Further insight into the coordination of 2,5-dicarbothioamidopyrroles: the case of Cu and Co complexes.

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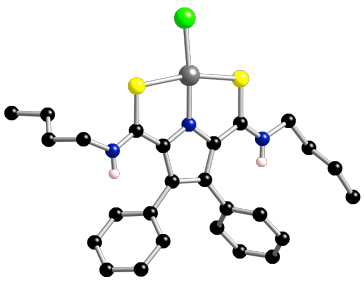
SUPPLEMENTARY INFORMATION

Table S1. Crystal data and structure refinement details for Complex **4**.



Empirical formula	$C_{26}H_{30}ClCuN_3S_2$
Formula weight	547.64
Temperature	120(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 14.9200(5) Å
	b = 9.0986(3) Å $\quad \beta$ = 90.731(2)°
	c = 18.6634(4) Å
Volume	2533.37(13) Å^3
Z	4
Density (calculated)	1.436 Mg / m^3
Absorption coefficient	1.152 mm^{-1}
F(000)	1140
Crystal	Block; Dark Green
Crystal size	0.2 × 0.15 × 0.09 mm^3
θ range for data collection	3.40 – 27.48°
Index ranges	$-19 \le h \le 19$, $-11 \le k \le 11$, $-24 \le l \le 24$
Reflections collected	43572
Independent reflections	5785 [R_{int} = 0.1149]
Completeness to θ = 27.48°	99.6 %
Absorption correction	Semi–empirical from equivalents
Max. and min. transmission	0.9034 and 0.8123
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5785 / 0 / 300
Goodness-of-fit on F^2	1.047
Final R indices [$F^2 > 2\sigma(F^2)$]	$R1$ = 0.0505, $wR2$ = 0.0997
R indices (all data)	$R1$ = 0.0844, $wR2$ = 0.1141
Largest diff. peak and hole	0.394 and –0.618 e Å^{-3}

Diffractometer: *Nonius KappaCCD* area detector (ϕ scans and ω scans to fill *asymmetric unit*). **Cell determination:** DirAx (Duisenberg, A.J.M.(1992). J. Appl. Cryst. 25, 92-96.) **Data collection:** Collect (Collect: Data collection software, R. Hooft, Nonius B.V., 1998). **Data reduction and cell refinement**: *Denzo* (Z. Otwinowski & W. Minor, *Methods in Enzymology* (1997) Vol. **276**: *Macromolecular Crystallography*, part A, pp. 307–326; C. W. Carter, Jr. & R. M. Sweet, Eds., Academic Press). **Absorption correction**: Sheldrick, G. M. SADABS - Bruker Nonius area detector scaling and absorption correction - V2.10 **Structure solution**: *SHELXS97* (G. M. Sheldrick, Acta Cryst. (1990) A**46** 467–473). **Structure refinement**: *SHELXL97* (G. M. Sheldrick (1997), University of Göttingen, Germany). **Graphics:** Cameron - A Molecular Graphics Package. (D. M. Watkin, L. Pearce and C. K. Prout, Chemical Crystallography Laboratory, University of Oxford, 1993).

Special details: All hydrogen atoms were placed in idealised positions and refined using a riding model.

Table S2. Complex **4:** Atomic coordinates [× 10^4], equivalent isotropic displacement parameters [Å^2 × 10^3] and site occupancy factors. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
C1	10576(2)	8376(4)	391(2)	34(1)	1
C2	9805(2)	7469(4)	84(2)	24(1)	1
C3	10023(2)	6786(4)	–639(2)	23(1)	1
C4	9300(2)	5752(4)	–931(2)	22(1)	1
C5	7739(2)	6500(3)	–667(2)	19(1)	1
C6	6955(2)	7330(3)	–887(2)	19(1)	1
C7	6728(2)	8247(3)	–1481(2)	19(1)	1
C8	5810(2)	8547(3)	–1430(2)	17(1)	1
C9	5518(2)	7848(3)	–792(2)	18(1)	1
C10	4706(2)	7891(3)	–376(2)	20(1)	1
C11	3224(2)	8996(4)	–160(2)	27(1)	1
C12	2621(2)	10071(4)	–561(2)	26(1)	1
C13	2169(2)	9409(4)	–1223(2)	35(1)	1
C14	1629(3)	10530(6)	–1642(2)	64(2)	1
C15	7368(2)	8781(3)	–2029(2)	19(1)	1
C16	8131(2)	9555(4)	–1819(2)	23(1)	1
C17	8774(2)	9959(4)	–2315(2)	25(1)	1
C18	8651(2)	9619(4)	–3033(2)	26(1)	1
C19	7886(2)	8875(4)	–3253(2)	26(1)	1
C20	7240(2)	8458(4)	–2759(2)	22(1)	1
C21	5215(2)	9406(4)	–1924(2)	20(1)	1
C22	5293(2)	10922(4)	–1991(2)	25(1)	1
C23	4667(2)	11727(4)	–2384(2)	30(1)	1
C24	3964(2)	11010(4)	–2726(2)	29(1)	1
C25	3892(2)	9498(4)	–2691(2)	31(1)	1
C26	4508(2)	8696(4)	–2284(2)	26(1)	1
N1	8460(2)	6522(3)	–1071(1)	20(1)	1
N2	6211(2)	7116(3)	–487(1)	19(1)	1
N3	4044(2)	8755(3)	–570(1)	23(1)	1
S1	7682(1)	5499(1)	108(1)	23(1)	1
S2	4664(1)	6857(1)	390(1)	24(1)	1
Cu1	6157(1)	5959(1)	360(1)	20(1)	1
Cl1	6182(1)	4863(1)	1410(1)	28(1)	1

Table S3. Complex **4:** Bond lengths [Å] and angles [°].

C1–C2	1.522(5)	C12–C13	1.523(5)
C2–C3	1.524(4)	C13–C14	1.512(6)
C3–C4	1.526(4)	C15–C16	1.391(4)
C4–N1	1.457(4)	C15–C20	1.404(4)
C5–N1	1.322(4)	C16–C17	1.392(4)
C5–C6	1.447(4)	C17–C18	1.386(5)
C5–S1	1.712(3)	C18–C19	1.385(5)
C6–N2	1.360(4)	C19–C20	1.395(4)
C6–C7	1.425(4)	C21–C22	1.389(5)
C7–C8	1.401(4)	C21–C26	1.401(5)
C7–C15	1.489(4)	C22–C23	1.388(5)
C8–C9	1.423(4)	C23–C24	1.385(5)
C8–C21	1.493(4)	C24–C25	1.381(5)
C9–N2	1.350(4)	C25–C26	1.391(5)
C9–C10	1.448(4)	N2–Cu1	1.902(2)
C10–N3	1.309(4)	S1–Cu1	2.3658(9)
C10–S2	1.714(3)	S2–Cu1	2.3746(9)
C11–N3	1.468(4)	Cu1–Cl1	2.1991(8)
C11–C12	1.519(5)		

C1–C2–C3	112.7(3)	C15–C16–C17	121.0(3)
C2–C3–C4	114.2(3)	C18–C17–C16	120.0(3)
N1–C4–C3	111.7(3)	C19–C18–C17	119.7(3)
N1–C5–C6	119.4(3)	C18–C19–C20	120.7(3)
N1–C5–S1	122.6(2)	C19–C20–C15	119.9(3)
C6–C5–S1	117.9(2)	C22–C21–C26	118.5(3)
N2–C6–C7	108.9(3)	C22–C21–C8	121.7(3)
N2–C6–C5	115.6(3)	C26–C21–C8	119.5(3)
C7–C6–C5	135.2(3)	C23–C22–C21	121.0(3)
C8–C7–C6	106.5(3)	C24–C23–C22	119.7(3)
C8–C7–C15	128.3(3)	C25–C24–C23	120.4(3)
C6–C7–C15	125.2(3)	C24–C25–C26	119.8(3)
C7–C8–C9	106.3(3)	C25–C26–C21	120.5(3)
C7–C8–C21	129.3(3)	C5–N1–C4	126.5(3)
C9–C8–C21	124.4(3)	C9–N2–C6	108.9(2)
N2–C9–C8	109.4(3)	C9–N2–Cu1	125.7(2)
N2–C9–C10	115.4(3)	C6–N2–Cu1	125.4(2)
C8–C9–C10	134.7(3)	C10–N3–C11	125.2(3)
N3–C10–C9	120.1(3)	C5–S1–Cu1	97.61(11)
N3–C10–S2	121.6(2)	C10–S2–Cu1	97.19(11)
C9–C10–S2	118.2(2)	N2–Cu1–Cl1	172.52(8)
N3–C11–C12	109.3(3)	N2–Cu1–S1	83.21(8)
C11–C12–C13	113.5(3)	Cl1–Cu1–S1	95.28(3)
C14–C13–C12	112.3(3)	N2–Cu1–S2	83.02(8)
C16–C15–C20	118.8(3)	Cl1–Cu1–S2	98.06(3)
C16–C15–C7	120.0(3)	S1–Cu1–S2	165.99(3)
C20–C15–C7	121.2(3)		

Table S4. Complex **4:** Anisotropic displacement parameters [Å^2× 10^3]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C1	25(2)	39(2)	37(2)	−7(2)	−3(2)	−1(2)
C2	15(2)	23(2)	33(2)	1(1)	0(1)	3(1)
C3	18(2)	25(2)	26(2)	3(1)	2(1)	2(1)
C4	18(2)	24(2)	24(2)	−2(1)	3(1)	0(1)
C5	18(2)	20(2)	18(2)	−3(1)	−2(1)	−2(1)
C6	18(2)	19(2)	19(2)	−2(1)	3(1)	−2(1)
C7	19(2)	21(2)	16(1)	−2(1)	1(1)	−2(1)
C8	21(2)	18(2)	13(1)	0(1)	−1(1)	−1(1)
C9	14(2)	23(2)	18(2)	0(1)	−1(1)	1(1)
C10	21(2)	22(2)	17(2)	−1(1)	2(1)	0(1)
C11	22(2)	37(2)	23(2)	2(1)	5(1)	7(2)
C12	18(2)	31(2)	29(2)	−3(1)	1(1)	5(2)
C13	25(2)	48(3)	30(2)	−10(2)	0(2)	3(2)
C14	50(3)	113(5)	30(2)	−5(2)	−6(2)	36(3)
C15	17(2)	19(2)	21(2)	2(1)	2(1)	3(1)
C16	24(2)	24(2)	21(2)	−1(1)	1(1)	2(1)
C17	22(2)	24(2)	29(2)	2(1)	6(1)	−2(1)
C18	27(2)	23(2)	29(2)	7(1)	10(1)	4(2)
C19	31(2)	28(2)	19(2)	2(1)	6(1)	5(2)
C20	22(2)	21(2)	23(2)	1(1)	1(1)	2(1)
C21	20(2)	23(2)	16(2)	2(1)	4(1)	3(1)
C22	28(2)	26(2)	22(2)	−2(1)	1(1)	1(2)
C23	39(2)	26(2)	27(2)	6(1)	2(2)	8(2)
C24	24(2)	40(2)	24(2)	14(2)	2(1)	11(2)
C25	24(2)	43(2)	24(2)	9(2)	−3(1)	−6(2)
C26	25(2)	27(2)	25(2)	6(1)	1(1)	0(2)
N1	15(1)	27(2)	17(1)	3(1)	1(1)	3(1)
N2	17(1)	21(1)	18(1)	1(1)	2(1)	0(1)
N3	19(1)	30(2)	21(1)	6(1)	6(1)	5(1)
S1	20(1)	29(1)	21(1)	6(1)	0(1)	2(1)
S2	22(1)	32(1)	19(1)	5(1)	4(1)	3(1)
Cu1	20(1)	25(1)	17(1)	4(1)	1(1)	1(1)
Cl1	32(1)	33(1)	18(1)	7(1)	1(1)	0(1)

Table S5. Complex 4: Hydrogen coordinates [× 10^4] and isotropic displacement parameters [Å^2 × 10^3].

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
H1A	11095	7738	477	51	1
H1B	10393	8826	843	51	1
H1C	10736	9148	49	51	1
H2A	9270	8104	29	28	1
H2B	9656	6676	426	28	1
H3A	10593	6235	–592	27	1
H3B	10116	7585	–990	27	1
H4A	9511	5297	–1380	26	1
H4B	9197	4956	–580	26	1
H11A	3378	9396	319	33	1
H11B	2906	8051	–94	33	1
H12A	2983	10929	–709	31	1
H12B	2153	10428	–233	31	1
H13A	2633	8987	–1537	42	1
H13B	1769	8600	–1073	42	1
H14A	1140	10897	–1345	97	1
H14B	1379	10069	–2075	97	1
H14C	2018	11350	–1777	97	1
H16	8214	9811	–1329	28	1
H17	9298	10468	–2161	30	1
H18	9089	9896	–3373	31	1
H19	7800	8645	–3746	31	1
H20	6714	7958	–2916	26	1
H22	5781	11414	–1765	30	1
H23	4721	12765	–2417	37	1
H24	3529	11561	–2987	35	1
H25	3424	9007	–2943	37	1
H26	4450	7659	–2250	31	1
H1	8429	7054	–1464	24	1
H3	4095	9230	–978	28	1

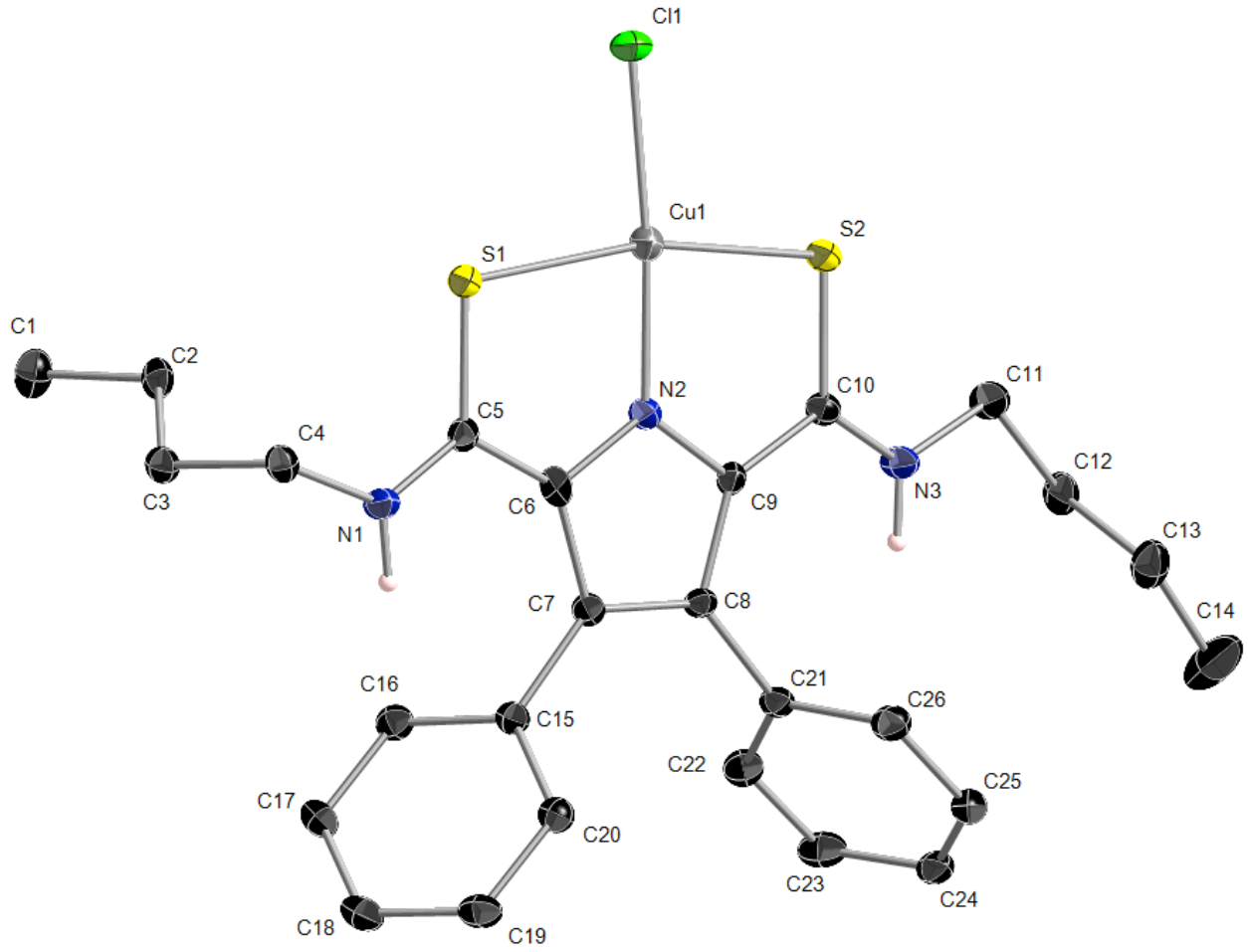
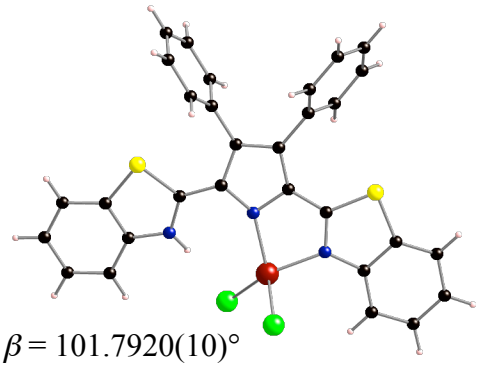


Figure S1. Complex **4.** Thermal ellipsoids drawn at the 35% probability level

Table S6. Complex **5:** Crystal data and structure refinement details.



Empirical formula	$C_{32}H_{22}Cl_2CuN_4S_2$
Formula weight	661.10
Temperature	120(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 12.7475(2) Å
	b = 8.48290(10) Å β = 101.7920(10)°
	c = 27.9445(4) Å
Volume	2958.03(7) Å^3
Z	4
Density (calculated)	1.484 Mg / m^3
Absorption coefficient	1.090 mm^{-1}
F(000)	1348
Crystal	Block; Dark Red
Crystal size	0.4 × 0.3 × 0.2 mm^3
θ range for data collection	2.91 – 27.48°
Index ranges	$-16 \le h \le 16$, $-10 \le k \le 11$, $-36 \le l \le 36$
Reflections collected	35352
Independent reflections	6752 [R_{int} = 0.0532]
Completeness to θ = 27.48°	99.8 %
Absorption correction	Semi–empirical from equivalents
Max. and min. transmission	0.8115 and 0.6596
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6752 / 1 / 375
Goodness-of-fit on F^2	1.022
Final R indices [$F^2 > 2\sigma(F^2)$]	$R1$ = 0.0431, $wR2$ = 0.1104
R indices (all data)	$R1$ = 0.0558, $wR2$ = 0.1174
Largest diff. peak and hole	0.490 and –0.721 e Å^{-3}

Diffractometer: *Nonius KappaCCD* area detector (ϕ scans and ω scans to fill *asymmetric unit*). **Cell determination:** DirAx (Duisenberg, A.J.M.(1992). J. Appl. Cryst. 25, 92-96.) **Data collection:** Collect (Collect: Data collection software, R. Hooft, Nonius B.V., 1998). **Data reduction and cell refinement**: *Denzo* (Z. Otwinowski & W. Minor, *Methods in Enzymology* (1997) Vol. **276**: *Macromolecular Crystallography*, part A, pp. 307–326; C. W. Carter, Jr. & R. M. Sweet, Eds., Academic Press). **Absorption correction**: Sheldrick, G. M. SADABS - Bruker Nonius area detector scaling and absorption correction - V2.10 S**tructure solution**: *SHELXS97* (G. M. Sheldrick, Acta Cryst. (1990) A**46** 467–473). S**tructure refinement**: *SHELXL97* (G. M. Sheldrick (1997), University of Göttingen, Germany). **Graphics:** Cameron - A Molecular Graphics Package. (D. M. Watkin, L. Pearce and C. K. Prout, Chemical Crystallography Laboratory, University of Oxford, 1993).

Special details: All CH hydrogen atoms were located from the difference map and then placed in idealised positions and refined using a riding model. The hydrogen of N1 was located in the difference map and then refined using a mild distance restrained.

