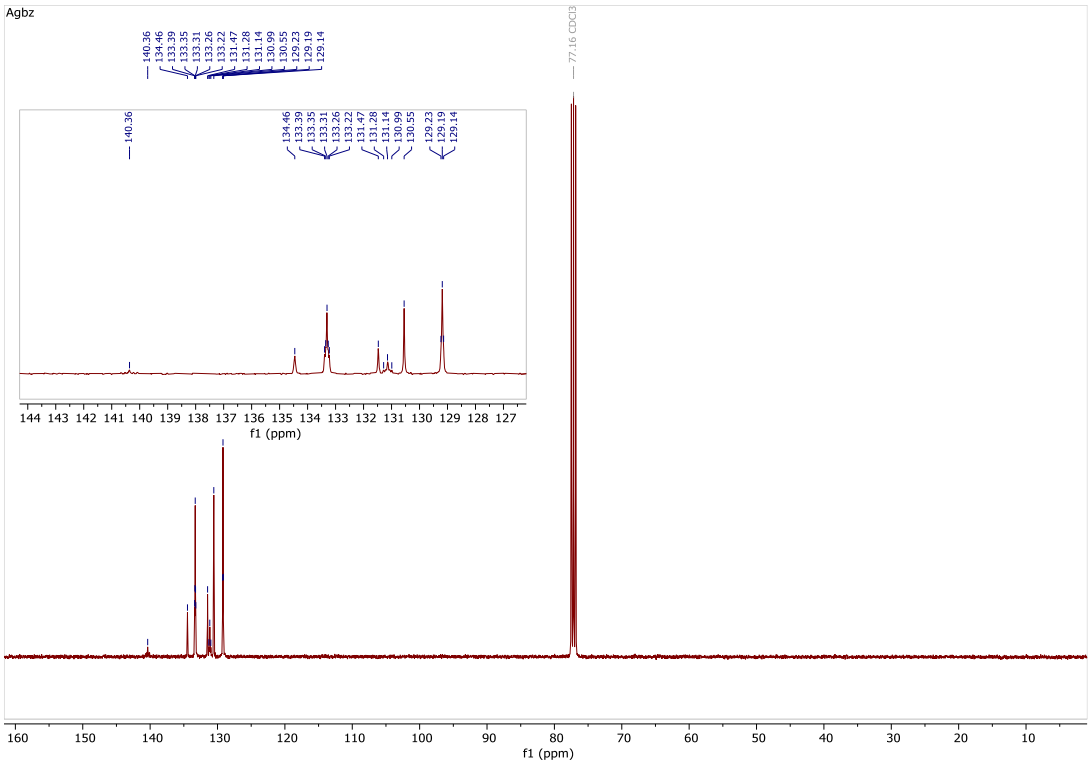
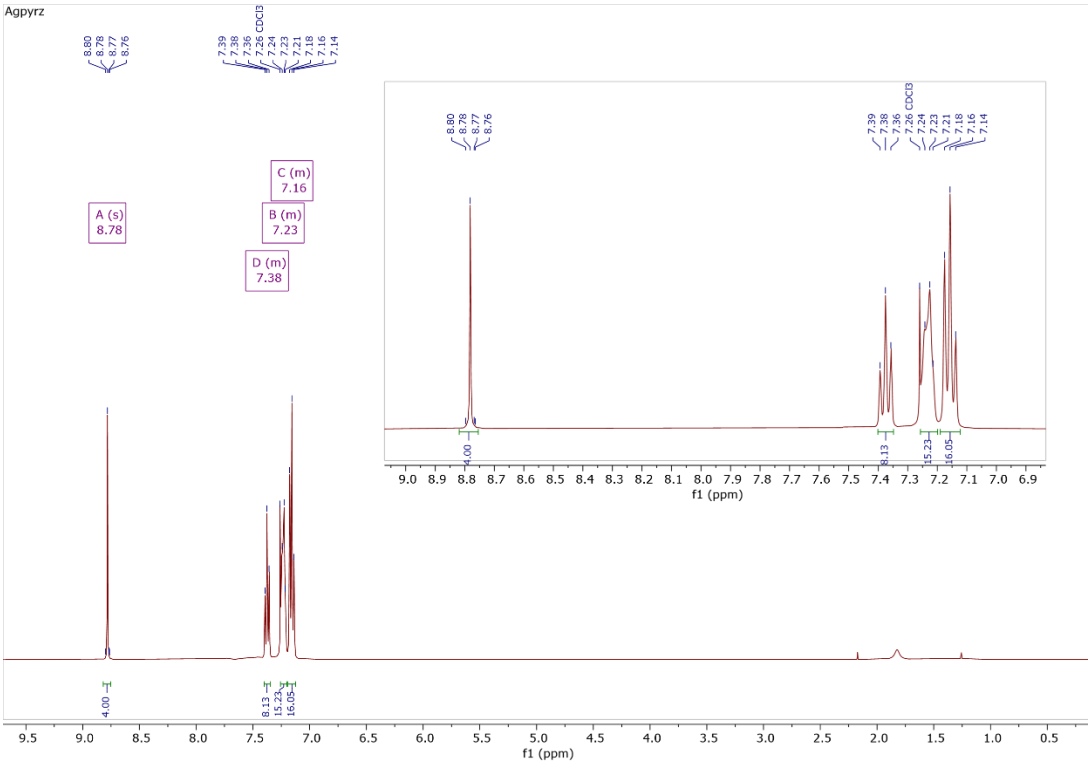


Figure S7. ^{1}H-, ^{31}P{^{1}H}- and ^{13}C{^{1}H}-NMR of **Ag^{bz}**.



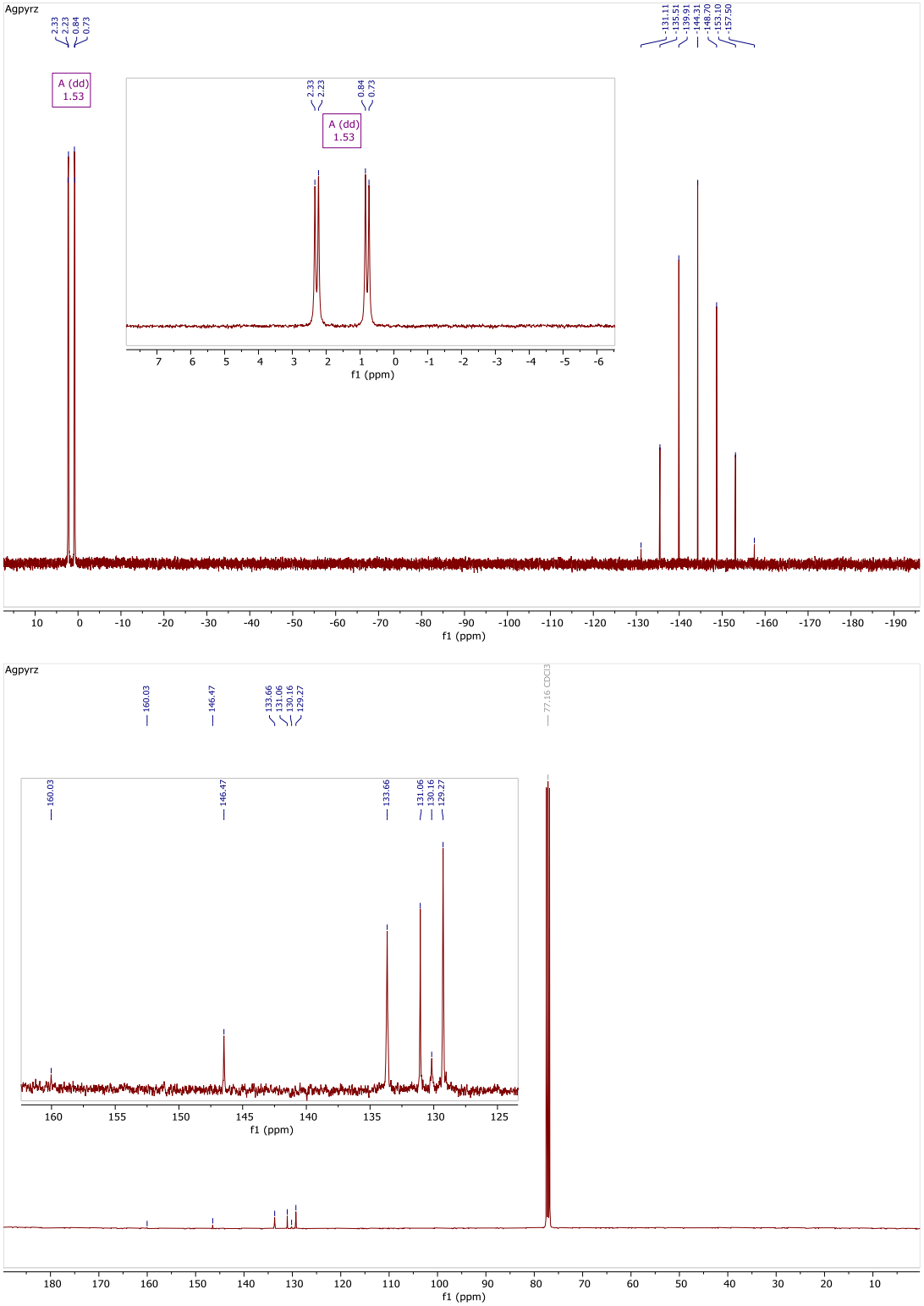
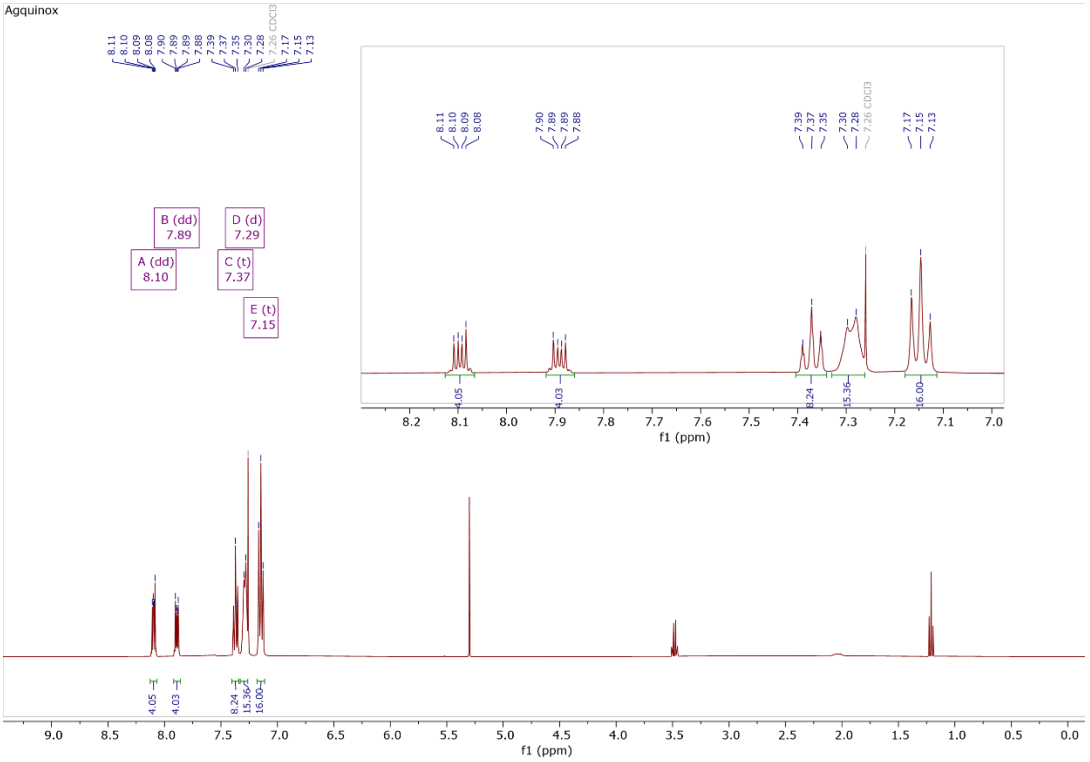
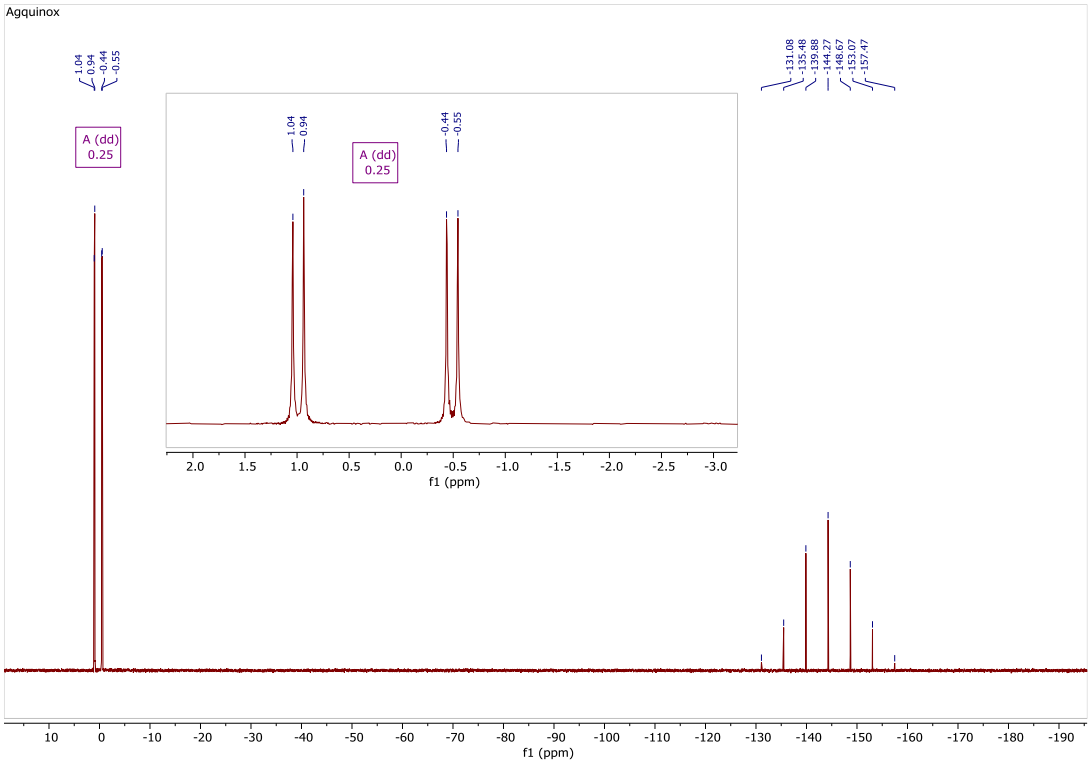


Figure S8. ^{1}H-, ^{31}P{^{1}H}- and ^{13}C{^{1}H}-NMR of **Ag^{pyrz}**.


Agquinox
B (dd)
7.89
D (d)
7.29
A (dd)
8.10
C (t)
7.37
E (t)
7.15
f1 (ppm)


Agquinox
A (dd)
0.25
A (dd)
0.25
f1 (ppm)

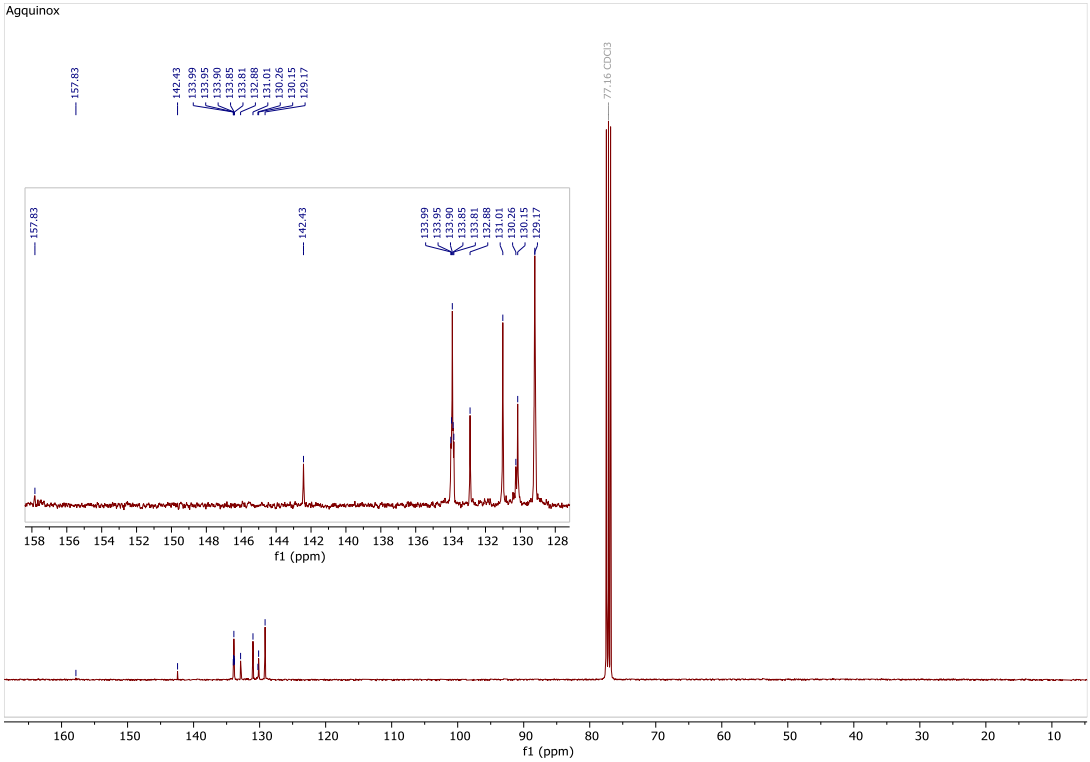


Figure S9. ^{1}H-, ^{31}P{^{1}H}- and ^{13}C{^{1}H}-NMR of **Ag^{quinox}**.

Table S1. Crystallographic data, data collection and structure refinement parameters.

	Cu^{bz}	**Ag^{pyrz}**	**Ag^{quinox}**
CCDC number	2406496	2425241	2406497
Chemical formula	$C_{60}H_{48}CuF_6P_5$	$C_{57}H_{45}AgCl_3F_6N_4P_5$	$C_{66}H_{50}AgCl_6F_6N_4P_5$
Formular weight	1101.37	1269.04	1488.52
Temperature	291(2)	173(2)	100(2)
Crystal size [mm^3]	0.213×0.225×0.398	0.2×0.2×0.1	0.027×0.088×0.401
Crystal color	colorless	yellow	orange
Crystal shape	block	block	needle
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2/n$ (13)	$P\ 2_1/c$ (14)	Pc (7)
Unit cell dimensions	*a* [Å] = 13.6792(3) b [Å] = 12.9093(3) c [Å] = 15.3195(4) β [°] = 98.5490(10)	*a* [Å] = 12.6263(4) b [Å] = 18.9307(6) c [Å] = 24.8789(9) β [°] = 91.952(2)	*a* [Å] = 16.5556(11) b [Å] = 19.9293(12) c [Å] = 19.8501(10) β [°] = 100.162(2)
Volume [Å^3]	2675.20(11)	5943.2(3)	6446.6(7)
Z	2	4	4
ρ (calc.) [gcm^{-3}]	1.367	1.418	1.533
μ [mm^{-1}]	0.617	0.667	0.748
F(000)	1132	2568	3008
Radiation source	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)
2Θ range [°]	4.15 to 52.79 (0.80 Å)	4.60 to 51.73 (0.81 Å)	4.09 to 50.79 (0.83 Å)
Index ranges	−17 ≤ h ≤ 17 −16 ≤ k ≤ 16 −19 ≤ l ≤ 19	−15 ≤ h ≤ 15 −23 ≤ k ≤ 23 −30 ≤ l ≤ 30	−19 ≤ h ≤ 19 −24 ≤ k ≤ 24 −23 ≤ l ≤ 23
Reflections collected	110611	11478	278397
Independent reflections	5480 R_{int} = 0.0384 R_{sigma} = 0.0116	10078 R_{int} = 0.1113 R_{sigma} = 0.0445	23592 R_{int} = 0.0826 R_{sigma} = 0.0344
Completeness	100.0 %	99.9%	99.9%
Data / restraints / parameters	5480 / 766 / 476	11478 / 6392 / 1125	23592 / 2 / 1586
Goodness-of-fit on F^2	1.049	1.065	1.018
Final *R* indexes [*I*≥2σ(*I*)]	R_1 = 0.0270 wR_2 = 0.0712	R_1 = 0.0650 wR_2 = 0.1729	R_1 = 0.0260 wR_2 = 0.0536
Final R indices [all data]	R_1 = 0.0311 wR_2 = 0.0743	R_1 = 0.0791 wR_2 = 0.1841	R_1 = 0.0325 wR_2 = 0.0558
Largest diff. peak and hole [eÅ^{-3}]	0.26/−0.30	1.72/−2.24	0.47/−0.45

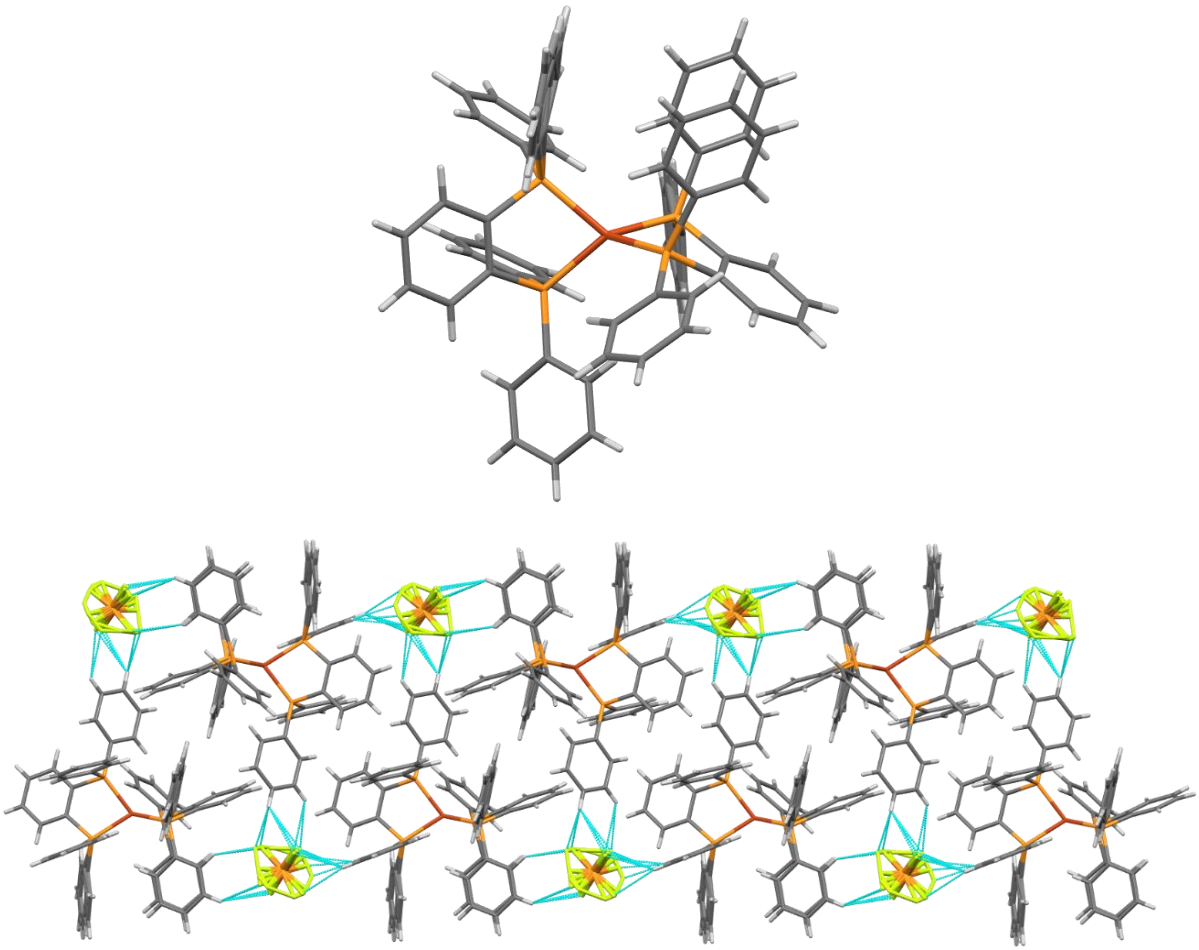


Figure S10. Top: X-ray structure of **Cu^{bz}**. The PF_6^- anion, solvent molecules, and hydrogen atoms are omitted for clarity. Bottom: View of the short contacts involving the cation and the PF_6^- anion in **Cu^{bz}**.

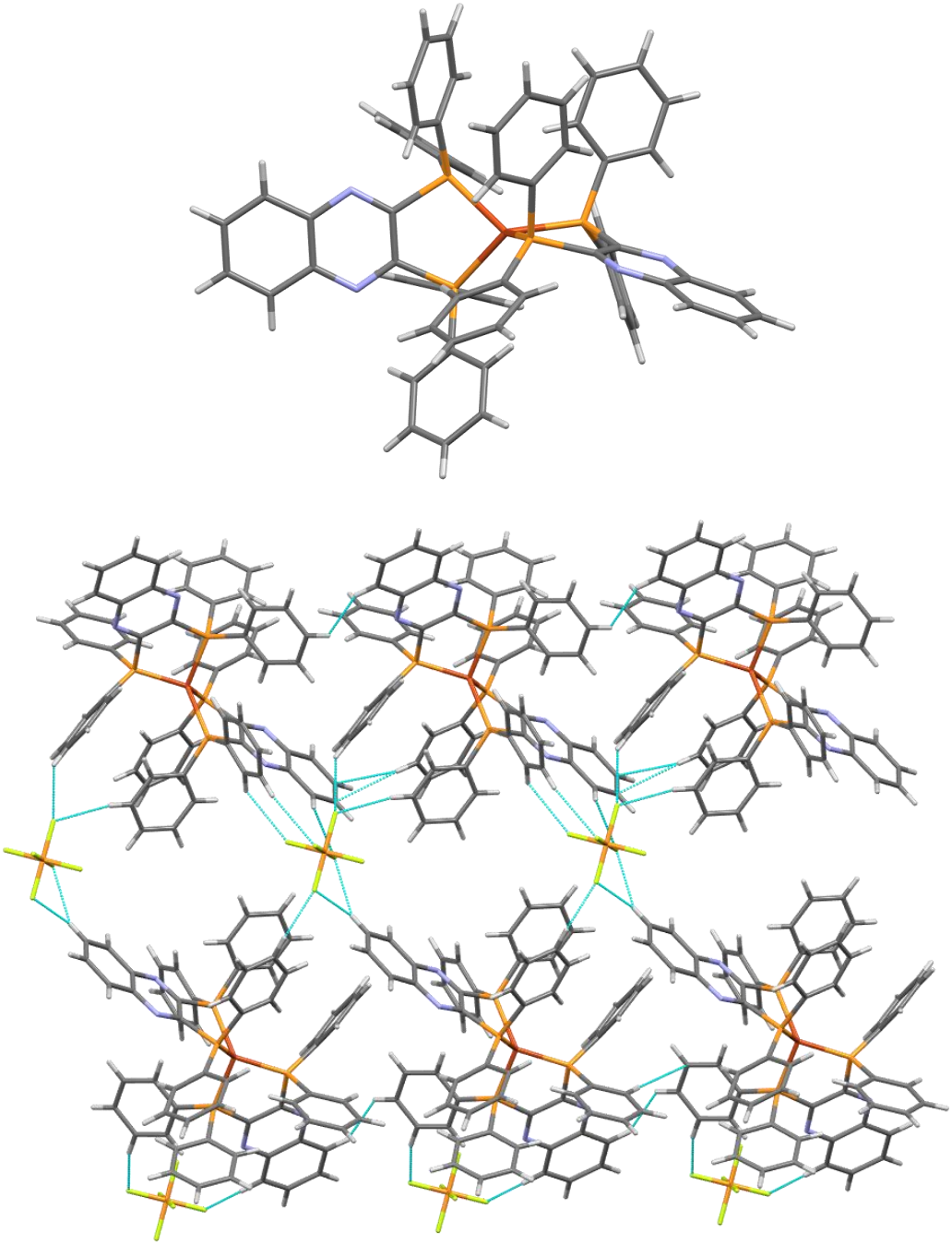


Figure S11. Top: X-ray structure of **Cu^{quinox}**. The PF_6^- anion, solvent molecules, and hydrogen atoms are omitted for clarity. Bottom: View of the short contacts involving the cation and the PF_6^- anion in **Cu^{quinox}**.

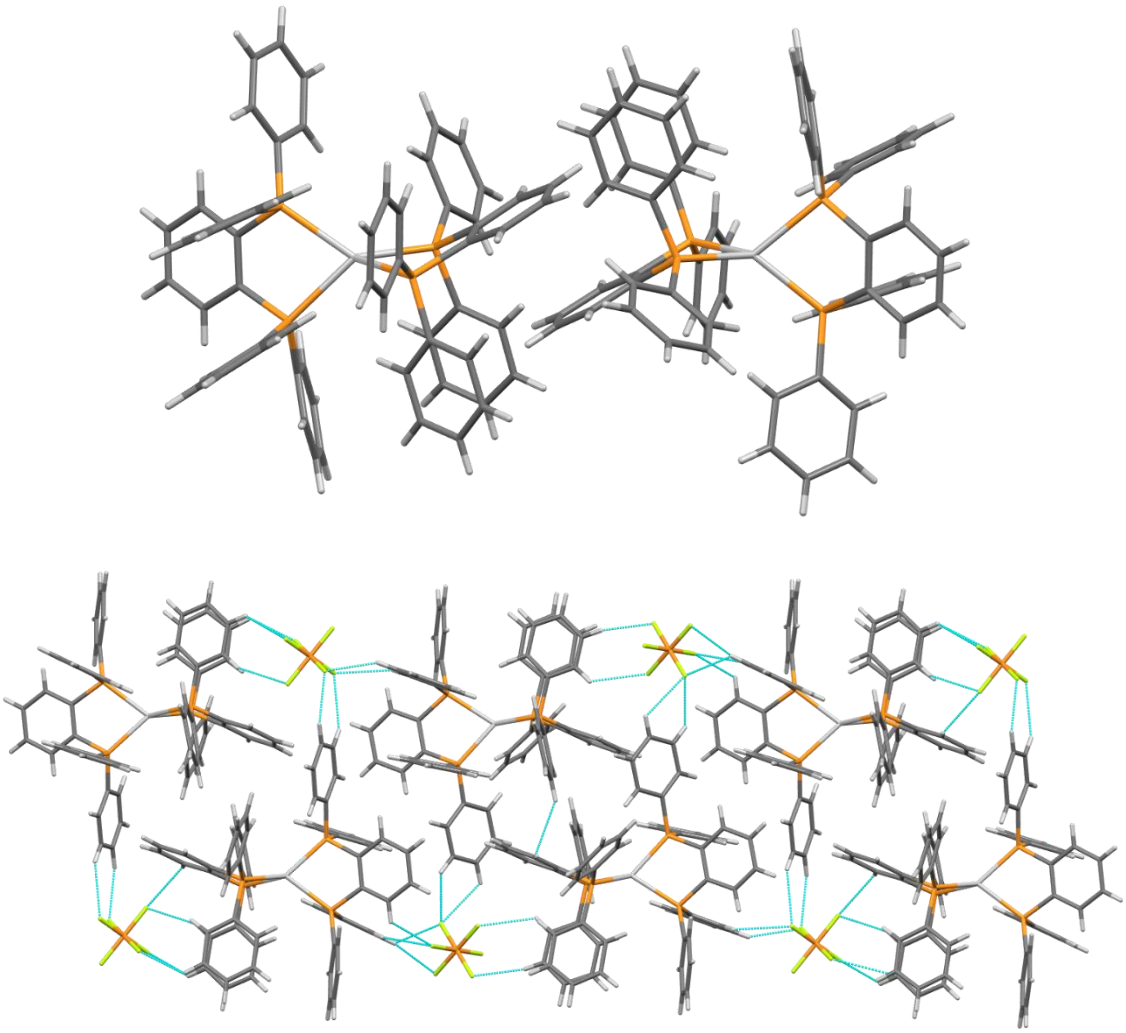


Figure S12. Top: X-ray structure of **Ag^{bz}**. The PF_6^- anion, solvent molecules, and hydrogen atoms are omitted for clarity. Bottom: View of the short contacts involving the cation and the PF_6^- anion in **Ag^{bz}**.

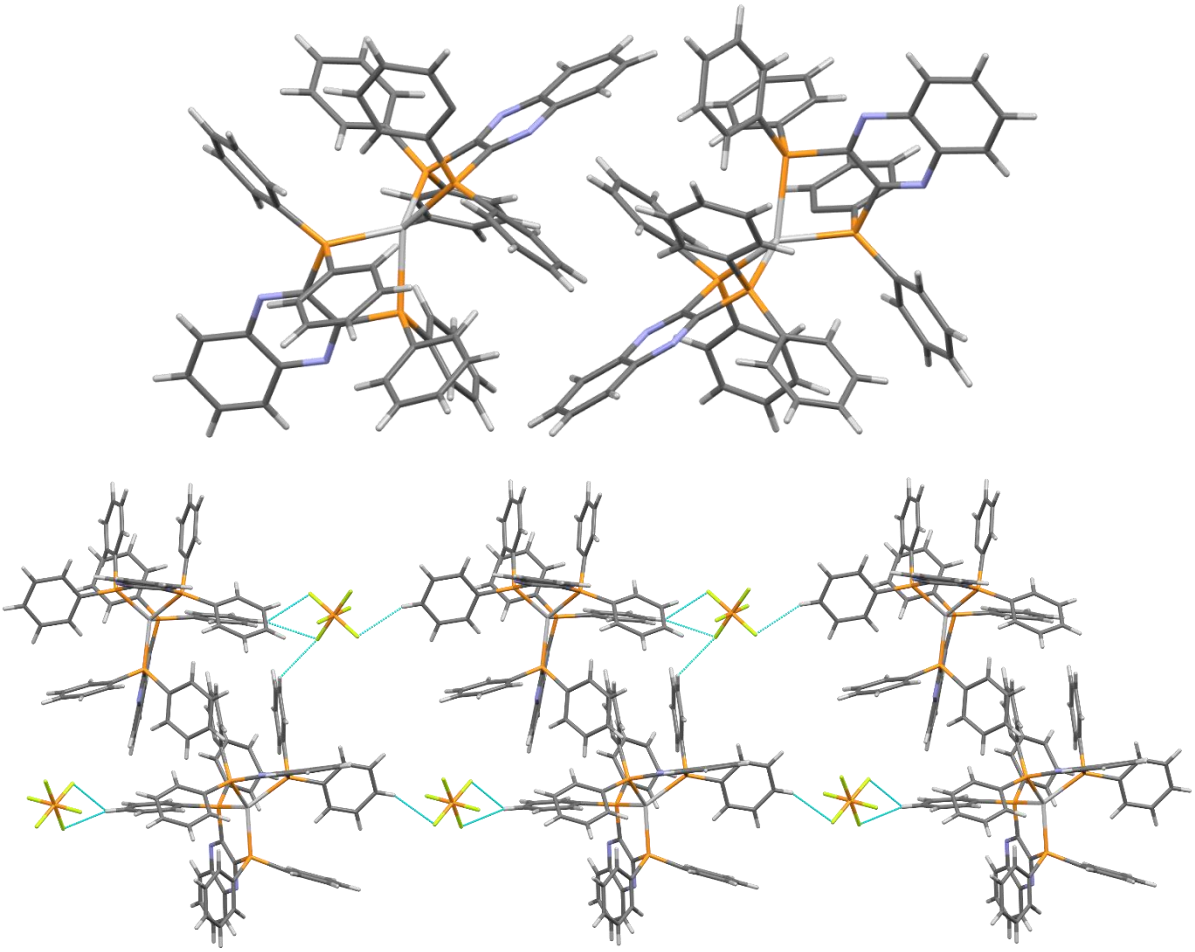


Figure S13. Top: X-ray structure of **Ag^{quinox}**. The PF_6^- anion, solvent molecules, and hydrogen atoms are omitted for clarity. Bottom: View of the short contacts involving the cation and the PF_6^- anion in **Ag^{quinox}**.

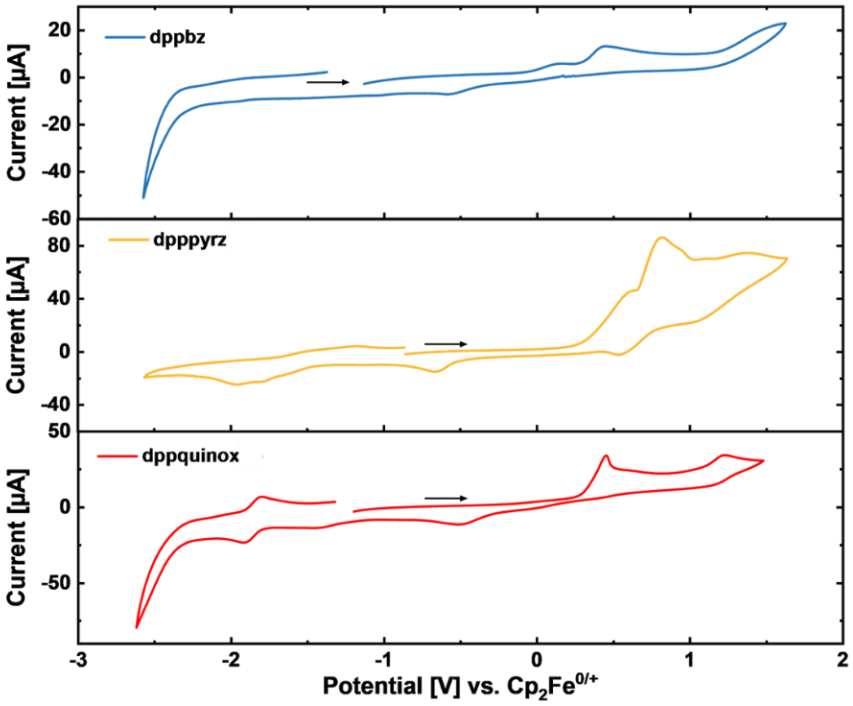


Figure S14. Cyclic voltammograms of the free ligands **dppbz** (blue), **dpppyrz** (yellow), **dppquinox** (red) in CH_3CN/NBu_4PF_6 (0.1 M) at room temperature using a Pt (WE), Pt (CE) and Ag wire (*quasi*-RE).

