Supplementary Material

Synthesis and Characterization of an Octanuclear Copper(I)

Methanediide Cluster

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The Supplementary Material contains:

- 1. Experimental Section
- 2. X-ray crystallographic data for compound **3**
- 3. Selected bond distances and angles for compound **3**
- 4. Absorption, emission and excitation spectra of compound **3**

Experimental Section

General procedures. All manipulations were carried out under an inert atmosphere of dinitrogen gas by standard Schlenk techniques. Solvents were dried over and distilled from Na (Et₂O and THF). [K{CH(${}^{i}Pr_{2}P$ -S)(C₉H₆N-2)}]_n was prepared according to the literature procedures.¹ CuCl was purchased from Aldrich Chemical Co. and used without further purification. The ¹H, ¹³C{¹H} and ³¹P{¹H} spectra were recorded on Bruker 400 spectrometer. The NMR spectra were recorded in C₆D₆, and the chemical shift are relative to SiMe₄ for ¹H and ¹³C{¹H} and 85% H₃PO₄ for ³¹P{¹H}, respectively.

Synthesis of 3

A solution of **1** (1.04 g, 3.16 mmol) in THF (30ml) was added to a solution of CuCl (0.31 g, 3.13 mmol) in THF (10ml) at 0 °C. The reaction mixture was stirred at room temperature for 12 hr and red mixture was formed. All the volatiles in the reaction mixture were removed under reduced pressure and the residue was extracted with Et₂O (20 ml). After filtration, THF (10 ml) was added to the filtrate and the filtrate was concentrated, compound **3** was isolated as red crystals. Yield: 0.36 g (55.2 %). Mp: 294.8 °C. Anal. Found: C, 46.33 ; H, 5.32 ; N, 3.36 Calcd. For C₆₄H₈₀Cu₈N₄P₄S₄: C, 46.14 ; H, 4.85 ; N, 3.36. ¹H NMR (C₆D₆, 25 °C): δ =

1.05-1.15 (m, 12H, CH*Me*₂), 1.81-2.16 (m, 2H, C*H*Me₂), 6.58 (d, 1H, $J_{H-H} = 8$ Hz, Qu), 6.96 (t, 1H, Qu), 7.28 (d, 1H, $J_{H-H} = 8$ Hz, Qu), 7.35 (t, 1H, $J_{H-H} = 8$ Hz, Qu), 7.48 (t, 1H, $J_{H-H} = 8$ Hz, Qu), 8.87 (d, 1H, $J_{H-H} = 12$ Hz, Qu) ¹³C{¹H} NMR (C₆D₆, 25 °C): $\delta = 18.9$ (CH*Me*₂), 30.4 (CHMe₂), 66.1 (CuCCu), 121.0, 122.3, 123.6, 126.8, 129.2, 133.6, 136.2, 147.7, 171.9 (Qu). ³¹P{¹H} NMR (C₆D₆, 25 °C): $\delta = 61.7$.

X-ray crystallography. Single crystals were sealed in Lindemann glass capillaries under nitrogen. X-ray data of **3** were collected on a Rigaku R-AXIS II imaging plate using graphite-monochromatized Mo K α radiation ($\lambda = 0.71073$ Å) from a rotating-anode generator operating at 50kV and 90mA. The structures were solved by direct phase determination using the computer program SHELXTL-PC on a PC 486 and refined by full-matrix least squares with anisotropic thermal parameters for the non-hydrogen atoms.² Hydrogen atoms were introduced in their idealized positions and included in structure factor calculations with assigned isotropic temperature factor calculations.

	3	
Formula	$C_{64}H_{80}Cu_8N_4P_4S_4$	
Fw	1665.76	
Color	Red	
Cryst. Syst.	Monoclinic	
Space Group	$P2_1/c$	
a (Å)	12.961(1)	
<i>b</i> (Å)	12.923(1)	
<i>c</i> (Å)	46.063(4)	
α (deg)	90	
β (deg)	90.277(2)	
γ (deg)	90	
$V(\text{\AA}^3)$	7715.1(1)	
Ζ	4	
d_{calcd} (g cm ⁻³)	1.434	
$\mu (\mathrm{mm}^{-1})$	2.389	
F(000)	3392	
Cryst size (mm)	0.50 x 0.40 x 0.30	
2θ range (deg)	0.88 to 25.25	
Index range	$-15 \le h \le 15$,	
	$-7 \le k \le 15$,	
	$-55 \le l \le 55$	
No. of rflns collected	60540	
No. of indep rflns	13971	
R1, wR2 ($I > 2(\sigma)I$)	0.0401, 0.0962	
R1, wR2 (all data)	0.0643, 0.1085	
Goodness of fit, F^2	1.053	
No. of data/restraints /params	3135 / 0 / 181	
Largest diff peaks ,eÅ ⁻³	0.724 to -0.521	

