Polymeric CuX coordination compounds assembled by acetylenic thioether ligands $RSCH_2C{\equiv}CCH_2R$ (R = C_6H_{11}, *t*-Bu): Effect of the RS-group, halide and stoichiometry on the network architecture and the luminescence properties

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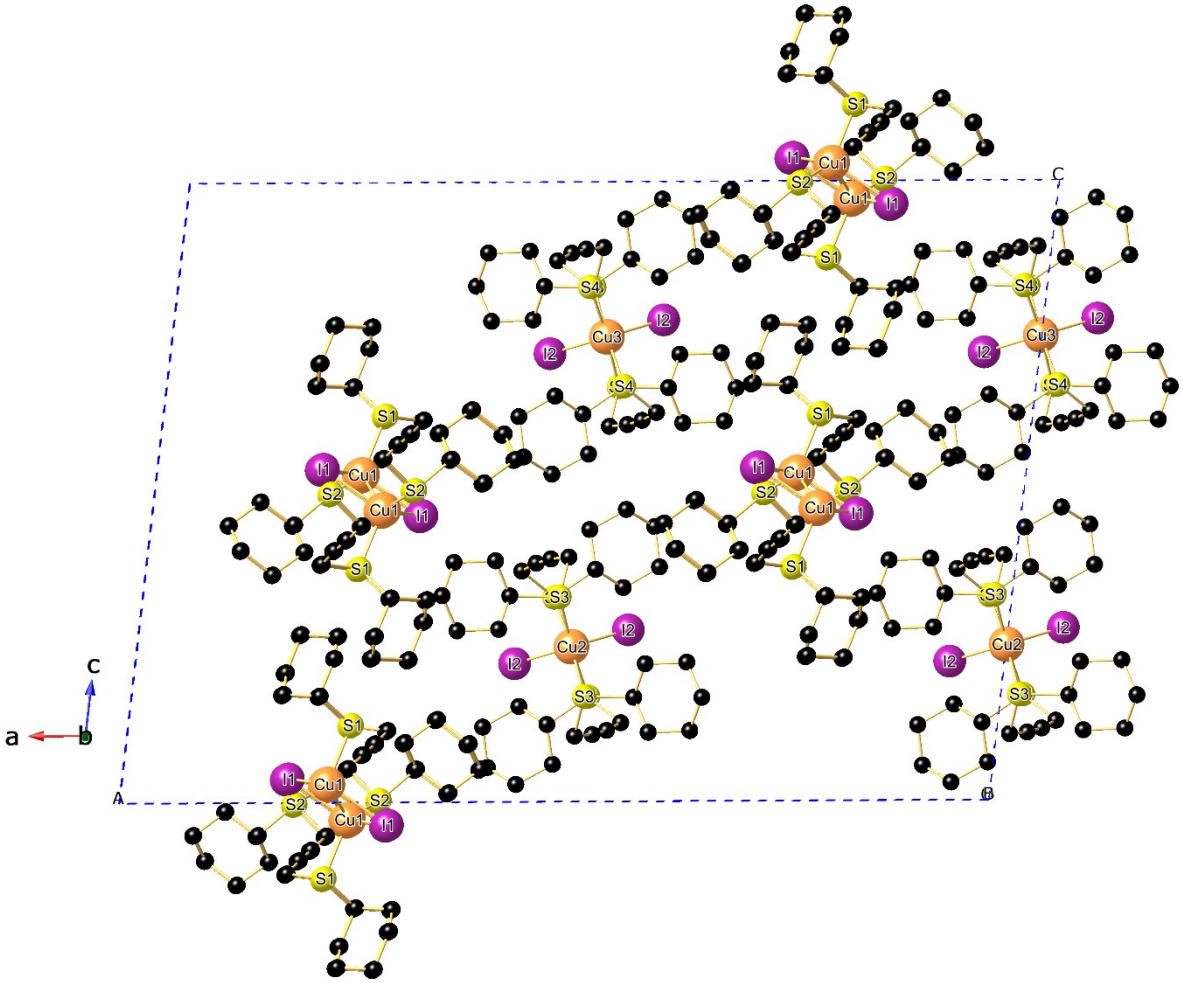


Figure S1. View of the [ac] plane down the *b* axis of $[\{Cu(\mu_2\text{-}I)_2Cu\}(\mu\text{-}\mathbf{L1})_2]_n$ (**CP2**) and co-crystallized discrete molecules of $[\{Cu(\mu_2\text{-}I)_2Cu\}(\mu\text{-}\mathbf{L1})_2]$ **D1**.

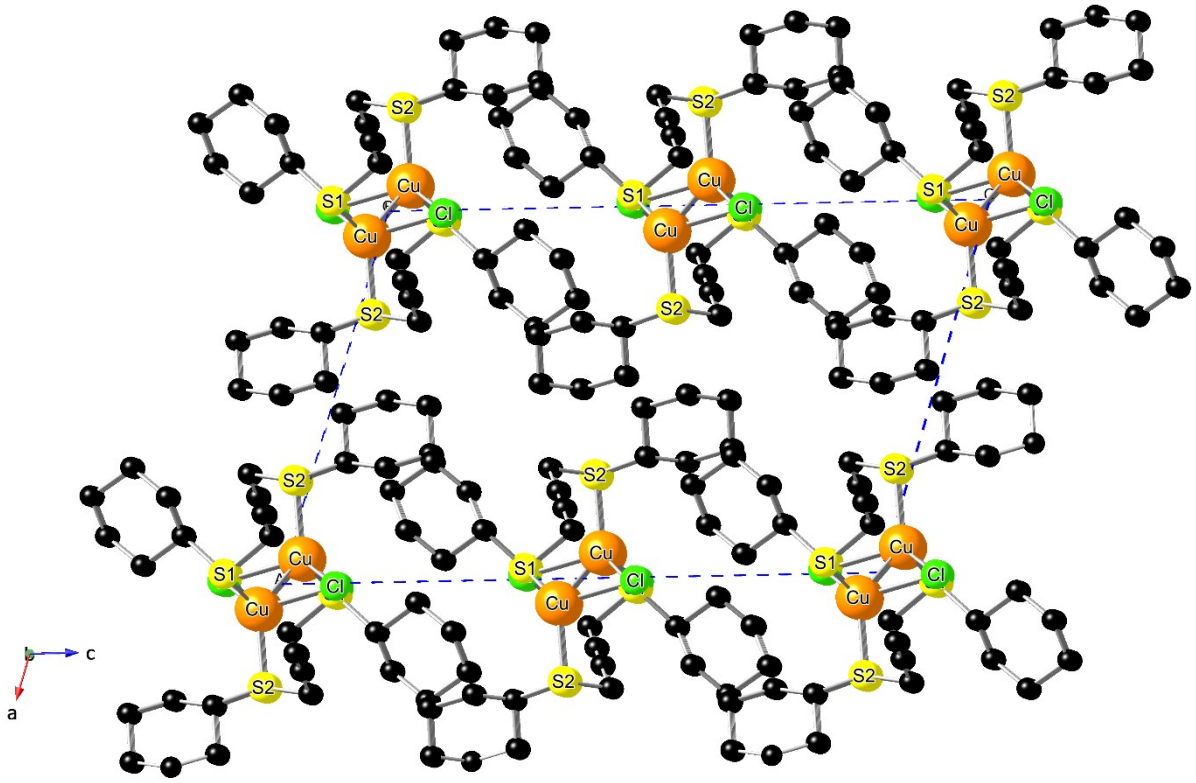


Figure S2. View of the [ac] plane down the *b* axis of $[\{Cu(\mu_2\text{-}Cl)_2Cu\}(\mu\text{-}\mathbf{L1})_2]_n$ (**CP4**).

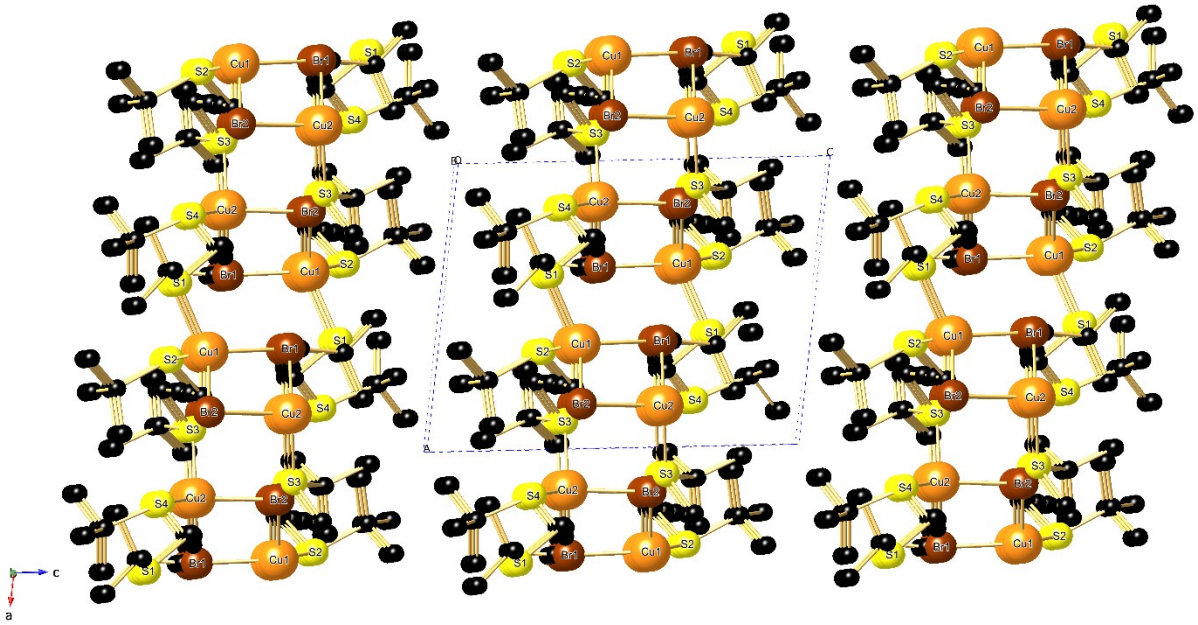


Figure S3. View of the [ac] plane down the *b* axis of $[\{Cu(\mu_2\text{-}Br)_2Cu\}(\mu\text{-}\mathbf{L2})_2]_n$ (**CP7**).

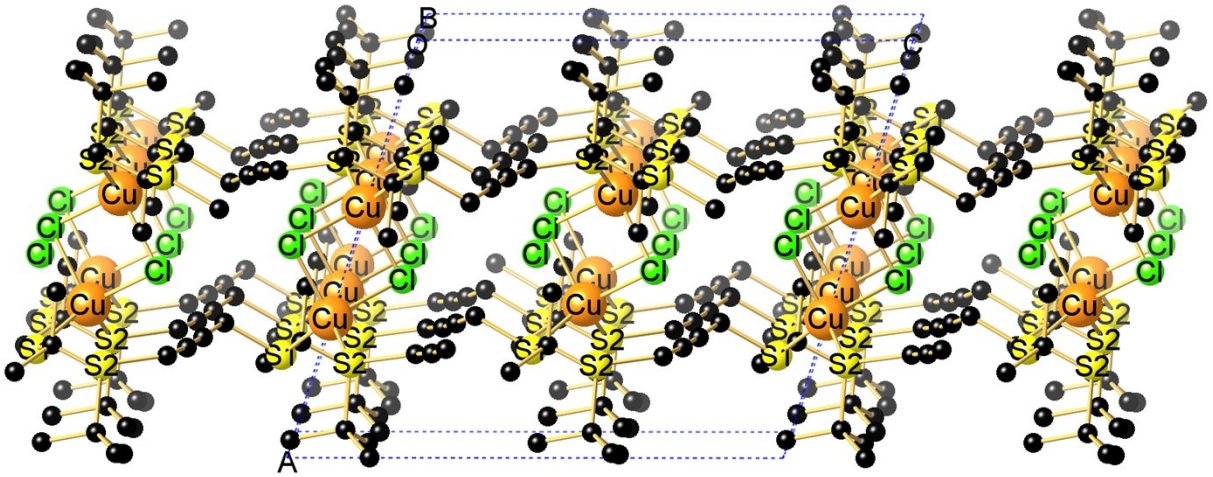


Figure S4. View of the [ac] plane down the *b* axis of $[\{Cu(\mu_2\text{-}Cl)_2Cu\}(\mu\text{-}\mathbf{L2})_2]_n$ (**CP8**).

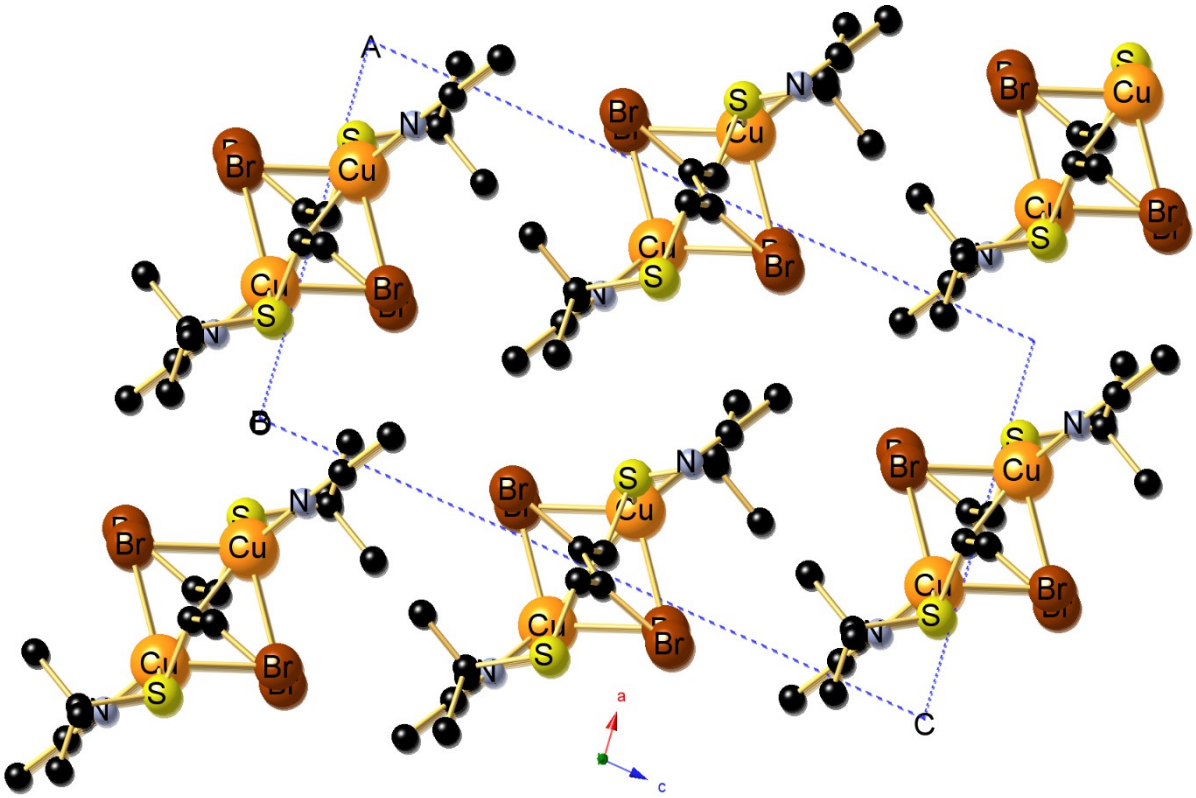


Figure S5. View of the [ac] plane down the *b* axis of $[\{Cu(\mu_2\text{-}Br)_2Cu\}(CH_3CN)(\mu\text{-}\mathbf{L3})_2]_n$ **CP9**.

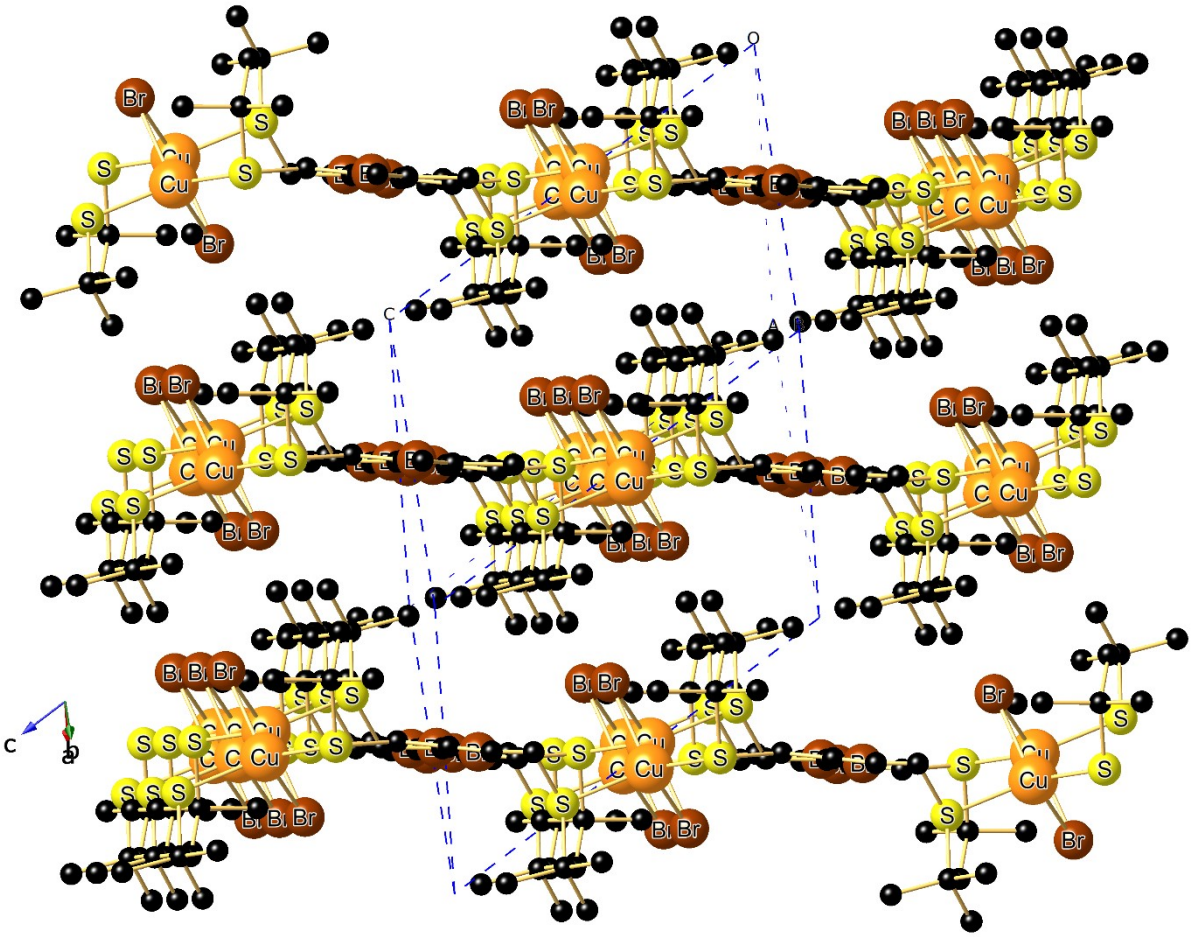


Figure S6. View of three layers of the 2D [{Cu(μ_2-Br)$_2$Cu}(μ-**L2**)(μ-**L3**)]$_n$ (**CP10**).

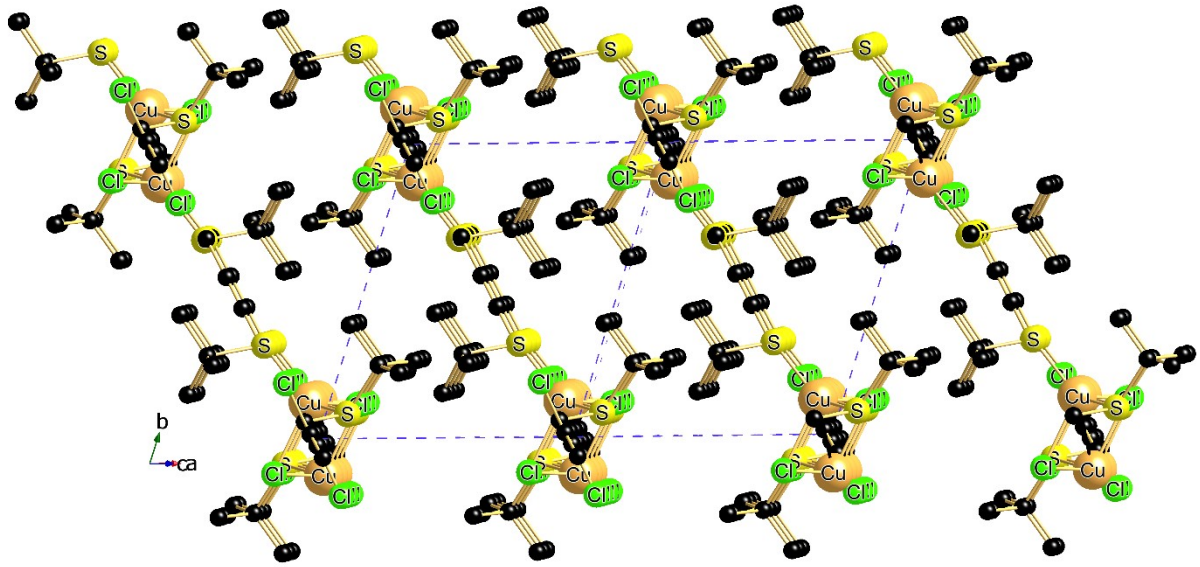


Figure S7. View of four layers of the 2D [{Cu(μ_2-Cl)$_2$Cu}(μ-**L2**)(μ-**L3**)]$_n$ (**CP11**).

Table S1 Comparison of the Cu···Cu distances within molecular $[S_2\{Cu(\mu_2\text{-}X)_2Cu\}S_2]$ compounds.

Compound name	Cu···Cu (Å)	Reference CSD	X
bis(μ_2-I)-bis(tris(((2-*t*-butyl-4-methylphenyl)thio)methyl)-amine-*S,S'*)dicopper	2.582	ENAWUM[1]	I
bis((μ_2-I)-(1,2,4,5-tetramethylmercaptobenzene))dicopper	2.616	PUGQIR[2]	I
bis((μ_2-I)(dimethyl-2-(4,5-bis(methylthio)-1,3-dithiol-2-ylidene)-1,3-dithiole-4,5-dicarboxylate))dicopper	2.647	MARFOB[3]	I
bis(μ_2-I)-bis(bis(tetrahydrothiophene)dicopper	2.675	FUHCEQ[4]	I
bis((μ_2-I)-bis(2,5-dioxa-8,11,14-trithia-1,6(1,2)dibenzenacyclo-pentadecaphane)dicopper	2.683	IGOBIQ[5]	I
bis(μ_2-I)-bis(7,8,16,17-tetrahydro-5H,10H-dibenzo[*e,m*][1,4,8,11]dioxadithiacyclotetradecine-*S,S'*)dicopper	2.688	HUWVOL[6]	I
bis((μ_2-I)-bis(3,14,25-trioxa-11,17-dithiatetracyclohentriconta 1(31),4,6,8,19,21,23,27,29-nonaene)dicopper	2.701	UJUWIG[7]	I
bis((μ_2-I)-(ethylenedithiobis(methylthio)tetrathiafulvalene)di-copper	2.734	NEZBOJ[8]	I
bis(μ_2-I)-bis(7,8,10,11,19,20,22,23-octahydro-5H,13H-dibenzo [*h,s*][1,4,7,14,11,17]tetraoxadithiacycloicosane)dicopper	2.846	POFZER[9]	I
bis(μ_2-I)-bis(1,4-dithia-7-oxacyclononane-1,4-diyl)dicopper	2.860	HALZOK[10]	I
bis((μ_2-I)-bis(methyltris(methylthiomethyl)silane-κ^2S,S')di-copper	2.863	TAKWIM[11]	I
bis(μ_2-I)-bis(μ_2-(1,1'-(but-2-yne-1,4-diylbis((sulfanediyl)methylene))dibenzene))dicopper	2.928	QUPXAC[12]	I
bis((μ_2-I)-(1,2-bis(cyclohexylthiomethyl)benzene))dicopper	2.956	BOBXUM[13]	I
bis((μ_2-Br)-bis(μ-(1,1'-(but-2-ene-1,4-diylbis(sulfanediyl))dibenzene))dicopper	2.740	KAKVIE[14]	Br
bis((μ_2-Br)-(1-oxa-4,7-dithiacyclononane)dicopper	2.852	NONWOC[15]	Br
bis(μ_2-Br)-bis(7,8,16,17-tetrahydro-5H,10H-dibenzo[*e,m*][1,4,8,11]dioxadithiacyclotetradecine-*S,S'*)dicopper	2.919	HUWVEB[6]	Br
bis((μ_2-Br)-tetrakis(phenylpropargyl sulfide)dicopper	3.006	VEQXUM[16]	Br
bis(μ_2-Br)-bis(μ_2-(1,1'-(but-2-yne-1,4-diylbis((sulfanediyl)methylene))dibenzene)dicopper	3.008	QUPXEG[12]	Br

Table S2 Crystal data, data collection, and structure refinement for **CP1.**

Internal Reference	**CP1_100K**	**CP1_150K**	**CP1_200K**	**CP1_250K**	**CP1_300K**
CCDC number	2326781	2326782	2356779	2326780	2326653
Empirical formula	$C_{64}H_{104}Cu_8I_8S_8$	$C_{64}H_{104}Cu_8I_8S_8$	$C_{64}H_{104}Cu_8I_8S_8$	$C_{64}H_{104}Cu_8I_8S_8$	$C_{64}H_{104}Cu_8I_8S_8$
Formula weight	2653.47	2653.47	2653.47	2653.47	2653.47
Temperature [K]	100.0(1)	150.0(1)	200.0(1)	250.0(1)	300.0(1)
Crystal system	triclinic	triclinic	triclinic	triclinic	triclinic
Space group (number)	$P\bar{1}$ (2)	$P\bar{1}$ (2)	$P\bar{1}$ (2)	$P\bar{1}$ (2)	$P\bar{1}$ (2)
a [Å]	11.7692(4)	11.7999(4)	11.8439(4)	11.8961(4)	11.9606(16)
b [Å]	18.6908(5)	18.7275(5)	18.8172(5)	18.9380(7)	19.095(3)
c [Å]	20.6753(6)	20.7647(6)	20.8187(6)	20.9008(7)	21.026(3)
α [°]	97.2090(10)	97.4108(10)	97.3254(10)	97.0884(14)	96.658(4)
β [°]	104.8990(10)	104.6354(10)	104.5536(10)	104.7460(13)	105.219(4)
γ [°]	103.0370(10)	103.1049(10)	103.6389(10)	104.3167(13)	105.342(4)
Volume [Å^3]	4199.8(2)	4238.8(2)	4277.4(2)	4324.1(3)	4378.9(10)
Z	2	2	2	2	2
ρ_{calc} [gcm^{-3}]	2.098	2.079	2.060	2.038	2.012
μ [mm^{-1}]	5.159	5.112	5.066	5.011	4.948
F(000)	2544	2544	2544	2544	2544
Crystal size [mm^3]	0.084×0.133×0.172	0.084×0.133×0.172	0.084×0.133×0.172	0.084×0.133×0.172	0.084×0.143×0.168
Crystal colour	clear light colourless	clear light colourless	clear light colourless	clear light colourless	clear light colourless
Crystal shape	block	block	block	block	block
Radiation	Mo K_{α} (λ=0.71073 Å)	Mo K_{α} (λ=0.71073 Å)	Mo K_{α} (λ=0.71073 Å)	Mo K_{α} (λ=0.71073 Å)	Mo K_{α} (λ=0.71073 Å)
2θ range [°]	4.33 to 55.00 (0.77 Å)	4.31 to 55.00 (0.77 Å)	4.30 to 55.00 (0.77 Å)	4.28 to 55.00 (0.77 Å)	2.05 to 50.00 (0.84 Å)
Index ranges	−15 ≤ h ≤ 15 −24 ≤ k ≤ 24 −26 ≤ l ≤ 26	−15 ≤ h ≤ 15 −24 ≤ k ≤ 24 −26 ≤ l ≤ 26	−15 ≤ h ≤ 15 −24 ≤ k ≤ 24 −27 ≤ l ≤ 27	−15 ≤ h ≤ 15 −24 ≤ k ≤ 24 −27 ≤ l ≤ 27	−14 ≤ h ≤ 14 −22 ≤ k ≤ 22 −24 ≤ l ≤ 24
Reflections collected	240995	509188	386877	260876	100554
Independent reflections	19283 R_{int} = 0.0305 R_{sigma} = 0.0131	19468 R_{int} = 0.0282 R_{sigma} = 0.0090	19652 R_{int} = 0.0300 R_{sigma} = 0.0110	19874 R_{int} = 0.0369 R_{sigma} = 0.0172	15416 R_{int} = 0.0941 R_{sigma} = 0.0442
Completeness to θ = 25.242°	99.9 %	99.9 %	99.9 %	99.9 %	99.9 %
Data / Restraints / Parameters	19283 / 736 / 914	19468 / 736 / 914	19652 / 737 / 914	19874 / 734 / 914	15416 / 675 / 910
Goodness-of-fit on F^2	1.025	1.086	1.080	1.067	1.040
Final R indexes [I≥2σ(I)]	R_1 = 0.0288 wR_2 = 0.0571	R_1 = 0.0289 wR_2 = 0.0568	R_1 = 0.0309 wR_2 = 0.0670	R_1 = 0.0397 wR_2 = 0.0899	R_1 = 0.0573 wR_2 = 0.1493
Final R indexes [all data]	R_1 = 0.0335 wR_2 = 0.0601	R_1 = 0.0334 wR_2 = 0.0604	R_1 = 0.0376 wR_2 = 0.0725	R_1 = 0.0557 wR_2 = 0.1021	R_1 = 0.0825 wR_2 = 0.1673
Largest peak/hole [eÅ^{-3}]	2.51/−2.88	1.80/−1.81	1.43/−1.23	1.61/−0.72	2.06/−0.63

Table S3 Crystal data, data collection, and structure refinement for **CP2-D1** at variable temperature.

Internal Reference	**CP2D1_100K**	**CP2D1_140K**	**CP2D1_180K**	**CP2D1_220K**	**CP2D1_260K**	**CP2D1_300k**
CCDC number	2326783	2326502	2326503	2326504	2326505	2326506
Empirical formula	$C_{16}H_{26}CuIS_2$	$C_{16}H_{26}CuIS_2$	$C_{16}H_{26}CuIS_2$	$C_{16}H_{26}CuIS_2$	$C_{16}H_{26}CuIS_2$	$C_{16}H_{26}CuIS_2$
Formula weight	472.93	472.93	472.93	472.93	472.93	472.93
Temperature [K]	100.0(1)	140.0(1)	180.0(1)	220.0(1)	260.0(1)	300.0(1)
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
Space group (number)	$C2/c$ (15)	$C2/c$ (15)	$C2/c$ (15)	$C2/c$ (15)	$C2/c$ (15)	$C2/c$ (15)
a [Å]	31.839(2)	31.853(2)	31.8836(12)	31.903(2)	31.932(2)	31.9681(8)
b [Å]	10.1369(7)	10.1612(6)	10.1900(4)	10.2246(7)	10.2558(7)	10.2932(2)
c [Å]	22.8562(15)	22.9100(14)	22.9758(9)	23.0547(15)	23.1217(16)	23.1990(7)
α [°]	90	90	90	90	90	90
β [°]	96.789(2)	96.804(2)	96.8390(10)	96.911(2)	96.952(3)	97.0950(10)
γ [°]	90	90	90	90	90	90
Volume [Å^3]	7325.0(9)	7363.0(8)	7411.6(5)	7465.8(9)	7516.5(9)	7575.3(3)
Z	16	16	16	16	16	16
ρ_{calc} [gcm^{-3}]	1.715	1.707	1.695	1.683	1.672	1.659
μ [mm^{-1}]	3.096	3.080	3.060	3.038	3.017	2.994
F(000)	3776	3776	3776	3776	3776	3776
Crystal size [mm^3]	0.247×0.279×0.481	0.247×0.279×0.481	0.247×0.279×0.481	0.247×0.279×0.481	0.247×0.279×0.481	0.247×0.279×0.481
Crystal colour	clear light yellow	clear light yellow	clear light yellow	clear light yellow	clear light yellow	clear light yellow
Crystal shape	block	block	block	block	block	block
Radiation	Mo K_{α} (λ=0.71073 Å)	Mo K_{α} (λ=0.71073 Å)	Mo K_{α} (λ=0.71073 Å)	Mo K_{α} (λ=0.71073 Å)	Mo K_{α} (λ=0.71073 Å)	Mo K_{α} (λ=0.71073 Å)
2θ range [°]	5.64 to 55.00 (0.77 Å)	5.43 to 54.99 (0.77 Å)	5.41 to 55.00 (0.77 Å)	5.39 to 55.00 (0.77 Å)	5.67 to 55.00 (0.77 Å)	5.52 to 55.00 (0.77 Å)
Index ranges	−41 ≤ h ≤ 41 −13 ≤ k ≤ 13 −29 ≤ l ≤ 29	−41 ≤ h ≤ 41 −13 ≤ k ≤ 13 −29 ≤ l ≤ 29	−41 ≤ h ≤ 41 −13 ≤ k ≤ 13 −29 ≤ l ≤ 29	−41 ≤ h ≤ 41 −13 ≤ k ≤ 13 −29 ≤ l ≤ 29	−41 ≤ h ≤ 41 −13 ≤ k ≤ 13 −30 ≤ l ≤ 30	−41 ≤ h ≤ 41 −13 ≤ k ≤ 13 −30 ≤ l ≤ 30
Reflections collected	96786	85404	85592	85128	67034	72825
Independent reflections	8412 R_{int} = 0.0284 R_{sigma} = 0.0127	8436 R_{int} = 0.0248 R_{sigma} = 0.0117	8493 R_{int} = 0.0236 R_{sigma} = 0.0122	8547 R_{int} = 0.0225 R_{sigma} = 0.0128	8597 R_{int} = 0.0242 R_{sigma} = 0.0151	8681 R_{int} = 0.0514 R_{sigma} = 0.0252
Completeness to θ = 25.242°	99.8 %	99.7 %	99.7 %	99.6 %	99.6 %	99.7 %
Data / Restraints / Parameters	8412 / 0 / 362	8436 / 0 / 362	8493 / 0 / 362	8547 / 0 / 363	8597 / 0 / 362	8681 / 12 / 362
Goodness-of-fit on F^2	1.169	1.147	1.157	1.163	1.124	1.041
Final R indexes [I≥2σ(I)]	R_1 = 0.0161 wR_2 = 0.0388	R_1 = 0.0162 wR_2 = 0.0390	R_1 = 0.0165 wR_2 = 0.0401	R_1 = 0.0165 wR_2 = 0.0411	R_1 = 0.0177 wR_2 = 0.0432	R_1 = 0.0198 wR_2 = 0.0511
Final R indexes [all data]	R_1 = 0.0163 wR_2 = 0.0389	R_1 = 0.0165 wR_2 = 0.0391	R_1 = 0.0169 wR_2 = 0.0403	R_1 = 0.0171 wR_2 = 0.0414	R_1 = 0.0189 wR_2 = 0.0438	R_1 = 0.0254 wR_2 = 0.0527
Largest peak/hole [eÅ^{-3}]	0.88/−0.52	0.64/−0.47	0.60/−0.50	0.67/−0.42	0.59/−0.49	0.64/−0.32

Table S4 Crystal data, data collection, and structure refinement for **CP3D2, CP4, CP5, CP6** and **CP7.**