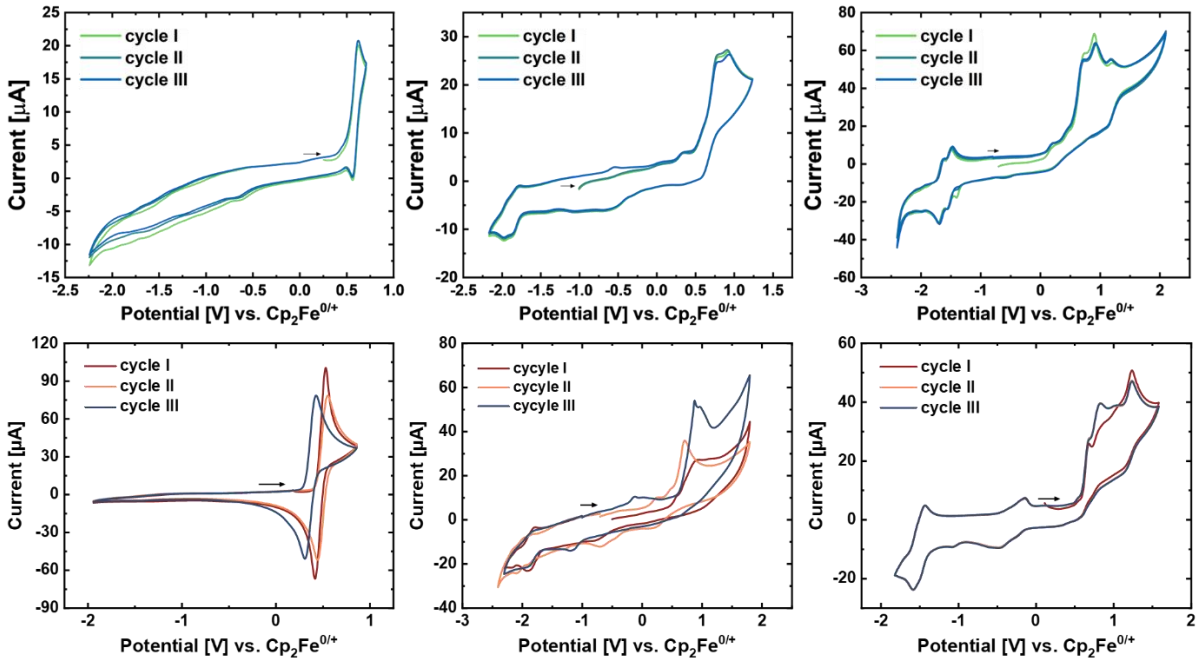


Figure S15. Top: Cyclic voltammograms of the first three cycles of **Cu^{bz}**, **Cu^{pyrz}** to **Cu^{quinox}** (from left to right). Bottom: Cyclic voltammograms of the first three cycles of **Ag^{bz}**, **Ag^{pyrz}** to **Ag^{quinox}** (from left to right). All measurements were performed in CH_3CN/NBu_4PF_6 (0.1 M) at room temperature using a Pt (WE), Pt (CE) and Ag wire (*quasi*-RE).

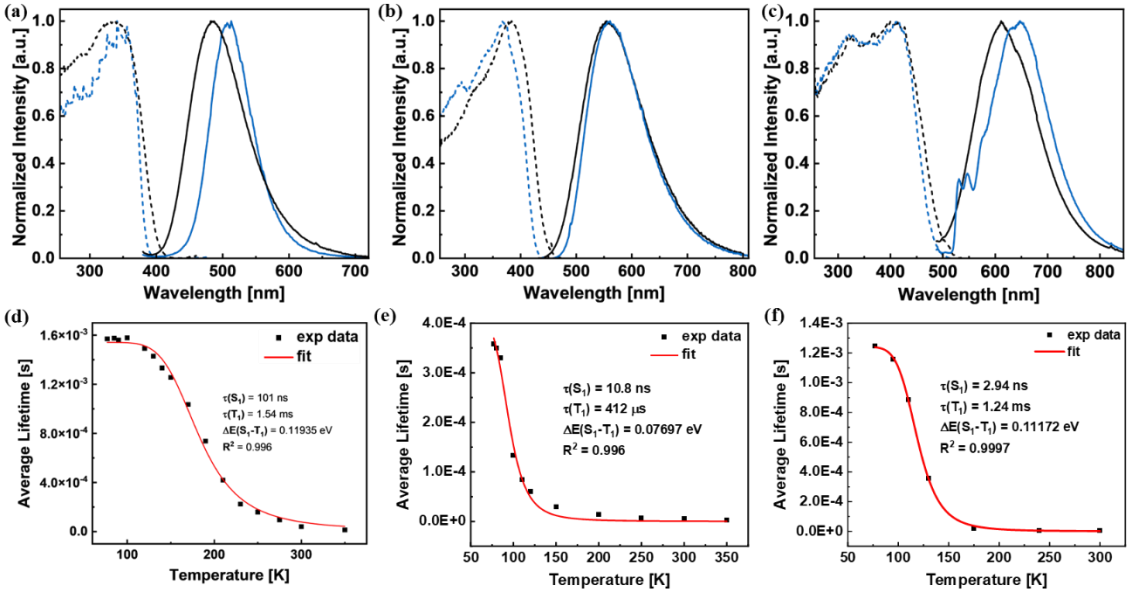


Figure S16. Excitation (dotted line) and emission (solid line) spectra of **Cu^{bz}** (a), **Cu^{pyrz}** (b), **Cu^{quinox}** (c) in the crystalline state at 298 K (black) and 77 K (blue). <τ> *vs.* T plots along the fitted equation (red) of **Cu^{bz}** (d), **Cu^{pyrz}** (e) and **Cu^{quinox}** (f) in the crystalline powder state.

Table S2. Vertical emission energies calculated at the equilibrium structure of S_1 (ΔE_{S1}, eV and nm) and T_1 (ΔE_{S1}, eV and nm), oscillator strengths and character of the states in terms of the weight of the largest singly excited configuration for the different complexes investigated with the ligands in tetrahedral-like arrangement obtained using TDDFT and the M06-2X/def2-TZVP level of theory.[a]

System	ΔE_{S1}	*f*	Character (%)	ΔE_{T1}	*f*	Character (%)
Cu^{bz}	2.97 (417)	0.022	H→L (95.4)	2.67 (465)	0.000	H→L (87.6)
Cu^{pyrz}	2.45 (505)	0.003	H→L (95.1)	2.33 (531)	0.000	H→L (90.9)
Cu^{quinox}	2.14 (579)	0.003	H→L (95.3)	2.03 (610)	0.000	H−3→L (51.8)
Ag^{bz}	2.84 (437)	0.019	H→L (95.8)	2.49 (498)	0.000	H→L (86.2)
Ag^{pyrz}	2.38 (521)	0.003	H→L (94.9)	2.12 (584)	0.000	H→L (91.9)
Ag^{quinox}	2.05 (603)	0.002	H→L (94.5)	2.03 (610)	0.000	H−3→L (40.8)

[a] H and L stand for highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), respectively.

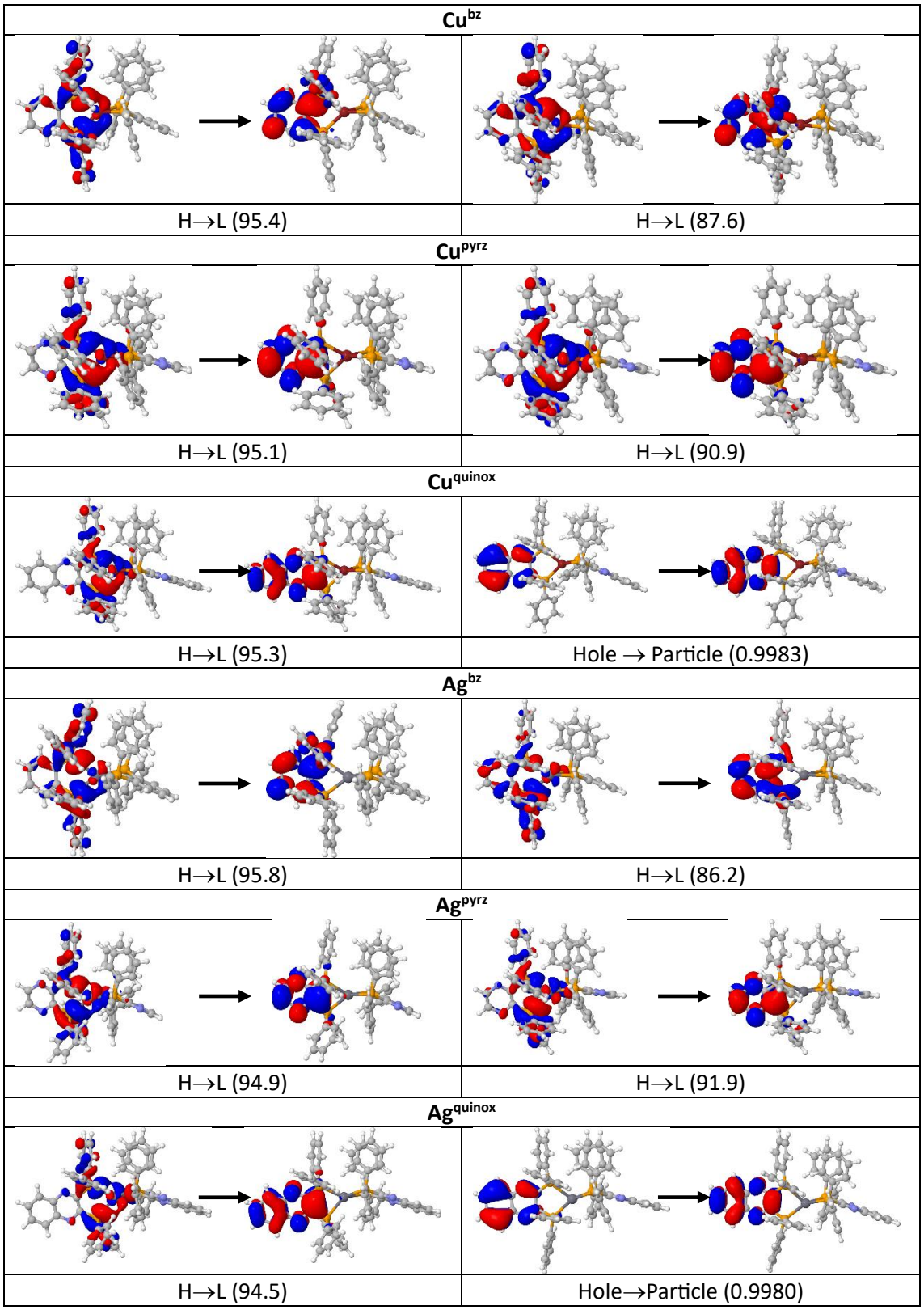


Figure S17. Canonical orbitals (cutoff 0.003) of the largest singly excited configuration of S_1 (left) and T_1 (right) obtained at the corresponding equilibrium structures for the different complexes investigated with the ligands in tetrahedral-like arrangement calculated using TDDFT and the M06-2X/def2-TZVP level of theory (H and L stand for highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), respectively, and the weight of the singly excited configuration is shown in parenthesis). For the T_1 states of

Cu^{quinox} and **Ag^{quinox}** we have used the hole and particle natural transition orbitals with the largest eigenvalue to characterize the state.

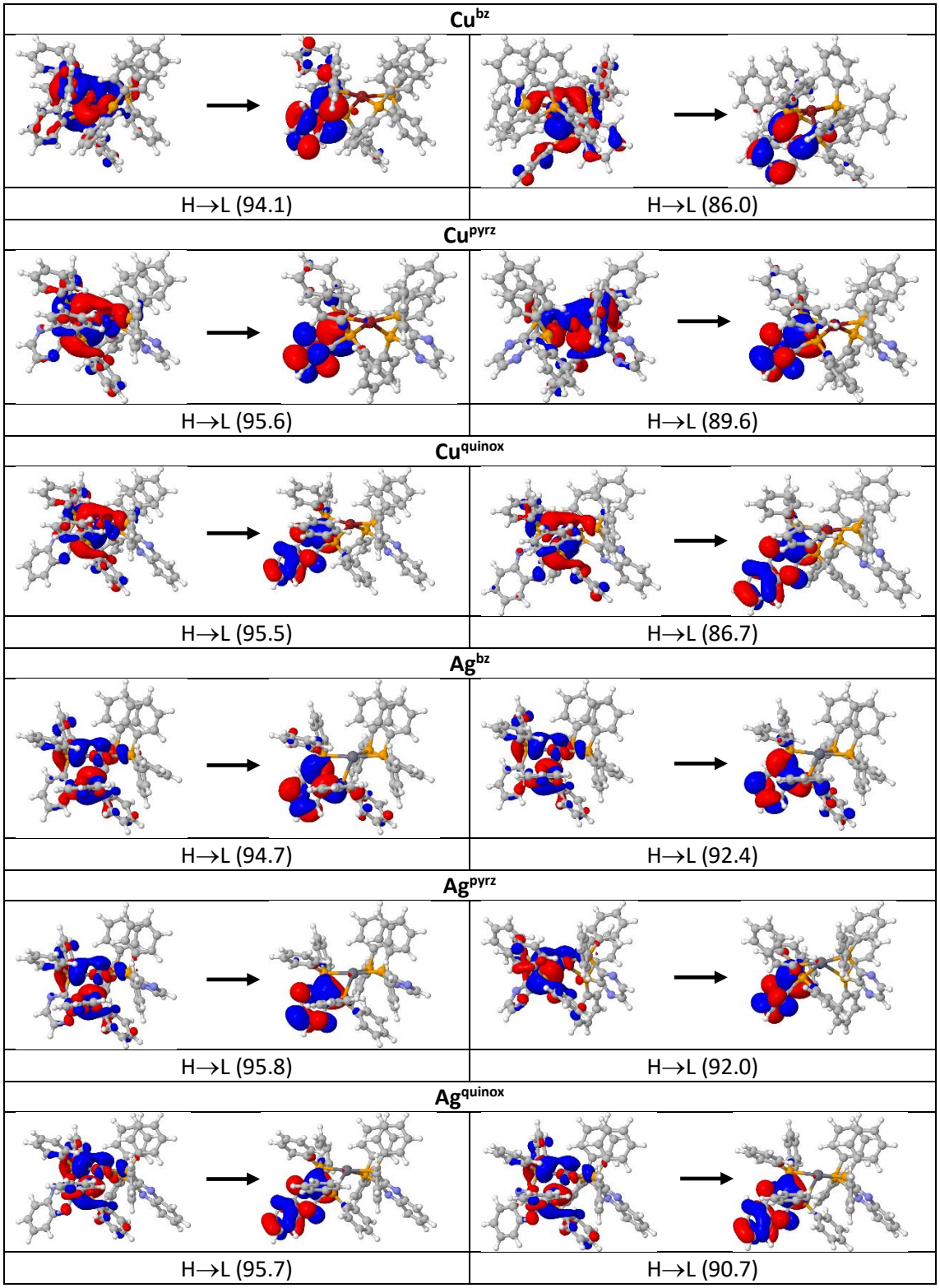


Figure S18. Canonical orbitals (cutoff 0.003) of the largest singly excited configuration of S_1 (left) and T_1 (right) obtained at the corresponding equilibrium structures for the different complexes investigated with the ligands in distorted tetrahedral arrangement calculated using TDDFT and the M06-2X/def2-TZVP level of theory (H and L stand for highest occupied

molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), respectively, , and the weight of the singly excited configuration is shown in parenthesis).

Table S3. Vertical emission energies calculated at the equilibrium structure of S1 (ΔE_{S1}, eV and nm) and T_1 (ΔE_{S1}, eV and nm), oscillator strengths and character of the states in terms of the weight of the largest singly excited configuration for the different complexes investigated with the ligands in distorted tetrahedral arrangement obtained using TDDFT and the M06-2X/def2-TZVP level of theory.[a]

System	ΔE_{S1}	*f*	Character (%)	ΔE_{T1}	*f*	Character (%)
Cu^{bz}	2.86 (434)	0.022	H→L (94.1)	2.50 (496)	0.000	H→L (86.0)
Cu^{pyrz}	2.29 (541)	0.001	H→L (95.6)	2.24 (554)	0.000	H→L (89.6)
Cu^{quinox}	1.97 (628)	0.002	H→L (95.5)	1.92 (647)	0.000	H→L (86.7)
Ag^{bz}	2.45 (507)	0.010	H→L (94.7)	2.32 (534)	0.000	H→L (92.4)
Ag^{pyrz}	2.22 (557)	0.001	H→L (95.8)	2.14 (580)	0.000	H→L (92.0)
Ag^{quinox}	1.91 (650)	0.002	H→L (95.7)	1.81 (686)	0.000	H→L (90.7)

[a] H and L stand for highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), respectively.

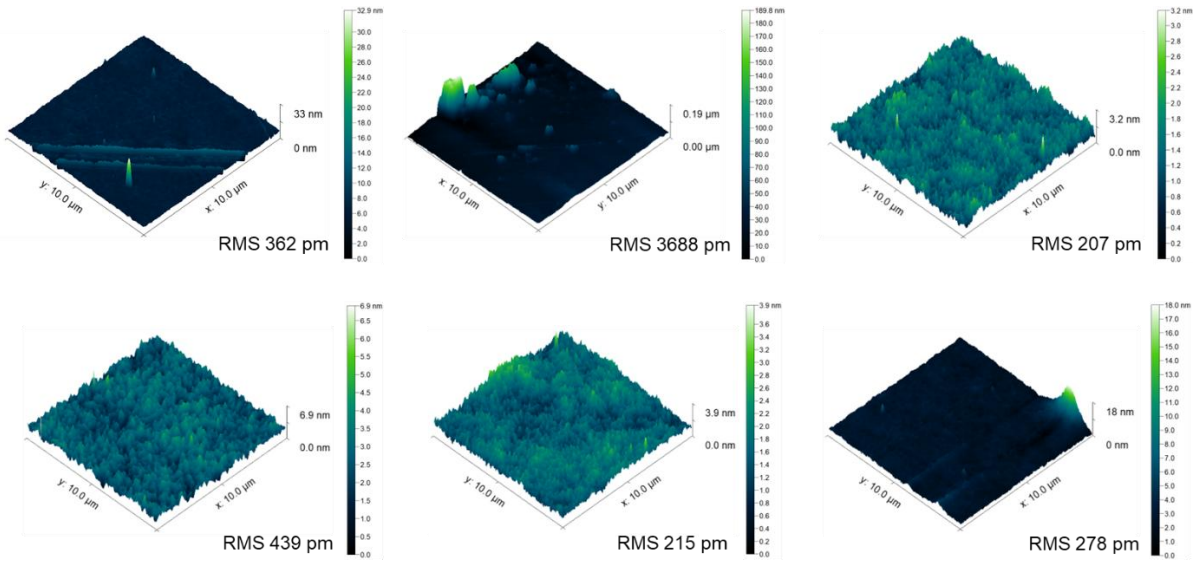


Figure S19. AFM images of **Cu^{bz}** (top left), **Ag^{bz}** (bottom left), **Cu^{pyrz}** (top middle), **Ag^{pyrz}** (bottom middle), **Cu^{quinox}** (top right) and **Ag^{quinox}** (bottom right) thin-films.

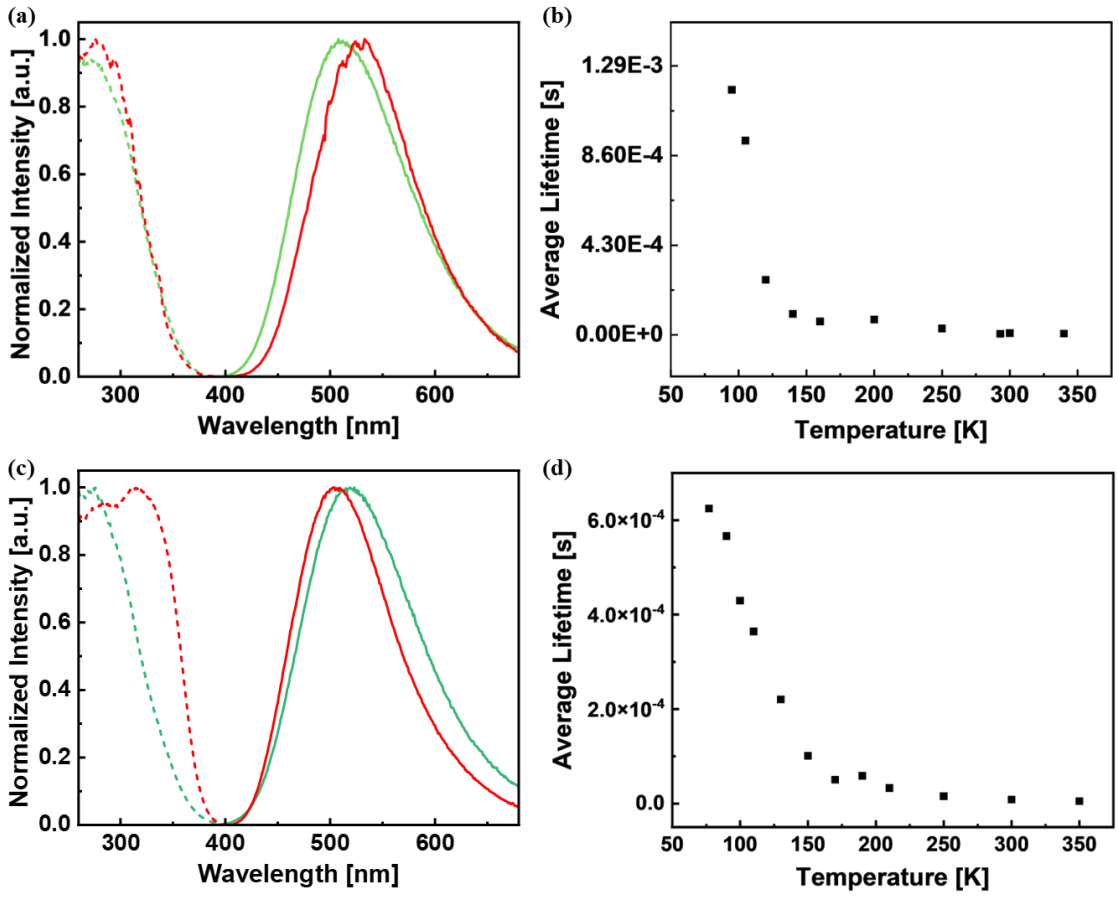


Figure S20. Excitation (dashed line) and emission (solid line) spectra of **Cu**^{bz} (a) and **Ag**^{bz} (c) in thin-film at 298 K (green) and at 77 K (red). <τ> vs. T plot **Cu**^{bz} (b) and **Ag**^{bz} (d) in thin-film.

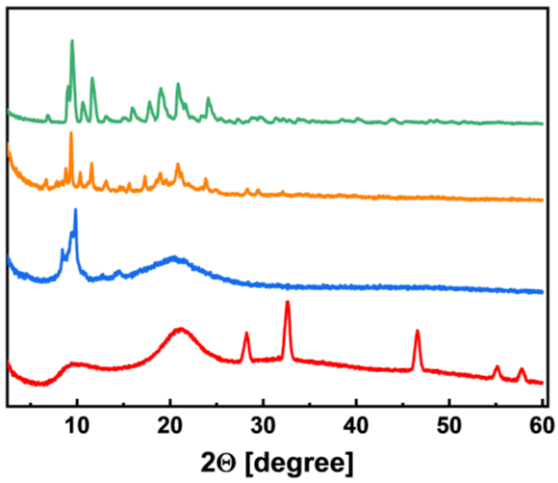


Figure S21. Powder X-ray diffraction pattern of **Cu**^{bz} (green), **Ag**^{bz} (orange), **Cu**^{pyrz} (blue) and **Ag**^{pyrz} (red) of the samples that were attempted to generate exclusively the amorphous powder.

Table S4. Absolute energies without including (E) and including (E+ZPE) the zero-point energy correction, internal energies (U), enthalpies (H) and Gibbs free energies (G) (in a.u.) evaluated at the ground state equilibrium structure for the different complexes investigated with the ligands in tetrahedral-like arrangement calculated at the M06-2X/def2-TZVP level of theory.[a]

System	E	E+ZPE	U	H	G
Cu^{bz}	-5320.964189	-5320.059205	-5320.001928	-5320.000983	-5320.154897
Cu^{pyrz}	-5385.106292	-5384.250859	-5384.193465	-5384.192521	-5384.349654
Cu^{quinox}	-5692.386482	-5691.436890	-5691.374305	-5691.373361	-5691.540799
Ag^{bz}	-3827.389471	-3826.485534	-3826.427727	-3826.426783	-3826.583848
Ag^{pyrz}	-3891.532096	-3890.677386	-3890.619702	-3890.618758	-3890.777201
Ag^{quinox}	-4198.812541	-4197.863515	-4197.800621	-4197.799677	-4197.968750

[a] The thermodynamic potentials were calculated at 298.15 K and 1 atm.

Table S5. In solution (acetonitrile, PCM model) absolute energies without including (E) and including (E+ZPE) the zero-point energy correction, internal energies (U), enthalpies (H) and Gibbs free energies (G) (in a.u.) evaluated at the ground state equilibrium structure for the different complexes investigated with the ligands in tetrahedral-like arrangement calculated at the M06-2X/def2-TZVP level of theory.[a]

System	E	E+ZPE	U	H	G
Cu^{bz}	-5321.011786	-5320.107899	-5320.050340	-5320.049396	-5320.205043
Cu^{pyrz}	-5385.160434	-5384.305488	-5384.247963	-5384.247019	-5384.404911
Cu^{quinox}	-5692.437680	-5691.488650	-5691.425993	-5691.425049	-5691.592458
Ag^{bz}	-3827.439288	-3826.535990	-3826.478163	-3826.477219	-3826.634110
Ag^{pyrz}	-3891.589353	-3890.734775	-3890.677203	-3890.676259	-3890.833250
Ag^{quinox}	-4198.867458	-4197.918707	-4197.855854	-4197.854910	-4198.023539

[a] The thermodynamic potentials were calculated at 298.15 K and 1 atm.

Table S6. Absolute energies without including (E) and including (E+ZPE) the zero-point energy correction, internal energies (U), enthalpies (H) and Gibbs free energies (G) (in a.u.) evaluated at the S_1 equilibrium structures for the different complexes investigated with the ligands in tetrahedral-like arrangement and calculated using TDDFT and the M06-2X/def2-TZVP level of theory.[a]

System	E	E+ZPE	U	H	G
Cu^{bz}	-5320.826778	-5319.925133	-5319.867206	-5319.866262	-5320.022629
Cu^{pyrz}	-5384.986607	-5384.133195	-5384.075652	-5384.074707	-5384.231529
Cu^{quinox}	-5692.279702	-5691.331520	-5691.268858	-5691.267914	-5691.435210
Ag^{bz}	-3827.254642	-3826.354082	-3826.295570	-3826.294626	-3826.454314
Ag^{pyrz}	-3891.414518	-3890.562298	-3890.504147	-3890.503203	-3890.663167
Ag^{quinox}	-4198.707396	-4197.760294	-4197.696948	-4197.696003	-4197.868000

[a] The thermodynamic potentials were calculated at 298.15 K and 1 atm.

Table S7. Absolute energies without including (E) and including (E+ZPE) the zero-point energy correction, internal energies (U), enthalpies (H) and Gibbs free energies (G) (in a.u.) evaluated at the T_1 equilibrium structures for the different complexes investigated with the ligands in tetrahedral-like arrangement and calculated using TDDFT and the M06-2X/def2-TZVP level of theory.[a]

System	E	E+ZPE	U	H	G
Cu^{bz}	-5320.834691	-5319.933905	-5319.875700	-5319.874756	-5320.032853
Cu^{pyrz}	-5384.991352	-5384.138415	-5384.080788	-5384.079844	-5384.236445
Cu^{quinox}	-5692.290274	-5691.346235	-5691.282855	-5691.281911	-5691.451610
Ag^{bz}	-3827.263549	-3826.363525	-3826.304874	-3826.303930	-3826.463866
Ag^{pyrz}	-3891.416944	-3890.565148	-3890.506913	-3890.505969	-3890.665538
Ag^{quinox}	-4198.716261	-4197.773427	-4197.709515	-4197.708571	-4197.881053

[a] The thermodynamic potentials were calculated at 298.15 K and 1 atm.

Table S8. Absolute energies without including (E) and including (E+ZPE) the zero-point energy correction, internal energies (U), enthalpies (H) and Gibbs free energies (G) (in a.u.) evaluated at the S_1 equilibrium structures for the different complexes investigated with the ligands in distorted tetrahedral arrangement and calculated using TDDFT and the M06-2X/def2-TZVP level of theory.[a]

System	E	E+ZPE	U	H	G
Cu^{bz}	-5320.835270	-5319.933978	-5319.876029	-5319.875085	-5320.031341
Cu^{pyrz}	-5384.991692	-5384.138337	-5384.080736	-5384.079791	-5384.236439
Cu^{quinox}	-5692.285970	-5691.337970	-5691.275202	-5691.274257	-5691.442226
Ag^{bz}	-3827.260740	-3826.359600	-3826.301287	-3826.300343	-3826.458048
Ag^{pyrz}	-3891.416767	-3890.564294	-3890.506280	-3890.505336	-3890.663753
Ag^{quinox}	-4198.710846	-4197.763302	-4197.700202	-4197.699258	-4197.868623

[a] The thermodynamic potentials were calculated at 298.15 K and 1 atm.

Table S9. Absolute energies without including (E) and including (E+ZPE) the zero-point energy correction, internal energies (U), enthalpies (H) and Gibbs free energies (G) (in a.u.) evaluated at the T_1 equilibrium structures for the different complexes investigated with the ligands in distorted tetrahedral arrangement and calculated using TDDFT and the M06-2X/def2-TZVP level of theory.[a]

System	E	E+ZPE	U	H	G
Cu^{bz}	-5320.844100	-5319.942750	-5319.884699	-5319.883755	-5320.039421
Cu^{pyrz}	-5384.997281	-5384.143648	-5384.086135	-5384.085191	-5384.240904
Cu^{quinox}	-5692.291909	-5691.345436	-5691.282318	-5691.281374	-5691.451012
Ag^{bz}	-3827.266230	-3826.365808	-3826.307255	-3826.306311	-3826.465915
Ag^{pyrz}	-3891.421923	-3890.569848	-3890.511722	-3890.510778	-3890.669379
Ag^{quinox}	-4198.716104	-4197.769836	-4197.706361	-4197.705417	-4197.769836

[a] The thermodynamic potentials were calculated at 298.15 K and 1 atm.

Table S10. Root mean square deviation of atomic positions (RMSD, in Å) between the tetrahedral-like (S_1 and T_1) and the distorted tetrahedral arrangement (S_1' and T_1') equilibrium structures for all the systems investigated calculated with respect to the corresponding ground state equilibrium structure.

System	RMSD (S_1)	RMSD (T_1)	RMSD (S_1')	RMSD (T_1')
Cu^{bz}	0.51650374	0.27502061	1.73699904	1.84389038
Cu^{pyrz}	0.65430573	0.64554732	1.72983681	1.79278462
Cu^{quinox}	1.47401604	0.12321897	1.91624296	1.78174255
Ag^{bz}	0.58423056	0.46605439	1.97320449	1.94024144
Ag^{pyrz}	1.36289237	0.96621427	2.09430779	2.10570923
Ag^{quinox}	1.32594572	0.14850569	2.23865505	2.28694646

Cartesian coordinates

In vacuo ground state equilibrium structures (cartesian coordinates, in Å) of the different complexes investigated calculated at the M06-2X/def2-TZVP theoretical level.

Cu^{bz}	X	Y	Z
Cu	-10.1495309010	8.0415786158	2.2946525139
P	-11.6803080342	7.0659891350	0.6747158417
P	-9.4830142067	9.3181433631	0.2499425978
P	-8.6401485492	7.0617709821	3.9319038575
P	-10.7884169566	9.3677810819	4.3166709569
C	-10.8187055713	7.1716911978	-0.9382013076
C	-11.1332561487	6.3053985974	-1.9836702934
C	-10.5122562125	6.4308321767	-3.2168957256
C	-9.5742601932	7.4326309506	-3.4209068061
C	-9.2522718390	8.3003198115	-2.3887049188
C	-9.8591899591	8.1793070400	-1.1391799558
C	-10.5934769319	10.7338740789	-0.0667909126
C	-10.6073181735	11.3867903951	-1.2997404514
C	-11.4884079367	12.4316348873	-1.5265291436
C	-12.3666864136	12.8328611858	-0.5253700495
C	-12.3602835612	12.1882433096	0.7018151545
C	-11.4743619736	11.1436044653	0.9299235912
C	-13.0759578133	8.2194535782	0.4764679120
C	-13.7637263109	8.5871244947	1.6329999336
C	-14.7858161667	9.5214103241	1.5781672439
C	-15.1226150933	10.1049128099	0.3629094694
C	-14.4406941306	9.7473223221	-0.7914046812
C	-13.4211186801	8.8059603051	-0.7387717949
C	-12.4047758271	5.4000419437	0.6753203780
C	-11.5406486536	4.3282321379	0.9067216210
C	-12.0238713687	3.0300553591	0.9095639465
C	-13.3777348895	2.7930093575	0.7000080424
C	-14.2414703516	3.8554488903	0.4800899518
C	-13.7583718863	5.1584848531	0.4623974296
C	-7.8203390413	9.9678347540	-0.1182828719
C	-7.5211653015	11.3121977109	0.0973709329
C	-6.2255731070	11.7806036782	-0.0851531653
C	-5.2194449515	10.9152274091	-0.4877269868
C	-5.5070071472	9.5703031941	-0.6907120421
C	-6.7955253104	9.0976262604	-0.4970118016
C	-9.4989449662	7.2143079971	5.5425577091
C	-9.2028369261	6.3599537074	6.6031334436
C	-9.8207009266	6.5203609928	7.8338714857
C	-10.7369066996	7.5455193739	8.0200988408
C	-11.0404194475	8.4016506995	6.9727626129
C	-10.4365340174	8.2456815783	5.7256390392
C	-9.6476006943	10.7645599224	4.6087578826
C	-9.6195036591	11.4386362306	5.8300268511
C	-8.7159590744	12.4679706952	6.0386430165
C	-7.8292805933	12.8323927876	5.0308343674
C	-7.8497635982	12.1665689232	3.8151827770
C	-8.7581310821	11.1375074451	3.6052489768
C	-7.2197837695	8.1880111856	4.1101720613
C	-6.5244880832	8.5204619365	2.9474959059
C	-5.4824067619	9.4332211157	2.9861528472
C	-5.1327759421	10.0304341251	4.1910847195

C	-5.8220095295	9.7079000623	5.3513663063
C	-6.8617381067	8.7880541170	5.3150317011
C	-7.9519903859	5.3807428635	3.9606326398
C	-8.8392739007	4.3240292841	3.7482002054
C	-8.3843469869	3.0158200968	3.7682944561
C	-7.0358678153	2.7531726582	3.9820142295
C	-6.1491870389	3.8003266165	4.1831201978
C	-6.6038793818	5.1136548795	4.1777919503
C	-12.4366134215	10.0595289896	4.6732239362
C	-12.7067846728	11.4060573379	4.4340656411
C	-13.9919329360	11.9054062555	4.6081879272
C	-15.0163993430	11.0690891429	5.0256566928
C	-14.7578525935	9.7220306171	5.2521596158
C	-13.4798657645	9.2183728506	5.0669500980
H	-11.8695826750	5.5260641133	-1.8314827902
H	-10.7636851518	5.7482529085	-4.0179507120
H	-9.0897300051	7.5381327026	-4.3826924326
H	-8.5103719004	9.0711706669	-2.5553598665
H	-9.9280497215	11.0776347170	-2.0854893399
H	-11.4930430017	12.9335234657	-2.4852483468
H	-13.0569126044	13.6463364434	-0.7078498553
H	-13.0506455314	12.4820516978	1.4826998616
H	-11.4920308831	10.6297563606	1.8835935562
H	-13.4906200409	8.1470263368	2.5857469068
H	-15.3047454123	9.8009066480	2.4859673694
H	-15.9119553556	10.8441604224	0.3174423702
H	-14.6961112386	10.2065713354	-1.7374505043
H	-12.8864129296	8.5455284874	-1.6437885647
H	-10.4839379429	4.5124073228	1.0731680920
H	-11.3467989613	2.2026241077	1.0777266704
H	-13.7571918180	1.7797376474	0.7088889426
H	-15.2952425954	3.6725404979	0.3157322127
H	-14.4356397090	5.9838615183	0.2812065717
H	-8.3032454587	12.0014869136	0.3939674181
H	-6.0088103329	12.8291775212	0.0734011683
H	-4.2145513848	11.2848515222	-0.6444386573
H	-4.7264169976	8.8883708764	-1.0023090557
H	-7.0088832951	8.0465425501	-0.6578274109
H	-8.4834656806	5.5624176918	6.4647585446
H	-9.5838148229	5.8467262197	8.6468421961
H	-11.2188300893	7.6782983335	8.9798136118
H	-11.7655398014	9.1910791813	7.1257447295
H	-10.3052540481	11.1581632178	6.6208932187
H	-8.7003626886	12.9864411921	6.9883809328
H	-7.1215773182	13.6338086374	5.1991798665
H	-7.1532968013	12.4315629450	3.0294248699
H	-8.7516872639	10.6067016028	2.6607688315
H	-6.8072868312	8.0698093185	2.0025408759
H	-4.9577569314	9.6855268632	2.0736892349
H	-4.3276090176	10.7531034929	4.2237446984
H	-5.5565029777	10.1779714366	6.2892839746
H	-7.4017397895	8.5551042299	6.2243841646
H	-9.8918029854	4.5281301140	3.5785264486
H	-9.0792887645	2.2004448800	3.6147810437
H	-6.6785032591	1.7319012531	3.9910507718
H	-5.0995711260	3.5975085552	4.3506814872

H	-5.9087868547	5.9272057048	4.3443670645
H	-11.9101003136	12.0730438190	4.1255810858
H	-14.1860698662	12.9554832484	4.4313217034
H	-16.0130590723	11.4629693073	5.1757160430
H	-15.5528955616	9.0626324453	5.5754969925
H	-13.2891754766	8.1659063831	5.2461554056