Table 1. Crystallographic Data for Compound 3

$\begin{array}{llllllllllllllllllllllllllllllllllll$				
Cu(1)-S(3)2.302(2) $Cu(5)$ -C(10)1.983(8) $Cu(1)$ -S(4)2.338(2) $Cu(5)$ -C(42)1.996(8) $Cu(1)$ -Cu(5)2.632(1) $Cu(5)$ -Cu(7)2.548(1) $Cu(1)$ -Cu(2)2.667(1) $Cu(5)$ -Cu(8)2.551(1) $Cu(1)$ -Cu(2)2.667(1) $Cu(5)$ -Cu(8)2.551(1) $Cu(1)$ -Cu(2)1.966(6) $Cu(6)$ -C(26)1.966(8) $Cu(2)$ -N(2)1.966(6) $Cu(6)$ -Cu(7)2.543(1) $Cu(2)$ -S(4)2.306(2) $Cu(6)$ -Cu(7)2.543(1) $Cu(2)$ -S(3)2.348(2) $Cu(6)$ -Cu(7)2.543(1) $Cu(2)$ -Cu(6)2.637(2) $Cu(7)$ -C(26)1.982(7) $Cu(2)$ -Cu(7)2.667(2) $Cu(7)$ -C(26)1.991(8) $Cu(3)$ -N(3)1.964(7) $Cu(8)$ -C(58)1.961(7) $Cu(3)$ -S(2)2.310(3) $Cu(8)$ -C(10)1.997(8) $Cu(3)$ -S(1)2.322(3)P(1)-C(10)1.753(8) $Cu(3)$ -S(1)2.322(3)P(1)-C(10)1.753(8) $Cu(3)$ -Cu(7)2.638(2)P(2)-C(26)1.751(8) $Cu(3)$ -Cu(5)2.648(2)P(2)-C(26)1.751(8) $Cu(3)$ -Cu(4)2.703(2)P(2)-S(2)2.033(3) $Cu(4)$ -N(4)1.949(7)P(3)-C(42)1.739(8) $Cu(4)$ -N(4)1.949(7)P(3)-C(42)1.739(8) $Cu(4)$ -S(1)2.315(3)P(3)-S(3)2.034(3) $Cu(4)$ -S(1)2.315(3)P(3)-S(3)2.034(3) $Cu(4)$ -S(1)2.315(3)P(3)-S(3)2.034(3) $Cu(4)$ -S(1)2.315(3)P(3)-S(4)1.75(8) <tr< td=""><td>Cu(1)-N(1)</td><td>1.974(6)</td><td>Cu(4)-Cu(6)</td><td>2.660(2)</td></tr<>	Cu(1)-N(1)	1.974(6)	Cu(4)-Cu(6)	2.660(2)
Cu(1)-S(4)2.338(2)Cu(5)-C(42)1.996(8)Cu(1)-Cu(5)2.632(1)Cu(5)-Cu(7)2.548(1)Cu(1)-Cu(2)2.667(1)Cu(5)-Cu(8)2.551(1)Cu(1)-Cu(8)2.673(2)Cu(6)-C(26)1.966(8)Cu(2)-N(2)1.966(6)Cu(6)-Cu(8)2.541(1)Cu(2)-S(4)2.306(2)Cu(6)-Cu(7)2.543(1)Cu(2)-S(3)2.348(2)Cu(6)-Cu(7)2.543(1)Cu(2)-S(3)2.348(2)Cu(7)-C(26)1.991(8)Cu(2)-Cu(7)2.667(2)Cu(7)-C(26)1.991(8)Cu(3)-N(3)1.964(7)Cu(8)-C(10)1.997(8)Cu(3)-N(3)1.964(7)Cu(8)-C(10)1.997(8)Cu(3)-S(1)2.322(3)P(1)-C(10)1.753(8)Cu(3)-S(1)2.322(3)P(1)-S(1)2.026(3)Cu(3)-Cu(7)2.638(2)P(1)-S(1)2.026(3)Cu(3)-Cu(4)2.703(2)P(2)-S(2)2.033(3)Cu(4)-N(4)1.949(7)P(3)-C(42)1.739(8)Cu(4)-S(1)2.315(3)P(3)-S(3)2.034(3)Cu(4)-S(1)2.315(3)P(3)-S(3)2.034(3)Cu(4)-S(1)2.315(3)P(3)-S(3)2.033(3)VN(1)-Cu(1)-S(3)131.3(2)Cu(7)-Cu(6)-Cu(4)107.0(2)S(3)-Cu(1)-S(4)93.6(8)C(58)-Cu(6)-Cu(4)107.0(2)S(3)-Cu(1)-S(4)93.6(8)C(58)-Cu(6)-Cu(4)49.6(2)S(4)-Cu(1)-Cu(5)53.8(6)C(26)-Cu(7)-Cu(6)49.6(2)S(4)-Cu(1)-Cu(2)55.8(6)C(26)-Cu(7)-Cu(3)104.5(2)S(3)-Cu(Cu(1)-S(3)	2.302(2)	Cu(5)-C(10)	1.983(8)
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Cu(2)-N(2)1.966(6) $Cu(6)-C(58)$ 1.973(8) $Cu(2)-S(4)$ 2.306(2) $Cu(6)-Cu(8)$ 2.541(1) $Cu(2)-S(3)$ 2.348(2) $Cu(6)-Cu(7)$ 2.543(1) $Cu(2)-Cu(6)$ 2.637(2) $Cu(7)-C(26)$ 1.982(7) $Cu(2)-Cu(7)$ 2.667(2) $Cu(7)-C(42)$ 1.991(8) $Cu(3)-N(3)$ 1.964(7) $Cu(8)-C(58)$ 1.961(7) $Cu(3)-S(2)$ 2.310(3) $Cu(8)-C(10)$ 1.997(8) $Cu(3)-S(1)$ 2.322(3) $P(1)-C(10)$ 1.753(8) $Cu(3)-S(1)$ 2.322(3) $P(1)-S(1)$ 2.026(3) $Cu(3)-Cu(7)$ 2.638(2) $P(2)-C(26)$ 1.751(8) $Cu(3)-Cu(4)$ 2.703(2) $P(2)-S(2)$ 2.033(3) $Cu(4)-N(4)$ 1.949(7) $P(3)-C(42)$ 1.739(8) $Cu(4)-S(1)$ 2.315(3) $P(3)-S(3)$ 2.034(3) $Cu(4)-S(1)$ 2.315(3) $P(3)-S(3)$ 2.034(3) $Cu(4)-S(2)$ 2.329(2) $P(4)-C(58)$ 1.775(8) $Cu(4)-Cu(8)$ 2.632(1) $P(4)-S(4)$ 2.033(3) $N(1)-Cu(1)-S(3)$ 131.3(2) $Cu(7)-Cu(6)-Cu(2)$ 61.9(4) $N(1)-Cu(1)-S(4)$ 124.6(2) $C(26)-Cu(7)-Cu(4)$ 40.8(4) $S(3)-Cu(1)-S(4)$ 93.6(8) $C(58)-Cu(6)-Cu(4)$ 40.8(4) $S(3)-Cu(1)-S(4)$ 93.6(8) $C(26)-Cu(7)-Cu(6)$ 49.6(2) $S(4)-Cu(1)-Cu(5)$ 54.4(6) $C(42)-Cu(7)-Cu(5)$ 50.4(2) $S(4)-Cu(1)-Cu(2)$ 54.4(6) $C(42)-Cu(7)-Cu(3)$ 77.8(2) $S(4)-Cu(1)-Cu(8)$ 85.6(7) $Cu(6)-Cu(7)-Cu(3)$ 61.4(4)	Cu(1)-Cu(8)	2.673(2)	Cu(6)-C(26)	1.966(8)
