Electronic Supplementary Information

Homoleptic polynuclear Cu^{I} and Ag^{I} complexes of *N*-thiophosphorylated thioureas *o*-$RO(O)CC_6H_4NHC(S)NHP(S)(O\textit{i}Pr)_2$ (R = Me, Et)

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Physical measurements

Infrared spectra (Nujol) were recorded with a Thermo Nicolet 380 FT-IR spectrometer in the range 400–3600 cm^{-1}. NMR spectra in $CDCl_3$ were obtained on a Bruker Avance 300 MHz spectrometer at 25 °C. ^1H and $^{31}P\{^1H\}$ NMR spectra were recorded at 299.948 and 121.420 MHz, respectively. Chemical shifts are reported with reference to $SiMe_4$ (^1H) and 85% H_3PO_4 ($^{31}P\{^1H\}$). Electronic spectra of absorption in 10^{-4} M solution were measured on a Lambda-35 spectrometer in the range 200–1000 nm. Elemental analyses were performed on a Thermoquest Flash EA 1112 Analyzer from CE Instruments.

Synthesis of $[Cu_3L^{I,II}{}_3]$, $[Ag_4L^{I}{}_4]$ and $[Ag_5L^{II}{}_5]$

A suspension of $HL^{I,II}$ (0.390 and 0.404 g, respectively; 1 mmol) in aqueous methanol (15 mL) was mixed with KOH (0.062 g, 1.1 mmol). The resulting mixture was added dropwise to a suspension of CuI or $AgNO_3$ (0.190 and 0.170 g, respectively; 1 mmol) in aqueous methanol (15 mL). The mixture was stirred at room temperature for 5 h. The resulting precipitate of KI or KNO_3 was filtered off and the solvent was then removed in vacuum. The residue was recrystallised from a CH_2Cl_2–*n*-hexane mixture (1 : 3, v/v).

$[Cu_3L^{I}{}_3]$: Yield: 0.412 g (91%). IR: 579 (P=S), 967 (POC), 1536 (SCN), 1707 (C=O), 3261 (NH) cm^{-1}. ^1H NMR: 1.28 (d, $^3J_{H,H}$ = 6.0 Hz, 18 H, CH_3, *i*Pr), 1.35 (d, $^3J_{H,H}$ = 6.1 Hz, 18 H, CH_3, *i*Pr), 3.91 (s, 9 H, CH_3, Me), 4.82 (d. sept, $^3J_{H,H}$ = 6.1 Hz, $^3J_{P,H}$ = 10.6 Hz, 6 H, OCH), 7.04 (d. t, $^3J_{H,H}$ = 7.5 Hz, $^4J_{H,H}$ = 1.2 Hz, 3 H, C_6H_4), 7.42 (d. t, $^3J_{H,H}$ = 7.5 Hz, $^4J_{H,H}$ = 1.6 Hz, 3 H, C_6H_4), 7.97 (d. d, $^3J_{H,H}$ = 7.9 Hz, $^4J_{H,H}$ = 1.4 Hz, 3 H, C_6H_4), 8.51 (d, $^3J_{H,H}$ = 8.4 Hz, $^4J_{H,H}$ = 1.4 Hz, 3 H, C_6H_4), 10.90 (d, $^4J_{PNCNH}$ = 6.3 Hz, 3 H, NH) ppm. $^{31}P\{^1H\}$ NMR: 52.9 ppm. *Anal.* Calc. for $C_{45}H_{66}Cu_3N_6O_{12}P_3S_6$ (1358.97): C 39.77, H 4.90, N 6.18. Found: C 39.92, H 4.83, N 6.26.