Cu^{pyrz}	X	Y	Z
Cu	9.3380231870	13.8138206249	9.4067859560
P	8.2681943986	15.7145761535	10.6291422430
P	9.8562168206	15.5738145078	7.8046076126
P	10.7600286856	12.0956675272	10.3860231789
P	7.8319882439	11.8575030969	9.0114520602
N	9.1988029469	18.3083302654	10.7524859736
N	10.5697174766	18.1675471694	8.3432872204
N	11.1275871217	9.5252666953	9.5002264654
N	8.6175925922	9.3007807451	8.3370411596
C	9.2159411907	17.1851409008	10.0377218791
C	9.9000237931	17.1172399654	8.8142191439
C	10.5630799749	19.2731504708	9.0713239121
C	9.8685914146	19.3464556457	10.2765098357
C	6.6031489627	16.1174623922	10.0053627619
C	5.9879603969	15.2646624183	9.0939255602
C	4.7420283772	15.5810442090	8.5685278683
C	4.1066780941	16.7504317172	8.9569612458
C	4.7159141224	17.6064187605	9.8692733272
C	5.9602037788	17.2947594456	10.3924938874
C	8.1487473945	15.9536663865	12.4274958228
C	6.9812200773	15.5887428340	13.0959081781
C	6.9129934597	15.6714273649	14.4807266794
C	8.0066240988	16.1191948120	15.2073491542
C	9.1779162732	16.4700800551	14.5467788708
C	9.2524597239	16.3810052372	13.1653116388
C	8.3809145361	15.8313605173	6.7725642396
C	7.7639046108	17.0692190197	6.6043016326
C	6.5845393182	17.1638160834	5.8780551986
C	6.0192374063	16.0295469646	5.3120153562
C	6.6356938520	14.7938135650	5.4649351531
C	7.8096537684	14.6975402735	6.1949518214
C	11.2992557470	15.7499553342	6.7254506407
C	11.2048622025	16.1393122993	5.3940694509
C	12.3549874462	16.2448743057	4.6232076347
C	13.5963583568	15.9732241487	5.1797754858
C	13.6933440705	15.5880228276	6.5114826155
C	12.5472102685	15.4669682019	7.2802116096
C	10.2684834999	10.5425939183	9.5201491702
C	9.0035045035	10.4326559084	8.9224175729
C	9.4792341036	8.2956926233	8.3213152484
C	10.7417941143	8.4112063408	8.8981680859
C	6.8581929131	11.3976910642	10.4825372193
C	6.8554554187	12.2371867608	11.5923482723
C	6.1614790421	11.8789525185	12.7406300935
C	5.4651100098	10.6808076464	12.7798317869
C	5.4626268767	9.8378837315	11.6727327313
C	6.1567225718	10.1913626382	10.5271187871

C	6.6978179150	11.5913609856	7.6156253124
C	5.3462019788	11.9019558230	7.7560907087
C	4.4881585597	11.7992819656	6.6686935543
C	4.9711843061	11.3854992962	5.4358214857
C	6.3207459657	11.0889802575	5.2869642557
C	7.1817222836	11.1982482821	6.3680395312
C	10.1722120906	11.7935892987	12.0804762329
C	9.9999849492	12.9113580806	12.8968421997
C	9.4749135941	12.7784218352	14.1723820360
C	9.1114141503	11.5215502492	14.6399101452
C	9.2855493804	10.4032453737	13.8364150242
C	9.8172701827	10.5347653688	12.5607735729
C	12.5670856355	11.9896585096	10.4216550758
C	13.2803494577	11.6134951644	11.5542805453
C	14.6673105760	11.5626754155	11.5105430659
C	15.3412259794	11.8758111045	10.3390698128
C	14.6300413746	12.2479203164	9.2046189586
C	13.2469563475	12.3144015715	9.2479651843
H	11.1173705384	20.1228047911	8.6904752473
H	9.8561903313	20.2577639898	10.8626898091
H	6.4882143904	14.3597476673	8.7710860470
H	4.2811790468	14.9136882370	7.8508541490
H	3.1352700625	17.0003225799	8.5503357695
H	4.2184321911	18.5185750659	10.1716591598
H	6.4379389225	17.9612569641	11.1016824094
H	6.1147783703	15.2563079961	12.5354912044
H	5.9968673472	15.3992870893	14.9888099567
H	7.9477223732	16.1976132670	16.2850300017
H	10.0338404810	16.8209747188	15.1084136739
H	10.1684425671	16.6648510581	12.6615963286
H	8.1944909960	17.9612046168	7.0412854053
H	6.1047751774	18.1264180399	5.7592959807
H	5.0954181831	16.1081561145	4.7535099425
H	6.2006850161	13.9016207652	5.0328113732
H	8.2775801963	13.7286741495	6.3291919140
H	10.2384619788	16.3612521556	4.9591016550
H	12.2798142588	16.5461501358	3.5867160902
H	14.4901186376	16.0609085651	4.5761076639
H	14.6608163761	15.3792423142	6.9492984564
H	12.6237015511	15.1586337840	8.3181780546
H	9.1637065461	7.3773179084	7.8404057348
H	11.4468894161	7.5887196494	8.8746636792
H	7.4142629210	13.1649726763	11.5751060487
H	6.1786222342	12.5367566549	13.6007473386
H	4.9224174473	10.3982508301	13.6726193210
H	4.9182549484	8.9032292964	11.7049013769
H	6.1582030917	9.5351820556	9.6640875366
H	4.9555100962	12.2072916258	8.7201608025
H	3.4376833573	12.0290105375	6.7920732276
H	4.2992762291	11.2913055674	4.5928020080
H	6.7029063392	10.7647733405	4.3277925821
H	8.2299970564	10.9567670860	6.2410431775
H	10.2641288250	13.8960157119	12.5275800109
H	9.3381474090	13.6582702517	14.7881198606
H	8.6890466580	11.4138923269	15.6306497296
H	9.0025390400	9.4241900074	14.2000572557

H	9.9476030243	9.6548910505	11.9436572638
H	12.7570980682	11.3592942072	12.4675019337
H	15.2211504137	11.2716049484	12.3933069486
H	16.4219484071	11.8307301349	10.3087779583
H	15.1530197455	12.4889859297	8.2882916874
H	12.6930527638	12.6125621484	8.3633260820

Cu^{quinox}	X	Y	Z
Cu	8.4066083962	9.9557221734	4.3966361811
P	8.0998200806	8.9894610597	2.1853075176
P	10.1665906703	11.2550693884	3.2108460124
P	8.7133422975	8.9896661389	6.6080491891
P	6.6466340322	11.2552251691	5.5822899068
N	10.1139995779	8.2231390676	0.5035327985
N	11.8902788789	10.2066775390	1.3527131721
N	6.6991342263	8.2235444633	8.2898790131
N	4.9228837260	10.2070114061	7.4404709139
C	9.7844073571	9.0748881223	1.4339059913
C	10.7023914434	10.0898323442	1.8777176606
C	12.2515125961	9.3261529136	0.3858364861
C	11.3546695179	8.3156491829	-0.0374954169
C	11.7530456924	7.4013194874	-1.0379446255
C	12.9983473417	7.5070124355	-1.5885049273
C	13.8938919029	8.5199910599	-1.1678294785
C	13.5342200372	9.4139448961	-0.2000074000
C	7.4593599429	7.3589261859	1.7313110357
C	7.2012944223	6.4498969468	2.7538445520
C	6.7046617148	5.1871616439	2.4581148951
C	6.4578242940	4.8368222605	1.1396655628
C	6.7016934915	5.7464089311	0.1159557571
C	7.2003045458	7.0047238459	0.4075420861
C	7.1759921355	10.1812209428	1.1620372693
C	5.9270225273	10.5733801026	1.6426559142
C	5.1747379976	11.5169503604	0.9624251185
C	5.6718448669	12.0837232802	-0.2047453695
C	6.9141279835	11.6995385504	-0.6891066748
C	7.6663800727	10.7489961567	-0.0114268742
C	11.7194346519	11.9018403622	3.9001197391
C	12.7788778298	11.0442515048	4.1966284341
C	13.9153607070	11.5291223315	4.8246909062
C	14.0022443806	12.8718585081	5.1737708525
C	12.9447900756	13.7255662131	4.8977450484
C	11.8065703522	13.2446093564	4.2628817334
C	9.5003051802	12.6428989233	2.2343861512
C	10.2660951548	13.2403199569	1.2323409149
C	9.7361561519	14.2789487030	0.4838408955
C	8.4427479905	14.7276690775	0.7303221215
C	7.6783718327	14.1368839509	1.7250719528
C	8.2069257636	13.0960028271	2.4763196831
C	7.0287484716	9.0751986723	7.3594268342
C	6.1107819019	10.0901097834	6.9155031043
C	4.5616250086	9.3265804118	8.4074240018
C	5.4584560734	8.3161176866	8.8308773192
C	5.0600567330	7.4018918174	9.8314119155
C	3.8147433295	7.5076431343	10.3819343477

C	2.9192085478	8.5205780163	9.9611333363
C	3.2789034975	9.4144324674	8.9932279254
C	9.3537424258	7.3591454535	7.0621771949
C	9.6117455406	6.4500129805	6.0397200043
C	10.1083266943	5.1872813519	6.3355518717
C	10.3551779324	4.8370493215	7.6540274507
C	10.1113724707	5.7467393034	8.6776602833
C	9.6128104981	7.0050501819	8.3859721849
C	9.6372060410	10.1814686359	7.6312358142
C	10.8861983839	10.5735370446	7.1506018718
C	11.6385195773	11.5171194685	7.8307744924
C	11.1414298921	12.0839935363	8.9979031573
C	9.8991221519	11.6999026262	9.4822766441
C	9.1468303851	10.7493521666	8.8046526423
C	5.0938249160	11.9020289935	4.8929670265
C	4.0343258692	11.0444855115	4.5965268280
C	2.8978704639	11.5293828875	3.9684344495
C	2.8110703348	12.8720981053	3.6192540072
C	3.8685811460	13.7257588354	3.8952097036
C	5.0067728599	13.2447762319	4.5301037097
C	7.3129740385	12.6430899146	6.5586647279
C	6.5472113473	13.2405823134	7.5606880649
C	7.0771848724	14.2792358674	8.3091287389
C	8.3706010406	14.7279115423	8.0626082209
C	9.1349500032	14.1370571139	7.0678785700
C	8.6063613613	13.0961499177	6.3166906791
H	11.0498984317	6.6368407990	-1.3405308169
H	13.3108249636	6.8114571256	-2.3560447822
H	14.8740423297	8.5802204625	-1.6219619988
H	14.2001754532	10.1953003777	0.1412741123
H	7.3764936866	6.7348106329	3.7853610957
H	6.5043914777	4.4847918749	3.2563981994
H	6.0659681404	3.8554332697	0.9060461790
H	6.4991960850	5.4721656502	-0.9109670215
H	7.3877272002	7.7146000293	-0.3879959057
H	5.5417647140	10.1426813767	2.5597860847
H	4.2098964816	11.8134218387	1.3539088487
H	5.0925656175	12.8288619919	-0.7345986215
H	7.3045331334	12.1433512239	-1.5956006477
H	8.6361878983	10.4628652393	-0.3996766135
H	12.7252105306	9.9972942661	3.9239959782
H	14.7379607914	10.8586237129	5.0367383485
H	14.8936933299	13.2496169411	5.6572771739
H	13.0074303134	14.7728128707	5.1637859421
H	10.9927629858	13.9235823104	4.0354475778
H	11.2746466477	12.8894479340	1.0442678063
H	10.3314291431	14.7412088085	-0.2927045702
H	8.0323458983	15.5378212923	0.1414579221
H	6.6659633496	14.4714398375	1.9130884935
H	7.5972586348	12.6222622975	3.2370640920
H	5.7631962344	6.6374434113	10.1340924233
H	3.5022477166	6.8121673694	11.1495389568
H	1.9390470248	8.5808540505	10.4152358759
H	2.6129568990	10.1957538825	8.6518508487
H	9.4365384633	6.7348436088	5.0081817799
H	10.3085476037	4.4848306821	5.5373273552

H	10.7469951092	3.8556638526	7.8877269961
H	10.3138816648	5.4725794282	9.7046030360
H	9.4254370137	7.7150059442	9.1814507588
H	11.2714481810	10.1427553561	6.2335076549
H	12.6033778278	11.8135195405	7.4392783297
H	11.7207416297	12.8291363966	9.5277147498
H	9.5087295074	12.1437935568	10.3887378691
H	8.1770041797	10.4632949228	9.1929105939
H	4.0879264894	9.9975459970	4.8692384123
H	2.0752263811	10.8589210178	3.7564410660
H	1.9196430085	13.2498769366	3.1357236380
H	3.8060077557	14.7729894679	3.6290901272
H	5.8206242759	13.9237151852	4.7574834547
H	5.5386533234	12.8897455148	7.7487915360
H	6.4819326572	14.7415501736	9.0856579617
H	8.7810308407	15.5380828111	8.6514269671
H	10.1473634420	14.4715798987	6.8798310229
H	9.2160068833	12.6223577674	5.5559608874

Ag^{bz}	X	Y	Z
Ag	10.3387128185	4.2021417609	9.2649623762
P	8.5451283799	2.5531219829	10.1830349939
P	8.3988660926	4.0887709608	7.3328833682
P	10.7211573339	6.7857562793	10.0940402618
P	12.8652038581	4.6886883024	8.8659011345
C	13.3908754710	5.9033620382	10.1363829030
C	8.7351044944	1.2233251072	11.4057653692
C	6.9608131616	5.1626094950	7.6742332365
C	7.2179355407	3.6176978061	10.8330170395
C	7.5893123928	4.6459314683	11.6991646473
C	8.6944052605	4.2958176757	5.5463664665
C	7.7699502569	1.7342083128	8.7358440473
C	12.9201844460	5.6419882022	7.3149525479
C	7.7008574079	2.3977987054	7.4947551272
C	12.4639989472	6.8195054003	10.6721141846
C	16.2870367135	2.6944631471	7.7720773244
C	9.7793851342	7.6036788295	11.4229219517
C	8.0159535537	-0.0406446574	13.3254338538
C	6.6385700724	5.5189347451	12.2045854390
C	13.5728353007	6.8668338595	7.1929499049
C	12.2270839269	5.1239998884	6.2210175173
C	14.7150455246	5.9416384261	10.5713210263
C	4.7871568296	6.8045638120	8.2574860251
C	7.0838173871	1.7598482056	6.4191246146
C	5.7413006636	4.9746707951	7.0226704510
C	10.1918174219	7.6356311156	7.4937242043
C	8.3087695844	5.4570616847	4.8794814691
C	10.7156580104	8.0015465604	8.7304156511
C	12.8983595868	7.7472119776	11.6183652917
C	9.9324561348	7.1683047081	12.7419445429
C	5.8800064335	3.4798337793	10.4696688179
C	9.8540000936	0.3976719881	11.2931626922
C	11.2455484268	10.1790695144	7.8390496216
C	15.2473557868	3.6151643275	7.7911148234
C	9.4263865117	3.3274340763	4.8540955837

C	9.1222615283	-0.8683553762	13.1995665583
C	7.2281335381	0.4550275984	8.8549727515
C	9.3217558507	4.6516308142	2.8482446373
C	8.8209138912	8.5742838800	11.1379735686
C	15.3474510580	1.5813427213	9.6859091596
C	9.1734038355	7.7247209376	13.7589681848
C	10.7161916705	9.8063865153	6.6082649849
C	14.2509753642	3.5191804894	8.7591019030
C	15.1277371684	6.8668118261	11.5184191143
C	14.2186464181	7.7733816255	12.0408259130
C	6.5491114320	0.4876533033	6.5530177309
C	5.3063129520	5.3744300814	11.8389745950
C	4.9294964693	4.3584960723	10.9713198412
C	7.0768073754	6.1754616814	8.6220652236
C	10.0414528199	-0.6500408063	12.1806186772
C	5.9935534125	6.9939738903	8.9135116907
C	12.8475729060	7.0324796925	4.9038082410
C	14.3013665116	2.4901516645	9.6997776312
C	11.2466773755	9.2814570479	8.8944627599
C	8.2321326913	8.7069016195	13.4696115357
C	7.8177166366	1.0021232380	12.4297065595
C	8.6241259951	5.6322665676	3.5367648010
C	6.6242747540	-0.1669261817	7.7724840855
C	8.0508142253	9.1203390785	12.1586622901
C	16.3406955860	1.6822719550	8.7194183034
C	4.6609664598	5.7923714585	7.3122433425
C	12.1933215656	5.8125263143	5.0184014024
C	10.1921706793	8.5347082637	6.4354225185
C	13.5331699076	7.5587085968	5.9900760132
C	9.7267204987	3.4985800926	3.5122294443
H	8.6846745791	8.9202394744	10.1202117466
H	7.3188641057	9.8831459678	11.9262761096
H	7.6434145696	9.1449640397	14.2648556508
H	9.3164167326	7.3926845661	14.7790714003
H	10.6655049419	6.4043506305	12.9781621915
H	8.6314060116	4.7727321531	11.9743092137
H	6.9442950897	6.3164503871	12.8695525597
H	4.5623822001	6.0610086906	12.2223219835
H	3.8935642699	4.2519531859	10.6768595927
H	5.5787498567	2.6974317652	9.7835445197
H	6.9503308190	1.6427441650	12.5297905331
H	7.3018893400	-0.2066633593	14.1213091600
H	9.2724288721	-1.6809040476	13.8981673819
H	10.9075519218	-1.2913483577	12.0837732938
H	10.5779738114	0.5758069854	10.5050120398
H	7.2802450423	-0.0637102943	9.8035909047
H	6.2128422368	-1.1612993273	7.8852801184
H	6.0771614959	0.0103949124	5.7042549277
H	7.0291326658	2.2580921504	5.4593917024
H	5.6350099946	4.1857535328	6.2873987896
H	3.7187977389	5.6406555837	6.8019349359
H	3.9406118877	7.4398064250	8.4840632261
H	6.0954014019	7.7670135762	9.6647982482
H	8.0092815068	6.3150308606	9.1573930318
H	7.7451589040	6.2211137563	5.4016442300
H	8.3073694970	6.5327848640	3.0265086761

H	9.5518306544	4.7824106953	1.7990245114
H	10.2767631087	2.7313843184	2.9829142686
H	9.7448505950	2.4236176026	5.3625068349
H	15.2123574066	4.4058730007	7.0519756791
H	17.0573259478	2.7713572473	7.0160288880
H	17.1532218848	0.9678871094	8.7025934993
H	15.3847771310	0.7896672739	10.4225492762
H	13.5192551256	2.4041720097	10.4467456646
H	14.1000689179	7.2908499686	8.0390656456
H	14.0337278478	8.5144681165	5.9053444732
H	12.8141375080	7.5788928925	3.9699492518
H	11.6444478681	5.4006301208	4.1812875411
H	11.7006415944	4.1792843389	6.3110835826
H	11.6637635875	9.5773809038	9.8498575056
H	11.6585089375	11.1701277107	7.9746286046
H	10.7195333094	10.5085488864	5.7845746095
H	9.7954964049	8.2293297969	5.4753238727
H	9.8021399151	6.6351705565	7.3427467496
H	15.4329517885	5.2390320224	10.1680367682
H	16.1593048177	6.8775754864	11.8448090725
H	14.5332489293	8.5002151983	12.7781508191
H	12.1940086919	8.4528885157	12.0405427423

Ag^{pyrz}	X	Y	Z
Ag	9.7511245776	13.8225594883	9.2741944802
P	8.4067501249	15.8436790830	10.5780366463
P	9.9392841952	15.8479013914	7.6474816925
P	10.9290035519	11.8264467926	10.4623629764
P	7.9787365929	11.7347502922	8.9709382647
N	9.2106081613	18.4704490817	10.6995152240
N	10.4752993822	18.4619424501	8.2347614510
N	11.1241238943	9.2280500749	9.6403636937
N	8.6629607758	9.1398209928	8.3717348640
C	9.2473311708	17.3670819932	9.9560012155
C	9.8865025286	17.3638714564	8.7026706443
C	10.4414936975	19.5500369682	8.9888773804
C	9.8037469885	19.5555405709	10.2250404928
C	6.7048420776	16.1226982955	9.9840577122
C	6.0755629978	15.1472800823	9.2165863445
C	4.7873940208	15.3531952917	8.7412147419
C	4.1246994137	16.5358830584	9.0318386467
C	4.7488908912	17.5159874859	9.7965962580
C	6.0339555278	17.3125317677	10.2730422572
C	8.3051062729	16.1026295100	12.3742640061
C	7.1340689935	15.8033242122	13.0670600522
C	7.0934218310	15.9141268439	14.4517577539
C	8.2178572273	16.3238886304	15.1523926814
C	9.3943162886	16.6059433982	14.4668993378
C	9.4412281183	16.4870640671	13.0871210201
C	8.3310830630	15.9109166786	6.7975390754
C	7.5611082759	17.0687476118	6.6985433823
C	6.3234842048	17.0288466427	6.0720607059
C	5.8496498284	15.8383093276	5.5374658957
C	6.6113544439	14.6807672698	5.6307533200
C	7.8449062542	14.7183339534	6.2619746737

C	11.1941244025	16.2424389517	6.4040982012
C	10.8920281942	16.9037439712	5.2169956403
C	11.9018068478	17.1910663073	4.3112892755
C	13.2130190590	16.8277019830	4.5891634001
C	13.5177226444	16.1679230867	5.7718243611
C	12.5085478698	15.8675924362	6.6741124509
C	10.3309671546	10.2965512304	9.6161083515
C	9.0826084430	10.2529530531	8.9687385961
C	9.4629615657	8.0845386829	8.3989646802
C	10.7000853578	8.1301590664	9.0332311045
C	6.9525562883	11.3973578133	10.4407253167
C	6.8500568349	12.3571183069	11.4431218452
C	6.0881455857	12.1073373361	12.5766381688
C	5.4265542055	10.8963134729	12.7111550307
C	5.5266812566	9.9317071585	11.7138671520
C	6.2855407992	10.1788969294	10.5812526764
C	6.8610962112	11.4497111020	7.5661421332
C	5.4950670467	11.6947310486	7.6878298968
C	4.6606766258	11.5652054170	6.5840487253
C	5.1823831073	11.1906660668	5.3549467699
C	6.5478988845	10.9630017075	5.2243805432
C	7.3842031289	11.1007790246	6.3206167628
C	10.1195009219	11.7116999657	12.0884696240
C	9.9899019489	12.8911069819	12.8217184725
C	9.3535971523	12.8886642959	14.0532264854
C	8.8339694862	11.7037054695	14.5578647135
C	8.9540265484	10.5258755888	13.8326110865
C	9.5964872744	10.5262028360	12.6025582127
C	12.6871570031	11.4963779994	10.7384742788
C	13.1580838193	10.8386929062	11.8713807327
C	14.5165236272	10.6020432681	12.0168093800
C	15.4059592148	11.0124872689	11.0324491677
C	14.9397939716	11.6688039238	9.9016185192
C	13.5833293185	11.9185172101	9.7587802280
H	10.9302490449	20.4369857837	8.6034753793
H	9.7727488294	20.4479071225	10.8389145568
H	6.5968553445	14.2301915698	8.9672825644
H	4.3143511589	14.5917379881	8.1337890383
H	3.1208614112	16.6994520961	8.6615846842
H	4.2308244382	18.4387272351	10.0229676739
H	6.5205748436	18.0724511749	10.8740995744
H	6.2438892958	15.5030481195	12.5264698980
H	6.1745267148	15.6937483049	14.9796576090
H	8.1807680460	16.4246298679	16.2291468272
H	10.2752902007	16.9244308006	15.0086547051
H	10.3613602605	16.7165066986	12.5622376188
H	7.9202790002	18.0032708710	7.1120426602
H	5.7270891249	17.9294364156	6.0064676552
H	4.8811986191	15.8111132930	5.0546467820
H	6.2458491852	13.7449761198	5.2273506596
H	8.4289295331	13.8076149104	6.3451035585
H	9.8711430179	17.1914776675	4.9994174990
H	11.6654347997	17.7025504945	3.3875970509
H	13.9980850420	17.0549041151	3.8799302254
H	14.5383893263	15.8803462390	5.9867359331
H	12.7419295853	15.3399840685	7.5926725671

H	9.1152112188	7.1840680505	7.9066815800
H	11.3557773519	7.2676981361	9.0512268231
H	7.3830342062	13.2967652366	11.3539693052
H	6.0277466746	12.8573806674	13.3553163605
H	4.8328248766	10.6985611248	13.5942818944
H	5.0098866481	8.9868242269	11.8197212468
H	6.3606145854	9.4309959783	9.7998732206
H	5.0747916063	11.9669674597	8.6491203010
H	3.5984862699	11.7431948612	6.6921440569
H	4.5296654443	11.0751651749	4.4996438464
H	6.9607239799	10.6721976877	4.2672720850
H	8.4459948368	10.9137434202	6.2092358261
H	10.3806669195	13.8226836259	12.4256497074
H	9.2550914883	13.8145270368	14.6055920318
H	8.3270840245	11.6993336807	15.5143163244
H	8.5426152040	9.6037217022	14.2217439593
H	9.6839232614	9.6012355656	12.0456834734
H	12.4664891187	10.5143230500	12.6387257821
H	14.8817719056	10.0933224784	12.8991313158
H	16.4652000484	10.8247477110	11.1495978425
H	15.6327687947	11.9930416742	9.1365670933
H	13.2180125413	12.4432968656	8.8825723293

Ag^{quinox}	X	Y	Z
Ag	12.7442657707	3.2785778187	9.2945500670
P	10.5148902908	1.8032451590	8.6038408884
P	13.1786024454	2.6292544983	6.8104757042
P	12.7764530319	5.1127120049	11.1427451078
P	13.8917358191	2.0063592577	11.4598500434
N	9.1813213148	2.0002991300	6.2268817835
N	11.4344816518	2.6865925417	4.7315777438
N	14.7859507221	5.7293271883	12.8599420980
N	15.7424533736	3.1226477035	13.1319473626
C	9.0777944019	2.2313208141	4.8948055230
C	10.2202242132	2.5834225246	4.1374282397
C	10.0937386564	2.8254951988	2.7513007722
C	8.8684195270	2.7128789414	2.1588036002
C	7.7255739579	2.3588373949	2.9165302087
C	7.8211893001	2.1224659174	4.2581822895
C	10.3538526580	2.1148714741	6.7868677203
C	11.5172930341	2.4646983442	6.0143618985
C	14.1725771414	3.4456988695	5.5366021711
C	14.8346350522	2.7393532214	4.5363822844
C	15.5669677830	3.4231162908	3.5777947574
C	15.6350253472	4.8098161959	3.6091832593
C	14.9759347882	5.5172930810	4.6050609468
C	14.2528844553	4.8358814755	5.5724765922
C	8.8231720405	2.0201906014	9.2350702441
C	8.0880361515	3.1544937361	8.8883516221
C	6.8316070262	3.3673357826	9.4329110016
C	6.3021082671	2.4601178886	10.3440073248
C	7.0396067841	1.3454272227	10.7135440083
C	8.2958775271	1.1237338293	10.1620580224
C	10.7699120838	-0.0036173716	8.6252859936
C	11.8655600066	-0.5368518600	9.2970496487

C	12.0772400483	-1.9089711307	9.3135279691
C	11.1933091117	-2.7522416984	8.6579449312
C	10.0980359602	-2.2253571325	7.9813213655
C	9.8846165932	-0.8563952058	7.9635216388
C	12.8147490585	6.9177469507	11.0096825400
C	12.2023774359	7.7504459927	11.9420431597
C	12.2813419415	9.1269786539	11.7948785647
C	12.9755591900	9.6759051145	10.7246943246
C	13.5874903496	8.8484906887	9.7932314128
C	13.4999350157	7.4713660145	9.9306223884
C	15.1534369322	0.6973518487	11.4147268946
C	16.4511655809	0.9918045035	10.9946311332
C	17.3942633458	-0.0167702218	10.8771395977
C	17.0480429774	-1.3335205135	11.1596464415
C	15.7524794626	-1.6360876781	11.5507533924
C	14.8067041330	-0.6258628701	11.6790361168
C	13.7500166148	0.9023507175	6.8767081370
C	14.7640331233	0.5996433722	7.7853256247
C	15.2310315508	-0.6991665067	7.9126918375
C	14.6787147723	-1.7090083840	7.1355373483
C	13.6650354749	-1.4179534691	6.2326387437
C	13.2018400571	-0.1164736371	6.0991964500
C	11.3660069556	4.7088622313	12.2200757798
C	11.4681007772	4.5948783252	13.6055755567
C	10.3550994537	4.2461577270	14.3577912530
C	9.1359688607	4.0154301408	13.7349184312
C	9.0258273698	4.1284720919	12.3551019323
C	10.1385780140	4.4695672966	11.6023354416
C	14.2241318120	4.7347402804	12.2300318909
C	15.8569946176	5.4687949231	13.6492875351
C	16.3399552229	4.1461161316	13.7907491781
C	14.7203967564	3.3902206439	12.3668680771
C	12.6991783499	1.4322922550	12.7162338039
C	11.3512191986	1.3247918769	12.3883630372
C	10.4313940402	0.8985471915	13.3370613286
C	10.8571934443	0.5783490596	14.6170599520
C	12.2028169516	0.6872155981	14.9524633045
C	13.1226712379	1.1122776530	14.0074174091
C	16.4943828599	6.5242029920	14.3390683543
C	17.5684741551	6.2527599489	15.1376850110
C	18.0506009407	4.9288458701	15.2805006541
C	17.4535865681	3.8918726205	14.6222421176
H	10.9826444973	3.0951473312	2.1967891822
H	8.7623341392	2.8953505482	1.0976533461
H	6.7676350067	2.2771552799	2.4202302788
H	6.9637962051	1.8527654295	4.8603683355
H	14.7807771793	1.6583450686	4.5077196596
H	16.0843017953	2.8724735631	2.8032227093
H	16.2076713694	5.3395344873	2.8591668248
H	15.0323506383	6.5974143206	4.6331238414
H	13.7475898512	5.3856734055	6.3591159256
H	8.4871320956	3.8634323025	8.1726033032
H	6.2617695855	4.2402482883	9.1422976163
H	5.3178628643	2.6241637879	10.7627642222
H	6.6330365491	0.6350912534	11.4219477436
H	8.8553009902	0.2383805361	10.4413876076

H	12.5727841833	0.1189201682	9.7915860292
H	12.9417596633	-2.3097197253	9.8278879634
H	11.3563959329	-3.8222268400	8.6685797672
H	9.4095265696	-2.8840418328	7.4683146906
H	11.6630567203	7.3252087865	12.7790659575
H	11.8014895714	9.7729445344	12.5182550713
H	13.0347372771	10.7507070158	10.6135714276
H	14.1244962225	9.2752277381	8.9564803033
H	13.9663364399	6.8226664222	9.1971007399
H	16.7343469363	2.0155703406	10.7804375365
H	18.4031345997	0.2252845193	10.5693483818
H	17.7876622648	-2.1188159571	11.0743124346
H	15.4765552806	-2.6590086482	11.7725885131
H	13.8025249067	-0.8700095014	12.0059102168
H	15.1884068458	1.3821434460	8.4057906753
H	16.0135816129	-0.9181645105	8.6279678329
H	15.0327705922	-2.7266521030	7.2397129047
H	13.2286038381	-2.2057880721	5.6327325035
H	12.4114296422	0.0998274873	5.3907659923
H	12.4141891028	4.7739519884	14.1018195063
H	10.4435012047	4.1501874804	15.4320436459
H	8.2721242347	3.7384516662	14.3255640391
H	8.0824335930	3.9389761102	11.8590534929
H	10.0507114806	4.5416042418	10.5232308914
H	11.0090011516	1.5959799572	11.3963383437
H	9.3832994723	0.8331172905	13.0729092007
H	10.1421144985	0.2465269179	15.3587706254
H	12.5341637956	0.4388507564	15.9522686551
H	14.1726341798	1.1947387464	14.2649145477
H	16.1060564542	7.5258155571	14.2113037855
H	18.0621388742	7.0545787216	15.6705748773
H	18.9034757455	4.7437046261	15.9200004497
H	17.8031831229	2.8719781974	14.7121693552
H	9.0298732847	-0.4431042692	7.4399460582

In solution (PCM, acetonitrile) ground state equilibrium structures (cartesian coordinates, in Å) of the different complexes investigated calculated at the M06-2X/def2-TZVP theoretical level.

Cu^{bz}	X	Y	Z
Cu	-10.1495104715	8.0608923534	2.2945906841
P	-11.6688322039	7.0693537546	0.6772282576
P	-9.4892960955	9.3445669505	0.2578139855
P	-8.6516539946	7.0652638409	3.9293683131
P	-10.7814596013	9.3940232593	4.3084339467
C	-10.8170997061	7.1960505821	-0.9393518671
C	-11.1310258981	6.3364453064	-1.9908523389
C	-10.5202375144	6.4789614900	-3.2276119715
C	-9.5933184201	7.4924227285	-3.4289723748
C	-9.2720379462	8.3534750869	-2.3906747415
C	-9.8682415392	8.2141468988	-1.1377248990
C	-10.5965716898	10.7643281156	-0.0595535612
C	-10.5677371200	11.4568613348	-1.2710122372
C	-11.4485219597	12.5026731399	-1.4982345101
C	-12.3682609164	12.8663953386	-0.5189582825

C	-12.4035542351	12.1829884667	0.6871648288
C	-11.5184808988	11.1365011686	0.9149291037
C	-13.0982570270	8.1822119048	0.4794375751
C	-13.7847717512	8.5456613765	1.6387025371
C	-14.8268985990	9.4583012870	1.5829101812
C	-15.1862675860	10.0240595187	0.3650477617
C	-14.5088608761	9.6663880194	-0.7924834130
C	-13.4683740813	8.7473464967	-0.7387794644
C	-12.3461106818	5.3824249585	0.6831654250
C	-11.4492972449	4.3379128161	0.9164710374
C	-11.8941518946	3.0256450252	0.9384423937
C	-13.2428836643	2.7471556749	0.7427119676
C	-14.1392919446	3.7824656358	0.5186324144
C	-13.6940169299	5.0991783101	0.4845672701
C	-7.8237923581	9.9918986435	-0.0998837224
C	-7.5156703237	11.3275251663	0.1566770232
C	-6.2157506214	11.7919783222	-0.0052191644
C	-5.2140836575	10.9305415845	-0.4290944787
C	-5.5111507603	9.5944592133	-0.6738725771
C	-6.8041945351	9.1251288342	-0.4998607267
C	-9.5001448956	7.2386384142	5.5433187746
C	-9.2046596141	6.3910121746	6.6097813190
C	-9.8119927022	6.5683396471	7.8437380325
C	-10.7167671352	7.6049584980	8.0271318466
C	-11.0195713089	8.4544213937	6.9738433333
C	-10.4267537798	8.2803120037	5.7236402802
C	-9.6437182775	10.7948819751	4.6010818176
C	-9.6573607312	11.5090016214	5.8002118675
C	-8.7541508440	12.5393675631	6.0092385645
C	-7.8269547371	12.8659217355	5.0239135826
C	-7.8066569470	12.1608789605	3.8299595518
C	-8.7141690715	11.1299209410	3.6204019438
C	-7.1984882321	8.1502830551	4.1078968470
C	-6.5045046880	8.4784505550	2.9425702366
C	-5.4428980874	9.3692059677	2.9825578763
C	-5.0711604831	9.9483230209	4.1903872933
C	-5.7559135106	9.6257039410	5.3538809349
C	-6.8160184777	8.7285507774	5.3160937823
C	-8.0109709664	5.3642549771	3.9531229805
C	-8.9301798738	4.3354287326	3.7379881228
C	-8.5137769889	3.0136751407	3.7391013741
C	-7.1713379655	2.7095922291	3.9399375212
C	-6.2527346256	3.7290669253	4.1460089098
C	-6.6694594685	5.0554846954	4.1569095723
C	-12.4325260661	10.0833445673	4.6544171809
C	-12.7117781053	11.4206130676	4.3744313316
C	-14.0013327001	11.9157992002	4.5279173636
C	-15.0212909727	11.0837577910	4.9666341993
C	-14.7531033927	9.7460658798	5.2348450334
C	-13.4705307210	9.2459406227	5.0693294647
H	-11.8606478664	5.5501289554	-1.8423984115
H	-10.7716674530	5.8019071969	-4.0333113689
H	-9.1170284717	7.6126101670	-4.3930537772
H	-8.5399130762	9.1333325714	-2.5573536253
H	-9.8549220757	11.1802994716	-2.0391453002
H	-11.4203494513	13.0345286018	-2.4402994705

H	-13.0576415782	13.6805193844	-0.7018483300
H	-13.1227609618	12.4514577719	1.4511466282
H	-11.5663352095	10.5937354572	1.8513925010
H	-13.4931038591	8.1218589934	2.5935669513
H	-15.3438537631	9.7371907200	2.4920938525
H	-15.9883356859	10.7495786182	0.3207469131
H	-14.7828292926	10.1096618792	-1.7411716595
H	-12.9378355325	8.4877857725	-1.6465311624
H	-10.3977525794	4.5541866228	1.0751939127
H	-11.1914600721	2.2215399394	1.1147004841
H	-13.5929554854	1.7234694969	0.7670372253
H	-15.1889047123	3.5679808442	0.3654388548
H	-14.3975573225	5.9019913320	0.3023264868
H	-8.2914238190	12.0140339841	0.4752456883
H	-5.9916454872	12.8321291678	0.1931439271
H	-4.2042441767	11.2953610018	-0.5637711466
H	-4.7337322479	8.9147652559	-0.9977677606
H	-7.0220794917	8.0797647045	-0.6867036869
H	-8.4922200382	5.5866390086	6.4752679684
H	-9.5750926689	5.9002361068	8.6612263091
H	-11.1901671696	7.7522821866	8.9888689343
H	-11.7346493584	9.2527115642	7.1266915109
H	-10.3758383772	11.2614044194	6.5729379846
H	-8.7706524785	13.0881360618	6.9418323357
H	-7.1201168581	13.6680466835	5.1926388327
H	-7.0819631939	12.4003214742	3.0615270339
H	-8.6782250919	10.5699197666	2.6936036616
H	-6.8054405786	8.0443803371	1.9952237880
H	-4.9202133091	9.6208906200	2.0687239910
H	-4.2536003631	10.6570135880	4.2221190173
H	-5.4722532538	10.0795117724	6.2947077563
H	-7.3518661691	8.4964555425	6.2281546936
H	-9.9768379204	4.5715497482	3.5753003886
H	-9.2337062021	2.2219698343	3.5768289854
H	-6.8434631446	1.6783145746	3.9336220458
H	-5.2079704325	3.4946790607	4.3031364443
H	-5.9487086683	5.8459849474	4.3251866247
H	-11.9214387955	12.0845189494	4.0440276634
H	-14.2029580621	12.9569116364	4.3113142424
H	-16.0229900586	11.4726066148	5.0947057735
H	-15.5449591940	9.0891015265	5.5704545337
H	-13.2752388247	8.1995493889	5.2745044419

Cu^{pyrz}	X	Y	Z
Cu	0.0001976800	0.4499532823	0.0006305156
P	1.1113224596	-0.8934697750	-1.7891037952
P	2.2143854934	1.4571674225	0.1308744657
P	-2.2123145743	1.4610905667	-0.1273722159
P	-1.1131565313	-0.8955904995	1.7874042154
N	2.9713581074	0.0333228697	-3.6057828004
N	3.8823592514	2.0770391853	-1.9639101910
N	-3.8792666782	2.0791137555	1.9687649499
N	-2.9716830821	0.0302558328	3.6061187426
C	2.4426739127	0.2312086490	-2.3990640809
C	2.9118403812	1.2556866528	-1.5640753147