Cu(2)-S(4)2.306(2) $Cu(6)$ -Cu(8)2.541(1) $Cu(2)$ -S(3)2.348(2) $Cu(6)$ -Cu(7)2.543(1) $Cu(2)$ -Cu(6)2.637(2) $Cu(7)$ -C(26)1.982(7) $Cu(2)$ -Cu(7)2.667(2) $Cu(7)$ -C(42)1.991(8) $Cu(3)$ -N(3)1.964(7) $Cu(8)$ -C(10)1.997(8) $Cu(3)$ -S(2)2.310(3) $Cu(8)$ -C(10)1.997(8) $Cu(3)$ -S(1)2.322(3)P(1)-C(10)1.753(8) $Cu(3)$ -Cu(7)2.638(2)P(1)-S(1)2.026(3) $Cu(3)$ -Cu(5)2.648(2)P(2)-C(26)1.751(8) $Cu(3)$ -Cu(4)2.703(2)P(2)-S(2)2.033(3) $Cu(4)$ -N(4)1.949(7)P(3)-C(42)1.739(8) $Cu(4)$ -N(4)1.949(7)P(3)-C(42)1.739(8) $Cu(4)$ -S(1)2.315(3)P(3)-S(3)2.034(3) $Cu(4)$ -S(2)2.329(2)P(4)-C(58)1.775(8) $Cu(4)$ -Cu(8)2.632(1)P(4)-S(4)2.033(3)N(1)-Cu(1)-S(3)131.3(2)Cu(7)-Cu(6)-Cu(2)61.9(4)N(1)-Cu(1)-S(4)124.6(2)C(26)-Cu(4)107.0(2)S(3)-Cu(1)-S(4)93.6(8)C(58)-Cu(6)-Cu(4)92.2(4)S(3)-Cu(1)-S(4)93.6(8)C(58)-Cu(6)-Cu(4)92.2(4)S(3)-Cu(1)-Cu(5)90.6(7)Cu(7)-Cu(6)-Cu(4)92.2(4)S(3)-Cu(1)-Cu(5)90.6(7)Cu(7)-Cu(6)-Cu(4)92.2(4)S(3)-Cu(1)-Cu(5)90.6(7)Cu(7)-Cu(5)50.4(2)Cu(5)-Cu(1)-Cu(2)55.8(6)C(26)-Cu(7)-Cu(5)50.4(2)Cu(5)-Cu(1)-Cu(2)55.8(6) <t< td=""><td>Cu(2)-N(2)</td><td>1.966(6)</td><td>Cu(6)-C(58)</td><td>1.973(8)</td></t<>	Cu(2)-N(2)	1.966(6)	Cu(6)-C(58)	1.973(8)
Cu(2)-S(3)2.348(2) $Cu(6)$ -Cu(7)2.543(1) $Cu(2)$ -Cu(6)2.637(2) $Cu(7)$ -C(26)1.982(7) $Cu(2)$ -Cu(7)2.667(2) $Cu(7)$ -C(42)1.991(8) $Cu(3)$ -N(3)1.964(7) $Cu(8)$ -C(58)1.961(7) $Cu(3)$ -S(2)2.310(3) $Cu(8)$ -C(10)1.997(8) $Cu(3)$ -S(1)2.322(3)P(1)-C(10)1.753(8) $Cu(3)$ -Cu(7)2.638(2)P(1)-S(1)2.026(3) $Cu(3)$ -Cu(5)2.648(2)P(2)-C(26)1.751(8) $Cu(3)$ -Cu(4)2.703(2)P(2)-S(2)2.033(3) $Cu(4)$ -N(4)1.949(7)P(3)-C(42)1.739(8) $Cu(4)$ -S(1)2.315(3)P(3)-S(3)2.034(3) $Cu(4)$ -S(1)2.315(3)P(3)-S(3)2.034(3) $Cu(4)$ -S(2)2.329(2)P(4)-C(58)1.775(8) $Cu(4)$ -S(2)2.329(2)P(4)-C(58)1.775(8) $Cu(4)$ -Cu(8)2.632(1)P(4)-S(4)2.033(3)N(1)-Cu(1)-S(3)131.3(2)Cu(7)-Cu(6)-Cu(2)61.9(4)N(1)-Cu(1)-S(4)124.6(2)C(26)-Cu(4)107.0(2)S(3)-Cu(1)-S(4)93.6(8)C(58)-Cu(6)-Cu(4)92.2(4)S(3)-Cu(1)-S(4)93.6(8)C(58)-Cu(6)-Cu(4)92.2(4)S(3)-Cu(1)-Cu(5)90.6(7)Cu(7)-Cu(6)-Cu(4)92.2(4)S(3)-Cu(1)-Cu(5)90.6(7)Cu(7)-Cu(6)-Cu(4)92.2(4)S(3)-Cu(1)-Cu(5)90.6(7)Cu(7)-Cu(5)50.4(2)Cu(5)-Cu(1)-Cu(2)55.8(6)C(26)-Cu(7)-Cu(5)50.4(2)Cu(5)-Cu(1)-Cu(2)55.8(6)C(Cu(2)-S(4)	2.306(2)	Cu(6)-Cu(8)	2.541(1)
Cu(2)-Cu(6) $2.637(2)$ Cu(7)-C(26) $1.982(7)$ Cu(2)-Cu(7) $2.667(2)$ Cu(7)-C(42) $1.991(8)$ Cu(3)-N(3) $1.964(7)$ Cu(8)-C(58) $1.961(7)$ Cu(3)-S(2) $2.310(3)$ Cu(8)-C(10) $1.997(8)$ Cu(3)-S(1) $2.322(3)$ P(1)-C(10) $1.753(8)$ Cu(3)-Cu(7) $2.638(2)$ P(1)-S(1) $2.026(3)$ Cu(3)-Cu(5) $2.648(2)$ P(2)-C(26) $1.751(8)$ Cu(3)-Cu(4) $2.703(2)$ P(2)-S(2) $2.033(3)$ Cu(4)-N(4) $1.949(7)$ P(3)-C(42) $1.739(8)$ Cu(4)-S(1) $2.315(3)$ P(3)-S(3) $2.034(3)$ Cu(4)-S(1) $2.315(3)$ P(3)-S(3) $2.034(3)$ Cu(4)-S(2) $2.329(2)$ P(4)-C(58) $1.775(8)$ Cu(4)-Cu(8) $2.632(1)$ P(4)-S(4) $2.033(3)$ N(1)-Cu(1)-S(4) $124.6(2)$ C(26)-Cu(6)-Cu(4) $107.0(2)$ S(3)-Cu(1)-S(4) $124.6(2)$ C(26)-Cu(6)-Cu(4) $107.0(2)$ S(3)-Cu(1)-S(4) $93.6(8)$ C(58)-Cu(6)-Cu(4) $76.6(2)$ N(1)-Cu(1)-S(4) $124.6(2)$ Cu(6)-Cu(7)-Cu(6) $49.6(2)$ S(3)-Cu(1)-Cu(5) $90.6(7)$ Cu(7)-Cu(6)-Cu(4) $92.2(4)$ S(3)-Cu(1)-S(4) $93.6(8)$ C(26)-Cu(7)-Cu(5) $90.4(4)$ S(3)-Cu(1)-Cu(2) $57.8(6)$ C(26)-Cu(7)-Cu(3) $77.8(2)$ S(4)-Cu(1)-Cu(8) $84.5(2)$ C(26)-Cu(7)-Cu(3) $71.4(4)$ Cu(5)-Cu(1)-Cu(8) $87.0(4)$ Cu(5)-Cu(7)-Cu(2) $73.(2)$ S(4)-Cu(1)-Cu(8) $87.0(4)$ Cu(5)-Cu(7)-	Cu(2)-S(3)	2.348(2)	Cu(6)-Cu(7)	2.543(1)