Table S7. Complex **5:** Atomic coordinates [× 10^4], equivalent isotropic displacement parameters [Å^2 × 10^3] and site occupancy factors. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
Cu1	2051(1)	550(1)	1106(1)	22(1)	1
Cl1	2608(1)	3039(1)	1197(1)	33(1)	1
Cl2	2946(1)	–323(1)	563(1)	31(1)	1
S1	–1773(1)	3766(1)	653(1)	20(1)	1
S2	1307(1)	–3476(1)	1977(1)	27(1)	1
N1	262(2)	3759(3)	836(1)	18(1)	1
N2	534(2)	565(2)	1220(1)	17(1)	1
N3	2181(2)	–1341(3)	1535(1)	22(1)	1
C1	–1107(2)	5431(3)	496(1)	20(1)	1
C2	–1539(2)	6830(3)	274(1)	23(1)	1
C3	–827(2)	7972(3)	191(1)	25(1)	1
C4	284(2)	7752(3)	319(1)	24(1)	1
C5	713(2)	6376(3)	537(1)	22(1)	1
C6	0(2)	5215(3)	625(1)	17(1)	1
C7	–564(2)	2846(3)	876(1)	18(1)	1
C8	–444(2)	1311(3)	1092(1)	17(1)	1
C9	–1246(2)	443(3)	1263(1)	18(1)	1
C10	–729(2)	–856(3)	1515(1)	18(1)	1
C11	344(2)	–754(3)	1473(1)	18(1)	1
C12	1260(2)	–1757(3)	1641(1)	20(1)	1
C13	2682(2)	–3613(4)	1995(1)	29(1)	1
C14	3410(3)	–4720(4)	2233(1)	38(1)	1
C15	4478(3)	–4523(4)	2209(1)	43(1)	1
C16	4814(3)	–3268(4)	1956(1)	41(1)	1
C17	4091(2)	–2159(4)	1715(1)	32(1)	1
C18	3016(2)	–2349(3)	1739(1)	25(1)	1
C19	–2396(2)	854(3)	1208(1)	19(1)	1
C20	–3116(2)	582(4)	770(1)	29(1)	1
C21	–4195(2)	957(4)	726(1)	39(1)	1
C22	–4558(2)	1607(4)	1118(1)	36(1)	1
C23	–3854(2)	1875(4)	1551(1)	35(1)	1
C24	–2769(2)	1498(3)	1600(1)	28(1)	1
C25	–1214(2)	–2052(3)	1789(1)	19(1)	1
C26	–2007(2)	–3064(3)	1548(1)	24(1)	1
C27	–2462(2)	–4180(4)	1810(1)	32(1)	1
C28	–2140(3)	–4270(4)	2313(1)	39(1)	1
C29	–1371(3)	–3240(4)	2556(1)	38(1)	1
C30	–898(2)	–2141(4)	2296(1)	28(1)	1
N4	6105(2)	5911(4)	533(1)	49(1)	1
C31	4120(3)	5670(5)	602(2)	49(1)	1
C32	5232(3)	5826(4)	563(1)	34(1)	1

Table S8. Complex **5:** Bond lengths [Å] and angles [°].

Cu1–N3	1.988(2)	C10–C11	1.399(3)
Cu1–N2	2.023(2)	C10–C25	1.480(3)
Cu1–Cl2	2.2060(7)	C11–C12	1.444(4)
Cu1–Cl1	2.2254(8)	C13–C14	1.390(4)
S1–C7	1.727(3)	C13–C18	1.404(4)
S1–C1	1.749(3)	C14–C15	1.385(5)
S2–C12	1.728(3)	C15–C16	1.394(5)
S2–C13	1.746(3)	C16–C17	1.391(4)
N1–C7	1.330(3)	C17–C18	1.395(4)
N1–C6	1.380(3)	C19–C24	1.392(4)
N2–C11	1.370(3)	C19–C20	1.392(4)
N2–C8	1.378(3)	C20–C21	1.391(4)
N3–C12	1.317(3)	C21–C22	1.388(5)
N3–C18	1.393(3)	C22–C23	1.371(5)
C1–C6	1.394(4)	C23–C24	1.399(4)
C1–C2	1.399(4)	C25–C26	1.392(4)
C2–C3	1.380(4)	C25–C30	1.394(4)
C3–C4	1.400(4)	C26–C27	1.394(4)
C4–C5	1.376(4)	C27–C28	1.382(5)
C5–C6	1.396(4)	C28–C29	1.383(5)
C7–C8	1.430(4)	C29–C30	1.392(4)
C8–C9	1.419(3)	N4–C32	1.135(4)
C9–C10	1.399(4)	C31–C32	1.449(5)
C9–C19	1.484(3)		

N3–Cu1–N2	82.82(9)	C3–C2–C1	117.2(3)
N3–Cu1–Cl2	98.78(7)	C2–C3–C4	121.9(3)
N2–Cu1–Cl2	139.11(6)	C5–C4–C3	121.1(3)
N3–Cu1–Cl1	135.35(7)	C4–C5–C6	117.5(3)
N2–Cu1–Cl1	105.60(6)	N1–C6–C1	111.9(2)
Cl2–Cu1–Cl1	101.50(3)	N1–C6–C5	126.6(2)
C7–S1–C1	90.72(12)	C1–C6–C5	121.5(2)
C12–S2–C13	89.74(14)	N1–C7–C8	123.2(2)
C7–N1–C6	115.5(2)	N1–C7–S1	111.68(19)
C11–N2–C8	105.2(2)	C8–C7–S1	125.08(19)
C11–N2–Cu1	110.55(16)	N2–C8–C9	110.5(2)
C8–N2–Cu1	143.61(17)	N2–C8–C7	122.7(2)
C12–N3–C18	112.7(2)	C9–C8–C7	126.3(2)
C12–N3–Cu1	112.57(17)	C10–C9–C8	106.2(2)
C18–N3–Cu1	134.75(19)	C10–C9–C19	126.2(2)
C6–C1–C2	120.8(2)	C8–C9–C19	127.5(2)
C6–C1–S1	110.26(19)	C9–C10–C11	106.1(2)
C2–C1–S1	128.9(2)	C9–C10–C25	126.6(2)

C11–C10–C25	127.2(2)	C24–C19–C20	119.2(3)
N2–C11–C10	111.9(2)	C24–C19–C9	120.0(2)
N2–C11–C12	115.7(2)	C20–C19–C9	120.8(2)
C10–C11–C12	132.4(2)	C21–C20–C19	120.2(3)
N3–C12–C11	117.8(2)	C22–C21–C20	120.2(3)
N3–C12–S2	114.5(2)	C23–C22–C21	120.0(3)
C11–C12–S2	127.6(2)	C22–C23–C24	120.3(3)
C14–C13–C18	121.1(3)	C19–C24–C23	120.1(3)
C14–C13–S2	128.9(3)	C26–C25–C30	119.3(2)
C18–C13–S2	110.0(2)	C26–C25–C10	120.7(2)
C15–C14–C13	117.6(3)	C30–C25–C10	119.9(2)
C14–C15–C16	121.6(3)	C25–C26–C27	120.2(3)
C17–C16–C15	121.4(3)	C28–C27–C26	120.2(3)
C16–C17–C18	117.3(3)	C27–C28–C29	119.8(3)
N3–C18–C17	125.9(3)	C28–C29–C30	120.5(3)
N3–C18–C13	113.0(2)	C29–C30–C25	120.0(3)
C17–C18–C13	121.1(3)	N4–C32–C31	178.4(4)

Table S9. Complex **5:** Anisotropic displacement parameters [Å^2× 10^3]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu1	18(1)	25(1)	24(1)	−1(1)	5(1)	0(1)
Cl1	18(1)	28(1)	50(1)	−2(1)	2(1)	−4(1)
Cl2	21(1)	46(1)	28(1)	−4(1)	8(1)	3(1)
S1	16(1)	19(1)	27(1)	5(1)	4(1)	1(1)
S2	30(1)	23(1)	28(1)	5(1)	3(1)	5(1)
N1	15(1)	19(1)	19(1)	1(1)	3(1)	0(1)
N2	17(1)	17(1)	17(1)	−1(1)	2(1)	0(1)
N3	19(1)	24(1)	21(1)	−3(1)	0(1)	4(1)
C1	22(1)	19(1)	18(1)	1(1)	4(1)	−2(1)
C2	24(1)	22(1)	23(1)	2(1)	3(1)	2(1)
C3	36(2)	18(1)	20(1)	2(1)	5(1)	−2(1)
C4	35(2)	20(1)	19(1)	−2(1)	7(1)	−9(1)
C5	23(1)	24(1)	19(1)	−2(1)	5(1)	−6(1)
C6	22(1)	17(1)	13(1)	−1(1)	3(1)	−2(1)
C7	15(1)	21(1)	18(1)	0(1)	5(1)	−1(1)
C8	16(1)	19(1)	17(1)	1(1)	2(1)	1(1)
C9	18(1)	19(1)	16(1)	−1(1)	4(1)	0(1)
C10	19(1)	18(1)	15(1)	−1(1)	3(1)	−1(1)
C11	19(1)	18(1)	15(1)	−1(1)	2(1)	1(1)
C12	23(1)	20(1)	16(1)	−3(1)	2(1)	2(1)
C13	32(2)	30(2)	24(1)	−6(1)	1(1)	7(1)
C14	43(2)	35(2)	31(2)	1(1)	−1(1)	16(2)
C15	41(2)	49(2)	33(2)	−5(2)	−6(2)	25(2)
C16	25(2)	55(2)	39(2)	−8(2)	−2(1)	15(2)
C17	26(2)	41(2)	29(2)	−4(1)	1(1)	7(1)
C18	23(1)	31(2)	20(1)	−7(1)	0(1)	9(1)
C19	16(1)	17(1)	24(1)	5(1)	6(1)	−1(1)
C20	21(1)	34(2)	31(2)	−7(1)	3(1)	−2(1)
C21	20(1)	46(2)	45(2)	−5(2)	−3(1)	0(1)
C22	18(1)	30(2)	63(2)	4(2)	13(1)	−1(1)
C23	30(2)	35(2)	45(2)	3(1)	21(1)	6(1)
C24	28(2)	30(2)	28(1)	3(1)	10(1)	2(1)
C25	21(1)	17(1)	22(1)	3(1)	8(1)	5(1)
C26	25(1)	23(1)	26(1)	2(1)	9(1)	−1(1)
C27	28(2)	27(2)	43(2)	7(1)	12(1)	−1(1)
C28	35(2)	36(2)	49(2)	23(2)	20(2)	6(1)
C29	46(2)	43(2)	27(2)	16(1)	12(1)	11(2)
C30	35(2)	29(2)	21(1)	5(1)	5(1)	5(1)
N4	33(2)	63(2)	49(2)	−6(2)	5(1)	−8(2)
C31	34(2)	60(2)	57(2)	−21(2)	19(2)	−10(2)
C32	35(2)	37(2)	28(2)	−6(1)	4(1)	−6(1)

Table S10. Complex **5:** Hydrogen coordinates [× 10^4] and isotropic displacement parameters [$Å^2$ × 10^3].

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
H901	907(16)	3500(40)	957(11)	32(9)	1
H2	–2292	6986	184	27	1
H3	–1098	8937	43	30	1
H4	749	8565	255	29	1
H5	1466	6222	623	26	1
H14	3185	–5581	2404	45	1
H15	4992	–5260	2370	51	1
H16	5552	–3168	1947	49	1
H17	4320	–1307	1541	39	1
H20	–2871	139	500	35	1
H21	–4684	767	426	46	1
H22	–5294	1867	1086	44	1
H23	–4104	2318	1819	42	1
H24	–2285	1682	1902	34	1
H26	–2240	–2995	1203	29	1
H27	–2995	–4880	1643	39	1
H28	–2447	–5037	2491	46	1
H29	–1164	–3284	2902	45	1
H30	–360	–1451	2465	34	1
H31A	3794	4784	400	74	1
H31B	3734	6643	488	74	1
H31C	4081	5478	943	74	1

Table S11. Complex **5:** Hydrogen bonds [Å and °].

D–H···*A*	*d*(*D*–H)	*d*(H···*A*)	*d*(*D*···*A*)	∠(*D*H*A*)
N1–H901···Cl1	0.850(18)	2.171(19)	3.016(2)	173(3)

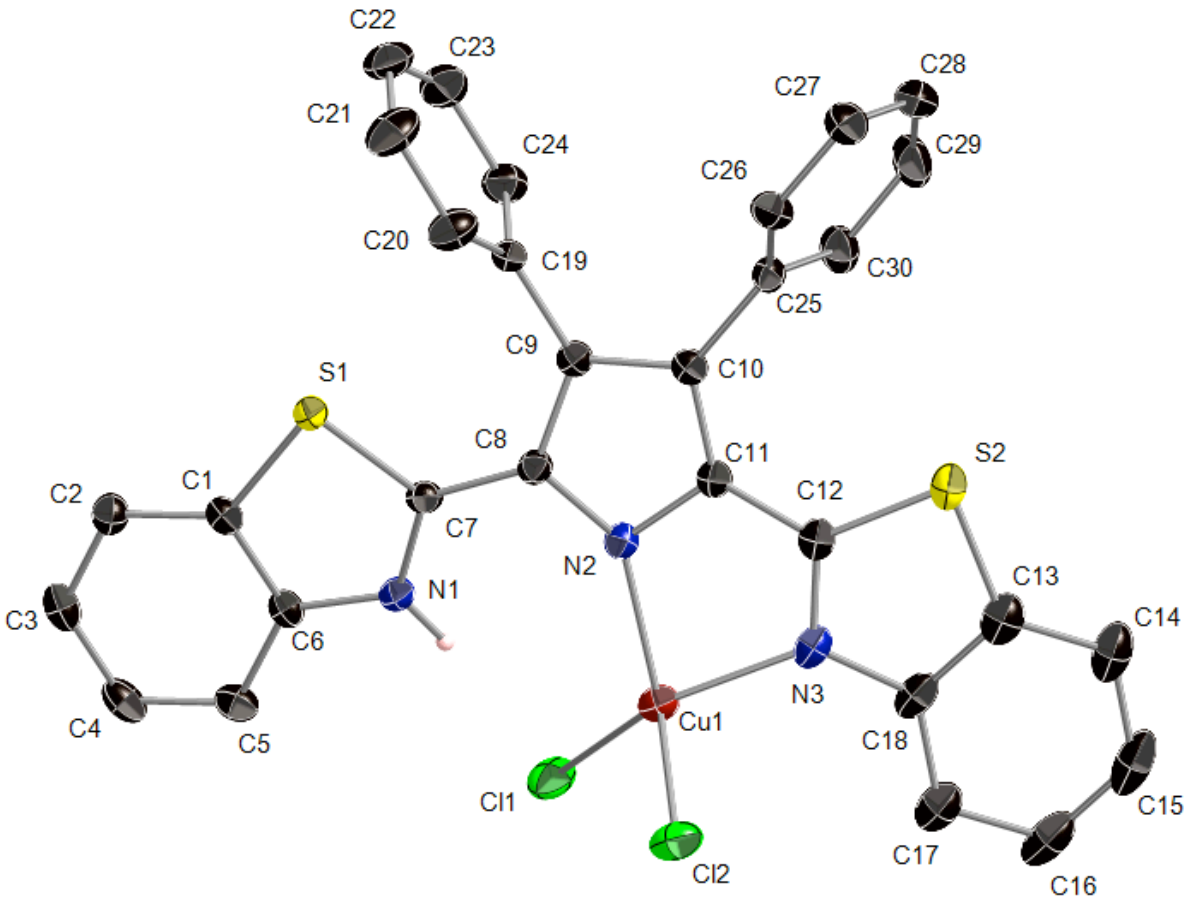
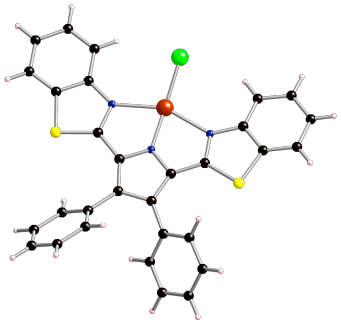


Figure S2. Complex **5**. Thermal ellipsoids drawn at the 50% probability level

Table S12. Complex **6**: Crystal data and structure refinement details.



Empirical formula	$C_{30}H_{18}ClCuN_3S_2$
Formula weight	583.58
Temperature	120(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 12.3901(2) Å
	b = 7.73120(10) Å β = 99.7560(10)°
	c = 24.4174(4) Å
Volume	2305.13(6) Å^3
Z	4
Density (calculated)	1.682 Mg / m^3
Absorption coefficient	1.273 mm^{-1}
$F(000)$	1188
Crystal	Plate; Orange
Crystal size	0.2 × 0.16 × 0.03 mm^3
θ range for data collection	3.12 – 26.37°
Index ranges	$-15 \le h \le 15$, $-9 \le k \le 9$, $-30 \le l \le 30$
Reflections collected	21672
Independent reflections	4702 [R_{int} = 0.0564]
Completeness to θ = 26.37°	99.7 %
Absorption correction	Semi–empirical from equivalents
Max. and min. transmission	0.963 and 0.767
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4702 / 0 / 334
Goodness-of-fit on F^2	1.650
Final R indices [$F^2 > 2\sigma(F^2)$]	$R1$ = 0.0465, $wR2$ = 0.0922
R indices (all data)	$R1$ = 0.0589, $wR2$ = 0.0972
Largest diff. peak and hole	0.490 and –0.556 e Å^{-3}

Diffractometer: *Nonius KappaCCD* area detector (ϕ scans and ω scans to fill *asymmetric unit*). **Cell determination:** DirAx (Duisenberg, A.J.M.(1992). J. Appl. Cryst. 25, 92-96.) **Data collection:** Collect (Collect: Data collection software, R. Hooft, Nonius B.V., 1998). **Data reduction and cell refinement**: *Denzo* (Z. Otwinowski & W. Minor, *Methods in Enzymology* (1997) Vol. **276**: *Macromolecular Crystallography*, part A, pp. 307–326; C. W. Carter, Jr. & R. M. Sweet, Eds., Academic Press). **Absorption correction**: Sheldrick, G. M. SADABS - Bruker Nonius area detector scaling and absorption correction - V2.10 S**tructure solution**: *SHELXS97* (G. M. Sheldrick, Acta Cryst. (1990) A**46** 467–473). S**tructure refinement**: *SHELXL97* (G. M. Sheldrick (1997), University of Göttingen, Germany). **Graphics:** Cameron - A Molecular Graphics Package. (D. M. Watkin, L. Pearce and C. K. Prout, Chemical Crystallography Laboratory, University of Oxford, 1993).

Special details: All hydrogen atoms were located in the difference map and then placed in geometrical positions and refined using a riding model.

Table S13. Complex **6**: Atomic coordinates [× 10^4], equivalent isotropic displacement parameters [Å^2 × 10^3] and site occupancy factors. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
Cu1	7694(1)	4923(1)	–34(1)	13(1)	1
Cl1	8442(1)	5497(1)	818(1)	16(1)	1
S1	4324(1)	2348(1)	–368(1)	14(1)	1
S2	8949(1)	7629(1)	–1467(1)	15(1)	1
N1	6288(2)	3341(3)	54(1)	13(1)	1
N2	6918(2)	4773(3)	–758(1)	12(1)	1
N3	8687(2)	6420(3)	–509(1)	12(1)	1
C1	4779(2)	1989(4)	335(1)	13(1)	1
C2	4213(3)	1215(4)	723(1)	16(1)	1
C3	4768(3)	1004(4)	1256(1)	18(1)	1
C4	5860(3)	1539(4)	1408(1)	17(1)	1
C5	6409(3)	2346(4)	1032(1)	15(1)	1
C6	5859(2)	2580(4)	487(1)	12(1)	1
C7	5575(2)	3268(4)	–417(1)	12(1)	1
C8	5928(2)	4017(4)	–906(1)	12(1)	1
C9	5577(2)	4234(4)	–1483(1)	12(1)	1
C10	6418(2)	5215(4)	–1675(1)	12(1)	1
C11	7231(2)	5506(4)	–1207(1)	11(1)	1
C12	8243(2)	6435(4)	–1046(1)	13(1)	1
C13	9924(2)	8153(4)	–890(1)	14(1)	1
C14	10851(2)	9177(4)	–874(1)	17(1)	1
C15	11519(3)	9390(4)	–370(1)	17(1)	1
C16	11269(2)	8607(4)	113(1)	17(1)	1
C17	10334(2)	7602(4)	96(1)	15(1)	1
C18	9653(2)	7379(4)	–414(1)	12(1)	1
C19	4608(2)	3430(4)	–1823(1)	12(1)	1
C20	3599(2)	3383(4)	–1645(1)	13(1)	1
C21	2715(3)	2483(4)	–1947(1)	18(1)	1
C22	2832(3)	1658(4)	–2435(1)	20(1)	1
C23	3817(3)	1730(4)	–2628(1)	19(1)	1
C24	4702(3)	2589(4)	–2321(1)	16(1)	1
C25	6408(2)	5882(4)	–2246(1)	12(1)	1
C26	5472(2)	6677(4)	–2536(1)	16(1)	1
C27	5457(3)	7331(4)	–3067(1)	18(1)	1
C28	6375(3)	7195(4)	–3317(1)	17(1)	1
C29	7314(3)	6409(4)	–3035(1)	16(1)	1
C30	7331(2)	5743(4)	–2502(1)	13(1)	1

Table S14. Complex **6**: Bond lengths [Å] and angles [°].