Internal Reference	**CP3D2**	**CP4**	**CP5**	**CP6**	**CP7**
CCDC number	2326258	2326259	2326261	2326262	2326263
Empirical formula	$C_{16}H_{26}BrCuS_2$	$C_{16}H_{26}ClCuS_2$	$C_{24}H_{44}Cu_4I_4S_4$	$C_{12}H_{22}CuIS_2$	$C_{24}H_{44}Br_2Cu_2S_4$
Formula weight	425.94	381.48	1222.59	420.85	747.73
Temperature [K]	150.0(1)	115.0(1)	100.0(1)	100.0(1)	115.00
Crystal system	monoclinic	monoclinic	orthorhombic	monoclinic	monoclinic
Space group (number)	$C2/c$ (15)	$P2_1/c$ (14)	$P2_12_12_1$ (19)	$P2_1/c$ (14)	$P2_1$ (4)
a [Å]	31.366(2)	11.3631(5)	9.9428(8)	11.4251(3)	8.7637(14)
b [Å]	10.0042(7)	9.2959(4)	18.9973(17)	16.2605(4)	15.977(2)
c [Å]	22.8146(17)	17.5929(7)	19.2437(15)	8.8793(2)	11.262(2)
α [°]	90	90	90	90	90
β [°]	96.959(8)	107.3267(13)	90	99.6380(10)	97.425(5)
γ [°]	90	90	90	90	90
Volume [Å^3]	7106.2(9)	1774.01(13)	3634.9(5)	1626.29(7)	1563.7(4)
Z	16	4	4	4	2
ρ_{calc} [gcm^{-3}]	1.592	1.428	2.234	1.719	1.588
μ [mm^{-1}]	3.703	1.606	5.950	3.474	4.194
F(000)	3488	800	2320	832	760
Crystal size [mm^3]	0.1×0.2×0.2	0.15×0.2×0.25	0.081×0.109×0.139	0.073×0.172×0.268	0.05×0.1×0.1
Crystal colour	clear light colourless	clear light colourless	clear light colourless	clear light colourless	clear light colourless
Crystal shape	block	prism	block	plate	needle
Radiation	MoK_α (λ=0.71073 Å)	Mo K_{α} (λ=0.71073 Å)	Mo K_{α} (λ=0.71073 Å)	Mo K_{α} (λ=0.71073 Å)	Mo K_{α} (λ=0.71073 Å)
2θ range [°]	4.28 to 50.00 (0.84 Å)	5.77 to 55.00 (0.77 Å)	4.29 to 55.00 (0.77 Å)	4.40 to 54.99 (0.77 Å)	4.69 to 55.06 (0.77 Å)
Index ranges	$-36 \le h \le 36$ $-11 \le k \le 11$ $-27 \le l \le 17$	$-14 \le h \le 14$ $-12 \le k \le 12$ $-16 \le l \le 22$	$-12 \le h \le 12$ $-24 \le k \le 24$ $-25 \le l \le 23$	$-14 \le h \le 14$ $-21 \le k \le 20$ $-11 \le l \le 11$	$-11 \le h \le 10$ $-20 \le k \le 19$ $-12 \le l \le 14$
Reflections collected	18548	33599	32078	25701	11046
Independent reflections	6118 R_{int} = 0.0301 R_{sigma} = 0.0556	4063 R_{int} = 0.0343 R_{sigma} = 0.0192	8319 R_{int} = 0.0437 R_{sigma} = 0.0395	3733 R_{int} = 0.0252 R_{sigma} = 0.0155	6598 R_{int} = 0.0465 R_{sigma} = 0.1257
Completeness to θ = 25(1)°	97.7 %	99.9 %	99.9 %	99.9 %	99.6 %
Data / Restraints / Parameters	6118 / 0 / 362	4063 / 0 / 181	8319 / 0 / 338	3733 / 0 / 151	6598 / 1 / 278
Goodness-of-fit on F^2	0.890	1.046	1.064	1.079	0.974
Final R indexes [$I \ge 2\sigma(I)$]	R_1 = 0.0301 wR_2 = 0.0636	R_1 = 0.0196 wR_2 = 0.0445	R_1 = 0.0296 wR_2 = 0.0720	R_1 = 0.0176 wR_2 = 0.0430	R_1 = 0.0538 wR_2 = 0.0609
Final R indexes [all data]	R_1 = 0.0483 wR_2 = 0.0653	R_1 = 0.0265 wR_2 = 0.0472	R_1 = 0.0314 wR_2 = 0.0732	R_1 = 0.0190 wR_2 = 0.0438	R_1 = 0.0964 wR_2 = 0.0694
Largest peak/hole [eÅ^{-3}]	1.22/−0.67	0.31/−0.23	2.08/−1.36	1.29/−0.39	0.75/−0.77
			-0.02(2)		0.437(14)

Table S5 Crystal data, data collection, and structure refinement for **CP8, CP9, CP10 and CP11.**

Internal Reference	**CP8**	**CP9**	**CP10**	**CP11**
CCDC number	2326264	2326265	2326266	2326267
Empirical formula	$C_{12}H_{22}ClCuS_2$	$C_8H_{14}Br_2CuNS$	$C_{12}H_{22}Br_2CuS_2$	$C_{12}H_{22}Cl_2CuS_2$
Formula weight	329.40	379.62	453.77	364.85
Temperature [K]	100.0(1)	100.0(1)	100.0(1)	115.0(1)
Crystal system	monoclinic	monoclinic	triclinic	triclinic
Space group (number)	$P2_1/c$ (14)	$P2_1/n$ (14)	$P\bar{1}$ (2)	$P\bar{1}$ (2)
a [Å]	12.0784(5)	8.1661(4)	9.1382(11)	8.7545(14)
b [Å]	9.6471(4)	10.2416(5)	9.9911(8)	10.0042(15)
c [Å]	13.6377(5)	15.1301(6)	11.2700(10)	11.2498(15)
α [°]	90	90	65.156(4)	64.220(6)
β [°]	107.3257(12)	98.034(2)	70.131(4)	70.764(6)
γ [°]	90	90	84.401(5)	82.779(7)
Volume [Å^3]	1516.98(11)	1252.97(10)	876.92(15)	837.5(2)
Z	4	4	2	2
ρ_{calc} [gcm^{-3}]	1.442	2.012	1.719	1.447
μ [mm^{-1}]	1.865	8.247	6.020	1.851
F(000)	688	736	450	378
Crystal size [mm^3]	0.16×0.18×0.32	0.192×0.334×0.436	0.138×0.263×0.508	0.1×0.15×0.2
Crystal colour	clear light colourless	clear light colourless	clear light colourless	clear light colourless
Crystal shape	prism	block	plate	prism
Radiation	Mo K_{α} (λ=0.71073 Å)	Mo K_{α} (λ=0.71073 Å)	Mo K_{α} (λ=0.71073 Å)	Mo K_{α} (λ=0.71073 Å)
2θ range [°]	5.79 to 55.04 (0.77 Å)	4.82 to 55.00 (0.77 Å)	4.22 to 55.00 (0.77 Å)	6.62 to 55.35 (0.77 Å)
Index ranges	−15 ≤ h ≤ 15 −12 ≤ k ≤ 12 −17 ≤ l ≤ 17	−9 ≤ h ≤ 10 −10 ≤ k ≤ 13 −19 ≤ l ≤ 19	−11 ≤ h ≤ 11 −12 ≤ k ≤ 12 −14 ≤ l ≤ 14	−11 ≤ h ≤ 11 −13 ≤ k ≤ 12 −14 ≤ l ≤ 14
Reflections collected	43880	10454	33300	27840
Independent reflections	3493 R_{int} = 0.0497 R_{sigma} = 0.0189	2860 R_{int} = 0.0354 R_{sigma} = 0.0369	4027 R_{int} = 0.0286 R_{sigma} = 0.0154	3875 R_{int} = 0.0413 R_{sigma} = 0.0261
Completeness to θ = 25(1)°	99.9 %	99.6 %	99.9 %	99.8 %
Data / Restraints / Parameters	3493 / 0 / 151	2860 / 0 / 122	4027 / 0 / 160	3875 / 0 / 160
Goodness-of-fit on F^2	1.077	1.062	1.048	1.063
Final R indexes [I≥2σ(I)]	R_1 = 0.0208 wR_2 = 0.0441	R_1 = 0.0258 wR_2 = 0.0554	R_1 = 0.0197 wR_2 = 0.0470	R_1 = 0.0256 wR_2 = 0.0638
Final R indexes [all data]	R_1 = 0.0290 wR_2 = 0.0470	R_1 = 0.0308 wR_2 = 0.0576	R_1 = 0.0216 wR_2 = 0.0479	R_1 = 0.0338 wR_2 = 0.0673
Largest peak/hole [eÅ^{-3}]	0.35/−0.25	0.54/−0.91	1.50/−0.80	0.43/−0.74

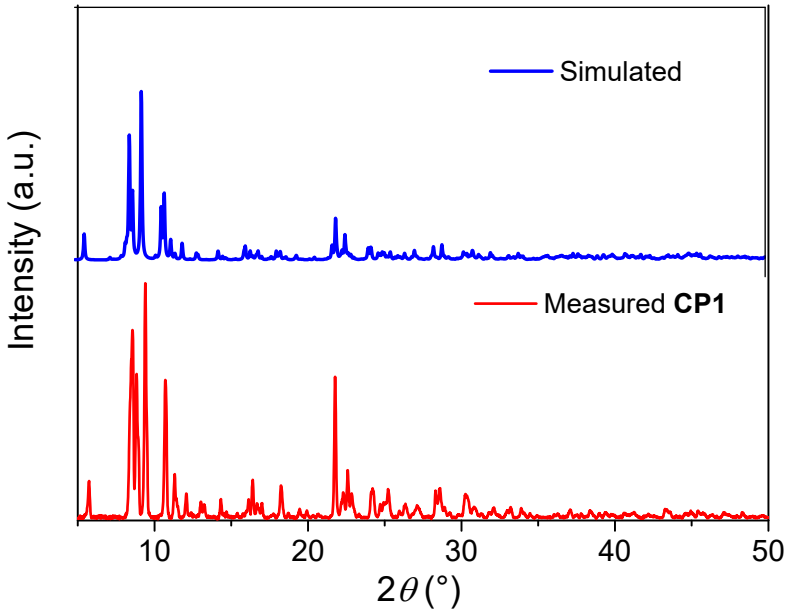


Figure S8: Experimental and simulated PXRD of **CP1**

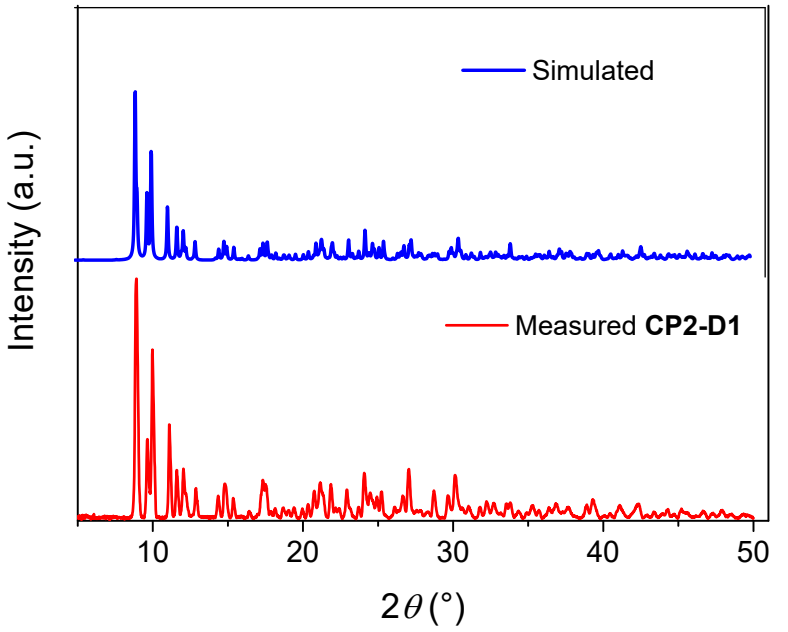


Figure S9: Experimental and simulated PXRD of **CP2-D1**

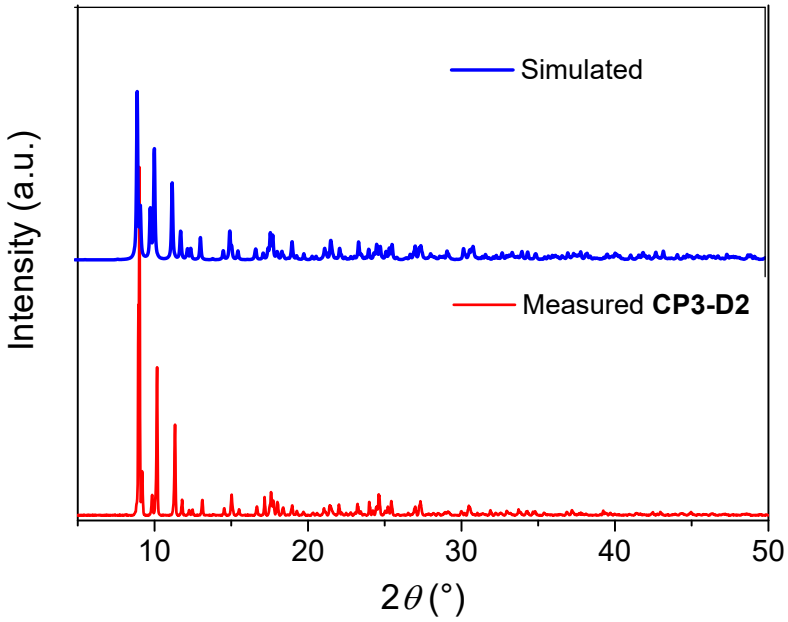


Figure S10: Experimental and simulated PXRD of **CP3-D2**

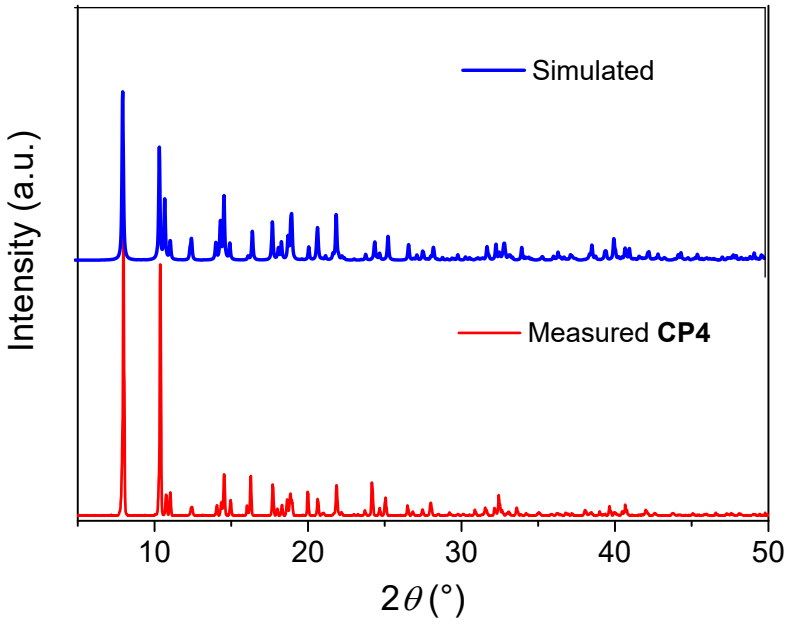


Figure S11: Experimental and simulated PXRD of **CP4**

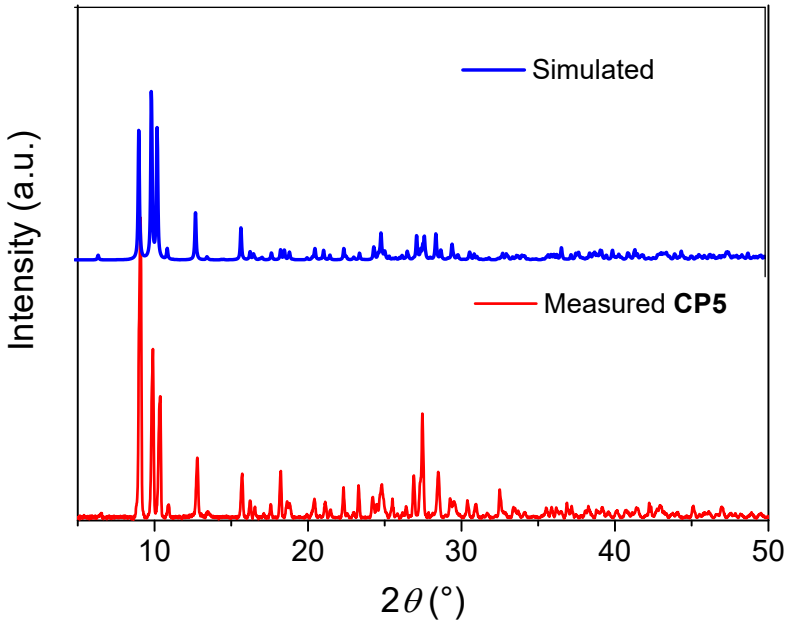


Figure S12: Experimental and simulated PXRD of **CP5**

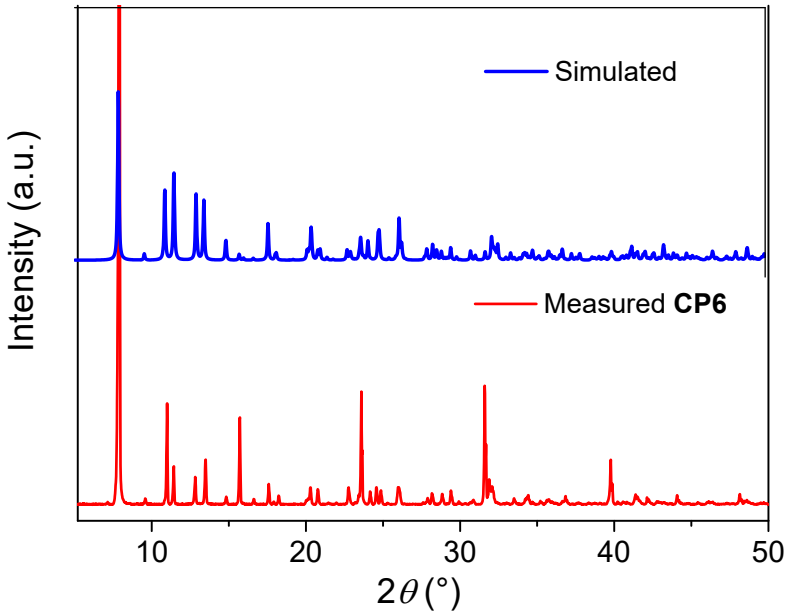


Figure S13: Experimental and simulated PXRD of **CP6**

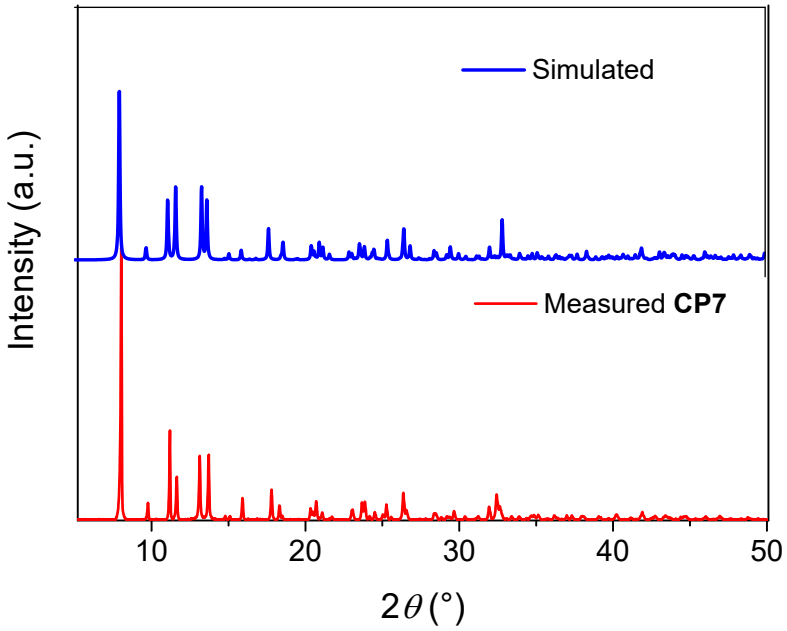


Figure S14: Experimental and simulated PXRD of **CP7**

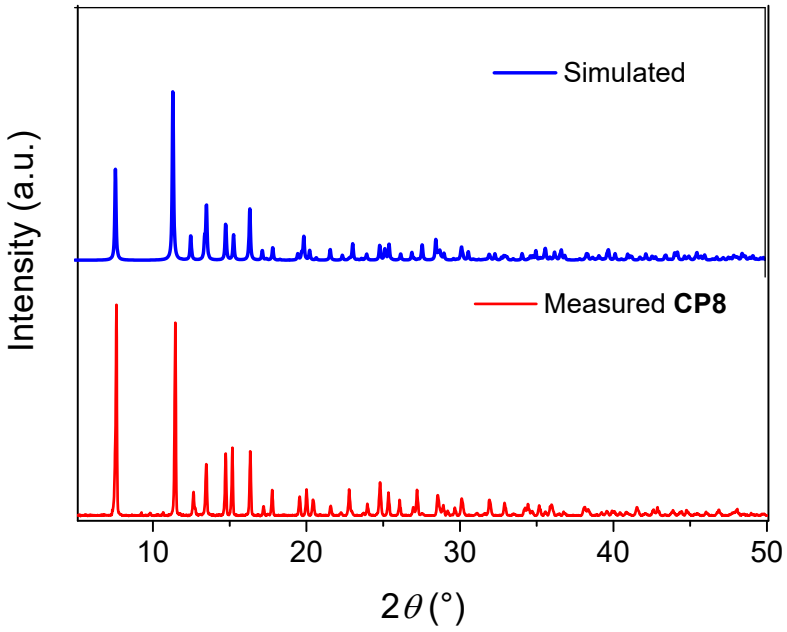


Figure S15: Experimental and simulated PXRD of **CP8**

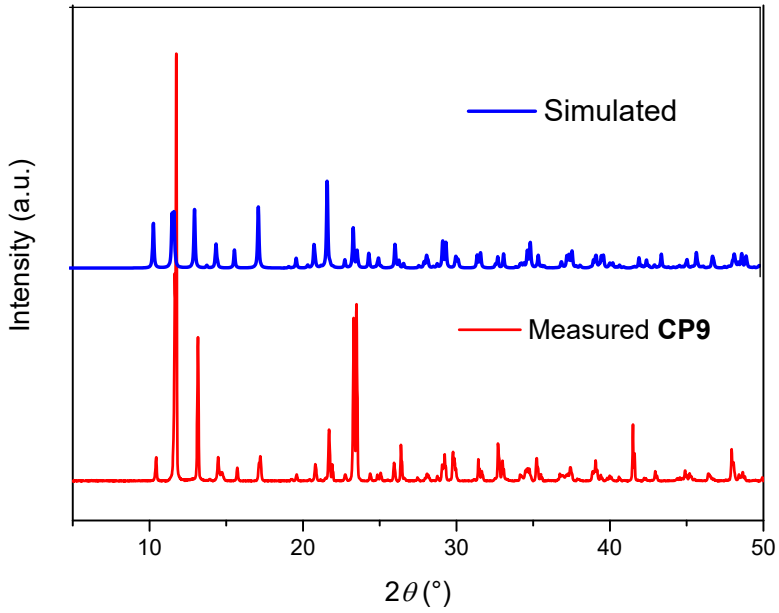


Figure S16: Experimental and simulated PXRD of **CP9**

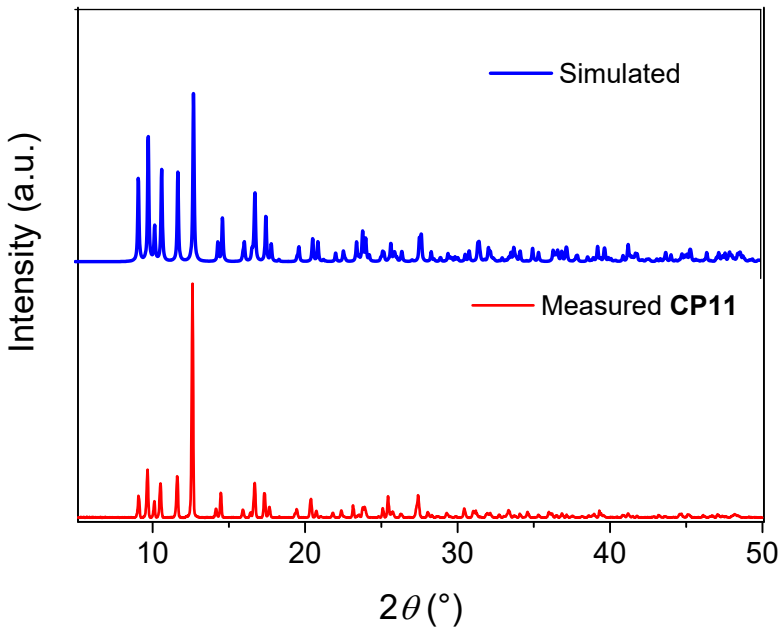


Figure S17: Experimental and simulated PXRD of **CP11**

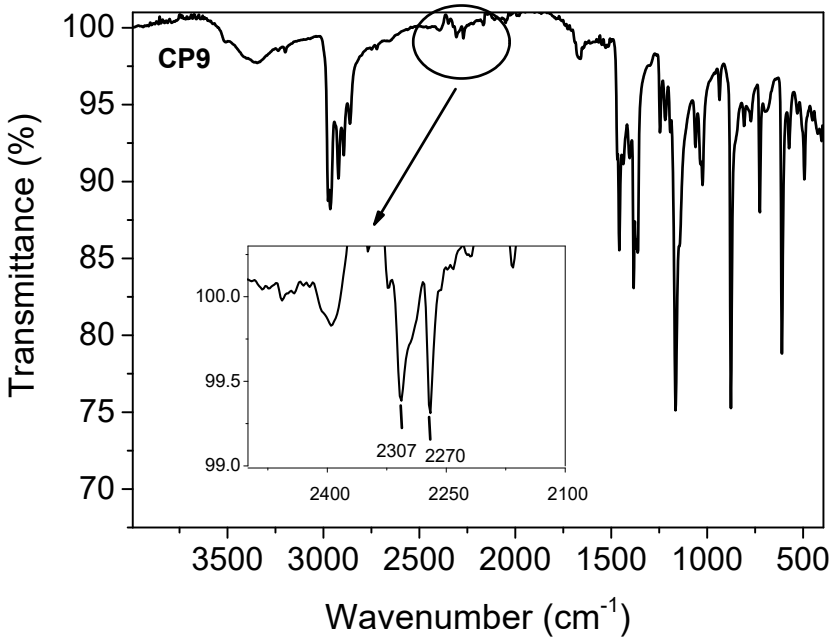


Figure S18: ATR-IR spectrum of **CP9**

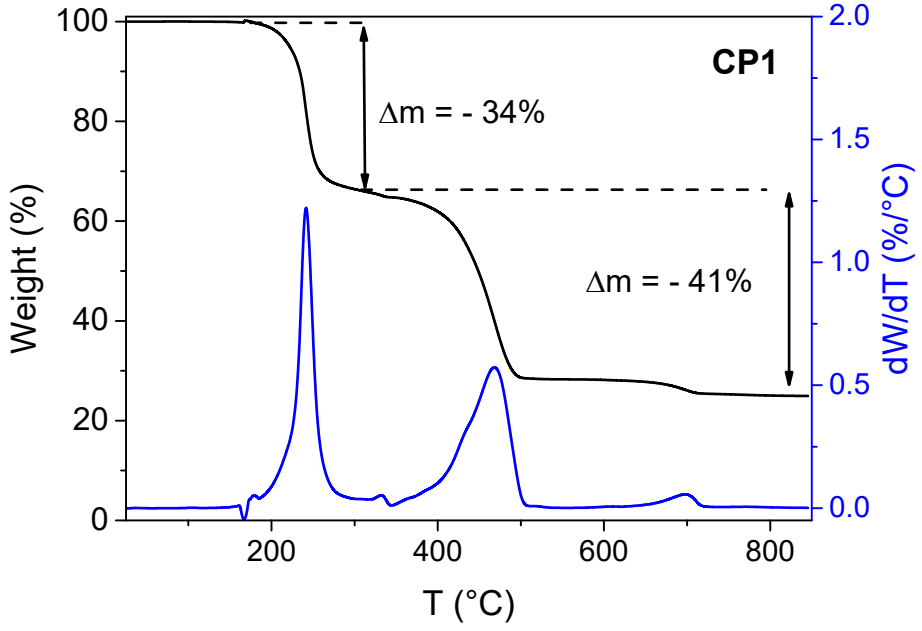


Figure S19. TGA traces and its first derivatives of **CP1** under air flow.

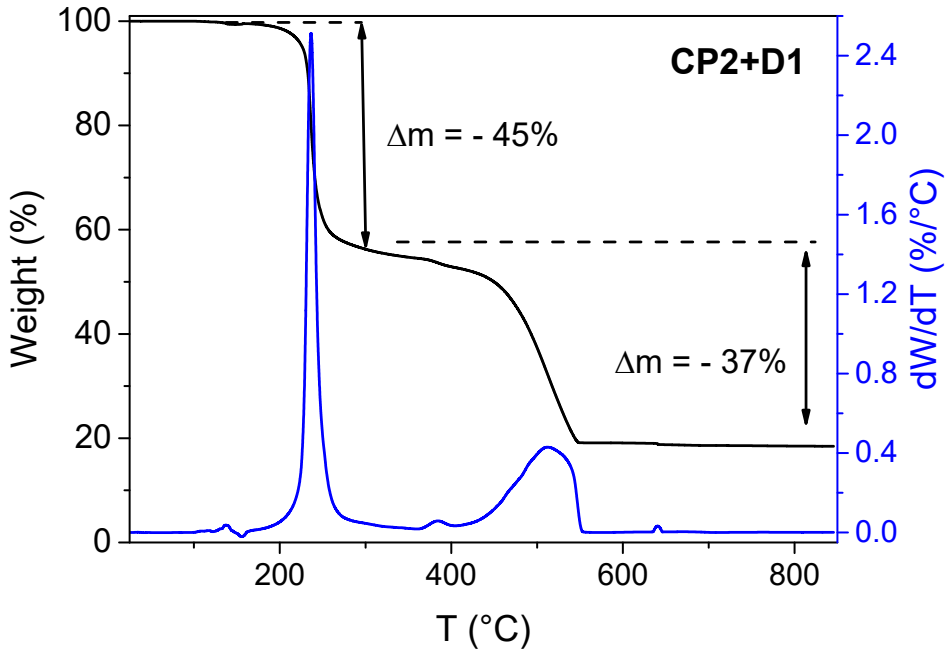


Figure S20. TGA traces and its first derivatives of **CP2- D1** under air flow.

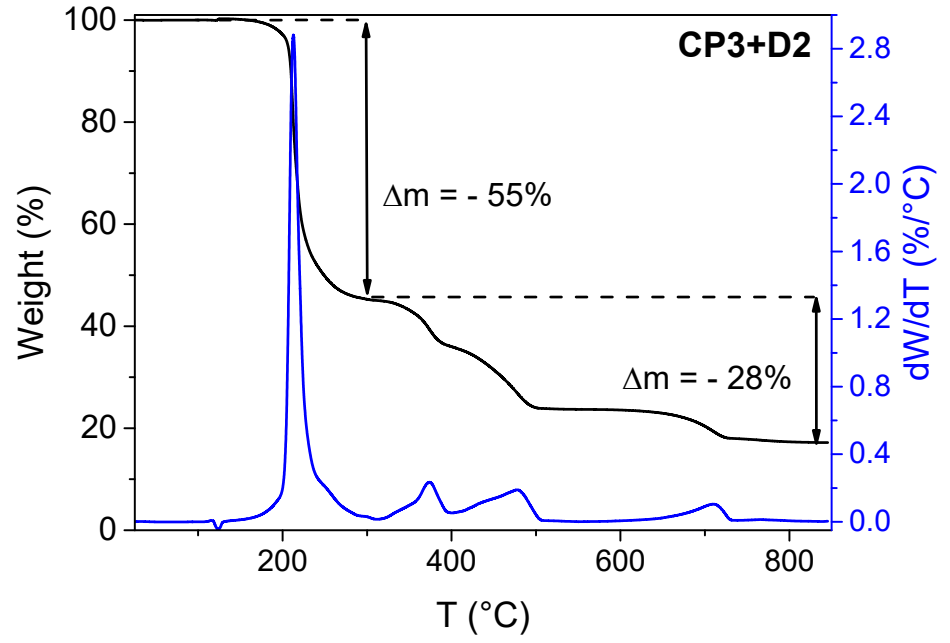


Figure S21. TGA traces and its first derivatives of **CP3- D2** under air flow.

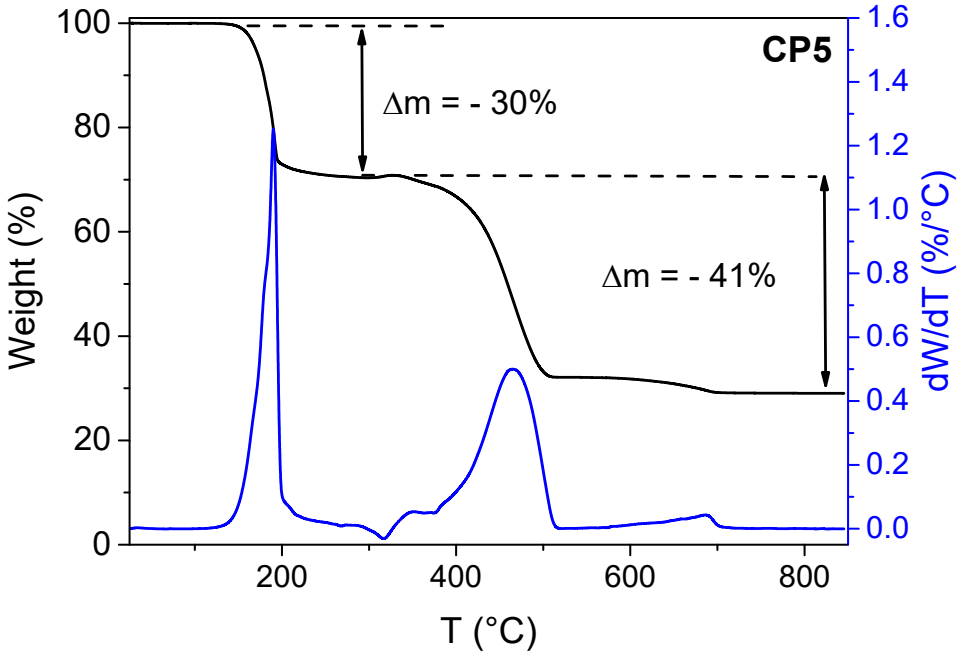


Figure S22. TGA traces and its first derivatives of **CP5** under air flow.

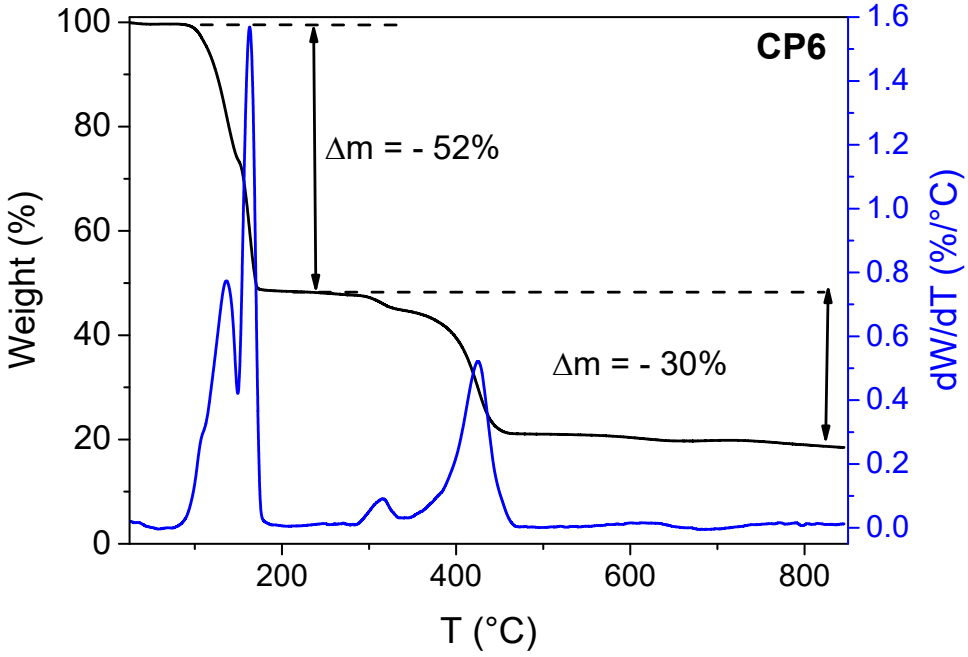


Figure S23. TGA trace and its first derivatives of **CP6** under air flow.

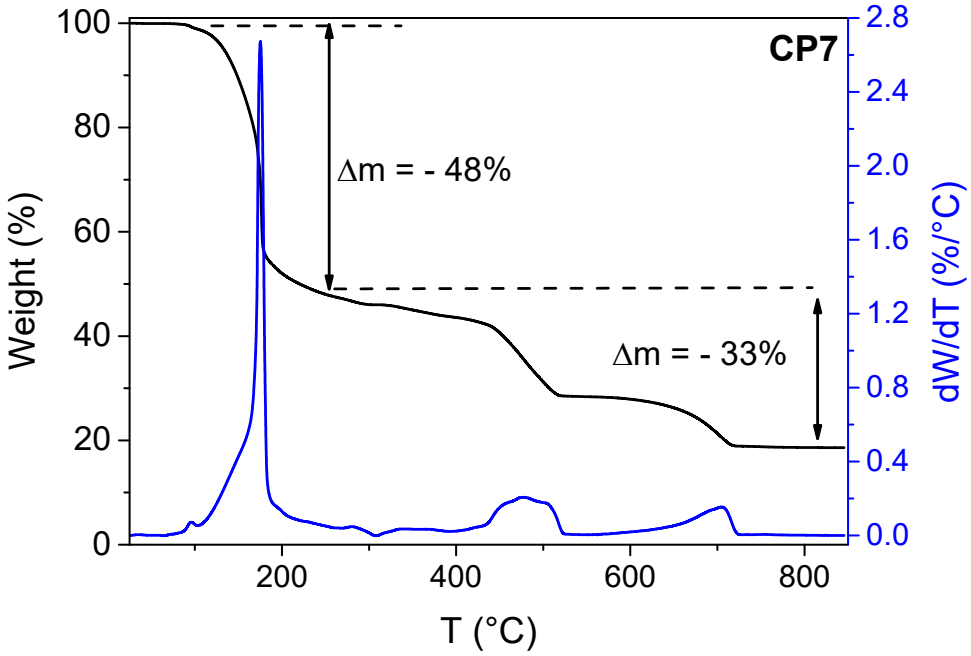


Figure S24. TGA trace and its first derivatives of **CP7** under air flow.