Cu(2)-Cu(7) $2.667(2)$ $Cu(7)-C(42)$ $1.991(8)$ $Cu(3)-N(3)$ $1.964(7)$ $Cu(8)-C(58)$ $1.961(7)$ $Cu(3)-S(2)$ $2.310(3)$ $Cu(8)-C(10)$ $1.997(8)$ $Cu(3)-S(1)$ $2.322(3)$ $P(1)-C(10)$ $1.753(8)$ $Cu(3)-Cu(7)$ $2.638(2)$ $P(1)-S(1)$ $2.026(3)$ $Cu(3)-Cu(5)$ $2.648(2)$ $P(2)-C(26)$ $1.751(8)$ $Cu(3)-Cu(4)$ $2.703(2)$ $P(2)-S(2)$ $2.033(3)$ $Cu(4)-N(4)$ $1.949(7)$ $P(3)-C(42)$ $1.739(8)$ $Cu(4)-S(1)$ $2.315(3)$ $P(3)-S(3)$ $2.034(3)$ $Cu(4)-S(1)$ $2.315(3)$ $P(3)-S(3)$ $2.034(3)$ $Cu(4)-S(2)$ $2.329(2)$ $P(4)-C(58)$ $1.775(8)$ $Cu(4)-Su(8)$ $2.632(1)$ $P(4)-S(4)$ $2.033(3)$ $N(1)-Cu(1)-S(4)$ $124.6(2)$ $C(26)-Cu(6)-Cu(4)$ $107.0(2)$ $S(3)-Cu(1)-S(4)$ $124.6(2)$ $C(26)-Cu(6)-Cu(4)$ $107.0(2)$ $S(3)-Cu(1)-S(4)$ $124.6(2)$ $Cu(7)-Cu(6)-Cu(4)$ $92.2(4)$ $S(3)-Cu(1)-S(4)$ $93.6(8)$ $C(58)-Cu(6)-Cu(4)$ $92.2(4)$ $S(3)-Cu(1)-Cu(5)$ $90.6(7)$ $Cu(7)-Cu(6)-Cu(4)$ $92.2(4)$ $S(3)-Cu(1)-Cu(2)$ $54.4(6)$ $C(42)-Cu(7)-Cu(5)$ $90.4(4)$ $N(1)-Cu(1)-Cu(8)$ $84.5(2)$ $C(26)-Cu(7)-Cu(3)$ $77.8(2)$ $S(4)-Cu(1)-Cu(8)$ $85.6(7)$ $Cu(6)-Cu(7)-Cu(3)$ $91.3(4)$ $Cu(2)-Cu(1)-Cu(8)$ $87.0(4)$ $Cu(2)-Cu(7)-Cu(2)$ $90.7(2)$ $N(2)-Cu(2)-S(3)$ $125.8(2)$ $C(42)-Cu(7$	Cu(2)-Cu(6)	2.637(2)	Cu(7)-C(26)	1.982(7)
Cu(3)-N(3) $1.964(7)$ Cu(8)-C(58) $1.961(7)$ Cu(3)-S(2) $2.310(3)$ Cu(8)-C(10) $1.997(8)$ Cu(3)-S(1) $2.322(3)$ P(1)-C(10) $1.753(8)$ Cu(3)-Cu(7) $2.638(2)$ P(1)-S(1) $2.026(3)$ Cu(3)-Cu(5) $2.648(2)$ P(2)-C(26) $1.751(8)$ Cu(3)-Cu(4) $2.703(2)$ P(2)-S(2) $2.033(3)$ Cu(4)-N(4) $1.949(7)$ P(3)-C(42) $1.739(8)$ Cu(4)-S(1) $2.315(3)$ P(3)-S(3) $2.034(3)$ Cu(4)-S(2) $2.329(2)$ P(4)-C(58) $1.775(8)$ Cu(4)-S(2) $2.329(2)$ P(4)-C(58) $1.775(8)$ Cu(4)-Cu(8) $2.632(1)$ P(4)-S(4) $2.033(3)$ N(1)-Cu(1)-S(3) $131.3(2)$ Cu(7)-Cu(6)-Cu(2) $61.9(4)$ N(1)-Cu(1)-S(4) $124.6(2)$ C(26)-Cu(6)-Cu(4) $107.0(2)$ S(3)-Cu(1)-Cu(5) $85.1(2)$ Cu(8)-Cu(6)-Cu(4) $76.6(2)$ N(1)-Cu(1)-S(4) $93.6(8)$ C(58)-Cu(6)-Cu(4) $76.6(2)$ N(1)-Cu(1)-Cu(5) $85.1(2)$ Cu(8)-Cu(7)-Cu(6) $49.6(2)$ S(4)-Cu(1)-Cu(2) $55.8(6)$ C(26)-Cu(7)-Cu(4) $92.2(4)$ S(3)-Cu(1)-Cu(2) $50.4(1)$ Cu(6)-Cu(7)-Cu(5) $50.4(2)$ Cu(5)-Cu(1)-Cu(2) $50.4(2)$ C(26)-Cu(7)-Cu(3) $104.5(2)$ S(3)-Cu(1)-Cu(8) $84.5(2)$ C(26)-Cu(7)-Cu(3) $104.5(2)$ S(3)-Cu(1)-Cu(8) $85.6(7)$ Cu(6)-Cu(7)-Cu(3) $91.3(4)$ Cu(2)-Cu(1)-Cu(8) $87.0(4)$ Cu(5)-Cu(7)-Cu(2) $77.3(2)$ N(2)-Cu(1)-Cu(8) $87.0(4$	Cu(2)-Cu(7)	2.667(2)	Cu(7)-C(42)	1.991(8)
Cu(3)-S(2) $2.310(3)$ $Cu(8)-C(10)$ $1.997(8)$ $Cu(3)-S(1)$ $2.322(3)$ $P(1)-C(10)$ $1.753(8)$ $Cu(3)-Cu(7)$ $2.638(2)$ $P(1)-S(1)$ $2.026(3)$ $Cu(3)-Cu(5)$ $2.648(2)$ $P(2)-C(26)$ $1.751(8)$ $Cu(3)-Cu(4)$ $2.703(2)$ $P(2)-S(2)$ $2.033(3)$ $Cu(4)-N(4)$ $1.949(7)$ $P(3)-C(42)$ $1.739(8)$ $Cu(4)-S(1)$ $2.315(3)$ $P(3)-S(3)$ $2.034(3)$ $Cu(4)-S(1)$ $2.329(2)$ $P(4)-C(58)$ $1.775(8)$ $Cu(4)-S(2)$ $2.329(2)$ $P(4)-C(58)$ $1.775(8)$ $Cu(4)-Cu(8)$ $2.632(1)$ $P(4)-S(4)$ $2.033(3)$ $N(1)-Cu(1)-S(3)$ $131.3(2)$ $Cu(7)-Cu(6)-Cu(2)$ $61.9(4)$ $N(1)-Cu(1)-S(4)$ $124.6(2)$ $C(26)-Cu(6)-Cu(4)$ $107.0(2)$ $S(3)-Cu(1)-S(4)$ $93.6(8)$ $C(58)-Cu(6)-Cu(4)$ $76.6(2)$ $N(1)-Cu(1)-S(4)$ $93.6(8)$ $C(58)-Cu(6)-Cu(4)$ $92.2(4)$ $S(3)-Cu(1)-Cu(5)$ $90.6(7)$ $Cu(7)-Cu(6)-Cu(4)$ $92.2(4)$ $S(3)-Cu(1)-Cu(2)$ $55.8(6)$ $C(26)-Cu(7)-Cu(5)$ $50.4(2)$ $Cu(5)-Cu(1)-Cu(2)$ $54.4(6)$ $C(42)-Cu(7)-Cu(5)$ $90.4(4)$ $N(1)-Cu(1)-Cu(8)$ $84.5(2)$ $C(26)-Cu(7)-Cu(3)$ $104.5(2)$ $S(3)-Cu(1)-Cu(8)$ $85.6(7)$ $Cu(6)-Cu(7)-Cu(3)$ $91.3(4)$ $Cu(5)-Cu(1)-Cu(8)$ $57.5(4)$ $Cu(5)-Cu(7)-Cu(2)$ $77.3(2)$ $N(2)-Cu(2)-S(3)$ $125.8(2)$ $C(42)-Cu(7)-Cu(2)$ $106.7(2)$	Cu(3)-N(3)	1.964(7)	Cu(8)-C(58)	1.961(7)
$\begin{array}{cccc} \mathrm{Cu}(3){\text{-}}\mathrm{S}(1) & 2.322(3) & \mathrm{P}(1){\text{-}}\mathrm{C}(10) & 1.753(8) \\ \mathrm{Cu}(3){\text{-}}\mathrm{Cu}(7) & 2.638(2) & \mathrm{P}(1){\text{-}}\mathrm{S}(1) & 2.026(3) \\ \mathrm{Cu}(3){\text{-}}\mathrm{Cu}(5) & 2.648(2) & \mathrm{P}(2){\text{-}}\mathrm{C}(26) & 1.751(8) \\ \mathrm{Cu}(3){\text{-}}\mathrm{Cu}(4) & 2.703(2) & \mathrm{P}(2){\text{-}}\mathrm{S}(2) & 2.033(3) \\ \mathrm{Cu}(4){\text{-}}\mathrm{N}(4) & 1.949(7) & \mathrm{P}(3){\text{-}}\mathrm{C}(42) & 1.739(8) \\ \mathrm{Cu}(4){\text{-}}\mathrm{N}(4) & 1.949(7) & \mathrm{P}(3){\text{-}}\mathrm{C}(42) & 