Cu1–N2	1.868(2)	C9–C19	1.476(4)
Cu1–N3	2.163(2)	C10–C11	1.408(4)
Cu1–N1	2.170(2)	C10–C25	1.483(4)
Cu1–Cl1	2.1742(8)	C11–C12	1.441(4)
S1–C7	1.729(3)	C13–C14	1.389(4)
S1–C1	1.735(3)	C13–C18	1.398(4)
S2–C12	1.726(3)	C14–C15	1.372(4)
S2–C13	1.742(3)	C15–C16	1.406(4)
N1–C7	1.328(4)	C16–C17	1.389(4)
N1–C6	1.391(4)	C17–C18	1.391(4)
N2–C11	1.347(4)	C19–C20	1.391(4)
N2–C8	1.352(4)	C19–C24	1.403(4)
N3–C12	1.332(4)	C20–C21	1.397(4)
N3–C18	1.393(4)	C21–C22	1.382(4)
C1–C6	1.404(4)	C22–C23	1.382(4)
C1–C2	1.405(4)	C23–C24	1.388(4)
C2–C3	1.375(4)	C25–C26	1.395(4)
C3–C4	1.404(4)	C25–C30	1.397(4)
C4–C5	1.382(4)	C26–C27	1.389(4)
C5–C6	1.399(4)	C27–C28	1.384(4)
C7–C8	1.457(4)	C28–C29	1.388(4)
C8–C9	1.413(4)	C29–C30	1.396(4)
C9–C10	1.430(4)		

N2–Cu1–N3	76.92(10)	C2–C1–S1	128.3(2)
N2–Cu1–N1	76.44(10)	C3–C2–C1	117.6(3)
N3–Cu1–N1	153.36(9)	C2–C3–C4	121.4(3)
N2–Cu1–Cl1	170.33(8)	C5–C4–C3	121.2(3)
N3–Cu1–Cl1	102.44(7)	C4–C5–C6	118.4(3)
N1–Cu1–Cl1	103.83(7)	N1–C6–C5	126.2(3)
C7–S1–C1	89.41(14)	N1–C6–C1	113.9(3)
C12–S2–C13	89.68(14)	C5–C6–C1	119.9(3)
C7–N1–C6	111.0(2)	N1–C7–C8	116.4(3)
C7–N1–Cu1	111.40(19)	N1–C7–S1	115.4(2)
C6–N1–Cu1	136.9(2)	C8–C7–S1	128.1(2)
C11–N2–C8	109.8(2)	N2–C8–C9	109.0(3)
C11–N2–Cu1	124.8(2)	N2–C8–C7	109.8(3)
C8–N2–Cu1	125.3(2)	C9–C8–C7	141.2(3)
C12–N3–C18	111.1(2)	C8–C9–C10	105.8(3)
C12–N3–Cu1	110.79(19)	C8–C9–C19	126.4(3)
C18–N3–Cu1	138.13(19)	C10–C9–C19	127.4(3)
C6–C1–C2	121.5(3)	C11–C10–C9	106.2(2)
C6–C1–S1	110.2(2)	C11–C10–C25	126.7(3)

C9–C10–C25	127.0(3)	C20–C19–C24	118.0(3)
N2–C11–C10	109.2(3)	C20–C19–C9	121.7(3)
N2–C11–C12	110.2(2)	C24–C19–C9	120.2(3)
C10–C11–C12	140.4(3)	C19–C20–C21	121.0(3)
N3–C12–C11	117.3(3)	C22–C21–C20	119.8(3)
N3–C12–S2	115.1(2)	C21–C22–C23	120.3(3)
C11–C12–S2	127.6(2)	C22–C23–C24	119.8(3)
C14–C13–C18	122.4(3)	C23–C24–C19	121.1(3)
C14–C13–S2	127.7(2)	C26–C25–C30	118.6(3)
C18–C13–S2	110.0(2)	C26–C25–C10	120.2(3)
C15–C14–C13	117.5(3)	C30–C25–C10	121.2(3)
C14–C15–C16	121.1(3)	C27–C26–C25	120.8(3)
C17–C16–C15	121.1(3)	C28–C27–C26	120.2(3)
C16–C17–C18	118.2(3)	C27–C28–C29	119.7(3)
C17–C18–N3	126.2(3)	C28–C29–C30	120.2(3)
C17–C18–C13	119.7(3)	C29–C30–C25	120.3(3)
N3–C18–C13	114.2(3)		

Table S15. Complex **6**: Anisotropic displacement parameters [Å^2× 10^3]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu1	12(1)	16(1)	9(1)	0(1)	1(1)	−1(1)
Cl1	15(1)	24(1)	10(1)	−2(1)	1(1)	−2(1)
S1	12(1)	16(1)	13(1)	0(1)	2(1)	−2(1)
S2	14(1)	18(1)	12(1)	2(1)	1(1)	−3(1)
N1	13(1)	15(1)	10(1)	0(1)	3(1)	1(1)
N2	7(1)	18(1)	11(1)	−1(1)	−1(1)	−3(1)
N3	12(1)	14(1)	10(1)	1(1)	1(1)	−1(1)
C1	14(2)	12(2)	12(1)	0(1)	2(1)	1(1)
C2	14(2)	17(2)	19(2)	−3(1)	6(1)	−2(1)
C3	28(2)	16(2)	14(2)	3(1)	11(1)	1(1)
C4	23(2)	17(2)	12(2)	0(1)	4(1)	3(1)
C5	16(2)	14(2)	14(2)	1(1)	4(1)	2(1)
C6	12(2)	10(2)	14(1)	−1(1)	5(1)	4(1)
C7	13(2)	12(2)	12(1)	−1(1)	2(1)	−1(1)
C8	11(2)	12(2)	15(2)	−1(1)	4(1)	2(1)
C9	12(2)	14(2)	12(1)	−2(1)	3(1)	1(1)
C10	12(2)	12(2)	10(1)	0(1)	1(1)	3(1)
C11	10(2)	13(2)	12(1)	1(1)	3(1)	3(1)
C12	15(2)	13(2)	12(1)	0(1)	5(1)	3(1)
C13	11(2)	15(2)	14(2)	−1(1)	−1(1)	2(1)
C14	15(2)	17(2)	20(2)	2(1)	6(1)	1(1)
C15	12(2)	17(2)	22(2)	−2(1)	2(1)	−3(1)
C16	13(2)	20(2)	16(2)	−5(1)	1(1)	0(1)
C17	13(2)	16(2)	16(2)	1(1)	3(1)	2(1)
C18	12(2)	11(2)	12(1)	1(1)	0(1)	3(1)
C19	14(2)	11(2)	10(1)	2(1)	−1(1)	1(1)
C20	14(2)	12(2)	13(1)	0(1)	0(1)	3(1)
C21	12(2)	19(2)	21(2)	1(1)	1(1)	2(1)
C22	16(2)	17(2)	23(2)	−2(1)	−6(1)	−2(1)
C23	25(2)	19(2)	12(2)	−4(1)	−1(1)	3(1)
C24	16(2)	18(2)	12(2)	−1(1)	3(1)	0(1)
C25	13(2)	13(2)	11(1)	−1(1)	2(1)	−3(1)
C26	14(2)	18(2)	16(2)	0(1)	4(1)	−1(1)
C27	17(2)	18(2)	15(2)	3(1)	−4(1)	−1(1)
C28	24(2)	16(2)	10(1)	1(1)	2(1)	−6(1)
C29	16(2)	17(2)	15(2)	−4(1)	7(1)	−3(1)
C30	13(2)	15(2)	12(1)	−2(1)	0(1)	0(1)

Table S16. Complex **6**: Hydrogen coordinates [× 10^4] and isotropic displacement parameters [Å^2 × 10^3].

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
H2	3474	850	620	20	1
H3	4404	485	1527	22	1
H4	6229	1343	1777	20	1
H5	7142	2732	1140	18	1
H14	11016	9709	–1201	20	1
H15	12161	10077	–347	20	1
H16	11747	8768	457	20	1
H17	10165	7081	423	18	1
H20	3510	3972	–1314	16	1
H21	2035	2438	–1816	21	1
H22	2233	1039	–2639	24	1
H23	3888	1194	–2970	23	1
H24	5382	2607	–2451	19	1
H26	4837	6772	–2368	19	1
H27	4815	7875	–3258	21	1
H28	6362	7637	–3681	20	1
H29	7947	6323	–3205	19	1
H30	7973	5193	–2313	16	1

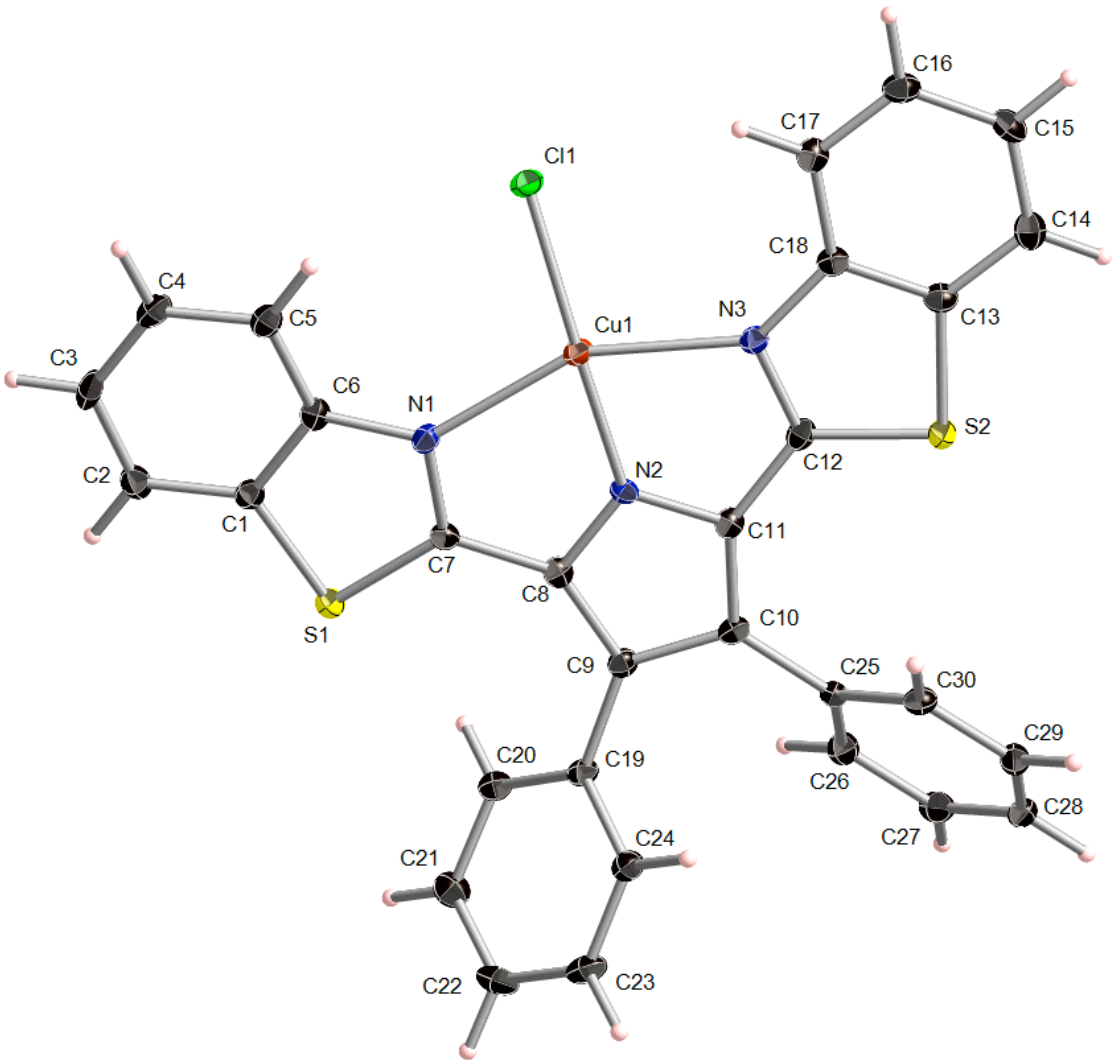
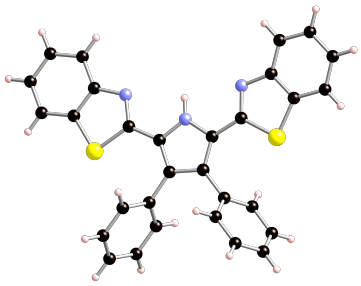


Fig S3. Complex **6**. Thermal ellipsoids drawn at the 50% probability level

Table S17. Ligand **3**: Crystal data and structure refinement details.



Empirical formula	$C_{30}H_{19}N_3S_2$	
Formula weight	485.60	
Temperature	120(2) K	
Wavelength	0.71069 Å	
Crystal system	Triclinic	
Space group	*P*–1	
Unit cell dimensions	a = 9.9600(2) Å	α = 89.652(1)°
	b = 13.5973(3) Å	β = 87.180(1)°
	c = 17.4476(3) Å	γ = 86.996(1)°
Volume	2356.79(8) Å^3	
Z	4 (Z'=2)	
Density (calculated)	1.369 Mg / m^3	
Absorption coefficient	0.251 mm-**1**	
F(000)	1008	
Crystal	Slab; Yellow	
Crystal size	0.22 × 0.18 × 0.03 mm^3	
θ range for data collection	3.00 – 27.48°	
Index ranges	$-12 \le h \le 12$, $-17 \le k \le 17$, $-22 \le l \le 22$	
Reflections collected	40153	
Independent reflections	10759 [R_{int} = 0.0504]	
Completeness to θ = 27.48°	99.4 %	
Absorption correction	Semi–empirical from equivalents	
Max. and min. transmission	0.9925 and 0.9468	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10759 / 0 / 639	
Goodness-of-fit on F^2	1.077	
Final *R* indices [$F^2 > 2\sigma(F^2)$]	*R1* = 0.0591, *wR2* = 0.1097	
R indices (all data)	*R1* = 0.0813, *wR2* = 0.1210	
Largest diff. peak and hole	0.318 and –0.349 e Å^{-3}	

Diffractometer: *Nonius KappaCCD* area detector (ϕ scans and ω scans to fill *asymmetric unit*). **Cell determination:** DirAx (Duisenberg, A.J.M.(1992). J. Appl. Cryst. 25, 92-96.) **Data collection:** Collect (Collect: Data collection software, R. Hooft, Nonius B.V., 1998). **Data reduction and cell refinement**: *Denzo* (Z. Otwinowski & W. Minor, *Methods in Enzymology* (1997) Vol. **276**: *Macromolecular Crystallography*, part A, pp. 307–326; C. W. Carter, Jr. & R. M. Sweet, Eds., Academic Press). **Absorption correction**: Sheldrick, G. M. SADABS - Bruker Nonius area detector scaling and absorption correction - V2.10 S**tructure solution**: *SHELXS97* (G. M. Sheldrick, Acta Cryst. (1990) A**46** 467–473). S**tructure refinement**: *SHELXL97* (G. M. Sheldrick (1997), University of Göttingen, Germany). **Graphics:** Cameron - A Molecular Graphics Package. (D. M. Watkin, L. Pearce and C. K. Prout, Chemical Crystallography Laboratory, University of Oxford, 1993).

Special details: All hydrogen atoms were placed in idealised positions and refined using a riding model, except those of the NH which were freely refined.

Table S18. Ligand **3**: Atomic coordinates [× 10^4], equivalent isotropic displacement parameters [Å^2 × 10^3] and site occupancy factors. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
S1	1236(1)	7352(1)	5812(1)	21(1)	1
S2	4130(1)	2082(1)	4629(1)	22(1)	1
N1	2938(2)	7052(2)	4644(1)	20(1)	1
N2	3274(2)	5021(2)	4794(1)	21(1)	1
N3	4709(2)	3664(2)	3858(1)	22(1)	1
C1	2651(2)	8061(2)	4688(1)	19(1)	1
C2	3192(3)	8758(2)	4186(2)	23(1)	1
C3	2802(3)	9743(2)	4296(2)	25(1)	1
C4	1911(3)	10041(2)	4905(2)	26(1)	1
C5	1375(3)	9362(2)	5406(2)	25(1)	1
C6	1750(2)	8366(2)	5292(1)	19(1)	1
C7	2267(2)	6601(2)	5192(1)	19(1)	1
C8	2396(2)	5540(2)	5279(1)	20(1)	1
C9	1816(2)	4882(2)	5793(1)	20(1)	1
C10	2393(2)	3931(2)	5608(1)	19(1)	1
C11	3282(3)	4043(2)	4977(1)	20(1)	1
C12	4058(2)	3357(2)	4475(1)	20(1)	1
C13	5137(2)	1944(2)	3792(2)	21(1)	1
C14	5709(3)	1084(2)	3452(2)	24(1)	1
C15	6440(3)	1164(2)	2765(2)	26(1)	1
C16	6615(3)	2082(2)	2421(2)	28(1)	1
C17	6078(3)	2937(2)	2761(2)	27(1)	1
C18	5323(2)	2871(2)	3457(1)	21(1)	1
C19	815(3)	5140(2)	6431(1)	20(1)	1
C20	–489(3)	5475(2)	6286(2)	24(1)	1
C21	–1395(3)	5759(2)	6884(2)	29(1)	1
C22	–1012(3)	5704(2)	7634(2)	33(1)	1
C23	274(3)	5347(2)	7784(2)	34(1)	1
C24	1184(3)	5062(2)	7186(2)	28(1)	1
C25	2071(3)	3002(2)	6011(1)	20(1)	1
C26	755(3)	2681(2)	6032(2)	25(1)	1
C27	458(3)	1813(2)	6416(2)	28(1)	1
C28	1449(3)	1266(2)	6779(2)	26(1)	1
C29	2749(3)	1585(2)	6767(2)	26(1)	1
C30	3058(3)	2452(2)	6387(1)	24(1)	1
S3	6825(1)	2792(1)	–388(1)	21(1)	1
S4	3192(1)	–1119(1)	2142(1)	24(1)	1
N4	8043(2)	1131(2)	–9(1)	20(1)	1
N5	5882(2)	351(2)	814(1)	20(1)	1
N6	5529(2)	–1529(2)	1443(1)	21(1)	1
C31	8929(2)	1612(2)	–504(1)	19(1)	1
C32	10214(3)	1245(2)	–754(2)	24(1)	1

C33	10943(3)	1786(2)	−1288(2)	26(1)	1
C34	10419(3)	2682(2)	−1574(2)	27(1)	1
C35	9169(3)	3070(2)	−1320(2)	24(1)	1
C36	8440(2)	2528(2)	−781(1)	20(1)	1
C37	6910(2)	1657(2)	92(1)	19(1)	1
C38	5783(2)	1303(2)	546(1)	18(1)	1
C39	4526(2)	1715(2)	794(1)	19(1)	1
C40	3867(2)	976(2)	1227(1)	18(1)	1
C41	4723(2)	142(2)	1224(1)	19(1)	1
C42	4603(2)	−825(2)	1557(1)	20(1)	1
C43	3914(3)	−2300(2)	2238(1)	23(1)	1
C44	3397(3)	−3104(2)	2635(2)	29(1)	1
C45	4142(3)	−3985(2)	2600(2)	33(1)	1
C46	5361(3)	−4082(2)	2167(2)	34(1)	1
C47	5882(3)	−3290(2)	1778(2)	29(1)	1
C48	5151(3)	−2383(2)	1819(2)	23(1)	1
C49	3913(3)	2710(2)	635(1)	20(1)	1
C50	2695(3)	2776(2)	271(2)	26(1)	1
C51	2069(3)	3688(2)	120(2)	30(1)	1
C52	2657(3)	4542(2)	323(2)	29(1)	1
C53	3860(3)	4488(2)	685(2)	27(1)	1
C54	4475(3)	3575(2)	846(1)	23(1)	1
C55	2555(2)	1109(2)	1666(1)	19(1)	1
C56	1363(3)	835(2)	1371(2)	27(1)	1
C57	159(3)	968(2)	1799(2)	31(1)	1
C58	137(3)	1365(2)	2531(2)	27(1)	1
C59	1316(3)	1633(2)	2826(2)	30(1)	1
C60	2523(3)	1515(2)	2396(2)	25(1)	1

Table S19. Ligand **3**: Bond lengths [Å] and angles [°].