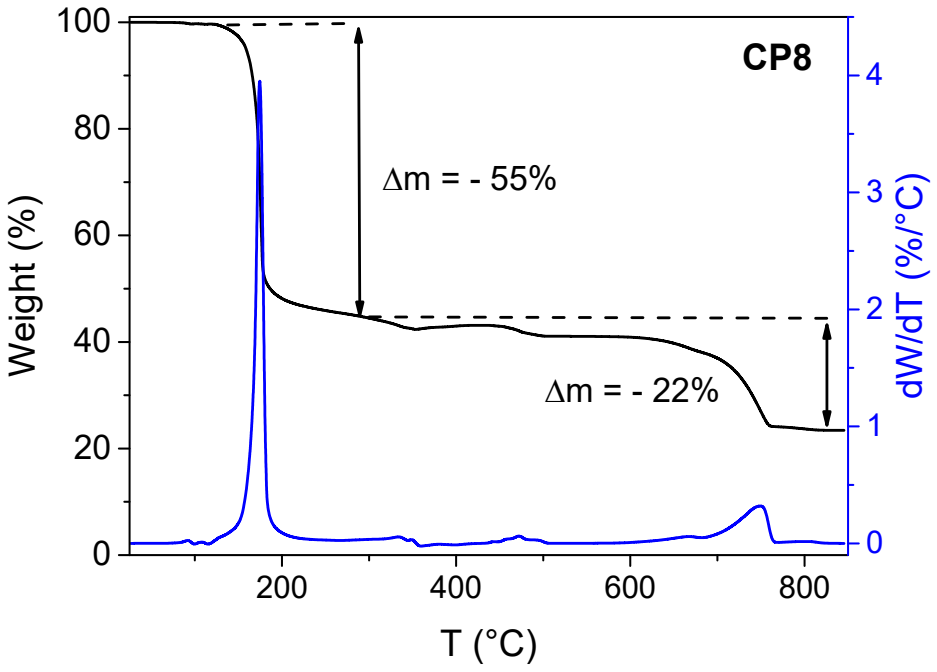


Figure S25. TGA trace and its first derivatives of **CP8** under air flow.

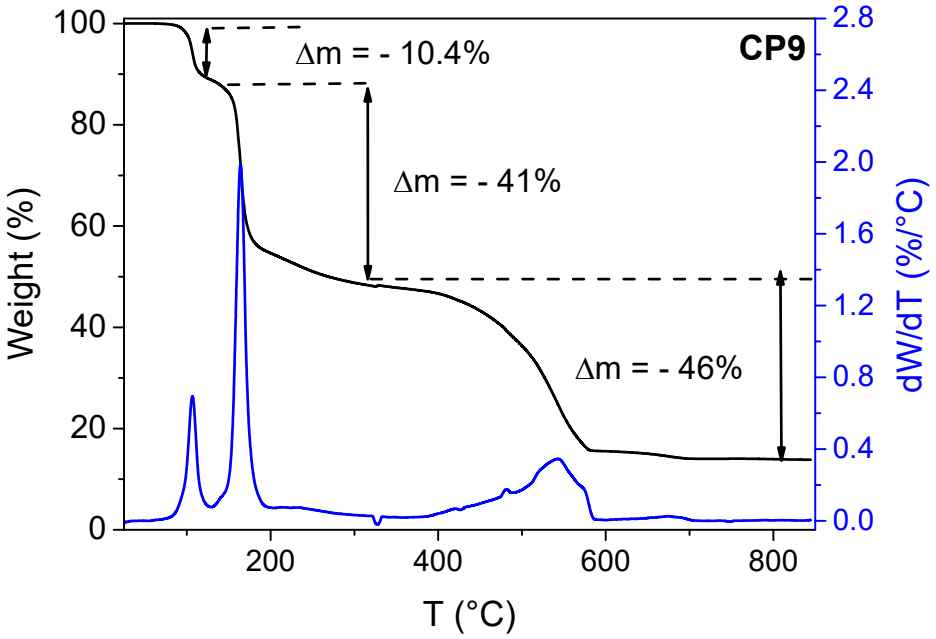


Figure S26. TGA trace and its first derivatives of **CP9** under air flow.

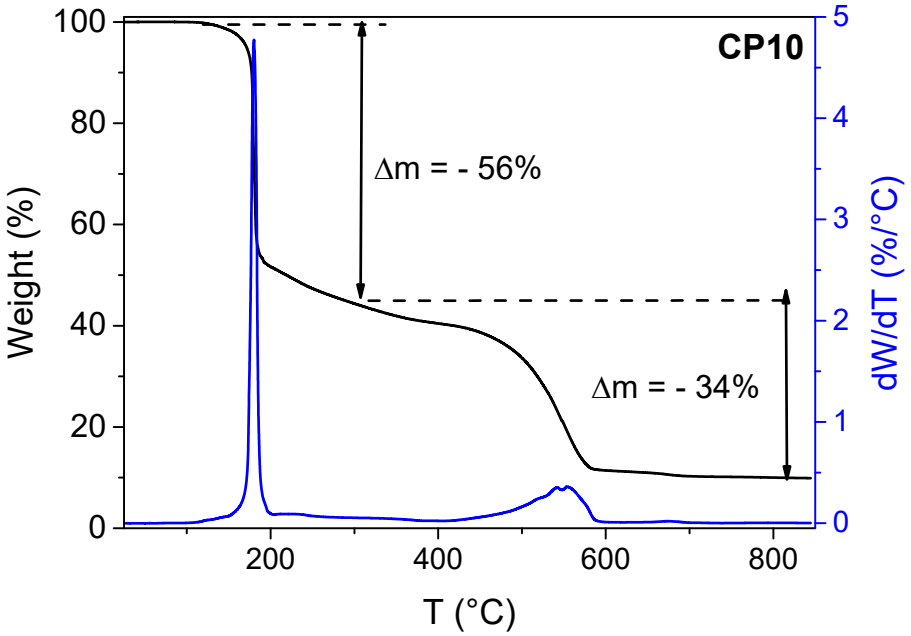


Figure S27. TGA trace and its first derivatives of **CP10** under air flow.

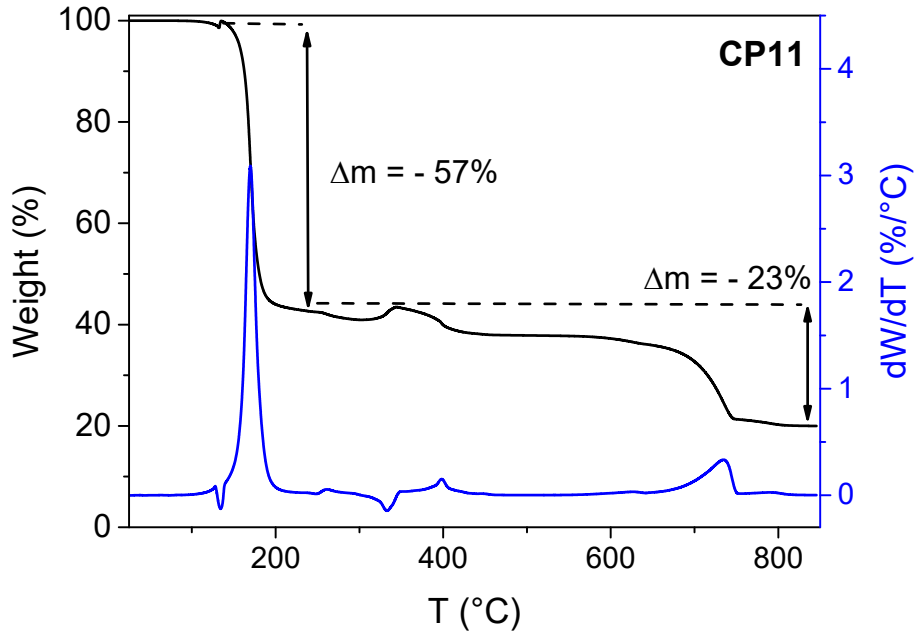


Figure S28. TGA trace and its first derivatives of **CP11** under air flow.

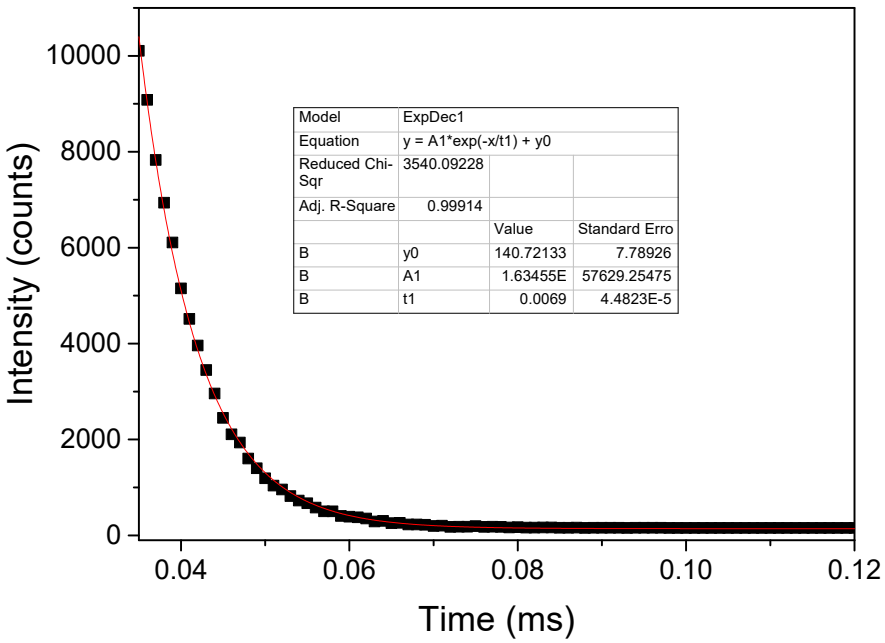


Figure S29. Solid-State Lifetime measurement of **CP1** (black) and the fitting curve (red) at 298K.

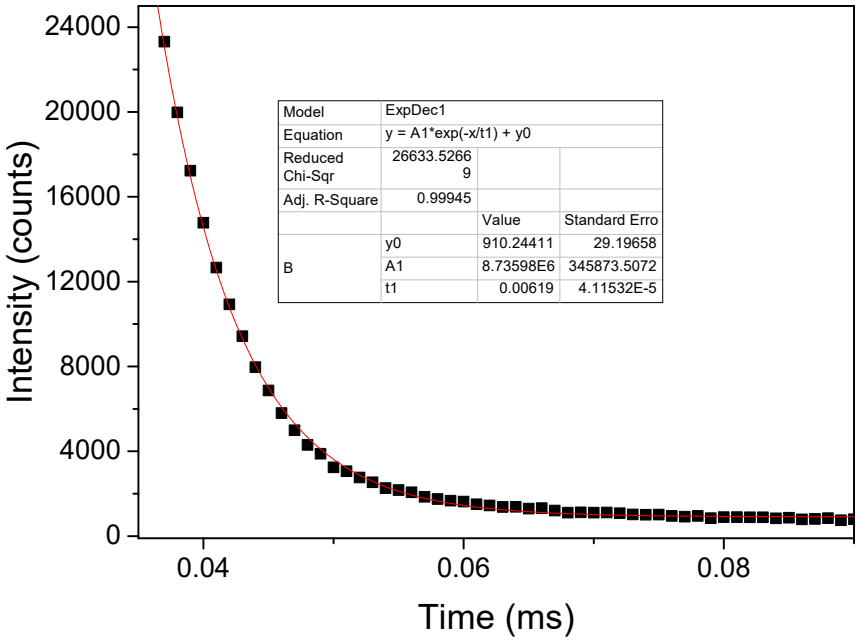


Figure S30. Solid-State Lifetime measurement of **CP5** (black) and the fitting curve (red) at 298K.

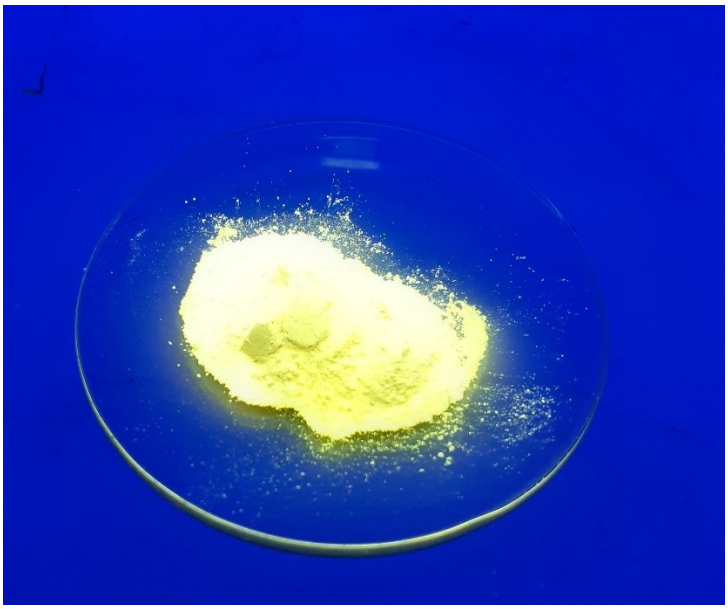


Figure S31. Yellow emission of **CP1** under UV light at 365 nm.

Noncovalent interactions and selected AIM studies.

There are several noncovalent interatomic (NCI) contacts shorter than the sums of Van der Waals (VdW) radii in all structures reported in this article. They led to the building of 3D macromolecular networks. This VdW criterion of atomic interactions is purely based on metric parameters. Generally, these interactions, like all chemical interacting systems have electronic origins and include the hydrogen bonds, the σ-hole interactions like halogen, chalcogen, pnicogen and tetrel bonds,[17, 18] the different types of π-π, X–π or n-π as well as the dipole-dipole (VdW) interactions. With a hope to detect a Cu···C≡C triple bond interaction we focused our attention on those involving the alkyne spacer's triple bonds and $Cu_2X_2S_4$ cores. The significant interactions for different CPs are depicted in Figures S32 to S38. The C-H···π (C≡C triple bond) interactions are present in the majority of coordination polymers except **CP5** and **CP9** in which all triple bonds are reduced to double bonds, **CP10** and **CP11** where half of triple bonds are reduced. The C-H donors for these interactions are provided by dithioether substituents (cyclohexyl, ^{t}Bu) or by CH_2 group of the SC_4S spacer. The C-H···X hydrogen bonding is observed in all compounds. The isostructural 1D coordination polymers **CP2** and **CP3** are interesting because all types (except C-H····H-C) of noncovalent interactions are present therein (Fig. S33). This Figure also contains a case of not frequently encountered C-H···S hydrogen bond. Note that the C-H donor for this last interaction is not provided by CH_2 group of C_4 spacer bound to the S atom. The connectivity in this latter compound between 1D CP and 0D molecular dimer occurs *via* an original tetrel interaction C-H····C^{sp3} which is shown on Figure S34. Independently, the **D1** (and also **D2**) molecules are interconnected by strong C-H····H-C interactions (Figure S35). We state that the metric criterion based on VdW radii did not allow us to find any Cu····π (C≡C) interaction in neither compound.

Consequently, we turned our attention to the Quantum Theory of Atoms In Molecules[19, 20] and Natural Bond Orbitals.[21] The topological analysis of electron density based on the wave function is a powerful tool for the study of weak interatomic forces such as hydrogen bonding,[22] σ–π, n–π and π–π interactions[23-25] as well for studying the nature of the metal–metal[26-28] and metal–ligand[24] interactions in addition to the classical case of covalent bonds. Various topological properties at *Bond Critical Points* (BCPs defined with (rank, signature) code (3,-1)) are used for these purposes.[19, 20] These topological parameters include the electronic charge density (ρ, $e^-/Å^3$), the Laplacian of electron density ($\nabla^2\rho$, $e^-/Å^5$), the local kinetic, potential and total energy densities (G, V and H, $Ha/Å^3$) as well as the derived quantities like the "bond

degree" ($|H|/\rho$, Ha/e^-), and a dimensionless ratio $|V|/G$ at the BCP. The integrations over atomic basins provide the useful information about atomic properties (e.g. charges …) and bond orders through the calculation of delocalization indexes DI. Wiberg bond indexes, which are related to the bond orders, calculated with NBO analysis are complementary to the AIM results.

All chemical interacting systems are classified within the QT-AIM frame into three main types depending on the values of parameters mentioned above. These are the:

1 - shared-shared (SS), covalent, $\nabla^2\rho < 0$, $H < 0$ and $|V|/G > 2$;

2 - shared-closed (SC), transit or intermediate, $\nabla^2\rho > 0$, $H < 0$ and $1 < |V|/G < 2$;

3 - closed-closed (CC), ionic, noncovalent…, $\nabla^2\rho > 0$, $H < 0$ and $|V|/G < 1$.

We selected for the AIM analyses the significant fragments from the structures of **CP6**, **CP7**, **CP3** and **CP4** exhibiting the interactions mentioned above and containing both ligands **L1** and **L2** and all three halogens. The parameters got for **CP3** and **CP7** both bearing X = Br offer the opportunity to directly compare the influence of ligands **L1** and **L2**. The bond paths were calculated, and the molecular graphs plotted.

First, we note that no BCP for an Cu–Cu interaction is observed. Instead, the RCPs (ring critical points) placed at midpoints of the Cu_2X_2 rhombi are present in all CPs. This confirms the discussions in the precedent part based on Cu–Cu distances. The S – C, C – C and C – H shared – shared covalent bonds (type 1 in classification above) present in the ligands are not discussed here. All other interactions have the positive values of Laplacian $\nabla^2\rho$ and belong so to the types 2 and 3. Among them, the Cu – X and Cu – S with negative values of total energy density H are typical coordination bonds whereas all other interactions with positive H values are non-covalent ones.

The AIM electronic approach to the nature of week interactions did not allow the detection of a Cu$\cdots\pi$ (C≡C) interaction. On the other hand, the electron density distribution in all CPs studied indicates the presence of BCPs, thus the occurrence of electronic interactions between one S atom with the triple C≡C bond of a neighboured ligand borne by another S atom. These interactions have topological parameters typical of the closed-closed systems and correspond from a crystal chemical point of view to n–π interactions.

The following interactions have been taken into account for each CP: Cu – X, Cu – S, CH – X, CH – π(C≡C), S – π(C≡C) and S – H. The calculated topological parameters at BCPs are

gathered in Table S10. The molecular graphs built on bond paths are shown in Figures S40 and S41.

We comment first the bonding within the $Cu_2X_2S_4$ cores. The covalent nature of the Cu – X bonds decreases, as expected, from X = I (**CP6**), through X = Br (**CP7** and **CP3**) to X = Cl **CP4**). All topological parameters argue for. The total energy density H is most negative for **CP6** (-0.0815 Ha/Å^3) and increases to -0.0455 and -0.0479 (**CP7** and **CP3**) and to -0.0415 for **CP4**; the $|H|/\rho$ ratio decreases in the same order 0.25 Ha/e$^-$ **CP6** > 0.14 **CP7** and **CP3** > 0.11 **CP4**; the $|V|/G$ ratio similarly decreases from 1.35 (for I) through 1.17 (for Br) to 1.11 (for Cl) and the $\nabla^2\rho$ is less positive for **CP6** (2.96 e$^-$/Å^5) than for **CP7** and **CP3** (3.28) reaching 4.92 for **CP4**. The DI values decrease from I (0.465)>Br (0.452 and 0.468)>Cl (0.455). However, the variations of DI's are very small. Finally, the Cu – I bonds are stronger than the Cu – Br ones which in turn are stronger than the Cu – Cl ones. Wiberg indexes related to the bond orders are in good agreement decreasing from 0.19 (I) to 0.17 (Br) and to 0.14 (Cl). Consequently, as it has been already suggested in the main text (page 24), the strengths of the Cu – S bonds should increase in an inverse order I < Br < Cl. It is confirmed by topological parameters: total energies H decrease -0.064 (I), -0.068 (Br), -0.070 (Cl); DI 0.52 (I), 0.54 (Br), 0.55 (Cl). The values of Wiberg indexes of 0.18, 0.20 and 0.21, respectively, confirm the trend.

The properties of CH – X BCPs found for all calculated coordination polymers correspond well to those of closed – closed hydrogen bonds. There is no clear and regular tendency for estimation of the influence of X on their strengths. Note also that CH – S hydrogen bonds have been observed in **CP6** and **CP7** with R – ^{t}Bu but not in **CP3** and **CP4** where R = C_6H_6.

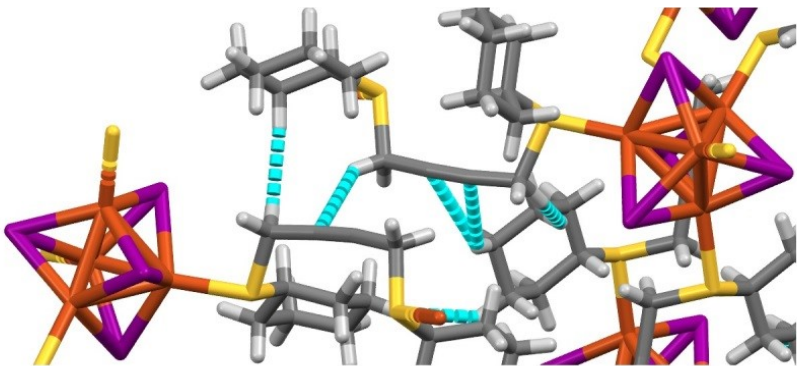
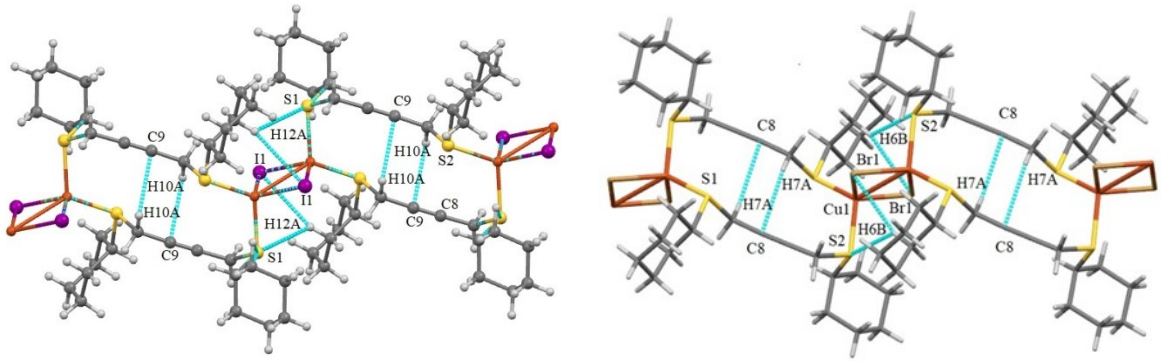


Figure S32. CP1: a fragment of the structure showing C-H···π(C≡C) and C-H···H-C interactions between the neighboured spacers.



(a) (b)

Figure S33. C-H···π, C-H···X and C-H···S interactions in isostructural **CP2** (a) and **CP3** (b). Interatomic distances (Å) together with their shortening (Å) relative to the sum of Van der Waals radii: **CP2**: C9····H10A 2.663 (-0.178), I1····H12A 3.087 (-0.093) and S1····H12A 2.958 (-0.042); **CP3**: C8····H7A 2.742 (-0.158), Br1····H6B 2.965 (-0.085) and S2····H6B 2.936 (-0.064).

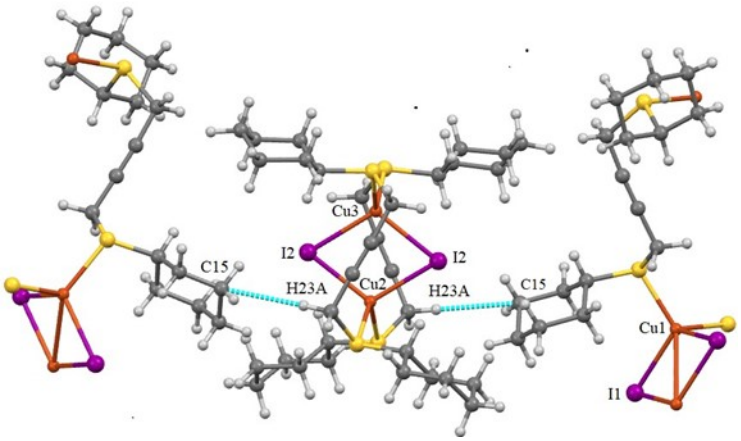


Figure S34. **CP2/D1**: C-H···C tetrel interaction connecting **CP2** and dinuclear discreet **D1**. H23A- C15 2.832 Å, -0.068Å with respect to the sum of the VdW radii.

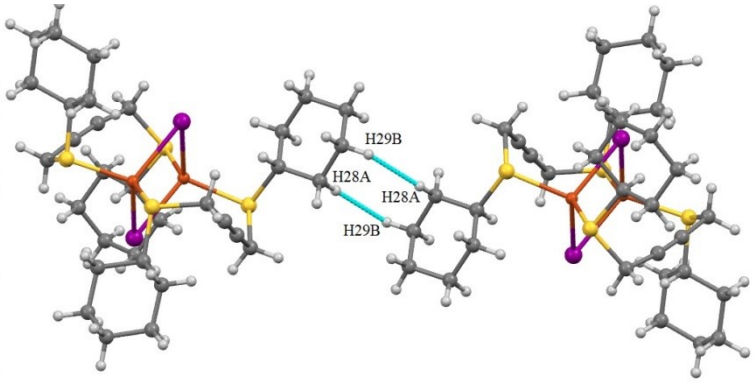


Figure S35. **CP2/D1**: C-H····H-C interactions connecting two **D1** molecules. H····H distance 2.252 (-0.148) Å.

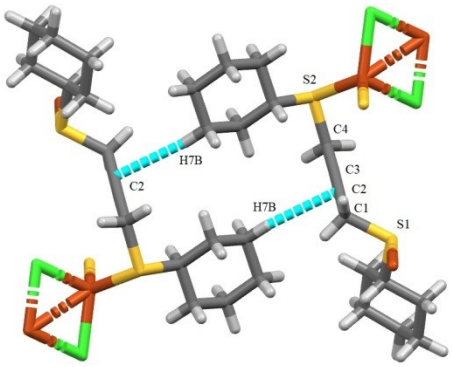


Figure S36. C-H···π interactions in **CP4**.

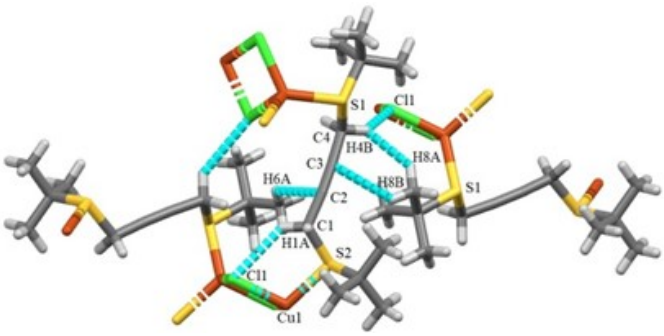


Figure S37. **CP8**: C-H····π(C≡C), C-H····Cl and C-H····H-C interactions present in the crystal structure of CP8. Interatomic distances (Å) together with their shortening (Å) relative to the sum of Van der Waals radii: C2····H6A 2.793 (-0.107), C3····H8B 2.826 (-0.074), Cl1····H1A 2.736 (-0.214), Cl1····H4B 2.946 (-0.004), H4B····H8A 2.318 (-0.082).

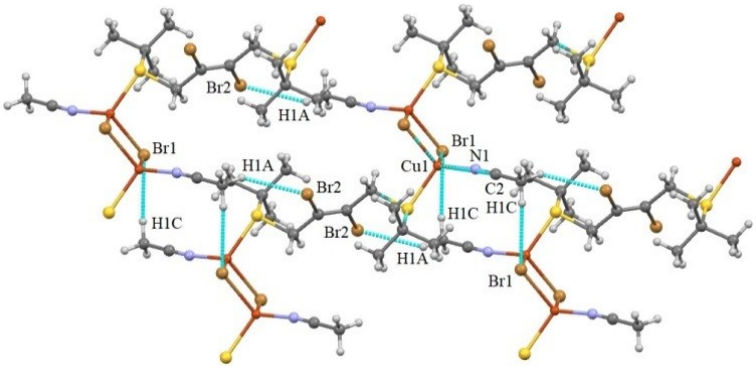


Figure S38. **CP9**: Br1····H1C 3.018(-0.032) Å, Br2····H1A 2.953(-0.097) Å.

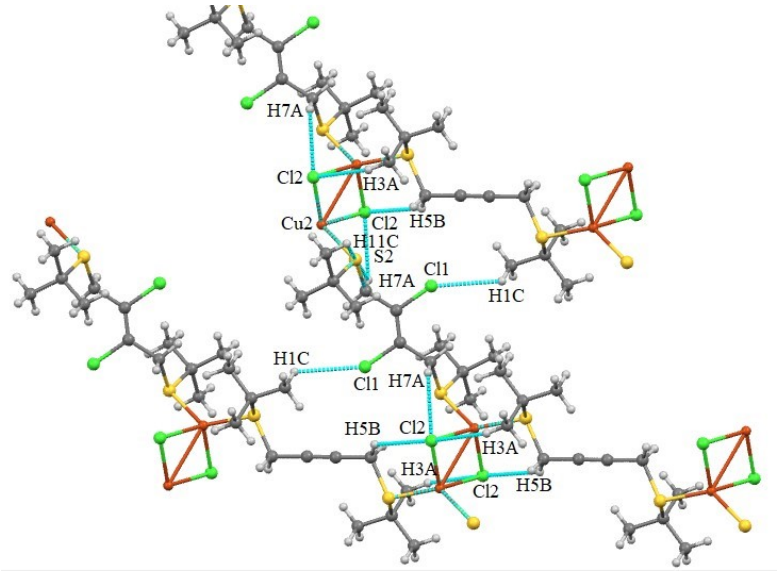


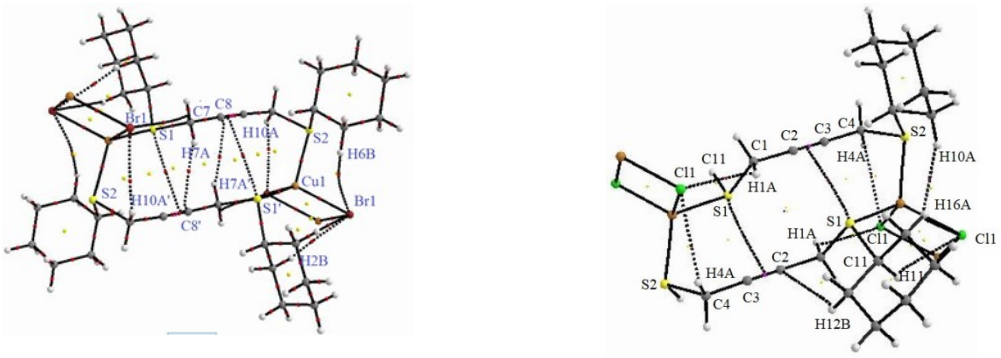
Figure S39. CP11: C-H···Cl and C-H···H-C interactions present in the crystal structure of **CP11**. Interatomic distances (Å) together with their shortening (Å) relative to the sum of the Van der Waals radii: Cl1···H1C 2.882 (-0.068), Cl2···H3A 2.745 (-0.205), Cl2···H5B 2.776 (-0.174), Cl2···H7A 2.849 (-0.101).

Table S6. Topological properties of bond critical points (mean values); d (distance), ρ (electron density), $\nabla^2\rho$ (Laplacian of ρ), H (total energy density), V potential energy density, G kinetic energy density, DI (delocalization index), Wiberg (bond index from NBO analysis).

Interaction	d (Å)	ρ ($e^-/Å^3$)	$\nabla^2\rho$ ($e^-/Å^5$)	H (Ha/$Å^3$)	|H|/ρ (Ha/e^-)	|V|/G	DI	Wiberg
Cu – X								
CP6 X=I	2.654	0.3309	2.96	-0.0815	0.246	1.348	0.465	0.186
CP7 X=Br	2.509	0.3208	3.28	-0.0455	0.140	1.164	0.452	0.166
CP3 X=Br	2.490	0.3329	3.28	-0.0479	0.144	1.174	0.468	0.177
CP4 X=Cl	2.358	0.3791	4.92	-0.0415	0.110	1.109	0.455	0.140
Cu – S								
CP6 X=I	2.341	0.432	5.28	-0.0637	0.147	1.147	0.522	0.186
CP7 X=Br	2.321	0.446	5.59	-0.0652	0.151	1.144	0.542	0.201
CP3 X=Br	2.304	0.466	5.88	-0.0710	0.152	1.146	0.545	0.207
CP4 X=Cl	2.306	0.464	5.86	-0.0700	0.151	1.146	0.553	0.210
CH – X								
CP6 (4a)	3.205	0.044	0.542	+0.0095	0.199	0.702	c	0.004
CP7 (8a)	3.142	0.043	0.438	+0.0047	0.124	0.798	c	0.006
CP3 (4a)	3.140	0.042	0.439	+0.0050	0.124	0.794	c	0.004
CP4 (4a)	2.852	0.053	0.696	+0.0011	0.197	0.725	c	0.002
CH– π(C≡C)								
CP6 (3a)	2.746	0.045	0.578	+0.0092	0.201	0.708	c	0.002
CP7 (4a,b)	2.766	0.046	0.566	+0.0088	0.193	0.713	c	0.001
CP3 (2a)	2.742	0.045	0.554	+0.0054	0.155	0.751	c	0.002
CP4 (1a)	2.836	0.051	0.665	+0.0105	0.207	0.709	c	0.002
S – π(C≡C)								
CP6 (1a)	3.712	0.034	0.342	+0.0051	0.152	0.729	c	0.002
CP7 (3a)	3.632	0.038	0.400	+0.0060	0.155	0.730	c	0.002
CP3 (1a)	3.610	0.033	0.369	+0.0054	0.155	0.751	c	0.002
CP4 (1a)	3.604	0.034	0.366	+0.0055	0.162	0.726	c	0.002

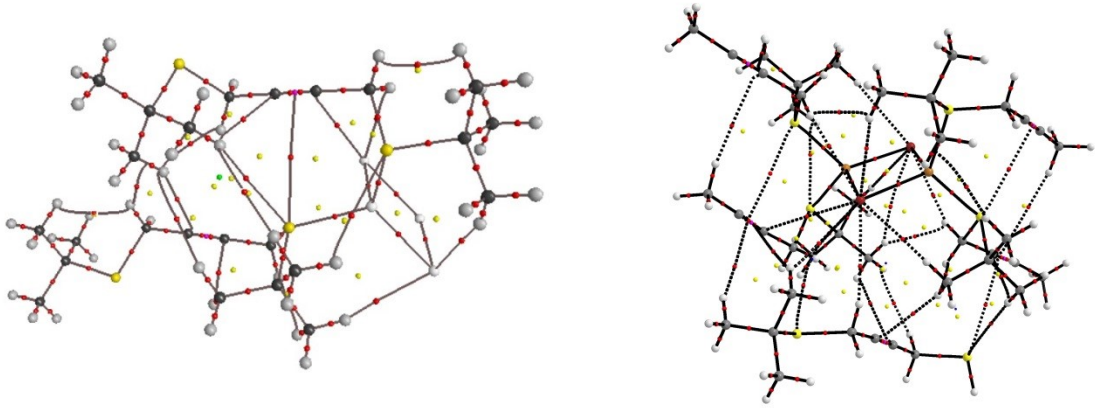
S – H								
CP6 (2a)	3.173	0.031	0.366	+0.0039	0.126	0.658	c	0.001
CP7 (3a)	3.104	0.040	0.547	+0.0037	0.093	0.675	c	0.002
CP3 (4a)						-	c	
CP4 (4a)							c	

a number of interactions, b four other BCPs with long H…C distances (mean 3.262 Å) have been detected but are not included here, c not detected. DI indexes for non-covalent interactions were not calculated.



(a) (b)

Figure S40. Molecular graphs showing the inter-ligand noncovalent interactions in 14 membered rings in the structures of (a) **CP3** and (b) **CP4**. **CP3**: S···π(C≡C), C-H···π(C≡C) and C-H···Br, **CP4**: S···π(C≡C) and C-H···Cl and exterior to the ring C-H···H–C bond paths.



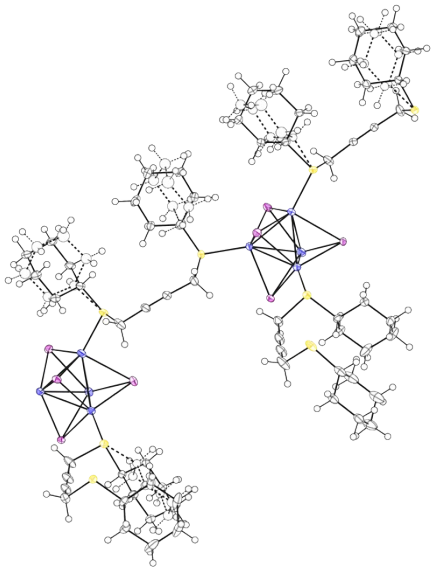
(a) (b)

Figure S41. Molecular graphs of (a) **CP6** and (b) **CP7**. **CP6**: S···π(C≡C), C-H···π(C≡C) C-H···H–C C-H···S and C-H···I bond paths; **CP7**: S···π(C≡C), C-H···π(C≡C) and C-H···Br, C-H···S and C-H···H–C bond paths.