$[Cu_3L^{II}{}_3]$: Yield: 0.392 g (84%). IR: 582, 585 (P=S), 974 (POC), 1540, 1543 (SCN), 1710 (C=O), 3273 (NH) cm^{-1}. ^1H NMR: 1.28 (d, $^3J_{H,H}$ = 6.2 Hz, 18 H, CH_3, *i*Pr), 1.35 (d, $^3J_{H,H}$ = 6.2 Hz, 18 H, CH_3, *i*Pr), 1.41 (t, $^3J_{H,H}$ = 7.0 Hz, 9 H, CH_3, Et), 4.37 (q, $^3J_{H,H}$ = 7.0 Hz, 6 H, CH_2, Et), 4.83 (d. sept, $^3J_{H,H}$ = 6.2 Hz, $^3J_{P,H}$ = 10.6 Hz, 6 H, OCH), 7.05 (t, $^3J_{H,H}$ = 7.5 Hz, 3 H, C_6H_4), 7.41 (t, $^3J_{H,H}$ = 7.5 Hz, 3 H, C_6H_4), 7.98 (d, $^3J_{H,H}$ = 7.9 Hz, 3 H,

C_6H_4), 8.50 (d, $^3J_{H,H}$ = 8.4 Hz, 3 H, C_6H_4), 10.95 (d, $^4J_{PNCNH}$ = 7.9 Hz, 3 H, NH) ppm. $^{31}P\{^1H\}$ NMR: 53.7 ppm. *Anal*. Calc. for $C_{48}H_{72}Cu_3N_6O_{12}P_3S_6$ (1401.05): C 41.15, H 5.18, N 6.00. Found: C 41.03, H 5.24, N 5.95.

[$Ag_4L^I_4$]: Yield: 0.433 g (87%). IR: 584 (P=S), 979 (POC), 1531 (SCN), 1703 (C=O), 3268 (NH) cm^{-1}. ^1H NMR: 1.30 (d, $^3J_{H,H}$ = 6.1 Hz, 24 H, CH_3, *i*Pr), 1.34 (d, $^3J_{H,H}$ = 6.0 Hz, 24 H, CH_3, *i*Pr), 3.90 (s, 12 H, CH_3, Me), 4.80 (d. sept, $^3J_{H,H}$ = 6.1 Hz, $^3J_{P,H}$ = 10.6 Hz, 8 H, OCH), 7.00 (br. s, 4 H, C_6H_4), 7.38 (br. s, 4 H, C_6H_4), 7.93 (br. s, 4 H, C_6H_4), 8.48 (br. s, 4 H, C_6H_4), 11.09 (br. s, 4 H, NH) ppm. $^{31}P\{^1H\}$ NMR: 55.4 ppm. *Anal*. Calc. for $C_{60}H_{88}Ag_4N_8O_{16}P_4S_8$ (1989.25): C 36.23, H 4.46, N 5.63. Found: C 36.38, H 4.39, N 5.70.

[$Ag_5L^{II}_5$]: Yield: 0.414 g (81%). IR: 580 (P=S), 991 (POC), 1537 (SCN), 1712 (C=O), 3257 (NH) cm^{-1}. ^1H NMR: 1.33 (d, $^3J_{H,H}$ = 6.0 Hz, 30 H, CH_3, *i*Pr), 1.37 (d, $^3J_{H,H}$ = 6.1 Hz, 30 H, CH_3, *i*Pr), 1.46 (t, $^3J_{H,H}$ = 7.1 Hz, 15 H, CH_3, Et), 4.42 (q, $^3J_{H,H}$ = 7.1 Hz, 10 H, CH_2, Et), 4.88 (d. sept, $^3J_{H,H}$ = 6.1 Hz, $^3J_{P,H}$ = 10.8 Hz, 10 H, OCH), 7.09 (br. s, 5 H, C_6H_4), 7.43 (br. s, 5 H, C_6H_4), 7.99 (br. s, 5 H, C_6H_4), 8.42 (br. s, 5 H, C_6H_4), 11.16 (br. s, 5 H, NH) ppm. $^{31}P\{^1H\}$ NMR: 56.1 ppm. *Anal*. Calc. for $C_{80}H_{120}Ag_5N_{10}O_{20}P_5S_{10}$ (2556.70): C 37.58, H 4.73, N 5.48. Found: C 37.71, H 4.65, N 5.54.