C	4.3853715375	1.8856868934	-3.1737628481
C	3.9349412660	0.8539519091	-3.9941176961
C	2.1049835072	-2.2831457833	-1.1483108098
C	1.9972786375	-2.6400991465	0.1928702833
C	2.7781286136	-3.6651526491	0.7119623077
C	3.6694304101	-4.3376632369	-0.1108185511
C	3.7820221439	-3.9862120471	-1.4529870061
C	3.0041676337	-2.9632165417	-1.9719604689
C	0.3453424640	-1.5397763341	-3.3056982163
C	-0.0695664231	-2.8693189841	-3.3637275002
C	-0.7604085338	-3.3389833796	-4.4743322374
C	-1.0380054829	-2.4872785108	-5.5339564828
C	-0.6366046422	-1.1572071746	-5.4755070234
C	0.0439173755	-0.6823517702	-4.3646456153
C	3.2827593305	0.3622539358	1.1167100573
C	4.4885592066	-0.1607431689	0.6535108221
C	5.1975213129	-1.0662102694	1.4322827302
C	4.7125216584	-1.4494654230	2.6755541913
C	3.5170552453	-0.9216579115	3.1487273129
C	2.8047255373	-0.0229705790	2.3696411357
C	2.6710572624	3.1577430592	0.5642813969
C	3.7202593188	3.4654860838	1.4242998790
C	3.9985466289	4.7925045211	1.7289299023
C	3.2375948411	5.8114988763	1.1726059135
C	2.1898947106	5.5066943971	0.3105553318
C	1.9021581542	4.1836156244	0.0137662349
C	-2.9101142168	1.2570313114	1.5671215351
C	-2.4426579447	0.2299309014	2.3998440037
C	-3.9339013822	0.8516294285	3.9962622692
C	-4.3826035678	1.8859282550	3.1781908313
C	-2.1090666471	-2.2822344435	1.1435409893
C	-2.0018701552	-2.6364391140	-0.1984096087
C	-2.7843633813	-3.6590807744	-0.7197775315
C	-3.6768101239	-4.3319251359	0.1014878186
C	-3.7889005003	-3.9832200009	1.4444142468
C	-3.0094038709	-2.9626311521	1.9656596288
C	-0.3482388532	-1.5464887911	3.3025703179
C	0.0644967881	-2.8768323878	3.3576703892
C	0.7545726839	-3.3500680107	4.4672348377
C	1.0335687010	-2.5011503953	5.5287270612
C	0.6343455415	-1.1702982727	5.4732060352
C	-0.0454066210	-0.6918891661	4.3633982220
C	-3.2824305626	0.3700329025	-1.1155951669
C	-2.8050826746	-0.0130529096	-2.3694438788
C	-3.5188303198	-0.9088901557	-3.1505117916
C	-4.7150514866	-1.4359736946	-2.6784401031
C	-5.1993612960	-1.0548347942	-1.4342509475
C	-4.4889681260	-0.1522179499	-0.6534765879
C	-2.6662550253	3.1633301185	-0.5571019933
C	-3.7151708819	3.4746220483	-1.4161955111
C	-3.9913553610	4.8027379247	-1.7179340872
C	-3.2285877503	5.8192980399	-1.1596420649
C	-2.1811689922	5.5109443612	-0.2985138331
C	-1.8955302807	4.1867660570	-0.0046098636
H	5.1665982727	2.5589799464	-3.5042469009
H	4.3627185525	0.6960322648	-4.9764105328

H	1.3175116134	-2.1058708049	0.8458352689
H	2.6910164890	-3.9269584533	1.7590843638
H	4.2810152268	-5.1352883974	0.2906604047
H	4.4787030845	-4.5103196181	-2.0940716029
H	3.0935416156	-2.6882020922	-3.0165901162
H	0.1541731793	-3.5470296265	-2.5479783102
H	-1.0736373119	-4.3742504914	-4.5106428864
H	-1.5693193913	-2.8553984519	-6.4018450127
H	-0.8543525256	-0.4871452340	-6.2969492839
H	0.3483130395	0.3566692690	-4.3287835002
H	4.8767712752	0.1243017983	-0.3162340398
H	6.1273995096	-1.4774901234	1.0616138314
H	5.2626811164	-2.1646264457	3.2733585105
H	3.1273264845	-1.2188668608	4.1140824475
H	1.8622769051	0.3716143497	2.7327225834
H	4.3200026722	2.6744863804	1.8569739463
H	4.8138623954	5.0285042318	2.4002290667
H	3.4577740352	6.8436416377	1.4120683812
H	1.5928976703	6.2983453739	-0.1232433548
H	1.0795223515	3.9463217774	-0.6528503079
H	-4.3619504613	0.6922488884	4.9782006500
H	-5.1627061002	2.5597925791	3.5101627608
H	-1.3211990746	-2.1018955383	-0.8501723586
H	-2.6976251917	-3.9187383736	-1.7674658039
H	-4.2896776864	-5.1276702095	-0.3017622222
H	-4.4864718598	-4.5075862938	2.0843179072
H	-3.0983828927	-2.6897543601	3.0108833379
H	-0.1603504024	-3.5523779758	2.5404314408
H	1.0661095116	-4.3859228171	4.5012663349
H	1.5642841159	-2.8720466787	6.3957994570
H	0.8531954159	-0.5024010495	6.2961169496
H	-0.3481030414	0.3477040935	4.3298216235
H	-1.8620735979	0.3809420098	-2.7317108687
H	-3.1296328889	-1.2044838149	-4.1165764327
H	-5.2663377053	-2.1489394842	-3.2778268857
H	-6.1298196672	-1.4655675585	-1.0644322580
H	-4.8766594623	0.1311629173	0.3169644764
H	-4.3163242915	2.6855272228	-1.8503894268
H	-4.8064544450	5.0415039004	-2.3885180489
H	-3.4471327125	6.8523073077	-1.3968546196
H	-1.5827599367	6.3006902754	0.1368091579
H	-1.0731128705	3.9467054081	0.6612840216

Cu^{quinox}	X	Y	Z
Cu	-0.0000084335	-0.2839363616	-0.0111748150
P	-1.7339321233	-1.2887488168	1.3737381828
P	-1.9321770137	1.0606529799	-0.8279904390
P	1.7342756378	-1.1752428629	-1.4714396055
P	1.9316431376	0.9922517575	0.9096727433
N	-4.2118830164	-2.0384868660	0.4836231330
N	-4.4182661801	0.0368892343	-1.3767334316
N	4.2126636770	-1.9920243878	-0.6437041243
N	4.4182596327	-0.0705934088	1.3753366980
C	-3.2520665597	-1.1703951638	0.3278154298
C	-3.3529550354	-0.1093838704	-0.6398175477

C	-5.4289108348	-0.8564853418	-1.2257265711
C	-5.3192045394	-1.9139883127	-0.2918415696
C	-6.3759422026	-2.8422557874	-0.1595596315
C	-7.4948557445	-2.7046272595	-0.9315406680
C	-7.6064480938	-1.6440023848	-1.8629477385
C	-6.5966161830	-0.7357171790	-2.0121335099
C	-1.8040193201	-2.9409356561	2.1150666738
C	-0.8250543238	-3.8618698790	1.7517176403
C	-0.8319003276	-5.1407394381	2.2953758034
C	-1.8127813994	-5.4955809239	3.2097998319
C	-2.7852590430	-4.5737557887	3.5863846036
C	-2.7822460229	-3.2992186400	3.0429796160
C	-2.1362654871	-0.1445215730	2.7354777555
C	-1.0831563014	0.2074992228	3.5803206664
C	-1.2800394667	1.1131702442	4.6107651296
C	-2.5334251528	1.6841997145	4.7984366830
C	-3.5857872463	1.3385887032	3.9619320859
C	-3.3924172829	0.4240153555	2.9341071660
C	-2.1450483018	1.7664302008	-2.4894524374
C	-2.4191454505	0.9389276223	-3.5793299914
C	-2.4604988366	1.4646494475	-4.8615681342
C	-2.2147897965	2.8173814900	-5.0714167446
C	-1.9231162574	3.6408950303	-3.9937923877
C	-1.8896230948	3.1195314854	-2.7058683707
C	-2.4180474219	2.4101236454	0.2985553613
C	-3.6757867895	3.0066459784	0.2007974619
C	-4.0337799942	4.0165909928	1.0799706019
C	-3.1401004646	4.4381668115	2.0596928746
C	-1.8884758758	3.8486193528	2.1607869366
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C	3.2524479368	-1.1394844127	-0.4194877608
C	3.3529391993	-0.1584957225	0.6292127073
C	5.4293167331	-0.9486874996	1.1538988959
C	5.3200085894	-1.9288650525	0.1391130935
C	6.3771786487	-2.8432045173	-0.0664356282
C	7.4961122856	-2.7666766532	0.7139449638
C	7.6073012658	-1.7831923562	1.7265140743
C	6.5970519173	-0.8900869647	1.9473219890
C	1.8054158119	-2.7632546046	-2.3417049758
C	0.8273670381	-3.7109967341	-2.0523555910
C	0.8351250800	-4.9426486583	-2.6958545034
C	1.8159968176	-5.2228923143	-3.6358392257
C	2.7875605320	-4.2732249471	-3.9382933380
C	2.7836400879	-3.0458686936	-3.2953903387
C	2.1358603893	0.0739282724	-2.7378465771
C	1.0823812295	0.4918446030	-3.5516296771
C	1.2786456887	1.4768834259	-4.5066145706
C	2.5317888739	2.0614923657	-4.6485025440
C	3.5845351978	1.6506038298	-3.8425539530
C	3.3917807840	0.6569030888	-2.8908917399
C	2.1439801869	1.5636470302	2.6220729726
C	2.4184786315	0.6521961526	3.6426717053
C	2.4593476812	1.0742178919	4.9626930858
C	2.2127640003	2.4058003861	5.2795070285
C	1.9207189349	3.3122992311	4.2707980899
C	1.8877088637	2.8950804014	2.9454608156

C	2.4170085338	2.4273581756	-0.1057651928
C	3.6744588570	3.0147657302	0.0394112009
C	4.0320540184	4.0917693119	-0.7563734639
C	3.1382546193	4.5897266424	-1.6994592191
C	1.8869228838	4.0095297733	-1.8474110982
C	1.5278547066	2.9296217284	-1.0516338851
H	-6.2695595393	-3.6435237292	0.5597943510
H	-8.3089362648	-3.4104963121	-0.8344157861
H	-8.5037457879	-1.5582876167	-2.4611711667
H	-6.6587756731	0.0808819663	-2.7192781686
H	-0.0482102114	-3.5734762546	1.0529627275
H	-0.0684119915	-5.8523174354	2.0099229347
H	-1.8179511502	-6.4894797642	3.6382396102
H	-3.5449407895	-4.8507838998	4.3055194199
H	-3.5369671881	-2.5808075847	3.3381885955
H	-0.1004367738	-0.2236851213	3.4265950501
H	-0.4505706053	1.3804661986	5.2532583924
H	-2.6873503487	2.4044127405	5.5916315870
H	-4.5612376538	1.7857661787	4.1029076258
H	-4.2235373984	0.1688199409	2.2880822737
H	-2.6069358908	-0.1171349786	-3.4281707036
H	-2.6843883938	0.8167685342	-5.6990227001
H	-2.2468717920	3.2249716236	-6.0733969868
H	-1.7265079324	4.6936460575	-4.1496543462
H	-1.6727476337	3.7747025067	-1.8701342021
H	-4.3718747854	2.6773487141	-0.5622560420
H	-5.0108488933	4.4754552497	1.0033942604
H	-3.4250939226	5.2240874447	2.7471602246
H	-1.1931130739	4.1644660082	2.9283516536
H	-0.5588852665	2.3621135695	1.3788127490
H	6.2710993288	-3.5849594560	-0.8470537444
H	8.3105218938	-3.4622214837	0.5610890770
H	8.5046232206	-1.7447473373	2.3295864028
H	6.6589005987	-0.1320984519	2.7169837667
H	0.0505305264	-3.4796971544	-1.3326723532
H	0.0723489536	-5.6753232088	-2.4675975504
H	1.8218705754	-6.1796254914	-4.1418524826
H	3.5472448986	-4.4916097249	-4.6773485198
H	3.5376564727	-2.3056274355	-3.5328188771
H	0.0998407273	0.0494599958	-3.4324844863
H	0.4488768100	1.7942994969	-5.1254828637
H	2.6852246516	2.8427538457	-5.3817463133
H	4.5598010809	2.1079260595	-3.9477089456
H	4.2231916441	0.3512671221	-2.2675308136
H	2.6069323013	-0.3883748296	3.4079832119
H	2.6835423448	0.3618721761	5.7459595347
H	2.2444624786	2.7323604903	6.3107573177
H	1.7234388851	4.3491862505	4.5099231390
H	1.6705347062	3.6145619719	2.1644876513
H	4.3706211766	2.6259928137	0.7738751454
H	5.0088957623	4.5435247632	-0.6433185973
H	3.4229223334	5.4281214881	-2.3220035514
H	1.1914770225	4.3852691303	-2.5874227530
H	0.5579591075	2.4647681613	-1.1866372586

Ag^{bz}	X	Y	Z
Ag	10.3867469449	4.1258629823	9.2989580418
P	8.5351187504	2.5226184060	10.1827552550
P	8.3911488519	4.0884415727	7.3530958419
P	10.7324069679	6.7805130045	10.0762600626
P	12.8941596331	4.6890432875	8.8796250239
C	13.4134267500	5.9293160384	10.1286288022
C	8.7068047646	1.1775730158	11.3954457089
C	6.9616984176	5.1782018772	7.6931675315
C	7.2218812245	3.5951468638	10.8514297999
C	7.6119409859	4.6182357241	11.7158850681
C	8.6854670362	4.3013469405	5.5661280925
C	7.7353060066	1.7272889183	8.7351124191
C	12.9423712182	5.6229865993	7.3151827322
C	7.6645349850	2.4066919536	7.5023135699
C	12.4778473479	6.8461860912	10.6486593625
C	16.3758794424	2.7578277711	7.8417213772
C	9.7864365643	7.6011392934	11.4017558864
C	7.9462839229	-0.1336669181	13.2692841053
C	6.6731160936	5.4974708241	12.2343133130
C	13.5947415620	6.8459898097	7.1724365961
C	12.2433102236	5.0899617699	6.2319794333
C	14.7371130213	5.9867409924	10.5638742147
C	4.8081666047	6.8499151754	8.2767001372
C	7.0297911132	1.7891615156	6.4247826320
C	5.7464900744	5.0216174934	7.0248932198
C	10.1991583731	7.6116385470	7.4701198723
C	8.3307084738	5.4791223772	4.9101013039
C	10.7096118901	7.9942832778	8.7077487717
C	12.9042977146	7.7940581282	11.5787087214
C	9.9548205338	7.1851245600	12.7253770551
C	5.8782204758	3.4686554042	10.5046253424
C	9.8525937196	0.3850548225	11.3187630386
C	11.1909014090	10.1811657899	7.8083862792
C	15.3293389136	3.6711097462	7.8559207739
C	9.3961406541	3.3231842806	4.8650340304
C	9.0816454840	-0.9280852099	13.1790758849
C	7.1786010942	0.4532062317	8.8431642643
C	9.3275175800	4.6708070695	2.8717658980
C	8.8032040248	8.5454165101	11.1102519400
C	15.3731103982	1.5698591009	9.6783150299
C	9.1881419592	7.7376675152	13.7393840169
C	10.6766833976	9.7906987389	6.5759253341
C	14.2976412662	3.5357854043	8.7823135842
C	15.1418999337	6.9315359645	11.4954760079
C	14.2243579891	7.8398299319	12.0013941951
C	6.4796957401	0.5220175027	6.5474946611
C	5.3350261433	5.3660200741	11.8833522726
C	4.9397965630	4.3537581485	11.0188416683
C	7.0838636186	6.1766409208	8.6559214450
C	10.0349152850	-0.6693249457	12.2013063324
C	6.0111383318	7.0100367646	8.9479145053
C	12.8552182743	6.9831173121	4.8854671168
C	14.3208768115	2.4735079729	9.6866458457
C	11.2079958549	9.2879841161	8.8683309802
C	8.2222833173	8.6941241811	13.4431133693

C	7.7555555696	0.9153678661	12.3789520022
C	8.6536418177	5.6620439779	3.5699022884
C	6.5577138270	-0.1488637013	7.7585538598
C	8.0240584713	9.0860390896	12.1273756701
C	16.4010819202	1.7108641363	8.7536003830
C	4.6761133011	5.8533718241	7.3147699944
C	12.2031862577	5.7634472633	5.0203598991
C	10.1826876598	8.5059088185	6.4068428517
C	13.5483018440	7.5229960354	5.9608395330
C	9.7023058375	3.5010140144	3.5249036152
H	8.6492513590	8.8732892314	10.0890412127
H	7.2682237141	9.8225550031	11.8867487801
H	7.6234245847	9.1240479738	14.2352755101
H	9.3416158273	7.4186643396	14.7621351457
H	10.7011895080	6.4364314994	12.9673020111
H	8.6594852930	4.7379363733	11.9734871099
H	6.9924235320	6.2928864794	12.8954795806
H	4.6024385457	6.0612825525	12.2730757739
H	3.8995379180	4.2562540815	10.7360447760
H	5.5620617320	2.6887613246	9.8222329670
H	6.8654660768	1.5282261017	12.4508006287
H	7.2048320693	-0.3310106978	14.0324891649
H	9.2271586702	-1.7450385094	13.8737629832
H	10.9242679902	-1.2819796812	12.1328231643
H	10.6044281578	0.5969007247	10.5661736364
H	7.2294001304	-0.0778222923	9.7848802763
H	6.1344261481	-1.1391476141	7.8635710827
H	5.9936187789	0.0622615533	5.6970777323
H	6.9710974659	2.2989725883	5.4715856958
H	5.6346396619	4.2473429634	6.2749167921
H	3.7371826385	5.7240114604	6.7922139003
H	3.9694713604	7.4949566569	8.5051021331
H	6.1172818769	7.7726687089	9.7096084364
H	8.0131971378	6.2928483406	9.2021506311
H	7.7890248915	6.2545304036	5.4386776048
H	8.3667055948	6.5793618928	3.0720685576
H	9.5680304638	4.8092240019	1.8258303261
H	10.2377784894	2.7273679931	2.9900424206
H	9.6979212136	2.4095539507	5.3653813375
H	15.3178244984	4.4887533113	7.1457486265
H	17.1732921830	2.8669797867	7.1182608988
H	17.2180801610	1.0012739217	8.7404844487
H	15.3860149234	0.7509631259	10.3855816538
H	13.5105420482	2.3538861226	10.3976812486
H	14.1288193670	7.2802715142	8.0091038600
H	14.0479853303	8.4779474028	5.8608216863
H	12.8114404795	7.5192581611	3.9460014218
H	11.6477800154	5.3424677971	4.1920567269
H	11.7135397384	4.1489632697	6.3410577907
H	11.6112557954	9.6001200727	9.8245873440
H	11.5804070808	11.1821017576	7.9418125113
H	10.6690098144	10.4881535718	5.7481854627
H	9.7956302954	8.1887770938	5.4462868516
H	9.8332043008	6.6017244473	7.3228729849
H	15.4629344122	5.2858867773	10.1722274416
H	16.1734274038	6.9569746882	11.8213094625

H	14.5316488939	8.5831409125	12.7252148030
H	12.1951431911	8.5021992976	11.9880655403

Ag^{pyrz}	X	Y	Z
Ag	9.8518372438	13.8248233208	9.2420623372
P	8.3994615491	15.8467834768	10.5441589905
P	9.9523263346	15.8771371053	7.6418202927
P	10.9440476510	11.7978458233	10.4590742919
P	7.9926892293	11.7319074864	9.0026436478
N	9.1525285377	18.4928478265	10.6764329910
N	10.4747626262	18.4979377655	8.2426564141
N	11.1204117262	9.1919760915	9.6339163113
N	8.6300565248	9.1155658807	8.4240152415
C	9.2175112663	17.3885795146	9.9342504054
C	9.8807308971	17.3941691936	8.6938453867
C	10.4141436494	19.5850489885	8.9972999774
C	9.7435458406	19.5849724612	10.2156250716
C	6.6886007357	16.1111149561	9.9620812325
C	6.0710960491	15.1293765789	9.1921263361
C	4.7755120682	15.3142969399	8.7259826314
C	4.0927216472	16.4832769298	9.0280471245
C	4.7049267463	17.4705349310	9.7943659131
C	5.9972783945	17.2867942873	10.2607214952
C	8.3001715498	16.1014103722	12.3429468958
C	7.1357331838	15.7928675974	13.0434693974
C	7.1047363092	15.8909473278	14.4300635755
C	8.2328114795	16.3006625476	15.1257092441
C	9.4032886187	16.5927695165	14.4327515010
C	9.4412129633	16.4829452202	13.0514008632
C	8.3454446482	15.9288840432	6.7855065854
C	7.5631887437	17.0787251572	6.6855842260
C	6.3271399012	17.0268163789	6.0555035178
C	5.8663493953	15.8314330980	5.5193312123
C	6.6418782416	14.6824104195	5.6121524254
C	7.8742219287	14.7314558733	6.2461534026
C	11.1966041447	16.2932249626	6.3886925156
C	10.8912548277	16.9972515267	5.2259737483
C	11.8917540177	17.2901624051	4.3106654948
C	13.1997737985	16.8870769337	4.5533390939
C	13.5079218470	16.1828270927	5.7097808722
C	12.5065934226	15.8788931304	6.6220810915
C	10.3325644631	10.2662190627	9.6262999299
C	9.0718759486	10.2306775220	9.0034898407
C	9.4205977582	8.0529652866	8.4413527468
C	10.6742186143	8.0940193267	9.0419940207
C	6.9517084044	11.4086426437	10.4681339939
C	6.8600464279	12.3750880925	11.4658993404
C	6.0858922869	12.1458195368	12.5964519287
C	5.4006473148	10.9476328433	12.7333627784
C	5.4903135105	9.9755161993	11.7415590604
C	6.2617857679	10.2034706459	10.6127164053
C	6.8752308962	11.4512401595	7.5945010023
C	5.5097394124	11.7058086540	7.7062159202
C	4.6815322344	11.5893419212	6.5954830809
C	5.2090018835	11.2148867826	5.3683294356

C	6.5743571590	10.9768732414	5.2471529477
C	7.4046861475	11.1052751752	6.3497414932
C	10.1389723738	11.6944397248	12.0897728431
C	10.0233762986	12.8793329580	12.8174019859
C	9.3893297306	12.8883899267	14.0506634101
C	8.8581469158	11.7113274943	14.5631882910
C	8.9670412250	10.5281085189	13.8442403088
C	9.6064770244	10.5163886335	12.6119664803
C	12.7001404383	11.4459278078	10.7488704743
C	13.1559790658	10.7452405782	11.8633448978
C	14.5126885979	10.5027011806	12.0217828038
C	15.4183859196	10.9529619652	11.0682310595
C	14.9684638042	11.6540644003	9.9572357599
C	13.6124072073	11.9076286191	9.8018663328
H	10.9057805735	20.4775318978	8.6302370296
H	9.6884268307	20.4795491703	10.8236005423
H	6.6091897305	14.2247624087	8.9326302564
H	4.3102065242	14.5486748576	8.1175202325
H	3.0844840759	16.6311697289	8.6631285214
H	4.1734896423	18.3841084593	10.0272350465
H	6.4736525654	18.0549735578	10.8590594102
H	6.2430656398	15.4884860522	12.5095100766
H	6.1926102609	15.6536728477	14.9623152557
H	8.2054311595	16.3864200294	16.2040957161
H	10.2891609174	16.9052175462	14.9702147941
H	10.3594236509	16.7102100811	12.5223019180
H	7.9085540392	18.0167976909	7.1032093396
H	5.7207874584	17.9209897521	5.9910131950
H	4.8967927193	15.7925848157	5.0394502710
H	6.2848711005	13.7431909140	5.2090469823
H	8.4677910052	13.8273290946	6.3340559036
H	9.8739647785	17.3156192636	5.0345381862
H	11.6510220699	17.8354307139	3.4074139938
H	13.9776995552	17.1172420554	3.8369930302
H	14.5239940693	15.8615379465	5.8974813218
H	12.7424015390	15.3143516045	7.5175810018
H	9.0567495380	7.1494245726	7.9678878690
H	11.3217519797	7.2258798679	9.0434001461
H	7.4131448571	13.3030228987	11.3752317504
H	6.0322964694	12.9002532935	13.3716113557
H	4.7995920775	10.7652617072	13.6148694086
H	4.9584062505	9.0392412539	11.8498850889
H	6.3303617752	9.4470431649	9.8393118297
H	5.0834907202	11.9820815033	8.6636091646
H	3.6216783267	11.7845419756	6.6963390237
H	4.5625894505	11.1147032216	4.5062758579
H	6.9933511462	10.6922099633	4.2907682306
H	8.4672525717	10.9202407865	6.2429201403
H	10.4191598872	13.8046913478	12.4117403368
H	9.2973006778	13.8180159147	14.5978448151
H	8.3482947998	11.7184733027	15.5180883644
H	8.5468627909	9.6119074835	14.2384402102
H	9.6805658986	9.5872777867	12.0597587480
H	12.4533428078	10.3902078360	12.6070775509
H	14.8638782047	9.9598871388	12.8896256328
H	16.4760811723	10.7620102772	11.1951721813

H	15.6721673543	12.0119987093	9.2172724224
H	13.2609717690	12.4695964446	8.9434275210

Ag^{quinox}	X	Y	Z
Ag	12.7648200610	3.3410603116	9.2641401700
P	10.5504136493	1.7860130760	8.5831657211
P	13.1864064425	2.6400284787	6.7875362185
P	12.7839646624	5.1315817007	11.1589395411
P	13.8512529688	2.0213937809	11.4743147488
N	9.2002542052	1.9626717945	6.2096361494
N	11.4286119539	2.7155530055	4.7098664735
N	14.8115937586	5.7312110397	12.8730478657
N	15.7034572393	3.1052495176	13.1722422233
C	9.0827221156	2.2103213105	4.8808715609
C	10.2104974309	2.6002542091	4.1225845625
C	10.0670054429	2.8657292206	2.7422853008
C	8.8397736445	2.7372907379	2.1551154365
C	7.7112252346	2.3432793311	2.9140397720
C	7.8241683508	2.0846440070	4.2509676804
C	10.3734640254	2.0903344956	6.7644394041
C	11.5267819512	2.4698837249	5.9872843528
C	14.1859744169	3.4456290649	5.5061226533
C	14.8128309047	2.7383269614	4.4825981588
C	15.5567905524	3.4156504253	3.5273682240
C	15.6744152299	4.7994583698	3.5864768660
C	15.0537362764	5.5079133923	4.6068263719
C	14.3173694933	4.8315738300	5.5699606948
C	8.8593356261	2.0132681894	9.2159548536
C	8.1427749945	3.1637867269	8.8802782855
C	6.8901757145	3.3930315050	9.4279301116
C	6.3472105020	2.4886901761	10.3350964833
C	7.0677540027	1.3600182636	10.6969355005
C	8.3186414408	1.1203044094	10.1389530431
C	10.7951206852	-0.0234960680	8.6147587440
C	11.8934909453	-0.5515184733	9.2872376169
C	12.0994441004	-1.9248058310	9.3251410175
C	11.2072384387	-2.7751350300	8.6890437881
C	10.1098672528	-2.2538502335	8.0102756205
C	9.9029377867	-0.8837618636	7.9721883079
C	12.8201531813	6.9416119574	11.0469592374
C	12.2457055045	7.7681888068	12.0101865890
C	12.3150912056	9.1466954326	11.8705526649
C	12.9607597026	9.7055045187	10.7736488436
C	13.5319110427	8.8851966706	9.8097389329
C	13.4548601693	7.5053205016	9.9417477540
C	15.1134328115	0.7113571895	11.4201003070
C	16.4054538516	1.0109641167	10.9834478224
C	17.3505070510	0.0055484862	10.8512875178
C	17.0113338907	-1.3144211934	11.1309813385
C	15.7206014159	-1.6227676626	11.5346466351
C	14.7741438043	-0.6146725095	11.6812361956
C	13.7549300077	0.9102349716	6.8475571593
C	14.7708212478	0.6059157720	7.7545972941
C	15.2345439491	-0.6947563121	7.8805493806
C	14.6780591701	-1.7049699769	7.1058047038

C	13.6647226883	-1.4111630517	6.2029355942
C	13.2044314231	-0.1079222750	6.0702294277
C	11.3720659180	4.7283320189	12.2375370933
C	11.4733710599	4.6019528834	13.6223367459
C	10.3591892255	4.2500712297	14.3724850823
C	9.1390412690	4.0277533504	13.7479065497
C	9.0294193829	4.1563387240	12.3687865703
C	10.1427939266	4.5005790674	11.6174696607
C	14.2248189164	4.7446926030	12.2532068056
C	15.8749772748	5.4518905875	13.6687549625
C	16.3218230294	4.1199228157	13.8270001682
C	14.6914794072	3.3886313194	12.4001481771
C	12.6576048648	1.4325943824	12.7251088420
C	11.3115029435	1.3272654260	12.3868980398
C	10.3857447714	0.8813071267	13.3216989787
C	10.8035615989	0.5399921079	14.5994373302
C	12.1470413100	0.6476192446	14.9460751079
C	13.0718469012	1.0919087061	14.0140030938
C	16.5383704586	6.4973324774	14.3493662043
C	17.6018689631	6.2076450414	15.1571151119
C	18.0469572711	4.8731654414	15.3181353116
C	17.4238596328	3.8456823502	14.6677291450
H	10.9430383034	3.1642662093	2.1816633821
H	8.7223817930	2.9370406630	1.0983625973
H	6.7513295803	2.2488627433	2.4240173152
H	6.9755574727	1.7846654864	4.8515625294
H	14.7213597141	1.6603994194	4.4314724450
H	16.0442935719	2.8631102449	2.7348093737
H	16.2560398359	5.3245332487	2.8399420508
H	15.1503583748	6.5843667455	4.6594684513
H	13.8459668778	5.3816362623	6.3769952839
H	8.5575745569	3.8765074864	8.1772423516
H	6.3369543485	4.2800805079	9.1479557394
H	5.3694033879	2.6695097827	10.7619923766
H	6.6563939124	0.6558312575	11.4086290257
H	8.8643660889	0.2262139178	10.4169987088
H	12.6080323349	0.1099513839	9.7636839543
H	12.9641203906	-2.3233673795	9.8412431987
H	11.3670441796	-3.8453599701	8.7148338920
H	9.4160491175	-2.9171251358	7.5103654885
H	11.7439277792	7.3367318936	12.8675007253
H	11.8659875567	9.7859729716	12.6193848591
H	13.0124767259	10.7813280856	10.6676233373
H	14.0281661312	9.3178008227	8.9509912244
H	13.8856895735	6.8633279989	9.1813125857
H	16.6795941961	2.0352489544	10.7600946462
H	18.3534401710	0.2518666607	10.5276506173
H	17.7502906732	-2.0980802663	11.0268004184
H	15.4460007196	-2.6482216216	11.7459657423
H	13.7737296187	-0.8662298342	12.0135232088
H	15.1950805239	1.3877229475	8.3759661287
H	16.0156949230	-0.9171071225	8.5963480713
H	15.0262156326	-2.7242214442	7.2142680895
H	13.2248639122	-2.1980831378	5.6041070059
H	12.4121114463	0.1072869696	5.3633996439
H	12.4197331306	4.7705831738	14.1219806108

H	10.4482171231	4.1429711556	15.4457606471
H	8.2755748769	3.7424259308	14.3351564565
H	8.0852904373	3.9720784588	11.8721241033
H	10.0563078961	4.5810602467	10.5388260430
H	10.9756437333	1.6166662534	11.3977223500
H	9.3392918178	0.8149091014	13.0506960914
H	10.0837455861	0.1950607099	15.3305109544
H	12.4724277303	0.3851953127	15.9443175251
H	14.1187185987	1.1740675099	14.2831114893
H	16.1804454025	7.5092802148	14.2125785204
H	18.1137894535	7.0025279176	15.6829685437
H	18.8910672210	4.6716780023	15.9641344923
H	17.7475889283	2.8186217615	14.7735303591
H	9.0471458972	-0.4774464034	7.4452834435

S_1 and T_1 equilibrium structures (cartesian coordinates, in Å) of the different complexes investigated with the ligands in tetrahedral-like arrangement calculated using TDDFT and the M06-2X/def2-TZVP level of theory.

S_1-Cu^{bz}	X	Y	Z
Cu	-0.1471046891	0.3307947615	-0.0757730150
P	2.1310222314	1.2261927148	-0.3454314255
P	0.9585870447	-1.5919200173	-1.2912022704
P	-1.4377744371	-0.0144345617	2.0336767146
P	-2.3481462430	1.2307790121	-0.5875381178
C	-3.1017241237	1.8623816588	0.8816625812
C	2.4852222731	2.9992815609	-0.5257436404
C	1.9771794517	-2.5545708220	-0.1246606687
C	3.3634627930	0.5932361808	0.8396829916
C	3.1696087106	0.8627898061	2.1954520878
C	0.2037187816	-2.8478136410	-2.3735780572
C	2.6927646599	0.5067295785	-1.9333338596
C	-3.2845524328	-0.2334799936	-1.0980723989
C	2.2300367132	-0.7616413362	-2.3257006130
C	-2.6828735556	1.2066621463	2.0854091230
C	-3.0727175750	3.2556303758	-4.0705094153
C	-0.2990099528	0.2975097150	3.4073939014
C	3.7343902383	5.0043038328	-0.0629247716
C	4.0729759984	0.3905252464	3.1362230716
C	-4.3931461313	-0.6530987635	-0.3650093255
C	-2.8001178267	-1.0254346384	-2.1392931045
C	-4.1797166314	2.7342696997	0.8758483952
C	3.6197723495	-3.8563638965	1.7058264615
C	2.7824627742	-1.3610566086	-3.4581058089
C	2.9160669234	-3.4876542395	-0.5648642019
C	-1.9917253767	-2.5907101920	1.1197106143
C	-0.1566699593	-4.0853103311	-1.8411043622
C	-1.9424847502	-1.7500369445	2.2356149289
C	-3.4716163940	1.4295199112	3.2600345480
C	-0.1242751946	1.6142853234	3.8461640225
C	4.4520685760	-0.1833260739	0.4461855909
C	1.6582125494	3.7245397932	-1.3849001333
C	-2.9910997069	-3.4796331994	3.5544024164
C	-3.0348545150	2.2458918949	-3.1184751177
C	-0.1266052050	-2.5578644394	-3.6989548190

C	2.9160381808	5.7194292435	-0.9241668179
C	3.6555575482	1.1574017927	-2.7033380342
C	-1.0964475389	-4.7447745613	-3.9572409442
C	0.4155362631	-0.7330798559	4.0274436331
C	-1.9232037253	4.7368316816	-2.5603021222
C	0.7410394050	1.8913139114	4.8930635122
C	-3.0263187284	-4.3127697283	2.4423402315
C	-2.4354649776	2.4814225374	-1.8819033485
C	-4.8913556159	2.9861625408	2.0430407341
C	-4.5266444954	2.3039660170	3.2244754130
C	3.7450170818	-0.7068942599	-4.2111101027
C	5.1549124700	-0.3835729052	2.7382836709
C	5.3368971560	-0.6765858889	1.3948122058
C	1.8662380705	-2.2874961920	1.2354710481
C	1.8787007946	5.0762724550	-1.5899199279
C	2.6886990751	-2.9303998392	2.1501932288
C	-4.5266901767	-2.6402291574	-1.7165109616
C	-1.8731090208	3.7332350838	-1.6090181021
C	-2.4484659067	-2.2079418077	3.4585014909
C	1.4388013674	0.8608035774	5.5105358634
C	3.5260877836	3.6443122025	0.1345431411
C	-0.8064766961	-5.0258357024	-2.6300744603
C	4.1730749883	0.5603001613	-3.8416016594
C	1.2754355295	-0.4496217869	5.0753492517
C	-2.5189618261	4.4973234949	-3.7946896613
C	3.7301258053	-4.1382176686	0.3479247829
C	-3.4220295725	-2.2242814789	-2.4503607387
C	-2.5223444947	-3.8661894261	1.2268630085
C	-5.0115489422	-1.8548506535	-0.6799803851
C	-0.7582607977	-3.5062101609	-4.4891999225
H	0.2750895043	-1.7585298521	3.7075170876
H	1.8131349176	-1.2529888246	5.5628391527
H	2.1036305024	1.0771459914	6.3371569811
H	0.8598201615	2.9103137841	5.2371089114
H	-0.6869571734	2.4110939903	3.3754562861
H	2.3148311003	1.4469249553	2.5221019645
H	3.9240549655	0.6230550956	4.1819116011
H	5.8528837549	-0.7595301327	3.4750734777
H	6.1723215759	-1.2876606163	1.0789676580
H	4.6103657313	-0.4194362280	-0.5981735180
H	4.1770938360	3.0901327726	0.7986905403
H	4.5439643717	5.5021554305	0.4543029344
H	3.0854596244	6.7768621020	-1.0787680752
H	1.2418109253	5.6279623336	-2.2691366012
H	0.8461149066	3.2269971343	-1.9057453789
H	4.0089118137	2.1362284700	-2.4036601863
H	4.9179417693	1.0783775624	-4.4310573036
H	4.1582410863	-1.1876127722	-5.0881216409
H	2.4543043320	-2.3464099633	-3.7622902807
H	3.0112083157	-3.7049962667	-1.6225524590
H	4.4556658743	-4.8627533692	0.0020995274
H	4.2647056846	-4.3594463627	2.4146020320
H	2.6082322405	-2.6955768048	3.2041931681
H	1.1509158134	-1.5518001932	1.5840746743
H	0.0825505858	-4.3225783879	-0.8109410572
H	-1.0709779161	-5.9866899518	-2.2079731098

H	-1.5855590398	-5.4857270715	-4.5757744417
H	-0.9878940712	-3.2769232428	-5.5217457232
H	0.1276540172	-1.5940206864	-4.1249625443
H	-3.4908440015	1.2876144999	-3.3299517611
H	-3.5488413530	3.0738473238	-5.0248519379
H	-2.5591367894	5.2837389899	-4.5368251349
H	-1.5081842590	5.7108330666	-2.3364117621
H	-1.4147632453	3.9212735449	-0.6441965023
H	-4.7606996373	-0.0495937923	0.4559518139
H	-5.8679002659	-2.1814045711	-0.1049896633
H	-5.0079122803	-3.5804517876	-1.9529699641
H	-3.0381476316	-2.8356664546	-3.2558398063
H	-1.9254667736	-0.7117879506	-2.6999345454
H	-2.4107879084	-1.5722413186	4.3355104378
H	-3.3833648987	-3.8242455402	4.5024315670
H	-3.4478635216	-5.3058296899	2.5243860794
H	-2.5525429234	-4.5042070363	0.3519950709
H	-1.6344165553	-2.2444433454	0.1549507594
H	-4.4693068184	3.2159514253	-0.0513741247
H	-5.7151331378	3.6838721674	2.0430342246
H	-5.0803248316	2.4905033480	4.1363531417
H	-3.2062477502	0.9407090860	4.1893950806