1.739(8) \\ \mathrm{Cu}(4){\text{-}}\mathrm{S}(1) & 2.315(3) & \mathrm{P}(3){\text{-}}\mathrm{S}(3) & 2.034(3) \\ \mathrm{Cu}(4){\text{-}}\mathrm{S}(2) & 2.329(2) & \mathrm{P}(4){\text{-}}\mathrm{C}(58) & 1.775(8) \\ \mathrm{Cu}(4){\text{-}}\mathrm{Cu}(8) & 2.632(1) & \mathrm{P}(4){\text{-}}\mathrm{S}(4) & 2.033(3) \\ \end{array}$ $\begin{array}{c} \mathrm{N}(1){\text{-}}\mathrm{Cu}(1){\text{-}}\mathrm{S}(3) & 131.3(2) & \mathrm{Cu}(7){\text{-}}\mathrm{Cu}(6){\text{-}}\mathrm{Cu}(4) & 107.0(2) \\ \mathrm{S}(3){\text{-}}\mathrm{Cu}(1){\text{-}}\mathrm{S}(4) & 23.6(8) & \mathrm{C}(58){\text{-}}\mathrm{Cu}(6){\text{-}}\mathrm{Cu}(4) & 107.0(2) \\ \mathrm{S}(3){\text{-}}\mathrm{Cu}(1){\text{-}}\mathrm{S}(4) & 93.6(8) & \mathrm{C}(58){\text{-}}\mathrm{Cu}(6){\text{-}}\mathrm{Cu}(4) & 60.8(4) \\ \mathrm{S}(3){\text{-}}\mathrm{Cu}(1){\text{-}}\mathrm{Cu}(5) & 90.6(7) & \mathrm{Cu}(7){\text{-}}\mathrm{Cu}(6){\text{-}}\mathrm{Cu}(4) & 92.2(4) \\ \mathrm{S}(3){\text{-}}\mathrm{Cu}(1){\text{-}}\mathrm{Cu}(2) & 55.8(6) & \mathrm{C}(26){\text{-}}\mathrm{Cu}(7){\text{-}}\mathrm{Cu}(5) & 90.4(4) \\ \mathrm{N}(1){\text{-}}\mathrm{Cu}(1){\text{-}}\mathrm{Cu}(2) & 55.8(6) & \mathrm{C}(26){\text{-}}\mathrm{Cu}(7){\text{-}}\mathrm{Cu}(5) & 90.4(4) \\ \mathrm{N}(1){\text{-}}\mathrm{Cu}(1){\text{-}}\mathrm{Cu}(8) & 84.5(2) & \mathrm{C}(26){\text{-}}\mathrm{Cu}(7){\text{-}}\mathrm{Cu}(3) & 104.5(2) \\ \\ \mathrm{S}(3){\text{-}}\mathrm{Cu}(1){\text{-}}\mathrm{Cu}(8) & 84.5(2) & \mathrm{C}(26){\text{-}}\mathrm{Cu}(7){\text{-}}\mathrm{Cu}(3) & 91.3(4) \\ \\ \mathrm{Cu}(5){\text{-}}\mathrm{Cu}(1){\text{-}}\mathrm{Cu}(8) & 85.6(7) & \mathrm{Cu}(6){\text{-}}\mathrm{Cu}(7){\text{-}}\mathrm{Cu}(3) & 91.3(4) \\ \\ \mathrm{Cu}(5){\text{-}}\mathrm{Cu}(1){\text{-}}\mathrm{Cu}(8) & 87.0(4) & \mathrm{Cu}(5){\text{-}}\mathrm{Cu}(7){\text{-}}\mathrm{Cu}(2) & 77.3(2) \\ \mathrm{N}(2){\text{-}}\mathrm{Cu}(2){\text{-}}\mathrm{S}(3) & 125.8(2) & \mathrm{C}(42){\text{-}}\mathrm{Cu}(7){\text{-}}\mathrm{Cu}(2) & 106.7(2) \\ \end{array}}$	Cu(3)-S(2)	2.310(3)	Cu(8)-C(10)	1.997(8)
$\begin{array}{c c} Cu(3)-Cu(7) & 2.638(2) & P(1)-S(1) & 2.026(3) \\ Cu(3)-Cu(5) & 2.648(2) & P(2)-C(26) & 1.751(8) \\ Cu(3)-Cu(4) & 2.703(2) & P(2)-S(2) & 2.033(3) \\ Cu(4)-N(4) & 1.949(7) & P(3)-C(42) & 1.739(8) \\ Cu(4)-S(1) & 2.315(3) & P(3)-S(3) & 2.034(3) \\ Cu(4)-S(2) & 2.329(2) & P(4)-C(58) & 1.775(8) \\ Cu(4)-Cu(8) & 2.632(1) & P(4)-S(4) & 2.033(3) \\ \end{array}$	Cu(3)-S(1)	2.322(3)	P(1)-C(10)	1.753(8)
Cu(3)-Cu(5) $2.648(2)$ P(2)-C(26) $1.751(8)$ Cu(3)-Cu(4) $2.703(2)$ P(2)-S(2) $2.033(3)$ Cu(4)-N(4) $1.949(7)$ P(3)-C(42) $1.739(8)$ Cu(4)-S(1) $2.315(3)$ P(3)-S(3) $2.034(3)$ Cu(4)-S(2) $2.329(2)$ P(4)-C(58) $1.775(8)$ Cu(4)-Cu(8) $2.632(1)$ P(4)-S(4) $2.033(3)$ N(1)-Cu(1)-S(3) $131.3(2)$ Cu(7)-Cu(6)-Cu(2) $61.9(4)$ N(1)-Cu(1)-S(4) $124.6(2)$ C(26)-Cu(6)-Cu(4) $107.0(2)$ S(3)-Cu(1)-S(4) $93.6(8)$ C(58)-Cu(6)-Cu(4) $76.6(2)$ N(1)-Cu(1)-S(4) $93.6(8)$ C(58)-Cu(6)-Cu(4) $92.2(4)$ S(3)-Cu(1)-Cu(5) $85.1(2)$ Cu(8)-Cu(6)-Cu(4) $92.2(4)$ S(3)-Cu(1)-Cu(5) $90.6(7)$ Cu(7)-Cu(6) $49.6(2)$ S(4)-Cu(1)-Cu(2) $55.8(6)$ C(26)-Cu(7)-Cu(5) $50.4(2)$ S(4)-Cu(1)-Cu(2) $54.4(6)$ C(42)-Cu(7)-Cu(3) $104.5(2)$ S(3)-Cu(1)-Cu(8) $84.5(2)$ C(26)-Cu(7)-Cu(3) $104.5(2)$ S(3)-Cu(1)-Cu(8) $132.0(7)$ C(42)-Cu(7)-Cu(3) $91.3(4)$ Cu(5)-Cu(1)-Cu(8) $85.6(7)$ Cu(6)-Cu(7)-Cu(3) $91.3(4)$ Cu(5)-Cu(1)-Cu(8) $87.0(4)$ Cu(5)-Cu(7)-Cu(2) $77.3(2)$ N(2)-Cu(1)-Cu(8) $87.0(4)$ C(26)-Cu(7)-Cu(2) $106.7(2)$	Cu(3)-Cu(7)	2.638(2)	P(1)-S(1)	2.026(3)