S1–C6	1.732(2)	S3–C36	1.738(2)
S1–C7	1.750(2)	S3–C37	1.752(3)
S2–C13	1.736(3)	S4–C43	1.735(3)
S2–C12	1.751(2)	S4–C42	1.756(2)
N1–C7	1.306(3)	N4–C37	1.308(3)
N1–C1	1.388(3)	N4–C31	1.390(3)
N2–C8	1.360(3)	N5–C41	1.370(3)
N2–C11	1.366(3)	N5–C38	1.374(3)
N3–C12	1.306(3)	N6–C42	1.303(3)
N3–C18	1.388(3)	N6–C48	1.390(3)
C1–C2	1.398(3)	C31–C32	1.399(3)
C1–C6	1.401(3)	C31–C36	1.404(3)
C2–C3	1.387(4)	C32–C33	1.385(4)
C3–C4	1.398(4)	C33–C34	1.399(4)
C4–C5	1.378(4)	C34–C35	1.380(4)
C5–C6	1.398(3)	C35–C36	1.392(3)
C7–C8	1.449(3)	C37–C38	1.443(3)
C8–C9	1.390(3)	C38–C39	1.394(3)
C9–C10	1.419(3)	C39–C40	1.422(3)
C9–C19	1.489(3)	C39–C49	1.485(3)
C10–C11	1.391(3)	C40–C41	1.383(3)
C10–C25	1.484(3)	C40–C55	1.485(3)
C11–C12	1.450(3)	C41–C42	1.443(3)
C13–C14	1.397(4)	C43–C44	1.399(4)
C13–C18	1.404(3)	C43–C48	1.401(4)
C14–C15	1.379(4)	C44–C45	1.377(4)
C15–C16	1.397(4)	C45–C46	1.398(4)
C16–C17	1.380(4)	C46–C47	1.380(4)
C17–C18	1.400(4)	C47–C48	1.399(4)
C19–C24	1.388(4)	C49–C54	1.389(3)
C19–C20	1.388(4)	C49–C50	1.395(4)
C20–C21	1.387(4)	C50–C51	1.388(4)
C21–C22	1.382(4)	C51–C52	1.384(4)
C22–C23	1.382(4)	C52–C53	1.380(4)
C23–C24	1.391(4)	C53–C54	1.389(4)
C25–C30	1.391(3)	C55–C56	1.387(4)
C25–C26	1.402(4)	C55–C60	1.390(4)
C26–C27	1.390(4)	C56–C57	1.385(4)
C27–C28	1.382(4)	C57–C58	1.388(4)
C28–C29	1.386(4)	C58–C59	1.373(4)
C29–C30	1.390(4)	C59–C60	1.387(4)
C6–S1–C7	88.69(12)	C13–S2–C12	88.79(12)

C7–N1–C1	110.2(2)	C22–C21–C20	120.3(3)
C8–N2–C11	110.0(2)	C21–C22–C23	119.4(3)
C12–N3–C18	110.3(2)	C22–C23–C24	120.4(3)
N1–C1–C2	125.0(2)	C19–C24–C23	120.3(3)
N1–C1–C6	115.2(2)	C30–C25–C26	119.2(2)
C2–C1–C6	119.9(2)	C30–C25–C10	120.7(2)
C3–C2–C1	118.5(2)	C26–C25–C10	120.1(2)
C2–C3–C4	121.1(2)	C27–C26–C25	119.8(2)
C5–C4–C3	121.0(2)	C28–C27–C26	120.6(3)
C4–C5–C6	118.2(2)	C27–C28–C29	119.9(2)
C5–C6–C1	121.3(2)	C28–C29–C30	120.1(2)
C5–C6–S1	128.8(2)	C29–C30–C25	120.4(3)
C1–C6–S1	109.83(18)	C36–S3–C37	88.97(12)
N1–C7–C8	121.3(2)	C43–S4–C42	88.48(12)
N1–C7–S1	116.16(18)	C37–N4–C31	110.4(2)
C8–C7–S1	122.56(18)	C41–N5–C38	109.8(2)
N2–C8–C9	108.1(2)	C42–N6–C48	110.2(2)
N2–C8–C7	118.5(2)	N4–C31–C32	125.5(2)
C9–C8–C7	133.4(2)	N4–C31–C36	115.3(2)
C8–C9–C10	107.1(2)	C32–C31–C36	119.2(2)
C8–C9–C19	126.0(2)	C33–C32–C31	118.6(2)
C10–C9–C19	126.9(2)	C32–C33–C34	121.2(2)
C11–C10–C9	106.9(2)	C35–C34–C33	121.1(2)
C11–C10–C25	127.4(2)	C34–C35–C36	117.5(2)
C9–C10–C25	125.7(2)	C35–C36–C31	122.3(2)
N2–C11–C10	107.9(2)	C35–C36–S3	128.2(2)
N2–C11–C12	117.9(2)	C31–C36–S3	109.45(18)
C10–C11–C12	133.8(2)	N4–C37–C38	121.9(2)
N3–C12–C11	121.0(2)	N4–C37–S3	115.89(18)
N3–C12–S2	116.14(19)	C38–C37–S3	122.19(19)
C11–C12–S2	122.81(19)	N5–C38–C39	107.8(2)
C14–C13–C18	121.3(2)	N5–C38–C37	117.9(2)
C14–C13–S2	129.2(2)	C39–C38–C37	134.3(2)
C18–C13–S2	109.56(19)	C38–C39–C40	106.8(2)
C15–C14–C13	118.2(2)	C38–C39–C49	129.0(2)
C14–C15–C16	121.0(2)	C40–C39–C49	124.2(2)
C17–C16–C15	121.2(3)	C41–C40–C39	107.7(2)
C16–C17–C18	118.7(2)	C41–C40–C55	126.1(2)
N3–C18–C17	125.1(2)	C39–C40–C55	126.0(2)
N3–C18–C13	115.2(2)	N5–C41–C40	107.9(2)
C17–C18–C13	119.6(2)	N5–C41–C42	119.2(2)
C24–C19–C20	118.8(2)	C40–C41–C42	132.8(2)
C24–C19–C9	120.0(2)	N6–C42–C41	122.1(2)
C20–C19–C9	121.2(2)	N6–C42–S4	116.24(18)
C21–C20–C19	120.7(2)	C41–C42–S4	121.62(19)

C44–C43–C48	121.4(2)	C51–C50–C49	120.5(2)
C44–C43–S4	128.7(2)	C52–C51–C50	120.2(3)
C48–C43–S4	109.90(18)	C53–C52–C51	119.9(2)
C45–C44–C43	117.8(3)	C52–C53–C54	119.9(3)
C44–C45–C46	121.3(3)	C49–C54–C53	121.0(2)
C47–C46–C45	121.3(3)	C56–C55–C60	119.0(2)
C46–C47–C48	118.3(3)	C56–C55–C40	122.0(2)
N6–C48–C47	124.9(2)	C60–C55–C40	119.0(2)
N6–C48–C43	115.1(2)	C57–C56–C55	120.3(3)
C47–C48–C43	120.0(2)	C56–C57–C58	120.3(3)
C54–C49–C50	118.5(2)	C59–C58–C57	119.5(2)
C54–C49–C39	123.2(2)	C58–C59–C60	120.5(3)
C50–C49–C39	118.3(2)	C59–C60–C55	120.3(2)

Table S20. Ligand **3**: Anisotropic displacement parameters [Å^2× 10^3]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S1	23(1)	16(1)	22(1)	−1(1)	4(1)	1(1)
S2	22(1)	16(1)	28(1)	−1(1)	1(1)	1(1)
N1	20(1)	17(1)	24(1)	0(1)	0(1)	0(1)
N2	24(1)	16(1)	22(1)	−1(1)	3(1)	0(1)
N3	22(1)	17(1)	27(1)	1(1)	−1(1)	2(1)
C1	20(1)	18(1)	20(1)	−2(1)	−3(1)	0(1)
C2	23(1)	22(1)	24(1)	0(1)	1(1)	−1(1)
C3	26(1)	19(1)	31(1)	3(1)	−1(1)	−4(1)
C4	25(1)	16(1)	38(2)	−1(1)	−3(1)	0(1)
C5	25(1)	19(1)	29(1)	−4(1)	1(1)	0(1)
C6	19(1)	18(1)	20(1)	0(1)	−3(1)	−3(1)
C7	19(1)	18(1)	19(1)	−2(1)	−2(1)	2(1)
C8	18(1)	19(1)	21(1)	−1(1)	−1(1)	−1(1)
C9	19(1)	17(1)	24(1)	0(1)	−4(1)	0(1)
C10	19(1)	17(1)	23(1)	0(1)	−4(1)	0(1)
C11	21(1)	14(1)	26(1)	−1(1)	−4(1)	0(1)
C12	18(1)	17(1)	24(1)	0(1)	−4(1)	0(1)
C13	17(1)	21(1)	26(1)	−1(1)	−3(1)	1(1)
C14	21(1)	19(1)	34(2)	−2(1)	−4(1)	1(1)
C15	20(1)	26(1)	32(1)	−8(1)	−2(1)	6(1)
C16	25(1)	31(2)	26(1)	−1(1)	1(1)	4(1)
C17	26(1)	25(1)	29(1)	4(1)	−2(1)	2(1)
C18	19(1)	20(1)	24(1)	−2(1)	−5(1)	1(1)
C19	24(1)	14(1)	24(1)	1(1)	1(1)	−2(1)
C20	23(1)	24(1)	24(1)	2(1)	1(1)	−1(1)
C21	21(1)	28(2)	38(2)	7(1)	5(1)	1(1)
C22	36(2)	32(2)	31(2)	1(1)	13(1)	−2(1)
C23	43(2)	40(2)	20(1)	1(1)	1(1)	−2(1)
C24	25(1)	32(2)	27(1)	1(1)	−4(1)	1(1)
C25	24(1)	16(1)	20(1)	−1(1)	−1(1)	0(1)
C26	26(1)	23(1)	28(1)	2(1)	−6(1)	1(1)
C27	27(1)	27(1)	32(2)	1(1)	1(1)	−7(1)
C28	41(2)	17(1)	21(1)	0(1)	−1(1)	−4(1)
C29	36(2)	20(1)	21(1)	2(1)	−5(1)	4(1)
C30	26(1)	22(1)	23(1)	−2(1)	−4(1)	2(1)
S3	20(1)	19(1)	25(1)	3(1)	2(1)	−1(1)
S4	25(1)	20(1)	26(1)	3(1)	6(1)	−1(1)
N4	18(1)	22(1)	20(1)	−1(1)	2(1)	−2(1)
N5	21(1)	18(1)	22(1)	1(1)	3(1)	1(1)
N6	18(1)	20(1)	25(1)	1(1)	−2(1)	−1(1)

C31	18(1)	21(1)	19(1)	−1(1)	−2(1)	−4(1)
C32	20(1)	28(1)	25(1)	−1(1)	−2(1)	1(1)
C33	18(1)	36(2)	26(1)	−2(1)	2(1)	−5(1)
C34	24(1)	32(2)	25(1)	2(1)	4(1)	−10(1)
C35	23(1)	25(1)	25(1)	3(1)	0(1)	−5(1)
C36	19(1)	19(1)	22(1)	−2(1)	1(1)	−2(1)
C37	20(1)	20(1)	18(1)	−2(1)	−2(1)	−2(1)
C38	19(1)	19(1)	17(1)	1(1)	−1(1)	−2(1)
C39	19(1)	18(1)	19(1)	−1(1)	−1(1)	−1(1)
C40	19(1)	18(1)	18(1)	−2(1)	0(1)	−1(1)
C41	18(1)	20(1)	19(1)	−1(1)	2(1)	−1(1)
C42	20(1)	22(1)	18(1)	0(1)	1(1)	−4(1)
C43	29(1)	19(1)	22(1)	2(1)	−4(1)	−2(1)
C44	36(2)	26(1)	27(1)	3(1)	−1(1)	−10(1)
C45	41(2)	23(1)	36(2)	10(1)	−12(1)	−10(1)
C46	36(2)	20(1)	47(2)	2(1)	−18(1)	−1(1)
C47	23(1)	21(1)	42(2)	0(1)	−9(1)	0(1)
C48	23(1)	22(1)	24(1)	2(1)	−6(1)	−4(1)
C49	23(1)	15(1)	20(1)	0(1)	4(1)	1(1)
C50	26(1)	22(1)	31(2)	−1(1)	−5(1)	−2(1)
C51	28(2)	27(1)	36(2)	−1(1)	−8(1)	5(1)
C52	36(2)	19(1)	31(2)	1(1)	0(1)	9(1)
C53	35(2)	17(1)	29(1)	−2(1)	2(1)	−2(1)
C54	24(1)	24(1)	21(1)	−2(1)	0(1)	−3(1)
C55	20(1)	16(1)	22(1)	3(1)	1(1)	1(1)
C56	24(1)	32(2)	26(1)	−7(1)	3(1)	−1(1)
C57	20(1)	37(2)	36(2)	−8(1)	0(1)	−4(1)
C58	21(1)	29(1)	31(2)	−5(1)	7(1)	0(1)
C59	26(1)	38(2)	24(1)	−7(1)	2(1)	2(1)
C60	18(1)	32(2)	25(1)	−3(1)	−1(1)	0(1)

Table S21. Ligand **3**: Hydrogen coordinates [× 10^4] and isotropic displacement parameters [$Å^2$ × 10^3].

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
H902	3740(30)	5280(20)	4421(17)	27(8)	1
H2	3815	8562	3779	28	1
H3	3145	10223	3952	30	1
H4	1672	10721	4974	31	1
H5	767	9565	5819	29	1
H14	5597	460	3688	29	1
H15	6829	587	2522	31	1
H16	7114	2118	1944	33	1
H17	6218	3559	2529	32	1
H20	–764	5511	5773	28	1
H21	–2283	5991	6776	35	1
H22	–1626	5911	8042	40	1
H23	537	5295	8300	41	1
H24	2063	4812	7296	33	1
H26	68	3054	5785	30	1
H27	–433	1595	6428	34	1
H28	1240	672	7037	32	1
H29	3430	1212	7020	31	1
H30	3949	2670	6383	28	1
H905	6510(30)	–70(20)	680(18)	39(9)	1
H32	10578	639	–561	29	1
H33	11815	1544	–1464	32	1
H34	10933	3030	–1948	32	1
H35	8819	3685	–1506	29	1
H44	2559	–3044	2920	35	1
H45	3823	–4538	2875	40	1
H46	5839	–4705	2140	40	1
H47	6715	–3359	1490	34	1
H50	2290	2192	126	32	1
H51	1235	3725	–123	36	1
H52	2233	5166	213	35	1
H53	4267	5073	823	32	1
H54	5293	3541	1105	28	1
H56	1371	555	873	33	1
H57	–656	786	1591	37	1
H58	–689	1451	2825	33	1
H59	1306	1901	3328	36	1
H60	3332	1712	2603	30	1

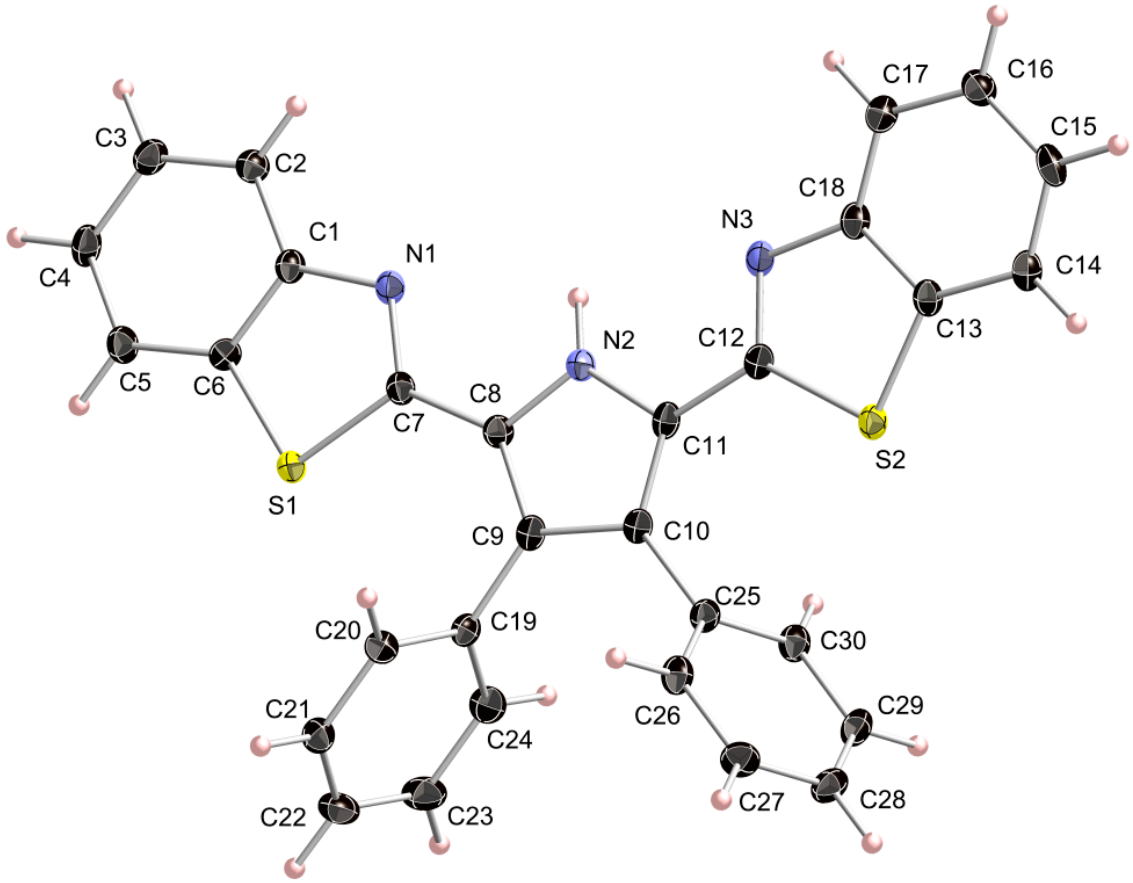
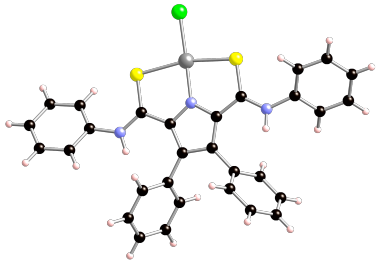


Figure S4. Ligand **3**. Thermal ellipsoids drawn at the 35% probability level, second molecule labelled in a similar fashion.

Figure S5. Ligand **3**. Overlay of the 2 independent molecules in the asymmetric unit

Table S22. Complex **7**: Crystal data and structure refinement details.



Empirical formula	$C_{31}H_{23}Cl_4CuN_3S_2$	
Formula weight	706.98	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*–1	
Unit cell dimensions	a = 8.98270(10) Å	α = 79.8410(10)°
	b = 12.2046(2) Å	β = 76.8820(10)°
	c = 14.5977(2) Å	γ = 84.9810(10)°
Volume	1532.27(4) Å^3	
Z	2	
Density (calculated)	1.532 Mg / m^3	
Absorption coefficient	1.225 mm-**1**	
F(000)	718	
Crystal	Fragment; Dark Green	
Crystal size	0.20 × 0.07 × 0.04 mm^3	
θ range for data collection	2.95 – 27.48°	
Index ranges	$-11 \le h \le 11$, $-15 \le k \le 15$, $-18 \le l \le 18$	
Reflections collected	28317	
Independent reflections	7002 [R_{int} = 0.0449]	
Completeness to θ = 27.48°	99.6 %	
Absorption correction	Semi–empirical from equivalents	
Max. and min. transmission	0.9526 and 0.7917	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7002 / 0 / 370	
Goodness-of-fit on F^2	1.051	
Final *R* indices [$F^2 > 2\sigma(F^2)$]	*R1* = 0.0470, *wR2* = 0.0907	
R indices (all data)	*R1* = 0.0590, *wR2* = 0.0973	
Largest diff. peak and hole	0.520 and –0.672 e Å^{-3}	

Diffractometer: *Nonius KappaCCD* area detector (ϕ scans and ω scans to fill *asymmetric unit*). **Cell determination:** DirAx (Duisenberg, A.J.M.(1992). J. Appl. Cryst. 25, 92-96.) **Data collection:** Collect (Collect: Data collection software, R. Hooft, Nonius B.V., 1998). **Data reduction and cell refinement**: *Denzo* (Z. Otwinowski & W. Minor, *Methods in Enzymology* (1997) Vol. **276**: *Macromolecular Crystallography*, part A, pp. 307–326; C. W. Carter, Jr. & R. M. Sweet, Eds., Academic Press). **Absorption correction**: Sheldrick, G. M. SADABS - Bruker Nonius area detector scaling and absorption correction - V2.10 **Structure solution**: *SHELXS97* (G. M. Sheldrick, Acta Cryst. (1990) A**46** 467–473). **Structure refinement**: *SHELXL97* (G. M. Sheldrick (1997), University of Göttingen, Germany). **Graphics:** Cameron - A Molecular Graphics Package. (D. M. Watkin, L. Pearce and C. K. Prout, Chemical Crystallography Laboratory, University of Oxford, 1993).

Special details: All hydrogen atoms were placed in idealised positions and refined using a riding model.