Synthesis of [Ag(phen)L^{II}]

Path A. A suspension of **phen** (0.090 g, 0.5 mmol) in anhydrous CH_2Cl_2 (10 mL) was added dropwise to a suspension of **[$Ag_5L^{II}_5$]** (0.256 g, 0.1 mmol) in anhydrous CH_2Cl_2 (10 mL). The mixture was stirred at room temperature for 4 h. The solvent was then removed in vacuum. The residue was recrystallised from a CH_2Cl_2–*n*-hexane mixture (1 : 5, v/v).

Path B. A suspension of **HL^{II}** (0.404 g, 1 mmol) in aqueous methanol (10 mL) was mixed with KOH (0.062 g, 1.1 mmol). The resulting mixture was added dropwise to a suspension of $AgNO_3$ (0.170 g, 1 mmol) and **phen** (0.180 g, 1 mmol) in anhydrous CH_2Cl_2 (10 mL). The mixture was stirred at room temperature for 4 h. The resulting precipitate of KNO_3 was filtered off and the solvent was then removed in vacuum. The residue was recrystallised from a CH_2Cl_2–*n*-hexane mixture (1 : 5, v/v).

[Ag(phen)L^{II}]: Yield: 0.332 g (96%, *Path A*); 0.609 g (88%, *Path B*). IR: 572 (P=S), 1003 (POC), 1516 (SCN), 1710 (C=O), 3269 (NH) cm^{-1}. ^1H NMR: 1.39 (d, $^3J_{H,H}$ = 6.1 Hz, 6 H, CH_3, *i*Pr), 1.44 (t, $^3J_{H,H}$ = 7.0 Hz, 3 H, CH_3, Et), 1.48 (d, $^3J_{H,H}$ = 6.1 Hz, 6 H, CH_3, *i*Pr), 4.47 (q, $^3J_{H,H}$ = 7.0 Hz, 2 H, CH_2, Et), 4.86–5.07 (m, 2 H, OCH), 7.16–9.37 (m, C_6H_4 + phen, overlapping with the solvent signal), 10.97 (br. s, 1 H, NH) ppm. $^{31}P\{^1H\}$ NMR: 58.0 ppm. *Anal*. Calc. for $C_{28}H_{32}AgN_4O_4PS_2$ (691.55): C 48.63, H 4.66, N 8.10. Found: C 48.49, H 4.71, N 8.02.

X-Ray crystallography

The X-ray data were collected on a STOE IPDS-II diffractometer with graphite-monochromatised Mo-K_α radiation generated by a fine-focus X-ray tube operated at 50 kV and 40 mA. The reflections of the images were indexed, integrated and scaled using the X-Area data reduction package.[1] Data were corrected for absorption using the PLATON program.[2] The structures were solved by direct methods using the SHELXS-97 program[3] and

refined first isotropically and then anisotropically using SHELXL-97.[3] Hydrogen atoms were revealed from $\Delta\rho$ maps and those bonded to C were refined using appropriate riding models. The NH hydrogen atoms in **[$Cu_3L^{I}_3$]** was freely refined whereas the same hydrogen atoms in **[$Cu_3L^{II}_3$]** and **[$Ag_4L^{I}_4$]** were geometrically positioned and refined using a riding model with N–H = 0.88 Å and U(H) = 1.2 U_{eq}(N). Figures were generated using the program Mercury.[4]

In **[$Cu_3L^{II}_3$]** the methyl groups of two *i*Pr and one O*i*Pr are disordered over two positions with site occupation factors of 0.752(8), 0.50(3) and 0.51(3) for the major occupied site. The disordered atoms have been refined isotropically. In **[$Ag_4L^{I}_4$]** one O*i*Pr and one $C(O)OCH_3$ groups are disordered over two positions with site occupation factors of 0.50(1) and 0.54(1), respectively, for the major occupied site. The disordered atoms have been refined isotropically.