T_1-**Cu^{bz}**	X	Y	Z
Cu	-0.0485662340	0.4107074133	-0.2214393190
P	2.2382658638	1.1978763263	-0.6651586426
P	0.8888796685	-1.6189127918	-1.3102775738
P	-1.2433480607	0.0665206192	2.1608421231
P	-2.2024685657	1.3889493060	-0.4566264937
C	-2.7428533349	2.1283892777	1.0903797461
C	2.7916115383	2.9014783387	-0.9689531316
C	1.8672364885	-2.6498975927	-0.1718813672
C	3.3589072682	0.5271904060	0.6016628046
C	3.0788948367	0.8401387872	1.9322397984
C	-0.0785948425	-2.7934730517	-2.3083126149
C	2.7270835030	0.2984130815	-2.1835445029
C	-3.4037299777	0.0826654722	-0.8333168854
C	2.1490188196	-0.9521965205	-2.4636537594
C	-2.1963943903	1.5664848676	2.2777395369
C	-3.4138394179	3.6651336609	-3.6506771971
C	-0.1375645018	0.0911693407	3.5863581846
C	4.2365909806	4.7894584645	-0.5883290116
C	3.8610502292	0.3228150969	2.9530921588
C	-4.4862940127	-0.1923062364	-0.0022891878
C	-3.1479679381	-0.7434646877	-1.9289038860
C	-3.7150677998	3.1051371790	1.1439500713
C	3.4312417664	-4.0957872779	1.6185857418
C	2.5752897955	-1.6623456457	-3.5859995708
C	2.7187617511	-3.6525807826	-0.6356678367
C	-2.0414898584	-2.3753647678	0.9763236127
C	-0.4792175066	-4.0161520662	-1.7737391323
C	-1.9268555622	-1.6376931630	2.1577866236
C	-2.7550488633	1.9927762423	3.5200163852
C	0.2925499068	1.3184114830	4.1115055527
C	4.4217530159	-0.3236724969	0.3069744094

C	2.0785549030	3.6487096506	-1.9087016240
C	-3.3560370398	-3.2429046292	3.2638531250
C	-3.3362251845	2.6346032332	-2.7211235454
C	-0.5336303894	-2.4219304606	-3.5758299509
C	3.5321975345	5.5249230754	-1.5292752093
C	3.7030491052	0.8095304061	-3.0379387043
C	-1.7330667577	-4.4972764771	-3.7724388966
C	0.3628919249	-1.0924862462	4.1444920392
C	-1.5818074423	4.7902679087	-2.5705519474
C	1.1355794721	1.3569328877	5.2083248062
C	-3.4503252606	-3.9789895806	2.0877982878
C	-2.3749625579	2.6807833184	-1.7153044387
C	-4.2313595544	3.5327416433	2.3739591204
C	-3.7489003821	2.9496120952	3.5459922130
C	3.5470918553	-1.1432802095	-4.4268707156
C	4.9166930491	-0.5292038024	2.6531887680
C	5.1929133460	-0.8533237922	1.3326837285
C	1.8042975762	-2.3828690070	1.1922390572
C	2.4541376611	4.9510384036	-2.1939134152
C	2.5867368205	-3.1004354099	2.0862831119
C	-5.0492192372	-2.0973871115	-1.3628759114
C	-1.4932662579	3.7626336201	-1.6480755962
C	-2.6008720819	-2.0825371249	3.3060040755
C	1.5894549572	0.1737747294	5.7823762738
C	3.8731207745	3.4771460404	-0.3097692660
C	-1.3050237354	-4.8617284910	-2.5047907398
C	4.1087351430	0.0962080253	-4.1549760679
C	1.2131447099	-1.0475481581	5.2377991425
C	-2.5412800778	4.7401182715	-3.5771147433
C	3.4950227359	-4.3736074827	0.2572354691
C	-3.9688140888	-1.8277614622	-2.1949209516
C	-2.7880123137	-3.5414611252	0.9467074431
C	-5.3049237628	-1.2813561038	-0.2702123179
C	-1.3463955305	-3.2733209406	-4.3068850084
H	0.0658026142	-2.0502265627	3.7360392866
H	1.5730572844	-1.9700605014	5.6750312141
H	2.2441572038	0.2052149798	6.6437737362
H	1.4388846826	2.3111905508	5.6188432738
H	-0.0527380081	2.2415621679	3.6625160640
H	2.2450983347	1.4917301898	2.1726683799
H	3.6382746137	0.5798913857	3.9796809276
H	5.5217265495	-0.9428076293	3.4496747831
H	6.0103898393	-1.5219734773	1.0966569216
H	4.6434966398	-0.5881239796	-0.7194233770
H	4.4351969661	2.9046294795	0.4173101017
H	5.0773483912	5.2331838937	-0.0715912172
H	3.8218515529	6.5443730731	-1.7473530257
H	1.9068028143	5.5194554835	-2.9346431461
H	1.2347414448	3.2054699166	-2.4278239784
H	4.1498093172	1.7730012710	-2.8268322531
H	4.8654999527	0.5071893299	-4.8100839538
H	3.8634616818	-1.7064036606	-5.2950351441
H	2.1357542614	-2.6254667923	-3.8130315549
H	2.7768813644	-3.8688438654	-1.6960392676
H	4.1533528737	-5.1512101531	-0.1072979352
H	4.0445631716	-4.6565177135	2.3120089526

H	2.5427434017	-2.8673491552	3.1427527867
H	1.1589262040	-1.5938959119	1.5608693579
H	-0.1437268034	-4.3137676698	-0.7872448393
H	-1.6022570947	-5.8135080169	-2.0836082497
H	-2.3641562673	-5.1640142613	-4.3453245217
H	-1.6775125196	-2.9825534002	-5.2955178941
H	-0.2370835641	-1.4693281291	-4.0011155404
H	-4.0284414907	1.8039455843	-2.7750460614
H	-4.1650331269	3.6284778402	-4.4285857413
H	-2.6093629442	5.5424897632	-4.2998514899
H	-0.9067145259	5.6335154573	-2.5023076974
H	-0.7451627156	3.8035815698	-0.8625682935
H	-4.6826847833	0.4328792811	0.8602309940
H	-6.1403024867	-1.4951615103	0.3833581947
H	-5.6880680544	-2.9474612736	-1.5642777972
H	-3.7573474818	-2.4642277138	-3.0443333112
H	-2.2970441448	-0.5438308030	-2.5722882347
H	-2.5334575944	-1.5180859192	4.2292043079
H	-3.8706798403	-3.5769859895	4.1556333501
H	-4.0417537882	-4.8844289300	2.0614378035
H	-2.8633075210	-4.0976583735	0.0201633666
H	-1.5684022227	-2.0271553551	0.0664694557
H	-4.0860951675	3.5400403558	0.2227369089
H	-4.9940929840	4.2966202575	2.4098304366
H	-4.1428781172	3.2671787421	4.5034469616
H	-2.3948933489	1.5678005488	4.4478817283

S_1-Cu^{pyrz}	X	Y	Z
Cu	0.0325024044	0.2541111143	0.0500375556
P	2.4887981035	0.4489634777	0.2696509909
P	0.6383056663	-1.7940607985	-1.2422476620
P	-1.9338177401	0.1530411265	1.4810928851
P	-1.1650418378	2.2904301053	-0.5352731901
N	-2.7107219957	4.0326082325	0.7969243577
N	2.9432457834	-2.4052617475	-2.5971297062
N	-3.5119602832	2.0028527850	2.6667492812
N	4.4746134492	-0.4209185680	-1.4088495117
C	-2.2047537507	2.7951640960	0.8222187418
C	3.6884342454	1.7895409674	0.4417483833
C	0.6895482094	-3.3224929566	-0.2624720624
C	2.7073065593	-0.6534719047	1.7033068975
C	1.9059158493	-0.4143968890	2.8209877497
C	-0.1451502085	-2.2640008263	-2.8145028221
C	3.1937723019	-0.5887197886	-1.0814389463
C	-2.1738135747	1.8446316727	-1.9612209285
C	2.4139338101	-1.5733759733	-1.7012368185
C	-2.5883868308	1.8158993861	1.7314781546
C	1.1610171492	4.9641729788	-2.5511043445
C	-1.6640400224	-0.5271999388	3.1359251849
C	5.6174361740	2.7997208486	1.4611750107
C	1.9573105571	-1.2629772962	3.9162696269
C	-3.5438403168	2.1110805257	-1.9525007703
C	-1.6217956788	1.0678541661	-2.9824619863
C	0.8285604711	-5.6077286735	1.3107624844
C	1.0079735411	-4.5507529197	-0.8447578502
C	-3.2156923858	-1.2032991923	-0.5806750080

C	-1.2849048671	-3.0671858321	-2.7829248749
C	-3.2748788434	-0.8251349097	0.7591754858
C	-1.3271053965	0.3270432516	4.1880401137
C	3.5713366974	-1.7479539742	1.7030606770
C	3.5955996780	2.8607125385	-0.4447117450
C	-5.4931779097	-1.7432570684	0.9143992390
C	0.2897977132	3.9201905373	-2.2810962609
C	0.3127409266	-1.7753413354	-4.0372045414
C	5.5367018224	3.8561705349	0.5639510737
C	-1.4716655923	-2.9188136112	-5.1772484014
C	-1.7826188964	-1.8982548984	3.3691981873
C	1.3518907975	5.4279382432	-0.1926148093
C	-1.1419479214	-0.1846181051	5.4626712044
C	-5.4271954760	-2.1263496366	-0.4202356162
C	-0.0510375200	3.6307326091	-0.9587504731
C	-3.6428608447	4.2428141010	1.7846609677
C	-4.0279839184	3.2808400264	2.6688364617
C	4.2189807647	-2.2415382956	-2.9062123428
C	2.8113616590	-2.3582536024	3.9025585739
C	3.6211028344	-2.5957298977	2.8002428282
C	0.4463438210	-3.2464030622	1.1056209205
C	4.5273360849	3.8853178129	-0.3887780503
C	0.5157217197	-4.3884424788	1.8920376507
C	-3.7946297396	0.8362930447	-3.9791536998
C	0.4929455533	4.3803899744	0.0879991165
C	-4.4223739993	-1.0946282385	1.5094476091
C	-1.2725928818	-1.5490782026	5.6936002706
C	4.6990415202	1.7624586729	1.3993062724
C	-1.9451618248	-3.3894831225	-3.9601426561
C	4.9822513256	-1.2304071686	-2.3236767008
C	-1.5848183942	-2.4050921069	4.6450603697
C	1.6868194486	5.7195443221	-1.5098045230
C	1.0750461912	-5.6877155425	-0.0564919770
C	-2.4324401130	0.5647085764	-3.9881909180
C	-4.2894637421	-1.8562931074	-1.1679517900
C	-4.3457624071	1.6119040069	-2.9666679054
C	-0.3427511796	-2.1113777958	-5.2128150855
H	-2.0580867385	-2.5661622751	2.5612081387
H	-1.6976460616	-3.4664684896	4.8247105377
H	-1.1388942734	-1.9436349004	6.6925157716
H	-0.9108067161	0.4849612447	6.2806957386
H	-1.2526347680	1.3933813824	4.0167253970
H	1.2295107666	0.4348276870	2.8337600688
H	1.3233822641	-1.0709364442	4.7712564818
H	2.8467386532	-3.0267062299	4.7531065205
H	4.2893997608	-3.4466199753	2.7899676199
H	4.2067565530	-1.9460834075	0.8492145317
H	4.7713856519	0.9341662261	2.0926530286
H	6.4011432783	2.7792168001	2.2067708554
H	6.2593379384	4.6603137229	0.6106660555
H	4.4577545219	4.7106468676	-1.0851118334
H	2.7962404051	2.8999817471	-1.1786324816
H	6.0205291145	-1.0831470932	-2.5969265364
H	4.6476157550	-2.9217379593	-3.6326140257
H	1.2020608946	-4.6096029165	-1.9089770603
H	1.3189502721	-6.6405190160	-0.5075251252

H	0.8804691386	-6.5008937605	1.9197100315
H	0.3287087946	-4.3140384369	2.9561347369
H	0.2165911795	-2.2940053975	1.5701770327
H	-1.6502801428	-3.4566918150	-1.8395016325
H	-2.8212783632	-4.0240583437	-3.9256191908
H	-1.9773753155	-3.1849317725	-6.0961150840
H	0.0334071746	-1.7448281291	-6.1591929990
H	1.1955136570	-1.1507316644	-4.0829623261
H	-0.1476839137	3.3566315856	-3.0950821138
H	1.4134425132	5.2016081001	-3.5760261228
H	2.3532836194	6.5445466624	-1.7264635405
H	1.7595008804	6.0200936282	0.6156882132
H	0.2192322688	4.1561918010	1.1118056399
H	-3.9752863680	2.7027292399	-1.1552072963
H	-5.4067074429	1.8235306675	-2.9605886436
H	-4.4285875703	0.4390395509	-4.7611319348
H	-2.0015045233	-0.0484567799	-4.7678646946
H	-0.5614810862	0.8321246199	-2.9813857612
H	-4.4768470642	-0.7801360951	2.5444031073
H	-6.3845117455	-1.9465610182	1.4931133887
H	-6.2677872573	-2.6322478592	-0.8770693166
H	-4.2328988859	-2.1412184120	-2.2112731016
H	-2.3415043758	-0.9747582488	-1.1801737182
H	-4.0828103290	5.2307391636	1.8196820277
H	-4.7797055776	3.4893626446	3.4181101988

T_1-**Cu^{pyrz}**	X	Y	Z
Cu	0.1037897034	0.2259696118	0.0340882307
P	2.4301542195	-0.3818037853	0.6083114498
P	0.1006918316	-2.0577722635	-0.9729204847
P	-1.9225680260	0.9980073927	1.1228662957
P	-0.1676361138	2.4853307849	-0.8804661138
N	-1.1109062425	4.8061746392	0.0779634719
N	2.1823894230	-3.6105053359	-1.8563873218
N	-2.8616829818	3.4255099755	1.8773051814
N	4.1649708230	-2.1016214382	-0.6367794727
C	-1.1128504192	3.4707682805	0.2470153131
C	3.9982531511	0.4812773030	0.8575248614
C	-0.5264841359	-3.3546257898	0.1338651079
C	2.0601903803	-1.2831189661	2.1489450841
C	1.2719741480	-0.6310404271	3.0989869421
C	-0.5950732300	-2.4522816928	-2.6063930540
C	2.8786231859	-1.7786000180	-0.5080042028
C	-1.0854150063	2.1714087415	-2.4027965289
C	1.8798844015	-2.5238194843	-1.1476191543
C	-1.9658137584	2.8113040722	1.1344044471
C	3.1461531570	3.9416829399	-2.7617502871
C	-2.1293264590	0.5126876223	2.8580642474
C	6.0209172455	0.9035639642	2.0868647960
C	0.8765579981	-1.2882966092	4.2539925142
C	-2.2866585532	2.8466064526	-2.6317458423
C	-0.7089935980	1.1197649345	-3.2427014244
C	-1.4273409065	-5.2957866321	1.9052552161
C	-0.5984931448	-4.6884546498	-0.2719442814
C	-3.3569956711	-0.0963566956	-0.9899238361

C	-1.9461646668	-2.7877271269	-2.6948860937
C	-3.4369081084	0.4656345517	0.2824772917
C	-1.6242823854	1.3314172682	3.8696417047
C	2.4579983153	-2.5998292794	2.3793078821
C	4.4025836393	1.3884280493	-0.1199855084
C	-5.8384257619	0.3782355445	0.1633881548
C	1.9366391298	3.3021278618	-2.5372586114
C	0.1606998554	-2.3489025384	-3.7730439650
C	6.4322114492	1.7918567241	1.1022776318
C	-1.7625297110	-2.9510221341	-5.0886102954
C	-2.7675882727	-0.6821166917	3.1913953032
C	3.2415560027	4.5968383700	-0.4428910026
C	-1.7874883702	0.9724492967	5.1984196635
C	-5.7543176653	-0.1905164451	-1.1026066719
C	1.3810650782	3.3079067891	-1.2570226680
C	-2.0324449188	5.4447893663	0.8571821173
C	-2.8744827578	4.7982747572	1.7131794868
C	3.4604299095	-3.9341031482	-1.9663791008
C	1.2658882698	-2.6041103113	4.4687167960
C	2.0606676037	-3.2555357393	3.5356126498
C	-0.9037268315	-3.0022279046	1.4263751647
C	5.6240738667	2.0325849274	-0.0005189162
C	-1.3540342116	-3.9722668035	2.3116841818
C	-2.7161222884	1.4269000552	-4.5269192354
C	2.0437671047	3.9465841187	-0.2054500181
C	-4.6860173443	0.7066994551	0.8595891526
C	-2.4351202674	-0.2125467936	5.5273386822
C	4.8078855426	0.2426797143	1.9650522350
C	-2.5257523219	-3.0323197215	-3.9316598270
C	4.4575590616	-3.1619228464	-1.3718529537
C	-2.9164903016	-1.0423184618	4.5231727386
C	3.7941179087	4.5919313984	-1.7183446036
C	-1.0490263686	-5.6527763340	0.6145362959
C	-1.5249547337	0.7490164502	-4.3001625088
C	-4.5148063583	-0.4270764227	-1.6795276856
C	-3.0903835289	2.4778187624	-3.6979195431
C	-0.4196595874	-2.6086654713	-5.0063100606
H	-3.1733662414	-1.3184574622	2.4133070407
H	-3.4298750313	-1.9609684133	4.7763929009
H	-2.5705165718	-0.4849226611	6.5659966276
H	-1.4200378061	1.6255677623	5.9790966480
H	-1.1378018134	2.2657583085	3.6188795054
H	0.9553946168	0.3940825642	2.9320237728
H	0.2570975045	-0.7740701738	4.9762097787
H	0.9498378468	-3.1217950831	5.3651668650
H	2.3675115402	-4.2795307910	3.7030491435
H	3.0752524467	-3.1217174118	1.6591816689
H	4.4945649282	-0.4582119537	2.7283544376
H	6.6486428671	0.7192988990	2.9485758414
H	7.3827008453	2.3004010688	1.1971822477
H	5.9388582802	2.7291692928	-0.7663831790
H	3.7662549808	1.5966700413	-0.9749288700
H	5.5052827226	-3.4142297975	-1.4859187119
H	3.7030470414	-4.8209109807	-2.5397811360
H	-0.3012162591	-4.9637961124	-1.2766853849
H	-1.1076061131	-6.6863804247	0.2999070775

H	-1.7807240905	-6.0545676885	2.5912938614
H	-1.6402493223	-3.6845645025	3.3157709842
H	-0.8351700284	-1.9718231313	1.7573957467
H	-2.5451372571	-2.8755223362	-1.7954606922
H	-3.5717900266	-3.3046281391	-3.9879648278
H	-2.2112789185	-3.1594005285	-6.0509244248
H	0.1813953947	-2.5471471098	-5.9043014588
H	1.2101306432	-2.0888355046	-3.7263078478
H	1.4141151057	2.8287267749	-3.3584530020
H	3.5730246767	3.9504844381	-3.7558356712
H	4.7299416023	5.1040722954	-1.9021699441
H	3.7467315236	5.1067520430	0.3663869434
H	1.6049640640	3.9495097387	0.7851366404
H	-2.5882446093	3.6522247400	-1.9743606262
H	-4.0170138602	3.0071856603	-3.8758167498
H	-3.3552907216	1.1329075403	-5.3492482228
H	-1.2362580645	-0.0760589686	-4.9368585683
H	0.2108783915	0.5720650316	-3.0582082795
H	-4.7479746626	1.1625399794	1.8400838817
H	-6.8060286604	0.5702317928	0.6078842879
H	-6.6589596669	-0.4443260175	-1.6397135660
H	-4.4392298121	-0.8593289353	-2.6697063018
H	-2.3936758772	-0.2614055129	-1.4605058634
H	-2.0743286210	6.5220011796	0.7568317843
H	-3.5964283507	5.3437445160	2.3044321213

S_1-**Cu^{quinox}**	X	Y	Z
Cu	0.0393294581	0.2656084606	0.0486897835
P	2.4940998464	0.4564528500	0.2213193155
P	0.6272656641	-1.7448751432	-1.3234170920
P	-1.8593073835	0.1581678930	1.5789434788
P	-1.2300204583	2.2834479038	-0.4982185311
N	-2.6705835737	4.0273272736	0.9223747469
N	2.8583405867	-2.2111035025	-2.8266771481
N	-3.3271302674	2.0187944639	2.8675355874
N	4.4055838258	-0.2444705386	-1.5864128528
C	-2.1651567924	2.8030602216	0.9246310386
C	3.6766846860	1.8037686088	0.4485206295
C	0.7639007413	-3.2646564194	-0.3369435118
C	2.7710285252	-0.7317420640	1.5738910750
C	2.0230965526	-0.5571164178	2.7393835080
C	-0.2220054026	-2.2540863235	-2.8495504547
C	3.1755023627	-0.4759057878	-1.2163031258
C	-2.3326444571	1.7845334345	-1.8342172445
C	2.3740091784	-1.4699107217	-1.8675628979
C	-2.4833202180	1.8223841965	1.8759676369
C	1.0523334240	4.8138790422	-2.7300819141
C	-1.5275194000	-0.5507677351	3.2100348829
C	5.5937357614	2.7969460862	1.5062392194
C	2.1260192738	-1.4636682769	3.7829934863
C	-3.7006731865	2.0398596556	-1.7276305787
C	-1.8522285965	0.9817121997	-2.8709580910
C	1.0144448632	-5.5360275939	1.2421412307
C	1.2176991474	-4.4580170131	-0.9011845179

C	-3.1837418701	-1.2612236955	-0.4213757832
C	-1.3126220115	-3.1179981656	-2.7524859581
C	-3.2312312899	-0.8053710827	0.8939060737
C	-1.0999766222	0.2783864952	4.2492726707
C	3.6314769988	-1.8241963758	1.4706676128
C	3.5521318483	2.9210631863	-0.3751540998
C	-5.4765992804	-1.6439701188	1.0982613886
C	0.1875618460	3.7923792365	-2.3720373539
C	0.1293869129	-1.7352016643	-4.0952099674
C	5.4785638126	3.9025359824	0.6748190537
C	-1.6604347763	-2.9689250614	-5.1288209882
C	-1.6889114554	-1.9182310238	3.4386247585
C	1.2612884538	5.4606371415	-0.4168245009
C	-0.8625650345	-0.2539234933	5.5065993538
C	-5.4237983149	-2.1022307728	-0.2135809133
C	-0.1410487657	3.6042153524	-1.0274716281
C	-3.5399915786	4.2886336228	1.9653622558
C	-3.8673630177	3.2935416916	2.9294848603
C	4.1361147184	-1.9929204272	-3.2201089236
C	2.9764412131	-2.5559117796	3.6673179922
C	3.7301962738	-2.7324994041	2.5150566063
C	0.4395108491	-3.2169867566	1.0148040008
C	4.4591185153	3.9631551006	-0.2662175150
C	0.5643598340	-4.3516411125	1.8049222567
C	-4.0918238002	0.7027507526	-3.6905587347
C	0.4091323393	4.4347042506	-0.0466528524
C	-4.3859846313	-0.9967636553	1.6570709918
C	-1.0356949443	-1.6143136957	5.7334650106
C	4.6976958698	1.7440184794	1.3926916974
C	-2.0288665119	-3.4701629666	-3.8881175130
C	4.9142968906	-0.9813235754	-2.6030559874
C	-1.4422248526	-2.4456349647	4.6975866132
C	1.5849789914	5.6496420819	-1.7548820412
C	1.3410964181	-5.5882440712	-0.1098838230
C	-2.7314747231	0.4411092344	-3.7958575031
C	-4.2785739060	-1.9109589748	-0.9734269924
C	-4.5723427457	1.5042964511	-2.6629145321
C	-0.5812622732	-2.1005155835	-5.2291269378
C	4.6944099089	-2.7694592454	-4.2610165034
C	6.2383583517	-0.7525983670	-3.0412537362
C	6.7528632625	-1.5151841154	-4.0499684978
C	5.9771190580	-2.5306552684	-4.6622996465
C	-4.1195299827	5.5558606944	2.0696889154
C	-4.7569011923	3.6081133539	3.9578217695
C	-4.9961310756	5.8456743754	3.0996464084
C	-5.3152798870	4.8714973798	4.0446383626
H	-2.0364314694	-2.5659975637	2.6420425782
H	-1.5897857778	-3.5031026317	4.8751567015
H	-0.8616649669	-2.0244432347	6.7198203723
H	-0.5583033470	0.3973867891	6.3153552300
H	-0.9945691298	1.3429953877	4.0835359233
H	1.3504051497	0.2896932193	2.8311466616
H	1.5348649129	-1.3182610055	4.6772422918
H	3.0515515819	-3.2707528700	4.4765842772
H	4.3942648838	-3.5820239096	2.4248798649
H	4.2258639027	-1.9732762156	0.5780857332

H	4.7954255586	0.8788246927	2.0361359922
H	6.3855746649	2.7509785085	2.2420888202
H	6.1818208534	4.7202432839	0.7633916080
H	4.3636397106	4.8258647893	-0.9126063343
H	2.7487909389	2.9802603823	-1.1033579502
H	1.4725665302	-4.4940095903	-1.9538891120
H	1.6915787510	-6.5143535438	-0.5461327114
H	1.1123722950	-6.4236630355	1.8535700029
H	0.3159607810	-4.2979548005	2.8576524142
H	0.1055157839	-2.2892166557	1.4645210404
H	-1.5955324170	-3.5314730714	-1.7909546939
H	-2.8654942267	-4.1515621518	-3.8029125664
H	-2.2088437693	-3.2577173172	-6.0158215153
H	-0.2870133913	-1.7087577879	-6.1942292006
H	0.9739461585	-1.0655446853	-4.1917812493
H	-0.2542809356	3.1660473411	-3.1363056926
H	1.2961200669	4.9709377254	-3.7723263551
H	2.2470027130	6.4567119976	-2.0414415902
H	1.6723741176	6.1152256291	0.3399937683
H	0.1445125189	4.2923345727	0.9931277711
H	-4.0762854557	2.6507636363	-0.9166626948
H	-5.6319056803	1.7070477983	-2.5815820240
H	-4.7798073210	0.2756876860	-4.4086119730
H	-2.3543344083	-0.1946743767	-4.5856041860
H	-0.7936738943	0.7512617094	-2.9423738846
H	-4.4287627626	-0.6231153981	2.6730427887
H	-6.3731022713	-1.7877685415	1.6867837702
H	-6.2803463046	-2.6058628797	-0.6424647338
H	-4.2315613057	-2.2551654737	-1.9992598744
H	-2.3026546750	-1.0950142562	-1.0303663532
H	4.0801201711	-3.5357676660	-4.7146675829
H	6.8095937577	0.0264582234	-2.5544715979
H	7.7663275643	-1.3486338654	-4.3901684820
H	6.4130217085	-3.1197438102	-5.4582254601
H	-4.9912620456	2.8359162878	4.6787303669
H	-3.8586037334	6.2944986118	1.3233279835
H	-5.4363930999	6.8312615199	3.1703660691
H	-6.0026716706	5.1024003480	4.8473274090

T_1-**Cu^{quinox}**	X	Y	Z
Cu	-0.0160195530	-0.0125124637	0.2571176135
P	1.7426956838	-1.4125887487	1.1737680924
P	1.9197293481	0.9847109849	-0.9213337516
P	-1.7954320179	1.3001252785	1.2715073494
P	-1.8950095436	-0.8701884561	-1.1205635930
N	4.2465842403	-0.6220321795	2.0219475692
N	4.4601962750	1.4294666045	0.0760561294
N	-4.2681137998	0.3471617727	1.9471415660
N	-4.3841974853	-1.4952971070	-0.1511498994
C	3.2206369972	-0.3323845928	1.1538188944
C	3.3077789122	0.6851916102	0.2330031988
C	5.4667939052	1.1420185612	0.9013351465
C	5.3557011180	0.1110041192	1.8954160445
C	6.4509408332	-0.1288977264	2.7487379332

C	7.6664373963	0.6396725753	2.6465403558
C	7.7743878031	1.6073710327	1.7053345654
C	6.6718625616	1.8719058931	0.8166702813
C	1.7610725180	-2.2661322679	2.7717077435
C	0.7235459213	-2.0079338006	3.6635596389
C	0.6852018618	-2.6438566751	4.8978283841
C	1.6804321271	-3.5472311663	5.2368295989
C	2.7113225986	-3.8200673089	4.3435367305
C	2.7538706760	-3.1840321139	3.1145838254
C	2.1760196355	-2.6854504853	-0.0586489112
C	1.1429846424	-3.5164569378	-0.4902172094
C	1.3621596808	-4.4533987219	-1.4874168595
C	2.6212192660	-4.5655736634	-2.0639867857
C	3.6553127061	-3.7440503351	-1.6376902804
C	3.4364847302	-2.8049877413	-0.6387780027
C	2.1025236533	2.7275945275	-1.3973021044
C	2.3876104116	3.6896923999	-0.4290471342
C	2.4225807467	5.0334555489	-0.7677873741
C	2.1660230073	5.4305139846	-2.0750275415
C	1.8680483391	4.4788560396	-3.0394713635
C	1.8351120972	3.1314824044	-2.7038017064
C	2.4352682646	0.0526635187	-2.4012659628
C	3.6666039476	0.2978695628	-3.0118530230
C	4.0613511191	-0.4627226553	-4.1010708481
C	3.2330917595	-1.4680960743	-4.5890261316
C	2.0083954523	-1.7140452168	-3.9868025487
C	1.6107837439	-0.9548117957	-2.8948435307
C	-3.2836208917	0.2198447952	1.1020525427
C	-3.3390597223	-0.7363948401	0.0279756972
C	-5.4168160332	-1.3780169942	0.7210052919
C	-5.3533121968	-0.4517341328	1.7898075800
C	-6.4338053305	-0.3525537266	2.6944296600
C	-7.5300159255	-1.1487905111	2.5230439152
C	-7.5953284235	-2.0722370519	1.4515896024
C	-6.5625764432	-2.1900687483	0.5657292009
C	-1.8865288021	1.9841405297	2.9450873310
C	-0.8598661438	1.6751180268	3.8333972383
C	-0.8772062209	2.1823433044	5.1262262916
C	-1.9172810771	3.0061665319	5.5277791689
C	-2.9375730821	3.3293868661	4.6392029198
C	-2.9246352410	2.8226823052	3.3508220211
C	-2.2134427503	2.6845640229	0.1622252909
C	-1.1782255716	3.5677708189	-0.1431775684
C	-1.3880531436	4.6232808150	-1.0156673103
C	-2.6365563429	4.7977507918	-1.5999682886
C	-3.6705843233	3.9213205188	-1.3032089361
C	-3.4643066834	2.8679683097	-0.4220131484
C	-2.0591134657	-2.5180243144	-1.8694647873
C	-2.3508091202	-3.6324313874	-1.0828162656
C	-2.3631304297	-4.8996449010	-1.6441651300
C	-2.0720604133	-5.0697135606	-2.9927206966
C	-1.7622124474	-3.9675739183	-3.7753518416
C	-1.7557571253	-2.6950766981	-3.2180901788
C	-2.3812105102	0.2796980919	-2.4489884156
C	-3.6173844525	0.1542005548	-3.0840905621
C	-3.9826831149	1.0563679443	-4.0703623890

C	-3.1191789273	2.0865281990	-4.4281706324
C	-1.8896461270	2.2147367873	-3.7998652045
C	-1.5208937313	1.3117213270	-2.8121725297
H	6.3547285299	-0.9197847321	3.4807595889
H	8.4814534104	0.4263673061	3.3234607121
H	8.6791604862	2.1904034964	1.6069838570
H	6.7358006179	2.6537666659	0.0715982813
H	-0.0655611499	-1.3176326335	3.3866054824
H	-0.1244550104	-2.4393768810	5.5858906920
H	1.6511422302	-4.0489436758	6.1953336884
H	3.4809262579	-4.5334072365	4.6077208475
H	3.5542843569	-3.3970100511	2.4175841075
H	0.1555486872	-3.4232490409	-0.0520816607
H	0.5452541496	-5.0822180442	-1.8179360206
H	2.7949709997	-5.2897386699	-2.8494131431
H	4.6353250127	-3.8262507593	-2.0893854887
H	4.2484189324	-2.1593366788	-0.3269214922
H	2.5933286401	3.3876748727	0.5916384678
H	2.6567096951	5.7720958525	-0.0122656298
H	2.2009059129	6.4793993608	-2.3393349121
H	1.6711587419	4.7821566076	-4.0596704635
H	1.6183181484	2.3927719518	-3.4670497239
H	4.3085647635	1.0828348522	-2.6288852452
H	5.0163430482	-0.2715790858	-4.5729917669
H	3.5471008879	-2.0595785692	-5.4393730384
H	1.3633315892	-2.5031356624	-4.3523271357
H	0.6635467429	-1.1685215920	-2.4129504922
H	-6.3580586823	0.3606666776	3.5043648920
H	-8.3623112510	-1.0781044532	3.2106866954
H	-8.4765524906	-2.6899035587	1.3397835030
H	-6.5858796251	-2.8893588056	-0.2594635650
H	-0.0370225583	1.0478355759	3.5088427672
H	-0.0764362804	1.9398376836	5.8123064121
H	-1.9316579906	3.4068538655	6.5330374717
H	-3.7423240717	3.9808694823	4.9534530225
H	-3.7160619310	3.0764320670	2.6573207822
H	-0.1987954911	3.4275985711	0.2999317214
H	-0.5720525164	5.2973641723	-1.2429336237
H	-2.8025462289	5.6149472754	-2.2900302212
H	-4.6423168909	4.0528075779	-1.7610321175
H	-4.2807193045	2.1907704927	-0.2030688199
H	-2.5846194827	-3.5116285651	-0.0321263106
H	-2.6059634239	-5.7561635908	-1.0288039178
H	-2.0891620858	-6.0593457711	-3.4303500700
H	-1.5370953818	-4.0928990201	-4.8265627473
H	-1.5288249741	-1.8379408667	-3.8416838153
H	-4.2877523407	-0.6502642396	-2.8027527493
H	-4.9416248431	0.9575379376	-4.5620446377
H	-3.4102869808	2.7907432527	-5.1968732687
H	-1.2187140489	3.0224953550	-4.0636250216
H	-0.5683381723	1.4292092901	-2.3082788598

S_1-Ag^{bz}	X	Y	Z
Ag	10.4056811626	4.5123209174	9.2838974375
P	8.5351879656	2.9325724692	10.2072201656

P	8.5754052831	4.2533357606	7.2382808995
P	11.0358222125	7.0091316468	10.0131861527
P	12.9132713626	4.7930950768	8.9236173122
C	13.5830178779	5.9111089954	10.1235662980
C	8.8999812546	1.6759814913	11.4669706169
C	7.1057449016	5.2799214184	7.5717914077
C	7.0255807656	3.7708321724	10.7866605910
C	7.1516426757	4.7120368387	11.8097095821
C	8.8596322235	4.4057886979	5.4469995069
C	7.9547425654	1.9695570962	8.7593132324
C	13.0227500902	5.6056522603	7.3056012251
C	7.9203009025	2.5516093452	7.4769319881
C	12.6872743829	6.9386147620	10.5726912099
C	15.4100534590	1.7502341788	7.8134886357
C	9.9544108395	7.3396497873	11.4196619169
C	8.3473727049	0.3504594829	13.3995441644
C	6.0287564074	5.3659368014	12.2947241120
C	13.6399357842	6.8472913096	7.1733700580
C	12.3647252801	5.0369406419	6.2144022186
C	14.9314882019	5.9504203667	10.4430023266
C	4.8518925522	6.7650986431	8.2506520876
C	7.3660516149	1.8245639333	6.4229177767
C	5.9059285274	5.0887753237	6.8859645049
C	10.3604089097	7.8455201415	7.4413745563
C	8.5019264950	5.5709568454	4.7708297163
C	10.5883175019	8.2453969941	8.7614318197
C	13.2619298241	8.0430855299	11.2826209958
C	10.3288702287	6.8704939713	12.6837687862
C	5.7711805038	3.5252572047	10.2316041024
C	10.1321800090	1.0267184376	11.3854829107
C	10.4612411333	10.5524070451	8.0627766660
C	14.6584843934	2.9179869673	7.7775405338
C	9.5595072172	3.4102053596	4.7604234809
C	9.5686657991	-0.3011467305	13.3066285493
C	7.4727564220	0.6731433854	8.9364897801
C	9.4711143661	4.7129539021	2.7398589703
C	8.7456340143	8.0287366122	11.2704768208
C	14.6592089036	1.3237878042	10.0611467502
C	9.5122179707	7.0985862460	13.7796616388
C	10.2256672179	10.1467689851	6.7543569356
C	13.9042947133	3.2885862971	8.8886217575
C	15.4556269810	6.9994960133	11.1901386040
C	14.5995366622	8.0484222537	11.5845786101
C	6.8826187233	0.5396721614	6.6158020331
C	4.7805770300	5.1157265730	11.7399285455
C	4.6558051901	4.2044369134	10.7016276713
C	7.1649563687	6.2226095014	8.5933137326
C	10.4610248890	0.0355051247	12.2959900655
C	6.0400773931	6.9593910973	8.9379617052
C	12.9444622232	6.9417964123	4.8711508882
C	13.9025841723	2.4814520004	10.0303863972
C	10.6361083038	9.6118093236	9.0655890547
C	8.3204231302	7.7969213175	13.6267108024
C	8.0082645558	1.3352242692	12.4804932018
C	8.8098345286	5.7220567120	3.4240046982
C	6.9466729816	-0.0425542562	7.8726132401