Table S23. Complex **7**: Atomic coordinates [× 10^4], equivalent isotropic displacement parameters [Å^2 × 10^3] and site occupancy factors. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
Cu1	958(1)	3594(1)	4438(1)	21(1)	1
Cl1	688(1)	4298(1)	2984(1)	23(1)	1
S1	−1581(1)	4039(1)	5205(1)	24(1)	1
S2	3497(1)	2854(1)	4007(1)	26(1)	1
N1	−2580(3)	3438(2)	7089(2)	21(1)	1
N2	1121(3)	2873(2)	5674(2)	18(1)	1
N3	4963(3)	1708(2)	5323(2)	22(1)	1
C1	−4963(3)	4054(2)	6526(2)	26(1)	1
C2	−6413(3)	4582(2)	6709(2)	31(1)	1
C3	−6931(4)	5059(3)	7522(3)	33(1)	1
C4	−5997(3)	5019(3)	8164(2)	33(1)	1
C5	−4556(3)	4494(3)	7996(2)	28(1)	1
C6	−4041(3)	4014(2)	7178(2)	21(1)	1
C7	−1439(3)	3425(2)	6328(2)	19(1)	1
C8	2(3)	2871(2)	6467(2)	18(1)	1
C9	562(3)	2288(2)	7262(2)	19(1)	1
C10	2073(3)	1927(2)	6907(2)	18(1)	1
C11	2380(3)	2316(2)	5908(2)	19(1)	1
C12	3691(3)	2254(2)	5125(2)	20(1)	1
C13	6376(3)	1449(2)	4715(2)	22(1)	1
C14	7125(3)	440(2)	5005(2)	24(1)	1
C15	8532(3)	137(3)	4462(2)	28(1)	1
C16	9199(3)	840(3)	3645(2)	30(1)	1
C17	8450(3)	1844(3)	3369(2)	31(1)	1
C18	7040(3)	2159(2)	3901(2)	26(1)	1
C19	−285(3)	2080(2)	8272(2)	19(1)	1
C20	−733(3)	2952(2)	8791(2)	26(1)	1
C21	−1555(4)	2753(3)	9724(2)	32(1)	1
C22	−1938(3)	1683(3)	10155(2)	32(1)	1
C23	−1491(4)	817(3)	9655(2)	35(1)	1
C24	−666(4)	1004(2)	8716(2)	30(1)	1
C25	3144(3)	1305(2)	7483(2)	20(1)	1
C26	3551(3)	1787(2)	8183(2)	24(1)	1
C27	4590(4)	1227(3)	8696(2)	30(1)	1
C28	5232(4)	190(3)	8520(2)	31(1)	1
C29	4818(3)	−302(2)	7838(2)	27(1)	1
C30	3764(3)	249(2)	7325(2)	23(1)	1
C31	2363(4)	3167(3)	1077(2)	36(1)	1
Cl2	1400(1)	4221(1)	419(1)	50(1)	1
Cl3	1589(1)	1883(1)	1131(1)	61(1)	1
Cl4	4342(1)	3114(1)	586(1)	43(1)	1

Table S24. Complex **7**: Bond lengths [Å] and angles [°].

Cu1–N2	1.894(2)	C10–C25	1.491(4)
Cu1–Cl1	2.2032(7)	C11–C12	1.449(4)
Cu1–S1	2.3634(8)	C13–C18	1.387(4)
Cu1–S2	2.3670(8)	C13–C14	1.396(4)
S1–C7	1.706(3)	C14–C15	1.389(4)
S2–C12	1.708(3)	C15–C16	1.386(4)
N1–C7	1.331(4)	C16–C17	1.386(4)
N1–C6	1.424(3)	C17–C18	1.388(4)
N2–C11	1.348(3)	C19–C20	1.392(4)
N2–C8	1.350(3)	C19–C24	1.393(4)
N3–C12	1.335(4)	C20–C21	1.386(4)
N3–C13	1.420(4)	C21–C22	1.382(5)
C1–C6	1.388(4)	C22–C23	1.371(5)
C1–C2	1.392(4)	C23–C24	1.391(4)
C2–C3	1.383(5)	C25–C30	1.395(4)
C3–C4	1.385(5)	C25–C26	1.396(4)
C4–C5	1.383(4)	C26–C27	1.387(4)
C5–C6	1.390(4)	C27–C28	1.386(5)
C7–C8	1.447(4)	C28–C29	1.381(4)
C8–C9	1.419(4)	C29–C30	1.394(4)
C9–C10	1.400(4)	C31–Cl3	1.752(4)
C9–C19	1.487(4)	C31–Cl2	1.753(3)
C10–C11	1.423(4)	C31–Cl4	1.759(4)

N2–Cu1–Cl1	174.97(7)	C1–C6–N1	123.2(3)
N2–Cu1–S1	83.68(7)	C5–C6–N1	116.1(2)
Cl1–Cu1–S1	95.91(3)	N1–C7–C8	117.9(2)
N2–Cu1–S2	83.20(7)	N1–C7–S1	123.6(2)
Cl1–Cu1–S2	96.89(3)	C8–C7–S1	118.5(2)
S1–Cu1–S2	166.51(3)	N2–C8–C9	109.0(2)
C7–S1–Cu1	96.95(10)	N2–C8–C7	115.7(2)
C12–S2–Cu1	97.30(10)	C9–C8–C7	135.2(3)
C7–N1–C6	129.8(2)	C10–C9–C8	106.5(2)
C11–N2–C8	109.2(2)	C10–C9–C19	126.3(2)
C11–N2–Cu1	125.71(19)	C8–C9–C19	127.2(2)
C8–N2–Cu1	125.07(18)	C9–C10–C11	106.2(2)
C12–N3–C13	130.9(2)	C9–C10–C25	126.0(2)
C6–C1–C2	118.7(3)	C11–C10–C25	127.8(2)
C3–C2–C1	120.9(3)	N2–C11–C10	109.1(2)
C2–C3–C4	119.8(3)	N2–C11–C12	115.6(2)
C5–C4–C3	120.1(3)	C10–C11–C12	135.2(2)
C4–C5–C6	119.9(3)	N3–C12–C11	117.8(2)
C1–C6–C5	120.6(3)	N3–C12–S2	124.1(2)

C11–C12–S2	118.0(2)	C23–C22–C21	119.6(3)
C18–C13–C14	120.5(3)	C22–C23–C24	120.7(3)
C18–C13–N3	123.4(3)	C23–C24–C19	120.2(3)
C14–C13–N3	116.0(3)	C30–C25–C26	119.2(3)
C15–C14–C13	119.6(3)	C30–C25–C10	121.0(2)
C16–C15–C14	120.2(3)	C26–C25–C10	119.7(2)
C17–C16–C15	119.7(3)	C27–C26–C25	119.9(3)
C16–C17–C18	120.9(3)	C28–C27–C26	120.7(3)
C13–C18–C17	119.1(3)	C29–C28–C27	119.9(3)
C20–C19–C24	118.5(3)	C28–C29–C30	119.9(3)
C20–C19–C9	121.1(2)	C29–C30–C25	120.4(3)
C24–C19–C9	120.4(3)	Cl3–C31–Cl2	109.6(2)
C21–C20–C19	120.6(3)	Cl3–C31–Cl4	110.65(18)
C22–C21–C20	120.3(3)	Cl2–C31–Cl4	111.42(18)

Table S25. Complex **7**: Anisotropic displacement parameters [Å^2× 10^3]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu1	26(1)	21(1)	16(1)	−1(1)	−5(1)	1(1)
Cl1	29(1)	24(1)	17(1)	−2(1)	−7(1)	−2(1)
S1	27(1)	26(1)	18(1)	1(1)	−8(1)	1(1)
S2	28(1)	30(1)	18(1)	0(1)	−3(1)	4(1)
N1	23(1)	21(1)	18(1)	2(1)	−7(1)	1(1)
N2	22(1)	16(1)	16(1)	−1(1)	−4(1)	2(1)
N3	26(1)	20(1)	19(1)	−1(1)	−3(1)	1(1)
C1	29(2)	23(1)	28(2)	3(1)	−12(1)	−5(1)
C2	26(2)	24(2)	43(2)	7(1)	−17(1)	−5(1)
C3	21(2)	26(2)	48(2)	5(1)	−6(1)	1(1)
C4	24(2)	35(2)	37(2)	−6(1)	0(1)	3(1)
C5	22(1)	34(2)	27(2)	−4(1)	−6(1)	0(1)
C6	19(1)	17(1)	27(2)	2(1)	−5(1)	−4(1)
C7	22(1)	14(1)	23(1)	−3(1)	−5(1)	−3(1)
C8	21(1)	15(1)	19(1)	−2(1)	−4(1)	−1(1)
C9	23(1)	14(1)	21(1)	0(1)	−6(1)	−2(1)
C10	21(1)	12(1)	22(1)	−2(1)	−5(1)	−1(1)
C11	25(1)	14(1)	19(1)	−3(1)	−6(1)	2(1)
C12	26(1)	14(1)	22(1)	−4(1)	−6(1)	0(1)
C13	23(1)	19(1)	28(2)	−9(1)	−7(1)	−1(1)
C14	24(1)	23(1)	28(2)	−5(1)	−9(1)	−3(1)
C15	24(2)	26(2)	39(2)	−10(1)	−13(1)	2(1)
C16	19(1)	34(2)	40(2)	−14(1)	−2(1)	−2(1)
C17	25(2)	30(2)	35(2)	−6(1)	0(1)	−8(1)
C18	26(2)	16(1)	34(2)	−4(1)	−4(1)	−3(1)
C19	17(1)	22(1)	17(1)	2(1)	−5(1)	0(1)
C20	31(2)	24(1)	22(1)	−1(1)	−3(1)	−3(1)
C21	34(2)	36(2)	24(2)	−5(1)	−3(1)	2(1)
C22	25(2)	47(2)	20(2)	4(1)	−2(1)	−2(1)
C23	38(2)	31(2)	31(2)	11(1)	−3(1)	−13(1)
C24	37(2)	21(1)	29(2)	3(1)	−7(1)	−8(1)
C25	20(1)	19(1)	17(1)	1(1)	−2(1)	−2(1)
C26	28(2)	21(1)	22(1)	−2(1)	−5(1)	−3(1)
C27	34(2)	35(2)	24(2)	−2(1)	−13(1)	−4(1)
C28	28(2)	36(2)	28(2)	5(1)	−12(1)	2(1)
C29	29(2)	21(1)	27(2)	6(1)	−6(1)	2(1)
C30	28(2)	19(1)	21(1)	2(1)	−7(1)	−3(1)
C31	44(2)	29(2)	30(2)	−2(1)	−2(2)	7(1)
Cl2	56(1)	37(1)	51(1)	6(1)	−15(1)	9(1)
Cl3	43(1)	29(1)	94(1)	−1(1)	14(1)	0(1)
Cl4	39(1)	43(1)	46(1)	−11(1)	−7(1)	−2(1)

Table S26. Complex **7**: Hydrogen coordinates [× 10^4] and isotropic displacement parameters [Å^2 × 10^3].

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
H1	–2405	3028	7617	25	1
H3	4918	1467	5933	27	1
H1A	–4611	3728	5966	31	1
H2	–7055	4614	6269	37	1
H3A	–7926	5412	7641	40	1
H4	–6346	5354	8720	39	1
H5	–3919	4460	8440	33	1
H14	6675	–37	5570	29	1
H15	9040	–554	4651	34	1
H16	10164	635	3276	36	1
H17	8907	2323	2808	37	1
H18	6537	2851	3710	31	1
H20	–473	3690	8501	31	1
H21	–1858	3356	10070	38	1
H22	–2506	1549	10795	39	1
H23	–1748	80	9951	42	1
H24	–362	396	8378	35	1
H26	3118	2498	8309	28	1
H27	4864	1557	9173	36	1
H28	5955	–182	8868	37	1
H29	5251	–1015	7719	32	1
H30	3467	–97	6864	28	1
H31	2202	3332	1741	43	1

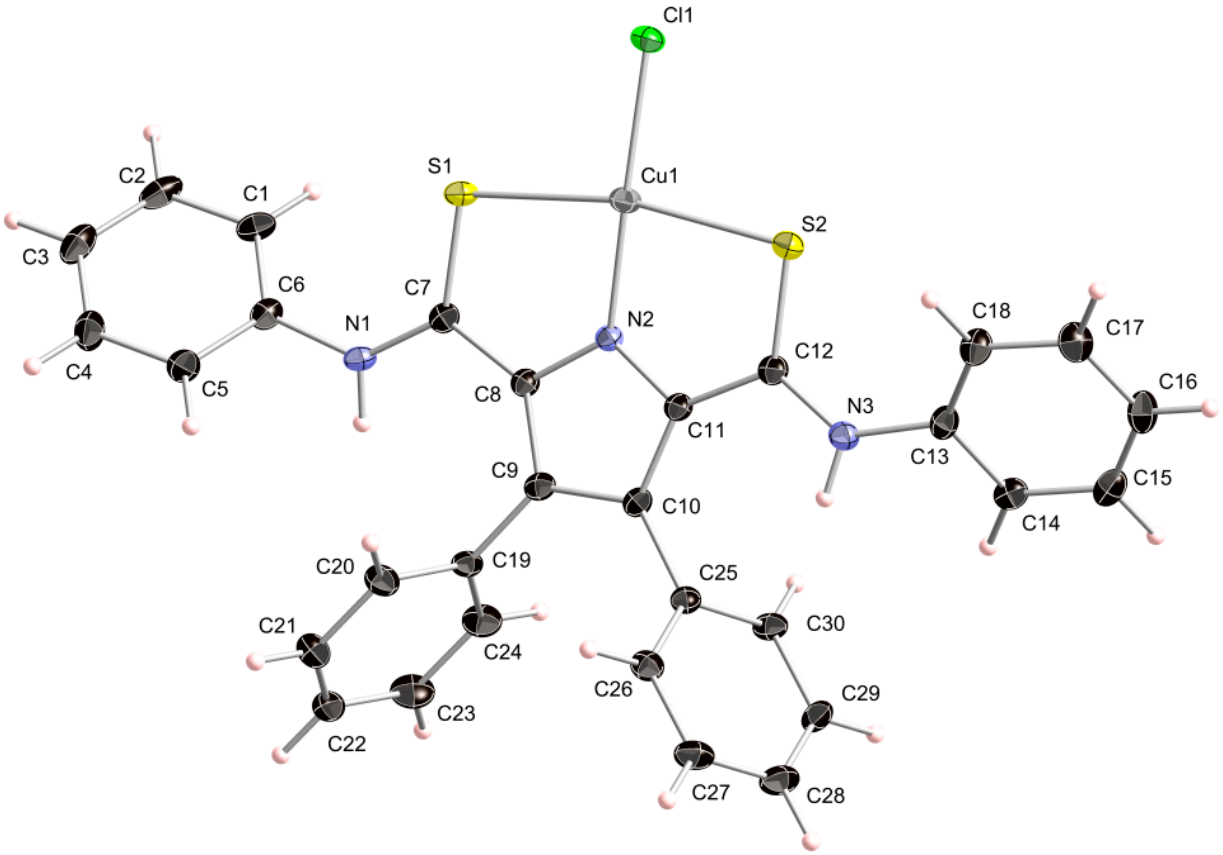
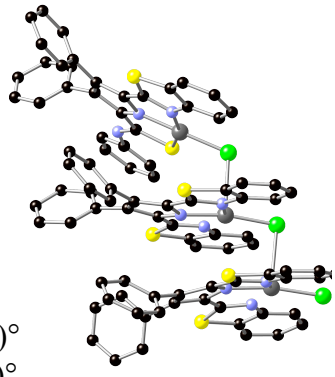


Figure S6. Complex **7**. Thermal ellipsoids drawn at the 35% probability level, solvent $CHCl_3$ omitted for clarity.

Table S27. Trimer **866**: Crystal data and structure refinement details.



Empirical formula	$C_{91.40}H_{57.40}Cl_{7.20}Cu_3N_9O_{0.60}S_6$ $C_{90}H_{56}Cl_3Cu_3N_9S_6$, 1.4($CHCl_3$), 0.6(O)	
Formula weight	1929.48	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*–1	
Unit cell dimensions	a = 13.4166(9) Å	α = 96.701(4)°
	b = 15.8954(10) Å	β = 95.457(4)°
	c = 19.7847(13) Å	γ = 95.884(4)°
Volume	4143.9(5) $Å^3$	
Z	2	
Density (calculated)	1.546 Mg / m^3	
Absorption coefficient	1.202 mm^{-1}	
F(000)	1958	
Crystal	Block; Brown	
Crystal size	0.12 × 0.08 × 0.02 mm^3	
θ range for data collection	2.92 – 25.02°	
Index ranges	$-15 \le h \le 15$, $-18 \le k \le 18$, $-23 \le l \le 22$	
Reflections collected	56588	
Independent reflections	14445 [R_{int} = 0.1338]	
Completeness to θ = 25.02°	98.7 %	
Absorption correction	Semi–empirical from equivalents	
Max. and min. transmission	0.9764 and 0.8692	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14445 / 989 / 1084	
Goodness-of-fit on F^2	1.084	
Final R indices [$F^2 > 2\sigma(F^2)$]	$R1$ = 0.1559, $wR2$ = 0.2671	
R indices (all data)	$R1$ = 0.2480, $wR2$ = 0.3124	
Largest diff. peak and hole	1.470 and –0.840 e $Å^{-3}$	

Diffractometer: *Nonius KappaCCD* area detector (ϕ scans and ω scans to fill *asymmetric unit*). **Cell determination:** DirAx (Duisenberg, A.J.M.(1992). J. Appl. Cryst. 25, 92-96.) **Data collection:** Collect (Collect: Data collection software, R. Hooft, Nonius B.V., 1998). **Data reduction and cell refinement**: *Denzo* (Z. Otwinowski & W. Minor, *Methods in Enzymology* (1997) Vol. **276**: *Macromolecular Crystallography*, part A, pp. 307–326; C. W. Carter, Jr. & R. M. Sweet, Eds., Academic Press). **Absorption correction**: Sheldrick, G. M. SADABS - Bruker Nonius area detector scaling and absorption correction - V2.10 S**tructure solution**: *SHELXS97* (G. M. Sheldrick, Acta Cryst. (1990) A**46** 467–473). S**tructure refinement**: *SHELXL97* (G. M. Sheldrick (1997), University of Göttingen, Germany). **Graphics:** Cameron - A Molecular Graphics Package. (D. M. Watkin, L. Pearce and C. K. Prout, Chemical Crystallography Laboratory, University of Oxford, 1993).

Special details: There is an area of mixed CHCl3 and H2O solvent that has been modelled as a partially occupied mixture of the two species. Thermal parameter restraints and constraints were used for the solvent, and mild thermal parameter restraints applied to the remainder of the structure. Hydrogen atoms were not located for the water, and the remainder were placed in calculated positions and refined using a riding model.

Table S28. Trimer **866**: Atomic coordinates [× 10^4], equivalent isotropic displacement parameters [Å^2 × 10^3] and site occupancy factors. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
Cu1	3254(1)	4661(1)	3635(1)	34(1)	1
Cl1	3823(3)	5909(2)	3368(2)	39(1)	1
S1	–163(3)	4046(2)	3741(2)	39(1)	1
S2	5328(3)	3144(2)	4864(2)	35(1)	1
N1	1604(9)	4703(7)	3505(6)	37(2)	1
N2	2720(9)	3689(7)	4013(6)	34(2)	1
N3	4573(9)	4241(6)	4159(5)	31(2)	1
C1	–86(11)	4964(9)	3316(7)	40(3)	1
C2	–873(12)	5398(9)	3100(8)	46(3)	1
C3	–613(12)	6113(10)	2790(8)	49(3)	1
C4	395(12)	6373(10)	2705(8)	51(3)	1
C5	1152(12)	5926(9)	2932(8)	46(3)	1
C6	908(11)	5203(9)	3237(8)	41(2)	1
C7	1126(11)	4076(9)	3765(7)	36(2)	1
C8	1726(11)	3493(8)	4080(7)	35(2)	1
C9	1638(11)	2846(8)	4505(7)	35(2)	1
C10	2638(11)	2686(8)	4723(7)	34(2)	1
C11	3287(10)	3235(8)	4413(7)	32(2)	1
C12	4324(10)	3550(8)	4441(6)	30(2)	1
C13	6144(11)	3964(8)	4663(7)	36(2)	1
C14	7173(11)	4136(9)	4834(7)	39(3)	1
C15	7667(12)	4852(9)	4610(7)	40(3)	1
C16	7128(11)	5368(9)	4227(7)	40(3)	1
C17	6108(11)	5200(8)	4045(7)	38(2)	1
C18	5595(11)	4491(8)	4269(7)	35(2)	1
C19	629(11)	2515(8)	4722(7)	36(2)	1
C20	138(11)	1743(9)	4407(7)	38(3)	1
C21	–795(11)	1438(10)	4578(8)	45(3)	1
C22	–1217(12)	1898(9)	5082(8)	44(3)	1
C23	–749(11)	2646(9)	5389(8)	43(3)	1
C24	191(11)	2976(9)	5223(7)	42(3)	1
C25	2889(11)	2084(8)	5200(7)	37(2)	1
C26	3608(11)	2308(9)	5760(7)	40(3)	1
C27	3903(12)	1747(10)	6202(8)	46(3)	1
C28	3460(11)	937(9)	6112(8)	43(3)	1
C29	2745(12)	657(9)	5553(8)	45(3)	1
C30	2464(11)	1222(8)	5094(8)	40(3)	1
Cu2	2871(1)	2610(1)	2615(1)	35(1)	1
Cl2	3418(3)	3880(2)	2374(2)	39(1)	1
S3	–528(3)	1717(2)	2463(2)	39(1)	1
S4	5047(3)	937(2)	3608(2)	41(1)	1
N4	1210(9)	2534(7)	2393(5)	32(2)	1