Crystal data for [$Cu_3L^{I}_3$]. $C_{45}H_{66}Cu_3N_6O_{12}P_3S_6$, M_r = 1358.93 g mol^{-1}, trigonal, space group *R*–3, *a* = 17.6497(2), *b* = 17.6497(2), *c* = 34.4980(5) Å, *V* = 9306.8(2) Å^3, *Z* = 6, ρ = 1.455 g cm^{-3}, μ(Mo-Kα) = 1.356 mm^{-1}, reflections: 25686 collected, 6312 unique, R_{int} = 0.0244, R_1(all) = 0.0473, wR_2(all) = 0.0960.

Crystal data for [$Cu_3L^{II}_3$]. $C_{48}H_{72}Cu_3N_6O_{12}P_3S_6$, M_r = 1401.01 g mol^{-1}, monoclinic, space group $P2_1/n$, *a* = 11.8107(4), *b* = 19.7508(5), *c* = 27.3802(10) Å, β = 90.034(3)°, *V* = 6387.0(4) Å^3, *Z* = 4, ρ = 1.457 g cm^{-3}, μ(Mo-Kα) = 1.319 mm^{-1}, reflections: 43431 collected, 12987 unique, R_{int} = 0.0449, R_1(all) = 0.0593, wR_2(all) = 0.1406.

Crystal data for [$Ag_4L^{I}_4$]. $C_{60}H_{88}Ag_4N_8O_{16}P_4S_8$, M_r = 1989.22 g mol^{-1}, tetragonal, space group $I4_1/a$, *a* = 27.4538(9, *b* = 27.4538(9), *c* = 10.7505(4) Å, *V* = 8102.8(5) Å^3, *Z* = 4, ρ = 1.631 g cm^{-3}, μ(Mo-Kα) = 1.301 mm^{-1}, reflections: 75564 collected, 4145 unique, R_{int} = 0.0751, R_1(all) = 0.0791, wR_2(all) = 0.1373.

CCDC 805255 (**[$Cu_3L^{I}_3$]**), 847766 (**[$Cu_3L^{II}_3$]**) and 813939 (**[$Ag_4L^{I}_4$]**) contain the supplementary crystallographic data. These data can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; or e-mail: deposit@ccdc.cam.ac.uk.

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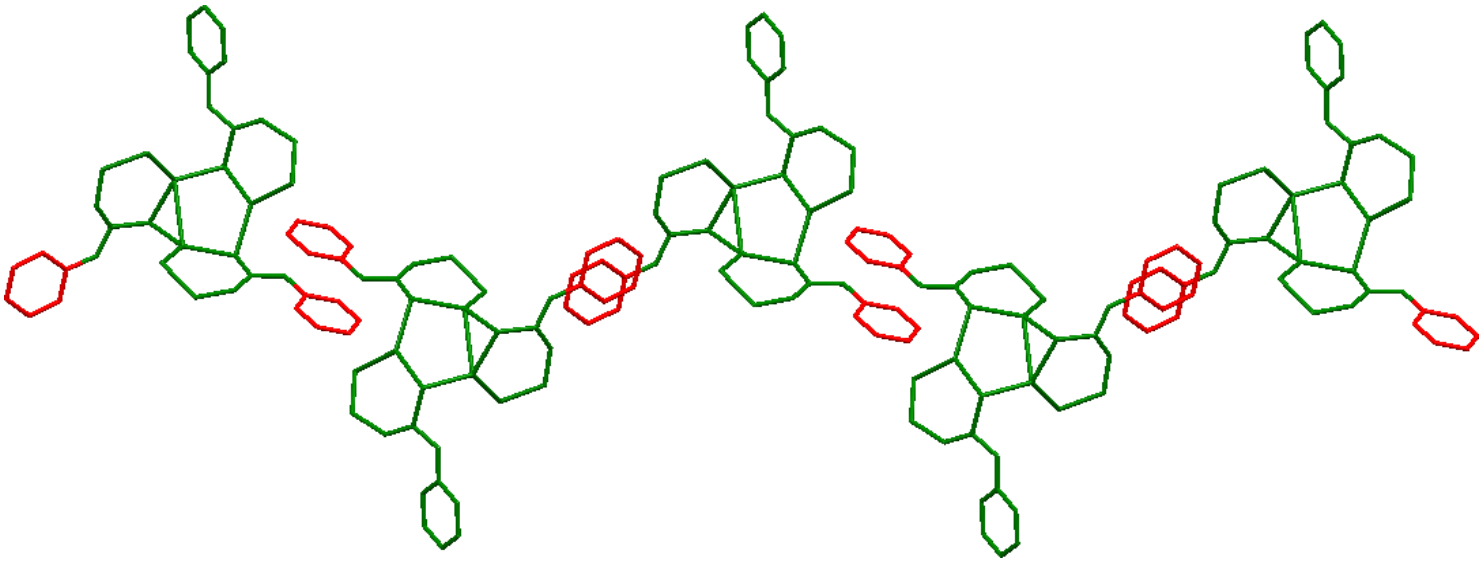