X-ray data and experimental refinement

Crystal structure of CP1_100K

Crystal Data and Experimental



Experimental: The data for CP1_100K were collected from a shock-cooled single crystal at 100.0(1) K on a Bruker D8 Venture four-circle diffractometer with a X-ray tube using a graphite as monochromator and a CPAD PHOTON II area detector detector. The diffractometer was equipped with an Oxford Cryostream 800 low temperature device and used Mo K_{α} radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.38A and a multi-scan absorption correction using SADABS 2016/2 was applied. [1,2] The structure was solved by direct methods with SHELXT and refined by full-matrix least-squares methods against F^2 using SHELXL.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters, excepted minor disordered parts. For each compound, some disorders were found in the crystal structure and some geometric parameters of disordered components in each group were restrained by using RIGU or DFIX restraints. For more detail see the .res file included in the cif files. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[5] CCDC 2326781 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures. This report and the CIF file were generated using FinalCif.[6]

Table S7. Crystal data and structure refinement for CP1_100K

Internal Reference	CP1_100K
CCDC number	2326781
Empirical formula	$C_{64}H_{104}Cu_8I_8S_8$
Formula weight	2653.47
Temperature [K]	100.0(1)
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	11.7692(4)
b [Å]	18.6908(5)
c [Å]	20.6753(6)
α [°]	97.2090(10)
β [°]	104.8990(10)
γ [°]	103.0370(10)
Volume [Å^3]	4199.8(2)
Z	2
ρ_{calc} [gcm^{-3}]	2.098
μ [mm^{-1}]	5.159
F(000)	2544
Crystal size [mm^3]	0.084×0.133×0.172
Crystal colour	clear light colourless
Crystal shape	block
Radiation	Mo K_{α} (λ=0.71073 Å)
2θ range [°]	4.33 to 55.00 (0.77 Å)
Index ranges	−15 ≤ h ≤ 15 −24 ≤ k ≤ 24 −26 ≤ l ≤ 26
Reflections collected	240995
Independent reflections	19283 R_{int} = 0.0305 R_{sigma} = 0.0131
Completeness to θ = 25.242°	99.9 %
Data / Restraints / Parameters	19283 / 736 / 914
Goodness-of-fit on F^2	1.025
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0288 wR_2 = 0.0571
Final *R* indexes [all data]	R_1 = 0.0335 wR_2 = 0.0601
Largest peak/hole [eÅ^{-3}]	2.51/−2.88

Table S8 Bond lengths and angles for CP1_100K

Atom–Atom	Length [Å]
I1–Cu1	2.7249(5)
I1–Cu2	2.6864(5)
I1–Cu3	2.6583(5)
I2–Cu1	2.7218(5)
I2–Cu2	2.6543(5)
I2–Cu4	2.6807(5)
I3–Cu1	2.6003(5)
I3–Cu3	2.6228(5)
I3–Cu4	2.7961(6)
I4–Cu2	2.6703(5)
I4–Cu3	2.7608(5)
I4–Cu4	2.6238(6)
I5–Cu5	2.6768(5)
I5–Cu6	2.6762(6)
I5–Cu7	2.6879(5)
I6–Cu5	2.7541(5)
I6–Cu6	2.6879(7)
I6–Cu8	2.6133(6)
I7–Cu5	2.6260(5)
I7–Cu7	2.6105(6)
I7–Cu8	2.8096(5)
I8–Cu6	2.6331(6)
I8–Cu7	2.6755(6)
I8–Cu8	2.7031(7)
Cu1–Cu2	2.6885(7)
Cu1–Cu3	2.5991(6)
Cu1–Cu4	2.7611(7)
Cu1–S1	2.2868(10)
Cu2–Cu3	2.7860(6)
Cu2–Cu4	2.6632(6)
Cu2–S8$^{\#1}$	2.2998(10)
Cu3–Cu4	2.7027(7)
Cu3–S2$^{\#2}$	2.2781(10)
Cu4–S3	2.3002(11)
Cu5–Cu6	2.8001(7)
Cu5–Cu7	2.6388(7)
Cu5–Cu8	2.6772(6)
Cu5–S5	2.2868(11)
Cu6–Cu7	2.7077(8)
Cu6–Cu8	2.6595(7)
Cu6–S4	2.3051(11)
Cu7–Cu8	2.7371(8)
Cu7–S6$^{\#2}$	2.2873(13)
Cu8–S7	2.2962(11)
S1–C1A	1.853(5)
S1–C1B	1.852(12)
S1–C7	1.824(4)
S2–C10	1.820(4)
S2–C11	1.825(4)
S3–C17A	1.864(6)
S3–C17B	1.877(13)
S3–C23	1.822(5)
S4–C26	1.822(5)
S4–C27	1.811(5)
S5–C33	1.824(4)
S5–C39	1.819(4)
S6–C42	1.835(5)
S6–C43	1.813(6)
S7–C49A	1.856(5)
S7–C49B	1.811(19)
S7–C55	1.809(5)
S8–C58	1.807(5)
S8–C59A	1.880(6)
S8–C59B	1.787(10)
C1A–H1A	1.0000
C1A–C2A	1.533(7)
C1A–C6A	1.523(8)
C1B–H1B	1.0000
C1B–C2B	1.518(17)
C1B–C6B	1.497(17)
C2A–H2AA	0.9900
C2A–H2AB	0.9900
C2A–C3A	1.534(9)
C2B–H2BA	0.9900
C2B–H2BB	0.9900
C2B–C3B	1.538(18)
C3A–H3AA	0.9900
C3A–H3AB	0.9900
C3A–C4A	1.526(10)
C3B–H3BA	0.9900
C3B–H3BB	0.9900
C3B–C4B	1.48(2)
C4A–H4AA	0.9900
C4A–H4AB	0.9900
C4A–C5A	1.540(13)
C4B–H4BA	0.9900
C4B–H4BB	0.9900
C4B–C5B	1.48(3)
C5A–H5AA	0.9900
C5A–H5AB	0.9900
C5A–C6A	1.526(11)
C5B–H5BA	0.9900
C5B–H5BB	0.9900
C5B–C6B	1.56(3)
C6A–H6AA	0.9900
C6A–H6AB	0.9900
C6B–H6BA	0.9900
C6B–H6BB	0.9900
C7–H7A	0.9900
C7–H7B	0.9900
C7–C8	1.460(6)
C8–C9	1.179(6)
C9–C10	1.459(5)
C10–H10A	0.9900
C10–H10B	0.9900
C11–H11	1.0000
C11–C12	1.528(6)
C11–C16	1.520(6)
C12–H12A	0.9900

C12–H12B	0.9900	C27–C28B	1.537(15)
C12–C13	1.533(7)	C27–C32A	1.519(9)
C13–H13A	0.9900	C27–C32B	1.467(14)
C13–H13B	0.9900	C28A–H28A	0.9900
C13–C14	1.494(11)	C28A–H28B	0.9900
C14–H14A	0.9900	C28A–C29A	1.500(10)
C14–H14B	0.9900	C28B–H28C	0.9900
C14–C15	1.528(8)	C28B–H28D	0.9900
C15–H15A	0.9900	C28B–C29B	1.52(2)
C15–H15B	0.9900	C29A–H29A	0.9900
C15–C16	1.534(7)	C29A–H29B	0.9900
C16–H16A	0.9900	C29A–C30A	1.470(10)
C16–H16B	0.9900	C29B–H29C	0.9900
C17A–H17A	1.0000	C29B–H29D	0.9900
C17A–C18A	1.523(8)	C29B–C30B	1.52(2)
C17A–C22A	1.527(8)	C30A–H30A	0.9900
C17B–H17B	1.0000	C30A–H30B	0.9900
C17B–C18B	1.502(16)	C30A–C31A	1.548(10)
C17B–C22B	1.532(17)	C30B–H30C	0.9900
C18A–H18A	0.9900	C30B–H30D	0.9900
C18A–H18B	0.9900	C30B–C31B	1.49(2)
C18A–C19A	1.531(8)	C31A–H31A	0.9900
C18B–H18C	0.9900	C31A–H31B	0.9900
C18B–H18D	0.9900	C31A–C32A	1.529(11)
C18B–C19B	1.534(18)	C31B–H31C	0.9900
C19A–H19A	0.9900	C31B–H31D	0.9900
C19A–H19B	0.9900	C31B–C32B	1.55(2)
C19A–C20A	1.505(9)	C32A–H32A	0.9900
C19B–H19C	0.9900	C32A–H32B	0.9900
C19B–H19D	0.9900	C32B–H32C	0.9900
C19B–C20B	1.53(2)	C32B–H32D	0.9900
C20A–H20A	0.9900	C33–H33	1.0000
C20A–H20B	0.9900	C33–C34	1.519(6)
C20A–C21A	1.526(11)	C33–C38	1.510(6)
C20B–H20C	0.9900	C34–H34A	0.9900
C20B–H20D	0.9900	C34–H34B	0.9900
C20B–C21B	1.48(2)	C34–C35	1.530(6)
C21A–H21A	0.9900	C35–H35A	0.9900
C21A–H21B	0.9900	C35–H35B	0.9900
C21A–C22A	1.547(10)	C35–C36	1.503(7)
C21B–H21C	0.9900	C36–H36A	0.9900
C21B–H21D	0.9900	C36–H36B	0.9900
C21B–C22B	1.51(2)	C36–C37	1.506(8)
C22A–H22A	0.9900	C37–H37A	0.9900
C22A–H22B	0.9900	C37–H37B	0.9900
C22B–H22C	0.9900	C37–C38	1.544(6)
C22B–H22D	0.9900	C38–H38A	0.9900
C23–H23A	0.9900	C38–H38B	0.9900
C23–H23B	0.9900	C39–H39A	0.9900
C23–C24	1.453(6)	C39–H39B	0.9900
C24–C25	1.174(6)	C39–C40	1.459(6)
C25–C26	1.452(6)	C40–C41	1.184(6)
C26–H26A	0.9900	C41–C42	1.460(6)
C26–H26B	0.9900	C42–H42A	0.9900
C27–H27	1.0000	C42–H42B	0.9900
C27–H27A	1.0000	C43–H43	1.0000
C27–C28A	1.429(7)	C43–C44	1.518(6)

C43–C48	1.527(6)
C44–H44A	0.9900
C44–H44B	0.9900
C44–C45	1.518(10)
C45–H45A	0.9900
C45–H45B	0.9900
C45–C46	1.533(9)
C46–H46A	0.9900
C46–H46B	0.9900
C46–C47	1.511(8)
C47–H47A	0.9900
C47–H47B	0.9900
C47–C48	1.523(7)
C48–H48A	0.9900
C48–H48B	0.9900
C49A–H49A	1.0000
C49A–C50A	1.484(9)
C49A–C54A	1.528(7)
C49B–H49B	1.0000
C49B–C50B	1.51(3)
C49B–C54B	1.49(3)
C50A–H50A	0.9900
C50A–H50B	0.9900
C50A–C51A	1.541(9)
C50B–H50C	0.9900
C50B–H50D	0.9900
C50B–C51B	1.54(3)
C51A–H51A	0.9900
C51A–H51B	0.9900
C51A–C52A	1.529(9)
C51B–H51C	0.9900
C51B–H51D	0.9900
C51B–C52B	1.54(3)
C52A–H52A	0.9900
C52A–H52B	0.9900
C52A–C53A	1.485(9)
C52B–H52C	0.9900
C52B–H52D	0.9900
C52B–C53B	1.45(3)
C53A–H53A	0.9900
C53A–H53B	0.9900
C53A–C54A	1.535(7)
C53B–H53C	0.9900
C53B–H53D	0.9900
C53B–C54B	1.61(3)
C54A–H54A	0.9900
C54A–H54B	0.9900
C54B–H54C	0.9900
C54B–H54D	0.9900
C55–H55A	0.9900
C55–H55B	0.9900
C55–C56	1.464(5)
C56–C57	1.188(6)
C57–C58	1.457(6)
C58–H58A	0.9900
C58–H58B	0.9900
C59A–H59A	1.0000
C59A–C60A	1.521(8)
C59A–C64A	1.525(8)
C59B–H59B	1.0000
C59B–C60B	1.518(15)
C59B–C64B	1.523(16)
C60A–H60A	0.9900
C60A–H60B	0.9900
C60A–C61A	1.530(8)
C60B–H60C	0.9900
C60B–H60D	0.9900
C60B–C61B	1.525(16)
C61A–H61A	0.9900
C61A–H61B	0.9900
C61A–C62A	1.513(10)
C61B–H61C	0.9900
C61B–H61D	0.9900
C61B–C62B	1.537(16)
C62A–H62A	0.9900
C62A–H62B	0.9900
C62A–C63A	1.512(9)
C62B–H62C	0.9900
C62B–H62D	0.9900
C62B–C63B	1.495(16)
C63A–H63A	0.9900
C63A–H63B	0.9900
C63A–C64A	1.528(8)
C63B–H63C	0.9900
C63B–H63D	0.9900
C63B–C64B	1.548(16)
C64A–H64A	0.9900
C64A–H64B	0.9900
C64B–H64C	0.9900
C64B–H64D	0.9900

Atom–Atom–Atom	**Angle [°]**
Cu2–I1–Cu1	59.577(15)
Cu3–I1–Cu1	57.722(14)
Cu3–I1–Cu2	62.831(15)
Cu2–I2–Cu1	59.996(15)
Cu2–I2–Cu4	59.890(15)
Cu4–I2–Cu1	61.467(15)
Cu1–I3–Cu3	59.683(15)
Cu1–I3–Cu4	61.423(15)
Cu3–I3–Cu4	59.733(16)
Cu2–I4–Cu3	61.696(14)
Cu4–I4–Cu2	60.395(15)
Cu4–I4–Cu3	60.191(16)
Cu5–I5–Cu7	58.928(16)
Cu6–I5–Cu5	63.079(16)
Cu6–I5–Cu7	60.634(17)
Cu6–I6–Cu5	61.918(16)
Cu8–I6–Cu5	59.772(15)
Cu8–I6–Cu6	60.203(17)
Cu5–I7–Cu8	58.899(15)
Cu7–I7–Cu5	60.518(16)
Cu7–I7–Cu8	60.529(17)
Cu6–I8–Cu7	61.329(17)

Cu6–I8–Cu8	59.771(17)	Cu4–Cu3–I4	57.391(15)
Cu7–I8–Cu8	61.177(17)	Cu4–Cu3–Cu2	58.029(16)
I1–Cu1–Cu4	106.849(19)	$S2^{\#2}$–Cu3–I1	111.73(3)
I2–Cu1–I1	112.417(18)	$S2^{\#2}$–Cu3–I3	108.46(3)
I2–Cu1–Cu4	58.534(15)	$S2^{\#2}$–Cu3–I4	96.77(3)
I3–Cu1–I1	114.313(18)	$S2^{\#2}$–Cu3–Cu1	154.54(3)
I3–Cu1–I2	112.251(18)	$S2^{\#2}$–Cu3–Cu2	141.28(3)
I3–Cu1–Cu2	112.587(19)	$S2^{\#2}$–Cu3–Cu4	135.49(3)
I3–Cu1–Cu4	62.783(15)	I2–Cu4–I3	107.570(18)
Cu2–Cu1–I1	59.499(14)	I2–Cu4–Cu1	59.999(15)
Cu2–Cu1–I2	58.757(15)	I2–Cu4–Cu3	108.907(19)
Cu2–Cu1–Cu4	58.490(17)	I4–Cu4–I2	114.190(19)
Cu3–Cu1–I1	59.854(15)	I4–Cu4–I3	114.12(2)
Cu3–Cu1–I2	110.79(2)	I4–Cu4–Cu1	107.93(2)
Cu3–Cu1–I3	60.589(15)	I4–Cu4–Cu2	60.668(16)
Cu3–Cu1–Cu2	63.565(17)	I4–Cu4–Cu3	62.419(16)
Cu3–Cu1–Cu4	60.467(18)	Cu1–Cu4–I3	55.794(15)
S1–Cu1–I1	105.63(3)	Cu2–Cu4–I2	59.564(15)
S1–Cu1–I2	96.52(3)	Cu2–Cu4–I3	107.38(2)
S1–Cu1–I3	114.24(3)	Cu2–Cu4–Cu1	59.391(17)
S1–Cu1–Cu2	132.64(3)	Cu2–Cu4–Cu3	62.553(18)
S1–Cu1–Cu3	152.21(3)	Cu3–Cu4–I3	56.946(15)
S1–Cu1–Cu4	144.84(3)	Cu3–Cu4–Cu1	56.797(17)
I1–Cu2–Cu1	60.924(15)	S3–Cu4–I2	109.04(4)
I1–Cu2–Cu3	58.092(14)	S3–Cu4–I3	92.91(3)
I2–Cu2–I1	115.893(18)	S3–Cu4–I4	116.83(4)
I2–Cu2–I4	113.526(18)	S3–Cu4–Cu1	133.40(4)
I2–Cu2–Cu1	61.247(15)	S3–Cu4–Cu2	158.80(4)
I2–Cu2–Cu3	107.221(19)	S3–Cu4–Cu3	137.18(4)
I2–Cu2–Cu4	60.547(16)	I5–Cu5–I6	108.086(18)
I4–Cu2–I1	108.989(17)	I5–Cu5–Cu6	58.449(16)
I4–Cu2–Cu1	108.724(19)	I5–Cu5–Cu8	108.90(2)
I4–Cu2–Cu3	60.749(15)	I6–Cu5–Cu6	57.880(17)
Cu1–Cu2–Cu3	56.654(16)	I7–Cu5–I5	113.43(2)
Cu4–Cu2–I1	110.89(2)	I7–Cu5–I6	115.947(18)
Cu4–Cu2–I4	58.936(15)	I7–Cu5–Cu6	109.29(2)
Cu4–Cu2–Cu1	62.118(18)	I7–Cu5–Cu7	59.450(16)
Cu4–Cu2–Cu3	59.417(17)	I7–Cu5–Cu8	63.973(16)
$S8^{\#1}$–Cu2–I1	100.31(3)	Cu7–Cu5–I5	60.746(16)
$S8^{\#1}$–Cu2–I2	102.92(3)	Cu7–Cu5–I6	108.39(2)
$S8^{\#1}$–Cu2–I4	114.50(3)	Cu7–Cu5–Cu6	59.628(19)
$S8^{\#1}$–Cu2–Cu1	136.62(3)	Cu7–Cu5–Cu8	61.97(2)
$S8^{\#1}$–Cu2–Cu3	148.49(3)	Cu8–Cu5–I6	57.501(16)
$S8^{\#1}$–Cu2–Cu4	148.60(3)	Cu8–Cu5–Cu6	58.046(17)
I1–Cu3–I4	107.145(18)	S5–Cu5–I5	109.52(3)
I1–Cu3–Cu2	59.076(14)	S5–Cu5–I6	97.27(3)
I1–Cu3–Cu4	110.531(19)	S5–Cu5–I7	111.36(3)
I3–Cu3–I1	115.828(19)	S5–Cu5–Cu6	138.75(3)
I3–Cu3–I4	115.336(19)	S5–Cu5–Cu7	154.24(3)
I3–Cu3–Cu2	108.840(19)	S5–Cu5–Cu8	139.15(3)
I3–Cu3–Cu4	63.321(16)	I5–Cu6–I6	110.09(2)
I4–Cu3–Cu2	57.554(14)	I5–Cu6–Cu5	58.472(15)
Cu1–Cu3–I1	62.424(15)	I5–Cu6–Cu7	59.898(16)
Cu1–Cu3–I3	59.729(15)	I6–Cu6–Cu5	60.202(16)
Cu1–Cu3–I4	108.657(19)	I6–Cu6–Cu7	108.33(2)
Cu1–Cu3–Cu2	59.781(17)	I8–Cu6–I5	113.22(2)
Cu1–Cu3–Cu4	62.736(18)	I8–Cu6–I6	114.03(2)

I8–Cu6–Cu5	107.266(19)	C1B–S1–Cu1	112.2(4)
I8–Cu6–Cu7	60.108(17)	C7–S1–Cu1	99.01(15)
I8–Cu6–Cu8	61.422(17)	C7–S1–C1A	94.7(3)
Cu7–Cu6–Cu5	57.224(18)	C7–S1–C1B	121.3(4)
Cu8–Cu6–I5	109.46(2)	C10–S2–Cu3$^{\#3}$	105.04(13)
Cu8–Cu6–I6	58.508(18)	C10–S2–C11	100.2(2)
Cu8–Cu6–Cu5	58.662(17)	C11–S2–Cu3$^{\#3}$	115.15(13)
Cu8–Cu6–Cu7	61.315(19)	C17A–S3–Cu4	116.48(19)
S4–Cu6–I5	101.02(3)	C17B–S3–Cu4	102.7(4)
S4–Cu6–I6	107.11(4)	C23–S3–Cu4	102.41(15)
S4–Cu6–I8	110.43(4)	C23–S3–C17A	92.7(3)
S4–Cu6–Cu5	141.98(4)	C23–S3–C17B	123.0(4)
S4–Cu6–Cu7	143.87(4)	C26–S4–Cu6	101.34(16)
S4–Cu6–Cu8	149.21(4)	C27–S4–Cu6	110.37(16)
I5–Cu7–Cu6	59.468(16)	C27–S4–C26	100.5(3)
I5–Cu7–Cu8	106.83(2)	C33–S5–Cu5	113.80(13)
I7–Cu7–I5	113.57(2)	C39–S5–Cu5	103.40(14)
I7–Cu7–I8	114.64(2)	C39–S5–C33	100.1(2)
I7–Cu7–Cu5	60.032(16)	C42–S6–Cu7$^{\#3}$	104.56(18)
I7–Cu7–Cu6	112.67(2)	C43–S6–Cu7$^{\#3}$	110.14(15)
I7–Cu7–Cu8	63.336(17)	C43–S6–C42	104.2(3)
I8–Cu7–I5	111.49(2)	C49A–S7–Cu8	109.59(18)
I8–Cu7–Cu6	58.562(17)	C49B–S7–Cu8	116.5(6)
I8–Cu7–Cu8	59.907(18)	C55–S7–Cu8	99.63(15)
Cu5–Cu7–I5	60.326(16)	C55–S7–C49A	105.8(3)
Cu5–Cu7–I8	110.86(2)	C55–S7–C49B	80.4(7)
Cu5–Cu7–Cu6	63.149(19)	C58–S8–Cu2$^{\#4}$	104.70(15)
Cu5–Cu7–Cu8	59.703(19)	C58–S8–C59A	109.1(3)
Cu6–Cu7–Cu8	58.474(19)	C59A–S8–Cu2$^{\#4}$	105.1(2)
S6$^{\#2}$–Cu7–I5	111.49(3)	C59B–S8–C58	87.7(4)
S6$^{\#2}$–Cu7–I7	107.16(4)	S1–C1A–H1A	109.1
S6$^{\#2}$–Cu7–I8	97.23(4)	C2A–C1A–S1	109.4(4)
S6$^{\#2}$–Cu7–Cu5	151.86(4)	C2A–C1A–H1A	109.1
S6$^{\#2}$–Cu7–Cu6	139.25(4)	C6A–C1A–S1	108.6(4)
S6$^{\#2}$–Cu7–Cu8	140.71(4)	C6A–C1A–H1A	109.1
I6–Cu8–I7	114.49(2)	C6A–C1A–C2A	111.4(5)
I6–Cu8–I8	114.18(2)	S1–C1B–H1B	107.5
I6–Cu8–Cu5	62.727(16)	C2B–C1B–S1	112.4(8)
I6–Cu8–Cu6	61.289(18)	C2B–C1B–H1B	107.5
I6–Cu8–Cu7	109.66(2)	C6B–C1B–S1	109.5(9)
I8–Cu8–I7	107.62(2)	C6B–C1B–H1B	107.5
I8–Cu8–Cu7	58.916(18)	C6B–C1B–C2B	112.3(11)
Cu5–Cu8–I7	57.128(15)	C1A–C2A–H2AA	109.5
Cu5–Cu8–I8	108.85(2)	C1A–C2A–H2AB	109.5
Cu5–Cu8–Cu7	58.323(18)	C1A–C2A–C3A	110.6(5)
Cu6–Cu8–I7	108.04(2)	H2AA–C2A–H2AB	108.1
Cu6–Cu8–I8	58.807(18)	C3A–C2A–H2AA	109.5
Cu6–Cu8–Cu5	63.292(18)	C3A–C2A–H2AB	109.5
Cu6–Cu8–Cu7	60.21(2)	C1B–C2B–H2BA	109.4
Cu7–Cu8–I7	56.134(16)	C1B–C2B–H2BB	109.4
S7–Cu8–I6	115.09(4)	C1B–C2B–C3B	111.0(11)
S7–Cu8–I7	93.75(3)	H2BA–C2B–H2BB	108.0
S7–Cu8–I8	109.78(3)	C3B–C2B–H2BA	109.4
S7–Cu8–Cu5	137.21(4)	C3B–C2B–H2BB	109.4
S7–Cu8–Cu6	157.47(3)	C2A–C3A–H3AA	109.3
S7–Cu8–Cu7	133.71(4)	C2A–C3A–H3AB	109.3
C1A–S1–Cu1	109.81(17)	H3AA–C3A–H3AB	108.0

C4A–C3A–C2A	111.5(6)	C9–C10–H10B	110.0
C4A–C3A–H3AA	109.3	H10A–C10–H10B	108.4
C4A–C3A–H3AB	109.3	S2–C11–H11	108.0
C2B–C3B–H3BA	109.2	C12–C11–S2	112.4(3)
C2B–C3B–H3BB	109.2	C12–C11–H11	108.0
H3BA–C3B–H3BB	107.9	C16–C11–S2	108.5(3)
C4B–C3B–C2B	112.2(14)	C16–C11–H11	108.0
C4B–C3B–H3BA	109.2	C16–C11–C12	111.8(4)
C4B–C3B–H3BB	109.2	C11–C12–H12A	109.7
C3A–C4A–H4AA	109.5	C11–C12–H12B	109.7
C3A–C4A–H4AB	109.5	C11–C12–C13	109.8(4)
C3A–C4A–C5A	110.7(7)	H12A–C12–H12B	108.2
H4AA–C4A–H4AB	108.1	C13–C12–H12A	109.7
C5A–C4A–H4AA	109.5	C13–C12–H12B	109.7
C5A–C4A–H4AB	109.5	C12–C13–H13A	109.4
C3B–C4B–H4BA	109.6	C12–C13–H13B	109.4
C3B–C4B–H4BB	109.6	H13A–C13–H13B	108.0
C3B–C4B–C5B	110.3(18)	C14–C13–C12	111.1(6)
H4BA–C4B–H4BB	108.1	C14–C13–H13A	109.4
C5B–C4B–H4BA	109.6	C14–C13–H13B	109.4
C5B–C4B–H4BB	109.6	C13–C14–H14A	109.1
C4A–C5A–H5AA	109.7	C13–C14–H14B	109.1
C4A–C5A–H5AB	109.7	C13–C14–C15	112.4(5)
H5AA–C5A–H5AB	108.2	H14A–C14–H14B	107.9
C6A–C5A–C4A	110.0(8)	C15–C14–H14A	109.1
C6A–C5A–H5AA	109.7	C15–C14–H14B	109.1
C6A–C5A–H5AB	109.7	C14–C15–H15A	109.5
C4B–C5B–H5BA	108.9	C14–C15–H15B	109.5
C4B–C5B–H5BB	108.9	C14–C15–C16	110.9(4)
C4B–C5B–C6B	113.4(18)	H15A–C15–H15B	108.1
H5BA–C5B–H5BB	107.7	C16–C15–H15A	109.5
C6B–C5B–H5BA	108.9	C16–C15–H15B	109.5
C6B–C5B–H5BB	108.9	C11–C16–C15	110.1(5)
C1A–C6A–C5A	110.7(6)	C11–C16–H16A	109.6
C1A–C6A–H6AA	109.5	C11–C16–H16B	109.6
C1A–C6A–H6AB	109.5	C15–C16–H16A	109.6
C5A–C6A–H6AA	109.5	C15–C16–H16B	109.6
C5A–C6A–H6AB	109.5	H16A–C16–H16B	108.2
H6AA–C6A–H6AB	108.1	S3–C17A–H17A	108.4
C1B–C6B–C5B	109.4(14)	C18A–C17A–S3	114.7(4)
C1B–C6B–H6BA	109.8	C18A–C17A–H17A	108.4
C1B–C6B–H6BB	109.8	C18A–C17A–C22A	110.8(5)
C5B–C6B–H6BA	109.8	C22A–C17A–S3	105.8(4)
C5B–C6B–H6BB	109.8	C22A–C17A–H17A	108.4
H6BA–C6B–H6BB	108.2	S3–C17B–H17B	109.0
S1–C7–H7A	109.1	C18B–C17B–S3	110.4(9)
S1–C7–H7B	109.1	C18B–C17B–H17B	109.0
H7A–C7–H7B	107.8	C18B–C17B–C22B	113.7(11)
C8–C7–S1	112.7(3)	C22B–C17B–S3	105.6(9)
C8–C7–H7A	109.1	C22B–C17B–H17B	109.0
C8–C7–H7B	109.1	C17A–C18A–H18A	109.3
C9–C8–C7	173.7(5)	C17A–C18A–H18B	109.3
C8–C9–C10	172.0(5)	C17A–C18A–C19A	111.4(5)
S2–C10–H10A	110.0	H18A–C18A–H18B	108.0
S2–C10–H10B	110.0	C19A–C18A–H18A	109.3
C9–C10–S2	108.4(3)	C19A–C18A–H18B	109.3
C9–C10–H10A	110.0	C17B–C18B–H18C	109.7

C17B–C18B–H18D	109.7	C24–C23–H23A	109.2
C17B–C18B–C19B	109.8(11)	C24–C23–H23B	109.2
H18C–C18B–H18D	108.2	C25–C24–C23	176.4(5)
C19B–C18B–H18C	109.7	C24–C25–C26	176.5(6)
C19B–C18B–H18D	109.7	S4–C26–H26A	108.9
C18A–C19A–H19A	109.3	S4–C26–H26B	108.9
C18A–C19A–H19B	109.3	C25–C26–S4	113.5(4)
H19A–C19A–H19B	107.9	C25–C26–H26A	108.9
C20A–C19A–C18A	111.7(6)	C25–C26–H26B	108.9
C20A–C19A–H19A	109.3	H26A–C26–H26B	107.7
C20A–C19A–H19B	109.3	S4–C27–H27	106.3
C18B–C19B–H19C	109.6	S4–C27–H27A	103.7
C18B–C19B–H19D	109.6	C28A–C27–S4	114.9(4)
H19C–C19B–H19D	108.1	C28A–C27–H27	106.3
C20B–C19B–C18B	110.5(12)	C28A–C27–C32A	113.9(5)
C20B–C19B–H19C	109.6	C28B–C27–S4	106.9(6)
C20B–C19B–H19D	109.6	C28B–C27–H27A	103.7
C19A–C20A–H20A	109.3	C32A–C27–S4	108.5(4)
C19A–C20A–H20B	109.3	C32A–C27–H27	106.3
C19A–C20A–C21A	111.8(6)	C32B–C27–S4	125.2(6)
H20A–C20A–H20B	107.9	C32B–C27–H27A	103.7
C21A–C20A–H20A	109.3	C32B–C27–C28B	111.3(9)
C21A–C20A–H20B	109.3	C27–C28A–H28A	109.4
C19B–C20B–H20C	108.9	C27–C28A–H28B	109.4
C19B–C20B–H20D	108.9	C27–C28A–C29A	111.2(6)
H20C–C20B–H20D	107.7	H28A–C28A–H28B	108.0
C21B–C20B–C19B	113.4(15)	C29A–C28A–H28A	109.4
C21B–C20B–H20C	108.9	C29A–C28A–H28B	109.4
C21B–C20B–H20D	108.9	C27–C28B–H28C	108.1
C20A–C21A–H21A	109.6	C27–C28B–H28D	108.1
C20A–C21A–H21B	109.6	H28C–C28B–H28D	107.3
C20A–C21A–C22A	110.3(5)	C29B–C28B–C27	116.7(12)
H21A–C21A–H21B	108.1	C29B–C28B–H28C	108.1
C22A–C21A–H21A	109.6	C29B–C28B–H28D	108.1
C22A–C21A–H21B	109.6	C28A–C29A–H29A	109.0
C20B–C21B–H21C	109.1	C28A–C29A–H29B	109.0
C20B–C21B–H21D	109.1	H29A–C29A–H29B	107.8
C20B–C21B–C22B	112.6(15)	C30A–C29A–C28A	113.0(7)
H21C–C21B–H21D	107.8	C30A–C29A–H29A	109.0
C22B–C21B–H21C	109.1	C30A–C29A–H29B	109.0
C22B–C21B–H21D	109.1	C28B–C29B–H29C	109.7
C17A–C22A–C21A	110.1(5)	C28B–C29B–H29D	109.7
C17A–C22A–H22A	109.6	H29C–C29B–H29D	108.2
C17A–C22A–H22B	109.6	C30B–C29B–C28B	109.8(14)
C21A–C22A–H22A	109.6	C30B–C29B–H29C	109.7
C21A–C22A–H22B	109.6	C30B–C29B–H29D	109.7
H22A–C22A–H22B	108.2	C29A–C30A–H30A	109.4
C17B–C22B–H22C	109.4	C29A–C30A–H30B	109.4
C17B–C22B–H22D	109.4	C29A–C30A–C31A	111.1(7)
C21B–C22B–C17B	111.2(13)	H30A–C30A–H30B	108.0
C21B–C22B–H22C	109.4	C31A–C30A–H30A	109.4
C21B–C22B–H22D	109.4	C31A–C30A–H30B	109.4
H22C–C22B–H22D	108.0	C29B–C30B–H30C	109.1
S3–C23–H23A	109.2	C29B–C30B–H30D	109.1
S3–C23–H23B	109.2	H30C–C30B–H30D	107.8
H23A–C23–H23B	107.9	C31B–C30B–C29B	112.7(15)
C24–C23–S3	112.2(3)	C31B–C30B–H30C	109.1

C31B–C30B–H30D	109.1	C33–C38–H38B	109.6
C30A–C31A–H31A	109.9	C37–C38–H38A	109.6
C30A–C31A–H31B	109.9	C37–C38–H38B	109.6
H31A–C31A–H31B	108.3	H38A–C38–H38B	108.2
C32A–C31A–C30A	108.9(7)	S5–C39–H39A	109.6
C32A–C31A–H31A	109.9	S5–C39–H39B	109.6
C32A–C31A–H31B	109.9	H39A–C39–H39B	108.1
C30B–C31B–H31C	110.0	C40–C39–S5	110.1(3)
C30B–C31B–H31D	110.0	C40–C39–H39A	109.6
C30B–C31B–C32B	108.3(15)	C40–C39–H39B	109.6
H31C–C31B–H31D	108.4	C41–C40–C39	174.3(5)
C32B–C31B–H31C	110.0	C40–C41–C42	174.7(6)
C32B–C31B–H31D	110.0	S6–C42–H42A	109.4
C27–C32A–C31A	108.9(7)	S6–C42–H42B	109.4
C27–C32A–H32A	109.9	C41–C42–S6	111.1(3)
C27–C32A–H32B	109.9	C41–C42–H42A	109.4
C31A–C32A–H32A	109.9	C41–C42–H42B	109.4
C31A–C32A–H32B	109.9	H42A–C42–H42B	108.0
H32A–C32A–H32B	108.3	S6–C43–H43	106.3
C27–C32B–C31B	115.6(12)	C44–C43–S6	111.1(4)
C27–C32B–H32C	108.4	C44–C43–H43	106.3
C27–C32B–H32D	108.4	C44–C43–C48	111.9(4)
C31B–C32B–H32C	108.4	C48–C43–S6	114.3(3)
C31B–C32B–H32D	108.4	C48–C43–H43	106.3
H32C–C32B–H32D	107.5	C43–C44–H44A	109.6
S5–C33–H33	107.8	C43–C44–H44B	109.6
C34–C33–S5	108.5(3)	H44A–C44–H44B	108.2
C34–C33–H33	107.8	C45–C44–C43	110.1(5)
C38–C33–S5	113.2(3)	C45–C44–H44A	109.6
C38–C33–H33	107.8	C45–C44–H44B	109.6
C38–C33–C34	111.5(4)	C44–C45–H45A	109.2
C33–C34–H34A	109.7	C44–C45–H45B	109.2
C33–C34–H34B	109.7	C44–C45–C46	112.0(5)
C33–C34–C35	109.9(3)	H45A–C45–H45B	107.9
H34A–C34–H34B	108.2	C46–C45–H45A	109.2
C35–C34–H34A	109.7	C46–C45–H45B	109.2
C35–C34–H34B	109.7	C45–C46–H46A	109.4
C34–C35–H35A	109.2	C45–C46–H46B	109.4
C34–C35–H35B	109.2	H46A–C46–H46B	108.0
H35A–C35–H35B	107.9	C47–C46–C45	111.2(5)
C36–C35–C34	111.8(4)	C47–C46–H46A	109.4
C36–C35–H35A	109.2	C47–C46–H46B	109.4
C36–C35–H35B	109.2	C46–C47–H47A	109.3
C35–C36–H36A	109.5	C46–C47–H47B	109.3
C35–C36–H36B	109.5	C46–C47–C48	111.5(6)
C35–C36–C37	110.8(5)	H47A–C47–H47B	108.0
H36A–C36–H36B	108.1	C48–C47–H47A	109.3
C37–C36–H36A	109.5	C48–C47–H47B	109.3
C37–C36–H36B	109.5	C43–C48–H48A	109.3
C36–C37–H37A	109.4	C43–C48–H48B	109.3
C36–C37–H37B	109.4	C47–C48–C43	111.5(4)
C36–C37–C38	111.2(5)	C47–C48–H48A	109.3
H37A–C37–H37B	108.0	C47–C48–H48B	109.3
C38–C37–H37A	109.4	H48A–C48–H48B	108.0
C38–C37–H37B	109.4	S7–C49A–H49A	106.0
C33–C38–C37	110.1(4)	C50A–C49A–S7	115.2(5)
C33–C38–H38A	109.6	C50A–C49A–H49A	106.0