$\begin{array}{cccc} \mathrm{Cu}(3){-}\mathrm{Cu}(4) & 2.703(2) & \mathrm{P}(2){-}\mathrm{S}(2) & 2.033(3) \\ \mathrm{Cu}(4){-}\mathrm{N}(4) & 1.949(7) & \mathrm{P}(3){-}\mathrm{C}(42) & 1.739(8) \\ \mathrm{Cu}(4){-}\mathrm{S}(1) & 2.315(3) & \mathrm{P}(3){-}\mathrm{S}(3) & 2.034(3) \\ \mathrm{Cu}(4){-}\mathrm{S}(2) & 2.329(2) & \mathrm{P}(4){-}\mathrm{C}(58) & 1.775(8) \\ \mathrm{Cu}(4){-}\mathrm{Cu}(8) & 2.632(1) & \mathrm{P}(4){-}\mathrm{S}(4) & 2.033(3) \\ \end{array}$	Cu(3)-Cu(5)	2.648(2)	P(2)-C(26)	1.751(8)
$\begin{array}{cccc} \mathrm{Cu}(4) \cdot \mathrm{N}(4) & 1.949(7) & \mathrm{P}(3) \cdot \mathrm{C}(42) & 1.739(8) \\ \mathrm{Cu}(4) \cdot \mathrm{S}(1) & 2.315(3) & \mathrm{P}(3) \cdot \mathrm{S}(3) & 2.034(3) \\ \mathrm{Cu}(4) \cdot \mathrm{S}(2) & 2.329(2) & \mathrm{P}(4) \cdot \mathrm{C}(58) & 1.775(8) \\ \mathrm{Cu}(4) \cdot \mathrm{Cu}(8) & 2.632(1) & \mathrm{P}(4) \cdot \mathrm{S}(4) & 2.033(3) \\ \end{array}$	Cu(3)-Cu(4)	2.703(2)	P(2)-S(2)	2.033(3)
$\begin{array}{cccc} Cu(4)-S(1) & 2.315(3) & P(3)-S(3) & 2.034(3) \\ Cu(4)-S(2) & 2.329(2) & P(4)-C(58) & 1.775(8) \\ Cu(4)-Cu(8) & 2.632(1) & P(4)-S(4) & 2.033(3) \\ \end{array}$	Cu(4)-N(4)	1.949(7)	P(3)-C(42)	1.739(8)
$\begin{array}{cccc} Cu(4)-S(2) & 2.329(2) & P(4)-C(58) & 1.775(8) \\ Cu(4)-Cu(8) & 2.632(1) & P(4)-S(4) & 2.033(3) \\ \\ \hline \\ N(1)-Cu(1)-S(3) & 131.3(2) & Cu(7)-Cu(6)-Cu(2) & 61.9(4) \\ N(1)-Cu(1)-S(4) & 124.6(2) & C(26)-Cu(6)-Cu(4) & 107.0(2) \\ S(3)-Cu(1)-S(4) & 93.6(8) & C(58)-Cu(6)-Cu(4) & 76.6(2) \\ N(1)-Cu(1)-Cu(5) & 85.1(2) & Cu(8)-Cu(6)-Cu(4) & 60.8(4) \\ S(3)-Cu(1)-Cu(5) & 90.6(7) & Cu(7)-Cu(6)-Cu(4) & 92.2(4) \\ S(3)-Cu(1)-Cu(2) & 55.8(6) & C(26)-Cu(7)-Cu(6) & 49.6(2) \\ S(4)-Cu(1)-Cu(2) & 54.4(6) & C(42)-Cu(7)-Cu(5) & 50.4(2) \\ Cu(5)-Cu(1)-Cu(2) & 90.4(4) & Cu(6)-Cu(7)-Cu(5) & 90.4(4) \\ N(1)-Cu(1)-Cu(8) & 84.5(2) & C(26)-Cu(7)-Cu(3) & 104.5(2) \\ S(3)-Cu(1)-Cu(8) & 132.0(7) & C(42)-Cu(7)-Cu(3) & 91.3(4) \\ Cu(5)-Cu(1)-Cu(8) & 85.6(7) & Cu(6)-Cu(7)-Cu(3) & 91.3(4) \\ Cu(5)-Cu(1)-Cu(8) & 87.0(4) & C(26)-Cu(7)-Cu(2) & 77.3(2) \\ N(2)-Cu(2)-S(3) & 125.8(2) & C(42)-Cu(7)-Cu(2) & 106.7(2) \\ \end{array}$	Cu(4)-S(1)	2.315(3)	P(3)-S(3)	2.034(3)
Cu(4)-Cu(8) $2.632(1)$ $P(4)-S(4)$ $2.033(3)$ $N(1)-Cu(1)-S(3)$ $131.3(2)$ $Cu(7)-Cu(6)-Cu(2)$ $61.9(4)$ $N(1)-Cu(1)-S(4)$ $124.6(2)$ $C(26)-Cu(6)-Cu(4)$ $107.0(2)$ $S(3)-Cu(1)-S(4)$ $93.6(8)$ $C(58)-Cu(6)-Cu(4)$ $76.6(2)$ $N(1)-Cu(1)-Cu(5)$ $85.1(2)$ $Cu(8)-Cu(6)-Cu(4)$ $60.8(4)$ $S(3)-Cu(1)-Cu(5)$ $90.6(7)$ $Cu(7)-Cu(6)-Cu(4)$ $92.2(4)$ $S(3)-Cu(1)-Cu(2)$ $55.8(6)$ $C(26)-Cu(7)-Cu(6)$ $49.6(2)$ $S(4)-Cu(1)-Cu(2)$ $54.4(6)$ $C(42)-Cu(7)-Cu(5)$ $50.4(2)$ $Cu(5)-Cu(1)-Cu(2)$ $90.4(4)$ $Cu(6)-Cu(7)-Cu(5)$ $90.4(4)$ $N(1)-Cu(1)-Cu(8)$ $84.5(2)$ $C(26)-Cu(7)-Cu(3)$ $104.5(2)$ $S(3)-Cu(1)-Cu(8)$ $132.0(7)$ $C(42)-Cu(7)-Cu(3)$ $77.8(2)$ $S(4)-Cu(1)-Cu(8)$ $85.6(7)$ $Cu(6)-Cu(7)-Cu(3)$ $91.3(4)$ $Cu(5)-Cu(1)-Cu(8)$ $57.5(4)$ $Cu(5)-Cu(7)-Cu(2)$ $77.3(2)$ $N(2)-Cu(2)-S(3)$ $125.8(2)$ $C(42)-Cu(7)-Cu(2)$ $106.7(2)$	Cu(4)-S(2)	2.329(2)	P(4)-C(58)	1.775(8)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Cu(4)-Cu(8)	2.632(1)	P(4)-S(4)	2.033(3)
N(1)-Cu(1)-S(3)131.3(2)Cu(7)-Cu(6)-Cu(2) $61.9(4)$ N(1)-Cu(1)-S(4)124.6(2)C(26)-Cu(6)-Cu(4) $107.0(2)$ S(3)-Cu(1)-S(4)93.6(8)C(58)-Cu(6)-Cu(4) $76.6(2)$ N(1)-Cu(1)-Cu(5)85.1(2)Cu(8)-Cu(6)-Cu(4) $60.8(4)$ S(3)-Cu(1)-Cu(5)90.6(7)Cu(7)-Cu(6)-Cu(4) $92.2(4)$ S(3)-Cu(1)-Cu(2)55.8(6)C(26)-Cu(7)-Cu(6) $49.6(2)$ S(4)-Cu(1)-Cu(2)54.4(6)C(42)-Cu(7)-Cu(5) $50.4(2)$ Cu(5)-Cu(1)-Cu(2)90.4(4)Cu(6)-Cu(7)-Cu(5) $90.4(4)$ N(1)-Cu(1)-Cu(8)84.5(2)C(26)-Cu(7)-Cu(3) $104.5(2)$ S(3)-Cu(1)-Cu(8)132.0(7)C(42)-Cu(7)-Cu(3) $77.8(2)$ S(4)-Cu(1)-Cu(8)85.6(7)Cu(6)-Cu(7)-Cu(3) $91.3(4)$ Cu(5)-Cu(1)-Cu(8) $57.5(4)$ Cu(5)-Cu(7)-Cu(2) $61.4(4)$ Cu(2)-Cu(1)-Cu(8) $87.0(4)$ C(26)-Cu(7)-Cu(2) $77.3(2)$ N(2)-Cu(2)-S(3)125.8(2)C(42)-Cu(7)-Cu(2) $106.7(2)$				