Fig. S1 $\pi\cdots\pi$ interactions in the structure of **[$Cu_3L^{II}_3$]**. Hydrogen atoms, *i*PrO and EtO(O)C groups are omitted for clarity.

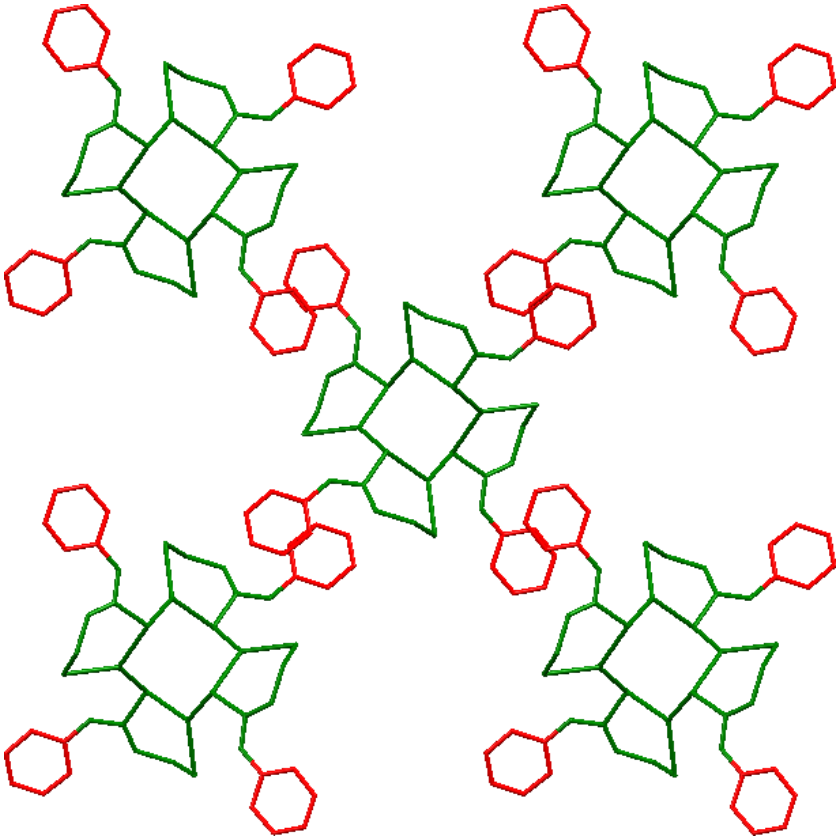

Fig. S2 $\pi\cdots\pi$ interactions in the structure of **[$Ag_4L^{I}_4$]**. Hydrogen atoms, *i*PrO and MeO(O)C groups are omitted for clarity.