C50A–C49A–C54A	112.5(5)	C49A–C54A–C53A	110.4(5)
C54A–C49A–S7	110.5(4)	C49A–C54A–H54A	109.6
C54A–C49A–H49A	106.0	C49A–C54A–H54B	109.6
S7–C49B–H49B	108.0	C53A–C54A–H54A	109.6
C50B–C49B–S7	120.6(14)	C53A–C54A–H54B	109.6
C50B–C49B–H49B	108.0	H54A–C54A–H54B	108.1
C54B–C49B–S7	98.8(15)	C49B–C54B–C53B	115(2)
C54B–C49B–H49B	108.0	C49B–C54B–H54C	108.4
C54B–C49B–C50B	112.5(19)	C49B–C54B–H54D	108.4
C49A–C50A–H50A	109.4	C53B–C54B–H54C	108.4
C49A–C50A–H50B	109.4	C53B–C54B–H54D	108.4
C49A–C50A–C51A	111.0(7)	H54C–C54B–H54D	107.5
H50A–C50A–H50B	108.0	S7–C55–H55A	108.5
C51A–C50A–H50A	109.4	S7–C55–H55B	108.5
C51A–C50A–H50B	109.4	H55A–C55–H55B	107.5
C49B–C50B–H50C	109.4	C56–C55–S7	115.1(3)
C49B–C50B–H50D	109.4	C56–C55–H55A	108.5
C49B–C50B–C51B	111.0(17)	C56–C55–H55B	108.5
H50C–C50B–H50D	108.0	C57–C56–C55	178.0(5)
C51B–C50B–H50C	109.4	C56–C57–C58	177.0(5)
C51B–C50B–H50D	109.4	S8–C58–H58A	109.1
C50A–C51A–H51A	109.7	S8–C58–H58B	109.1
C50A–C51A–H51B	109.7	C57–C58–S8	112.6(3)
H51A–C51A–H51B	108.2	C57–C58–H58A	109.1
C52A–C51A–C50A	110.0(5)	C57–C58–H58B	109.1
C52A–C51A–H51A	109.7	H58A–C58–H58B	107.8
C52A–C51A–H51B	109.7	S8–C59A–H59A	106.9
C50B–C51B–H51C	109.2	C60A–C59A–S8	110.6(4)
C50B–C51B–H51D	109.2	C60A–C59A–H59A	106.9
H51C–C51B–H51D	107.9	C60A–C59A–C64A	112.1(6)
C52B–C51B–C50B	112(2)	C64A–C59A–S8	113.0(4)
C52B–C51B–H51C	109.2	C64A–C59A–H59A	106.9
C52B–C51B–H51D	109.2	S8–C59B–H59B	109.7
C51A–C52A–H52A	109.7	C60B–C59B–S8	105.3(7)
C51A–C52A–H52B	109.7	C60B–C59B–H59B	109.7
H52A–C52A–H52B	108.2	C60B–C59B–C64B	112.2(10)
C53A–C52A–C51A	109.9(6)	C64B–C59B–S8	110.1(8)
C53A–C52A–H52A	109.7	C64B–C59B–H59B	109.7
C53A–C52A–H52B	109.7	C59A–C60A–H60A	109.6
C51B–C52B–H52C	108.3	C59A–C60A–H60B	109.6
C51B–C52B–H52D	108.3	C59A–C60A–C61A	110.2(5)
H52C–C52B–H52D	107.4	H60A–C60A–H60B	108.1
C53B–C52B–C51B	116(2)	C61A–C60A–H60A	109.6
C53B–C52B–H52C	108.3	C61A–C60A–H60B	109.6
C53B–C52B–H52D	108.3	C59B–C60B–H60C	109.4
C52A–C53A–H53A	109.2	C59B–C60B–H60D	109.4
C52A–C53A–H53B	109.2	C59B–C60B–C61B	111.0(9)
C52A–C53A–C54A	111.9(5)	H60C–C60B–H60D	108.0
H53A–C53A–H53B	107.9	C61B–C60B–H60C	109.4
C54A–C53A–H53A	109.2	C61B–C60B–H60D	109.4
C54A–C53A–H53B	109.2	C60A–C61A–H61A	109.3
C52B–C53B–H53C	109.8	C60A–C61A–H61B	109.3
C52B–C53B–H53D	109.8	H61A–C61A–H61B	107.9
C52B–C53B–C54B	109(2)	C62A–C61A–C60A	111.8(5)
H53C–C53B–H53D	108.3	C62A–C61A–H61A	109.3
C54B–C53B–H53C	109.8	C62A–C61A–H61B	109.3
C54B–C53B–H53D	109.8	C60B–C61B–H61C	109.5

C60B–C61B–H61D	109.5
C60B–C61B–C62B	110.7(10)
H61C–C61B–H61D	108.1
C62B–C61B–H61C	109.5
C62B–C61B–H61D	109.5
C61A–C62A–H62A	109.4
C61A–C62A–H62B	109.4
H62A–C62A–H62B	108.0
C63A–C62A–C61A	111.0(6)
C63A–C62A–H62A	109.4
C63A–C62A–H62B	109.4
C61B–C62B–H62C	109.4
C61B–C62B–H62D	109.4
H62C–C62B–H62D	108.0
C63B–C62B–C61B	111.1(10)
C63B–C62B–H62C	109.4
C63B–C62B–H62D	109.4
C62A–C63A–H63A	109.4
C62A–C63A–H63B	109.4
C62A–C63A–C64A	111.0(6)
H63A–C63A–H63B	108.0
C64A–C63A–H63A	109.4
C64A–C63A–H63B	109.4
C62B–C63B–H63C	109.2
C62B–C63B–H63D	109.2
C62B–C63B–C64B	112.0(10)
H63C–C63B–H63D	107.9
C64B–C63B–H63C	109.2
C64B–C63B–H63D	109.2
C59A–C64A–C63A	110.7(5)
C59A–C64A–H64A	109.5
C59A–C64A–H64B	109.5
C63A–C64A–H64A	109.5
C63A–C64A–H64B	109.5
H64A–C64A–H64B	108.1
C59B–C64B–C63B	109.8(10)
C59B–C64B–H64C	109.7
C59B–C64B–H64D	109.7
C63B–C64B–H64C	109.7
C63B–C64B–H64D	109.7
H64C–C64B–H64D	108.2

Symmetry transformations used to generate equivalent atoms:
#1: -1+X, -1+Y, -1+Z; #2: 1+X, +Y, +Z; #3: -1+X, +Y, +Z; #4: 1+X, 1+Y, 1+Z;

Table S9 Torsion angles for CP1_100K

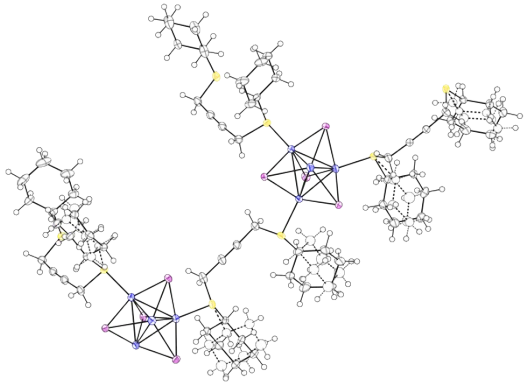
Atom–Atom–Atom–Atom	Torsion Angle [°]
Cu1–S1–C1A–C2A	174.3(4)
Cu1–S1–C1A–C6A	52.5(4)
Cu1–S1–C1B–C2B	−179.8(8)
Cu1–S1–C1B–C6B	−54.3(10)
Cu1–S1–C7–C8	−160.4(4)
Cu2$^{\#1}$–S8–C58–C57	159.4(3)
Cu2$^{\#1}$–S8–C59A–C60A	174.4(4)
Cu2$^{\#1}$–S8–C59A–C64A	47.8(6)
Cu2$^{\#1}$–S8–C59B–C60B	−97.8(7)
Cu2$^{\#1}$–S8–C59B–C64B	23.3(10)
Cu3$^{\#2}$–S2–C10–C9	157.7(3)
Cu3$^{\#2}$–S2–C11–C12	33.7(4)
Cu3$^{\#2}$–S2–C11–C16	−90.4(3)
Cu4–S3–C17A–C18A	30.8(5)
Cu4–S3–C17A–C22A	−91.7(4)
Cu4–S3–C17B–C18B	49.1(9)
Cu4–S3–C17B–C22B	172.4(8)
Cu4–S3–C23–C24	150.9(3)
Cu5–S5–C33–C34	85.4(3)
Cu5–S5–C33–C38	−39.0(4)
Cu5–S5–C39–C40	−172.9(3)
Cu6–S4–C26–C25	−165.3(4)
Cu6–S4–C27–C28A	173.2(4)
Cu6–S4–C27–C28B	99.7(7)
Cu6–S4–C27–C32A	44.6(5)
Cu6–S4–C27–C32B	−33.1(9)
Cu7$^{\#2}$–S6–C42–C41	139.1(4)
Cu7$^{\#2}$–S6–C43–C44	173.1(3)
Cu7$^{\#2}$–S6–C43–C48	45.2(4)
Cu8–S7–C49A–C50A	−40.8(5)
Cu8–S7–C49A–C54A	−169.6(4)
Cu8–S7–C49B–C50B	−25(2)
Cu8–S7–C49B–C54B	98.3(15)
Cu8–S7–C55–C56	−155.4(3)
S1–C1A–C2A–C3A	−175.3(5)
S1–C1A–C6A–C5A	178.0(5)
S1–C1B–C2B–C3B	178.1(10)
S1–C1B–C6B–C5B	−178.4(11)
S2–C11–C12–C13	−179.6(4)
S2–C11–C16–C15	−178.7(3)
S3–C17A–C18A–C19A	−175.7(4)
S3–C17A–C22A–C21A	−177.8(5)
S3–C17B–C18B–C19B	173.2(9)
S3–C17B–C22B–C21B	−173.6(11)
S4–C27–C28A–C29A	178.6(5)
S4–C27–C28B–C29B	176.5(10)
S4–C27–C32A–C31A	−172.8(6)
S4–C27–C32B–C31B	178.6(10)
S5–C33–C34–C35	178.0(3)
S5–C33–C38–C37	179.3(4)
S6–C43–C44–C45	175.4(3)
S6–C43–C48–C47	−177.5(3)
S7–C49A–C50A–C51A	177.2(5)
S7–C49A–C54A–C53A	−176.6(4)
S7–C49B–C50B–C51B	168.6(16)
S7–C49B–C54B–C53B	−179(2)
S8–C59A–C60A–C61A	178.4(5)
S8–C59A–C64A–C63A	−179.0(5)
S8–C59B–C60B–C61B	175.7(8)
S8–C59B–C64B–C63B	−171.6(8)
C1A–S1–C7–C8	88.7(4)
C1A–C2A–C3A–C4A	54.7(8)

C1B–S1–C7–C8	76.7(6)
C1B–C2B–C3B–C4B	−55.2(17)
C2A–C1A–C6A–C5A	57.4(7)
C2A–C3A–C4A–C5A	−56.2(10)
C2B–C1B–C6B–C5B	−52.8(16)
C2B–C3B–C4B–C5B	56(2)
C3A–C4A–C5A–C6A	57.5(10)
C3B–C4B–C5B–C6B	−56(2)
C4A–C5A–C6A–C1A	−58.1(9)
C4B–C5B–C6B–C1B	55(2)
C6A–C1A–C2A–C3A	−55.2(7)
C6B–C1B–C2B–C3B	54.1(15)
C7–S1–C1A–C2A	−84.3(4)
C7–S1–C1A–C6A	153.9(4)
C7–S1–C1B–C2B	−63.4(10)
C7–S1–C1B–C6B	62.1(10)
C10–S2–C11–C12	−78.3(4)
C10–S2–C11–C16	157.5(3)
C11–S2–C10–C9	−82.6(3)
C11–C12–C13–C14	56.2(7)
C12–C11–C16–C15	56.8(5)
C12–C13–C14–C15	−56.0(8)
C13–C14–C15–C16	55.3(8)
C14–C15–C16–C11	−54.6(7)
C16–C11–C12–C13	−57.3(6)
C17A–S3–C23–C24	−91.2(4)
C17A–C18A–C19A–C20A	54.5(8)
C17B–S3–C23–C24	−94.8(6)
C17B–C18B–C19B–C20B	−54.7(16)
C18A–C17A–C22A–C21A	57.3(7)
C18A–C19A–C20A–C21A	−54.8(8)
C18B–C17B–C22B–C21B	−52.5(17)
C18B–C19B–C20B–C21B	55.4(19)
C19A–C20A–C21A–C22A	56.1(8)
C19B–C20B–C21B–C22B	−54(2)
C20A–C21A–C22A–C17A	−57.1(8)
C20B–C21B–C22B–C17B	51(2)
C22A–C17A–C18A–C19A	−55.9(7)
C22B–C17B–C18B–C19B	54.7(15)
C23–S3–C17A–C18A	−74.5(5)
C23–S3–C17A–C22A	163.0(4)
C23–S3–C17B–C18B	−65.1(10)
C23–S3–C17B–C22B	58.3(10)
C26–S4–C27–C28A	−80.4(5)
C26–S4–C27–C28B	−153.9(7)
C26–S4–C27–C32A	151.0(5)
C26–S4–C27–C32B	73.3(8)
C27–S4–C26–C25	81.3(5)
C27–C28A–C29A–C30A	53.8(9)
C27–C28B–C29B–C30B	46.9(18)
C28A–C27–C32A–C31A	57.9(9)
C28A–C29A–C30A–C31A	−54.4(11)
C28B–C27–C32B–C31B	47.5(15)
C28B–C29B–C30B–C31B	−56(2)
C29A–C30A–C31A–C32A	55.9(12)
C29B–C30B–C31B–C32B	59(2)
C30A–C31A–C32A–C27	−55.7(11)
C30B–C31B–C32B–C27	−56.2(19)
C32A–C27–C28A–C29A	−55.5(8)
C32B–C27–C28B–C29B	−43.5(15)
C33–S5–C39–C40	69.5(4)
C33–C34–C35–C36	56.3(5)
C34–C33–C38–C37	56.6(6)
C34–C35–C36–C37	−56.4(6)
C35–C36–C37–C38	55.9(6)
C36–C37–C38–C33	−56.0(7)
C38–C33–C34–C35	−56.6(5)
C39–S5–C33–C34	−165.0(3)
C39–S5–C33–C38	70.6(4)
C42–S6–C43–C44	61.4(4)
C42–S6–C43–C48	−66.4(4)
C43–S6–C42–C41	−105.3(5)
C43–C44–C45–C46	55.7(6)
C44–C43–C48–C47	55.0(6)
C44–C45–C46–C47	−55.7(8)
C45–C46–C47–C48	54.2(7)
C46–C47–C48–C43	−54.1(5)
C48–C43–C44–C45	−55.5(6)
C49A–S7–C55–C56	91.0(4)
C49A–C50A–C51A–C52A	57.2(11)
C49B–S7–C55–C56	89.2(7)
C49B–C50B–C51B–C52B	−53(3)
C50A–C49A–C54A–C53A	53.1(7)
C50A–C51A–C52A–C53A	−58.6(10)
C50B–C49B–C54B–C53B	−51(3)
C50B–C51B–C52B–C53B	54(3)
C51A–C52A–C53A–C54A	58.2(8)
C51B–C52B–C53B–C54B	−49(4)
C52A–C53A–C54A–C49A	−54.9(7)
C52B–C53B–C54B–C49B	48(3)
C54A–C49A–C50A–C51A	−54.9(8)
C54B–C49B–C50B–C51B	53(3)
C55–S7–C49A–C50A	65.8(5)
C55–S7–C49A–C54A	−63.0(5)
C55–S7–C49B–C50B	71.4(17)
C55–S7–C49B–C54B	−165.7(15)
C58–S8–C59A–C60A	62.6(5)
C58–S8–C59A–C64A	−64.0(6)
C58–S8–C59B–C60B	156.4(8)
C58–S8–C59B–C64B	−82.5(8)
C59A–S8–C58–C57	−88.6(4)
C59A–C60A–C61A–C62A	55.1(8)
C59B–S8–C58–C57	−79.2(5)
C59B–C60B–C61B–C62B	−55.6(13)
C60A–C59A–C64A–C63A	55.3(8)
C60A–C61A–C62A–C63A	−56.7(8)
C60B–C59B–C64B–C63B	−54.7(13)
C60B–C61B–C62B–C63B	56.3(14)
C61A–C62A–C63A–C64A	56.7(8)
C61B–C62B–C63B–C64B	−56.4(14)
C62A–C63A–C64A–C59A	−55.8(9)
C62B–C63B–C64B–C59B	55.2(13)
C64A–C59A–C60A–C61A	−54.5(8)
C64B–C59B–C60B–C61B	56.0(13)

Symmetry transformations used to generate equivalent atoms:
#1: 1+X, 1+Y, 1+Z; #2: -1+X, +Y, +Z;

Crystal structure of CP1_150K

Crystal Data and Experimental



Experimental: The data for CP1_150K were collected from a shock-cooled single crystal at 150.0(1) K on a Bruker D8 Venture four-circle diffractometer with a X-ray tube using a graphite as monochromator and a CPAD PHOTON II area detector detector. The diffractometer was equipped with an Oxford Cryostream 800 low temperature device and used Mo K_{α} radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.38A and a multi-scan absorption correction using SADABS 2016/2 was applied. [1,2] The structure was solved by direct methods with SHELXT and refined by full-matrix least-squares methods against F^2 using SHELXL.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters, excepted minor disordered parts. For each compound, some disorders were found in the crystal structure and some geometric parameters of disordered components in each group were restrained by using RIGU or DFIX restraints. For more detail see the .res file included in the cif files. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[5] CCDC 2326782 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures. This report and the CIF file were generated using FinalCif.[6]

Table S10 Crystal data and structure refinement for CP1_150K

Internal Reference	CP1_150K
CCDC number	2326782
Empirical formula	$C_{64}H_{104}Cu_8I_8S_8$
Formula weight	2653.47
Temperature [K]	150.0(1)
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	11.7999(4)
b [Å]	18.7275(5)
c [Å]	20.7647(6)
α [°]	97.4108(10)
β [°]	104.6354(10)
γ [°]	103.1049(10)
Volume [Å^3]	4238.8(2)
Z	2
ρ_{calc} [gcm^{-3}]	2.079
μ [mm^{-1}]	5.112
F(000)	2544
Crystal size [mm^3]	0.084×0.133×0.172
Crystal colour	clear light colourless
Crystal shape	block
Radiation	Mo K_{α} (λ=0.71073 Å)
2θ range [°]	4.31 to 55.00 (0.77 Å)
Index ranges	−15 ≤ h ≤ 15 −24 ≤ k ≤ 24 −26 ≤ l ≤ 26
Reflections collected	509188
Independent reflections	19468 R_{int} = 0.0282 R_{sigma} = 0.0090
Completeness to θ = 25.242°	99.9 %
Data / Restraints / Parameters	19468 / 736 / 914
Goodness-of-fit on F^2	1.086
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0289 wR_2 = 0.0568
Final *R* indexes [all data]	R_1 = 0.0334 wR_2 = 0.0604
Largest peak/hole [eÅ^{-3}]	1.80/−1.81

Table S11 Bond lengths and angles for CP1_150K

Atom–Atom	Length [Å]
I1–Cu1	2.7276(5)
I1–Cu2	2.6870(5)
I1–Cu3	2.6631(5)
I2–Cu1	2.7264(5)
I2–Cu2	2.6572(6)
I2–Cu4	2.6801(6)
I3–Cu1	2.6002(5)
I3–Cu3	2.6244(6)
I3–Cu4	2.8024(6)
I4–Cu2	2.6722(5)
I4–Cu3	2.7659(6)
I4–Cu4	2.6250(6)
I5–Cu5	2.6810(5)
I5–Cu6	2.6785(5)
I5–Cu7	2.6903(5)
I6–Cu5	2.7616(5)
I6–Cu6	2.6911(6)
I6–Cu8	2.6147(6)
I7–Cu5	2.6272(5)
I7–Cu7	2.6129(6)
I7–Cu8	2.8187(6)
I8–Cu6	2.6368(6)
I8–Cu7	2.6789(6)
I8–Cu8	2.7058(6)
Cu1–Cu2	2.7018(7)
Cu1–Cu3	2.6030(7)
Cu1–Cu4	2.7793(7)
Cu1–S1	2.2895(10)
Cu2–Cu3	2.7966(7)
Cu2–Cu4	2.6763(7)
Cu2–S8$^{\#1}$	2.3037(10)
Cu3–Cu4	2.7236(7)
Cu3–S2$^{\#2}$	2.2818(10)
Cu4–S3	2.3047(11)
Cu5–Cu6	2.8164(7)
Cu5–Cu7	2.6480(7)
Cu5–Cu8	2.6972(7)
Cu5–S5	2.2906(10)
Cu6–Cu7	2.7266(7)
Cu6–Cu8	2.6693(7)
Cu6–S4	2.3058(10)
Cu7–Cu8	2.7517(7)
Cu7–S6$^{\#2}$	2.2941(12)
Cu8–S7	2.2972(10)
S1–C7	1.821(4)
S1–C1A	1.868(5)
S1–C1B	1.799(13)
S2–C10	1.821(4)
S2–C11	1.825(4)
S3–C23	1.833(5)
S3–C17A	1.852(5)
S3–C17B	1.919(16)
S4–C26	1.820(5)
S4–C27	1.817(4)
S5–C33	1.825(4)
S5–C39	1.822(4)
S6–C42	1.832(4)
S6–C43	1.816(5)
S7–C55	1.805(5)
S7–C49A	1.861(6)
S7–C49B	1.848(16)
S8–C58	1.811(5)
S8–C59A	1.862(5)
S8–C59B	1.823(13)
C7–H7A	0.9900
C7–H7B	0.9900
C7–C8	1.455(5)
C8–C9	1.180(6)
C9–C10	1.463(5)
C10–H10A	0.9900
C10–H10B	0.9900
C11–H11	1.0000
C11–C12	1.515(6)
C11–C16	1.527(6)
C12–H12A	0.9900
C12–H12B	0.9900
C12–C13	1.529(7)
C13–H13A	0.9900
C13–H13B	0.9900
C13–C14	1.520(9)
C14–H14A	0.9900
C14–H14B	0.9900
C14–C15	1.497(10)
C15–H15A	0.9900
C15–H15B	0.9900
C15–C16	1.536(7)
C16–H16A	0.9900
C16–H16B	0.9900
C23–H23A	0.9900
C23–H23B	0.9900
C23–C24	1.454(6)
C24–C25	1.170(6)
C25–C26	1.460(6)
C26–H26A	0.9900
C26–H26B	0.9900
C27–H27	1.0000
C27–H27A	1.0000
C27–C28A	1.449(7)
C27–C32A	1.514(9)
C27–C28B	1.53(2)
C27–C32B	1.426(19)
C33–H33	1.0000
C33–C34	1.513(6)
C33–C38	1.511(6)
C34–H34A	0.9900
C34–H34B	0.9900
C34–C35	1.523(6)
C35–H35A	0.9900
C35–H35B	0.9900

C35–C36	1.499(7)	C17A–H17A	1.0000
C36–H36A	0.9900	C17A–C18A	1.520(7)
C36–H36B	0.9900	C17A–C22A	1.525(8)
C36–C37	1.502(8)	C18A–H18A	0.9900
C37–H37A	0.9900	C18A–H18B	0.9900
C37–H37B	0.9900	C18A–C19A	1.529(8)
C37–C38	1.540(6)	C19A–H19A	0.9900
C38–H38A	0.9900	C19A–H19B	0.9900
C38–H38B	0.9900	C19A–C20A	1.511(9)
C39–H39A	0.9900	C20A–H20A	0.9900
C39–H39B	0.9900	C20A–H20B	0.9900
C39–C40	1.458(6)	C20A–C21A	1.514(11)
C40–C41	1.191(6)	C21A–H21A	0.9900
C41–C42	1.460(6)	C21A–H21B	0.9900
C42–H42A	0.9900	C21A–C22A	1.555(9)
C42–H42B	0.9900	C22A–H22A	0.9900
C43–H43	1.0000	C22A–H22B	0.9900
C43–C44	1.526(6)	C28A–H28A	0.9900
C43–C48	1.523(6)	C28A–H28B	0.9900
C44–H44A	0.9900	C28A–C29A	1.500(9)
C44–H44B	0.9900	C29A–H29A	0.9900
C44–C45	1.518(8)	C29A–H29B	0.9900
C45–H45A	0.9900	C29A–C30A	1.459(11)
C45–H45B	0.9900	C30A–H30A	0.9900
C45–C46	1.528(8)	C30A–H30B	0.9900
C46–H46A	0.9900	C30A–C31A	1.545(10)
C46–H46B	0.9900	C31A–H31A	0.9900
C46–C47	1.514(7)	C31A–H31B	0.9900
C47–H47A	0.9900	C31A–C32A	1.522(10)
C47–H47B	0.9900	C32A–H32A	0.9900
C47–C48	1.531(7)	C32A–H32B	0.9900
C48–H48A	0.9900	C49A–H49A	1.0000
C48–H48B	0.9900	C49A–C50A	1.481(9)
C55–H55A	0.9900	C49A–C54A	1.521(7)
C55–H55B	0.9900	C50A–H50A	0.9900
C55–C56	1.463(6)	C50A–H50B	0.9900
C56–C57	1.190(6)	C50A–C51A	1.548(9)
C57–C58	1.458(6)	C51A–H51A	0.9900
C58–H58A	0.9900	C51A–H51B	0.9900
C58–H58B	0.9900	C51A–C52A	1.518(10)
C1A–H1A	1.0000	C52A–H52A	0.9900
C1A–C2A	1.517(7)	C52A–H52B	0.9900
C1A–C6A	1.535(7)	C52A–C53A	1.483(10)
C2A–H2AA	0.9900	C53A–H53A	0.9900
C2A–H2AB	0.9900	C53A–H53B	0.9900
C2A–C3A	1.544(13)	C53A–C54A	1.532(8)
C3A–H3AA	0.9900	C54A–H54A	0.9900
C3A–H3AB	0.9900	C54A–H54B	0.9900
C3A–C4A	1.513(15)	C59A–H59A	1.0000
C4A–H4AA	0.9900	C59A–C60A	1.516(8)
C4A–H4AB	0.9900	C59A–C64A	1.527(8)
C4A–C5A	1.534(10)	C60A–H60A	0.9900
C5A–H5AA	0.9900	C60A–H60B	0.9900
C5A–H5AB	0.9900	C60A–C61A	1.533(9)
C5A–C6A	1.532(9)	C61A–H61A	0.9900
C6A–H6AA	0.9900	C61A–H61B	0.9900
C6A–H6AB	0.9900	C61A–C62A	1.494(10)

C62A–H62A	0.9900
C62A–H62B	0.9900
C62A–C63A	1.514(9)
C63A–H63A	0.9900
C63A–H63B	0.9900
C63A–C64A	1.528(8)
C64A–H64A	0.9900
C64A–H64B	0.9900
C1B–H1B	1.0000
C1B–C2B	1.50(2)
C1B–C6B	1.52(2)
C2B–H2BA	0.9900
C2B–H2BB	0.9900
C2B–C3B	1.53(4)
C3B–H3BA	0.9900
C3B–H3BB	0.9900
C3B–C4B	1.54(4)
C4B–H4BA	0.9900
C4B–H4BB	0.9900
C4B–C5B	1.48(2)
C5B–H5BA	0.9900
C5B–H5BB	0.9900
C5B–C6B	1.51(2)
C6B–H6BA	0.9900
C6B–H6BB	0.9900
C17B–H17B	1.0000
C17B–C18B	1.49(2)
C17B–C22B	1.53(2)
C18B–H18C	0.9900
C18B–H18D	0.9900
C18B–C19B	1.55(2)
C19B–H19C	0.9900
C19B–H19D	0.9900
C19B–C20B	1.50(3)
C20B–H20C	0.9900
C20B–H20D	0.9900
C20B–C21B	1.47(3)
C21B–H21C	0.9900
C21B–H21D	0.9900
C21B–C22B	1.53(3)
C22B–H22C	0.9900
C22B–H22D	0.9900
C28B–H28C	0.9900
C28B–H28D	0.9900
C28B–C29B	1.53(3)
C29B–H29C	0.9900
C29B–H29D	0.9900
C29B–C30B	1.51(3)
C30B–H30C	0.9900
C30B–H30D	0.9900
C30B–C31B	1.47(3)
C31B–H31C	0.9900
C31B–H31D	0.9900
C31B–C32B	1.56(3)
C32B–H32C	0.9900
C32B–H32D	0.9900
C49B–H49B	1.0000
C49B–C50B	1.50(2)
C49B–C54B	1.50(2)
C50B–H50C	0.9900
C50B–H50D	0.9900
C50B–C51B	1.54(2)
C51B–H51C	0.9900
C51B–H51D	0.9900
C51B–C52B	1.57(2)
C52B–H52C	0.9900
C52B–H52D	0.9900
C52B–C53B	1.43(3)
C53B–H53C	0.9900
C53B–H53D	0.9900
C53B–C54B	1.58(3)
C54B–H54C	0.9900
C54B–H54D	0.9900
C59B–H59B	1.0000
C59B–C60B	1.494(18)
C59B–C64B	1.52(2)
C60B–H60C	0.9900
C60B–H60D	0.9900
C60B–C61B	1.51(2)
C61B–H61C	0.9900
C61B–H61D	0.9900
C61B–C62B	1.53(2)
C62B–H62C	0.9900
C62B–H62D	0.9900
C62B–C63B	1.49(2)
C63B–H63C	0.9900
C63B–H63D	0.9900
C63B–C64B	1.53(2)
C64B–H64C	0.9900
C64B–H64D	0.9900

Atom–Atom–Atom	**Angle [°]**
Cu2–I1–Cu1	59.859(15)
Cu3–I1–Cu1	57.731(15)
Cu3–I1–Cu2	63.028(15)
Cu2–I2–Cu1	60.228(15)
Cu2–I2–Cu4	60.186(16)
Cu4–I2–Cu1	61.863(15)
Cu1–I3–Cu3	59.762(16)
Cu1–I3–Cu4	61.786(15)
Cu3–I3–Cu4	60.143(16)
Cu2–I4–Cu3	61.867(15)
Cu4–I4–Cu2	60.684(15)
Cu4–I4–Cu3	60.626(16)
Cu5–I5–Cu7	59.074(16)
Cu6–I5–Cu5	63.403(15)
Cu6–I5–Cu7	61.041(16)
Cu6–I6–Cu5	62.182(15)
Cu8–I6–Cu5	60.149(15)
Cu8–I6–Cu6	60.390(17)
Cu5–I7–Cu8	59.250(15)
Cu7–I7–Cu5	60.707(16)
Cu7–I7–Cu8	60.736(16)
Cu6–I8–Cu7	61.712(16)

Cu6–I8–Cu8	59.934(16)	Cu4–Cu3–I4	57.127(16)
Cu7–I8–Cu8	61.461(16)	Cu4–Cu3–Cu2	57.982(17)
I1–Cu1–Cu4	106.841(19)	$S2^{\#2}$–Cu3–I1	111.80(3)
I2–Cu1–I1	112.103(18)	$S2^{\#2}$–Cu3–I3	108.42(3)
I2–Cu1–Cu4	58.250(16)	$S2^{\#2}$–Cu3–I4	97.21(3)
I3–Cu1–I1	114.576(19)	$S2^{\#2}$–Cu3–Cu1	154.17(3)
I3–Cu1–I2	111.989(18)	$S2^{\#2}$–Cu3–Cu2	141.46(3)
I3–Cu1–Cu2	112.42(2)	$S2^{\#2}$–Cu3–Cu4	135.62(3)
I3–Cu1–Cu3	60.582(16)	I2–Cu4–I3	107.298(18)
I3–Cu1–Cu4	62.687(16)	I2–Cu4–Cu1	59.887(15)
Cu2–Cu1–I1	59.325(15)	I2–Cu4–Cu3	108.48(2)
Cu2–Cu1–I2	58.617(15)	I4–Cu4–I2	114.188(19)
Cu2–Cu1–Cu4	58.434(17)	I4–Cu4–I3	113.73(2)
Cu3–Cu1–I1	59.891(16)	I4–Cu4–Cu1	107.56(2)
Cu3–Cu1–I2	110.71(2)	I4–Cu4–Cu2	60.530(16)
Cu3–Cu1–Cu2	63.600(18)	I4–Cu4–Cu3	62.248(17)
Cu3–Cu1–Cu4	60.695(18)	Cu1–Cu4–I3	55.527(15)
S1–Cu1–I1	105.73(3)	Cu2–Cu4–I2	59.483(15)
S1–Cu1–I2	96.43(3)	Cu2–Cu4–I3	107.07(2)
S1–Cu1–I3	114.51(3)	Cu2–Cu4–Cu1	59.333(17)
S1–Cu1–Cu2	132.49(3)	Cu2–Cu4–Cu3	62.376(18)
S1–Cu1–Cu3	152.37(4)	Cu3–Cu4–I3	56.687(15)
S1–Cu1–Cu4	144.55(3)	Cu3–Cu4–Cu1	56.449(17)
I1–Cu2–Cu1	60.816(15)	S3–Cu4–I2	109.13(4)
I1–Cu2–Cu3	58.067(15)	S3–Cu4–I3	93.06(3)
I2–Cu2–I1	115.680(19)	S3–Cu4–I4	117.23(4)
I2–Cu2–I4	113.387(18)	S3–Cu4–Cu1	133.29(4)
I2–Cu2–Cu1	61.155(16)	S3–Cu4–Cu2	158.93(4)
I2–Cu2–Cu3	107.008(19)	S3–Cu4–Cu3	137.33(4)
I2–Cu2–Cu4	60.331(16)	I5–Cu5–I6	107.885(18)
I4–Cu2–I1	109.034(18)	I5–Cu5–Cu6	58.255(15)
I4–Cu2–Cu1	108.479(19)	I5–Cu5–Cu8	108.52(2)
I4–Cu2–Cu3	60.713(15)	I6–Cu5–Cu6	57.681(16)
I4–Cu2–Cu4	58.785(16)	I7–Cu5–I5	113.497(19)
Cu1–Cu2–Cu3	56.480(17)	I7–Cu5–I6	115.594(18)
Cu4–Cu2–I1	111.09(2)	I7–Cu5–Cu6	109.202(19)
Cu4–Cu2–Cu1	62.233(18)	I7–Cu5–Cu7	59.379(16)
Cu4–Cu2–Cu3	59.642(18)	I7–Cu5–Cu8	63.914(16)
$S8^{\#1}$–Cu2–I1	100.64(3)	Cu7–Cu5–I5	60.638(16)
$S8^{\#1}$–Cu2–I2	102.60(3)	Cu7–Cu5–I6	108.25(2)
$S8^{\#1}$–Cu2–I4	114.86(3)	Cu7–Cu5–Cu6	59.769(18)
$S8^{\#1}$–Cu2–Cu1	136.54(3)	Cu7–Cu5–Cu8	61.960(19)
$S8^{\#1}$–Cu2–Cu3	149.00(4)	Cu8–Cu5–I6	57.224(16)
$S8^{\#1}$–Cu2–Cu4	148.02(3)	Cu8–Cu5–Cu6	57.863(17)
I1–Cu3–I4	106.979(18)	S5–Cu5–I5	109.54(3)
I1–Cu3–Cu2	58.904(14)	S5–Cu5–I6	97.94(3)
I1–Cu3–Cu4	110.36(2)	S5–Cu5–I7	111.24(3)
I3–Cu3–I1	115.968(19)	S5–Cu5–Cu6	138.99(3)
I3–Cu3–I4	114.96(2)	S5–Cu5–Cu7	153.71(3)
I3–Cu3–Cu2	108.71(2)	S5–Cu5–Cu8	139.57(3)
I3–Cu3–Cu4	63.171(16)	I5–Cu6–I6	110.063(19)
I4–Cu3–Cu2	57.419(15)	I5–Cu6–Cu5	58.342(14)
Cu1–Cu3–I1	62.378(16)	I5–Cu6–Cu7	59.693(16)
Cu1–Cu3–I3	59.657(16)	I6–Cu6–Cu5	60.138(16)
Cu1–Cu3–I4	108.59(2)	I6–Cu6–Cu7	108.04(2)
Cu1–Cu3–Cu2	59.920(18)	I8–Cu6–I5	112.77(2)
Cu1–Cu3–Cu4	62.856(18)	I8–Cu6–I6	114.05(2)