N(1)-Cu(1)-S(4) $124.6(2)$ $C(26)-Cu(6)-Cu(4)$ $107.0(2)$ $S(3)-Cu(1)-S(4)$ $93.6(8)$ $C(58)-Cu(6)-Cu(4)$ $76.6(2)$ $N(1)-Cu(1)-Cu(5)$ $85.1(2)$ $Cu(8)-Cu(6)-Cu(4)$ $60.8(4)$ $S(3)-Cu(1)-Cu(5)$ $90.6(7)$ $Cu(7)-Cu(6)-Cu(4)$ $92.2(4)$ $S(3)-Cu(1)-Cu(2)$ $55.8(6)$ $C(26)-Cu(7)-Cu(6)$ $49.6(2)$ $S(4)-Cu(1)-Cu(2)$ $54.4(6)$ $C(42)-Cu(7)-Cu(5)$ $50.4(2)$ $Cu(5)-Cu(1)-Cu(2)$ $90.4(4)$ $Cu(6)-Cu(7)-Cu(5)$ $90.4(4)$ $N(1)-Cu(1)-Cu(8)$ $84.5(2)$ $C(26)-Cu(7)-Cu(3)$ $104.5(2)$ $S(3)-Cu(1)-Cu(8)$ $132.0(7)$ $C(42)-Cu(7)-Cu(3)$ $77.8(2)$ $S(4)-Cu(1)-Cu(8)$ $85.6(7)$ $Cu(6)-Cu(7)-Cu(3)$ $91.3(4)$ $Cu(5)-Cu(1)-Cu(8)$ $57.5(4)$ $Cu(5)-Cu(7)-Cu(2)$ $61.4(4)$ $Cu(2)-Cu(1)-Cu(8)$ $87.0(4)$ $C(26)-Cu(7)-Cu(2)$ $77.3(2)$ $N(2)-Cu(2)-S(3)$ $125.8(2)$ $C(42)-Cu(7)-Cu(2)$ $106.7(2)$	N(1)-Cu(1)-S(3)	131.3(2)	Cu(7)-Cu(6)-Cu(2)	61.9(4)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	N(1)-Cu(1)-S(4)	124.6(2)	C(26)-Cu(6)-Cu(4)	107.0(2)
N(1)-Cu(1)-Cu(5) $85.1(2)$ $Cu(8)-Cu(6)-Cu(4)$ $60.8(4)$ $S(3)-Cu(1)-Cu(5)$ $90.6(7)$ $Cu(7)-Cu(6)-Cu(4)$ $92.2(4)$ $S(3)-Cu(1)-Cu(2)$ $55.8(6)$ $C(26)-Cu(7)-Cu(6)$ $49.6(2)$ $S(4)-Cu(1)-Cu(2)$ $54.4(6)$ $C(42)-Cu(7)-Cu(5)$ $50.4(2)$ $Cu(5)-Cu(1)-Cu(2)$ $90.4(4)$ $Cu(6)-Cu(7)-Cu(5)$ $90.4(4)$ $N(1)-Cu(1)-Cu(8)$ $84.5(2)$ $C(26)-Cu(7)-Cu(3)$ $104.5(2)$ $S(3)-Cu(1)-Cu(8)$ $132.0(7)$ $C(42)-Cu(7)-Cu(3)$ $77.8(2)$ $S(4)-Cu(1)-Cu(8)$ $85.6(7)$ $Cu(6)-Cu(7)-Cu(3)$ $91.3(4)$ $Cu(5)-Cu(1)-Cu(8)$ $57.5(4)$ $Cu(5)-Cu(7)-Cu(3)$ $61.4(4)$ $Cu(2)-Cu(1)-Cu(8)$ $87.0(4)$ $C(26)-Cu(7)-Cu(2)$ $77.3(2)$ $N(2)-Cu(2)-S(3)$ $125.8(2)$ $C(42)-Cu(7)-Cu(2)$ $106.7(2)$	S(3)-Cu(1)-S(4)	93.6(8)	C(58)-Cu(6)-Cu(4)	76.6(2)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	N(1)-Cu(1)-Cu(5)	85.1(2)	Cu(8)-Cu(6)-Cu(4)	60.8(4)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	S(3)-Cu(1)-Cu(5)	90.6(7)	Cu(7)-Cu(6)-Cu(4)	92.2(4)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	S(3)-Cu(1)-Cu(2)	55.8(6)	C(26)-Cu(7)-Cu(6)	49.6(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	S(4)-Cu(1)-Cu(2)	54.4(6)	C(42)-Cu(7)-Cu(5)	50.4(2)
N(1)-Cu(1)-Cu(8)84.5(2) $C(26)-Cu(7)-Cu(3)$ 104.5(2) $S(3)-Cu(1)-Cu(8)$ 132.0(7) $C(42)-Cu(7)-Cu(3)$ 77.8(2) $S(4)-Cu(1)-Cu(8)$ 85.6(7) $Cu(6)-Cu(7)-Cu(3)$ 91.3(4) $Cu(5)-Cu(1)-Cu(8)$ 57.5(4) $Cu(5)-Cu(7)-Cu(3)$ 61.4(4) $Cu(2)-Cu(1)-Cu(8)$ 87.0(4) $C(26)-Cu(7)-Cu(2)$ 77.3(2) $N(2)-Cu(2)-S(3)$ 125.8(2) $C(42)-Cu(7)-Cu(2)$ 106.7(2)	Cu(5)-Cu(1)-Cu(2)	90.4(4)	Cu(6)-Cu(7)-Cu(5)	90.4(4)
S(3)-Cu(1)-Cu(8) $132.0(7)$ $C(42)-Cu(7)-Cu(3)$ $77.8(2)$ $S(4)-Cu(1)-Cu(8)$ $85.6(7)$ $Cu(6)-Cu(7)-Cu(3)$ $91.3(4)$ $Cu(5)-Cu(1)-Cu(8)$ $57.5(4)$ $Cu(5)-Cu(7)-Cu(3)$ $61.4(4)$ $Cu(2)-Cu(1)-Cu(8)$ $87.0(4)$ $C(26)-Cu(7)-Cu(2)$ $77.3(2)$ $N(2)-Cu(2)-S(3)$ $125.8(2)$ $C(42)-Cu(7)-Cu(2)$ $106.7(2)$	N(1)-Cu(1)-Cu(8)	84.5(2)	C(26)-Cu(7)-Cu(3)	104.5(2)
S(4)-Cu(1)-Cu(8) 85.6(7) Cu(6)-Cu(7)-Cu(3) 91.3(4) Cu(5)-Cu(1)-Cu(8) 57.5(4) Cu(5)-Cu(7)-Cu(3) 61.4(4) Cu(2)-Cu(1)-Cu(8) 87.0(4) C(26)-Cu(7)-Cu(2) 77.3(2) N(2)-Cu(2)-S(3) 125.8(2) C(42)-Cu(7)-Cu(2) 106.7(2)	S(3)-Cu(1)-Cu(8)	132.0(7)	C(42)-Cu(7)-Cu(3)	77.8(2)
Cu(5)-Cu(1)-Cu(8)57.5(4)Cu(5)-Cu(7)-Cu(3)61.4(4)Cu(2)-Cu(1)-Cu(8)87.0(4)C(26)-Cu(7)-Cu(2)77.3(2)N(2)-Cu(2)-S(3)125.8(2)C(42)-Cu(7)-Cu(2)106.7(2)	S(4)-Cu(1)-Cu(8)	85.6(7)	Cu(6)-Cu(7)-Cu(3)	91.3(4)
Cu(2)-Cu(1)-Cu(8)87.0(4)C(26)-Cu(7)-Cu(2)77.3(2)N(2)-Cu(2)-S(3)125.8(2)C(42)-Cu(7)-Cu(2)106.7(2)	Cu(5)-Cu(1)-Cu(8)	57.5(4)	Cu(5)-Cu(7)-Cu(3)	61.4(4)
N(2)-Cu(2)-S(3) 125.8(2) C(42)-Cu(7)-Cu(2) 106.7(2)	Cu(2)-Cu(1)-Cu(8)	87.0(4)	C(26)-Cu(7)-Cu(2)	77.3(2)
	N(2)-Cu(2)-S(3)	125.8(2)	C(42)-Cu(7)-Cu(2)	106.7(2)