Table S1. Selected bond lengths (Å) and angles (°) for **[$Cu_3L^I_3$]**

Bond lengths					
Cu(1)–S(1)	2.2236(5)	N(2)–C(1)	1.3582(19)	P(1)–O(2)	1.5699(12)
Cu(1)–S(2)	2.2410(4)	P(1)–N(1)	1.6132(14)	P(1)–S(1)	1.9829(6)
Cu(1)–S(2)#1	2.1981(4)	P(1)–O(1)	1.5656(13)	S(2)–C(1)	1.7687(16)
N(1)–C(1)	1.2972(19)				
Bond angles					
Cu(1)#1–S(2)–Cu(1)	113.007(19)	P(1)–S(1)–Cu(1)	90.77(2)	O(1)–P(1)–N(1)	106.72(7)
S(1)–Cu(1)–S(2)	113.407(17)	C(1)–N(1)–P(1)	129.08(12)	O(1)–P(1)–O(2)	102.04(7)
S(2)#1–Cu(1)–S(1)	132.780(17)	N(1)–C(1)–N(2)	120.73(14)	O(1)–P(1)–S(1)	114.57(5)
S(2)#1–Cu(1)–S(2)	113.68(2)	N(1)–C(1)–S(2)	124.48(12)	O(2)–P(1)–N(1)	105.87(7)
C(1)–S(2)–Cu(1)	106.77(5)	N(1)–P(1)–S(1)	116.68(6)	O(2)–P(1)–S(1)	109.64(5)
C(1)–S(2)–Cu(1)#1	115.82(5)	N(2)–C(1)–S(2)	114.74(11)		
Symmetry operator: #1 $-x + y, -x + 1, z$					