N5	2382(9)	1635(6)	2984(5)	32(2)	1
N6	4262(9)	2151(7)	3037(6)	36(2)	1
C31	–474(12)	2652(9)	2088(7)	41(3)	1
C32	–1295(13)	3023(9)	1799(7)	47(3)	1
C33	–1036(13)	3784(9)	1524(8)	49(3)	1
C34	–48(13)	4153(9)	1544(8)	49(3)	1
C35	759(12)	3776(8)	1826(7)	43(3)	1
C36	512(12)	3018(8)	2102(7)	39(2)	1
C37	789(10)	1835(8)	2595(6)	32(2)	1
C38	1423(10)	1278(8)	2897(7)	31(2)	1
C39	1368(10)	450(8)	3108(6)	30(2)	1
C40	2377(10)	342(8)	3334(6)	31(2)	1
C41	2991(10)	1086(8)	3236(7)	32(2)	1
C42	4030(11)	1408(8)	3287(7)	36(2)	1
C43	5861(11)	1788(9)	3417(8)	43(3)	1
C44	6895(12)	1904(10)	3523(8)	50(3)	1
C45	7382(13)	2629(10)	3337(8)	52(3)	1
C46	6829(12)	3211(10)	3034(8)	52(3)	1
C47	5798(12)	3094(9)	2918(8)	43(3)	1
C48	5302(11)	2368(9)	3114(7)	40(2)	1
C49	451(11)	–154(8)	3122(7)	34(2)	1
C50	338(11)	–534(8)	3701(7)	37(2)	1
C51	–506(11)	–1135(9)	3723(8)	41(3)	1
C52	–1180(11)	–1354(9)	3156(8)	44(3)	1
C53	–1052(12)	–988(10)	2561(8)	47(3)	1
C54	–238(11)	–374(9)	2563(8)	40(3)	1
C55	2739(11)	–447(8)	3548(7)	33(2)	1
C56	2405(11)	–1245(8)	3182(7)	36(3)	1
C57	2802(11)	–1960(8)	3369(7)	39(3)	1
C58	3497(11)	–1907(9)	3931(7)	40(3)	1
C59	3830(11)	–1129(9)	4295(7)	40(3)	1
C60	3467(10)	–403(8)	4113(7)	33(2)	1
Cu3	2345(2)	446(1)	1312(1)	45(1)	1
Cl3	3036(3)	1778(2)	1395(2)	45(1)	1
S5	692(3)	755(2)	1007(2)	46(1)	1
S6	4225(4)	–1726(3)	1632(3)	71(1)	1
N7	–890(9)	–495(7)	703(6)	41(2)	1
N8	1697(10)	–675(8)	1206(6)	46(2)	1
N9	3610(9)	–226(7)	1570(5)	34(2)	1
C61	–2586(11)	–515(9)	282(7)	42(3)	1
C62	–3446(12)	–132(9)	101(8)	47(3)	1
C63	–3407(12)	723(10)	165(8)	47(3)	1
C64	–2501(12)	1246(10)	424(8)	47(3)	1
C65	–1669(12)	864(9)	612(7)	42(3)	1
C66	–1716(12)	–18(9)	544(7)	43(2)	1
C67	118(12)	–261(9)	869(7)	45(2)	1
C68	734(13)	–940(9)	987(7)	44(2)	1

C69	604(12)	−1846(9)	881(7)	44(2)	1
C70	1547(13)	−2105(9)	1077(7)	46(2)	1
C71	2225(13)	−1349(10)	1280(7)	45(2)	1
C72	3276(12)	−1080(9)	1484(7)	44(2)	1
C73	5123(14)	−847(12)	1786(9)	63(3)	1
C74	6129(15)	−791(13)	1948(9)	69(3)	1
C75	6708(15)	36(12)	2034(10)	72(3)	1
C76	6214(14)	770(13)	1929(9)	69(3)	1
C77	5203(14)	717(12)	1768(9)	64(3)	1
C78	4597(13)	−87(11)	1691(9)	56(3)	1
C79	−394(13)	−2408(10)	696(8)	49(3)	1
C80	−865(13)	−2534(10)	17(8)	53(3)	1
C81	−1787(14)	−3041(10)	−137(9)	56(3)	1
C82	−2214(14)	−3421(11)	352(9)	63(3)	1
C83	−1764(15)	−3282(12)	989(10)	72(3)	1
C84	−854(14)	−2770(11)	1179(9)	62(3)	1
C85	1788(13)	−3015(10)	1027(8)	51(3)	1
C86	1445(14)	−3588(10)	455(8)	57(3)	1
C87	1680(14)	−4409(10)	404(9)	60(3)	1
C88	2264(14)	−4683(11)	942(9)	60(3)	1
C89	2626(14)	−4117(10)	1499(8)	55(3)	1
C90	2374(13)	−3291(10)	1551(8)	54(3)	1
C91	5782(17)	5838(16)	2147(11)	52(4)	0.70
Cl4	6515(5)	4983(4)	2026(3)	59(2)	0.70
Cl5	5397(6)	6181(5)	1370(4)	83(2)	0.70
Cl6	6488(7)	6684(4)	2664(4)	87(2)	0.70
O2W	4930(30)	5400(30)	1170(20)	82(2)	0.30
C92	5080(20)	6916(17)	−633(14)	80(2)	0.70
Cl7	5186(7)	5869(5)	−541(5)	96(3)	0.70
Cl8	4116(6)	7166(4)	−1131(4)	81(2)	0.70
Cl9	5427(5)	7607(4)	106(3)	56(2)	0.70
O1W	3630(30)	6390(30)	−150(20)	82(2)	0.30

Table S29. Trimer **866**: Bond lengths [Å] and angles [°].

Cu1–N2	1.899(11)	C28–C29	1.39(2)
Cu1–N3	2.169(11)	C29–C30	1.404(19)
Cu1–Cl1	2.192(4)	Cu2–N5	1.875(11)
Cu1–N1	2.213(12)	Cu2–Cl2	2.197(4)
Cu1–Cl2	2.693(4)	Cu2–N6	2.200(11)
S1–C7	1.722(15)	Cu2–N4	2.218(11)
S1–C1	1.765(14)	Cu2–Cl3	2.654(4)
S2–C13	1.722(14)	S3–C31	1.735(14)
S2–C12	1.738(13)	S3–C37	1.749(14)
N1–C7	1.312(17)	S4–C42	1.728(14)
N1–C6	1.393(17)	S4–C43	1.749(16)
N2–C8	1.361(18)	N4–C37	1.317(16)
N2–C11	1.363(16)	N4–C36	1.397(16)
N3–C12	1.316(16)	N5–C38	1.338(17)
N3–C18	1.378(18)	N5–C41	1.359(16)
C1–C6	1.38(2)	N6–C42	1.351(17)
C1–C2	1.381(19)	N6–C48	1.392(18)
C2–C3	1.38(2)	C31–C36	1.39(2)
C3–C4	1.41(2)	C31–C32	1.41(2)
C4–C5	1.37(2)	C32–C33	1.41(2)
C5–C6	1.385(19)	C33–C34	1.39(2)
C7–C8	1.444(18)	C34–C35	1.39(2)
C8–C9	1.405(18)	C35–C36	1.403(19)
C9–C10	1.428(19)	C37–C38	1.429(17)
C9–C19	1.52(2)	C38–C39	1.424(17)
C10–C11	1.402(19)	C39–C40	1.418(18)
C10–C25	1.462(18)	C39–C49	1.487(19)
C11–C12	1.424(19)	C40–C41	1.415(18)
C13–C14	1.38(2)	C40–C55	1.482(17)
C13–C18	1.422(19)	C41–C42	1.424(19)
C14–C15	1.40(2)	C43–C44	1.37(2)
C15–C16	1.389(19)	C43–C48	1.40(2)
C16–C17	1.37(2)	C44–C45	1.37(2)
C17–C18	1.397(19)	C45–C46	1.40(2)
C19–C24	1.38(2)	C46–C47	1.37(2)
C19–C20	1.381(19)	C47–C48	1.39(2)
C20–C21	1.38(2)	C49–C54	1.360(19)
C21–C22	1.37(2)	C49–C50	1.369(18)
C22–C23	1.34(2)	C50–C51	1.412(19)
C23–C24	1.40(2)	C51–C52	1.36(2)
C25–C26	1.38(2)	C52–C53	1.39(2)
C25–C30	1.413(19)	C53–C54	1.39(2)
C26–C27	1.381(18)	C55–C56	1.394(18)
C27–C28	1.35(2)	C55–C60	1.403(19)

C56–C57	1.377(18)	C70–C71	1.42(2)
C57–C58	1.37(2)	C70–C85	1.51(2)
C58–C59	1.366(19)	C71–C72	1.44(2)
C59–C60	1.369(18)	C73–C74	1.35(2)
Cu3–N8	1.880(13)	C73–C78	1.48(2)
Cu3–N9	2.149(11)	C74–C75	1.44(3)
Cu3–Cl3	2.203(4)	C75–C76	1.43(2)
Cu3–S5	2.358(5)	C76–C77	1.36(2)
S5–C67	1.697(15)	C77–C78	1.43(2)
S6–C73	1.73(2)	C79–C84	1.34(2)
S6–C72	1.741(16)	C79–C80	1.41(2)
N7–C67	1.362(19)	C80–C81	1.39(2)
N7–C66	1.436(19)	C81–C82	1.34(2)
N8–C68	1.331(19)	C82–C83	1.33(2)
N8–C71	1.358(19)	C83–C84	1.39(2)
N9–C78	1.31(2)	C85–C86	1.38(2)
N9–C72	1.371(18)	C85–C90	1.38(2)
C61–C66	1.36(2)	C86–C87	1.37(2)
C61–C62	1.40(2)	C87–C88	1.40(2)
C62–C63	1.35(2)	C88–C89	1.36(2)
C63–C64	1.42(2)	C89–C90	1.38(2)
C64–C65	1.37(2)	C91–Cl6	1.73(3)
C65–C66	1.387(19)	C91–Cl5	1.74(2)
C67–C68	1.45(2)	C91–Cl4	1.77(2)
C68–C69	1.42(2)	C92–Cl8	1.66(3)
C69–C70	1.40(2)	C92–Cl7	1.72(3)
C69–C79	1.52(2)	C92–Cl9	1.72(3)

N2–Cu1–N3	76.5(4)	C11–N2–Cu1	123.7(9)
N2–Cu1–Cl1	170.0(4)	C12–N3–C18	111.7(11)
N3–Cu1–Cl1	103.4(3)	C12–N3–Cu1	110.8(9)
N2–Cu1–N1	75.8(4)	C18–N3–Cu1	137.5(9)
N3–Cu1–N1	150.0(4)	C6–C1–C2	124.0(14)
Cl1–Cu1–N1	102.0(3)	C6–C1–S1	109.0(10)
N2–Cu1–Cl2	97.7(3)	C2–C1–S1	127.0(12)
N3–Cu1–Cl2	97.6(3)	C1–C2–C3	115.9(15)
Cl1–Cu1–Cl2	92.27(13)	C2–C3–C4	121.3(14)
N1–Cu1–Cl2	97.2(3)	C5–C4–C3	120.7(14)
C7–S1–C1	88.4(7)	C4–C5–C6	119.0(15)
C13–S2–C12	90.0(7)	C1–C6–C5	119.1(13)
C7–N1–C6	109.3(12)	C1–C6–N1	116.1(13)
C7–N1–Cu1	111.4(9)	C5–C6–N1	124.8(14)
C6–N1–Cu1	139.3(10)	N1–C7–C8	117.6(13)
C8–N2–C11	109.8(11)	N1–C7–S1	117.1(10)
C8–N2–Cu1	124.3(9)	C8–C7–S1	125.2(11)

N2–C8–C9	108.3(12)	Cl2–Cu2–N4	104.0(3)
N2–C8–C7	110.8(12)	N6–Cu2–N4	153.1(4)
C9–C8–C7	140.4(14)	N5–Cu2–Cl3	94.6(3)
C8–C9–C10	106.7(12)	Cl2–Cu2–Cl3	96.22(14)
C8–C9–C19	121.9(12)	N6–Cu2–Cl3	90.3(3)
C10–C9–C19	130.9(12)	N4–Cu2–Cl3	91.7(3)
C11–C10–C9	106.4(11)	Cu2–Cl2–Cu1	93.94(13)
C11–C10–C25	128.9(13)	C31–S3–C37	89.4(7)
C9–C10–C25	124.6(12)	C42–S4–C43	89.6(7)
N2–C11–C10	108.6(12)	C37–N4–C36	113.2(12)
N2–C11–C12	109.7(11)	C37–N4–Cu2	109.4(8)
C10–C11–C12	141.1(13)	C36–N4–Cu2	137.5(9)
N3–C12–C11	119.0(12)	C38–N5–C41	109.9(11)
N3–C12–S2	114.8(10)	C38–N5–Cu2	125.3(9)
C11–C12–S2	126.1(10)	C41–N5–Cu2	123.0(9)
C14–C13–C18	121.7(13)	C42–N6–C48	110.1(11)
C14–C13–S2	128.9(11)	C42–N6–Cu2	109.4(9)
C18–C13–S2	109.4(11)	C48–N6–Cu2	140.4(9)
C13–C14–C15	117.8(14)	C36–C31–C32	122.0(14)
C16–C15–C14	120.3(14)	C36–C31–S3	111.2(10)
C17–C16–C15	122.5(14)	C32–C31–S3	126.8(13)
C16–C17–C18	118.3(13)	C31–C32–C33	115.0(15)
N3–C18–C17	126.6(13)	C34–C33–C32	122.9(14)
N3–C18–C13	114.1(12)	C33–C34–C35	121.6(14)
C17–C18–C13	119.3(13)	C34–C35–C36	116.1(15)
C24–C19–C20	119.3(14)	C31–C36–N4	112.7(12)
C24–C19–C9	121.2(13)	C31–C36–C35	122.4(13)
C20–C19–C9	119.5(13)	N4–C36–C35	124.9(14)
C19–C20–C21	120.9(14)	N4–C37–C38	118.7(12)
C22–C21–C20	119.1(15)	N4–C37–S3	113.5(10)
C23–C22–C21	120.4(15)	C38–C37–S3	127.8(10)
C22–C23–C24	121.7(15)	N5–C38–C39	109.7(11)
C19–C24–C23	118.4(14)	N5–C38–C37	110.0(11)
C26–C25–C30	115.7(13)	C39–C38–C37	140.2(13)
C26–C25–C10	122.0(13)	C40–C39–C38	105.0(11)
C30–C25–C10	122.1(13)	C40–C39–C49	127.3(11)
C27–C26–C25	123.8(14)	C38–C39–C49	127.7(12)
C28–C27–C26	119.8(16)	C41–C40–C39	107.4(11)
C27–C28–C29	119.9(14)	C41–C40–C55	125.9(12)
C28–C29–C30	120.2(14)	C39–C40–C55	126.3(12)
C29–C30–C25	120.5(15)	N5–C41–C40	108.0(12)
N5–Cu2–Cl2	169.1(3)	N5–C41–C42	112.2(11)
N5–Cu2–N6	77.4(5)	C40–C41–C42	139.7(12)
Cl2–Cu2–N6	102.5(3)	N6–C42–C41	117.3(12)
N5–Cu2–N4	75.7(4)	N6–C42–S4	115.3(11)

C41–C42–S4	127.4(10)	C62–C63–C64	120.7(15)
C44–C43–C48	122.4(15)	C65–C64–C63	118.6(14)
C44–C43–S4	127.8(12)	C64–C65–C66	120.3(15)
C48–C43–S4	109.8(11)	C61–C66–C65	120.6(15)
C45–C44–C43	117.8(15)	C61–C66–N7	113.7(13)
C44–C45–C46	120.1(16)	C65–C66–N7	125.6(14)
C47–C46–C45	122.4(16)	N7–C67–C68	116.7(13)
C46–C47–C48	117.7(15)	N7–C67–S5	125.6(12)
C47–C48–N6	125.3(13)	C68–C67–S5	117.6(12)
C47–C48–C43	119.6(14)	N8–C68–C69	108.8(14)
N6–C48–C43	115.1(13)	N8–C68–C67	114.5(13)
C54–C49–C50	119.8(14)	C69–C68–C67	136.5(15)
C54–C49–C39	121.5(12)	C70–C69–C68	106.2(14)
C50–C49–C39	118.5(13)	C70–C69–C79	127.3(13)
C49–C50–C51	120.0(14)	C68–C69–C79	125.9(14)
C52–C51–C50	119.3(14)	C69–C70–C71	106.8(13)
C51–C52–C53	120.8(15)	C69–C70–C85	125.4(15)
C54–C53–C52	118.6(15)	C71–C70–C85	127.6(15)
C49–C54–C53	121.3(14)	N8–C71–C70	107.5(14)
C56–C55–C60	118.1(12)	N8–C71–C72	111.6(14)
C56–C55–C40	121.5(12)	C70–C71–C72	140.6(15)
C60–C55–C40	120.4(12)	N9–C72–C71	119.0(13)
C57–C56–C55	120.0(14)	N9–C72–S6	113.8(12)
C58–C57–C56	121.1(13)	C71–C72–S6	127.2(12)
C59–C58–C57	119.4(13)	C74–C73–C78	122.2(18)
C58–C59–C60	121.0(14)	C74–C73–S6	130.5(15)
C59–C60–C55	120.3(13)	C78–C73–S6	107.3(13)
N8–Cu3–N9	80.2(5)	C73–C74–C75	118.8(18)
N8–Cu3–Cl3	176.7(4)	C76–C75–C74	119.6(18)
N9–Cu3–Cl3	102.8(3)	C77–C76–C75	121.8(19)
N8–Cu3–S5	82.1(4)	C76–C77–C78	120.5(18)
N9–Cu3–S5	162.2(3)	N9–C78–C77	126.9(16)
Cl3–Cu3–S5	95.02(15)	N9–C78–C73	115.9(15)
Cu3–Cl3–Cu2	110.88(16)	C77–C78–C73	117.1(16)
C67–S5–Cu3	97.9(6)	C84–C79–C80	119.1(16)
C73–S6–C72	90.9(8)	C84–C79–C69	120.4(14)
C67–N7–C66	132.5(12)	C80–C79–C69	120.6(14)
C68–N8–C71	110.6(13)	C81–C80–C79	119.4(16)
C68–N8–Cu3	127.7(11)	C82–C81–C80	120.3(16)
C71–N8–Cu3	121.3(11)	C83–C82–C81	119.2(18)
C78–N9–C72	111.7(13)	C82–C83–C84	123.3(18)
C78–N9–Cu3	139.7(11)	C79–C84–C83	118.7(17)
C72–N9–Cu3	107.7(9)	C86–C85–C90	118.2(14)
C66–C61–C62	119.5(14)	C86–C85–C70	121.1(14)
C63–C62–C61	120.2(15)	C90–C85–C70	120.7(14)

C87–C86–C85	121.2(16)	Cl6–C91–Cl4	109.5(13)
C86–C87–C88	120.0(16)	Cl5–C91–Cl4	111.1(11)
C89–C88–C87	119.2(15)	Cl8–C92–Cl7	120.0(17)
C88–C89–C90	120.3(16)	Cl8–C92–Cl9	115.0(14)
C85–C90–C89	121.0(16)	Cl7–C92–Cl9	113.9(15)
Cl6–C91–Cl5	108.3(14)		

Table S30. Trimer **866**: Anisotropic displacement parameters [Å^2× 10^3]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu1	40(1)	25(1)	39(1)	10(1)	1(1)	7(1)
Cl1	49(2)	24(2)	45(2)	8(2)	1(2)	4(2)
S1	38(2)	37(2)	44(2)	11(2)	6(2)	9(2)
S2	38(2)	29(2)	40(2)	12(2)	1(2)	7(2)
N1	44(5)	30(5)	38(5)	0(4)	7(4)	13(4)
N2	43(4)	25(5)	36(5)	9(4)	1(4)	9(4)
N3	46(5)	20(4)	32(5)	2(4)	11(4)	13(4)
C1	47(5)	34(5)	40(6)	10(5)	0(5)	9(4)
C2	46(6)	42(6)	52(7)	11(5)	1(5)	14(5)
C3	50(6)	44(6)	60(7)	19(5)	−1(6)	23(5)
C4	54(6)	43(6)	60(7)	23(5)	−1(6)	10(5)
C5	47(6)	36(6)	57(7)	15(5)	−1(5)	7(5)
C6	46(5)	34(5)	44(5)	10(4)	1(5)	10(4)
C7	41(5)	33(5)	35(6)	3(4)	5(5)	10(4)
C8	43(4)	29(5)	35(5)	5(4)	4(4)	8(4)
C9	43(4)	27(5)	34(5)	6(4)	1(4)	2(4)
C10	42(4)	26(4)	37(5)	7(4)	8(4)	9(4)
C11	41(4)	25(5)	32(5)	5(4)	8(4)	10(4)
C12	42(4)	23(5)	28(5)	5(4)	10(4)	12(4)
C13	47(5)	27(5)	34(6)	−2(4)	7(5)	7(4)
C14	46(5)	32(5)	40(6)	−4(5)	8(5)	10(5)
C15	44(6)	35(6)	41(6)	−5(5)	7(5)	10(4)
C16	48(5)	35(6)	39(6)	1(5)	9(5)	8(5)
C17	46(5)	29(5)	41(6)	5(4)	8(5)	12(5)
C18	45(5)	24(4)	39(5)	1(4)	11(4)	11(4)
C19	43(5)	30(5)	36(5)	10(4)	2(4)	4(4)
C20	44(6)	34(5)	36(6)	8(5)	0(5)	4(5)
C21	46(6)	42(6)	47(6)	8(5)	0(5)	2(5)
C22	41(6)	45(6)	47(6)	15(5)	4(5)	6(5)
C23	46(6)	40(6)	46(6)	13(5)	8(5)	9(5)
C24	50(6)	36(6)	41(6)	10(5)	4(5)	5(5)
C25	44(5)	30(4)	42(5)	13(4)	14(4)	11(4)
C26	44(6)	38(5)	44(6)	23(5)	13(5)	11(5)
C27	48(6)	47(6)	52(6)	25(5)	11(5)	13(5)
C28	48(7)	41(5)	51(6)	23(5)	20(5)	19(5)
C29	54(7)	35(5)	54(6)	20(5)	19(5)	7(5)
C30	49(6)	31(5)	45(6)	11(5)	14(5)	11(5)
Cu2	47(1)	24(1)	35(1)	8(1)	4(1)	9(1)
Cl2	54(2)	22(2)	42(2)	5(1)	4(2)	4(2)
S3	40(2)	39(2)	38(2)	8(2)	0(2)	12(2)
S4	39(2)	32(2)	56(2)	8(2)	3(2)	12(2)
N4	47(5)	26(4)	26(5)	7(4)	3(4)	12(4)
N5	46(4)	24(4)	29(5)	6(4)	6(4)	11(4)