I8–Cu6–Cu5	107.056(19)	C7–S1–C1A	95.6(2)
I8–Cu6–Cu7	59.905(16)	C1A–S1–Cu1	110.20(16)
I8–Cu6–Cu8	61.317(17)	C1B–S1–Cu1	112.4(4)
Cu7–Cu6–Cu5	57.046(17)	C1B–S1–C7	121.9(5)
Cu8–Cu6–I5	109.43(2)	C10–S2–Cu3$^{\#3}$	104.90(13)
Cu8–Cu6–I6	58.387(17)	C10–S2–C11	100.6(2)
Cu8–Cu6–Cu5	58.828(17)	C11–S2–Cu3$^{\#3}$	115.33(13)
Cu8–Cu6–Cu7	61.312(18)	C23–S3–Cu4	102.42(15)
S4–Cu6–I5	101.57(3)	C23–S3–C17A	94.6(2)
S4–Cu6–I6	106.71(4)	C23–S3–C17B	124.4(5)
S4–Cu6–I8	110.79(3)	C17A–S3–Cu4	116.28(17)
S4–Cu6–Cu5	141.87(4)	C17B–S3–Cu4	101.9(5)
S4–Cu6–Cu7	144.57(4)	C26–S4–Cu6	101.27(15)
S4–Cu6–Cu8	148.63(4)	C27–S4–Cu6	110.07(16)
I5–Cu7–Cu6	59.266(15)	C27–S4–C26	100.7(3)
I5–Cu7–Cu8	106.67(2)	C33–S5–Cu5	113.89(13)
I7–Cu7–I5	113.66(2)	C39–S5–Cu5	103.48(14)
I7–Cu7–I8	114.63(2)	C39–S5–C33	99.9(2)
I7–Cu7–Cu5	59.914(16)	C42–S6–Cu7$^{\#3}$	104.39(15)
I7–Cu7–Cu6	112.45(2)	C43–S6–Cu7$^{\#3}$	110.49(14)
I7–Cu7–Cu8	63.332(17)	C43–S6–C42	104.2(2)
I8–Cu7–I5	111.063(19)	C55–S7–Cu8	99.74(15)
I8–Cu7–Cu6	58.383(16)	C55–S7–C49A	107.8(3)
I8–Cu7–Cu8	59.751(17)	C55–S7–C49B	82.3(6)
Cu5–Cu7–I5	60.288(16)	C49A–S7–Cu8	109.17(18)
Cu5–Cu7–I8	110.86(2)	C49B–S7–Cu8	117.9(5)
Cu5–Cu7–Cu6	63.185(19)	C58–S8–Cu2$^{\#4}$	104.81(15)
Cu5–Cu7–Cu8	59.898(18)	C58–S8–C59A	108.6(3)
Cu6–Cu7–Cu8	58.318(18)	C58–S8–C59B	86.6(5)
S6$^{\#2}$–Cu7–I5	111.74(3)	C59A–S8–Cu2$^{\#4}$	105.76(18)
S6$^{\#2}$–Cu7–I7	107.47(3)	S1–C7–H7A	109.0
S6$^{\#2}$–Cu7–I8	97.02(4)	S1–C7–H7B	109.0
S6$^{\#2}$–Cu7–Cu5	152.07(4)	H7A–C7–H7B	107.8
S6$^{\#2}$–Cu7–Cu6	139.08(4)	C8–C7–S1	113.0(3)
S6$^{\#2}$–Cu7–Cu8	140.47(4)	C8–C7–H7A	109.0
I6–Cu8–I7	114.09(2)	C8–C7–H7B	109.0
I6–Cu8–I8	114.29(2)	C9–C8–C7	174.3(5)
I6–Cu8–Cu5	62.627(17)	C8–C9–C10	172.3(5)
I6–Cu8–Cu6	61.223(17)	S2–C10–H10A	110.0
I6–Cu8–Cu7	109.53(2)	S2–C10–H10B	110.0
I8–Cu8–I7	107.44(2)	C9–C10–S2	108.4(3)
I8–Cu8–Cu7	58.788(17)	C9–C10–H10A	110.0
Cu5–Cu8–I7	56.836(15)	C9–C10–H10B	110.0
Cu5–Cu8–I8	108.55(2)	H10A–C10–H10B	108.4
Cu5–Cu8–Cu7	58.142(18)	S2–C11–H11	107.9
Cu6–Cu8–I7	107.92(2)	C12–C11–S2	108.6(3)
Cu6–Cu8–I8	58.749(17)	C12–C11–H11	107.9
Cu6–Cu8–Cu5	63.309(18)	C12–C11–C16	112.1(4)
Cu6–Cu8–Cu7	60.369(19)	C16–C11–S2	112.3(3)
Cu7–Cu8–I7	55.931(15)	C16–C11–H11	107.9
S7–Cu8–I6	115.42(4)	C11–C12–H12A	109.6
S7–Cu8–I7	93.70(3)	C11–C12–H12B	109.6
S7–Cu8–I8	109.90(3)	C11–C12–C13	110.5(5)
S7–Cu8–Cu5	137.15(4)	H12A–C12–H12B	108.1
S7–Cu8–Cu6	157.63(3)	C13–C12–H12A	109.6
S7–Cu8–Cu7	133.40(4)	C13–C12–H12B	109.6
C7–S1–Cu1	99.20(14)	C12–C13–H13A	109.5

C12–C13–H13B	109.5	C33–C34–C35	110.1(4)
H13A–C13–H13B	108.1	H34A–C34–H34B	108.1
C14–C13–C12	110.8(5)	C35–C34–H34A	109.6
C14–C13–H13A	109.5	C35–C34–H34B	109.6
C14–C13–H13B	109.5	C34–C35–H35A	109.3
C13–C14–H14A	109.0	C34–C35–H35B	109.3
C13–C14–H14B	109.0	H35A–C35–H35B	108.0
H14A–C14–H14B	107.8	C36–C35–C34	111.7(4)
C15–C14–C13	112.7(5)	C36–C35–H35A	109.3
C15–C14–H14A	109.0	C36–C35–H35B	109.3
C15–C14–H14B	109.0	C35–C36–H36A	109.4
C14–C15–H15A	109.4	C35–C36–H36B	109.4
C14–C15–H15B	109.4	C35–C36–C37	111.0(4)
C14–C15–C16	111.1(5)	H36A–C36–H36B	108.0
H15A–C15–H15B	108.0	C37–C36–H36A	109.4
C16–C15–H15A	109.4	C37–C36–H36B	109.4
C16–C15–H15B	109.4	C36–C37–H37A	109.4
C11–C16–C15	109.6(4)	C36–C37–H37B	109.4
C11–C16–H16A	109.8	C36–C37–C38	111.3(5)
C11–C16–H16B	109.8	H37A–C37–H37B	108.0
C15–C16–H16A	109.8	C38–C37–H37A	109.4
C15–C16–H16B	109.8	C38–C37–H37B	109.4
H16A–C16–H16B	108.2	C33–C38–C37	110.1(4)
S3–C23–H23A	109.3	C33–C38–H38A	109.6
S3–C23–H23B	109.3	C33–C38–H38B	109.6
H23A–C23–H23B	107.9	C37–C38–H38A	109.6
C24–C23–S3	111.7(3)	C37–C38–H38B	109.6
C24–C23–H23A	109.3	H38A–C38–H38B	108.2
C24–C23–H23B	109.3	S5–C39–H39A	109.6
C25–C24–C23	175.9(5)	S5–C39–H39B	109.6
C24–C25–C26	176.8(5)	H39A–C39–H39B	108.1
S4–C26–H26A	108.9	C40–C39–S5	110.2(3)
S4–C26–H26B	108.9	C40–C39–H39A	109.6
C25–C26–S4	113.5(4)	C40–C39–H39B	109.6
C25–C26–H26A	108.9	C41–C40–C39	174.2(5)
C25–C26–H26B	108.9	C40–C41–C42	175.1(5)
H26A–C26–H26B	107.7	S6–C42–H42A	109.5
S4–C27–H27	106.1	S6–C42–H42B	109.5
S4–C27–H27A	103.1	C41–C42–S6	110.9(3)
C28A–C27–S4	115.0(4)	C41–C42–H42A	109.5
C28A–C27–H27	106.1	C41–C42–H42B	109.5
C28A–C27–C32A	113.1(5)	H42A–C42–H42B	108.0
C32A–C27–S4	109.8(4)	S6–C43–H43	106.4
C32A–C27–H27	106.1	C44–C43–S6	111.4(3)
C28B–C27–S4	104.9(8)	C44–C43–H43	106.4
C28B–C27–H27A	103.1	C48–C43–S6	114.1(3)
C32B–C27–S4	125.7(9)	C48–C43–H43	106.4
C32B–C27–H27A	103.1	C48–C43–C44	111.6(4)
C32B–C27–C28B	114.2(12)	C43–C44–H44A	109.6
S5–C33–H33	107.8	C43–C44–H44B	109.6
C34–C33–S5	108.7(3)	H44A–C44–H44B	108.1
C34–C33–H33	107.8	C45–C44–C43	110.4(5)
C38–C33–S5	113.4(3)	C45–C44–H44A	109.6
C38–C33–H33	107.8	C45–C44–H44B	109.6
C38–C33–C34	111.2(4)	C44–C45–H45A	109.4
C33–C34–H34A	109.6	C44–C45–H45B	109.4
C33–C34–H34B	109.6	C44–C45–C46	111.4(4)

H45A–C45–H45B	108.0	C5A–C4A–H4AA	109.6
C46–C45–H45A	109.4	C5A–C4A–H4AB	109.6
C46–C45–H45B	109.4	C4A–C5A–H5AA	109.2
C45–C46–H46A	109.3	C4A–C5A–H5AB	109.2
C45–C46–H46B	109.3	H5AA–C5A–H5AB	107.9
H46A–C46–H46B	108.0	C6A–C5A–C4A	112.0(5)
C47–C46–C45	111.4(4)	C6A–C5A–H5AA	109.2
C47–C46–H46A	109.3	C6A–C5A–H5AB	109.2
C47–C46–H46B	109.3	C1A–C6A–H6AA	109.5
C46–C47–H47A	109.4	C1A–C6A–H6AB	109.5
C46–C47–H47B	109.4	C5A–C6A–C1A	110.5(6)
C46–C47–C48	111.0(5)	C5A–C6A–H6AA	109.5
H47A–C47–H47B	108.0	C5A–C6A–H6AB	109.5
C48–C47–H47A	109.4	H6AA–C6A–H6AB	108.1
C48–C47–H47B	109.4	S3–C17A–H17A	108.3
C43–C48–C47	111.3(4)	C18A–C17A–S3	114.9(4)
C43–C48–H48A	109.4	C18A–C17A–H17A	108.3
C43–C48–H48B	109.4	C18A–C17A–C22A	111.1(5)
C47–C48–H48A	109.4	C22A–C17A–S3	105.8(4)
C47–C48–H48B	109.4	C22A–C17A–H17A	108.3
H48A–C48–H48B	108.0	C17A–C18A–H18A	109.3
S7–C55–H55A	108.5	C17A–C18A–H18B	109.3
S7–C55–H55B	108.5	C17A–C18A–C19A	111.5(5)
H55A–C55–H55B	107.5	H18A–C18A–H18B	108.0
C56–C55–S7	115.1(4)	C19A–C18A–H18A	109.3
C56–C55–H55A	108.5	C19A–C18A–H18B	109.3
C56–C55–H55B	108.5	C18A–C19A–H19A	109.4
C57–C56–C55	177.4(5)	C18A–C19A–H19B	109.4
C56–C57–C58	177.6(5)	H19A–C19A–H19B	108.0
S8–C58–H58A	109.0	C20A–C19A–C18A	111.3(6)
S8–C58–H58B	109.0	C20A–C19A–H19A	109.4
C57–C58–S8	112.8(4)	C20A–C19A–H19B	109.4
C57–C58–H58A	109.0	C19A–C20A–H20A	109.3
C57–C58–H58B	109.0	C19A–C20A–H20B	109.3
H58A–C58–H58B	107.8	C19A–C20A–C21A	111.6(6)
S1–C1A–H1A	109.0	H20A–C20A–H20B	108.0
C2A–C1A–S1	108.9(4)	C21A–C20A–H20A	109.3
C2A–C1A–H1A	109.0	C21A–C20A–H20B	109.3
C2A–C1A–C6A	111.5(5)	C20A–C21A–H21A	109.5
C6A–C1A–S1	109.4(4)	C20A–C21A–H21B	109.5
C6A–C1A–H1A	109.0	C20A–C21A–C22A	110.6(6)
C1A–C2A–H2AA	109.7	H21A–C21A–H21B	108.1
C1A–C2A–H2AB	109.7	C22A–C21A–H21A	109.5
C1A–C2A–C3A	110.1(7)	C22A–C21A–H21B	109.5
H2AA–C2A–H2AB	108.2	C17A–C22A–C21A	109.9(5)
C3A–C2A–H2AA	109.6	C17A–C22A–H22A	109.7
C3A–C2A–H2AB	109.7	C17A–C22A–H22B	109.7
C2A–C3A–H3AA	109.5	C21A–C22A–H22A	109.7
C2A–C3A–H3AB	109.5	C21A–C22A–H22B	109.7
H3AA–C3A–H3AB	108.1	H22A–C22A–H22B	108.2
C4A–C3A–C2A	110.6(10)	C27–C28A–H28A	109.3
C4A–C3A–H3AA	109.5	C27–C28A–H28B	109.3
C4A–C3A–H3AB	109.5	C27–C28A–C29A	111.7(6)
C3A–C4A–H4AA	109.6	H28A–C28A–H28B	107.9
C3A–C4A–H4AB	109.6	C29A–C28A–H28A	109.3
C3A–C4A–C5A	110.1(7)	C29A–C28A–H28B	109.3
H4AA–C4A–H4AB	108.1	C28A–C29A–H29A	108.9

C28A–C29A–H29B	108.9	C53A–C54A–H54B	109.5
H29A–C29A–H29B	107.7	H54A–C54A–H54B	108.1
C30A–C29A–C28A	113.5(7)	S8–C59A–H59A	107.0
C30A–C29A–H29A	108.9	C60A–C59A–S8	111.1(4)
C30A–C29A–H29B	108.9	C60A–C59A–H59A	107.0
C29A–C30A–H30A	109.4	C60A–C59A–C64A	111.7(5)
C29A–C30A–H30B	109.4	C64A–C59A–S8	112.7(4)
C29A–C30A–C31A	111.2(6)	C64A–C59A–H59A	107.0
H30A–C30A–H30B	108.0	C59A–C60A–H60A	109.6
C31A–C30A–H30A	109.4	C59A–C60A–H60B	109.6
C31A–C30A–H30B	109.4	C59A–C60A–C61A	110.1(5)
C30A–C31A–H31A	109.8	H60A–C60A–H60B	108.2
C30A–C31A–H31B	109.8	C61A–C60A–H60A	109.6
H31A–C31A–H31B	108.3	C61A–C60A–H60B	109.6
C32A–C31A–C30A	109.3(7)	C60A–C61A–H61A	109.1
C32A–C31A–H31A	109.8	C60A–C61A–H61B	109.1
C32A–C31A–H31B	109.8	H61A–C61A–H61B	107.9
C27–C32A–C31A	110.5(7)	C62A–C61A–C60A	112.3(6)
C27–C32A–H32A	109.6	C62A–C61A–H61A	109.1
C27–C32A–H32B	109.6	C62A–C61A–H61B	109.1
C31A–C32A–H32A	109.6	C61A–C62A–H62A	109.5
C31A–C32A–H32B	109.6	C61A–C62A–H62B	109.5
H32A–C32A–H32B	108.1	C61A–C62A–C63A	110.5(6)
S7–C49A–H49A	105.9	H62A–C62A–H62B	108.1
C50A–C49A–S7	114.9(5)	C63A–C62A–H62A	109.5
C50A–C49A–H49A	105.9	C63A–C62A–H62B	109.5
C50A–C49A–C54A	112.8(5)	C62A–C63A–H63A	109.4
C54A–C49A–S7	110.8(4)	C62A–C63A–H63B	109.4
C54A–C49A–H49A	105.9	C62A–C63A–C64A	111.1(6)
C49A–C50A–H50A	109.3	H63A–C63A–H63B	108.0
C49A–C50A–H50B	109.3	C64A–C63A–H63A	109.4
C49A–C50A–C51A	111.4(7)	C64A–C63A–H63B	109.4
H50A–C50A–H50B	108.0	C59A–C64A–C63A	110.3(5)
C51A–C50A–H50A	109.3	C59A–C64A–H64A	109.6
C51A–C50A–H50B	109.3	C59A–C64A–H64B	109.6
C50A–C51A–H51A	109.7	C63A–C64A–H64A	109.6
C50A–C51A–H51B	109.7	C63A–C64A–H64B	109.6
H51A–C51A–H51B	108.2	H64A–C64A–H64B	108.1
C52A–C51A–C50A	109.9(6)	S1–C1B–H1B	107.4
C52A–C51A–H51A	109.7	C2B–C1B–S1	108.7(10)
C52A–C51A–H51B	109.7	C2B–C1B–H1B	107.4
C51A–C52A–H52A	109.6	C2B–C1B–C6B	112.6(13)
C51A–C52A–H52B	109.6	C6B–C1B–S1	113.0(10)
H52A–C52A–H52B	108.1	C6B–C1B–H1B	107.4
C53A–C52A–C51A	110.3(7)	C1B–C2B–H2BA	109.8
C53A–C52A–H52A	109.6	C1B–C2B–H2BB	109.8
C53A–C52A–H52B	109.6	C1B–C2B–C3B	109(2)
C52A–C53A–H53A	109.2	H2BA–C2B–H2BB	108.3
C52A–C53A–H53B	109.2	C3B–C2B–H2BA	109.8
C52A–C53A–C54A	111.8(5)	C3B–C2B–H2BB	109.8
H53A–C53A–H53B	107.9	C2B–C3B–H3BA	109.3
C54A–C53A–H53A	109.2	C2B–C3B–H3BB	109.3
C54A–C53A–H53B	109.2	C2B–C3B–C4B	112(3)
C49A–C54A–C53A	110.6(5)	H3BA–C3B–H3BB	108.0
C49A–C54A–H54A	109.5	C4B–C3B–H3BA	109.3
C49A–C54A–H54B	109.5	C4B–C3B–H3BB	109.3
C53A–C54A–H54A	109.5	C3B–C4B–H4BA	110.0

C3B–C4B–H4BB	110.0	C29B–C28B–H28C	108.8
H4BA–C4B–H4BB	108.3	C29B–C28B–H28D	108.8
C5B–C4B–C3B	109(3)	C28B–C29B–H29C	109.8
C5B–C4B–H4BA	110.0	C28B–C29B–H29D	109.8
C5B–C4B–H4BB	110.0	H29C–C29B–H29D	108.2
C4B–C5B–H5BA	109.4	C30B–C29B–C28B	110(2)
C4B–C5B–H5BB	109.4	C30B–C29B–H29C	109.8
C4B–C5B–C6B	111.0(16)	C30B–C29B–H29D	109.8
H5BA–C5B–H5BB	108.0	C29B–C30B–H30C	108.5
C6B–C5B–H5BA	109.4	C29B–C30B–H30D	108.5
C6B–C5B–H5BB	109.4	H30C–C30B–H30D	107.5
C1B–C6B–H6BA	109.3	C31B–C30B–C29B	115(2)
C1B–C6B–H6BB	109.3	C31B–C30B–H30C	108.5
C5B–C6B–C1B	111.7(14)	C31B–C30B–H30D	108.5
C5B–C6B–H6BA	109.3	C30B–C31B–H31C	110.6
C5B–C6B–H6BB	109.3	C30B–C31B–H31D	110.6
H6BA–C6B–H6BB	107.9	C30B–C31B–C32B	106(2)
S3–C17B–H17B	109.1	H31C–C31B–H31D	108.8
C18B–C17B–S3	110.1(11)	C32B–C31B–H31C	110.6
C18B–C17B–H17B	109.1	C32B–C31B–H31D	110.6
C18B–C17B–C22B	114.6(13)	C27–C32B–C31B	113.9(17)
C22B–C17B–S3	104.8(10)	C27–C32B–H32C	108.8
C22B–C17B–H17B	109.1	C27–C32B–H32D	108.8
C17B–C18B–H18C	109.7	C31B–C32B–H32C	108.8
C17B–C18B–H18D	109.7	C31B–C32B–H32D	108.8
C17B–C18B–C19B	109.8(14)	H32C–C32B–H32D	107.7
H18C–C18B–H18D	108.2	S7–C49B–H49B	109.1
C19B–C18B–H18C	109.7	C50B–C49B–S7	118.6(11)
C19B–C18B–H18D	109.7	C50B–C49B–H49B	109.1
C18B–C19B–H19C	109.8	C54B–C49B–S7	98.4(12)
C18B–C19B–H19D	109.8	C54B–C49B–H49B	109.1
H19C–C19B–H19D	108.2	C54B–C49B–C50B	112.0(15)
C20B–C19B–C18B	109.5(17)	C49B–C50B–H50C	109.7
C20B–C19B–H19C	109.8	C49B–C50B–H50D	109.7
C20B–C19B–H19D	109.8	C49B–C50B–C51B	109.8(14)
C19B–C20B–H20C	108.7	H50C–C50B–H50D	108.2
C19B–C20B–H20D	108.7	C51B–C50B–H50C	109.7
H20C–C20B–H20D	107.6	C51B–C50B–H50D	109.7
C21B–C20B–C19B	114(2)	C50B–C51B–H51C	109.1
C21B–C20B–H20C	108.7	C50B–C51B–H51D	109.1
C21B–C20B–H20D	108.7	C50B–C51B–C52B	112.4(16)
C20B–C21B–H21C	109.3	H51C–C51B–H51D	107.9
C20B–C21B–H21D	109.3	C52B–C51B–H51C	109.1
C20B–C21B–C22B	111.8(19)	C52B–C51B–H51D	109.1
H21C–C21B–H21D	107.9	C51B–C52B–H52C	108.6
C22B–C21B–H21C	109.3	C51B–C52B–H52D	108.6
C22B–C21B–H21D	109.3	H52C–C52B–H52D	107.6
C17B–C22B–C21B	109.5(15)	C53B–C52B–C51B	114.5(19)
C17B–C22B–H22C	109.8	C53B–C52B–H52C	108.6
C17B–C22B–H22D	109.8	C53B–C52B–H52D	108.6
C21B–C22B–H22C	109.8	C52B–C53B–H53C	109.5
C21B–C22B–H22D	109.8	C52B–C53B–H53D	109.5
H22C–C22B–H22D	108.2	C52B–C53B–C54B	111(2)
C27–C28B–H28C	108.8	H53C–C53B–H53D	108.1
C27–C28B–H28D	108.8	C54B–C53B–H53C	109.5
H28C–C28B–H28D	107.7	C54B–C53B–H53D	109.5
C29B–C28B–C27	113.8(16)	C49B–C54B–C53B	115.0(18)

C49B–C54B–H54C	108.5
C49B–C54B–H54D	108.5
C53B–C54B–H54C	108.5
C53B–C54B–H54D	108.5
H54C–C54B–H54D	107.5
S8–C59B–H59B	109.4
C60B–C59B–S8	105.0(9)
C60B–C59B–H59B	109.4
C60B–C59B–C64B	112.9(12)
C64B–C59B–S8	110.6(10)
C64B–C59B–H59B	109.4
C59B–C60B–H60C	109.2
C59B–C60B–H60D	109.2
C59B–C60B–C61B	112.0(12)
H60C–C60B–H60D	107.9
C61B–C60B–H60C	109.2
C61B–C60B–H60D	109.2
C60B–C61B–H61C	109.6
C60B–C61B–H61D	109.6
C60B–C61B–C62B	110.2(14)
H61C–C61B–H61D	108.1
C62B–C61B–H61C	109.6
C62B–C61B–H61D	109.6
C61B–C62B–H62C	109.2
C61B–C62B–H62D	109.2
H62C–C62B–H62D	107.9
C63B–C62B–C61B	112.2(14)
C63B–C62B–H62C	109.2
C63B–C62B–H62D	109.2
C62B–C63B–H63C	109.2
C62B–C63B–H63D	109.2
C62B–C63B–C64B	111.8(13)
H63C–C63B–H63D	107.9
C64B–C63B–H63C	109.2
C64B–C63B–H63D	109.2
C59B–C64B–C63B	110.5(13)
C59B–C64B–H64C	109.5
C59B–C64B–H64D	109.5
C63B–C64B–H64C	109.5
C63B–C64B–H64D	109.5
H64C–C64B–H64D	108.1

Symmetry transformations used to generate equivalent atoms:
#1: -1+X, -1+Y, -1+Z; #2: 1+X, +Y, +Z; #3: -1+X, +Y, +Z; #4: 1+X, 1+Y, 1+Z;

Table S12. Torsion angles for CP1_150K

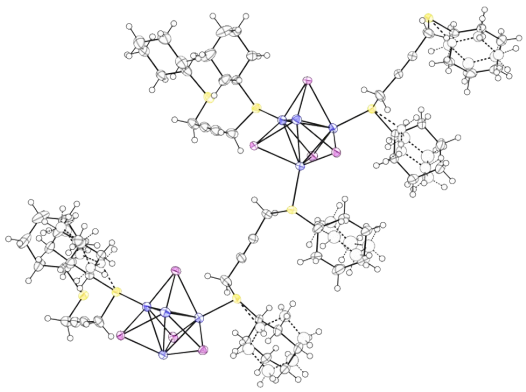
Atom–Atom–Atom–Atom	Torsion Angle [°]
Cu1–S1–C7–C8	−159.2(3)
Cu1–S1–C1A–C2A	51.8(4)
Cu1–S1–C1A–C6A	173.9(4)
Cu1–S1–C1B–C2B	−52.7(12)
Cu1–S1–C1B–C6B	−178.4(10)
Cu2$^{\#1}$–S8–C58–C57	158.9(3)
Cu2$^{\#1}$–S8–C59A–C60A	174.5(4)
Cu2$^{\#1}$–S8–C59A–C64A	48.2(5)
Cu2$^{\#1}$–S8–C59B–C60B	−98.6(9)
Cu2$^{\#1}$–S8–C59B–C64B	23.5(12)
Cu3$^{\#2}$–S2–C10–C9	158.4(3)
Cu3$^{\#2}$–S2–C11–C12	−90.2(3)
Cu3$^{\#2}$–S2–C11–C16	34.4(4)
Cu4–S3–C23–C24	151.1(3)
Cu4–S3–C17A–C18A	31.5(5)
Cu4–S3–C17A–C22A	−91.5(4)
Cu5–S5–C33–C34	85.0(3)
Cu5–S5–C33–C38	−39.2(4)
Cu5–S5–C39–C40	−172.1(3)
Cu6–S4–C26–C25	−165.2(3)
Cu6–S4–C27–C28A	174.5(4)
Cu6–S4–C27–C32A	45.7(5)
Cu6–S4–C27–C28B	99.2(9)
Cu6–S4–C27–C32B	−36.3(12)
Cu7$^{\#2}$–S6–C42–C41	139.3(3)
Cu7$^{\#2}$–S6–C43–C44	172.4(3)
Cu7$^{\#2}$–S6–C43–C48	44.9(3)
Cu8–S7–C55–C56	−156.1(3)
Cu8–S7–C49A–C50A	−41.6(6)
Cu8–S7–C49A–C54A	−170.8(4)
Cu8–S7–C49B–C50B	−23.5(16)
Cu8–S7–C49B–C54B	97.3(11)
S1–C1A–C2A–C3A	177.9(6)
S1–C1A–C6A–C5A	−175.5(5)
S1–C1B–C2B–C3B	−179(2)
S1–C1B–C6B–C5B	177.6(12)
S2–C11–C12–C13	−178.7(3)
S2–C11–C16–C15	−179.3(4)
S3–C17A–C18A–C19A	−176.0(4)
S3–C17A–C22A–C21A	−178.2(5)
S3–C17B–C18B–C19B	172.8(12)
S3–C17B–C22B–C21B	−173.8(13)
S4–C27–C28A–C29A	179.3(5)
S4–C27–C32A–C31A	−174.3(6)
S4–C27–C28B–C29B	174.3(15)
S4–C27–C32B–C31B	−176.6(13)
S5–C33–C34–C35	177.5(3)
S5–C33–C38–C37	179.4(4)
S6–C43–C44–C45	175.4(3)
S6–C43–C48–C47	−177.4(3)
S7–C49A–C50A–C51A	178.1(6)
S7–C49A–C54A–C53A	−177.2(4)
S7–C49B–C50B–C51B	168.0(12)
S7–C49B–C54B–C53B	−178.3(17)
S8–C59A–C60A–C61A	178.6(5)
S8–C59A–C64A–C63A	−178.5(5)
S8–C59B–C60B–C61B	175.8(11)
S8–C59B–C64B–C63B	−170.6(10)
C7–S1–C1A–C2A	153.8(4)
C7–S1–C1A–C6A	−84.1(4)
C7–S1–C1B–C2B	64.8(12)
C7–S1–C1B–C6B	−60.9(12)

C10–S2–C11–C12	157.6(3)
C10–S2–C11–C16	−77.8(4)
C11–S2–C10–C9	−81.6(3)
C11–C12–C13–C14	−54.4(7)
C12–C11–C16–C15	−56.8(6)
C12–C13–C14–C15	54.9(8)
C13–C14–C15–C16	−55.7(7)
C14–C15–C16–C11	55.5(7)
C16–C11–C12–C13	56.7(5)
C23–S3–C17A–C18A	−74.8(4)
C23–S3–C17A–C22A	162.3(4)
C26–S4–C27–C28A	−79.2(5)
C26–S4–C27–C32A	152.0(5)
C26–S4–C27–C28B	−154.5(9)
C26–S4–C27–C32B	70.0(12)
C27–S4–C26–C25	81.6(4)
C27–C28A–C29A–C30A	53.6(10)
C27–C28B–C29B–C30B	44(3)
C33–S5–C39–C40	70.2(4)
C33–C34–C35–C36	56.7(5)
C34–C33–C38–C37	56.5(6)
C34–C35–C36–C37	−56.4(6)
C35–C36–C37–C38	55.7(6)
C36–C37–C38–C33	−55.8(7)
C38–C33–C34–C35	−57.0(5)
C39–S5–C33–C34	−165.4(3)
C39–S5–C33–C38	70.4(4)
C42–S6–C43–C44	60.8(3)
C42–S6–C43–C48	−66.7(3)
C43–S6–C42–C41	−104.8(4)
C43–C44–C45–C46	56.1(6)
C44–C43–C48–C47	55.3(5)
C44–C45–C46–C47	−56.4(7)
C45–C46–C47–C48	55.0(6)
C46–C47–C48–C43	−54.6(5)
C48–C43–C44–C45	−55.8(5)
C55–S7–C49A–C50A	65.9(6)
C55–S7–C49A–C54A	−63.3(5)
C55–S7–C49B–C50B	73.5(14)
C55–S7–C49B–C54B	−165.7(12)
C58–S8–C59A–C60A	62.5(5)
C58–S8–C59A–C64A	−63.8(5)
C58–S8–C59B–C60B	156.1(10)
C58–S8–C59B–C64B	−81.8(10)
C1A–S1–C7–C8	89.3(4)
C1A–C2A–C3A–C4A	−58.8(11)
C2A–C1A–C6A–C5A	−55.0(7)
C2A–C3A–C4A–C5A	57.8(12)
C3A–C4A–C5A–C6A	−56.2(10)
C4A–C5A–C6A–C1A	54.2(8)
C6A–C1A–C2A–C3A	57.1(8)
C17A–S3–C23–C24	−90.7(4)
C17A–C18A–C19A–C20A	54.8(7)
C18A–C17A–C22A–C21A	56.5(7)
C18A–C19A–C20A–C21A	−55.5(8)
C19A–C20A–C21A–C22A	56.6(9)
C20A–C21A–C22A–C17A	−56.8(8)
C22A–C17A–C18A–C19A	−55.9(7)
C28A–C27–C32A–C31A	55.9(9)
C28A–C29A–C30A–C31A	−54.4(12)
C29A–C30A–C31A–C32A	55.1(13)
C30A–C31A–C32A–C27	−54.8(11)
C32A–C27–C28A–C29A	−53.5(9)
C49A–S7–C55–C56	90.0(4)
C49A–C50A–C51A–C52A	55.9(11)
C50A–C49A–C54A–C53A	52.5(8)
C50A–C51A–C52A–C53A	−58.1(11)
C51A–C52A–C53A–C54A	58.5(9)
C52A–C53A–C54A–C49A	−54.8(8)
C54A–C49A–C50A–C51A	−53.7(9)
C59A–S8–C58–C57	−88.4(4)
C59A–C60A–C61A–C62A	55.6(8)
C60A–C59A–C64A–C63A	55.6(8)
C60A–C61A–C62A–C63A	−56.8(9)
C61A–C62A–C63A–C64A	57.0(8)
C62A–C63A–C64A–C59A	−56.3(9)
C64A–C59A–C60A–C61A	−54.6(8)
C1B–S1–C7–C8	77.0(6)
C1B–C2B–C3B–C4B	57(4)
C2B–C1B–C6B–C5B	54.0(19)
C2B–C3B–C4B–C5B	−60(4)
C3B–C4B–C5B–C6B	59(3)
C4B–C5B–C6B–C1B	−57(2)
C6B–C1B–C2B–C3B	−53(2)
C17B–S3–C23–C24	−94.8(6)
C17B–C18B–C19B–C20B	−54(2)
C18B–C17B–C22B–C21B	−53(2)
C18B–C19B–C20B–C21B	57(3)
C19B–C20B–C21B–C22B	−56(3)
C20B–C21B–C22B–C17B	51(2)
C22B–C17B–C18B–C19B	55(2)
C28B–C27–C32B–C31B	51(2)
C28B–C29B–C30B–C31B	−56(3)
C29B–C30B–C31B–C32B	61(3)
C30B–C31B–C32B–C27	−58(3)
C32B–C27–C28B–C29B	−44(2)
C49B–S7–C55–C56	86.8(6)
C49B–C50B–C51B–C52B	−54(2)
C50B–C49B–C54B–C53B	−53(2)
C50B–C51B–C52B–C53B	53(3)
C51B–C52B–C53B–C54B	−48(3)
C52B–C53B–C54B–C49B	49(3)
C54B–C49B–C50B–C51B	54(2)
C59B–S8–C58–C57	−79.4(5)
C59B–C60B–C61B–C62B	−54.5(18)
C60B–C59B–C64B–C63B	−53.3(17)
C60B–C61B–C62B–C63B	55.1(19)
C61B–C62B–C63B–C64B	−54.9(19)
C62B–C63B–C64B–C59B	53.2(17)
C64B–C59B–C60B–C61B	55.1(17)

Symmetry transformations used to generate equivalent atoms:
#1: 1+X, 1+Y, 1+Z; #2: -1+X, +Y, +Z;

Crystal structure of CP1_200K

Crystal Data and Experimental



Experimental: The data for CP1_200K were collected from a shock-cooled single crystal at 200.0(1) K on a Bruker D8 Venture four-circle diffractometer with a X-ray tube using a graphite as monochromator and a CPAD PHOTON II area detector detector. The diffractometer was equipped with an Oxford Cryostream 800 low temperature device and used Mo K_{α} radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.38A and a multi-scan absorption correction using SADABS 2016/2 was applied. [1,2] The structure was solved by direct methods with SHELXT and refined by full-matrix least-squares methods against F^2 using SHELXL.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters, excepted minor disordered parts. For each compound, some disorders were found in the crystal structure and some geometric parameters of disordered components in each group were restrained by using RIGU or DFIX restraints. For more detail see the .res file included in the cif files.The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[5] CCDC 2356779 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures. This report and the CIF file were generated using FinalCif.[6]

Table S13. Crystal data and structure refinement for CP1_200K

Internal Reference	CP1_200K
CCDC number	2356779
Empirical formula	$C_{64}H_{104}Cu_8I_8S_8$
Formula weight	2653.47
Temperature [K]	200.0(1)
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	11.8439(4)
b [Å]	18.8172(5)
c [Å]	20.8187(6)
α [°]	97.3254(10)
β [°]	104.5536(10)
γ [°]	103.6389(10)
Volume [Å^3]	4277.4(2)
Z	2
ρ_{calc} [gcm^{-3}]	2.060
μ [mm^{-1}]	5.066
F(000)	2544
Crystal size [mm^3]	0.084×0.133×0.172
Crystal colour	clear light colourless
Crystal shape	block
Radiation	Mo K_{α} (λ=0.71073 Å)
2θ range [°]	4.30 to 55.00 (0.77 Å)
Index ranges	−15 ≤ h ≤ 15 −24 ≤ k ≤ 24 −27 ≤ l ≤ 27
Reflections collected	386877
Independent reflections	19652 R_{int} = 0.0300 R_{sigma} = 0.0110
Completeness to θ = 25.242°	99.9 %
Data / Restraints / Parameters	19652 / 737 / 914
Goodness-of-fit on F^2	1.080
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0309 wR_2 = 0.0670
Final *R* indexes [all data]	R_1 = 0.0376 wR_2 = 0.0725
Largest peak/hole [eÅ^{-3}]	1.43/−1.23