Table S2. Selected bond lengths (Å) and angles (°) for **[$Cu_3L^{II}_3$]**

Bond lengths					
Cu(1A)–Cu(1B)	2.8073(6)	N(2)–C(1)	1.354(4)	P(1A)–O(2A)	1.665(4)
Cu(1)–S(1)	2.2349(10)	N(1A)–C(1A)	1.292(5)	P(1B)–O(2B)	1.567(3)
Cu(1)–S(2)	2.2303(10)	N(2A)–C(1A)	1.352(5)	P(1B)–O(1B)	1.587(3)
Cu(1)–S(2B)	2.2302(9)	N(1B)–C(1B)	1.287(4)	P(1B)–O(1")	1.643(16)
Cu(1A)–S(1A)	2.2433(13)	N(2B)–C(1B)	1.362(4)	P(1)–S(1)	1.9780(12)
Cu(1A)–S(2A)	2.2096(10)	P(1)–N(1)	1.616(3)	P(1A)–S(1A)	1.9631(17)
Cu(1B)–S(1B)	2.2492(12)	P(1A)–N(1A)	1.585(3)	P(1B)–S(1B)	1.9735(14)
Cu(1B)–S(2B)	2.2032(9)	P(1B)–N(1B)	1.608(3)	S(2)–C(1)	1.771(3)
S(2)–Cu(1A)	2.2278(11)	P(1)–O(1)	1.567(2)	S(2A)–C(1A)	1.785(4)
S(2A)–Cu(1B)	2.2510(10)	P(1)–O(2)	1.570(2)	S(2B)–C(1B)	1.778(3)
N(1)–C(1)	1.299(4)	P(1A)–O(1A)	1.552(3)		
Bond angles					
Cu(1A)–S(2)–Cu(1)	94.74(4)	C(1A)–S(2A)–Cu(1A)	106.56(12)	N(1A)–P(1A)–S(1A)	121.54(13)
Cu(1A)–S(2A)–Cu(1B)	78.00(3)	C(1A)–S(2A)–Cu(1B)	98.76(12)	N(1B)–P(1B)–S(1B)	120.88(13)
Cu(1B)–S(2B)–Cu(1)	95.56(3)	C(1B)–S(2B)–Cu(1)	107.72(11)	O(1)–P(1)–N(1)	110.89(15)
S(1A)–Cu(1A)–Cu(1B)	111.51(4)	C(1B)–S(2B)–Cu(1B)	107.78(11)	O(2)–P(1)–N(1)	103.67(14)
S(1B)–Cu(1B)–Cu(1A)	117.24(3)	P(1)–S(1)–Cu(1)	95.20(4)	O(1A)–P(1A)–N(1A)	105.59(19)
S(2)–Cu(1A)–Cu(1B)	102.28(3)	P(1A)–S(1A)–Cu(1A)	97.05(6)	O(2A)–P(1A)–N(1A)	97.51(18)
S(2A)–Cu(1B)–Cu(1A)	50.34(3)	P(1B)–S(1B)–Cu(1B)	96.23(5)	O(1B)–P(1B)–N(1B)	104.20(17)
S(2A)–Cu(1A)–Cu(1B)	51.66(3)	C(1)–N(1)–P(1)	129.1(2)	O(2B)–P(1B)–N(1B)	104.27(16)
S(2B)–Cu(1B)–Cu(1A)	104.77(3)	C(1A)–N(1A)–P(1A)	135.0(3)	O(1")–P(1B)–N(1B)	110.1(6)
S(1B)–Cu(1B)–S(2A)	120.58(4)	C(1B)–N(1B)–P(1B)	134.3(3)	O(1)–P(1)–O(2)	102.52(14)
S(2)–Cu(1)–S(1)	114.40(4)	N(1)–C(1)–N(2)	120.8(3)	O(1A)–P(1A)–O(2A)	98.98(19)
S(2)–Cu(1A)–S(1A)	125.65(4)	N(1A)–C(1A)–N(2A)	121.4(3)	O(2B)–P(1B)–O(1B)	98.14(18)
S(2A)–Cu(1A)–S(1A)	116.53(4)	N(1B)–C(1B)–N(2B)	120.5(3)	O(2B)–P(1B)–O(1")	119.8(6)
S(2A)–Cu(1A)–S(2)	117.82(4)	N(1)–C(1)–S(2)	126.8(3)	O(1)–P(1)–S(1)	108.86(10)
S(2B)–Cu(1)–S(1)	126.22(4)	N(1A)–C(1A)–S(2A)	128.4(3)	O(2)–P(1)–S(1)	110.70(11)
S(2B)–Cu(1)–S(2)	119.38(4)	N(1B)–C(1B)–S(2B)	127.6(3)	O(1A)–P(1A)–S(1A)	118.48(16)
S(2B)–Cu(1B)–S(1B)	115.28(4)	N(2)–C(1)–S(2)	112.3(2)	O(2A)–P(1A)–S(1A)	110.49(14)
S(2B)–Cu(1B)–S(2A)	124.11(4)	N(2A)–C(1A)–S(2A)	110.2(3)	O(1B)–P(1B)–S(1B)	112.76(15)
C(1)–S(2)–Cu(1)	105.69(11)	N(2B)–C(1B)–S(2B)	111.7(2)	O(2B)–P(1B)–S(1B)	113.77(12)
C(1)–S(2)–Cu(1A)	105.82(12)	N(1)–P(1)–S(1)	118.90(11)	O(1")–P(1B)–S(1B)	88.5(6)