C	7.9391670348	8.2594765147	12.3722503571
C	15.4111301865	0.9552260378	8.9495792126
C	4.7860469999	5.8322195518	7.2209707411
C	12.3281784393	5.7020215388	4.9990055265
C	10.1716347517	8.7925230044	6.4478099491
C	13.5995434802	7.5102400697	5.9542088369
C	9.8491183962	3.5566217882	3.4129292146
H	8.4544528400	8.4064573890	10.2978389519
H	7.0134107964	8.8086362132	12.2558830562
H	7.6922282841	7.9881255014	14.4874796004
H	9.8130431840	6.7457560541	14.7572688315
H	11.2709988465	6.3487653315	12.7998752638
H	8.1265445929	4.9343823730	12.2347878703
H	6.1329137667	6.0772568817	13.1026204261
H	3.9074045581	5.6342836520	12.1142051875
H	3.6877261650	4.0148970561	10.2566208141
H	5.6587975109	2.8119211137	9.4249805216
H	7.0508620798	1.8360813732	12.5535089314
H	7.6526158353	0.0905613869	14.1873086494
H	9.8279937279	-1.0690596904	14.0234514012
H	11.4148687463	-0.4702724034	12.2222344053
H	10.8338690586	1.2950949661	10.6019696779
H	7.5049846181	0.2194520345	9.9189807572
H	6.5799042496	-1.0483592816	8.0290618886
H	6.4593211953	-0.0053106452	5.7822486099
H	7.3167983475	2.2628473857	5.4346011389
H	5.8476168487	4.3541506016	6.0908685786
H	3.8584519193	5.6815587115	6.6843716297
H	3.9721910196	7.3363344067	8.5176510688
H	6.0916240185	7.6730381530	9.7505952466
H	8.0890081645	6.3672538605	9.1428546250
H	7.9695999524	6.3581721796	5.2915811744
H	8.5167082761	6.6265968832	2.9070124504
H	9.6941881082	4.8252319665	1.6870281344
H	10.3721605224	2.7681824998	2.8874234174
H	9.8612784292	2.5050144604	5.2758607669
H	14.6707832133	3.5437088762	6.8943974133
H	16.0024970124	1.4682174876	6.9532260068
H	16.0013246964	0.0486614105	8.9740349168
H	14.6682861927	0.7085168426	10.9512214017
H	13.3204903691	2.7753453577	10.8974254482
H	14.1361549964	7.2992293866	8.0237949050
H	14.0728539242	8.4782863222	5.8564574647
H	12.9089226484	7.4662857544	3.9249724407
H	11.8107639052	5.2576737814	4.1589873940
H	11.8665983851	4.0775880391	6.3174291556
H	10.8022740252	9.9374544180	10.0858847936
H	10.5028672740	11.6065562833	8.3045004991
H	10.0864010962	10.8859913621	5.9766943475
H	9.9956228682	8.4666439509	5.4300475489
H	10.3472756069	6.7916587392	7.1804597130
H	15.5814965409	5.1547312051	10.0964126477
H	16.5021929637	7.0142133452	11.4546596243
H	14.9994294514	8.8710557716	12.1644814280
H	12.6283511618	8.8514439320	11.6265045228

T_1-**Ag^{bz}**	X	Y	Z
Ag	0.0059974681	0.4287856624	0.0685427887
P	2.5366141278	0.9117698091	0.5579037692
P	1.3563640505	-1.3873463063	-1.4077629180
P	-2.0755731955	-0.1938112954	1.4386599650
P	-2.0037698553	2.2000974454	-0.7076488015
C	-2.8555002066	2.4295754148	0.7564851817
C	3.3865963794	2.4154778535	1.1137165731
C	1.6638806728	-2.8736515466	-0.3931572161
C	2.8507363208	-0.3438011909	1.8414976820
C	1.9742307288	-0.3833716985	2.9271379933
C	0.8325004860	-2.0332661954	-3.0276847388
C	3.5319701755	0.3133972536	-0.8601720699
C	-2.7395463975	1.0349536530	-1.8852466835
C	3.0334173684	-0.7004534065	-1.7015835828
C	-3.0745749322	1.2757562162	1.6422879664
C	-1.3521334844	5.1421449598	-3.4347355504
C	-1.7430002120	-0.8562746247	3.1032536813
C	4.9239295355	3.6070983378	2.5328155325
C	2.1174473744	-1.3482738629	3.9118576118
C	-4.0677091709	0.6514189528	-1.6939877698
C	-1.9593157146	0.4036691151	-2.8575265434
C	-3.5690996586	3.6519721208	1.0393209681
C	2.1331437018	-5.0882165318	1.2301721478
C	3.8363127931	-1.1743325992	-2.7393095117
C	2.5924055334	-3.8423970064	-0.7755452984
C	-2.5249572627	-2.2421874744	-0.3985012610
C	0.1621538802	-3.2515681246	-3.1234525240
C	-3.0743072513	-1.5053872808	0.6468809581
C	-4.0342252520	1.3929028860	2.6441756003
C	-1.4684651959	0.0148042743	4.1599859033
C	3.8681641499	-1.2914661510	1.7502620042
C	3.0950290257	3.6046068152	0.4444413997
C	-5.1194630898	-2.7653954548	0.4312540558
C	-1.7757253924	3.9578651438	-2.8518880006
C	0.9852862371	-1.2500942410	-4.1744997613
C	4.6425510801	4.7843018694	1.8543786675
C	4.8059676047	0.8292122691	-1.0955883826
C	-0.1405985839	-2.9210732596	-5.4898091322
C	-1.6946995167	-2.2329758470	3.3261096680
C	-0.4013035932	5.8493909988	-1.3357660312
C	-1.1768918275	-0.4842455517	5.4206585869
C	-4.5584894533	-3.5061899121	-0.6044428288
C	-1.5134960762	3.7195594428	-1.5011825349
C	-4.4819995849	3.7105496638	2.0412969645
C	-4.7428791431	2.5643820893	2.8570152204
C	5.1028716352	-0.6553813270	-2.9583441807
C	3.1332576303	-2.2906941873	3.8128651860
C	4.0048353452	-2.2623920344	2.7332249434
C	0.9756667736	-3.0261160161	0.8080581649
C	3.7285692406	4.7824038487	0.8076111947
C	1.2106588756	-4.1290004333	1.6183946518
C	-3.8426456154	-0.9565726796	-3.4661657984
C	-0.8157062076	4.6689710394	-0.7449645815
C	-4.3825790633	-1.7709328393	1.0537226990
C	-1.1468114241	-1.8563007800	5.6403064668

C	4.3014250725	2.4218698146	2.1634599797
C	-0.3236903159	-3.6896759550	-4.3496149792
C	5.5859371475	0.3526354315	-2.1382850424
C	-1.3982649452	-2.7273055595	4.5895975543
C	-0.6675299170	6.0859148313	-2.6804765139
C	2.8242515805	-4.9442367451	0.0317881703
C	-2.5133757285	-0.5856797288	-3.6506712896
C	-3.2630395822	-3.2425000886	-1.0196107021
C	-4.6167647193	-0.3412270775	-2.4931669248
C	0.5140651550	-1.6978875452	-5.3989183459
H	-1.9138183944	-2.9222340793	2.5186749628
H	-1.3833371205	-3.7969253589	4.7558322201
H	-0.9334036362	-2.2432760470	6.6281900541
H	-0.9847890413	0.2007876464	6.2363038918
H	-1.5116862251	1.0857932256	3.9998979157
H	1.1669283620	0.3385896437	3.0022710639
H	1.4258333950	-1.3684047112	4.7437690476
H	3.2400380827	-3.0532272867	4.5736872151
H	4.7910000187	-3.0014144062	2.6497506116
H	4.5465377960	-1.2854306475	0.9058031266
H	4.5267586470	1.5042384488	2.6928394036
H	5.6319351654	3.6086702162	3.3510692650
H	5.1312321782	5.7052902576	2.1437991316
H	3.5052482324	5.7003888677	0.2798396920
H	2.3712492167	3.6061799643	-0.3640882557
H	6.5711866997	0.7676073958	-2.3053112691
H	5.7077190167	-1.0369344716	-3.7703897475
H	3.1376967222	-3.7348973014	-1.7057205317
H	3.5455394139	-5.6917541632	-0.2715915587
H	2.3197889672	-5.9481343779	1.8603613841
H	0.6785785248	-4.2232847651	2.5568176317
H	0.2634019541	-2.2744152975	1.1320969954
H	0.0337060050	-3.8702039814	-2.2428143579
H	-0.8316347462	-4.6432991578	-4.4139246257
H	-0.5046978274	-3.2717939317	-6.4464584429
H	0.6575905566	-1.0914886312	-6.2838022557
H	1.4958852307	-0.2952789995	-4.1147584647
H	-2.3215486610	3.2279694608	-3.4360320384
H	-1.5656511692	5.3329457785	-4.4779422581
H	-0.3430681322	7.0103555629	-3.1397950871
H	0.1278893355	6.5881023472	-0.7484177865
H	-0.6104925473	4.4771775220	0.3019931317
H	-4.6575767602	1.1243769484	-0.9176160584
H	-5.6456210166	-0.6417119716	-2.3449553238
H	-4.2704672541	-1.7405861856	-4.0778321444
H	-1.9079473042	-1.0762663579	-4.4017400887
H	-0.9169184384	0.6809298098	-2.9867278543
H	-4.8290635837	-1.1935728676	1.8539703564
H	-6.1326788504	-2.9662035698	0.7543195888
H	-5.1367159009	-4.2831117736	-1.0876216232
H	-2.8261145651	-3.8006850086	-1.8382767454
H	-1.5207117873	-2.0269813964	-0.7492172898
H	-5.0078700953	4.6359794515	2.2327368471
H	-5.4579693481	2.6237526730	3.6645271461
H	5.1943569925	1.6116686042	-0.4562958846
H	3.4627735033	-1.9505614921	-3.3952372939

H	-3.3874288993	4.5210388453	0.4191026879
H	-4.1953169672	0.5591236075	3.3193519647

S_1-Ag^{pyrz}	X	Y	Z
Ag	-0.0384007925	0.3044538259	-0.0583958111
P	2.6036620577	0.0235133103	0.1106993372
P	0.4313177923	-2.0000650618	-1.3167010238
P	-2.1345076849	0.3239009205	1.4202649612
P	-1.0711029484	2.5786377668	-0.5227847034
N	-2.7058346258	4.2564784625	0.7590802315
N	2.5017504911	-2.6159140904	-2.9994930935
N	-3.6629747489	2.2146678419	2.5294417011
N	4.3247388124	-0.8958525942	-1.8131852846
C	-2.2522109293	3.0021894418	0.7559998937
C	3.9945008645	1.1468147889	0.3710036302
C	0.4853389893	-3.4819617666	-0.2734120490
C	2.6762884559	-1.2050410650	1.4559902984
C	1.9801914268	-0.9082581996	2.6289007290
C	-0.5347234072	-2.4464525774	-2.7844772812
C	3.0815617650	-0.9980887947	-1.3490915794
C	-1.8903181302	2.6289779104	-2.1309489267
C	2.1564243326	-1.8641762813	-1.9572195036
C	-2.7192601216	2.0124379502	1.6135653166
C	1.8588983047	5.1299171813	-1.7376271119
C	-1.7358296276	-0.2720279725	3.0770991044
C	6.2544001680	1.5994868471	1.0562077332
C	1.9699737989	-1.8054390230	3.6858408228
C	-2.4328578892	3.8348020590	-2.5831510404
C	-2.0397694946	1.4682414870	-2.8864472507
C	0.5654605158	-5.7043504107	1.3885194933
C	0.9983293808	-4.6891305699	-0.7504033261
C	-3.3942580508	-1.3682495966	-0.4001530661
C	-1.4926343473	-3.4558712719	-2.7366215211
C	-3.4874433874	-0.7125126620	0.8253440619
C	-1.1599769893	0.6122341672	3.9926289366
C	3.3540411447	-2.4192427901	1.3532906592
C	3.8196432878	2.4907522036	0.0510762576
C	-5.7202315285	-1.5586665618	1.1066447548
C	0.8417415196	4.1874967871	-1.7427599046
C	-0.4033671237	-1.6752084286	-3.9402982246
C	6.0820673917	2.9392008952	0.7258173797
C	-2.1570398271	-2.9398916594	-4.9923600527
C	-1.9675306507	-1.5983052999	3.4468021238
C	1.6095239997	5.3924060501	0.6453768889
C	-0.8443320560	0.1791640713	5.2695586430
C	-5.6218138575	-2.2177190045	-0.1131667061
C	0.1981185749	3.8531182513	-0.5500006245
C	-3.6826298804	4.4747211912	1.7007807072
C	-4.1387895993	3.5061842674	2.5417021708
C	3.7423752014	-2.5078359831	-3.4509379692
C	2.6460888088	-3.0133852060	3.5742097327
C	3.3351202964	-3.3196687155	2.4088111517
C	0.0165609748	-3.3942493809	1.0334441035
C	4.8681461755	3.3841279933	0.2250415262
C	0.0549843221	-4.5056471070	1.8637544507

C	-3.2653188736	2.7045924826	-4.5396211599
C	0.5932920155	4.4517399723	0.6480309893
C	-4.6571635729	-0.8090746445	1.5849331716
C	-1.0932113466	-1.1380242489	5.6399909172
C	5.2146078918	0.7030031786	0.8795744774
C	-2.2998716102	-3.6995180713	-3.8409617080
C	4.6538331917	-1.6378528046	-2.8597903322
C	-1.6480587419	-2.0255983813	4.7270585412
C	2.2387475797	5.7350738398	-0.5462382716
C	1.0378888893	-5.7955116317	0.0829708036
C	-2.7230176062	1.5075336489	-4.0927435323
C	-4.4595949999	-2.1247880623	-0.8659416477
C	-3.1223152528	3.8631479112	-3.7853194717
C	-1.2058180979	-1.9271814157	-5.0408805133
H	-2.4270919934	-2.2863088926	2.7467864686
H	-1.8519199152	-3.0476439001	5.0190852984
H	-0.8598426355	-1.4700170632	6.6434208334
H	-0.4222269968	0.8735121603	5.9839848289
H	-0.9918851025	1.6453617987	3.7105241577
H	1.4426794798	0.0308697608	2.7213580033
H	1.4278136334	-1.5597327827	4.5891539396
H	2.6329930085	-3.7189902795	4.3948748973
H	3.8583622088	-4.2625648532	2.3183899659
H	3.8949110838	-2.6716969064	0.4491094693
H	5.3482188692	-0.3399423903	1.1386330712
H	7.2010666173	1.2557480341	1.4514426326
H	6.8971423921	3.6371641109	0.8662987192
H	4.7287977237	4.4271959023	-0.0257037404
H	2.8660831894	2.8442274218	-0.3271746566
H	5.6647502142	-1.5417144940	-3.2379175377
H	4.0182771797	-3.1208879400	-4.3005446882
H	1.3591879345	-4.7567536259	-1.7703815747
H	1.4344279714	-6.7326021655	-0.2851429266
H	0.5983707808	-6.5723580414	2.0341550453
H	-0.3026253647	-4.4254531264	2.8825765190
H	-0.3604805869	-2.4515356261	1.4147862419
H	-1.6074991925	-4.0567437599	-1.8425215735
H	-3.0349088083	-4.4930071653	-3.8015892234
H	-2.7807530868	-3.1386014179	-5.8538347815
H	-1.0852421203	-1.3367000269	-5.9398897245
H	0.3361002105	-0.8831540618	-3.9866901014
H	0.5362728300	3.7255115242	-2.6736938225
H	2.3483486866	5.3984228805	-2.6643699185
H	3.0228623529	6.4814570048	-0.5467310810
H	1.9032384925	5.8693686795	1.5708909081
H	0.0866676662	4.1969994562	1.5710378544
H	-2.3268177943	4.7317326085	-1.9855242457
H	-3.5517494657	4.7931676662	-4.1336073774
H	-3.8043803774	2.7363400808	-5.4774155790
H	-2.8350940095	0.6012484106	-4.6737286627
H	-1.6290144232	0.5263962436	-2.5362394363
H	-4.7304522663	-0.2848923858	2.5296924005
H	-6.6302656243	-1.6269995645	1.6879113911
H	-6.4562368852	-2.8024106802	-0.4777914398
H	-4.3788341626	-2.6319651996	-1.8186888020
H	-2.4952859093	-1.2857953288	-1.0005777069

H	-4.0876742046	5.4770340026	1.7423857402
H	-4.9136442209	3.7214735614	3.2649472035

T_1-Ag^{pyrz}	X	Y	Z
Ag	0.1067549582	0.3244006166	0.0738042641
P	2.6868802093	-0.1081075644	0.2836738186
P	0.4159860384	-1.9390308668	-1.3158590938
P	-1.9895557070	0.6377160032	1.4934894339
P	-0.8188328689	2.7078264347	-0.5126310027
N	-2.0167917464	4.6533368384	0.8772961264
N	2.5876740596	-2.9942593956	-2.6045484529
N	-3.1833987099	2.7521309476	2.6751455790
N	4.4656728046	-1.3938075258	-1.3454583323
C	-1.7436499331	3.3165142756	0.8488888984
C	4.1334790105	0.9473735559	0.5102904406
C	0.1155502907	-3.4266157855	-0.3167709237
C	2.5846272937	-1.2395823927	1.7124711016
C	1.7937382831	-0.8394504054	2.7924925188
C	-0.4041749679	-2.2483653958	-2.9070375529
C	3.1702539563	-1.2858696795	-1.0530407577
C	-1.8205027317	2.3017114523	-1.9579571484
C	2.2163707161	-2.0817550828	-1.7076170139
C	-2.3341362001	2.4102578046	1.7434269836
C	2.0562541807	4.7644004366	-2.5315109609
C	-1.8829912388	-0.0909930407	3.1455171927
C	6.3202249314	1.4060977087	1.3958722209
C	1.5870588722	-1.6891076871	3.8677833698
C	-3.1502589883	2.7274333272	-1.9987716621
C	-1.3514469110	1.3946791813	-2.9133048778
C	-0.3000484762	-5.6561681915	1.2880581140
C	0.2647331933	-4.7075898983	-0.8511868954
C	-3.4018821703	-0.5536472816	-0.5835776622
C	-1.6909934494	-2.7875969360	-2.8985150260
C	-3.4687990798	-0.0561064175	0.7164171242
C	-1.3572335479	0.6527422825	4.2031295243
C	3.1754002771	-2.5025577880	1.7343901936
C	4.1182890210	2.1976799814	-0.1052399083
C	-5.8312957311	-0.5066417912	0.7636904608
C	0.9635925953	3.9563309308	-2.2613566428
C	0.1645195449	-1.8565541048	-4.1179441989
C	6.3092523343	2.6478874432	0.7717250137
C	-1.8061796895	-2.5841704469	-5.2935856438
C	-2.2685127613	-1.4155490675	3.3545721698
C	2.2644471206	5.2845270824	-0.1854294240
C	-1.2508174171	0.0837548817	5.4628019793
C	-5.7606211551	-1.0048874834	-0.5327053541
C	0.5234485574	3.8075587512	-0.9440447554
C	-2.9071293298	4.9945759706	1.8392253910
C	-3.4770519083	4.1079660011	2.7097684813
C	3.8776974083	-3.1020144865	-2.8785316593
C	2.1714571217	-2.9494018863	3.8750494598
C	2.9690198821	-3.3515412536	2.8130036314
C	-0.2418154636	-3.2708976764	1.0199521592
C	5.2109421391	3.0432131629	0.0216615663
C	-0.4481555458	-4.3851791316	1.8220356079

C	-3.5232233417	1.3527575847	-3.9387087678
C	1.1825797710	4.4689850217	0.0969511737
C	-4.6910288206	-0.0321193735	1.3922261647
C	-1.6510177350	-1.2306743495	5.6724316629
C	5.2360011456	0.5535823924	1.2651918238
C	-2.3871671509	-2.9527326607	-4.0874925094
C	4.8192655855	-2.2842097270	-2.2581818308
C	-2.1518096464	-1.9807558691	4.6164886898
C	2.7045805139	5.4284521419	-1.4964380730
C	0.0558235717	-5.8165044767	-0.0476442816
C	-2.2033566229	0.9200506675	-3.8978713875
C	-4.5479074206	-1.0280554734	-1.2062541083
C	-3.9911756328	2.2604451936	-2.9960449747
C	-0.5310645906	-2.0348606530	-5.3054948441
H	-2.6848201127	-1.9966642366	2.5394066387
H	-2.4729836148	-3.0015094882	4.7792389301
H	-1.5784925908	-1.6671591713	6.6600940203
H	-0.8685362937	0.6728547424	6.2860691087
H	-1.0684239022	1.6849340223	4.0499146020
H	1.3260165467	0.1408176321	2.7927929226
H	0.9603480218	-1.3678990688	4.6892741072
H	2.0036570711	-3.6187128631	4.7089329491
H	3.4261340965	-4.3322899213	2.8175519541
H	3.7932495434	-2.8338709213	0.9090513276
H	5.2439636453	-0.4145768101	1.7503987670
H	7.1760816908	1.1024848356	1.9839804505
H	7.1583266462	3.3105980038	0.8768214976
H	5.1969329815	4.0126584187	-0.4590228334
H	3.2525475990	2.5165632730	-0.6780649173
H	5.8733050084	-2.3579793011	-2.4988595475
H	4.1725311990	-3.8487334755	-3.6062053503
H	0.5439208276	-4.8282383168	-1.8912205290
H	0.1690281280	-6.8097019996	-0.4618435763
H	-0.4629019622	-6.5271515134	1.9094665231
H	-0.7190238596	-4.2503188007	2.8618181193
H	-0.3481634399	-2.2799916800	1.4494191409
H	-2.1444139328	-3.0971999379	-1.9632473820
H	-3.3787104962	-3.3865387644	-4.0717535178
H	-2.3431738526	-2.7289727426	-6.2217535984
H	-0.0723865759	-1.7478745389	-6.2428325426
H	1.1603062113	-1.4334927990	-4.1444329536
H	0.4405655838	3.4634596449	-3.0708409530
H	2.3933301038	4.8895458133	-3.5517916754
H	3.5494642123	6.0689751711	-1.7147767748
H	2.7642177431	5.8108489367	0.6168450263
H	0.8302634933	4.3553585712	1.1145025214
H	-3.5201242076	3.4139983731	-1.2473203102
H	-5.0186867510	2.5975271114	-3.0291760768
H	-4.1897267572	0.9766307236	-4.7039606629
H	-1.8394653002	0.2030485689	-4.6218045859
H	-0.3264534274	1.0360156694	-2.8758926531
H	-4.7423041324	0.3698312719	2.3969396077
H	-6.7792742250	-0.4845306425	1.2847605216
H	-6.6557980437	-1.3729434842	-1.0169827691
H	-4.4860827384	-1.4048385188	-2.2196903270
H	-2.4620032820	-0.5593939899	-1.1262159224

H	-3.1640559066	6.0460421238	1.8932587550
H	-4.1834356461	4.4283392529	3.4610623541

S_1-Ag^{quinox}	X	Y	Z
Ag	-0.1337622068	0.0923359581	-0.0403015464
P	1.9439847499	1.4781654794	0.8761862111
P	1.9271702938	-1.5629984136	-0.4087710110
P	-2.3064337187	-1.0057811138	0.7900714691
P	-1.9461547645	1.2484963394	-1.4061935376
N	-4.5345514590	1.7701473764	-1.0859828003
N	4.4287365085	-0.9341236073	-1.2774153693
N	-4.8608290932	-0.2659993931	0.9035579066
N	4.4365750954	1.6430372194	-0.2018135064
C	-3.5418207402	1.0296840563	-0.6263139200
C	2.2928180878	3.2277670306	1.1599954547
C	2.3638197581	-2.6127343617	1.0041961986
C	2.1483183034	0.6426202410	2.4836906087
C	1.0206875944	0.5425469921	3.3005713787
C	1.9811871098	-2.6372177197	-1.8690035255
C	3.4092108041	0.8526862335	-0.0556375249
C	-1.9982391356	0.6070735514	-3.0935199016
C	3.4046887217	-0.4720206462	-0.6144566364
C	-3.7019305251	0.0318427795	0.3470622093
C	-0.5275658850	4.8616159448	-2.6224486007
C	-2.3024895739	-1.1308515475	2.5899053884
C	3.4726049437	5.0008403534	2.2759782338
C	1.0956704145	-0.1007316419	4.5261818763
C	-2.8878531862	1.1737165631	-4.0101117073
C	-1.2073664046	-0.4770637719	-3.4659321811
C	2.9724637724	-4.1949147441	3.2029403306
C	3.5848086340	-3.2861683256	1.0599246355
C	-1.6590378135	-3.2637163071	-0.7106913993
C	1.7839276349	-4.0112965045	-1.7597764492
C	-2.5681455976	-2.6809682749	0.1685697670
C	-2.6638932261	-0.0133183865	3.3466061247
C	3.3510271600	0.0793735536	2.9086882935
C	1.5914399886	4.1656451699	0.4066186982
C	-3.9490108026	-4.6446165485	0.0389253628
C	-0.8259113946	3.5088395760	-2.5696291190
C	2.0922393972	-2.0560334186	-3.1332694305
C	2.7790626354	5.9360071515	1.5158549157
C	1.8368393395	-4.2165011365	-4.1579954965
C	-1.9270708542	-2.3117195326	3.2334588148
C	-1.7790636807	5.2212145155	-0.5940115419
C	-2.6719673603	-0.0866335489	4.7295000223
C	-3.0370072201	-5.2259406335	-0.8346647731
C	-1.6131794223	3.0106463324	-1.5294299451
C	-5.7712608191	1.4964922439	-0.5300248170
C	-5.9340968781	0.4846473319	0.4561478156
C	5.5052679778	-0.1256230965	-1.4385765524
C	2.2968208828	-0.6618615622	4.9400542181
C	3.4213745137	-0.5735230216	4.1311654951
C	1.4557202360	-2.7333183702	2.0509876768
C	1.8409866620	5.5198086942	0.5833249936

C	1.7589942377	-3.5258029506	3.1492650323
C	-2.1839286161	-0.4338473827	-5.6585307444
C	-2.0810925837	3.8708774895	-0.5339778843
C	-3.7202895329	-3.3760738361	0.5475637850
C	-2.3142798047	-1.2697631274	5.3668083759
C	3.2326625819	3.6486433730	2.0995232638
C	1.7133020063	-4.7961255315	-2.9043883852
C	5.5056057939	1.1833315708	-0.8978160324
C	-1.9370259649	-2.3777071108	4.6187806920
C	-1.0076158666	5.7174580919	-1.6386985189
C	3.8852850773	-4.0736843173	2.1598715098
C	-1.2980394963	-0.9948862284	-4.7496353730
C	-1.8919758449	-4.5376297930	-1.2087367999
C	-2.9774072572	0.6458779467	-5.2883214400
C	2.0278456144	-2.8439174128	-4.2706067954
C	6.6312693459	-0.5888045739	-2.1554319046
C	6.6323496381	2.0152249640	-1.0820874335
C	7.7090848351	1.5435963555	-1.7773150767
C	7.7089029301	0.2341958126	-2.3170134476
C	-6.8853832525	2.2298187261	-0.9447554798
C	-7.2037547482	0.2466812867	0.9866449725
C	-8.1335995147	1.9778150837	-0.4051627978
C	-8.2931853492	0.9852513099	0.5615322764
H	-1.6602056571	-3.1870863009	2.6527596610
H	-1.6704719707	-3.3020811574	5.1146456694
H	-2.3366382850	-1.3290154494	6.4473255218
H	-2.9765406633	0.7731242592	5.3115108891
H	-2.9713253692	0.8982703844	2.8475462498
H	0.0758217495	0.9716310286	2.9806589811
H	0.2135246497	-0.1674160896	5.1488239292
H	2.3557350081	-1.1729862556	5.8923490481
H	4.3565650175	-1.0149854518	4.4498708407
H	4.2364096543	0.1428421069	2.2874262835
H	3.7718089269	2.9202139185	2.6923661873
H	4.2000521576	5.3280112386	3.0070210723
H	2.9680796244	6.9920962210	1.6580628731
H	1.2942563053	6.2453490928	-0.0041688822
H	0.8466268873	3.8431684906	-0.3135284312
H	4.2903235153	-3.1925500129	0.2422371826
H	4.8312628719	-4.5971533412	2.2047444153
H	3.2128178793	-4.8121110027	4.0589232987
H	1.0503066153	-3.6052700585	3.9639985495
H	0.5169465949	-2.1910595596	2.0226483668
H	1.6909387547	-4.4730150305	-0.7841845730
H	1.5710165152	-5.8651035406	-2.8118447018
H	1.7906144724	-4.8316415586	-5.0469053686
H	2.1324218298	-2.3874203556	-5.2464020291
H	2.2429959137	-0.9865873507	-3.2306031881
H	-0.4631828546	2.8432642821	-3.3436288063
H	0.0713346922	5.2492188188	-3.4358047519
H	-0.7857829418	6.7757754503	-1.6900456052
H	-2.1563366501	5.8903523482	0.1677530782
H	-2.7005292172	3.4846792225	0.2657482036
H	-3.5119797177	2.0070487594	-3.7114603100
H	-3.6718653123	1.0766636225	-5.9973756134
H	-2.2607149505	-0.8397849864	-6.6587096020

H	-0.6809446249	-1.8386495447	-5.0303201755
H	-0.5195407305	-0.9273971291	-2.7572762519
H	-4.4314920176	-2.9124553494	1.2200937426
H	-4.8445037411	-5.1810542557	0.3235328549
H	-3.2236914976	-6.2173736473	-1.2261685240
H	-1.1800564004	-4.9824289062	-1.8920178155
H	-0.7693378599	-2.7259539137	-1.0172691659
H	6.6038524491	-1.5916259895	-2.5603516469
H	6.6062405438	3.0112277181	-0.6607091213
H	8.5767534116	2.1735533719	-1.9218862559
H	8.5759635504	-0.1115201448	-2.8640157399
H	-7.3034085843	-0.5268661634	1.7366566700
H	-6.7378841221	2.9950994018	-1.6953280065
H	-8.9886602282	2.5525259333	-0.7349795978
H	-9.2716288801	0.7916670717	0.9802179939

T_1-**Ag^{quinox}**	X	Y	Z
Ag	0.0173955590	-0.0875527374	0.6524559002
P	2.1613521365	-1.4667035775	1.1951161767
P	1.9739123376	1.1282807068	-0.8566463504
P	-1.9794386712	-0.8833016369	-1.0520481284
P	-2.1183021901	1.0859083604	1.5555102791
N	-4.6773350089	0.1615529993	1.8397055863
N	4.5293490191	1.6337021934	-0.0260813570
N	-4.5750630585	-1.5492975912	-0.4158672669
N	4.6727423426	-0.5638084023	1.6869939884
C	-3.5374603876	0.0292349139	1.0788995260
C	2.6068635331	-2.4359210408	2.6578749079
C	2.3612049503	0.2568713858	-2.4124254418
C	2.3493094335	-2.5787699885	-0.2333759974
C	1.2230028775	-3.3006593140	-0.6277758496
C	2.0770297474	2.8899069290	-1.2956733313
C	3.5956048736	-0.3171150388	0.9938184041
C	-2.3294677766	2.5644823392	0.5146641331
C	3.5198411706	0.8191633816	0.1127280210
C	-3.4810715872	-0.8106555441	-0.0091765625
C	-3.3779536899	3.1331533527	4.8779304413
C	-2.0962661486	-2.4984435062	-1.8762326125
C	3.7102744161	-4.2750003828	3.7450507744
C	1.2763464930	-4.1455873734	-1.7251403036
C	-3.5364984307	2.8926651901	-0.1006057571
C	-1.2045651751	3.3541160237	0.2789997440
C	2.9415172579	-1.1027168367	-4.7677829236
C	3.5515324058	0.5143977821	-3.0943780847
C	-1.5358800717	1.4076213508	-2.5803582383
C	1.7331903714	3.3153007035	-2.5771394719
C	-2.3809486847	0.3236423856	-2.3609086423
C	-2.3836459836	-3.6356068572	-1.1208551652
C	3.5330503198	-2.7077097237	-0.9581716021
C	2.1486916690	-1.9853644743	3.8939219854
C	-3.8642578526	1.1516268303	-4.0693921909
C	-3.1000803952	2.8115402147	3.5568996198
C	2.3796347122	3.8398462247	-0.3193990347
C	3.2628876085	-3.8160792583	4.9771655136

C	2.0489374074	5.6085540090	-1.9174175179
C	-1.7995388729	-2.6366643982	-3.2303456422
C	-2.4849881131	1.0165760823	5.5914438846
C	-2.4072942278	-4.8857361839	-1.7187937555
C	-3.0147887967	2.2320932322	-4.2840658657
C	-2.5086255883	1.5901100510	3.2510959460
C	-5.7391628291	-0.5477347927	1.4511819848
C	-5.6877871620	-1.4114217696	0.3054717028
C	5.6550167030	1.3933829783	0.6908615076
C	2.4585278869	-4.2667186284	-2.4440309044
C	3.5830589796	-3.5474727133	-2.0621083754
C	1.4689444771	-0.6843627573	-2.9166939521
C	2.4838239528	-2.6697560616	5.0526065388
C	1.7588563190	-1.3632875536	-4.0927586354
C	-2.4855395809	4.7751430465	-1.1702761125
C	-2.1927749226	0.6983733460	4.2745242471
C	-3.5516733736	0.1995690467	-3.1124727608
C	-2.1290861584	-5.0161221998	-3.0749151347
C	3.3876371066	-3.5860721861	2.5857340562
C	1.7191827526	4.6705524979	-2.8842195885
C	5.7257797040	0.2806743535	1.5623639857
C	-1.8174274186	-3.8921050505	-3.8256906386
C	-3.0755197588	2.2367863924	5.8935824587
C	3.8384544429	-0.1645763856	-4.2675337580
C	-1.2804862181	4.4568526161	-0.5581738818
C	-1.8522603922	2.3607035893	-3.5394315737
C	-3.6108467192	3.9942819038	-0.9408550125
C	2.3749899914	5.1899434681	-0.6322410242
C	6.9040386466	0.0474844017	2.3061887478
C	6.7641762147	2.2603381017	0.5704256588
C	7.9629784182	0.8992214368	2.1715708164
C	7.8928042772	2.0118990844	1.2982358521
C	-6.8450344688	-2.1374010556	-0.0470478868
C	-6.9417127731	-0.4574605802	2.1797211243
C	-8.0598649008	-2.0307925054	0.7194229328
C	-8.1071755131	-1.2168220992	1.8009990163
H	-1.5761413531	-1.7613608883	-3.8293525365
H	-1.6000099125	-3.9874065103	-4.8818103504
H	-2.1547894206	-5.9919176018	-3.5420518531
H	-2.6483386638	-5.7596816831	-1.1277823324
H	-2.6109985223	-3.5411742302	-0.0648672966
H	0.2927264859	-3.1973411513	-0.0789026090
H	0.3910100386	-4.6940002557	-2.0206496770
H	2.5015608246	-4.9164844165	-3.3087752756
H	4.5020598209	-3.6353536339	-2.6267603440
H	4.4166131820	-2.1522140584	-0.6680108531
H	3.7406380253	-3.9439011897	1.6266771169
H	4.3142748564	-5.1709155386	3.6871241068
H	3.5177092131	-4.3563021742	5.8795635572
H	2.1308055173	-2.3139974688	6.0115249083
H	1.5289020256	-1.0969411450	3.9490591672
H	4.2469389707	1.2486093288	-2.7034509980
H	4.7617540269	0.0377023177	-4.7945007335
H	3.1701994677	-1.6317749475	-5.6839601022
H	1.0633608422	-2.1039510910	-4.4671996706
H	0.5526059144	-0.9073402657	-2.3821390561

H	1.4938646379	2.5888430364	-3.3452342433
H	1.4640813050	4.9895385733	-3.8866450832
H	2.0525899171	6.6627844722	-2.1615305081
H	2.6310144718	5.9173256186	0.1270758708
H	2.6433279108	3.5247984547	0.6831350386
H	-3.3443857271	3.5101447098	2.7666530606
H	-3.8352354559	4.0851605030	5.1135929398
H	-3.2950014479	2.4909311548	6.9223116722
H	-2.2446203373	0.3182077468	6.3822406818
H	-1.7193376252	-0.2489401501	4.0388544216
H	-4.4172601557	2.2852498631	0.0690193581
H	-4.5484802070	4.2382908729	-1.4229678163
H	-2.5464428150	5.6284549432	-1.8335526259
H	-0.3945732322	5.0517414917	-0.7402700419
H	-0.2559891387	3.0992307726	0.7404047620
H	-4.2104612296	-0.6444234431	-2.9430681613
H	-4.7716636666	1.0523164920	-4.6507805491
H	-3.2641147948	2.9735282967	-5.0321607794
H	-1.1924066705	3.2063192991	-3.6889384302
H	-0.6368654870	1.5267024816	-1.9862487654
H	6.9295466685	-0.8090635615	2.9665476629
H	8.8695882628	0.7282266260	2.7367280698
H	8.7472031575	2.6700855658	1.2121595542
H	6.6839004058	3.1041447682	-0.1019225644
H	-6.7885923807	-2.7886133322	-0.9091845567
H	-6.9629132514	0.2035482807	3.0359584039
H	-8.9239486794	-2.6050166105	0.4163903775
H	-9.0096666218	-1.1216505667	2.3879653927

S_1 and T_1 equilibrium structures (cartesian coordinates, in Å) of the different complexes investigated with the ligands in distorted tetrahedrale arrangement calculated using TDDFT and the M06-2X/def2-TZVP level of theory.