Table S14. Bond lengths and angles for CP1_200K

Atom–Atom	Length [Å]
I1–Cu1	2.7261(6)
I1–Cu2	2.6912(6)
I1–Cu3	2.6659(6)
I2–Cu1	2.7302(6)
I2–Cu2	2.6535(6)
I2–Cu4	2.6819(6)
I3–Cu1	2.5999(6)
I3–Cu3	2.6279(6)
I3–Cu4	2.8000(6)
I4–Cu2	2.6725(6)
I4–Cu3	2.7699(6)
I4–Cu4	2.6282(6)
I5–Cu5	2.6812(6)
I5–Cu6	2.6814(6)
I5–Cu7	2.6937(6)
I6–Cu5	2.7662(6)
I6–Cu6	2.6915(7)
I6–Cu8	2.6176(7)
I7–Cu5	2.6259(6)
I7–Cu7	2.6133(6)
I7–Cu8	2.8266(6)
I8–Cu6	2.6402(6)
I8–Cu7	2.6827(6)
I8–Cu8	2.7015(7)
Cu1–Cu2	2.7155(7)
Cu1–Cu3	2.6116(7)
Cu1–Cu4	2.7870(7)
Cu1–S1	2.2900(11)
Cu2–Cu3	2.8132(7)
Cu2–Cu4	2.6899(7)
Cu2–S8$^{\#1}$	2.3070(11)
Cu3–Cu4	2.7386(8)
Cu3–S2$^{\#2}$	2.2832(11)
Cu4–S3	2.3027(12)
Cu5–Cu6	2.8288(7)
Cu5–Cu7	2.6591(8)
Cu5–Cu8	2.7224(7)
Cu5–S5	2.2906(12)
Cu6–Cu7	2.7478(8)
Cu6–Cu8	2.6811(7)
Cu6–S4	2.3085(11)
Cu7–Cu8	2.7683(8)
Cu7–S6$^{\#2}$	2.2974(13)
Cu8–S7	2.2971(11)
S1–C1A	1.887(6)
S1–C1B	1.777(13)
S1–C7	1.818(5)
S2–C10	1.819(5)
S2–C11	1.826(4)
S3–C17A	1.853(6)
S3–C17B	1.916(14)
S3–C23	1.825(6)
S4–C26	1.817(5)
S4–C27	1.812(5)
S5–C33	1.820(4)
S5–C39	1.820(5)
S6–C42	1.826(5)
S6–C43	1.809(5)
S7–C49A	1.871(8)
S7–C49B	1.859(11)
S7–C55	1.811(6)
S8–C58	1.808(6)
S8–C59A	1.853(6)
S8–C59B	1.836(14)
C1A–H1A	1.0000
C1A–C2A	1.516(9)
C1A–C6A	1.532(9)
C1B–H1B	1.0000
C1B–C2B	1.507(19)
C1B–C6B	1.51(2)
C2A–H2AA	0.9900
C2A–H2AB	0.9900
C2A–C3A	1.574(18)
C2B–H2BA	0.9900
C2B–H2BB	0.9900
C2B–C3B	1.51(4)
C3A–H3AA	0.9900
C3A–H3AB	0.9900
C3A–C4A	1.52(2)
C3B–H3BA	0.9900
C3B–H3BB	0.9900
C3B–C4B	1.50(4)
C4A–H4AA	0.9900
C4A–H4AB	0.9900
C4A–C5A	1.305(16)
C4B–H4BA	0.9900
C4B–H4BB	0.9900
C4B–C5B	1.62(3)
C5A–H5AA	0.9900
C5A–H5AB	0.9900
C5A–C6A	1.547(11)
C5B–H5BA	0.9900
C5B–H5BB	0.9900
C5B–C6B	1.51(2)
C6A–H6AA	0.9900
C6A–H6AB	0.9900
C6B–H6BA	0.9900
C6B–H6BB	0.9900
C7–H7A	0.9900
C7–H7B	0.9900
C7–C8	1.449(6)
C8–C9	1.180(6)
C9–C10	1.457(6)
C10–H10A	0.9900
C10–H10B	0.9900
C11–H11	1.0000
C11–C12	1.520(7)
C11–C16	1.517(7)
C12–H12A	0.9900

C12–H12B	0.9900	C27–C28B	1.53(2)
C12–C13	1.524(7)	C27–C32A	1.518(10)
C13–H13A	0.9900	C27–C32B	1.38(2)
C13–H13B	0.9900	C28A–H28A	0.9900
C13–C14	1.512(10)	C28A–H28B	0.9900
C14–H14A	0.9900	C28A–C29A	1.488(11)
C14–H14B	0.9900	C28B–H28C	0.9900
C14–C15	1.495(11)	C28B–H28D	0.9900
C15–H15A	0.9900	C28B–C29B	1.52(3)
C15–H15B	0.9900	C29A–H29A	0.9900
C15–C16	1.537(8)	C29A–H29B	0.9900
C16–H16A	0.9900	C29A–C30A	1.444(12)
C16–H16B	0.9900	C29B–H29C	0.9900
C17A–H17A	1.0000	C29B–H29D	0.9900
C17A–C18A	1.528(9)	C29B–C30B	1.50(3)
C17A–C22A	1.517(9)	C30A–H30A	0.9900
C17B–H17B	1.0000	C30A–H30B	0.9900
C17B–C18B	1.465(19)	C30A–C31A	1.543(11)
C17B–C22B	1.536(19)	C30B–H30C	0.9900
C18A–H18A	0.9900	C30B–H30D	0.9900
C18A–H18B	0.9900	C30B–C31B	1.46(3)
C18A–C19A	1.519(9)	C31A–H31A	0.9900
C18B–H18C	0.9900	C31A–H31B	0.9900
C18B–H18D	0.9900	C31A–C32A	1.516(12)
C18B–C19B	1.54(2)	C31B–H31C	0.9900
C19A–H19A	0.9900	C31B–H31D	0.9900
C19A–H19B	0.9900	C31B–C32B	1.56(3)
C19A–C20A	1.518(12)	C32A–H32A	0.9900
C19B–H19C	0.9900	C32A–H32B	0.9900
C19B–H19D	0.9900	C32B–H32C	0.9900
C19B–C20B	1.52(2)	C32B–H32D	0.9900
C20A–H20A	0.9900	C33–H33	1.0000
C20A–H20B	0.9900	C33–C34	1.509(6)
C20A–C21A	1.489(13)	C33–C38	1.503(7)
C20B–H20C	0.9900	C34–H34A	0.9900
C20B–H20D	0.9900	C34–H34B	0.9900
C20B–C21B	1.50(3)	C34–C35	1.527(7)
C21A–H21A	0.9900	C35–H35A	0.9900
C21A–H21B	0.9900	C35–H35B	0.9900
C21A–C22A	1.566(12)	C35–C36	1.484(8)
C21B–H21C	0.9900	C36–H36A	0.9900
C21B–H21D	0.9900	C36–H36B	0.9900
C21B–C22B	1.52(2)	C36–C37	1.495(10)
C22A–H22A	0.9900	C37–H37A	0.9900
C22A–H22B	0.9900	C37–H37B	0.9900
C22B–H22C	0.9900	C37–C38	1.550(7)
C22B–H22D	0.9900	C38–H38A	0.9900
C23–H23A	0.9900	C38–H38B	0.9900
C23–H23B	0.9900	C39–H39A	0.9900
C23–C24	1.449(6)	C39–H39B	0.9900
C24–C25	1.178(6)	C39–C40	1.461(6)
C25–C26	1.455(6)	C40–C41	1.190(6)
C26–H26A	0.9900	C41–C42	1.453(6)
C26–H26B	0.9900	C42–H42A	0.9900
C27–H27	1.0000	C42–H42B	0.9900
C27–H27A	1.0000	C43–H43	1.0000
C27–C28A	1.450(8)	C43–C44	1.516(7)

C43–C48	1.517(7)
C44–H44A	0.9900
C44–H44B	0.9900
C44–C45	1.535(9)
C45–H45A	0.9900
C45–H45B	0.9900
C45–C46	1.512(9)
C46–H46A	0.9900
C46–H46B	0.9900
C46–C47	1.506(9)
C47–H47A	0.9900
C47–H47B	0.9900
C47–C48	1.540(7)
C48–H48A	0.9900
C48–H48B	0.9900
C49A–H49A	1.0000
C49A–C50A	1.469(13)
C49A–C54A	1.517(10)
C49B–H49B	1.0000
C49B–C50B	1.503(18)
C49B–C54B	1.463(16)
C50A–H50A	0.9900
C50A–H50B	0.9900
C50A–C51A	1.549(13)
C50B–H50C	0.9900
C50B–H50D	0.9900
C50B–C51B	1.57(2)
C51A–H51A	0.9900
C51A–H51B	0.9900
C51A–C52A	1.526(15)
C51B–H51C	0.9900
C51B–H51D	0.9900
C51B–C52B	1.44(2)
C52A–H52A	0.9900
C52A–H52B	0.9900
C52A–C53A	1.472(13)
C52B–H52C	0.9900
C52B–H52D	0.9900
C52B–C53B	1.54(2)
C53A–H53A	0.9900
C53A–H53B	0.9900
C53A–C54A	1.530(11)
C53B–H53C	0.9900
C53B–H53D	0.9900
C53B–C54B	1.529(17)
C54A–H54A	0.9900
C54A–H54B	0.9900
C54B–H54C	0.9900
C54B–H54D	0.9900
C55–H55A	0.9900
C55–H55B	0.9900
C55–C56	1.471(6)
C56–C57	1.178(6)
C57–C58	1.452(6)
C58–H58A	0.9900
C58–H58B	0.9900
C59A–H59A	1.0000
C59A–C60A	1.520(9)
C59A–C64A	1.533(10)
C59B–H59B	1.0000
C59B–C60B	1.51(2)
C59B–C64B	1.45(2)
C60A–H60A	0.9900
C60A–H60B	0.9900
C60A–C61A	1.528(11)
C60B–H60C	0.9900
C60B–H60D	0.9900
C60B–C61B	1.52(2)
C61A–H61A	0.9900
C61A–H61B	0.9900
C61A–C62A	1.473(13)
C61B–H61C	0.9900
C61B–H61D	0.9900
C61B–C62B	1.49(2)
C62A–H62A	0.9900
C62A–H62B	0.9900
C62A–C63A	1.509(12)
C62B–H62C	0.9900
C62B–H62D	0.9900
C62B–C63B	1.50(2)
C63A–H63A	0.9900
C63A–H63B	0.9900
C63A–C64A	1.536(10)
C63B–H63C	0.9900
C63B–H63D	0.9900
C63B–C64B	1.53(2)
C64A–H64A	0.9900
C64A–H64B	0.9900
C64B–H64C	0.9900
C64B–H64D	0.9900

Atom–Atom–Atom	**Angle [°]**
Cu2–I1–Cu1	60.164(16)
Cu3–I1–Cu1	57.927(17)
Cu3–I1–Cu2	63.354(17)
Cu2–I2–Cu1	60.563(17)
Cu2–I2–Cu4	60.548(17)
Cu4–I2–Cu1	61.981(17)
Cu1–I3–Cu3	59.939(17)
Cu1–I3–Cu4	62.013(17)
Cu3–I3–Cu4	60.501(17)
Cu2–I4–Cu3	62.219(16)
Cu4–I4–Cu2	60.981(17)
Cu4–I4–Cu3	60.903(17)
Cu5–I5–Cu6	63.675(17)
Cu5–I5–Cu7	59.303(17)
Cu6–I5–Cu7	61.488(17)
Cu6–I6–Cu5	62.420(17)
Cu8–I6–Cu5	60.675(17)
Cu8–I6–Cu6	60.643(18)
Cu5–I7–Cu8	59.771(17)
Cu7–I7–Cu5	61.000(18)
Cu7–I7–Cu8	61.031(18)
Cu6–I8–Cu7	62.152(17)

Cu6–I8–Cu8	60.241(18)	Cu4–Cu3–I4	56.992(17)
Cu7–I8–Cu8	61.882(18)	Cu4–Cu3–Cu2	57.941(18)
I1–Cu1–I2	111.78(2)	$S2^{\#2}$–Cu3–I1	112.08(4)
I1–Cu1–Cu4	106.90(2)	$S2^{\#2}$–Cu3–I3	108.45(4)
I2–Cu1–Cu4	58.158(17)	$S2^{\#2}$–Cu3–I4	97.65(3)
I3–Cu1–I1	114.69(2)	$S2^{\#2}$–Cu3–Cu1	153.98(4)
I3–Cu1–I2	111.94(2)	$S2^{\#2}$–Cu3–Cu2	141.68(4)
I3–Cu1–Cu2	112.35(2)	$S2^{\#2}$–Cu3–Cu4	135.73(4)
I3–Cu1–Cu3	60.563(18)	I2–Cu4–I3	107.37(2)
I3–Cu1–Cu4	62.523(17)	I2–Cu4–Cu1	59.861(17)
Cu2–Cu1–I1	59.281(16)	I2–Cu4–Cu2	59.203(17)
Cu2–Cu1–I2	58.320(17)	I2–Cu4–Cu3	108.28(2)
Cu2–Cu1–Cu4	58.511(18)	I4–Cu4–I2	113.82(2)
Cu3–Cu1–I1	59.880(18)	I4–Cu4–I3	113.61(2)
Cu3–Cu1–I2	110.63(2)	I4–Cu4–Cu1	107.34(2)
Cu3–Cu1–Cu2	63.72(2)	I4–Cu4–Cu2	60.323(18)
Cu3–Cu1–Cu4	60.86(2)	I4–Cu4–Cu3	62.105(18)
S1–Cu1–I1	106.53(3)	Cu1–Cu4–I3	55.464(16)
S1–Cu1–I2	96.29(3)	Cu2–Cu4–I3	107.09(2)
S1–Cu1–I3	114.08(3)	Cu2–Cu4–Cu1	59.416(19)
S1–Cu1–Cu2	132.84(4)	Cu2–Cu4–Cu3	62.42(2)
S1–Cu1–Cu3	152.70(4)	Cu3–Cu4–I3	56.637(17)
S1–Cu1–Cu4	143.75(4)	Cu3–Cu4–Cu1	56.404(19)
I1–Cu2–Cu1	60.555(17)	S3–Cu4–I2	109.54(4)
I1–Cu2–Cu3	57.884(16)	S3–Cu4–I3	93.61(3)
I2–Cu2–I1	115.40(2)	S3–Cu4–I4	116.88(4)
I2–Cu2–I4	113.30(2)	S3–Cu4–Cu1	133.90(4)
I2–Cu2–Cu1	61.116(18)	S3–Cu4–Cu2	158.48(4)
I2–Cu2–Cu3	106.91(2)	S3–Cu4–Cu3	137.48(4)
I2–Cu2–Cu4	60.249(18)	I5–Cu5–I6	107.842(19)
I4–Cu2–I1	108.96(2)	I5–Cu5–Cu6	58.167(16)
I4–Cu2–Cu1	108.17(2)	I5–Cu5–Cu8	108.22(2)
I4–Cu2–Cu3	60.589(17)	I6–Cu5–Cu6	57.495(17)
I4–Cu2–Cu4	58.696(17)	I7–Cu5–I5	113.55(2)
Cu1–Cu2–Cu3	56.343(19)	I7–Cu5–I6	115.15(2)
Cu4–Cu2–I1	110.79(2)	I7–Cu5–Cu6	109.14(2)
Cu4–Cu2–Cu1	62.072(19)	I7–Cu5–Cu7	59.266(18)
Cu4–Cu2–Cu3	59.64(2)	I7–Cu5–Cu8	63.780(17)
$S8^{\#1}$–Cu2–I1	100.62(3)	Cu7–Cu5–I5	60.583(17)
$S8^{\#1}$–Cu2–I2	103.08(4)	Cu7–Cu5–I6	108.15(2)
$S8^{\#1}$–Cu2–I4	114.89(4)	Cu7–Cu5–Cu6	60.00(2)
$S8^{\#1}$–Cu2–Cu1	136.79(4)	Cu7–Cu5–Cu8	61.90(2)
$S8^{\#1}$–Cu2–Cu3	148.59(4)	Cu8–Cu5–I6	56.962(18)
$S8^{\#1}$–Cu2–Cu4	148.36(4)	Cu8–Cu5–Cu6	57.722(19)
I1–Cu3–I4	106.84(2)	S5–Cu5–I5	109.75(3)
I1–Cu3–Cu2	58.763(16)	S5–Cu5–I6	97.89(3)
I1–Cu3–Cu4	110.07(2)	S5–Cu5–I7	111.51(3)
I3–Cu3–I1	115.81(2)	S5–Cu5–Cu6	138.72(4)
I3–Cu3–I4	114.61(2)	S5–Cu5–Cu7	153.87(4)
I3–Cu3–Cu2	108.46(2)	S5–Cu5–Cu8	139.56(4)
I3–Cu3–Cu4	62.862(18)	I5–Cu6–I6	110.06(2)
I4–Cu3–Cu2	57.192(16)	I5–Cu6–Cu5	58.159(16)
Cu1–Cu3–I1	62.192(18)	I5–Cu6–Cu7	59.476(17)
Cu1–Cu3–I3	59.498(17)	I6–Cu6–Cu5	60.084(18)
Cu1–Cu3–I4	108.33(2)	I6–Cu6–Cu7	107.75(2)
Cu1–Cu3–Cu2	59.939(19)	I8–Cu6–I5	112.36(2)
Cu1–Cu3–Cu4	62.73(2)	I8–Cu6–I6	113.93(2)

I8–Cu6–Cu5	106.85(2)	C1B–S1–Cu1	112.3(4)
I8–Cu6–Cu7	59.682(18)	C1B–S1–C7	121.2(5)
I8–Cu6–Cu8	61.013(19)	C7–S1–Cu1	99.64(16)
Cu7–Cu6–Cu5	56.935(19)	C7–S1–C1A	95.0(3)
Cu8–Cu6–I5	109.44(2)	C10–S2–Cu3$^{\#3}$	104.95(15)
Cu8–Cu6–I6	58.315(19)	C10–S2–C11	100.5(2)
Cu8–Cu6–Cu5	59.146(19)	C11–S2–Cu3$^{\#3}$	115.25(15)
Cu8–Cu6–Cu7	61.30(2)	C17A–S3–Cu4	116.8(2)
S4–Cu6–I5	101.97(3)	C17B–S3–Cu4	102.6(4)
S4–Cu6–I6	107.25(4)	C23–S3–Cu4	102.74(16)
S4–Cu6–I8	110.49(4)	C23–S3–C17A	93.3(3)
S4–Cu6–Cu5	142.34(4)	C23–S3–C17B	122.1(5)
S4–Cu6–Cu7	144.39(4)	C26–S4–Cu6	101.43(16)
S4–Cu6–Cu8	148.34(4)	C27–S4–Cu6	110.05(19)
I5–Cu7–Cu6	59.036(16)	C27–S4–C26	101.0(3)
I5–Cu7–Cu8	106.53(2)	C33–S5–Cu5	114.30(15)
I7–Cu7–I5	113.55(2)	C39–S5–Cu5	103.76(16)
I7–Cu7–I8	114.55(2)	C39–S5–C33	100.3(2)
I7–Cu7–Cu5	59.733(17)	C42–S6–Cu7$^{\#3}$	104.51(17)
I7–Cu7–Cu6	112.04(2)	C43–S6–Cu7$^{\#3}$	110.64(16)
I7–Cu7–Cu8	63.291(18)	C43–S6–C42	105.0(2)
I8–Cu7–I5	110.64(2)	C49A–S7–Cu8	107.7(3)
I8–Cu7–Cu6	58.166(17)	C49B–S7–Cu8	117.5(4)
I8–Cu7–Cu8	59.394(19)	C55–S7–Cu8	99.84(17)
Cu5–Cu7–I5	60.114(17)	C55–S7–C49A	111.8(4)
Cu5–Cu7–I8	110.67(2)	C55–S7–C49B	87.4(4)
Cu5–Cu7–Cu6	63.07(2)	C58–S8–Cu2$^{\#4}$	104.61(16)
Cu5–Cu7–Cu8	60.17(2)	C58–S8–C59A	109.2(3)
Cu6–Cu7–Cu8	58.161(19)	C58–S8–C59B	87.7(5)
S6$^{\#2}$–Cu7–I5	111.99(4)	C59A–S8–Cu2$^{\#4}$	106.0(2)
S6$^{\#2}$–Cu7–I7	107.84(4)	S1–C1A–H1A	108.9
S6$^{\#2}$–Cu7–I8	97.11(4)	C2A–C1A–S1	108.7(4)
S6$^{\#2}$–Cu7–Cu5	152.19(4)	C2A–C1A–H1A	108.9
S6$^{\#2}$–Cu7–Cu6	139.10(4)	C2A–C1A–C6A	111.9(5)
S6$^{\#2}$–Cu7–Cu8	140.26(4)	C6A–C1A–S1	109.4(5)
I6–Cu8–I7	113.41(2)	C6A–C1A–H1A	108.9
I6–Cu8–I8	114.34(2)	S1–C1B–H1B	107.6
I6–Cu8–Cu5	62.363(19)	C2B–C1B–S1	109.5(10)
I6–Cu8–Cu6	61.042(19)	C2B–C1B–H1B	107.6
I6–Cu8–Cu7	109.30(2)	C6B–C1B–S1	112.4(10)
I8–Cu8–I7	107.39(2)	C6B–C1B–H1B	107.6
I8–Cu8–Cu5	108.20(2)	C6B–C1B–C2B	111.9(12)
I8–Cu8–Cu7	58.724(18)	C1A–C2A–H2AA	110.4
Cu5–Cu8–I7	56.449(16)	C1A–C2A–H2AB	110.4
Cu5–Cu8–Cu7	57.92(2)	C1A–C2A–C3A	106.8(10)
Cu6–Cu8–I7	107.63(2)	H2AA–C2A–H2AB	108.6
Cu6–Cu8–I8	58.747(19)	C3A–C2A–H2AA	110.4
Cu6–Cu8–Cu5	63.132(19)	C3A–C2A–H2AB	110.4
Cu6–Cu8–Cu7	60.54(2)	C1B–C2B–H2BA	109.6
Cu7–Cu8–I7	55.678(17)	C1B–C2B–H2BB	109.6
S7–Cu8–I6	116.02(4)	C1B–C2B–C3B	110(3)
S7–Cu8–I7	93.69(3)	H2BA–C2B–H2BB	108.2
S7–Cu8–I8	109.93(4)	C3B–C2B–H2BA	109.6
S7–Cu8–Cu5	137.23(4)	C3B–C2B–H2BB	109.6
S7–Cu8–Cu6	157.90(4)	C2A–C3A–H3AA	109.6
S7–Cu8–Cu7	132.92(4)	C2A–C3A–H3AB	109.6
C1A–S1–Cu1	109.98(19)	H3AA–C3A–H3AB	108.2

C4A–C3A–C2A	110.1(15)	C9–C10–H10B	109.9
C4A–C3A–H3AA	109.6	H10A–C10–H10B	108.3
C4A–C3A–H3AB	109.6	S2–C11–H11	108.0
C2B–C3B–H3BA	107.4	C12–C11–S2	108.3(3)
C2B–C3B–H3BB	107.4	C12–C11–H11	108.0
H3BA–C3B–H3BB	106.9	C16–C11–S2	112.6(3)
C4B–C3B–C2B	120(3)	C16–C11–H11	108.0
C4B–C3B–H3BA	107.4	C16–C11–C12	111.9(4)
C4B–C3B–H3BB	107.4	C11–C12–H12A	109.6
C3A–C4A–H4AA	108.2	C11–C12–H12B	109.6
C3A–C4A–H4AB	108.2	C11–C12–C13	110.2(5)
H4AA–C4A–H4AB	107.4	H12A–C12–H12B	108.1
C5A–C4A–C3A	116.2(15)	C13–C12–H12A	109.6
C5A–C4A–H4AA	108.2	C13–C12–H12B	109.6
C5A–C4A–H4AB	108.2	C12–C13–H13A	109.4
C3B–C4B–H4BA	109.7	C12–C13–H13B	109.4
C3B–C4B–H4BB	109.7	H13A–C13–H13B	108.0
C3B–C4B–C5B	110(3)	C14–C13–C12	111.4(5)
H4BA–C4B–H4BB	108.2	C14–C13–H13A	109.4
C5B–C4B–H4BA	109.7	C14–C13–H13B	109.4
C5B–C4B–H4BB	109.7	C13–C14–H14A	109.2
C4A–C5A–H5AA	109.0	C13–C14–H14B	109.2
C4A–C5A–H5AB	109.0	H14A–C14–H14B	107.9
C4A–C5A–C6A	113.0(9)	C15–C14–C13	112.1(6)
H5AA–C5A–H5AB	107.8	C15–C14–H14A	109.2
C6A–C5A–H5AA	109.0	C15–C14–H14B	109.2
C6A–C5A–H5AB	109.0	C14–C15–H15A	109.3
C4B–C5B–H5BA	107.0	C14–C15–H15B	109.3
C4B–C5B–H5BB	107.0	C14–C15–C16	111.5(6)
H5BA–C5B–H5BB	106.8	H15A–C15–H15B	108.0
C6B–C5B–C4B	121.3(17)	C16–C15–H15A	109.3
C6B–C5B–H5BA	107.0	C16–C15–H15B	109.3
C6B–C5B–H5BB	107.0	C11–C16–C15	109.4(5)
C1A–C6A–C5A	109.9(7)	C11–C16–H16A	109.8
C1A–C6A–H6AA	109.7	C11–C16–H16B	109.8
C1A–C6A–H6AB	109.7	C15–C16–H16A	109.8
C5A–C6A–H6AA	109.7	C15–C16–H16B	109.8
C5A–C6A–H6AB	109.7	H16A–C16–H16B	108.2
H6AA–C6A–H6AB	108.2	S3–C17A–H17A	108.4
C1B–C6B–C5B	111.8(14)	C18A–C17A–S3	114.7(4)
C1B–C6B–H6BA	109.3	C18A–C17A–H17A	108.4
C1B–C6B–H6BB	109.3	C22A–C17A–S3	105.6(5)
C5B–C6B–H6BA	109.3	C22A–C17A–H17A	108.4
C5B–C6B–H6BB	109.3	C22A–C17A–C18A	111.2(6)
H6BA–C6B–H6BB	107.9	S3–C17B–H17B	108.3
S1–C7–H7A	108.9	C18B–C17B–S3	111.0(11)
S1–C7–H7B	108.9	C18B–C17B–H17B	108.3
H7A–C7–H7B	107.7	C18B–C17B–C22B	115.5(13)
C8–C7–S1	113.3(3)	C22B–C17B–S3	105.2(9)
C8–C7–H7A	108.9	C22B–C17B–H17B	108.3
C8–C7–H7B	108.9	C17A–C18A–H18A	109.4
C9–C8–C7	174.3(5)	C17A–C18A–H18B	109.4
C8–C9–C10	172.9(5)	H18A–C18A–H18B	108.0
S2–C10–H10A	109.9	C19A–C18A–C17A	111.2(6)
S2–C10–H10B	109.9	C19A–C18A–H18A	109.4
C9–C10–S2	108.9(3)	C19A–C18A–H18B	109.4
C9–C10–H10A	109.9	C17B–C18B–H18C	109.4

C17B–C18B–H18D	109.4	C24–C23–H23A	109.1
C17B–C18B–C19B	111.0(14)	C24–C23–H23B	109.1
H18C–C18B–H18D	108.0	C25–C24–C23	176.2(5)
C19B–C18B–H18C	109.4	C24–C25–C26	177.0(5)
C19B–C18B–H18D	109.4	S4–C26–H26A	108.9
C18A–C19A–H19A	109.4	S4–C26–H26B	108.9
C18A–C19A–H19B	109.4	C25–C26–S4	113.5(4)
H19A–C19A–H19B	108.0	C25–C26–H26A	108.9
C20A–C19A–C18A	111.2(7)	C25–C26–H26B	108.9
C20A–C19A–H19A	109.4	H26A–C26–H26B	107.7
C20A–C19A–H19B	109.4	S4–C27–H27	105.6
C18B–C19B–H19C	109.6	S4–C27–H27A	101.2
C18B–C19B–H19D	109.6	C28A–C27–S4	115.9(5)
H19C–C19B–H19D	108.1	C28A–C27–H27	105.6
C20B–C19B–C18B	110.1(16)	C28A–C27–C32A	112.6(5)
C20B–C19B–H19C	109.6	C28B–C27–S4	103.6(10)
C20B–C19B–H19D	109.6	C28B–C27–H27A	101.2
C19A–C20A–H20A	109.2	C32A–C27–S4	110.7(5)
C19A–C20A–H20B	109.2	C32A–C27–H27	105.6
H20A–C20A–H20B	107.9	C32B–C27–S4	125.4(10)
C21A–C20A–C19A	112.2(7)	C32B–C27–H27A	101.2
C21A–C20A–H20A	109.2	C32B–C27–C28B	119.7(14)
C21A–C20A–H20B	109.2	C27–C28A–H28A	109.1
C19B–C20B–H20C	109.4	C27–C28A–H28B	109.1
C19B–C20B–H20D	109.4	C27–C28A–C29A	112.5(7)
H20C–C20B–H20D	108.0	H28A–C28A–H28B	107.8
C21B–C20B–C19B	111.1(17)	C29A–C28A–H28A	109.1
C21B–C20B–H20C	109.4	C29A–C28A–H28B	109.1
C21B–C20B–H20D	109.4	C27–C28B–H28C	109.3
C20A–C21A–H21A	109.7	C27–C28B–H28D	109.3
C20A–C21A–H21B	109.7	H28C–C28B–H28D	107.9
C20A–C21A–C22A	109.9(7)	C29B–C28B–C27	111.8(19)
H21A–C21A–H21B	108.2	C29B–C28B–H28C	109.3
C22A–C21A–H21A	109.7	C29B–C28B–H28D	109.3
C22A–C21A–H21B	109.7	C28A–C29A–H29A	108.7
C20B–C21B–H21C	108.8	C28A–C29A–H29B	108.7
C20B–C21B–H21D	108.8	H29A–C29A–H29B	107.6
C20B–C21B–C22B	114.0(17)	C30A–C29A–C28A	114.1(8)
H21C–C21B–H21D	107.7	C30A–C29A–H29A	108.7
C22B–C21B–H21C	108.8	C30A–C29A–H29B	108.7
C22B–C21B–H21D	108.8	C28B–C29B–H29C	109.4
C17A–C22A–C21A	110.4(7)	C28B–C29B–H29D	109.4
C17A–C22A–H22A	109.6	H29C–C29B–H29D	108.0
C17A–C22A–H22B	109.6	C30B–C29B–C28B	111(2)
C21A–C22A–H22A	109.6	C30B–C29B–H29C	109.4
C21A–C22A–H22B	109.6	C30B–C29B–H29D	109.4
H22A–C22A–H22B	108.1	C29A–C30A–H30A	109.3
C17B–C22B–H22C	110.0	C29A–C30A–H30B	109.3
C17B–C22B–H22D	110.0	C29A–C30A–C31A	111.8(8)
C21B–C22B–C17B	108.5(14)	H30A–C30A–H30B	107.9
C21B–C22B–H22C	110.0	C31A–C30A–H30A	109.3
C21B–C22B–H22D	110.0	C31A–C30A–H30B	109.3
H22C–C22B–H22D	108.4	C29B–C30B–H30C	108.9
S3–C23–H23A	109.1	C29B–C30B–H30D	108.9
S3–C23–H23B	109.1	H30C–C30B–H30D	107.7
H23A–C23–H23B	107.9	C31B–C30B–C29B	114(3)
C24–C23–S3	112.4(4)	C31B–C30B–H30C	108.9

C31B–C30B–H30D	108.9	C33–C38–H38B	109.7
C30A–C31A–H31A	109.9	C37–C38–H38A	109.7
C30A–C31A–H31B	109.9	C37–C38–H38B	109.7
H31A–C31A–H31B	108.3	H38A–C38–H38B	108.2
C32A–C31A–C30A	109.0(8)	S5–C39–H39A	109.6
C32A–C31A–H31A	109.9	S5–C39–H39B	109.6
C32A–C31A–H31B	109.9	H39A–C39–H39B	108.1
C30B–C31B–H31C	110.2	C40–C39–S5	110.3(4)
C30B–C31B–H31D	110.2	C40–C39–H39A	109.6
C30B–C31B–C32B	107(3)	C40–C39–H39B	109.6
H31C–C31B–H31D	108.5	C41–C40–C39	174.7(6)
C32B–C31B–H31C	110.2	C40–C41–C42	175.2(6)
C32B–C31B–H31D	110.2	S6–C42–H42A	109.3
C27–C32A–H32A	109.3	S6–C42–H42B	109.3
C27–C32A–H32B	109.3	C41–C42–S6	111.4(3)
C31A–C32A–C27	111.5(8)	C41–C42–H42A	109.3
C31A–C32A–H32A	109.3	C41–C42–H42B	109.3
C31A–C32A–H32B	109.3	H42A–C42–H42B	108.0
H32A–C32A–H32B	108.0	S6–C43–H43	106.3
C27–C32B–C31B	111.6(19)	C44–C43–S6	111.9(4)
C27–C32B–H32C	109.3	C44–C43–H43	106.3
C27–C32B–H32D	109.3	C44–C43–C48	111.6(4)
C31B–C32B–H32C	109.3	C48–C43–S6	113.9(3)
C31B–C32B–H32D	109.3	C48–C43–H43	106.3
H32C–C32B–H32D	108.0	C43–C44–H44A	109.6
S5–C33–H33	107.7	C43–C44–H44B	109.6
C34–C33–S5	108.7(3)	C43–C44–C45	110.2(5)
C34–C33–H33	107.7	H44A–C44–H44B	108.1
C38–C33–S5	113.1(3)	C45–C44–H44A	109.6
C38–C33–H33	107.7	C45–C44–H44B	109.6
C38–C33–C34	111.6(4)	C44–C45–H45A	109.3
C33–C34–H34A	109.6	C44–C45–H45B	109.3
C33–C34–H34B	109.6	H45A–C45–H45B	108.0
C33–C34–C35	110.3(4)	C46–C45–C44	111.5(5)
H34A–C34–H34B	108.1	C46–C45–H45A	109.3
C35–C34–H34A	109.6	C46–C45–H45B	109.3
C35–C34–H34B	109.6	C45–C46–H46A	109.3
C34–C35–H35A	109.3	C45–C46–H46B	109.3
C34–C35–H35B	109.3	H46A–C46–H46B	107.9
H35A–C35–H35B	108.0	C47–C46–C45	111.7(5)
C36–C35–C34	111.4(4)	C47–C46–H46A	109.3
C36–C35–H35A	109.3	C47–C46–H46B	109.3
C36–C35–H35B	109.3	C46–C47–H47A	109.5
C35–C36–H36A	109.3	C46–C47–H47B	109.5
C35–C36–H36B	109.3	C46–C47–C48	110.7(5)
C35–C36–C37	111.4(6)	H47A–C47–H47B	108.1
H36A–C36–H36B	108.0	C48–C47–H47A	109.5
C37–C36–H36A	109.3	C48–C47–H47B	109.5
C37–C36–H36B	109.3	C43–C48–C47	111.2(4)
C36–C37–H37A	109.4	C43–C48–H48A	109.4
C36–C37–H37B	109.4	C43–C48–H48B	109.4
C36–C37–C38	111.0(6)	C47–C48–H48A	109.4
H37A–C37–H37B	108.0	C47–C48–H48B	109.4
C38–C37–H37A	109.4	H48A–C48–H48B	108.0
C38–C37–H37B	109.4	S7–C49A–H49A	105.7
C33–C38–C37	109.8(4)	C50A–C49A–S7	114.8(7)
C33–C38–H38A	109.7	C50A–C49A–H49A	105.7

C50A–C49A–C54A	113.8(7)	C49A–C54A–C53A	110.4(7)
C54A–C49A–S7	110.1(6)	C49A–C54A–H54A	109.6
C54A–C49A–H49A	105.7	C49A–C54A–H54B	109.6
S7–C49B–H49B	108.5	C53A–C54A–H54A	109.6
C50B–C49B–S7	100.1(9)	C53A–C54A–H54B	109.6
C50B–C49B–H49B	108.5	H54A–C54A–H54B	108.1
C54B–C49B–S7	118.4(8)	C49B–C54B–C53B	111.6(11)
C54B–C49B–H49B	108.5	C49B–C54B–H54C	109.3
C54B–C49B–C50B	112.3(11)	C49B–C54B–H54D	109.3
C49A–C50A–H50A	109.6	C53B–C54B–H54C	109.3
C49A–C50A–H50B	109.6	C53B–C54B–H54D	109.3
C49A–C50A–C51A	110.5(10)	H54C–C54B–H54D	108.0
H50A–C50A–H50B	108.1	S7–C55–H55A	108.7
C51A–C50A–H50A	109.6	S7–C55–H55B	108.7
C51A–C50A–H50B	109.6	H55A–C55–H55B	107.6
C49B–C50B–H50C	109.1	C56–C55–S7	114.2(4)
C49B–C50B–H50D	109.1	C56–C55–H55A	108.7
C49B–C50B–C51B	112.4(13)	C56–C55–H55B	108.7
H50C–C50B–H50D	107.9	C57–C56–C55	177.3(5)
C51B–C50B–H50C	109.1	C56–C57–C58	176.9(5)
C51B–C50B–H50D	109.1	S8–C58–H58A	109.0
C50A–C51A–H51A	109.7	S8–C58–H58B	109.0
C50A–C51A–H51B	109.7	C57–C58–S8	113.1(4)
H51A–C51A–H51B	108.2	C57–C58–H58A	109.0
C52A–C51A–C50A	109.7(8)	C57–C58–H58B	109.0
C52A–C51A–H51A	109.7	H58A–C58–H58B	107.8
C52A–C51A–H51B	109.7	S8–C59A–H59A	107.0
C50B–C51B–H51C	109.2	C60A–C59A–S8	111.3(5)
C50B–C51B–H51D	109.2	C60A–C59A–H59A	107.0
H51C–C51B–H51D	107.9	C60A–C59A–C64A	111.5(6)
C52B–C51B–C50B	112.2(16)	C64A–C59A–S8	112.6(5)
C52B–C51B–H51C	109.2	C64A–C59A–H59A	107.0
C52B–C51B–H51D	109.2	S8–C59B–H59B	108.5
C51A–C52A–H52A	109.8	C60B–C59B–S8	105.4(11)
C51A–C52A–H52B	109.8	C60B–C59B–H59B	108.5
H52A–C52A–H52B	108.2	C64B–C59B–S8	112.9(12)
C53A–C52A–C51A	109.4(9)	C64B–C59B–H59B	108.5
C53A–C52A–H52A	109.8	C64B–C59B–C60B	113.0(14)
C53A–C52A–H52B	109.8	C59A–C60A–H60A	109.7
C51B–C52B–H52C	109.0	C59A–C60A–H60B	109.7
C51B–C52B–H52D	109.0	C59A–C60A–C61A	110.0(6)
C51B–C52B–C53B	112.8(14)	H60A–C60A–H60B	108.2
H52C–C52B–H52D	107.8	C61A–C60A–H60A	109.7
C53B–C52B–H52C	109.0	C61A–C60A–H60B	109.7
C53B–C52B–H52D	109.0	C59B–C60B–H60C	109.2
C52A–C53A–H53A	109.0	C59B–C60B–H60D	109.2
C52A–C53A–H53B	109.0	C59B–C60B–C61B	112.1(14)
C52A–C53A–C54A	112.9(8)	H60C–C60B–H60D	107.9
H53A–C53A–H53B	107.8	C61B–C60B–H60C	109.2
C54A–C53A–H53A	109.0	C61B–C60B–H60D	109.2
C54A–C53A–H53B	109.0	C60A–C61A–H61A	109.0
C52B–C53B–H53C	109.4	C60A–C61A–H61B	109.0
C52B–C53B–H53D	109.4	H61A–C61A–H61B	107.8
H53C–C53B–H53D	108.0	C62A–C61A–C60A	112.7(7)
C54B–C53B–C52B	111.1(12)	C62A–C61A–H61A	109.0
C54B–C53B–H53C	109.4	C62A–C61A–H61B	109.0
C54B–C53B–H53D	109.4	C60B–C61B–H61C	109.4