N6	42(5)	28(5)	39(5)	7(4)	3(4)	9(4)
C31	57(5)	31(5)	36(6)	4(4)	−2(5)	16(4)
C32	62(6)	38(6)	42(6)	5(5)	−4(5)	18(5)
C33	62(6)	35(6)	50(6)	6(5)	−8(6)	21(5)
C34	66(6)	30(6)	52(7)	5(5)	−5(6)	16(5)
C35	58(6)	27(5)	45(6)	8(5)	−3(5)	16(5)
C36	55(5)	29(5)	34(5)	4(4)	1(5)	18(4)
C37	43(5)	28(5)	26(5)	7(4)	3(5)	8(4)
C38	43(4)	23(4)	28(5)	3(4)	8(4)	12(4)
C39	44(4)	19(4)	29(5)	−1(4)	12(4)	12(3)
C40	45(4)	21(4)	28(5)	3(4)	8(4)	9(4)
C41	42(4)	25(4)	30(5)	6(4)	7(4)	10(4)
C42	43(4)	29(5)	36(6)	5(5)	2(5)	8(4)
C43	43(5)	32(5)	51(6)	−4(5)	−2(5)	7(4)
C44	42(5)	42(6)	62(7)	−6(5)	−1(6)	7(5)
C45	44(6)	45(6)	63(7)	−6(6)	3(6)	4(5)
C46	52(6)	42(6)	57(7)	−3(5)	3(6)	−1(5)
C47	49(5)	33(5)	46(6)	−1(5)	3(5)	3(5)
C48	44(5)	31(5)	43(5)	−2(4)	3(5)	5(4)
C49	41(5)	29(5)	38(5)	11(4)	10(4)	14(4)
C50	40(6)	32(5)	43(6)	13(5)	11(5)	11(4)
C51	40(6)	41(6)	49(6)	18(5)	13(5)	11(5)
C52	39(6)	42(6)	54(6)	12(5)	11(5)	8(5)
C53	43(6)	47(6)	51(6)	6(5)	5(5)	7(5)
C54	43(6)	37(6)	44(6)	13(5)	9(5)	9(5)
C55	48(5)	27(4)	29(5)	7(4)	10(4)	13(4)
C56	51(6)	26(5)	34(6)	4(4)	9(5)	11(5)
C57	54(7)	24(5)	42(6)	1(5)	10(5)	8(5)
C58	54(7)	28(5)	41(6)	13(5)	10(5)	9(5)
C59	47(6)	34(5)	41(6)	10(5)	7(5)	11(5)
C60	42(6)	30(5)	30(5)	8(4)	11(4)	11(5)
Cu3	58(1)	36(1)	41(1)	2(1)	5(1)	8(1)
Cl3	56(2)	36(2)	42(2)	1(2)	5(2)	6(2)
S5	62(3)	32(2)	44(2)	4(2)	7(2)	5(2)
S6	86(3)	50(3)	83(4)	16(2)	15(3)	24(2)
N7	61(5)	29(5)	34(5)	2(4)	10(5)	5(4)
N8	65(5)	44(5)	29(5)	2(5)	7(5)	6(4)
N9	43(5)	34(4)	27(5)	8(4)	8(4)	15(4)
C61	55(6)	30(5)	41(6)	2(5)	12(5)	0(4)
C62	54(6)	39(5)	48(6)	5(5)	10(5)	1(5)
C63	52(6)	44(5)	47(6)	3(5)	7(5)	13(5)
C64	57(6)	38(5)	46(6)	3(5)	0(6)	10(5)
C65	56(6)	33(5)	34(6)	1(5)	0(5)	6(5)
C66	61(5)	30(5)	36(5)	−2(5)	2(5)	5(4)
C67	63(5)	34(4)	37(5)	4(4)	8(5)	2(4)
C68	65(5)	36(4)	32(5)	3(5)	8(5)	9(4)
C69	66(5)	38(4)	28(5)	6(4)	9(5)	8(4)
C70	66(5)	42(4)	34(5)	6(4)	9(5)	14(4)

C71	66(5)	42(5)	29(5)	4(5)	9(5)	9(4)
C72	62(5)	45(5)	27(6)	8(5)	10(5)	10(4)
C73	65(5)	64(6)	61(7)	7(6)	5(6)	19(5)
C74	72(6)	70(7)	67(7)	10(7)	−2(7)	21(5)
C75	69(7)	75(7)	71(8)	13(7)	1(7)	14(5)
C76	64(6)	71(7)	71(8)	10(7)	−2(7)	9(6)
C77	63(6)	64(6)	63(7)	10(6)	−3(7)	6(5)
C78	60(5)	56(5)	52(6)	7(5)	4(6)	11(4)
C79	65(5)	46(5)	36(5)	8(5)	2(5)	10(4)
C80	73(7)	44(6)	42(6)	8(5)	−2(5)	8(5)
C81	73(7)	48(7)	46(6)	10(5)	−12(6)	9(6)
C82	71(7)	63(7)	52(7)	5(6)	−6(6)	−1(6)
C83	76(7)	80(8)	54(6)	12(6)	0(6)	−12(6)
C84	68(7)	69(7)	47(6)	12(6)	−2(6)	−6(6)
C85	74(6)	40(4)	40(5)	10(4)	5(5)	15(5)
C86	80(7)	42(5)	47(6)	7(5)	−3(6)	15(6)
C87	88(8)	43(6)	51(6)	7(5)	1(6)	19(6)
C88	90(8)	43(6)	52(7)	13(5)	5(6)	21(6)
C89	85(8)	39(6)	45(6)	17(5)	10(6)	19(6)
C90	84(7)	41(5)	41(6)	12(5)	6(5)	19(6)
C91	44(13)	85(12)	35(8)	1(7)	25(8)	29(6)
Cl4	71(4)	49(3)	58(4)	10(2)	−7(3)	23(3)
Cl5	81(5)	94(5)	91(4)	51(4)	12(3)	43(4)
Cl6	135(7)	53(3)	75(4)	−2(3)	39(4)	5(4)
O2W	80(5)	93(6)	89(5)	51(4)	13(4)	43(4)
C92	103(6)	66(3)	66(5)	−11(4)	−25(4)	44(4)
Cl7	105(6)	70(4)	108(6)	21(4)	−35(5)	22(4)
Cl8	103(6)	68(3)	66(4)	−12(3)	−26(4)	44(4)
Cl9	62(4)	55(4)	51(4)	6(3)	−2(3)	13(3)
O1W	80(5)	93(6)	89(5)	51(4)	13(4)	43(4)

Table S31. Trimer **866**: Hydrogen coordinates [× 10^4] and isotropic displacement parameters [Å² × 10^3].

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
H2	−1538	5221	3160	55	1
H3	−1116	6427	2635	59	1
H4	550	6855	2493	61	1
H5	1820	6105	2882	56	1
H14	7526	3785	5090	47	1
H15	8359	4985	4717	48	1
H16	7472	5846	4090	49	1
H17	5767	5548	3780	45	1
H20	439	1425	4076	45	1
H21	−1132	927	4353	54	1
H22	−1833	1688	5211	53	1
H23	−1057	2957	5722	51	1
H24	512	3494	5446	51	1
H26	3910	2869	5842	48	1
H27	4406	1929	6562	56	1
H28	3630	566	6423	52	1
H29	2452	93	5484	54	1
H30	1996	1028	4716	48	1
H32	−1959	2784	1791	57	1
H33	−1549	4052	1320	59	1
H34	78	4664	1364	59	1
H35	1423	4013	1831	51	1
H44	7253	1503	3715	60	1
H45	8081	2733	3413	62	1
H46	7174	3695	2907	62	1
H47	5444	3488	2714	52	1
H50	817	−396	4080	44	1
H51	−601	−1378	4120	50	1
H52	−1733	−1754	3166	53	1
H53	−1503	−1151	2170	56	1
H54	−161	−107	2174	48	1
H56	1913	−1296	2810	43	1
H57	2596	−2486	3111	47	1
H58	3739	−2397	4064	48	1
H59	4311	−1091	4671	48	1
H60	3704	122	4366	39	1
H7	−1065	−1032	692	49	1
H61	−2607	−1106	225	50	1
H62	−4047	−468	−65	56	1
H63	−3982	973	38	57	1
H64	−2473	1837	466	57	1

H65	−1068	1197	785	50	1
H74	6442	−1278	2002	83	1
H75	7400	91	2158	86	1
H76	6595	1300	1971	83	1
H77	4901	1208	1707	77	1
H80	−562	−2281	−324	64	1
H81	−2108	−3117	−582	68	1
H82	−2816	−3778	246	76	1
H83	−2074	−3540	1326	86	1
H84	−570	−2680	1633	75	1
H86	1047	−3415	98	68	1
H87	1452	−4785	10	72	1
H88	2401	−5247	917	72	1
H89	3047	−4284	1848	66	1
H90	2602	−2917	1945	65	1
H91	5187	5654	2367	63	0.70
H92	5637	7050	−899	96	0.70

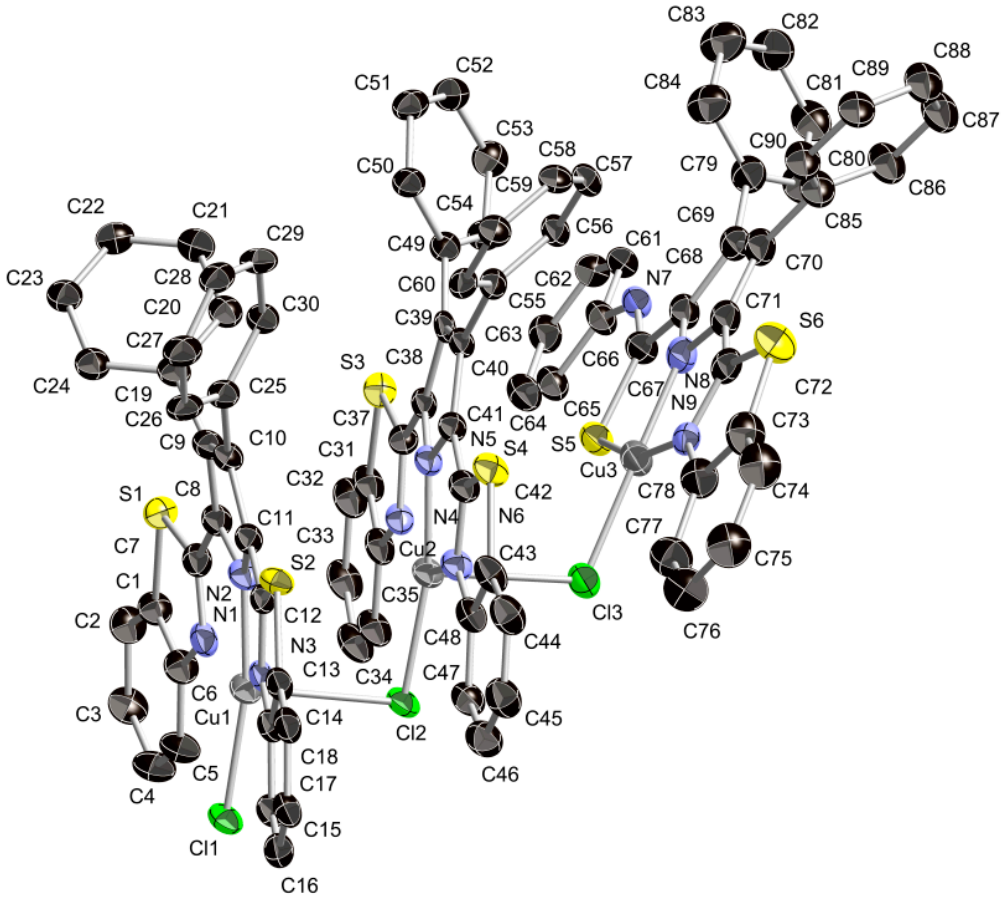
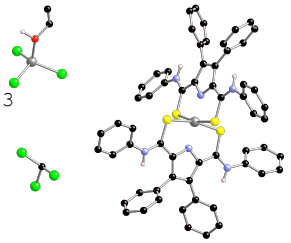


Figure S7. Trimer **866**. Thermal ellipsoids drawn at the 35% probability level, solvent and hydrogen atom s omitted for clarity.

Table S32. Complex **9**: Crystal data and structure refinement details.



Empirical formula	$C_{63}H_{51}Cl_6Co_2N_6OS_4$ $C_{60}H_{44}CoN_6S_4$, $C_2H_6Cl_3CoO$, $CHCl_3$
Formula weight	1366.90
Temperature	120(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 17.8652(3) Å b = 20.1328(3) Å β = 108.8240(10)° c = 18.0402(3) Å
Volume	6141.58(17) Å^3
Z	4
Density (calculated)	1.478 Mg / m^3
Absorption coefficient	0.985 mm-**1**
$F(000)$	2796
Crystal	Plate; Pale Brown
Crystal size	0.20 × 0.07 × 0.01 mm^3
θ range for data collection	2.97 – 25.03°
Index ranges	$-19 \le h \le 21$, $-23 \le k \le 22$, $-21 \le l \le 21$
Reflections collected	64380
Independent reflections	10813 [R_{int} = 0.1061]
Completeness to θ = 25.03°	99.8 %
Absorption correction	Semi–empirical from equivalents
Max. and min. transmission	0.9902 and 0.8274
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10813 / 1 / 744
Goodness-of-fit on F^2	1.133
Final R indices [$F^2 > 2\sigma(F^2)$]	$R1$ = 0.0776, $wR2$ = 0.1364
R indices (all data)	$R1$ = 0.1155, $wR2$ = 0.1528
Largest diff. peak and hole	1.037 and –0.601 e Å^{-3}

Diffractometer: *Nonius KappaCCD* area detector (ϕ scans and ω scans to fill *asymmetric unit*). **Cell determination:** DirAx (Duisenberg, A.J.M.(1992). J. Appl. Cryst. 25, 92-96.) **Data collection:** Collect (Collect: Data collection software, R. Hooft, Nonius B.V., 1998). **Data reduction and cell refinement**: *Denzo* (Z. Otwinowski & W. Minor, *Methods in Enzymology* (1997) Vol. **276**: *Macromolecular Crystallography*, part A, pp. 307–326; C. W. Carter, Jr. & R. M. Sweet, Eds., Academic Press). **Absorption correction**: Sheldrick, G. M. SADABS - Bruker Nonius area detector scaling and absorption correction - V2.10 **Structure solution**: *SHELXS97* (G. M. Sheldrick, Acta Cryst. (1990) A**46** 467–473). **Structure refinement**: *SHELXL97* (G. M. Sheldrick (1997), University of Göttingen, Germany). **Graphics:** Cameron - A Molecular Graphics Package. (D. M. Watkin, L. Pearce and C. K. Prout, Chemical Crystallography Laboratory, University of Oxford, 1993).

Special details: All hydrogen atoms were placed in idealised positions and refined using a riding model, except the OH which was refined using a distance restraint.

Table S33. Complex **9**: Atomic coordinates [× 10^4], equivalent isotropic displacement parameters [Å² × 10^3] and site occupancy factors. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
Co1	2488(1)	5172(1)	6454(1)	18(1)	1
S1	3010(1)	4788(1)	7708(1)	22(1)	1
S2	2243(1)	5625(1)	5220(1)	19(1)	1
N1	4583(3)	4765(2)	8474(3)	22(1)	1
N2	3539(3)	5390(2)	6580(3)	18(1)	1
N3	3419(3)	6118(2)	4742(3)	23(1)	1
C1	3999(4)	4495(4)	9508(4)	32(2)	1
C2	4072(4)	4165(4)	10202(4)	39(2)	1
C3	4727(4)	3787(3)	10566(4)	37(2)	1
C4	5327(5)	3725(4)	10239(4)	41(2)	1
C5	5254(4)	4046(4)	9546(4)	36(2)	1
C6	4585(4)	4421(3)	9174(4)	24(1)	1
C7	3985(3)	4934(3)	7846(3)	21(1)	1
C8	4175(3)	5252(3)	7223(3)	20(1)	1
C9	4868(3)	5453(3)	7064(3)	20(1)	1
C10	4634(3)	5727(3)	6308(3)	18(1)	1
C11	3794(3)	5674(3)	6026(3)	18(1)	1
C12	3192(3)	5828(3)	5296(3)	18(1)	1
C13	2984(3)	6330(3)	3966(3)	20(1)	1
C14	3214(3)	6932(3)	3732(4)	27(2)	1
C15	2854(4)	7146(3)	2966(4)	31(2)	1
C16	2268(3)	6772(3)	2457(4)	26(1)	1
C17	2048(4)	6172(3)	2692(4)	29(2)	1
C18	2405(3)	5943(3)	3456(4)	23(1)	1
C19	5708(3)	5455(3)	7599(3)	20(1)	1
C20	6125(3)	4875(3)	7872(4)	27(1)	1
C21	6909(4)	4895(4)	8344(4)	32(2)	1
C22	7289(4)	5492(4)	8543(4)	31(2)	1
C23	6883(3)	6077(3)	8274(4)	26(1)	1
C24	6103(3)	6063(3)	7813(4)	27(1)	1
C25	5164(3)	5985(3)	5891(3)	19(1)	1
C26	5688(3)	5556(3)	5706(4)	24(1)	1
C27	6179(4)	5795(3)	5310(4)	30(2)	1
C28	6157(4)	6462(3)	5107(4)	30(2)	1
C29	5640(4)	6881(3)	5276(4)	30(2)	1
C30	5147(3)	6645(3)	5683(4)	24(1)	1
S3	2560(1)	4133(1)	5966(1)	20(1)	1
S4	2123(1)	6153(1)	6919(1)	21(1)	1
N4	1345(3)	3279(2)	5554(3)	23(1)	1
N5	1455(3)	4916(2)	6361(3)	18(1)	1
N6	687(3)	6295(2)	7119(3)	21(1)	1
C31	2449(4)	2518(3)	5705(4)	28(2)	1

C32	2808(4)	2039(3)	5372(4)	38(2)	1
C33	2479(4)	1846(3)	4615(4)	38(2)	1
C34	1772(4)	2123(3)	4164(4)	35(2)	1
C35	1396(4)	2592(3)	4479(4)	31(2)	1
C36	1754(3)	2786(3)	5251(4)	22(1)	1
C37	1623(3)	3871(3)	5849(3)	18(1)	1
C38	1111(3)	4322(3)	6072(3)	17(1)	1
C39	341(3)	4302(3)	6139(3)	17(1)	1
C40	231(3)	4901(3)	6470(3)	19(1)	1
C41	931(3)	5272(3)	6594(3)	18(1)	1
C42	1205(3)	5926(3)	6889(3)	21(1)	1
C43	703(3)	6963(3)	7383(3)	21(1)	1
C44	191(4)	7109(3)	7800(4)	29(2)	1
C45	127(4)	7749(3)	8038(4)	36(2)	1
C46	574(4)	8256(3)	7853(4)	34(2)	1
C47	1076(4)	8105(3)	7444(4)	30(2)	1
C48	1153(3)	7461(3)	7207(4)	24(1)	1
C49	–231(3)	3740(3)	5905(3)	18(1)	1
C50	–475(3)	3476(3)	5157(3)	23(1)	1
C51	–992(3)	2938(3)	4972(4)	29(2)	1
C52	–1269(3)	2668(3)	5533(4)	29(2)	1
C53	–1041(4)	2932(3)	6279(4)	28(2)	1
C54	–520(3)	3465(3)	6469(4)	22(1)	1
C55	–473(3)	5161(3)	6660(3)	18(1)	1
C56	–1050(3)	5517(3)	6099(4)	23(1)	1
C57	–1651(3)	5820(3)	6299(4)	27(2)	1
C58	–1688(4)	5780(3)	7047(4)	31(2)	1
C59	–1123(4)	5417(3)	7598(4)	32(2)	1
C60	–521(3)	5105(3)	7410(3)	23(1)	1
Co2	–75(1)	6139(1)	473(1)	30(1)	1
Cl1	174(1)	6806(1)	1518(1)	34(1)	1
Cl2	1080(1)	5637(1)	550(1)	40(1)	1
Cl3	–756(1)	6548(1)	–701(1)	38(1)	1
O1	–699(3)	5391(2)	730(3)	36(1)	1
C62	–1392(5)	5487(4)	963(6)	56(2)	1
C63	–1719(6)	4820(5)	1093(6)	78(3)	1
C61	3638(4)	7663(3)	7011(4)	33(2)	1
Cl4	3945(1)	6999(1)	7655(2)	66(1)	1
Cl5	3063(1)	8233(1)	7331(1)	51(1)	1
Cl6	3101(1)	7377(1)	6065(1)	43(1)	1

Table S34. Complex **9**: Bond lengths [Å] and angles [°].