Table S3. Selected bond lengths (Å) and angles (°) for **[Ag$_4$L$^{I}_4$]**

Bond lengths					
Ag(1)–S(1)	2.477(2)	C(1)–N(2)	1.358(6)	P(1)–O(2)	1.680(11)
Ag(1)–S(2)	2.5134(15)	C(1)–S(2)	1.767(5)	P(1)–O(2')	1.548(8)
Ag(1)–S(2)#1	2.4182(16)	P(1)–N(1)	1.616(5)	P(1)–S(1)	1.951(3)
C(1)–N(1)	1.283(7)	P(1)–O(1)	1.560(5)		
Bond angles					
Ag(1)#2–S(2)–Ag(1)	92.15(5)	C(1)–N(1)–P(1)	128.9(4)	N(1)–P(1)–S(1)	117.0(2)
S(1)–Ag(1)–S(2)	104.21(6)	N(1)–C(1)–N(2)	120.5(5)	O(1)–P(1)–O(2)	94.9(4)
S(2)#1–Ag(1)–S(1)	134.84(6)	N(1)–C(1)–S(2)	125.5(4)	O(1)–P(1)–O(2')	112.4(4)
S(2)#1–Ag(1)–S(2)	120.93(6)	N(2)–C(1)–S(2)	114.0(4)	O(1)–P(1)–S(1)	115.4(2)
C(1)–S(2)–Ag(1)	102.27(18)	N(1)–P(1)–O(1)	107.1(3)	O(2)–P(1)–S(1)	120.9(4)
C(1)–S(2)–Ag(1)#2	111.14(19)	N(1)–P(1)–O(2)	98.2(4)	O(2')–P(1)–S(1)	94.9(4)
P(1)–S(1)–Ag(1)	94.49(8)	N(1)–P(1)–O(2')	109.7(3)		
Symmetry operators: #1 –*y* + 5/4, *x* + 1/4, –*z* + 1/4; #2 *y* – 1/4, –*x* + 5/4, –*z* + 1/4					

Table S4. Hydrogen bond lengths (Å) and angles (°) for **[Cu$_3$L$^{I,II}_3$]** and **[Ag$_4$L$^{I}_4$]**

Complex	D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠(DHA)
[Cu$_3$L$^{I}_3$]	N(2)–H(2)···O(3)	0.81(2)	2.05(2)	2.6794(19)	133.8(19)
[Cu$_3$L$^{II}_3$]	N(2)–H(2)···O(3)	0.88	2.07	2.664(4)	124
	N(2A)–H(2A1)···O(3A)	0.88	1.91	2.649(4)	141
	N(2B)–H(2B)···O(3B)	0.88	1.98	2.647(4)	132
[Ag$_4$L$^{I}_4$]	N(2)–H(2)···O(3)	0.88	2.00	2.692(9)	135
	N(2)–H(2)···O(3')	0.88	1.92	2.653(9)	140

Table S5. Selected $\pi\cdots\pi$ interactions for **[Cu$_3$L$^{II}_3$]** and **[Ag$_4$L$^{I}_4$]**

	Cg(*I*)[a]	Cg(*J*)[a]	Cg–Cg[b] (Å)	Dihedral angle (°)	Beta[c] (°)
[Cu$_3$L$^{II}_3$][d]	Cg(8)	Cg(8)#1	4.263(2)	0.03	38.23
	Cg(9)	Cg(9)#2	3.896(2)	0.03	25.65
[Ag$_4$L$^{I}_4$][e]	Cg(2)	Cg(2)#1	3.941(5)	0.00	26.43

[a] Cg refers to the ring center of gravity and the numbers represent the rings involved in the interactions.
[b] Cg–Cg: distance between ring centroids.
[c] Beta: angle Cg(*I*) → Cg(*J*) vector and normal to plane *I*.
[d] Cg(8): C(11A)–C(12A)–C(13A)–C(14A)–C(15A)–C(16A). Cg(9): C(11B)–C(12B)–C(13B)–C(14B)–C(15B)–C(16B). Symmetry code: #1 – *x*, 1 – *y*, 1 – *z*; #2 1 – *x*, 2 – *y*, 1 – *z*.

[e] Cg(2): C(11)–C(12)–C(13)–C(14)–C(15)–C(16). Symmetry code: #1 3/2 – *x*, 3/2 – *y*, 1/2 – *z*.