S_1-Cu^{bz}	X	Y	Z
Cu	-10.0998365314	8.8018543417	2.4093567050
P	-11.9411278672	7.7598228725	1.1638074114
P	-9.2641430768	9.1234933416	0.1661760340
P	-8.3824903287	7.6607020709	3.6575654234
P	-10.8002940298	9.1750954980	4.6677573705
C	-11.0136297481	6.9844330642	-0.2104206838
C	-11.4576075867	5.8097812920	-0.8121498406
C	-10.7556465838	5.2515656283	-1.8714881294
C	-9.6085173502	5.8715154904	-2.3454767193
C	-9.1523394835	7.0395172253	-1.7506906275
C	-9.8365512060	7.6001896922	-0.6745636722
C	-10.1236724741	10.4620793111	-0.7147318426
C	-10.0614146927	10.5722356403	-2.1038606627
C	-10.7810718006	11.5611977435	-2.7542713878
C	-11.5696155919	12.4429516345	-2.0226905301
C	-11.6345699361	12.3396775255	-0.6413896872
C	-10.9109422940	11.3511674988	0.0117673813
C	-13.1337964480	8.8596290962	0.3501814724
C	-13.9425161543	9.6377708295	1.1805031310
C	-14.8273356136	10.5519795525	0.6319369228
C	-14.8989755062	10.7088744961	-0.7473796961

C	-14.0902845360	9.9431056273	-1.5748116605
C	-13.2110901415	9.0154674542	-1.0311676317
C	-12.9149682465	6.4237726761	1.9103093957
C	-12.2987582938	5.6438158377	2.8908905192
C	-12.9980620847	4.6188459252	3.5093088202
C	-14.3221217689	4.3769949686	3.1627953963
C	-14.9422875953	5.1559324029	2.1951126974
C	-14.2422104204	6.1776813573	1.5667122395
C	-7.5038722682	9.3065886708	-0.2315416837
C	-6.9797247782	10.5761006564	-0.4752651634
C	-5.6089617989	10.7516701511	-0.6051869087
C	-4.7519649416	9.6656681505	-0.4923876495
C	-5.2691639961	8.3991068071	-0.2511910327
C	-6.6370495722	8.2171424192	-0.1154584546
C	-9.2743966706	6.9046196151	4.9986033125
C	-8.8463839463	5.7652732170	5.6550402701
C	-9.4975399016	5.3280493149	6.8085388744
C	-10.5592949532	6.0981903228	7.3188870203
C	-10.9983309088	7.2393595322	6.6905872296
C	-10.4057795775	7.6573994309	5.4592816826
C	-10.0970944446	10.6691665413	5.4405327015
C	-10.2428483248	10.9038676821	6.8113040339
C	-9.5640715244	11.9523573362	7.4109824063
C	-8.7387011488	12.7780256177	6.6537918367
C	-8.5901714239	12.5498000964	5.2926671453
C	-9.2601712237	11.4953030026	4.6898999879
C	-7.1763638376	8.8189648281	4.3348265517
C	-6.3921697335	9.5707152301	3.4562101916
C	-5.5273502813	10.5324768742	3.9542660587
C	-5.4564473108	10.7613506494	5.3234934613
C	-6.2449767442	10.0236099976	6.1960753829
C	-7.1037362362	9.0499436277	5.7072710390
C	-7.5152607476	6.4097803410	2.6911210335
C	-8.2757139853	5.5878598365	1.8524040581
C	-7.6555902624	4.6616521352	1.0333078553
C	-6.2668153218	4.5502759561	1.0405796534
C	-5.5090875158	5.3557113710	1.8777223135
C	-6.1270363280	6.2884467496	2.7027296621
C	-12.5907898572	9.4379376786	4.7244996008
C	-13.1081406767	10.7345691046	4.6472773146
C	-14.4792078979	10.9347991311	4.6015559214
C	-15.3445034032	9.8467489372	4.6315900304
C	-14.8359584914	8.5560876416	4.7119984759
C	-13.4648763499	8.3480960976	4.7554829193
H	-12.3572562283	5.3285664638	-0.4481109524
H	-11.1094948281	4.3371407930	-2.3292881710
H	-9.0634451972	5.4450137385	-3.1773757265
H	-8.2495404050	7.5089922102	-2.1205984657
H	-9.4528098693	9.8815376606	-2.6764101612
H	-10.7304018440	11.6445438796	-3.8319749042
H	-12.1361404355	13.2103325287	-2.5341078606
H	-12.2532429737	13.0201434855	-0.0716110157
H	-10.9772100828	11.2608016010	1.0917955658
H	-13.8830580546	9.5254214497	2.2577195356
H	-15.4561210918	11.1445827311	1.2841250131
H	-15.5847294892	11.4281286623	-1.1759730815

H	-14.1407204104	10.0657926031	-2.6488689919
H	-12.5813208238	8.4260771800	-1.6862590678
H	-11.2817768535	5.8574995621	3.2050426867
H	-12.5138743510	4.0243404613	4.2729844629
H	-14.8723796562	3.5839584221	3.6521185749
H	-15.9742771596	4.9697198760	1.9279912455
H	-14.7313614818	6.7878166625	0.8172263102
H	-7.6412536132	11.4290960109	-0.5642755345
H	-5.2121003825	11.7394127673	-0.7993496574
H	-3.6840274186	9.8047160600	-0.5969032181
H	-4.6089021623	7.5459293473	-0.1639860798
H	-7.0247121713	7.2239547271	0.0806667091
H	-7.9941889329	5.2168187574	5.2692613047
H	-9.1762877199	4.4286986286	7.3121327095
H	-11.0556598083	5.7796043424	8.2273390985
H	-11.8267529382	7.7989272749	7.1074225983
H	-10.8850892135	10.2656322752	7.4071398260
H	-9.6824365914	12.1312674751	8.4718924350
H	-8.2108236889	13.5952531040	7.1273861261
H	-7.9436738381	13.1853264569	4.7012783451
H	-9.1147539400	11.3020469619	3.6306617746
H	-6.4545515846	9.4033450282	2.3848744788
H	-4.9130593017	11.1059593835	3.2723301946
H	-4.7868336288	11.5186714785	5.7100313699
H	-6.1964433462	10.2079607338	7.2610619921
H	-7.7235703602	8.4773007368	6.3870251054
H	-9.3563410202	5.6823288819	1.8321908020
H	-8.2517708246	4.0317538823	0.3861601107
H	-5.7795971839	3.8290943948	0.3975008159
H	-4.4312612197	5.2583100589	1.8945611423
H	-5.5309286410	6.9196823613	3.3490581862
H	-12.4356739230	11.5838496535	4.6349626068
H	-14.8737906055	11.9411931820	4.5492753587
H	-16.4146121043	10.0056621436	4.6004505466
H	-15.5063285778	7.7071668498	4.7448600787
H	-13.0701102855	7.3425442562	4.8217085053

T_1-**Cu^{bz}**	X	Y	Z
Cu	-0.1098141558	0.1143963658	0.3724753218
P	2.1079910909	-0.1957086914	-0.6968382507
P	0.1666668209	-2.2458155366	0.7729028385
P	-2.1412934823	0.2988686690	-1.1906424654
P	-0.5820157548	2.4334679276	0.4975721860
C	1.9483376723	-1.8949026905	-1.3600509317
C	2.6387206752	-2.2999008269	-2.5000408525
C	2.5188484395	-3.5979018762	-2.9764619682
C	1.7171981024	-4.5099801915	-2.3056672270
C	1.0184676342	-4.1177744593	-1.1730568297
C	1.1086349751	-2.8110316686	-0.6972753861
C	1.2750502170	-2.5995910741	2.1714366012
C	1.8352008375	-3.8645499191	2.3485110937
C	2.7106975854	-4.0956345918	3.3968504304
C	3.0360461764	-3.0644350221	4.2713599261
C	2.4832108709	-1.8044488064	4.0998740112
C	1.6017416679	-1.5728616074	3.0524746965

C	3.4375380672	-0.3300164520	0.5391763329
C	3.6363708458	0.7665343089	1.3807203815
C	4.6013358304	0.7175368840	2.3744579084
C	5.3585800305	-0.4334775951	2.5527754720
C	5.1522672694	-1.5322043267	1.7308348258
C	4.1992135777	-1.4815755164	0.7218868203
C	2.7863161358	0.8005061714	-2.0538412924
C	1.8793338891	1.3963202625	-2.9330071948
C	2.3351463329	2.1949034428	-3.9709710633
C	3.6984810784	2.4129137276	-4.1297860891
C	4.6034244505	1.8306939174	-3.2521693246
C	4.1516698574	1.0252685749	-2.2146942733
C	-1.2250126430	-3.3987932173	0.9554653272
C	-1.6517503227	-3.7607075284	2.2333253106
C	-2.8182527609	-4.4944157560	2.3986196861
C	-3.5682570420	-4.8724679140	1.2933400616
C	-3.1465292773	-4.5167128837	0.0187399771
C	-1.9843788804	-3.7795737812	-0.1527001567
C	-1.6521297259	1.7383864239	-1.9861413246
C	-1.8688362992	1.9710137962	-3.3855171760
C	-1.5963404062	3.1812594319	-3.9405257522
C	-1.0877233357	4.2523506118	-3.1334386502
C	-0.8386931132	4.0474060997	-1.7909619706
C	-1.0629528716	2.8122639416	-1.1762520722
C	-1.8277544577	3.0461189687	1.6780159057
C	-2.4201199230	4.2997077390	1.5319757442
C	-3.3934182862	4.7153547895	2.4266342630
C	-3.7831004773	3.8819466484	3.4702025147
C	-3.2018803595	2.6313541913	3.6158479340
C	-2.2285802784	2.2126006015	2.7177446671
C	-3.5599704132	0.4261161412	-0.0795588276
C	-3.8476295544	-0.6042428249	0.8197370144
C	-4.8712463664	-0.4447576959	1.7380561516
C	-5.5901655821	0.7465316972	1.7788516189
C	-5.2930866832	1.7764546813	0.8975902120
C	-4.2771617426	1.6214387479	-0.0346143625
C	-2.3379558473	-1.0857146660	-2.3035853849
C	-1.2228487338	-1.5106618935	-3.0366802116
C	-1.3106512287	-2.6300594195	-3.8453045595
C	-2.5128596155	-3.3262881489	-3.9393436401
C	-3.6259999378	-2.8969218740	-3.2283776425
C	-3.5424898758	-1.7845798789	-2.4035357818
C	0.9321075867	3.3670511107	0.8831452497
C	1.2199323432	3.6911755621	2.2104919386
C	2.4345904117	4.2743631548	2.5396818558
C	3.3725632292	4.5428729152	1.5497648051
C	3.0888270905	4.2299431502	0.2275975228
C	1.8767933148	3.6413034417	-0.1074938851
H	3.2754278632	-1.5931732540	-3.0181584627
H	3.0598235862	-3.8973514992	-3.8646882053
H	1.6305263184	-5.5272913146	-2.6643679754
H	0.3850765515	-4.8345376514	-0.6659467303
H	1.5881519808	-4.6685452760	1.6647945131
H	3.1422572551	-5.0786486432	3.5322414569
H	3.7245692495	-3.2461156162	5.0863830827
H	2.7411658359	-0.9988323912	4.7743825229

H	1.1805502555	-0.5824286051	2.9119707147
H	3.0361083163	1.6621350153	1.2618650498
H	4.7531402658	1.5778264018	3.0137640302
H	6.1049119568	-0.4759933268	3.3355036241
H	5.7337665756	-2.4338357656	1.8727660733
H	4.0443085942	-2.3464745942	0.0884639173
H	0.8107961155	1.2672060896	-2.7911679500
H	1.6208409474	2.6577096898	-4.6396376128
H	4.0555133416	3.0436840236	-4.9333880229
H	5.6646246329	2.0051524024	-3.3727367855
H	4.8598000171	0.5809416330	-1.5255719157
H	-1.0724459018	-3.4704420725	3.1013993890
H	-3.1374602398	-4.7750495825	3.3937416943
H	-4.4754104617	-5.4474829142	1.4243144948
H	-3.7221213378	-4.8112677256	-0.8493182743
H	-1.6702235637	-3.5057354190	-1.1532962349
H	-2.2678555415	1.1693661155	-3.9958717917
H	-1.7691276683	3.3394474708	-4.9963091639
H	-0.8786393536	5.2139287082	-3.5799288232
H	-0.4101248644	4.8562303372	-1.2090179340
H	-2.1269068085	4.9447806531	0.7119013968
H	-3.8491595510	5.6903606470	2.3127797517
H	-4.5443168065	4.2095164302	4.1663797661
H	-3.5124615188	1.9767247046	4.4197809245
H	-1.7898316145	1.2244374690	2.8156693281
H	-3.2750195012	-1.5267106596	0.7980009120
H	-5.1056369779	-1.2462210836	2.4264995215
H	-6.3816650177	0.8722516279	2.5063623494
H	-5.8481794074	2.7043136005	0.9375107426
H	-4.0320260438	2.4222122934	-0.7223642875
H	-0.2872484099	-0.9676399210	-2.9655213427
H	-0.4426101930	-2.9593797380	-4.4010501459
H	-2.5826343576	-4.1988229874	-4.5756508929
H	-4.5647296496	-3.4279556605	-3.3182556490
H	-4.4079442951	-1.4581360570	-1.8412792715
H	0.4909414094	3.4913924717	2.9869926259
H	2.6456889514	4.5266636791	3.5707507241
H	4.3177865406	5.0018221074	1.8085832947
H	3.8113525911	4.4395775755	-0.5504692550
H	1.6699692602	3.3957768482	-1.1410192333

S_1-**Cu^{pyrz}**	X	Y	Z
Cu	-0.0648932559	-0.1311946121	-0.1232386615
P	2.2517732195	-0.1839335447	0.7685128639
P	0.5297080691	2.1658319477	-0.6204376404
P	-2.2389882501	-0.0327233748	0.9771486090
P	-0.9506223720	-2.2998174471	-0.5012486452
N	3.3038807171	1.8200660210	2.3270898440
N	1.8591351627	3.8526495573	1.1016798441
N	-3.2037376795	-1.8059552508	2.7588916845
N	-2.0621711649	-4.0052613999	1.3030623792
C	2.4462013213	1.5565017576	1.3446906930
C	3.4320806414	3.0844634159	2.7018073116
C	2.7160304374	4.1048090968	2.0801537683
C	1.7049988590	2.5827695198	0.7370676691

C	1.5803097021	2.2903289963	-2.0950860630
C	2.2903789498	3.4592503020	-2.3720567102
C	3.1351767028	3.5074868022	-3.4692823082
C	3.2753400532	2.3935692789	-4.2905450790
C	2.5688975502	1.2309868470	-4.0201601997
C	1.7201079980	1.1796649249	-2.9232146932
C	3.5339496294	-0.3304136872	-0.5099622886
C	3.5720156104	-1.5324616611	-1.2187176962
C	4.4784649488	-1.7018272169	-2.2529181462
C	5.3429763454	-0.6693824376	-2.5965912592
C	5.3054882771	0.5279547740	-1.8965421625
C	4.4072868743	0.6991074273	-0.8515841319
C	2.8007357773	-1.1969758408	2.1622102561
C	1.8300168513	-1.7586570039	2.9899734337
C	2.2058438213	-2.5309262314	4.0798245270
C	3.5518313527	-2.7514443817	4.3366498916
C	4.5221506274	-2.1996993493	3.5083504544
C	4.1509334339	-1.4216847187	2.4232543213
C	-0.6408333912	3.5411252822	-0.6910380336
C	-1.1448768989	3.9401709464	-1.9284638243
C	-2.1799887911	4.8620042732	-1.9918800810
C	-2.7167242531	5.3875117130	-0.8240187334
C	-2.2127942568	4.9938689505	0.4091577194
C	-1.1807076495	4.0706120641	0.4807807777
C	-2.4075166217	-1.6655203916	1.7116913016
C	-3.4000532166	-3.1270980604	3.1090281352
C	-2.8592742785	-4.1636442812	2.4096663613
C	-1.8358453427	-2.7221331960	1.0020972357
C	-2.0721601560	-2.4841995306	-1.9049764268
C	-2.7427758729	-3.6940371583	-2.1021691489
C	-3.6830711035	-3.7954414743	-3.1159568950
C	-3.9505828300	-2.7044561527	-3.9354966223
C	-3.2822605640	-1.5032349394	-3.7419267901
C	-2.3476054356	-1.3904505839	-2.7232567824
C	-3.6902545563	0.3347463615	-0.0154385027
C	-3.7895480717	1.5757338417	-0.6518079506
C	-4.8321910979	1.8171654358	-1.5320801003
C	-5.7754714248	0.8276292297	-1.7819411169
C	-5.6770784832	-0.4060356909	-1.1506347978
C	-4.6339508749	-0.6603221553	-0.2745692715
C	-2.0775203054	1.2368272647	2.2526239907
C	-0.8643109608	1.3230376898	2.9404618817
C	-0.6718574069	2.3020806085	3.9003496570
C	-1.6924532064	3.2050566688	4.1794287621
C	-2.9047315241	3.1140066850	3.5089125002
C	-3.1015369888	2.1352168093	2.5450044766
C	0.3835472689	-3.4889376372	-0.7316343253
C	0.8129512227	-3.8249058431	-2.0166032070
C	1.9110960073	-4.6558881650	-2.1822368597
C	2.5902584771	-5.1420840257	-1.0715027825
C	2.1638874567	-4.8080785009	0.2092485112
C	1.0618390815	-3.9860265250	0.3827134556
H	4.1227627499	3.2958974149	3.5095485158
H	2.8387945057	5.1390914475	2.3789830300
H	2.1781764313	4.3242955093	-1.7278796507
H	3.6851712357	4.4137237587	-3.6863085242

H	3.9388659099	2.4349886247	-5.1445776208
H	2.6817898403	0.3627848010	-4.6556132210
H	1.1796051946	0.2638547555	-2.7038552205
H	2.8959831966	-2.3398292459	-0.9580581179
H	4.5050981240	-2.6410171158	-2.7905429555
H	6.0469370785	-0.7995631307	-3.4081850615
H	5.9772357422	1.3339433874	-2.1614113891
H	4.3910936237	1.6395318225	-0.3152340352
H	0.7759167540	-1.6135399225	2.7725405012
H	1.4486965987	-2.9659955961	4.7187196054
H	3.8470677639	-3.3588169184	5.1822964431
H	5.5705136466	-2.3749858682	3.7104495882
H	4.9062117248	-0.9902787799	1.7782485785
H	-0.7301861750	3.5323044113	-2.8426042805
H	-2.5632832633	5.1726278133	-2.9549603576
H	-3.5223782493	6.1081358321	-0.8746591731
H	-2.6241463145	5.4040113520	1.3222697419
H	-0.8029599854	3.7653114311	1.4492653888
H	-4.0328376030	-3.3050558967	3.9674611489
H	-3.0591318963	-5.1852825921	2.7064111922
H	-2.5339709917	-4.5382259614	-1.4553658637
H	-4.2075032672	-4.7295158672	-3.2689422191
H	-4.6840018262	-2.7922945270	-4.7263930461
H	-3.4953267754	-0.6521199459	-4.3751020395
H	-1.8475787788	-0.4422131038	-2.5510348112
H	-3.0577830804	2.3535164518	-0.4597318304
H	-4.9051500347	2.7798122096	-2.0211940068
H	-6.5892100808	1.0186185446	-2.4693325059
H	-6.4119788908	-1.1760534734	-1.3438308330
H	-4.5531220282	-1.6268753629	0.2072902448
H	-0.0692488653	0.6139785194	2.7327867285
H	0.2673774393	2.3548446483	4.4357305364
H	-1.5461221087	3.9710538430	4.9296791473
H	-3.7059614276	3.8031422946	3.7419815873
H	-4.0499630827	2.0661777460	2.0291104929
H	0.2819263236	-3.4475077726	-2.8825038735
H	2.2337820721	-4.9280010093	-3.1787449716
H	3.4471646641	-5.7897909840	-1.2031964191
H	2.6842516424	-5.1960251923	1.0750607330
H	0.7135613035	-3.7469907465	1.3787272999

T_1-**Cu^{pyrz}**	X	Y	Z
Cu	-0.0944063915	-0.1264356407	-0.0654160349
P	2.2633047687	-0.4573954218	0.6828111573
P	0.7435382720	2.0827471691	-0.5991067783
P	-2.2619732536	0.3100912384	0.9676188428
P	-1.2176250893	-2.1822457333	-0.4196651200
N	3.6434584145	1.4032801048	2.1582736975
N	2.3545121513	3.5973445744	1.0412052010
N	-3.4997985315	-1.2824972257	2.7472358583
N	-2.5694739248	-3.6429755688	1.4422275623
C	2.6951329097	1.2470713657	1.2383478289
C	3.9394185899	2.6416952657	2.5248219453
C	3.2988186365	3.7417195677	1.9594050736
C	2.0364142888	2.3561498204	0.6837008282

C	1.7252701769	2.0451264241	-2.1267528478
C	2.5854001665	3.0970433400	-2.4444758771
C	3.3724907066	3.0237626773	-3.5823612136
C	3.3052393234	1.9041631642	-4.4050968599
C	2.4493334385	0.8580526802	-4.0945681787
C	1.6584927487	0.9286008155	-2.9560071735
C	3.4382433851	-0.7643626165	-0.6666351007
C	3.2922982354	-1.9710215642	-1.3531366368
C	4.1111704935	-2.2599830870	-2.4330729093
C	5.0702223815	-1.3418826557	-2.8440355529
C	5.2155247396	-0.1404407448	-2.1653409646
C	4.4064178673	0.1491577557	-1.0746571163
C	2.7941163652	-1.5196090078	2.0523406002
C	1.8762986834	-1.8196310094	3.0580846404
C	2.2490468207	-2.6233871597	4.1249602670
C	3.5365242765	-3.1401904494	4.1851274975
C	4.4516627127	-2.8480568487	3.1822749346
C	4.0853663138	-2.0372517151	2.1183178378
C	-0.2314751615	3.6040024944	-0.6554348988
C	-0.7019449965	4.0613521087	-1.8861932993
C	-1.5947720574	5.1219750698	-1.9381508757
C	-2.0220803287	5.7302116169	-0.7654985211
C	-1.5508310120	5.2790869000	0.4609405558
C	-0.6621466620	4.2164970057	0.5215128084
C	-2.6685279955	-1.2700111419	1.7146397688
C	-3.8332931135	-2.5428191312	3.1692055341
C	-3.3845363584	-3.6706095154	2.5474918816
C	-2.2073608806	-2.4261665761	1.0727162261
C	-2.3412259006	-2.3669155329	-1.8260894192
C	-3.0766161260	-3.5446172360	-1.9828158118
C	-3.9972924964	-3.6437484210	-3.0141128717
C	-4.1819217482	-2.5808270750	-3.8918313064
C	-3.4507661630	-1.4115296815	-3.7382117959
C	-2.5343619091	-1.3017314682	-2.7018400197
C	-3.6343461626	0.8776691538	-0.0487204946
C	-3.5803518672	2.1430055680	-0.6438457088
C	-4.5590298882	2.5237619692	-1.5477314082
C	-5.5941635150	1.6519936119	-1.8637510678
C	-5.6490539778	0.3940697562	-1.2753157784
C	-4.6693984330	0.0000417866	-0.3788855738
C	-1.9716071660	1.5634134184	2.2457520304
C	-0.7610819369	1.5317464933	2.9420719085
C	-0.4842991964	2.4821352490	3.9111428734
C	-1.4157053662	3.4752878087	4.1910931498
C	-2.6268526419	3.5027905296	3.5122319941
C	-2.9081664938	2.5524094027	2.5415192150
C	-0.0444348742	-3.5517335141	-0.5112692213
C	0.3166240291	-4.1127899918	-1.7357624508
C	1.3208090282	-5.0698396054	-1.7865372013
C	1.9772262204	-5.4548846523	-0.6242135617
C	1.6181482122	-4.8963276065	0.5977003495
C	0.6055463145	-3.9525887443	0.6563594843
H	4.7054479892	2.7663420812	3.2809451146
H	3.5548752247	4.7526191579	2.2537293720
H	2.6343528110	3.9678324282	-1.7999858122
H	4.0386799506	3.8396800750	-3.8300204561

H	3.9244764464	1.8494142014	-5.2910828147
H	2.4011897065	-0.0155331925	-4.7308931617
H	1.0013566948	0.1013307396	-2.7063796206
H	2.5428773640	-2.6894377783	-1.0375040344
H	3.9963414544	-3.2021321540	-2.9535161238
H	5.7056719549	-1.5646869141	-3.6912498674
H	5.9618292371	0.5762849361	-2.4821963553
H	4.5339380022	1.0897737389	-0.5537355421
H	0.8587414012	-1.4472430166	3.0003246364
H	1.5319540779	-2.8533933501	4.9018912293
H	3.8261004105	-3.7734209893	5.0135435823
H	5.4552553560	-3.2496357655	3.2297753793
H	4.8021800203	-1.8094815834	1.3397210014
H	-0.3733666150	3.5898910609	-2.8044332237
H	-1.9521422119	5.4752834502	-2.8965010673
H	-2.7163296967	6.5592170642	-0.8071819110
H	-1.8766854912	5.7526012064	1.3778210468
H	-0.3119943605	3.8686289199	1.4856599864
H	-4.4912165251	-2.6041121251	4.0257800632
H	-3.6766464208	-4.6505330300	2.9006085045
H	-2.9305021536	-4.3669729797	-1.2921830772
H	-4.5719794498	-4.5525950419	-3.1349665369
H	-4.9007403256	-2.6659601600	-4.6963530419
H	-3.6001165189	-0.5817006114	-4.4162462814
H	-1.9853711523	-0.3760183652	-2.5606091492
H	-2.7802806469	2.8332345531	-0.3993439929
H	-4.5113284053	3.5049178008	-2.0022068213
H	-6.3588943832	1.9528745018	-2.5677755369
H	-6.4555373564	-0.2850692719	-1.5178699370
H	-4.7091993438	-0.9866596351	0.0663257278
H	-0.0323050318	0.7567048464	2.7321903129
H	0.4535497281	2.4449206611	4.4502251704
H	-1.2024970940	4.2194933716	4.9472901972
H	-3.3612951285	4.2629249419	3.7446722608
H	-3.8569785660	2.5754221089	2.0224449342
H	-0.1896321837	-3.8091567734	-2.6440969460
H	1.5900492788	-5.5156268765	-2.7352511303
H	2.7635395652	-6.1970128376	-0.6685423976
H	2.1214022315	-5.1988154711	1.5070489928
H	0.3106671038	-3.5323114868	1.6097884249

S_1-**Cu^{quinox}**	X	Y	Z
Cu	0.1513149676	-0.0680521490	0.6102099964
P	1.5228786340	1.5952890534	-0.5673277303
P	2.3478978193	-0.9205214796	0.8473923794
P	-1.3670847402	-1.7449477931	-0.4214232462
P	-1.9356971053	1.0146545738	1.1734474911
N	3.2901336914	1.0308938664	-2.5040409280
N	4.1679655140	-1.3310403424	-1.1211032647
N	-3.4149441695	-0.9616138518	-2.0515339357
N	-3.9592722897	1.3831097848	-0.6261107521
C	2.7279465107	0.5676768746	-1.4069469545
C	3.1473453043	-0.5912912194	-0.7266478212
C	4.7727039892	-0.9078793781	-2.2933458358

C	4.3395680095	0.2616411881	-2.9809455459
C	4.9900867814	0.6462148560	-4.1544960713
C	6.0427330167	-0.1014355752	-4.6526599814
C	6.4680012008	-1.2460898969	-3.9806251562
C	5.8401213227	-1.6431831935	-2.8128152980
C	0.4098885214	2.3873293963	-1.7450481632
C	-0.4951304755	1.5753643835	-2.4352457494
C	-1.4173048353	2.1352913937	-3.3025601730
C	-1.4332564184	3.5131385156	-3.4967330347
C	-0.5180063376	4.3205125027	-2.8344198301
C	0.3989913411	3.7651698677	-1.9530519135
C	2.3349506943	2.8621144194	0.4131998490
C	1.5617802694	3.7296114162	1.1905796541
C	2.1827403619	4.6127488918	2.0592407733
C	3.5689697663	4.6311688096	2.1599938424
C	4.3372235755	3.7667369990	1.3905055973
C	3.7259059508	2.8761350264	0.5221312369
C	2.2900759238	-2.7004771501	1.1133779304
C	2.1424519072	-3.5620558460	0.0245342583
C	1.9697977514	-4.9203250149	0.2403931134
C	1.9448340786	-5.4243651052	1.5356699778
C	2.0985942839	-4.5690921496	2.6206321334
C	2.2661767011	-3.2082494850	2.4138408500
C	3.3461634287	-0.2005605290	2.1692611090
C	4.7101015880	-0.4912394433	2.2419204740
C	5.4925706361	0.1412099886	3.1956321643
C	4.9226033890	1.0552565396	4.0749294159
C	3.5666968545	1.3433277692	4.0038916932
C	2.7782323772	0.7187156835	3.0486013582
C	-2.7313988389	-0.6383848244	-0.9894873486
C	-2.9986274506	0.5779288939	-0.2708384956
C	-4.6794999201	1.0650158925	-1.7307142352
C	-4.3938095848	-0.1151363771	-2.4608978940
C	-5.1367401720	-0.4139110902	-3.6246884810
C	-6.1253907574	0.4379787131	-4.0285229590
C	-6.4144600805	1.6145073032	-3.2953075973
C	-5.7094607330	1.9273878611	-2.1679660465
C	-0.9965792402	-2.7865180541	-1.8519092119
C	0.0951561747	-2.4450788583	-2.6488782291
C	0.4087960023	-3.2083494017	-3.7644772891
C	-0.3620614787	-4.3191831498	-4.0782391214
C	-1.4465878762	-4.6664942442	-3.2813164010
C	-1.7672067976	-3.9025372780	-2.1701983699
C	-2.1848585871	-2.8108836192	0.8018484353
C	-1.3608180451	-3.6440421469	1.5605405720
C	-1.9058123240	-4.4521015653	2.5456409772
C	-3.2728279593	-4.4215720274	2.7930566993
C	-4.0942963788	-3.5889069798	2.0466173366
C	-3.5556406655	-2.7882775915	1.0482084338
C	-2.0964575921	2.8047452861	1.3760918670
C	-2.1114322985	3.6518836728	0.2689038743
C	-2.0416527246	5.0252503433	0.4497254594
C	-1.9517283933	5.5608295745	1.7279401172
C	-1.9387750877	4.7188396394	2.8322960542
C	-2.0095930882	3.3441392105	2.6594670735
C	-2.8133003457	0.2526393041	2.5668628033

C	-4.1596703973	0.5361341458	2.7978149745
C	-4.8271742396	-0.0941441893	3.8354574366
C	-4.1565651294	-1.0074031304	4.6420891944
C	-2.8174901392	-1.2900642817	4.4161706595
C	-2.1445850552	-0.6589435670	3.3792096761
H	4.6437337983	1.5407517710	-4.6550327849
H	6.5378386968	0.2056095858	-5.5640812857
H	7.2936895571	-1.8258649233	-4.3710736130
H	6.1554269598	-2.5270667919	-2.2740129990
H	-0.4678085787	0.4985966633	-2.3052979431
H	-2.1129559464	1.4984999930	-3.8348524873
H	-2.1508045440	3.9537785971	-4.1764568799
H	-0.5143699247	5.3890111839	-3.0062507217
H	1.1062077938	4.3997696367	-1.4355211478
H	0.4784207846	3.7158873313	1.1210654504
H	1.5814725889	5.2842124571	2.6582840180
H	4.0512796535	5.3205611208	2.8406993999
H	5.4161077330	3.7811894767	1.4691254338
H	4.3245123805	2.1949741605	-0.0700245429
H	2.1852143135	-3.1735663743	-0.9838096567
H	1.8622451007	-5.5865199252	-0.6054543629
H	1.8147538340	-6.4861753283	1.6993768595
H	2.0941180730	-4.9632301955	3.6284633744
H	2.3902912267	-2.5414426725	3.2591851455
H	5.1492515982	-1.1964654359	1.5456703212
H	6.5503322607	-0.0793955083	3.2532998003
H	5.5399044021	1.5453800585	4.8165043001
H	3.1248029723	2.0604654943	4.6829834872
H	1.7233196051	0.9637115513	2.9732934187
H	-4.8975172068	-1.3202689931	-4.1647693062
H	-6.7000518887	0.2156649160	-4.9178492170
H	-7.2046488709	2.2693174052	-3.6379444169
H	-5.9079707261	2.8209454789	-1.5912128127
H	0.7180574485	-1.5940169346	-2.3891203198
H	1.2588573001	-2.9403133359	-4.3779876239
H	-0.1144942583	-4.9201470896	-4.9435319510
H	-2.0436188121	-5.5347491515	-3.5271769784
H	-2.6119093539	-4.1728994539	-1.5487309654
H	-0.2914439741	-3.6653068909	1.3789827401
H	-1.2591414045	-5.1017533124	3.1214975657
H	-3.6974167603	-5.0467691733	3.5677810391
H	-5.1589802204	-3.5614733046	2.2381485113
H	-4.2095878234	-2.1475336276	0.4698929261
H	-2.1781434612	3.2468107834	-0.7327825691
H	-2.0572060265	5.6767940258	-0.4144501340
H	-1.8988060978	6.6330731029	1.8638220774
H	-1.8782046181	5.1314954171	3.8307510281
H	-1.9992844874	2.6914670724	3.5245093923
H	-4.6778648141	1.2467515752	2.1636638212
H	-5.8710639090	0.1254577471	4.0167752001
H	-4.6827684965	-1.4998642490	5.4495414349
H	-2.2975463536	-2.0050033547	5.0397685962
H	-1.1006178402	-0.8907894334	3.1929954040

T_1-**Cu^{quinox}**	X	Y	Z
Cu	-0.0767686439	-0.1300439213	-0.4249062255
P	2.1776820407	0.1347491789	0.5976604367
P	0.2133470853	2.2011583809	-0.9524355068
P	-2.1072466365	-0.2616925738	1.0213129376
P	-0.6343962346	-2.4258692477	-0.5728220091
N	2.6930944561	2.2347001323	2.2660869415
N	1.0561878143	4.0365914216	0.8887884282
N	-2.1335746756	-1.9047273461	3.1344419089
N	-1.0159479310	-4.0446668803	1.5832081235
C	2.0413845364	1.8764566504	1.1952174092
C	2.5389481368	3.5077780372	2.7103500985
C	1.7220777204	4.4250184455	2.0050298962
C	1.1820770807	2.7989564757	0.5014316138
C	1.3149537108	2.5561422844	-2.3500490364
C	1.8262501723	3.8402765240	-2.5397088523
C	2.6981766998	4.0852147205	-3.5880842771
C	3.0619840459	3.0534972590	-4.4469886552
C	2.5535198754	1.7763770301	-4.2617604588
C	1.6783636914	1.5268790122	-3.2135586289
C	3.4730781253	0.2362607552	-0.6738848654
C	3.6234813530	-0.8688226732	-1.5142305677
C	4.5658258250	-0.8475719486	-2.5304996520
C	5.3484857701	0.2827846967	-2.7300556997
C	5.1944767666	1.3878897373	-1.9050151433
C	4.2648961454	1.3649961856	-0.8739980469
C	2.8893093747	-0.7646873881	1.9972570462
C	2.0182532993	-1.4143597461	2.8719939127
C	2.5181334886	-2.1117323557	3.9621663776
C	3.8890299303	-2.1719233128	4.1736715411
C	4.7594439043	-1.5329801375	3.2994243979
C	4.2635190897	-0.8278103773	2.2132546314
C	-1.1892443164	3.3345161378	-1.1111948359
C	-1.7143193247	3.5650790385	-2.3829758548
C	-2.8981013999	4.2731319088	-2.5292833341
C	-3.5657088369	4.7519156783	-1.4093951646
C	-3.0426323317	4.5264097920	-0.1431494587
C	-1.8591760226	3.8190292998	0.0109814844
C	-1.7280460554	-1.7764769268	1.8646714317
C	-2.0346704795	-3.1767908566	3.6453505004
C	-1.4799633281	-4.2437471712	2.8789542630
C	-1.1439037196	-2.8201581947	1.1194336603
C	-1.9469647197	-2.9790911412	-1.6864346084
C	-2.4638556434	-4.2711086049	-1.5771670247
C	-3.5190781946	-4.6562559157	-2.3895545839
C	-4.0559371082	-3.7620857235	-3.3093613316
C	-3.5414770570	-2.4779506170	-3.4196225790
C	-2.4886725890	-2.0843425611	-2.6059789590
C	-3.6543321022	-0.3253505670	0.1074521130
C	-3.9839037560	0.7282442317	-0.7501807894
C	-5.1134072260	0.6363526711	-1.5477401456
C	-5.9079730168	-0.5032972221	-1.5011198045
C	-5.5764576124	-1.5530950943	-0.6539074153
C	-4.4491657497	-1.4712505845	0.1480064065
C	-2.1520428487	1.1195581178	2.1705285657

C	-0.9701913203	1.4303252736	2.8511434681
C	-0.9163163354	2.5344808243	3.6844872009
C	-2.0453076774	3.3310854459	3.8498833480
C	-3.2277088006	3.0107109123	3.1954060601
C	-3.2844967913	1.9119900055	2.3503709086
C	0.8339922143	-3.4166150882	-0.9277125000
C	1.1320896338	-3.7539814920	-2.2483679971
C	2.3314131567	-4.3828682551	-2.5483730743
C	3.2384203532	-4.6725033867	-1.5359854973
C	2.9417982104	-4.3398410059	-0.2202106829
C	1.7446794522	-3.7106518649	0.0876601889
C	-2.4652370438	-3.4286538723	4.9524174359
C	-1.3748453795	-5.5065778438	3.4493637458
C	-1.8112648735	-5.7359925414	4.7517157301
C	-2.3534208014	-4.6983704940	5.4999317055
C	3.1977174289	3.9215957763	3.8895454301
C	1.5788437520	5.7467309028	2.4830476491
C	2.2263233397	6.1220482436	3.6259150372
C	3.0394461654	5.2038137401	4.3337133043
H	1.5400487816	4.6401091756	-1.8659606782
H	3.0949282667	5.0807195589	-3.7375814543
H	3.7450858050	3.2488934576	-5.2634336469
H	2.8406235216	0.9725159886	-4.9264664787
H	1.2901471980	0.5255289308	-3.0591848593
H	3.0053033644	-1.7497020316	-1.3741419603
H	4.6818893139	-1.7136898928	-3.1693197952
H	6.0772953090	0.3030287382	-3.5299768838
H	5.8002434183	2.2709991070	-2.0603621572
H	4.1609500753	2.2306804255	-0.2316611537
H	0.9470016237	-1.3964949587	2.6954592319
H	1.8370064575	-2.6157904524	4.6353229994
H	4.2809796304	-2.7228415002	5.0186722663
H	5.8276328752	-1.5833897990	3.4646442528
H	4.9429995674	-0.3304616793	1.5323002381
H	-1.1971270377	3.1940281155	-3.2601199226
H	-3.2956820241	4.4548688259	-3.5191011961
H	-4.4877878774	5.3064198493	-1.5245155236
H	-3.5543702764	4.9027372101	0.7332847043
H	-1.4605437847	3.6525193465	1.0032450332
H	-2.0440689396	-4.9591583195	-0.8524819407
H	-3.9234606686	-5.6564932466	-2.3064853480
H	-4.8791272929	-4.0694594542	-3.9412709882
H	-3.9639604574	-1.7802115783	-4.1306220663
H	-2.1000863541	-1.0733548758	-2.6711409382
H	-3.3610377330	1.6169822693	-0.7968418450
H	-5.3696451052	1.4544337287	-2.2082363713
H	-6.7867433429	-0.5740755813	-2.1288180006
H	-6.1942631137	-2.4405674675	-0.6194815497
H	-4.1829486111	-2.2935651192	0.8009510611
H	-0.0960438896	0.7981438393	2.7392387305
H	-0.0003201015	2.7680893852	4.2125667203
H	-2.0049678772	4.1942370695	4.5014134287
H	-4.1114632197	3.6170938884	3.3454810522
H	-4.2056689660	1.6703158181	1.8363510109
H	0.4232466116	-3.5335522439	-3.0382284809
H	2.5547340869	-4.6531728694	-3.5721680483

H	4.1730316764	-5.1643078018	-1.7720821060
H	3.6421758155	-4.5703663514	0.5718511809
H	1.5151825057	-3.4615612275	1.1146939738
H	-2.8875002552	-2.6052841151	5.5131675606
H	-0.9411098074	-6.2989949606	2.8535619259
H	-1.7279860411	-6.7262309029	5.1788605290
H	-2.6933946470	-4.8798166159	6.5106718213
H	3.8148171908	3.2008352747	4.4093037038
H	0.9496443298	6.4273244041	1.9249262242
H	2.1210994211	7.1317072692	4.0002508789
H	3.5407443154	5.5288343743	5.2357537928