Co1–N5	1.870(5)	C28–C29	1.356(9)
Co1–N2	1.871(4)	C29–C30	1.399(8)
Co1–S1	2.2863(17)	S3–C37	1.702(6)
Co1–S3	2.2885(17)	S4–C42	1.686(6)
Co1–S2	2.3134(17)	N4–C37	1.334(7)
Co1–S4	2.3208(17)	N4–C36	1.441(7)
S1–C7	1.704(6)	N5–C41	1.348(7)
S2–C12	1.705(6)	N5–C38	1.369(7)
N1–C7	1.327(7)	N6–C42	1.353(7)
N1–C6	1.438(7)	N6–C43	1.425(7)
N2–C11	1.350(7)	C31–C36	1.360(8)
N2–C8	1.365(7)	C31–C32	1.395(9)
N3–C12	1.329(7)	C32–C33	1.360(10)
N3–C13	1.429(7)	C33–C34	1.381(10)
C1–C6	1.376(8)	C34–C35	1.384(9)
C1–C2	1.385(9)	C35–C36	1.388(9)
C2–C3	1.373(10)	C37–C38	1.436(8)
C3–C4	1.386(10)	C38–C39	1.420(8)
C4–C5	1.376(9)	C39–C40	1.388(8)
C5–C6	1.390(9)	C39–C49	1.491(8)
C7–C8	1.427(8)	C40–C41	1.413(8)
C8–C9	1.416(8)	C40–C55	1.499(8)
C9–C10	1.404(8)	C41–C42	1.444(8)
C9–C19	1.500(8)	C43–C48	1.384(8)
C10–C11	1.426(8)	C43–C44	1.390(8)
C10–C25	1.480(8)	C44–C45	1.376(9)
C11–C12	1.440(8)	C45–C46	1.401(10)
C13–C18	1.382(8)	C46–C47	1.367(9)
C13–C14	1.389(8)	C47–C48	1.384(9)
C14–C15	1.392(9)	C49–C50	1.384(8)
C15–C16	1.373(9)	C49–C54	1.394(8)
C16–C17	1.378(9)	C50–C51	1.391(8)
C17–C18	1.397(9)	C51–C52	1.374(9)
C19–C20	1.386(8)	C52–C53	1.380(9)
C19–C24	1.404(9)	C53–C54	1.390(8)
C20–C21	1.385(9)	C55–C60	1.387(8)
C21–C22	1.370(10)	C55–C56	1.389(8)
C22–C23	1.387(9)	C56–C57	1.380(8)
C23–C24	1.374(8)	C57–C58	1.375(9)
C25–C30	1.379(8)	C58–C59	1.375(10)
C25–C26	1.391(8)	C59–C60	1.379(8)
C26–C27	1.383(8)	Co2–O1	2.016(5)
C27–C28	1.390(9)	Co2–Cl3	2.2310(19)

Co2–Cl1	2.2394(19)	C61–Cl4	1.741(7)
Co2–Cl2	2.2632(19)	C61–Cl5	1.756(7)
O1–C62	1.443(8)	C61–Cl6	1.764(7)
C62–C63	1.512(12)		

N5–Co1–N2	177.0(2)	C9–C10–C25	126.4(5)
N5–Co1–S1	94.08(15)	C11–C10–C25	128.1(5)
N2–Co1–S1	83.43(15)	N2–C11–C10	109.6(5)
N5–Co1–S3	83.72(15)	N2–C11–C12	116.0(5)
N2–Co1–S3	94.71(15)	C10–C11–C12	134.4(5)
S1–Co1–S3	90.90(6)	N3–C12–C11	117.6(5)
N5–Co1–S2	98.54(15)	N3–C12–S2	125.5(5)
N2–Co1–S2	83.95(15)	C11–C12–S2	116.8(4)
S1–Co1–S2	167.38(6)	C18–C13–C14	121.3(6)
S3–Co1–S2	90.42(6)	C18–C13–N3	122.5(5)
N5–Co1–S4	83.26(15)	C14–C13–N3	116.0(5)
N2–Co1–S4	98.31(15)	C13–C14–C15	119.1(6)
S1–Co1–S4	90.13(6)	C16–C15–C14	120.1(6)
S3–Co1–S4	166.98(6)	C15–C16–C17	120.4(6)
S2–Co1–S4	91.41(6)	C16–C17–C18	120.6(6)
C7–S1–Co1	99.1(2)	C13–C18–C17	118.4(6)
C12–S2–Co1	98.2(2)	C20–C19–C24	118.2(5)
C7–N1–C6	130.3(5)	C20–C19–C9	122.5(6)
C11–N2–C8	109.2(5)	C24–C19–C9	119.3(5)
C11–N2–Co1	125.0(4)	C21–C20–C19	120.9(6)
C8–N2–Co1	125.7(4)	C22–C21–C20	120.3(6)
C12–N3–C13	131.7(5)	C21–C22–C23	119.6(6)
C6–C1–C2	118.8(6)	C24–C23–C22	120.5(6)
C3–C2–C1	121.1(6)	C23–C24–C19	120.4(6)
C2–C3–C4	120.2(6)	C30–C25–C26	119.4(5)
C5–C4–C3	119.1(7)	C30–C25–C10	120.9(5)
C4–C5–C6	120.6(6)	C26–C25–C10	119.7(5)
C1–C6–C5	120.3(6)	C27–C26–C25	119.7(6)
C1–C6–N1	123.1(6)	C26–C27–C28	120.3(6)
C5–C6–N1	116.4(6)	C29–C28–C27	120.2(6)
N1–C7–C8	117.2(5)	C28–C29–C30	119.9(6)
N1–C7–S1	125.7(5)	C25–C30–C29	120.4(6)
C8–C7–S1	117.0(4)	C37–S3–Co1	98.9(2)
N2–C8–C9	108.1(5)	C42–S4–Co1	98.1(2)
N2–C8–C7	114.6(5)	C37–N4–C36	126.7(5)
C9–C8–C7	137.2(5)	C41–N5–C38	108.2(5)
C10–C9–C8	107.7(5)	C41–N5–Co1	126.1(4)
C10–C9–C19	123.1(5)	C38–N5–Co1	125.7(4)
C8–C9–C19	129.0(5)	C42–N6–C43	132.7(5)
C9–C10–C11	105.4(5)	C36–C31–C32	118.2(6)

C33–C32–C31	121.4(7)	C47–C46–C45	119.4(6)
C32–C33–C34	119.5(6)	C46–C47–C48	121.5(6)
C33–C34–C35	120.5(6)	C47–C48–C43	119.0(6)
C34–C35–C36	118.4(6)	C50–C49–C54	119.1(5)
C31–C36–C35	121.9(6)	C50–C49–C39	122.5(5)
C31–C36–N4	121.4(5)	C54–C49–C39	118.4(5)
C35–C36–N4	116.7(5)	C49–C50–C51	120.5(6)
N4–C37–C38	119.2(5)	C52–C51–C50	120.1(6)
N4–C37–S3	123.5(4)	C51–C52–C53	120.1(6)
C38–C37–S3	117.4(4)	C52–C53–C54	120.1(6)
N5–C38–C39	108.7(5)	C53–C54–C49	120.1(6)
N5–C38–C37	114.2(5)	C60–C55–C56	119.1(5)
C39–C38–C37	136.8(5)	C60–C55–C40	121.0(5)
C40–C39–C38	106.7(5)	C56–C55–C40	119.6(5)
C40–C39–C49	127.0(5)	C57–C56–C55	119.7(6)
C38–C39–C49	126.3(5)	C58–C57–C56	121.3(6)
C39–C40–C41	106.6(5)	C57–C58–C59	118.9(6)
C39–C40–C55	130.3(5)	C58–C59–C60	120.9(6)
C41–C40–C55	123.0(5)	C59–C60–C55	120.1(6)
N5–C41–C40	109.7(5)	O1–Co2–Cl3	108.77(15)
N5–C41–C42	114.4(5)	O1–Co2–Cl1	103.20(15)
C40–C41–C42	135.9(5)	Cl3–Co2–Cl1	118.54(7)
N6–C42–C41	115.4(5)	O1–Co2–Cl2	102.29(14)
N6–C42–S4	126.6(5)	Cl3–Co2–Cl2	115.49(8)
C41–C42–S4	118.0(4)	Cl1–Co2–Cl2	106.66(7)
C48–C43–C44	120.2(6)	C62–O1–Co2	123.8(4)
C48–C43–N6	123.9(5)	O1–C62–C63	109.6(7)
C44–C43–N6	115.7(5)	Cl4–C61–Cl5	112.0(4)
C45–C44–C43	120.1(6)	Cl4–C61–Cl6	110.5(4)
C44–C45–C46	119.7(6)	Cl5–C61–Cl6	109.8(4)

Table S35. Complex **9**: Anisotropic displacement parameters [Å^2× 10^3]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co1	15(1)	18(1)	23(1)	2(1)	9(1)	−1(1)
S1	18(1)	23(1)	27(1)	4(1)	10(1)	−1(1)
S2	16(1)	21(1)	22(1)	2(1)	8(1)	−1(1)
N1	18(2)	27(3)	25(3)	9(2)	12(2)	3(2)
N2	14(2)	19(3)	24(3)	0(2)	10(2)	0(2)
N3	16(2)	27(3)	23(3)	4(2)	4(2)	−4(2)
C1	20(3)	47(4)	35(4)	5(3)	18(3)	8(3)
C2	35(4)	59(5)	30(4)	4(4)	18(3)	−9(4)
C3	55(5)	35(4)	24(4)	1(3)	17(3)	−12(4)
C4	55(5)	37(4)	35(4)	9(3)	19(4)	22(4)
C5	31(4)	49(5)	29(4)	6(3)	12(3)	14(3)
C6	29(3)	18(3)	23(3)	2(3)	4(3)	0(3)
C7	18(3)	21(3)	26(3)	1(3)	9(3)	4(2)
C8	19(3)	15(3)	25(3)	0(3)	6(3)	2(2)
C9	16(3)	20(3)	29(3)	−2(3)	13(3)	0(2)
C10	18(3)	18(3)	20(3)	−2(2)	9(2)	1(2)
C11	12(3)	18(3)	27(3)	0(3)	8(2)	2(2)
C12	21(3)	11(3)	24(3)	1(2)	10(3)	0(2)
C13	17(3)	23(3)	20(3)	0(3)	9(3)	5(2)
C14	19(3)	31(4)	32(4)	7(3)	9(3)	−7(3)
C15	29(4)	27(4)	41(4)	11(3)	16(3)	0(3)
C16	19(3)	39(4)	24(3)	7(3)	10(3)	1(3)
C17	23(3)	37(4)	25(4)	−4(3)	7(3)	−1(3)
C18	20(3)	23(3)	29(4)	−2(3)	13(3)	−1(3)
C19	13(3)	32(3)	18(3)	2(3)	9(2)	8(3)
C20	22(3)	31(4)	30(4)	7(3)	10(3)	3(3)
C21	20(3)	43(4)	34(4)	13(3)	9(3)	8(3)
C22	14(3)	58(5)	21(3)	7(3)	5(3)	1(3)
C23	20(3)	34(4)	27(4)	−5(3)	11(3)	−10(3)
C24	17(3)	36(4)	29(4)	−5(3)	10(3)	−7(3)
C25	16(3)	26(3)	15(3)	0(2)	5(2)	−4(2)
C26	20(3)	22(3)	29(4)	0(3)	7(3)	1(3)
C27	23(3)	28(4)	48(4)	−3(3)	26(3)	1(3)
C28	25(3)	35(4)	37(4)	−1(3)	20(3)	−1(3)
C29	32(4)	21(3)	43(4)	7(3)	24(3)	1(3)
C30	23(3)	25(3)	30(4)	0(3)	17(3)	3(3)
S3	18(1)	19(1)	29(1)	0(1)	13(1)	0(1)
S4	19(1)	19(1)	27(1)	−3(1)	10(1)	−2(1)
N4	18(3)	22(3)	31(3)	−1(2)	13(2)	−2(2)
N5	19(2)	19(3)	18(3)	3(2)	11(2)	4(2)
N6	20(3)	19(3)	27(3)	−3(2)	11(2)	−2(2)
C31	24(3)	28(4)	33(4)	−8(3)	9(3)	3(3)

C32	26(4)	32(4)	53(5)	−6(3)	9(3)	2(3)
C33	48(4)	27(4)	53(5)	−11(3)	36(4)	0(3)
C34	48(4)	28(4)	29(4)	−6(3)	16(3)	−5(3)
C35	36(4)	28(4)	29(4)	−3(3)	11(3)	1(3)
C36	17(3)	25(3)	28(3)	−4(3)	13(3)	−1(3)
C37	16(3)	17(3)	20(3)	5(2)	4(2)	0(2)
C38	16(3)	15(3)	20(3)	2(2)	6(2)	−1(2)
C39	16(3)	19(3)	15(3)	−2(2)	3(2)	−4(2)
C40	20(3)	21(3)	15(3)	5(2)	6(2)	5(2)
C41	21(3)	16(3)	21(3)	−3(2)	13(2)	2(2)
C42	21(3)	21(3)	20(3)	2(3)	7(3)	6(3)
C43	19(3)	22(3)	21(3)	−8(3)	3(3)	−1(3)
C44	26(3)	24(4)	42(4)	−8(3)	17(3)	−4(3)
C45	33(4)	37(4)	47(5)	−10(3)	23(3)	−1(3)
C46	34(4)	20(3)	46(4)	−16(3)	11(3)	5(3)
C47	31(4)	17(3)	39(4)	−2(3)	8(3)	−8(3)
C48	22(3)	23(3)	27(3)	−3(3)	9(3)	−1(3)
C49	16(3)	18(3)	20(3)	−3(2)	6(2)	3(2)
C50	22(3)	26(3)	20(3)	−2(3)	8(3)	−2(3)
C51	21(3)	22(3)	36(4)	−11(3)	0(3)	4(3)
C52	16(3)	21(3)	47(4)	−4(3)	8(3)	−3(3)
C53	27(3)	24(3)	33(4)	7(3)	12(3)	0(3)
C54	21(3)	23(3)	27(3)	−6(3)	16(3)	0(3)
C55	13(3)	15(3)	27(3)	1(3)	9(2)	−3(2)
C56	16(3)	22(3)	30(4)	0(3)	9(3)	−5(3)
C57	15(3)	26(3)	39(4)	5(3)	6(3)	0(3)
C58	30(4)	20(3)	51(5)	−9(3)	24(3)	−1(3)
C59	32(4)	39(4)	33(4)	−8(3)	24(3)	−5(3)
C60	19(3)	31(3)	20(3)	0(3)	6(3)	−2(3)
Co2	27(1)	31(1)	31(1)	6(1)	10(1)	4(1)
Cl1	32(1)	42(1)	28(1)	2(1)	9(1)	6(1)
Cl2	27(1)	37(1)	54(1)	−3(1)	11(1)	2(1)
Cl3	49(1)	32(1)	28(1)	6(1)	5(1)	7(1)
O1	31(3)	34(3)	45(3)	0(2)	17(2)	−2(2)
C62	42(5)	51(5)	88(7)	−4(5)	40(5)	5(4)
C63	67(6)	105(9)	75(7)	5(6)	43(6)	−4(6)
C61	25(3)	30(4)	40(4)	−1(3)	7(3)	−2(3)
Cl4	41(1)	59(1)	77(2)	26(1)	−9(1)	−9(1)
Cl5	49(1)	58(1)	52(1)	−21(1)	26(1)	0(1)
Cl6	44(1)	44(1)	41(1)	−16(1)	14(1)	−7(1)

Table S36. Complex **9**: Hydrogen coordinates [× 10^4] and isotropic displacement parameters [Å^2 × 10^3].

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
H901	5053	4882	8461	26	1
H903	3931	6193	4877	27	1
H1	3552	4767	9268	38	1
H2	3663	4202	10429	47	1
H3	4769	3566	11043	44	1
H4	5781	3464	10489	49	1
H5	5665	4011	9320	43	1
H14	3612	7194	4089	32	1
H15	3013	7553	2794	37	1
H16	2013	6928	1939	32	1
H17	1651	5913	2331	34	1
H18	2253	5531	3620	28	1
H20	5868	4458	7735	33	1
H21	7184	4493	8529	38	1
H22	7828	5505	8864	38	1
H23	7147	6491	8410	32	1
H24	5828	6468	7639	32	1
H26	5710	5101	5852	29	1
H27	6531	5502	5176	36	1
H28	6506	6626	4848	36	1
H29	5612	7333	5119	35	1
H30	4798	6942	5818	29	1
H4A	862	3180	5544	27	1
H6	253	6079	7103	25	1
H31	2684	2653	6234	34	1
H32	3293	1845	5682	45	1
H33	2733	1521	4397	46	1
H34	1542	1991	3633	41	1
H35	904	2778	4174	37	1
H44	–114	6765	7921	35	1
H45	–220	7848	8327	44	1
H46	530	8700	8011	41	1
H47	1380	8449	7319	36	1
H48	1508	7363	6928	29	1
H50	–289	3664	4766	27	1
H51	–1152	2757	4459	35	1
H52	–1620	2300	5407	34	1
H53	–1240	2749	6663	33	1
H54	–359	3643	6984	26	1
H56	–1032	5551	5580	27	1
H57	–2046	6061	5913	33	1
H58	–2098	5999	7182	37	1

H59	−1147	5382	8114	38	1
H60	−140	4851	7794	28	1
H99	−850(40)	5020(20)	330(30)	36(19)	1
H62A	−1798	5735	551	67	1
H62B	−1252	5751	1452	67	1
H63A	−1938	4591	590	117	1
H63B	−2136	4886	1329	117	1
H63C	−1293	4551	1443	117	1
H61	4119	7900	6981	39	1

Table S37. Complex **9**: Hydrogen bonds [Å and °].

D–H···*A*	*d*(*D*–H)	*d*(H···*A*)	*d*(*D*···*A*)	∠(*D*H*A*)
O1–H99···Cl2^{i}	1.02(2)	2.00(2)	3.010(5)	172(6)

Symmetry transformations used to generate equivalent atoms:
(i) −x,−y+1,−z

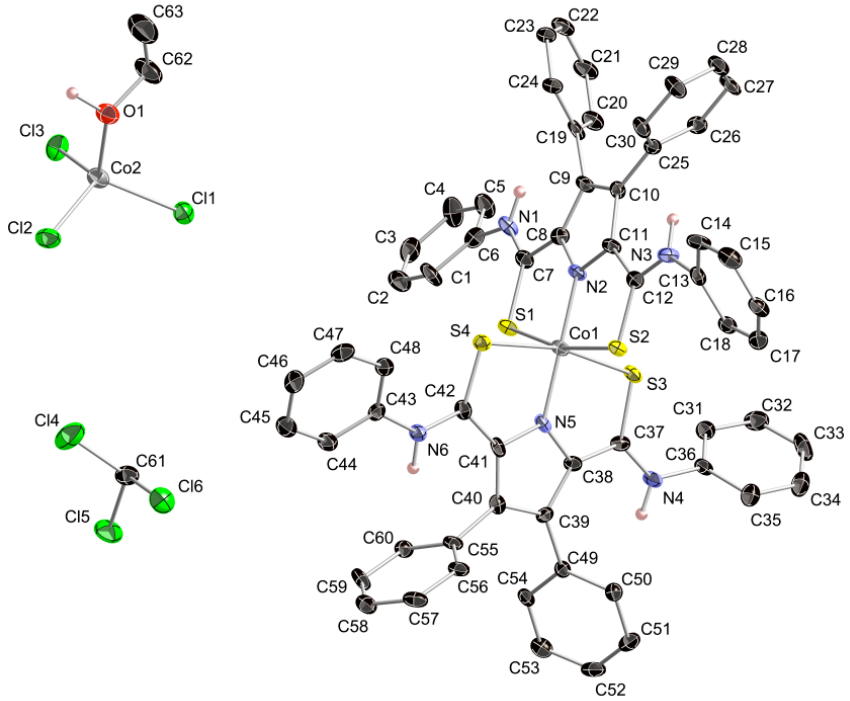


Figure S8. Complex **9**. Thermal ellipsoids drawn at the 35% probability level, selected hydrogens omitted for clarity.