Table 1 Selected Bond Distances (Å) and Angles (deg) for Compound 3

N(2)-Cu(2)-S(4)	130.8(2)	Cu(6)-Cu(7)-Cu(2)	60.8(4)
S(4)-Cu(2)-S(3)	93.2(8)	Cu(5)-Cu(7)-Cu(2)	92.2(4)
N(2)-Cu(2)-Cu(6)	84.7(2)	C(58)-Cu(8)-Cu(6)	50.0(2)
S(3)-Cu(2)-Cu(6)	131.7(7)	C(10)-Cu(8)-Cu(5)	49.9(2)
S(4)-Cu(2)-Cu(6)	90.0(7)	Cu(6)-Cu(8)-Cu(5)	90.4(4)
S(3)-Cu(2)-Cu(1)	54.2(6)	C(58)-Cu(8)-Cu(4)	77.4(2)
S(4)-Cu(2)-Cu(1)	55.5(6)	C(10)-Cu(8)-Cu(4)	104.0(2)
Cu(6)-Cu(2)-Cu(1)	90.3(5)	Cu(6)-Cu(8)-Cu(4)	61.9(4)
N(2)-Cu(2)-Cu(7)	84.8(2)	Cu(5)-Cu(8)-Cu(4)	90.9(4)
S(3)-Cu(2)-Cu(7)	86.2(7)	C(58)-Cu(8)-Cu(1)	107.7(2)
S(4)-Cu(2)-Cu(7)	131.4(7)	C(10)-Cu(8)-Cu(1)	77.1(2)
Cu(1)-Cu(2)-Cu(7)	87.0(4)	Cu(6)-Cu(8)-Cu(1)	92.2(4)
Cu(6)-Cu(2)-Cu(7)	57.3(4)	Cu(5)-Cu(8)-Cu(1)	60.4(4)
N(3)-Cu(3)-S(1)	128.0(2)	C(10)-P(1)-S(1)	111.6(3)
N(3)-Cu(3)-S(2)	129.3(2)	C(26)-P(2)-S(2)	110.6(3)
S(2)-Cu(3)-S(1)	92.7(9)	C(42)-P(3)-S(3)	111.9(3)
N(3)-Cu(3)-Cu(7)	84.9(2)	C(58)-P(4)-S(4)	111.0(3)
S(1)-Cu(3)-Cu(7)	131.2(8)	P(1)-S(1)-Cu(4)	106.6(1)
S(2)-Cu(3)-Cu(7)	88.8(7)	P(1)-S(1)-Cu(3)	112.4(1)
N(3)-Cu(3)-Cu(5)	85.8(2)	Cu(4)-S(1)-Cu(3)	71.3(8)
S(1)-Cu(3)-Cu(5)	86.6(7)	P(2)-S(2)-Cu(3)	107.7(1)
S(2)-Cu(3)-Cu(5)	131.0(8)	P(2)-S(2)-Cu(4)	112.7(1)
Cu(7)-Cu(3)-Cu(5)	57.6(4)	Cu(3)-S(2)-Cu(4)	71.3(7)
S(1)-Cu(3)-Cu(4)	54.2(7)	P(3)-S(3)-Cu(1)	106.8(1)
S(2)-Cu(3)-Cu(4)	54.7(7)	P(3)-S(3)-Cu(2)	111.8(1)
Cu(5)-Cu(3)-Cu(4)	87.4(5)	Cu(1)-S(3)-Cu(2)	70.0(7)
N(4)-Cu(4)-S(1)	130.2(2)	P(4)-S(4)-Cu(2)	107.0(1)
N(4)-Cu(4)-S(2)	127.8(2)	P(4)-S(4)-Cu(1)	112.8(1)
S(1)-Cu(4)-S(2)	92.3(9)	Cu(2)-S(4)-Cu(1)	70.09(7)
N(4)-Cu(4)-Cu(8)	84.4(2)	C(1)-N(1)-Cu(1)	116.9(5)
S(1)-Cu(4)-Cu(8)	89.8(7)	C(17)-N(2)-Cu(2)	117.5(5)
S(2)-Cu(4)-Cu(8)	130.5(7)	C(33)-N(3)-Cu(3)	117.0(5)
N(4)-Cu(4)-Cu(6)	85.1(2)	C(49)-N(4)-Cu(4)	118.4(5)
S(1)-Cu(4)-Cu(6)	131.3(8)	C(1)-C(10)-P(1)	121.9(6)
S(2)-Cu(4)-Cu(6)	86.0(7)	C(1)-C(10)-Cu(5)	115.5(6)
Cu(8)-Cu(4)-Cu(6)	57.4(4)	P(1)-C(10)-Cu(5)	110.2(4)
S(1)-Cu(4)-Cu(3)	54.5(7)	C(1)-C(10)-Cu(8)	112.5(6)
S(2)-Cu(4)-Cu(3)	54.0(7)	P(1)-C(10)-Cu(8)	109.1(4)

Cu(6)-Cu(4)-Cu(3)	87.4(5)	Cu(5)-C(10)-Cu(8)	79.7(3)
Cu(8)-Cu(4)-Cu(3)	89.3(5)	C(17)-C(26)-P(2)	119.7(6)
C(42)-Cu(5)-Cu(7)	50.2(2)	C(17)-C(26)-Cu(6)	114.7(5)
C(10)-Cu(5)-Cu(8)	50.4(2)	P(2)-C(26)-Cu(6)	110.9(4)
Cu(7)-Cu(5)-Cu(8)	89.4(4)	C(17)-C(26)-Cu(7)	115.3(6)
C(10)-Cu(5)-Cu(1)	78.4(2)	P(2)-C(26)-Cu(7)	109.4(4)
C(42)-Cu(5)-Cu(1)	103.1(2)	Cu(6)-C(26)-Cu(7)	80.2(3)
Cu(7)-Cu(5)-Cu(1)	90.3(4)	C(33)-C(42)-P(3)	120.6(6)
Cu(8)-Cu(5)-Cu(1)	62.1(4)	C(33)-C(42)-Cu(7)	115.0(5)
C(10)-Cu(5)-Cu(3)	107.0(2)	P(3)-C(42)-Cu(7)	110.1(4)
C(42)-Cu(5)-Cu(3)	77.5(2)	C(33)-C(42)-Cu(5)	114.0(6)
Cu(7)-Cu(5)-Cu(3)	61.0(4)	P(3)-C(42)-Cu(5)	110.5(4)
Cu(8)-Cu(5)-Cu(3)	92.3(4)	Cu(7)-C(42)-Cu(5)	79.4(3)
C(58)-Cu(6)-Cu(8)	49.6(2)	C(49)-C(58)-P(4)	118.1(6)
C(26)-Cu(6)-Cu(7)	50.2(2)	C(49)-C(58)-Cu(8)	117.2(6)
Cu(8)-Cu(6)-Cu(7)	89.8(4)	P(4)-C(58)-Cu(8)	109.6(4)
C(26)-Cu(6)-Cu(2)	78.2(2)	C(49)-C(58)-Cu(6)	115.7(6)
C(58)-Cu(6)-Cu(2)	104.0(2)	P(4)-C(58)-Cu(6)	109.8(4)
Cu(8)-Cu(6)-Cu(2)	90.4(4)	Cu(8)-C(58)-Cu(6)	80.4(3)





Emission spectrum of compound 3







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