S_1-**Ag^{bz}**	X	Y	Z
Ag	-0.2269295316	-0.1531418925	-0.3441100522
P	2.3936797576	-0.1885947347	0.6401835356
P	0.6339495046	2.2720443949	-0.5733083994
P	-2.5364562404	-0.0561984262	1.0386783498
P	-1.0591479786	-2.5159405885	-0.3972355510
C	2.6210087600	1.5161707081	1.2788670566
C	1.8612297483	2.5810970577	0.7524549713
C	2.9800187875	4.1132783958	2.2563471271
C	3.7123739450	3.0637377393	2.7883799060
C	3.3203693527	-1.2430720311	1.7990912581
C	2.6782552871	-1.6404405106	2.9730347866
C	3.3174750029	-2.4759408375	3.8756739481
C	4.6026582431	-2.9328195649	3.6063571581
C	5.2443796278	-2.5465557209	2.4381237292
C	4.6079046416	-1.7035526224	1.5355051008
C	3.3855714224	-0.2202729808	-0.8854044714
C	3.2011017496	-1.3209155592	-1.7235982939
C	3.9059930597	-1.4182490724	-2.9138736250
C	4.7859650053	-0.4086294832	-3.2830131640
C	4.9666302331	0.6919873285	-2.4563440376
C	4.2744064540	0.7856201570	-1.2564120495
C	-0.5669364161	3.6328766876	-0.4765294015
C	-1.0665374754	4.0570752310	0.7559622153
C	-2.0907308133	4.9909807756	0.8083873049
C	-2.6379167605	5.4965543023	-0.3638015053
C	-2.1518547934	5.0691926992	-1.5923527253
C	-1.1196946697	4.1434111160	-1.6515030417
C	1.5448057587	2.5413723434	-2.1247488321
C	2.3230335503	3.6819974175	-2.3204423011
C	3.0249825258	3.8493485985	-3.5032338485
C	2.9554467099	2.8794779670	-4.4972781240
C	2.1836011935	1.7430975297	-4.3086001759
C	1.4793792301	1.5745468874	-3.1240780692
C	3.5379565413	1.7782230128	2.2962646641
C	2.0644286014	3.8703175044	1.2435060506
C	-2.7387530788	-1.6790919011	1.6156789000
C	-1.9095983524	-2.7610214363	1.1295452173
C	-2.9842893842	-4.2837752480	2.6826996829
C	-3.8353208204	-3.2292462097	3.1307756141
C	-2.0203030621	1.1540935272	2.2885923448
C	-0.7136435226	1.0848228836	2.7845542662
C	-0.2832665794	1.9551408468	3.7700375438

C	-1.1641980277	2.8958601581	4.2964819285
C	-2.4707935089	2.9536527416	3.8305465053
C	-2.9001720582	2.0964960392	2.8259575247
C	-3.9816064604	0.6160360584	0.2069459330
C	-3.9768855525	1.9388071067	-0.2516131881
C	-5.0440415089	2.4162586772	-0.9925941390
C	-6.1189482665	1.5828368987	-1.2844293725
C	-6.1195146879	0.2658072200	-0.8444534187
C	-5.0491919964	-0.2250890210	-0.1114942149
C	0.3704901221	-3.6120521604	-0.4876131410
C	1.1820734588	-3.7317699781	0.6433588619
C	2.3873265330	-4.4110081960	0.5727210694
C	2.7874169041	-4.9909245630	-0.6256722005
C	1.9787837776	-4.8879174870	-1.7507248346
C	0.7787274023	-4.1929379903	-1.6897894783
C	-2.1496760909	-2.9172497040	-1.7904497683
C	-2.5355865370	-4.2377568584	-2.0385102459
C	-3.4687661848	-4.5137713809	-3.0219878341
C	-4.0389416758	-3.4762794483	-3.7551467762
C	-3.6711415724	-2.1639994280	-3.5046481021
C	-2.7258488026	-1.8837173836	-2.5252308254
C	-3.7165201220	-1.9738142229	2.6145960252
C	-2.0699127125	-4.0436096940	1.6907715741
H	4.4277751224	3.2429398013	3.5803218538
H	3.1180983243	5.1206867569	2.6262391552
H	1.6667178196	-1.3048103962	3.1785732390
H	2.8111594969	-2.7779763689	4.7830180156
H	5.1002935918	-3.5912302381	4.3062262609
H	6.2447524057	-2.9008812908	2.2263192286
H	5.1133387710	-1.4116511145	0.6234719311
H	2.5117271559	-2.1099686008	-1.4382131902
H	3.7639404678	-2.2805126530	-3.5527114097
H	5.3296741951	-0.4784959036	-4.2162902984
H	5.6481332753	1.4816770576	-2.7448005076
H	4.4204624920	1.6485980292	-0.6177627938
H	-0.6611926225	3.6596753742	1.6788688732
H	-2.4641771671	5.3161059412	1.7709013902
H	-3.4374623396	6.2245082689	-0.3197246237
H	-2.5703857994	5.4624886352	-2.5095622829
H	-0.7436024875	3.8200841441	-2.6145194821
H	2.3836296354	4.4384151277	-1.5468570848
H	3.6269397668	4.7362674844	-3.6514847689
H	3.5068456290	3.0117320706	-5.4191268636
H	2.1334479146	0.9832703095	-5.0771505212
H	0.8874966879	0.6774475755	-2.9743862646
H	-4.5725321604	-3.4227773445	3.8982937113
H	-3.0641411773	-5.2678433670	3.1219383665
H	-0.0288638301	0.3378450098	2.3972856043
H	0.7386651697	1.9011023301	4.1253023510
H	-0.8342916457	3.5735849822	5.0726927328
H	-3.1639071272	3.6715443593	4.2502981258
H	-3.9181202230	2.1607049939	2.4633923660
H	-3.1398279557	2.5926957689	-0.0315054965
H	-5.0341337205	3.4397190416	-1.3445791375
H	-6.9533826822	1.9598298883	-1.8612840488
H	-6.9531927752	-0.3838370982	-1.0757246306

H	-5.0349483630	-1.2579151768	0.2144652932
H	0.8668281227	-3.2842036890	1.5782113005
H	3.0137610852	-4.4793879079	1.4541312740
H	3.7270850542	-5.5244945953	-0.6824145661
H	2.2847134548	-5.3470591489	-2.6818109640
H	0.1637994120	-4.0987332187	-2.5760336283
H	-2.1068129124	-5.0461153132	-1.4569921506
H	-3.7599818945	-5.5377899709	-3.2154994956
H	-4.7727476512	-3.6965657281	-4.5192784922
H	-4.1171647438	-1.3555567198	-4.0690093825
H	-2.4425602926	-0.8541955074	-2.3296815943
H	-4.3565499448	-1.1784790871	2.9808509772
H	-1.4474687153	-4.8555386445	1.3291305178
H	4.1253727678	0.9676800160	2.7080195610
H	1.4912129294	4.6955915728	0.8409067752

T_1-**Ag^{bz}**	X	Y	Z
Ag	-0.1986090727	-0.1641208856	-0.2844771092
P	2.4079998357	-0.1872572525	0.6534496506
P	0.6428716793	2.2648951924	-0.5660087410
P	-2.5307708732	-0.0974344151	1.0476294446
P	-1.0619989172	-2.5285390663	-0.3621983373
C	2.6312536872	1.5193689705	1.2878635455
C	1.8642863096	2.5809572649	0.7634635354
C	2.9691634135	4.1155610573	2.2748552840
C	3.7099812113	3.0699925483	2.8029539684
C	3.3344369741	-1.2441233363	1.8095867321
C	2.6886529303	-1.6515947433	2.9780606210
C	3.3263401238	-2.4924268288	3.8769035575
C	4.6136432469	-2.9439825527	3.6092640027
C	5.2593000610	-2.5473871872	2.4466021573
C	4.6242275737	-1.6996381928	1.5475157504
C	3.3900569430	-0.2285070277	-0.8779698535
C	3.1912571283	-1.3258410551	-1.7177195224
C	3.8907546413	-1.4275720859	-2.9108440034
C	4.7792705552	-0.4260829990	-3.2813916468
C	4.9732128312	0.6716660272	-2.4539475148
C	4.2863616196	0.7697963830	-1.2513628565
C	-0.5634013336	3.6218393782	-0.4871002843
C	-1.0880024206	4.0386285336	0.7375498775
C	-2.1218465723	4.9625033953	0.7742470928
C	-2.6534559752	5.4659714920	-0.4059638757
C	-2.1411672588	5.0475188779	-1.6267483052
C	-1.0996189701	4.1313827534	-1.6702720760
C	1.5616178944	2.5293284078	-2.1138806534
C	2.3486394195	3.6646965107	-2.3046397645
C	3.0520639096	3.8318449088	-3.4865985944
C	2.9747244772	2.8671786566	-4.4850141935
C	2.1943131984	1.7358058097	-4.3010692542
C	1.4890190084	1.5671306497	-3.1171767425
C	3.5454548035	1.7847061553	2.3067017164
C	2.0560420416	3.8694317059	1.2603477865
C	-2.7513404365	-1.7334494095	1.6183097843
C	-1.9043371894	-2.8057908499	1.1604153974
C	-2.7988200081	-4.2724586474	2.8626369301

C	-3.6857690290	-3.2415579006	3.2766131096
C	-2.0633321142	1.1547616159	2.2775628599
C	-0.7677465589	1.1106237720	2.8108913564
C	-0.3744228544	2.0002895695	3.7936599110
C	-1.2817993118	2.9348283740	4.2873412552
C	-2.5786630431	2.9653658716	3.7894507329
C	-2.9703368530	2.0909435893	2.7858367037
C	-3.9749354155	0.5401208231	0.1872892002
C	-3.9616670844	1.8474549076	-0.3150626264
C	-5.0184898165	2.3037692178	-1.0840548133
C	-6.0924364206	1.4646252493	-1.3618694115
C	-6.1016438278	0.1620949109	-0.8787169091
C	-5.0413398649	-0.3076045548	-0.1187409771
C	0.3463508572	-3.6419637081	-0.5085289967
C	1.2017314887	-3.7536432217	0.5914864652
C	2.3988959607	-4.4409907542	0.4814903535
C	2.7505071839	-5.0302300269	-0.7279419523
C	1.9012154707	-4.9300624746	-1.8224866620
C	0.7053663456	-4.2313893765	-1.7211013747
C	-2.1844534335	-2.8185248923	-1.7576834476
C	-2.6751128692	-4.1029976184	-2.0040695383
C	-3.6013519075	-4.3080094113	-3.0118405600
C	-4.0598625976	-3.2318353248	-3.7666742045
C	-3.5873508376	-1.9534252139	-3.5168366772
C	-2.6458092691	-1.7464996675	-2.5155921536
C	-3.6647740468	-2.0140970710	2.6801445490
C	-1.9434382263	-4.0480455958	1.8101018973
H	4.4234044410	3.2519586499	3.5960303922
H	3.0985418207	5.1224365081	2.6493033125
H	1.6758151494	-1.3187543978	3.1820510448
H	2.8173239489	-2.8022473869	4.7800824773
H	5.1101571661	-3.6062853410	4.3062470803
H	6.2614130927	-2.8976672428	2.2363217819
H	5.1321054507	-1.3999894819	0.6393201632
H	2.4944342563	-2.1087924707	-1.4326382835
H	3.7374541205	-2.2868477257	-3.5510630413
H	5.3186670038	-0.4996111513	-4.2168865521
H	5.6605021473	1.4557000634	-2.7440660272
H	4.4417673778	1.6306807082	-0.6120015433
H	-0.6956265800	3.6425950835	1.6666089621
H	-2.5151351526	5.2807360290	1.7310715746
H	-3.4611158716	6.1855276892	-0.3740660390
H	-2.5467369759	5.4399791207	-2.5501331134
H	-0.7037916881	3.8147101364	-2.6274689370
H	2.4148841204	4.4171110291	-1.5275822294
H	3.6608808588	4.7147406134	-3.6308947636
H	3.5269618625	2.9991909705	-5.4064023543
H	2.1385884263	0.9797725954	-5.0730171836
H	0.8905776454	0.6738262025	-2.9707361004
H	-4.3806579567	-3.4265591389	4.0852353536
H	-2.8083916210	-5.2306207316	3.3616702034
H	-0.0624456659	0.3675757171	2.4530321428
H	0.6390309448	1.9659970105	4.1745988298
H	-0.9814826691	3.6261200480	5.0634891726
H	-3.2924893402	3.6774002927	4.1839433052
H	-3.9799625635	2.1353460163	2.3977273611

H	-3.1252683656	2.5062425163	-0.1048856906
H	-5.0013495078	3.3155341521	-1.4682573129
H	-6.9186269611	1.8246214250	-1.9609695226
H	-6.9346662016	-0.4924665068	-1.0984378931
H	-5.0328524481	-1.3302989941	0.2380637464
H	0.9304135860	-3.2905493755	1.5326431194
H	3.0580729737	-4.5051664769	1.3389257943
H	3.6856030894	-5.5673372114	-0.8171549071
H	2.1709299471	-5.3953027171	-2.7616451551
H	0.0567193417	-4.1412859202	-2.5835177367
H	-2.3352944894	-4.9369340087	-1.4001687728
H	-3.9755998673	-5.3046795833	-3.2050147628
H	-4.7910966915	-3.3949462804	-4.5475425652
H	-3.9507510920	-1.1145887862	-4.0957012852
H	-2.2819544810	-0.7431281489	-2.3183126928
H	-4.3311867387	-1.2330342138	3.0290274848
H	-1.2953876020	-4.8457034631	1.4633769592
H	4.1376549255	0.9768169330	2.7170340653
H	1.4757785825	4.6912171442	0.8604287130

S_1-**Ag^{pyrz}**	X	Y	Z
Ag	-0.2530815472	-0.0865877537	-0.4121242760
P	2.2534059999	-0.7936755371	0.6502358951
P	1.1569227790	2.0497759947	-0.6655436951
P	-2.3535231070	0.5588217735	1.0314038710
P	-1.7144031839	-2.1191843136	-0.4879303374
N	3.7126321979	0.8533885668	2.2849530149
N	2.8488459422	3.2187605569	1.1291865452
N	-3.7185960787	-0.8965031008	2.7897148666
N	-3.1197802371	-3.3585724117	1.4395835231
C	2.8493581217	0.8386091815	1.2707847354
C	2.3915595794	2.0439553599	0.7054842109
C	3.7186735967	3.2184681633	2.1283581559
C	4.1361123715	2.0307052068	2.7203370447
C	2.8987652116	-1.9854926544	1.8556473257
C	2.1516787089	-2.2052695123	3.0124691254
C	2.5616842895	-3.1475134149	3.9421991005
C	3.7150038192	-3.8883794152	3.7132477526
C	4.4578640852	-3.6776504067	2.5600848079
C	4.0539618714	-2.7275081635	1.6315117133
C	3.2536793670	-1.0344127295	-0.8497762822
C	2.8163534099	-2.0185639683	-1.7376551474
C	3.5184413088	-2.2636636195	-2.9085891629
C	4.6495151491	-1.5153842497	-3.2087052816
C	5.0849227030	-0.5307276955	-2.3319027783
C	4.3954428506	-0.2945097745	-1.1510157761
C	0.3076709579	3.6448898067	-0.5339675263
C	-0.0359642338	4.1782628513	0.7071626070
C	-0.8225827738	5.3187343576	0.7755211375
C	-1.2799712779	5.9259250860	-0.3866363774
C	-0.9436918890	5.3930287666	-1.6241551711
C	-0.1516449141	4.2565157458	-1.7002933442
C	2.1847507480	2.1471206207	-2.1574671454
C	3.1575187662	3.1391645643	-2.2867337408
C	3.9511445418	3.1796014000	-3.4217617201

C	3.7748000136	2.2379350872	-4.4301521436
C	2.8049846409	1.2543645253	-4.3061122713
C	2.0104101507	1.2073381519	-3.1689869654
C	-2.9215259942	-0.9878152384	1.7181836320
C	-2.6369732794	-2.1842982250	1.0619468862
C	-3.9264948212	-3.2838005125	2.5575464078
C	-4.2154000407	-2.1129106619	3.1887494333
C	-1.6351488702	1.5935075066	2.3282605340
C	-0.3920563269	1.2229652044	2.8466686767
C	0.2151747659	1.9847353110	3.8302569420
C	-0.4227694323	3.1235548815	4.3112864502
C	-1.6672038705	3.4858463159	3.8130235399
C	-2.2747120207	2.7294789762	2.8204147142
C	-3.6722437765	1.4760045370	0.2398157126
C	-3.4086609682	2.7513640730	-0.2714384760
C	-4.3905948866	3.4235921661	-0.9793347818
C	-5.6307597649	2.8293962979	-1.1838487410
C	-5.8887865263	1.5581909616	-0.6856055624
C	-4.9109975839	0.8728473588	0.0181800775
C	-0.5770107883	-3.5184479275	-0.5160472333
C	0.1568820825	-3.7917319219	0.6391082486
C	1.1660152627	-4.7394158249	0.6152975846
C	1.4393683523	-5.4303011903	-0.5605171579
C	0.7008072812	-5.1728821258	-1.7086193869
C	-0.3008337742	-4.2115240404	-1.6944149793
C	-2.9080898786	-2.3475782301	-1.8197349329
C	-3.6200861948	-3.5463952124	-1.9097896329
C	-4.5960372537	-3.6878015860	-2.8838885502
C	-4.8617456841	-2.6461432550	-3.7649392234
C	-4.1567684692	-1.4539175177	-3.6733208929
C	-3.1815864721	-1.3019555775	-2.6984037324
H	4.8292968499	2.0310045312	3.5534367952
H	4.0880647496	4.1789359039	2.4673344100
H	1.2365795595	-1.6482779179	3.1853346095
H	1.9775591193	-3.3115763571	4.8380332358
H	4.0316161708	-4.6314970902	4.4332889415
H	5.3566728313	-4.2531643977	2.3815379894
H	4.6357068829	-2.5721431897	0.7318681085
H	1.9309950309	-2.6035907686	-1.5054271217
H	3.1790415116	-3.0367222809	-3.5859534160
H	5.1925109506	-1.6994160214	-4.1267075833
H	5.9649156070	0.0541889406	-2.5654006212
H	4.7506355074	0.4692595215	-0.4698916861
H	0.3064556673	3.7114160663	1.6221945066
H	-1.0787837576	5.7301708819	1.7431927355
H	-1.8921387864	6.8164004743	-0.3282116603
H	-1.2910724287	5.8657969638	-2.5334044697
H	0.1122367440	3.8490877771	-2.6690621248
H	3.2865593975	3.8746826599	-1.5009091170
H	4.7056805135	3.9484154010	-3.5238497561
H	4.3959551913	2.2748557644	-5.3156557934
H	2.6692570003	0.5194918789	-5.0884558025
H	1.2629197338	0.4281511217	-3.0651781385
H	-4.8695225341	-2.0984393445	4.0506846096
H	-4.3400146451	-4.2190631867	2.9092203895
H	0.0956044371	0.3248563110	2.4829851964

H	1.1777989215	1.6852004663	4.2260237336
H	0.0445741482	3.7202854261	5.0836509440
H	-2.1737842924	4.3584513940	4.2044795144
H	-3.2464518381	3.0152801849	2.4402648702
H	-2.4406319702	3.2174697206	-0.1173569190
H	-4.1841836838	4.4106242118	-1.3722696465
H	-6.3974916515	3.3576024451	-1.7353613486
H	-6.8552498504	1.0987764064	-0.8439865650
H	-5.1080249361	-0.1184457634	0.4068609345
H	-0.0648586060	-3.2598936619	1.5573220811
H	1.7392684862	-4.9337864754	1.5140253219
H	2.2259184502	-6.1731809260	-0.5799937191
H	0.9055875357	-5.7204428110	-2.6193332035
H	-0.8675279249	-4.0049384257	-2.5941137320
H	-3.4169473553	-4.3481982519	-1.2102620107
H	-5.1530500041	-4.6127324188	-2.9540567694
H	-5.6236796635	-2.7646193692	-4.5242130311
H	-4.3671556643	-0.6424634228	-4.3571912448
H	-2.6410153519	-0.3653164301	-2.6126993649

T_1-**Ag^{pyrz}**	X	Y	Z
Ag	-0.2424442157	-0.0782975055	-0.4370823571
P	2.2441034351	-0.7922253989	0.6447650850
P	1.1614613392	2.0599620774	-0.6648608205
P	-2.3218060143	0.5519720865	1.0775679835
P	-1.7293216282	-2.1011067633	-0.5331369678
N	3.7033943365	0.8443156514	2.2905394228
N	2.8454140450	3.2170099775	1.1453129861
N	-3.5876317693	-0.9421044132	2.8699635172
N	-3.0473218266	-3.3650809307	1.4508022345
C	2.8430586987	0.8358543073	1.2737035415
C	2.3883172238	2.0450591074	0.7135720389
C	3.7121067113	3.2102498025	2.1471988053
C	4.1269701775	2.0188034894	2.7335020241
C	2.8637432284	-1.9890790736	1.8581627374
C	2.0774499952	-2.2361522319	2.9829849472
C	2.4700808608	-3.1814838547	3.9175120985
C	3.6451203106	-3.8978242010	3.7245267821
C	4.4271197602	-3.6601519439	2.6026609435
C	4.0406690784	-2.7069368351	1.6701427261
C	3.2592636798	-1.0395850893	-0.8441359182
C	2.8169603351	-2.0144564457	-1.7400156437
C	3.5252797500	-2.2635680906	-2.9061450763
C	4.6678414877	-1.5281206303	-3.1941309265
C	5.1078773510	-0.5520120415	-2.3100692508
C	4.4118817259	-0.3119113205	-1.1336791902
C	0.3176729094	3.6586129492	-0.5370963300
C	-0.0312470929	4.1969147437	0.7004449322
C	-0.8170553366	5.3385428864	0.7605831880
C	-1.2684507240	5.9420709909	-0.4056988534
C	-0.9264424292	5.4045462283	-1.6396935498
C	-0.1354261682	4.2669503424	-1.7076694571
C	2.2059462627	2.1612341608	-2.1454107051
C	3.1738855921	3.1598658870	-2.2612980412
C	3.9833104920	3.2056568211	-3.3847989219

C	3.8284693375	2.2619445362	-4.3947833698
C	2.8639260017	1.2715726086	-4.2839288837
C	2.0525564934	1.2198934413	-3.1587044000
C	-2.8473905453	-1.0026563451	1.7475140816
C	-2.5950480578	-2.1968040867	1.0603565771
C	-3.7951259886	-3.3214983856	2.6138814200
C	-4.0541464045	-2.1578396999	3.2754498587
C	-1.6292109547	1.6252506269	2.3569418281
C	-0.3826299658	1.2870651494	2.8894508516
C	0.2053541317	2.0813383957	3.8594386727
C	-0.4544565454	3.2191467611	4.3117021304
C	-1.7015402971	3.5508330887	3.7978123507
C	-2.2893985765	2.7630034250	2.8188337473
C	-3.6274598494	1.4507562981	0.2409085327
C	-3.3597796077	2.7155826463	-0.2965971464
C	-4.3238053863	3.3580176428	-1.0549138332
C	-5.5518254494	2.7472972457	-1.2831720091
C	-5.8154850650	1.4877405545	-0.7569839590
C	-4.8545339205	0.8309336811	-0.0058097762
C	-0.5958547108	-3.5056821701	-0.5903597533
C	0.1527542147	-3.7925577869	0.5517404271
C	1.1644494178	-4.7370410478	0.5032052211
C	1.4244629097	-5.4124739893	-0.6842799814
C	0.6709340509	-5.1416794929	-1.8194414801
C	-0.3326031561	-4.1827170710	-1.7802847504
C	-2.9879036589	-2.3513227506	-1.8016030850
C	-3.6646016644	-3.5705907559	-1.8838788545
C	-4.6808622867	-3.7257371507	-2.8131953187
C	-5.0232246396	-2.6752570516	-3.6570638600
C	-4.3544193696	-1.4622679936	-3.5727460381
C	-3.3369888413	-1.2980796433	-2.6434054756
H	4.8179100077	2.0138679077	3.5684858204
H	4.0809291848	4.1684890269	2.4931014492
H	1.1439297906	-1.7004306918	3.1244258243
H	1.8552810916	-3.3674848461	4.7881856064
H	3.9482274155	-4.6435129319	4.4477468298
H	5.3424383610	-4.2173174226	2.4520049662
H	4.6525073944	-2.5299568372	0.7947030790
H	1.9218014833	-2.5885705775	-1.5185213018
H	3.1815561370	-3.0296350595	-3.5892835353
H	5.2160485807	-1.7151857353	-4.1084279007
H	5.9964556614	0.0233688805	-2.5346048905
H	4.7702298951	0.4451705663	-0.4467315463
H	0.3047015375	3.7329608624	1.6192843649
H	-1.0772948116	5.7538502359	1.7255173712
H	-1.8802146170	6.8331805494	-0.3532332668
H	-1.2686731662	5.8745124755	-2.5523692734
H	0.1319999310	3.8552650858	-2.6736677926
H	3.2867383523	3.8964851479	-1.4740231678
H	4.7335870330	3.9799331527	-3.4765110004
H	4.4621800459	2.3025232062	-5.2711979010
H	2.7447610984	0.5351718387	-5.0675175008
H	1.3082300134	0.4364131754	-3.0658397253
H	-4.6580225052	-2.1601392573	4.1741789948
H	-4.1778575988	-4.2663675073	2.9723621841
H	0.1240771285	0.3919895678	2.5464013252

H	1.1708050113	1.8079603078	4.2667018897
H	-0.0017282487	3.8403860082	5.0734283866
H	-2.2242071557	4.4237802901	4.1666798666
H	-3.2627302771	3.0245911557	2.4253505869
H	-2.4022356502	3.1963121244	-0.1235156438
H	-4.1133062565	4.3359006632	-1.4680764988
H	-6.3044135670	3.2529421871	-1.8738434418
H	-6.7727758176	1.0153687663	-0.9324115060
H	-5.0537461614	-0.1537490111	0.3989820567
H	-0.0585354761	-3.2739249833	1.4798377305
H	1.7485907692	-4.9415114553	1.3926648367
H	2.2118102270	-6.1536968492	-0.7231815345
H	0.8651246752	-5.6770376048	-2.7396990157
H	-0.9108041272	-3.9658135495	-2.6703391601
H	-3.4022365431	-4.3789042688	-1.2121258945
H	-5.2101346106	-4.6672173544	-2.8772575804
H	-5.8168058876	-2.8039887689	-4.3815248803
H	-4.6241274156	-0.6441834503	-4.2273132098
H	-2.8220130709	-0.3466629098	-2.5639277809

S_1-**Ag^{quinox}**	X	Y	Z
Ag	8.2669131950	11.1837419031	4.5778380380
P	7.6525075968	9.7347541985	2.2452451939
P	10.4171380138	11.3401064302	3.1788164087
P	8.9087514637	9.9796312043	6.8326085992
P	6.1890497009	11.3194481568	5.9710634549
N	9.3911664452	7.9434411905	1.1585016014
N	11.6997234319	9.3357685385	1.8797400942
N	7.4754159173	8.2855191582	8.2773278212
N	4.9849046596	9.4746700986	7.4956029079
C	9.3196834272	9.0796836355	1.7967470903
C	10.5150737403	9.7819442260	2.1899960829
C	11.7891706736	8.1587105132	1.2122862822
C	10.6179399485	7.4448678215	0.8636453095
C	10.7284457119	6.2047407137	0.1963008157
C	11.9664963436	5.7141541089	-0.1093123765
C	13.1377280197	6.4321311945	0.2338548731
C	13.0576936186	7.6318556102	0.8822263131
C	6.5141888848	8.4157567312	1.7414054881
C	6.2836142103	7.3789773036	2.6450092048
C	5.3793357736	6.3737368228	2.3414702734
C	4.6878530777	6.4064922064	1.1362357301
C	4.9099786286	7.4393762363	0.2364260581
C	5.8219786666	8.4432046752	0.5349687007
C	7.4080138845	11.0701353271	1.0355337715
C	6.3975281827	11.9902377062	1.3193343860
C	6.1408514121	13.0368329736	0.4460283512
C	6.9048656140	13.1825412804	-0.7047347592
C	7.9173584701	12.2752430984	-0.9874365291
C	8.1644021135	11.2156130667	-0.1259433216
C	11.9838590259	11.4284668807	4.0878637285
C	12.5717085754	10.2901422959	4.6376579233
C	13.6802087292	10.4148123445	5.4625071880
C	14.2022042291	11.6682808606	5.7531405723

C	13.6150235625	12.8041000238	5.2111509584
C	12.5100305115	12.6868467731	4.3804905808
C	10.4926795644	12.6533304814	1.9291957388
C	11.5015721275	12.6550684718	0.9654106398
C	11.5362494154	13.6567659601	0.0089043188
C	10.5717015202	14.6588155259	0.0133721899
C	9.5703929448	14.6608477388	0.9729898044
C	9.5289497891	13.6568584802	1.9306858315
C	7.3707818411	9.2705284022	7.4022256860
C	6.1521627266	9.8569934155	7.0182562507
C	5.0361167053	8.4292511575	8.4036285602
C	6.2719721136	7.8455460236	8.7989993467
C	6.2699853477	6.8055840754	9.7313312540
C	5.0801578973	6.3396825012	10.2612972249
C	3.8683530564	6.9084614699	9.8712480008
C	3.8482518825	7.9432663101	8.9525231567
C	10.0402709001	8.6801070750	6.2962870182
C	9.7364193529	7.9995391951	5.1142124346
C	10.5799775767	7.0119579839	4.6352605907
C	11.7332410081	6.6890265566	5.3435511436
C	12.0278868065	7.3467024853	6.5306493540
C	11.1907165391	8.3458230790	7.0078338045
C	9.7131808878	10.9651494356	8.0930580872
C	10.9448821173	11.5640568232	7.8075620009
C	11.5272639666	12.4108884069	8.7352520426
C	10.8848915341	12.6685441136	9.9413914098
C	9.6567936373	12.0822676454	10.2198685284
C	9.0616958366	11.2362467580	9.2965771911
C	4.8248064991	11.2039302612	4.7987682019
C	4.5732897159	9.9695851888	4.1983511589
C	3.6564473750	9.8717154136	3.1652244559
C	2.9726123680	11.0042167280	2.7365867498
C	3.2067068686	12.2320409481	3.3436504988
C	4.1386540179	12.3392275093	4.3666811949
C	5.8945641674	12.7538071474	7.0241203944
C	4.6678666953	12.8837430908	7.6799797746
C	4.4692636858	13.9425003256	8.5517813411
C	5.4834342895	14.8675987287	8.7713007855
C	6.7043028807	14.7351821730	8.1246531770
C	6.9126023622	13.6764442749	7.2522416455
H	9.8180989143	5.6790269452	-0.0592729489
H	12.0600305823	4.7664462171	-0.6228857707
H	14.1043664577	6.0196922294	-0.0230925901
H	13.9363583054	8.1990850014	1.1593417830
H	6.8017534246	7.3609502138	3.5983784278
H	5.2060080087	5.5727162616	3.0478513957
H	3.9737619414	5.6279873842	0.9017560326
H	4.3723893461	7.4656195055	-0.7023582518
H	5.9852692761	9.2492055128	-0.1690817246
H	5.8003631172	11.8785632255	2.2197320622
H	5.3464426960	13.7379837847	0.6674071253
H	6.7120586515	14.0043831191	-1.3821805929
H	8.5149653832	12.3895537087	-1.8823370103
H	8.9477316824	10.5057250110	-0.3630389543
H	12.1730774427	9.3059576522	4.4274422073
H	14.1337078540	9.5250713911	5.8799707063

H	15.0682380030	11.7596229809	6.3956252399
H	14.0207581416	13.7835168713	5.4279590794
H	12.0604979625	13.5768863319	3.9561977016
H	12.2540532344	11.8747974678	0.9703033134
H	12.3180506974	13.6601026334	-0.7391691800
H	10.6039442234	15.4403474511	-0.7346195930
H	8.8171980083	15.4375449409	0.9742884767
H	8.7367612456	13.6488621199	2.6714904340
H	7.2227895437	6.3803271374	10.0175856577
H	5.0907969542	5.5318374994	10.9806667989
H	2.9404451874	6.5415634636	10.2891072769
H	2.9200193726	8.4011960024	8.6370347946
H	8.8267840531	8.2395315688	4.5744033922
H	10.3338625496	6.4892887465	3.7189134084
H	12.3946915589	5.9160341152	4.9746595333
H	12.9124340599	7.0775164930	7.0931788195
H	11.4264298927	8.8552220172	7.9328979155
H	11.4463414830	11.3705760437	6.8642830068
H	12.4809961176	12.8715108074	8.5130765535
H	11.3424351716	13.3302024257	10.6652240590
H	9.1598824514	12.2823548528	11.1596697937
H	8.1052972165	10.7761616337	9.5109764847
H	5.0957073792	9.0856654261	4.5438483161
H	3.4803131121	8.9108989444	2.6963517121
H	2.2528091462	10.9286486136	1.9321829460
H	2.6636945448	13.1099892711	3.0188105964
H	4.3282049887	13.2999703039	4.8298555266
H	3.8881367303	12.1497726351	7.5156539223
H	3.5219427801	14.0443825349	9.0644701734
H	5.3208447609	15.6928811785	9.4521585531
H	7.4946026537	15.4528592757	8.3002487425
H	7.8713172088	13.5614023801	6.7575878442

T_1-**Ag^{quinox}**	X	Y	Z
Ag	-0.2048618081	0.1030670169	-0.9499392625
P	1.4273993686	-1.7960077153	0.2896020117
P	2.1254117392	1.1456333349	-1.1129976135
P	-1.6307323029	1.6303729691	0.7058499323
P	-2.5269711725	-0.8539698458	-1.0351514451
N	3.3294920544	-1.0699082202	2.0999342660
N	3.9478127759	1.3630766513	0.8811763424
N	-3.2628438773	0.7663819875	2.6023599904
N	-4.1929627482	-1.4212718034	1.0002306260
C	2.7317072333	-0.6976557859	1.0009807128
C	3.0372174381	0.5714598240	0.3889293180
C	4.5776980665	0.9881542224	2.0217973283
C	4.2512624910	-0.2383954262	2.6474813633
C	1.2412940373	-3.1044734427	1.5303220458
C	0.2982696184	-2.9103627910	2.5392201290
C	0.0901729539	-3.8885679112	3.4993289298
C	0.8135668096	-5.0735020278	3.4465227257
C	1.7466393523	-5.2747032933	2.4383487544
C	1.9636757934	-4.2929910430	1.4816722248
C	2.2825007588	-2.5675636279	-1.1186109387

C	1.4760029976	-3.1679684673	-2.0872818216
C	2.0496468149	-3.7768041257	-3.1936029037
C	3.4296311812	-3.7713830695	-3.3508708327
C	4.2362636523	-3.1659696882	-2.3965434089
C	3.6672277297	-2.5724580578	-1.2784753821
C	2.2162823748	2.9557897430	-1.0625192232
C	2.0935407958	3.6550762293	0.1373402010
C	1.9927480426	5.0385773007	0.1233374500
C	2.0059730686	5.7316052737	-1.0799585985
C	2.1264594704	5.0370089483	-2.2763516246
C	2.2309734770	3.6535584735	-2.2700336172
C	3.1912032679	0.6276453343	-2.4864709643
C	4.5478612088	0.9539871887	-2.4883303803
C	5.3536266125	0.5357801314	-3.5348074469
C	4.8103808074	-0.2026438742	-4.5807961963
C	3.4615049806	-0.5247912844	-4.5822102495
C	2.6506557810	-0.1112445135	-3.5340145315
C	-2.7793356584	0.4685049533	1.3946891612
C	-3.2266712454	-0.6194786192	0.6188538968
C	-4.7646165529	-1.1241166605	2.2321883109
C	-4.3019651486	-0.0344514058	3.0224776949
C	-0.5165475159	2.2714874029	1.9623889132
C	0.3702518329	1.3684844616	2.5569999452
C	1.2947945983	1.8083365343	3.4888740423
C	1.3354463405	3.1546908376	3.8374887138
C	0.4430738309	4.0515189769	3.2636573664
C	-0.4785938733	3.6178589524	2.3218623051
C	-2.4000676220	2.9988490740	-0.1610950114
C	-1.5902329898	3.9189263968	-0.8365520287
C	-2.1747307509	4.9138719387	-1.6019708736
C	-3.5598112672	4.9915729543	-1.7032219732
C	-4.3629180050	4.0730294798	-1.0392380769
C	-3.7887198752	3.0701311319	-0.2732729455
C	-2.3013476132	-2.6333252172	-1.2450186476
C	-1.8803062456	-3.3895251809	-0.1509615391
C	-1.5208815960	-4.7172188373	-0.3191115341
C	-1.5944605921	-5.3016181732	-1.5780711567
C	-2.0282392378	-4.5560137448	-2.6677713800
C	-2.3728890227	-3.2210180806	-2.5079762110
C	-3.7730352680	-0.3115450116	-2.2237006430
C	-4.9888603751	-0.9923328816	-2.3190382293
C	-5.9667396424	-0.5266451584	-3.1831126955
C	-5.7385110800	0.6113630511	-3.9489149651
C	-4.5326540387	1.2908090844	-3.8514225652
C	-3.5483389959	0.8309175700	-2.9877620010
C	5.5458075608	1.8377585326	2.6018650669
C	4.8921508781	-0.5989799924	3.8536181969
C	5.8223423439	0.2411977759	4.3977404598
C	6.1523690164	1.4657912453	3.7679989944
C	-5.8024490283	-1.9195711692	2.7087559164
C	-4.9060502422	0.2160816823	4.2584733637
C	-5.9398850435	-0.5863650437	4.7114444021
C	-6.3890632428	-1.6534300747	3.9386754986
H	-0.2914663125	-1.9987445274	2.5671823163
H	-0.6434882247	-3.7313824483	4.2788909350
H	0.6449908295	-5.8425461741	4.1889466108

H	2.3082010072	-6.1987461320	2.3958668170
H	2.6897976275	-4.4561984128	0.6952620561
H	0.3960269869	-3.1686243439	-1.9707090465
H	1.4168872573	-4.2509967639	-3.9328509144
H	3.8775970237	-4.2375119212	-4.2189950550
H	5.3113002538	-3.1572419426	-2.5202647895
H	4.3063372852	-2.1139300719	-0.5333886877
H	2.0814172017	3.1287864811	1.0832549390
H	1.9045775350	5.5738208757	1.0599946588
H	1.9302123643	6.8110737317	-1.0852102215
H	2.1464399706	5.5716620368	-3.2168813065
H	2.3287163196	3.1176395636	-3.2068223920
H	4.9647580456	1.5337334991	-1.6727515024
H	6.4058336494	0.7880776817	-3.5382241993
H	5.4433575198	-0.5261166273	-5.3969210200
H	3.0393124093	-1.1033376663	-5.3931336679
H	1.5992568126	-0.3766282033	-3.5260958857
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H	0.4609621059	5.0937995501	3.5545648111
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H	-4.0133650317	5.7698880536	-2.3028654892
H	-5.4400326266	4.1351146252	-1.1183363740
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H	-1.8403568304	-2.9406600844	0.8329624891
H	-1.1849847600	-5.2907392334	0.5360452104
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H	-6.1319296017	-2.7467739984	2.0938353369
H	-4.5401686865	1.0512319454	4.8409301213
H	-6.4002460443	-0.3809259068	5.6685851996
H	-7.1977877300	-2.2770418270	4.2950980968