C60B–C61B–H61D	109.4
H61C–C61B–H61D	108.0
C62B–C61B–C60B	111.2(17)
C62B–C61B–H61C	109.4
C62B–C61B–H61D	109.4
C61A–C62A–H62A	109.3
C61A–C62A–H62B	109.3
C61A–C62A–C63A	111.4(7)
H62A–C62A–H62B	108.0
C63A–C62A–H62A	109.3
C63A–C62A–H62B	109.3
C61B–C62B–H62C	109.2
C61B–C62B–H62D	109.2
C61B–C62B–C63B	112.1(15)
H62C–C62B–H62D	107.9
C63B–C62B–H62C	109.2
C63B–C62B–H62D	109.2
C62A–C63A–H63A	109.6
C62A–C63A–H63B	109.6
C62A–C63A–C64A	110.5(7)
H63A–C63A–H63B	108.1
C64A–C63A–H63A	109.6
C64A–C63A–H63B	109.6
C62B–C63B–H63C	109.3
C62B–C63B–H63D	109.3
C62B–C63B–C64B	111.7(15)
H63C–C63B–H63D	107.9
C64B–C63B–H63C	109.3
C64B–C63B–H63D	109.3
C59A–C64A–C63A	109.6(7)
C59A–C64A–H64A	109.7
C59A–C64A–H64B	109.7
C63A–C64A–H64A	109.7
C63A–C64A–H64B	109.7
H64A–C64A–H64B	108.2
C59B–C64B–C63B	113.0(16)
C59B–C64B–H64C	109.0
C59B–C64B–H64D	109.0
C63B–C64B–H64C	109.0
C63B–C64B–H64D	109.0
H64C–C64B–H64D	107.8

Symmetry transformations used to generate equivalent atoms:
#1: -1+X, -1+Y, -1+Z; #2: 1+X, +Y, +Z; #3: -1+X, +Y, +Z; #4: 1+X, 1+Y, 1+Z;

Table S15. Torsion angles for CP1_200K

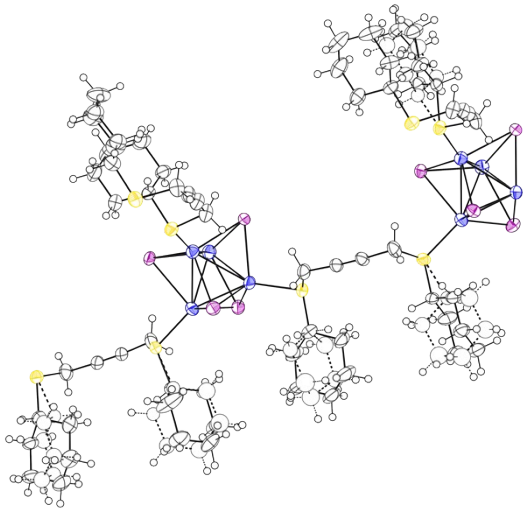
Atom–Atom–Atom–Atom	Torsion Angle [°]
Cu1–S1–C1A–C2A	51.9(5)
Cu1–S1–C1A–C6A	174.4(4)
Cu1–S1–C1B–C2B	−51.8(11)
Cu1–S1–C1B–C6B	−176.8(9)
Cu1–S1–C7–C8	−157.9(4)
Cu2$^{\#1}$–S8–C58–C57	159.1(4)
Cu2$^{\#1}$–S8–C59A–C60A	175.1(5)
Cu2$^{\#1}$–S8–C59A–C64A	49.0(6)
Cu2$^{\#1}$–S8–C59B–C60B	−99.6(10)
Cu2$^{\#1}$–S8–C59B–C64B	24.2(14)
Cu3$^{\#2}$–S2–C10–C9	159.6(3)
Cu3$^{\#2}$–S2–C11–C12	−90.0(3)
Cu3$^{\#2}$–S2–C11–C16	34.3(4)
Cu4–S3–C17A–C18A	30.4(6)
Cu4–S3–C17A–C22A	−92.4(5)
Cu4–S3–C23–C24	150.2(4)
Cu5–S5–C33–C34	84.8(3)
Cu5–S5–C33–C38	−39.7(4)
Cu5–S5–C39–C40	−172.1(4)
Cu6–S4–C26–C25	−165.0(4)
Cu6–S4–C27–C28A	175.8(5)
Cu6–S4–C27–C28B	100.4(11)
Cu6–S4–C27–C32A	46.1(6)
Cu6–S4–C27–C32B	−42.5(13)
Cu7$^{\#2}$–S6–C42–C41	139.3(4)
Cu7$^{\#2}$–S6–C43–C44	172.8(3)
Cu7$^{\#2}$–S6–C43–C48	45.1(4)
Cu8–S7–C49A–C50A	−43.1(9)
Cu8–S7–C49A–C54A	−173.1(6)
Cu8–S7–C49B–C50B	94.9(8)
Cu8–S7–C49B–C54B	−27.5(11)
Cu8–S7–C55–C56	−158.0(4)
S1–C1A–C2A–C3A	177.1(10)
S1–C1A–C6A–C5A	−175.6(6)
S1–C1B–C2B–C3B	173(2)
S1–C1B–C6B–C5B	177.1(11)
S2–C11–C12–C13	−178.5(4)
S2–C11–C16–C15	−179.2(5)
S3–C17A–C18A–C19A	−175.0(5)
S3–C17A–C22A–C21A	−179.1(6)
S3–C17B–C18B–C19B	174.2(12)
S3–C17B–C22B–C21B	−174.3(12)
S4–C27–C28A–C29A	179.7(7)
S4–C27–C28B–C29B	174.7(18)
S4–C27–C32A–C31A	−174.3(8)
S4–C27–C32B–C31B	−174.8(15)
S5–C33–C34–C35	178.0(4)
S5–C33–C38–C37	179.0(5)
S6–C43–C44–C45	175.3(4)
S6–C43–C48–C47	−176.4(4)
S7–C49A–C50A–C51A	177.8(9)
S7–C49A–C54A–C53A	−178.3(7)
S7–C49B–C50B–C51B	−178.5(12)
S7–C49B–C54B–C53B	171.1(9)
S8–C59A–C60A–C61A	178.7(7)
S8–C59A–C64A–C63A	−177.7(6)
S8–C59B–C60B–C61B	175.8(13)
S8–C59B–C64B–C63B	−170.7(12)
C1A–S1–C7–C8	90.9(4)
C1A–C2A–C3A–C4A	−53.6(18)
C1B–S1–C7–C8	78.5(6)
C1B–C2B–C3B–C4B	52(5)

C2A–C1A–C6A–C5A	−55.1(9)
C2A–C3A–C4A–C5A	57(2)
C2B–C1B–C6B–C5B	53.4(18)
C2B–C3B–C4B–C5B	−31(6)
C3A–C4A–C5A–C6A	−55.6(19)
C3B–C4B–C5B–C6B	22(4)
C4A–C5A–C6A–C1A	53.6(13)
C4B–C5B–C6B–C1B	−34(2)
C6A–C1A–C2A–C3A	56.2(12)
C6B–C1B–C2B–C3B	−62(3)
C7–S1–C1A–C2A	154.1(4)
C7–S1–C1A–C6A	−83.4(5)
C7–S1–C1B–C2B	65.6(11)
C7–S1–C1B–C6B	−59.3(12)
C10–S2–C11–C12	157.9(3)
C10–S2–C11–C16	−77.9(4)
C11–S2–C10–C9	−80.5(4)
C11–C12–C13–C14	−54.7(8)
C12–C11–C16–C15	−57.0(6)
C12–C13–C14–C15	54.9(9)
C13–C14–C15–C16	−55.5(9)
C14–C15–C16–C11	55.9(8)
C16–C11–C12–C13	56.9(6)
C17A–S3–C23–C24	−91.4(4)
C17A–C18A–C19A–C20A	54.4(9)
C17B–S3–C23–C24	−95.9(6)
C17B–C18B–C19B–C20B	−55(2)
C18A–C17A–C22A–C21A	55.9(9)
C18A–C19A–C20A–C21A	−56.6(10)
C18B–C17B–C22B–C21B	−51.6(19)
C18B–C19B–C20B–C21B	56(2)
C19A–C20A–C21A–C22A	57.0(11)
C19B–C20B–C21B–C22B	−56(2)
C20A–C21A–C22A–C17A	−56.7(10)
C20B–C21B–C22B–C17B	51(2)
C22A–C17A–C18A–C19A	−55.3(8)
C22B–C17B–C18B–C19B	55(2)
C23–S3–C17A–C18A	−75.6(5)
C23–S3–C17A–C22A	161.6(5)
C26–S4–C27–C28A	−77.6(6)
C26–S4–C27–C28B	−153.0(11)
C26–S4–C27–C32A	152.7(6)
C26–S4–C27–C32B	64.1(13)
C27–S4–C26–C25	81.7(5)
C27–C28A–C29A–C30A	52.7(13)
C27–C28B–C29B–C30B	40(3)
C28A–C27–C32A–C31A	54.2(12)
C28A–C29A–C30A–C31A	−53.9(16)
C28B–C27–C32B–C31B	48(3)
C28B–C29B–C30B–C31B	−56(4)
C29A–C30A–C31A–C32A	54.4(16)
C29B–C30B–C31B–C32B	62(4)
C30A–C31A–C32A–C27	−53.9(14)
C30B–C31B–C32B–C27	−57(3)
C32A–C27–C28A–C29A	−51.4(11)
C32B–C27–C28B–C29B	−40(3)
C33–S5–C39–C40	69.5(4)
C33–C34–C35–C36	56.3(7)
C34–C33–C38–C37	56.1(7)
C34–C35–C36–C37	−56.7(8)
C35–C36–C37–C38	56.3(8)
C36–C37–C38–C33	−55.6(8)
C38–C33–C34–C35	−56.6(6)
C39–S5–C33–C34	−164.9(3)
C39–S5–C33–C38	70.6(4)
C42–S6–C43–C44	60.6(4)
C42–S6–C43–C48	−67.1(4)
C43–S6–C42–C41	−104.2(4)
C43–C44–C45–C46	55.7(7)
C44–C43–C48–C47	55.8(6)
C44–C45–C46–C47	−56.3(8)
C45–C46–C47–C48	55.4(7)
C46–C47–C48–C43	−55.1(6)
C48–C43–C44–C45	−55.7(6)
C49A–S7–C55–C56	88.3(5)
C49A–C50A–C51A–C52A	57.4(16)
C49B–S7–C55–C56	84.6(5)
C49B–C50B–C51B–C52B	50(2)
C50A–C49A–C54A–C53A	51.1(12)
C50A–C51A–C52A–C53A	−59.3(16)
C50B–C49B–C54B–C53B	55.2(15)
C50B–C51B–C52B–C53B	−51(2)
C51A–C52A–C53A–C54A	58.3(14)
C51B–C52B–C53B–C54B	54(2)
C52A–C53A–C54A–C49A	−53.2(12)
C52B–C53B–C54B–C49B	−55.2(16)
C54A–C49A–C50A–C51A	−54.0(14)
C54B–C49B–C50B–C51B	−52.0(17)
C55–S7–C49A–C50A	65.6(8)
C55–S7–C49A–C54A	−64.4(8)
C55–S7–C49B–C50B	−165.4(9)
C55–S7–C49B–C54B	72.3(10)
C58–S8–C59A–C60A	62.9(6)
C58–S8–C59A–C64A	−63.2(6)
C58–S8–C59B–C60B	154.8(11)
C58–S8–C59B–C64B	−81.5(12)
C59A–S8–C58–C57	−87.8(5)
C59A–C60A–C61A–C62A	54.9(11)
C59B–S8–C58–C57	−79.9(6)
C59B–C60B–C61B–C62B	−53(2)
C60A–C59A–C64A–C63A	56.4(10)
C60A–C61A–C62A–C63A	−56.8(11)
C60B–C59B–C64B–C63B	−51(2)
C60B–C61B–C62B–C63B	54(2)
C61A–C62A–C63A–C64A	57.5(11)
C61B–C62B–C63B–C64B	−53(2)
C62A–C63A–C64A–C59A	−56.8(11)
C62B–C63B–C64B–C59B	52(2)
C64A–C59A–C60A–C61A	−54.6(10)
C64B–C59B–C60B–C61B	52(2)

Symmetry transformations used to generate equivalent atoms:
#1: 1+X, 1+Y, 1+Z; #2: -1+X, +Y, +Z;

Crystal structure of CP1_250K

Crystal Data and Experimental



Experimental: The data for CP1_250K were collected from a shock-cooled single crystal at 250.0(1) K on a Bruker D8 Venture four-circle diffractometer with a X-ray tube using a graphite as monochromator and a CPAD PHOTON II area detector detector. The diffractometer was equipped with an Oxford Cryostream 800 low temperature device and used Mo K_{α} radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.38A and a multi-scan absorption correction using SADABS 2016/2 was applied. [1,2] The structure was solved by direct methods with XT and refined by full-matrix least-squares methods against F^2 using SHELXL.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters, excepted minor disordered parts. For each compound, some disorders were found in the crystal structure and some geometric parameters of disordered components in each group were restrained by using RIGU or DFIX restraints. For more detail see the .res file included in the cif files.The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[5] CCDC 2326780 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures. This report and the CIF file were generated using FinalCif.[6]

Table S16. Crystal data and structure refinement for CP1_250K

Internal Reference	CP1_250K
CCDC number	2326780
Empirical formula	$C_{64}H_{104}Cu_8I_8S_8$
Formula weight	2653.47
Temperature [K]	250.0(1)
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	11.8961(4)
b [Å]	18.9380(7)
c [Å]	20.9008(7)
α [°]	97.0884(14)
β [°]	104.7460(13)
γ [°]	104.3167(13)
Volume [Å^3]	4324.1(3)
Z	2
ρ_{calc} [gcm^{-3}]	2.038
μ [mm^{-1}]	5.011
F(000)	2544
Crystal size [mm^3]	0.084×0.133×0.172
Crystal colour	clear light colourless
Crystal shape	block
Radiation	Mo K_{α} (λ=0.71073 Å)
2θ range [°]	4.28 to 55.00 (0.77 Å)
Index ranges	−15 ≤ h ≤ 15 −24 ≤ k ≤ 24 −27 ≤ l ≤ 27
Reflections collected	260876
Independent reflections	19874 R_{int} = 0.0369 R_{sigma} = 0.0172
Completeness to θ = 25.242°	99.9 %
Data / Restraints / Parameters	19874 / 734 / 914
Goodness-of-fit on F^2	1.067
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0397 wR_2 = 0.0899
Final *R* indexes [all data]	R_1 = 0.0557 wR_2 = 0.1021
Largest peak/hole [eÅ^{-3}]	1.61/−0.72

Table S17. Bond lengths and angles for CP1_250K

Atom–Atom	Length [Å]
I1–Cu1	2.7214(8)
I1–Cu2	2.6972(8)
I1–Cu3	2.6694(8)
I2–Cu1	2.7350(8)
I2–Cu2	2.6469(8)
I2–Cu4	2.6828(9)
I3–Cu1	2.5997(8)
I3–Cu3	2.6301(9)
I3–Cu4	2.7957(8)
I4–Cu2	2.6760(8)
I4–Cu3	2.7720(8)
I4–Cu4	2.6317(9)
I5–Cu5	2.6819(8)
I5–Cu6	2.6867(8)
I5–Cu7	2.6970(8)
I6–Cu5	2.7704(8)
I6–Cu6	2.6919(9)
I6–Cu8	2.6213(9)
I7–Cu5	2.6229(8)
I7–Cu7	2.6141(9)
I7–Cu8	2.8250(8)
I8–Cu6	2.6426(9)
I8–Cu7	2.6890(9)
I8–Cu8	2.6957(10)
Cu1–Cu2	2.7326(10)
Cu1–Cu3	2.6218(10)
Cu1–Cu4	2.7962(10)
Cu1–S1	2.2912(15)
Cu2–Cu3	2.8302(10)
Cu2–Cu4	2.7029(10)
Cu2–S8$^{\#1}$	2.3087(15)
Cu3–Cu4	2.7507(11)
Cu3–S2$^{\#2}$	2.2863(16)
Cu4–S3	2.3019(16)
Cu5–Cu6	2.8416(10)
Cu5–Cu7	2.6683(11)
Cu5–Cu8	2.7429(10)
Cu5–S5	2.2928(17)
Cu6–Cu7	2.7660(10)
Cu6–Cu8	2.6962(10)
Cu6–S4	2.3114(15)
Cu7–Cu8	2.7876(11)
Cu7–S6$^{\#2}$	2.2967(18)
Cu8–S7	2.2997(16)
S1–C7	1.811(6)
S1–C1A	1.902(9)
S1–C1B	1.748(16)
S2–C10	1.809(7)
S2–C11	1.820(6)
S3–C23	1.828(8)
S3–C17A	1.845(9)
S3–C17B	1.911(18)
S4–C26	1.812(7)
S4–C27	1.809(7)
S5–C33	1.815(6)
S5–C39	1.810(7)
S6–C42	1.825(7)
S6–C43	1.803(8)
S7–C55	1.806(8)
S7–C49A	1.833(10)
S7–C49B	1.921(17)
S8–C58	1.801(7)
S8–C59A	1.844(9)
S8–C59B	1.83(2)
C7–H7A	0.9800
C7–H7B	0.9800
C7–C8	1.452(8)
C8–C9	1.175(8)
C9–C10	1.456(8)
C10–H10A	0.9800
C10–H10B	0.9800
C11–H11	0.9900
C11–C12	1.513(9)
C11–C16	1.510(9)
C12–H12A	0.9800
C12–H12B	0.9800
C12–C13	1.521(10)
C13–H13A	0.9800
C13–H13B	0.9800
C13–C14	1.501(14)
C14–H14A	0.9800
C14–H14B	0.9800
C14–C15	1.471(15)
C15–H15A	0.9800
C15–H15B	0.9800
C15–C16	1.558(11)
C16–H16A	0.9800
C16–H16B	0.9800
C23–H23A	0.9800
C23–H23B	0.9800
C23–C24	1.457(8)
C24–C25	1.167(8)
C25–C26	1.465(8)
C26–H26A	0.9800
C26–H26B	0.9800
C27–H27	0.9900
C27–H27A	0.9900
C27–C28A	1.436(11)
C27–C32A	1.513(14)
C27–C28B	1.51(3)
C27–C32B	1.34(2)
C33–H33	0.9900
C33–C34	1.497(9)
C33–C38	1.485(9)
C34–H34A	0.9800
C34–H34B	0.9800
C34–C35	1.537(10)
C35–H35A	0.9800
C35–H35B	0.9800

C35–C36	1.466(12)	C17A–H17A	0.9900
C36–H36A	0.9800	C17A–C18A	1.527(12)
C36–H36B	0.9800	C17A–C22A	1.498(14)
C36–C37	1.492(14)	C18A–H18A	0.9800
C37–H37A	0.9800	C18A–H18B	0.9800
C37–H37B	0.9800	C18A–C19A	1.518(13)
C37–C38	1.553(10)	C19A–H19A	0.9800
C38–H38A	0.9800	C19A–H19B	0.9800
C38–H38B	0.9800	C19A–C20A	1.505(18)
C39–H39A	0.9800	C20A–H20A	0.9800
C39–H39B	0.9800	C20A–H20B	0.9800
C39–C40	1.466(9)	C20A–C21A	1.497(19)
C40–C41	1.184(9)	C21A–H21A	0.9800
C41–C42	1.454(9)	C21A–H21B	0.9800
C42–H42A	0.9800	C21A–C22A	1.564(16)
C42–H42B	0.9800	C22A–H22A	0.9800
C43–H43	0.9900	C22A–H22B	0.9800
C43–C44	1.497(10)	C28A–H28A	0.9800
C43–C48	1.478(10)	C28A–H28B	0.9800
C44–H44A	0.9800	C28A–C29A	1.475(15)
C44–H44B	0.9800	C29A–H29A	0.9800
C44–C45	1.545(13)	C29A–H29B	0.9800
C45–H45A	0.9800	C29A–C30A	1.402(17)
C45–H45B	0.9800	C30A–H30A	0.9800
C45–C46	1.495(13)	C30A–H30B	0.9800
C46–H46A	0.9800	C30A–C31A	1.516(16)
C46–H46B	0.9800	C31A–H31A	0.9800
C46–C47	1.492(12)	C31A–H31B	0.9800
C47–H47A	0.9800	C31A–C32A	1.503(19)
C47–H47B	0.9800	C32A–H32A	0.9800
C47–C48	1.551(10)	C32A–H32B	0.9800
C48–H48A	0.9800	C49A–H49A	0.9900
C48–H48B	0.9800	C49A–C50A	1.475(14)
C55–H55A	0.9800	C49A–C54A	1.484(19)
C55–H55B	0.9800	C50A–H50A	0.9800
C55–C56	1.467(8)	C50A–H50B	0.9800
C56–C57	1.172(8)	C50A–C51A	1.532(15)
C57–C58	1.467(8)	C51A–H51A	0.9800
C58–H58A	0.9800	C51A–H51B	0.9800
C58–H58B	0.9800	C51A–C52A	1.52(2)
C1A–H1A	0.9900	C52A–H52A	0.9800
C1A–C2A	1.529(13)	C52A–H52B	0.9800
C1A–C6A	1.521(13)	C52A–C53A	1.41(2)
C2A–H2AA	0.9800	C53A–H53A	0.9800
C2A–H2AB	0.9800	C53A–H53B	0.9800
C2A–C3A	1.50(2)	C53A–C54A	1.59(2)
C3A–H3AA	0.9800	C54A–H54A	0.9800
C3A–H3AB	0.9800	C54A–H54B	0.9800
C3A–C4A	1.52(2)	C59A–H59A	0.9900
C4A–H4AA	0.9800	C59A–C60A	1.501(14)
C4A–H4AB	0.9800	C59A–C64A	1.514(14)
C4A–C5A	1.51(2)	C60A–H60A	0.9800
C5A–H5AA	0.9800	C60A–H60B	0.9800
C5A–H5AB	0.9800	C60A–C61A	1.541(16)
C5A–C6A	1.522(17)	C61A–H61A	0.9800
C6A–H6AA	0.9800	C61A–H61B	0.9800
C6A–H6AB	0.9800	C61A–C62A	1.444(18)

C62A–H62A	0.9800
C62A–H62B	0.9800
C62A–C63A	1.474(18)
C63A–H63A	0.9800
C63A–H63B	0.9800
C63A–C64A	1.525(15)
C64A–H64A	0.9800
C64A–H64B	0.9800
C1B–H1B	0.9900
C1B–C2B	1.50(2)
C1B–C6B	1.48(2)
C2B–H2BA	0.9800
C2B–H2BB	0.9800
C2B–C3B	1.57(4)
C3B–H3BA	0.9800
C3B–H3BB	0.9800
C3B–C4B	1.49(4)
C4B–H4BA	0.9800
C4B–H4BB	0.9800
C4B–C5B	1.49(3)
C5B–H5BA	0.9800
C5B–H5BB	0.9800
C5B–C6B	1.54(3)
C6B–H6BA	0.9800
C6B–H6BB	0.9800
C17B–H17B	0.9900
C17B–C18B	1.43(2)
C17B–C22B	1.54(2)
C18B–H18C	0.9800
C18B–H18D	0.9800
C18B–C19B	1.51(3)
C19B–H19C	0.9800
C19B–H19D	0.9800
C19B–C20B	1.51(3)
C20B–H20C	0.9800
C20B–H20D	0.9800
C20B–C21B	1.47(3)
C21B–H21C	0.9800
C21B–H21D	0.9800
C21B–C22B	1.49(3)
C22B–H22C	0.9800
C22B–H22D	0.9800
C28B–H28C	0.9800
C28B–H28D	0.9800
C28B–C29B	1.51(3)
C29B–H29C	0.9800
C29B–H29D	0.9800
C29B–C30B	1.50(4)
C30B–H30C	0.9800
C30B–H30D	0.9800
C30B–C31B	1.43(4)
C31B–H31C	0.9800
C31B–H31D	0.9800
C31B–C32B	1.55(3)
C32B–H32C	0.9800
C32B–H32D	0.9800
C49B–H49B	0.9900
C49B–C50B	1.46(2)
C49B–C54B	1.498(19)
C50B–H50C	0.9800
C50B–H50D	0.9800
C50B–C51B	1.52(3)
C51B–H51C	0.9800
C51B–H51D	0.9800
C51B–C52B	1.61(3)
C52B–H52C	0.9800
C52B–H52D	0.9800
C52B–C53B	1.44(2)
C53B–H53C	0.9800
C53B–H53D	0.9800
C53B–C54B	1.49(2)
C54B–H54C	0.9800
C54B–H54D	0.9800
C59B–H59B	0.9900
C59B–C60B	1.56(3)
C59B–C64B	1.41(3)
C60B–H60C	0.9800
C60B–H60D	0.9800
C60B–C61B	1.53(3)
C61B–H61C	0.9800
C61B–H61D	0.9800
C61B–C62B	1.43(3)
C62B–H62C	0.9800
C62B–H62D	0.9800
C62B–C63B	1.55(4)
C63B–H63C	0.9800
C63B–H63D	0.9800
C63B–C64B	1.55(3)
C64B–H64C	0.9800
C64B–H64D	0.9800

Atom–Atom–Atom	**Angle [°]**
Cu2–I1–Cu1	60.57(2)
Cu3–I1–Cu1	58.19(2)
Cu3–I1–Cu2	63.65(2)
Cu2–I2–Cu1	61.00(2)
Cu2–I2–Cu4	60.94(2)
Cu4–I2–Cu1	62.14(2)
Cu1–I3–Cu3	60.17(2)
Cu1–I3–Cu4	62.31(2)
Cu3–I3–Cu4	60.83(2)
Cu2–I4–Cu3	62.57(2)
Cu4–I4–Cu2	61.22(2)
Cu4–I4–Cu3	61.13(2)
Cu5–I5–Cu6	63.91(2)
Cu5–I5–Cu7	59.48(2)
Cu6–I5–Cu7	61.83(2)
Cu6–I6–Cu5	62.67(2)
Cu8–I6–Cu5	61.08(2)
Cu8–I6–Cu6	60.97(2)
Cu5–I7–Cu8	60.33(2)
Cu7–I7–Cu5	61.26(2)
Cu7–I7–Cu8	61.52(2)
Cu6–I8–Cu7	62.49(2)

Cu6–I8–Cu8	60.66(2)	Cu4–Cu3–I4	56.91(2)
Cu7–I8–Cu8	62.35(2)	Cu4–Cu3–Cu2	57.91(2)
I1–Cu1–I2	111.39(3)	$S2^{\#2}$–Cu3–I1	112.34(5)
I1–Cu1–Cu2	59.28(2)	$S2^{\#2}$–Cu3–I3	108.56(5)
I1–Cu1–Cu4	106.93(3)	$S2^{\#2}$–Cu3–I4	97.95(5)
I2–Cu1–Cu4	58.02(2)	$S2^{\#2}$–Cu3–Cu1	153.78(5)
I3–Cu1–I1	114.79(3)	$S2^{\#2}$–Cu3–Cu2	141.79(5)
I3–Cu1–I2	111.81(3)	$S2^{\#2}$–Cu3–Cu4	135.88(5)
I3–Cu1–Cu2	112.17(3)	I2–Cu4–I3	107.50(3)
I3–Cu1–Cu3	60.49(2)	I2–Cu4–Cu1	59.85(2)
I3–Cu1–Cu4	62.28(2)	I2–Cu4–Cu2	58.87(2)
Cu2–Cu1–I2	57.91(2)	I2–Cu4–Cu3	108.09(3)
Cu2–Cu1–Cu4	58.52(2)	I3–Cu4–Cu1	55.41(2)
Cu3–Cu1–I1	59.91(2)	I4–Cu4–I2	113.49(3)
Cu3–Cu1–I2	110.37(3)	I4–Cu4–I3	113.46(3)
Cu3–Cu1–Cu2	63.78(3)	I4–Cu4–Cu1	107.22(3)
Cu3–Cu1–Cu4	60.92(3)	I4–Cu4–Cu2	60.20(2)
S1–Cu1–I1	107.49(5)	I4–Cu4–Cu3	61.95(2)
S1–Cu1–I2	96.30(5)	Cu2–Cu4–I3	107.19(3)
S1–Cu1–I3	113.53(5)	Cu2–Cu4–Cu1	59.56(3)
S1–Cu1–Cu2	133.39(5)	Cu2–Cu4–Cu3	62.52(3)
S1–Cu1–Cu3	153.07(5)	Cu3–Cu4–I3	56.61(2)
S1–Cu1–Cu4	142.89(5)	Cu3–Cu4–Cu1	56.41(3)
I1–Cu2–Cu1	60.15(2)	S3–Cu4–I2	109.90(5)
I1–Cu2–Cu3	57.69(2)	S3–Cu4–I3	94.26(4)
I1–Cu2–Cu4	110.38(3)	S3–Cu4–I4	116.43(6)
I2–Cu2–I1	115.00(3)	S3–Cu4–Cu1	134.54(6)
I2–Cu2–I4	113.21(3)	S3–Cu4–Cu2	157.85(5)
I2–Cu2–Cu1	61.09(2)	S3–Cu4–Cu3	137.72(5)
I2–Cu2–Cu3	106.80(3)	I5–Cu5–I6	107.74(3)
I2–Cu2–Cu4	60.18(2)	I5–Cu5–Cu6	58.12(2)
I4–Cu2–I1	108.85(3)	I5–Cu5–Cu8	108.13(3)
I4–Cu2–Cu1	107.81(3)	I6–Cu5–Cu6	57.31(2)
I4–Cu2–Cu3	60.38(2)	I7–Cu5–I5	113.69(3)
I4–Cu2–Cu4	58.58(2)	I7–Cu5–I6	114.71(3)
Cu1–Cu2–Cu3	56.21(3)	I7–Cu5–Cu6	108.99(3)
Cu4–Cu2–Cu1	61.92(3)	I7–Cu5–Cu7	59.20(2)
Cu4–Cu2–Cu3	59.57(3)	I7–Cu5–Cu8	63.49(2)
$S8^{\#1}$–Cu2–I1	100.58(4)	Cu7–Cu5–I5	60.54(2)
$S8^{\#1}$–Cu2–I2	104.06(5)	Cu7–Cu5–I6	108.08(3)
$S8^{\#1}$–Cu2–I4	114.54(5)	Cu7–Cu5–Cu6	60.17(3)
$S8^{\#1}$–Cu2–Cu1	137.41(5)	Cu7–Cu5–Cu8	62.00(3)
$S8^{\#1}$–Cu2–Cu3	147.78(5)	Cu8–Cu5–I6	56.77(2)
$S8^{\#1}$–Cu2–Cu4	148.88(5)	Cu8–Cu5–Cu6	57.70(2)
I1–Cu3–I4	106.86(3)	S5–Cu5–I5	110.07(5)
I1–Cu3–Cu2	58.65(2)	S5–Cu5–I6	97.77(5)
I1–Cu3–Cu4	109.76(3)	S5–Cu5–I7	111.70(5)
I3–Cu3–I1	115.55(3)	S5–Cu5–Cu6	138.57(5)
I3–Cu3–I4	114.29(3)	S5–Cu5–Cu7	154.07(5)
I3–Cu3–Cu2	108.24(3)	S5–Cu5–Cu8	139.24(6)
I3–Cu3–Cu4	62.56(2)	I5–Cu6–I6	109.94(3)
I4–Cu3–Cu2	57.06(2)	I5–Cu6–Cu5	57.96(2)
Cu1–Cu3–I1	61.90(2)	I5–Cu6–Cu7	59.27(2)
Cu1–Cu3–I3	59.34(2)	I5–Cu6–Cu8	109.38(3)
Cu1–Cu3–I4	108.22(3)	I6–Cu6–Cu5	60.02(2)
Cu1–Cu3–Cu2	60.02(3)	I6–Cu6–Cu7	107.54(3)
Cu1–Cu3–Cu4	62.67(3)	I6–Cu6–Cu8	58.22(3)

I8–Cu6–I5	112.21(3)	C7–S1–C1A	93.9(4)
I8–Cu6–I6	113.65(3)	C1A–S1–Cu1	109.7(3)
I8–Cu6–Cu5	106.56(3)	C1B–S1–Cu1	113.2(5)
I8–Cu6–Cu7	59.57(2)	C1B–S1–C7	119.5(7)
I8–Cu6–Cu8	60.64(3)	C10–S2–Cu3$^{\#3}$	104.9(2)
Cu7–Cu6–Cu5	56.81(3)	C10–S2–C11	100.6(3)
Cu8–Cu6–Cu5	59.31(3)	C11–S2–Cu3$^{\#3}$	115.2(2)
Cu8–Cu6–Cu7	61.36(3)	C23–S3–Cu4	102.7(2)
S4–Cu6–I5	102.11(5)	C23–S3–C17A	92.6(4)
S4–Cu6–I6	108.18(5)	C23–S3–C17B	120.1(6)
S4–Cu6–I8	110.06(5)	C17A–S3–Cu4	117.1(3)
S4–Cu6–Cu5	142.99(5)	C17B–S3–Cu4	104.0(5)
S4–Cu6–Cu7	143.73(6)	C26–S4–Cu6	101.6(2)
S4–Cu6–Cu8	148.36(5)	C27–S4–Cu6	110.2(3)
I5–Cu7–Cu6	58.90(2)	C27–S4–C26	101.1(4)
I5–Cu7–Cu8	106.42(3)	C33–S5–Cu5	114.7(2)
I7–Cu7–I5	113.48(3)	C39–S5–Cu5	103.7(2)
I7–Cu7–I8	114.04(3)	C39–S5–C33	101.2(3)
I7–Cu7–Cu5	59.53(2)	C42–S6–Cu7$^{\#3}$	104.3(2)
I7–Cu7–Cu6	111.59(3)	C43–S6–Cu7$^{\#3}$	110.6(2)
I7–Cu7–Cu8	62.97(3)	C43–S6–C42	106.5(4)
I8–Cu7–I5	110.44(3)	C55–S7–Cu8	100.3(2)
I8–Cu7–Cu6	57.93(2)	C55–S7–C49A	92.7(5)
I8–Cu7–Cu8	58.94(3)	C55–S7–C49B	117.1(6)
Cu5–Cu7–I5	59.98(2)	C49A–S7–Cu8	116.0(4)
Cu5–Cu7–I8	110.34(3)	C49B–S7–Cu8	107.6(4)
Cu5–Cu7–Cu6	63.02(3)	C58–S8–Cu2$^{\#4}$	104.0(2)
Cu5–Cu7–Cu8	60.32(3)	C58–S8–C59A	109.3(5)
Cu6–Cu7–Cu8	58.09(3)	C58–S8–C59B	88.1(7)
S6$^{\#2}$–Cu7–I5	112.05(5)	C59A–S8–Cu2$^{\#4}$	106.6(3)
S6$^{\#2}$–Cu7–I7	108.40(5)	S1–C7–H7A	108.8
S6$^{\#2}$–Cu7–I8	97.33(5)	S1–C7–H7B	108.8
S6$^{\#2}$–Cu7–Cu5	152.30(6)	H7A–C7–H7B	107.7
S6$^{\#2}$–Cu7–Cu6	138.95(6)	C8–C7–S1	113.7(4)
S6$^{\#2}$–Cu7–Cu8	140.22(6)	C8–C7–H7A	108.8
I6–Cu8–I7	112.96(3)	C8–C7–H7B	108.8
I6–Cu8–I8	114.22(3)	C9–C8–C7	174.3(7)
I6–Cu8–Cu5	62.14(3)	C8–C9–C10	173.2(8)
I6–Cu8–Cu6	60.81(3)	S2–C10–H10A	109.7
I6–Cu8–Cu7	108.94(3)	S2–C10–H10B	109.7
I8–Cu8–I7	107.35(3)	C9–C10–S2	109.9(5)
I8–Cu8–Cu5	107.91(3)	C9–C10–H10A	109.7
I8–Cu8–Cu6	58.70(3)	C9–C10–H10B	109.7
I8–Cu8–Cu7	58.70(3)	H10A–C10–H10B	108.2
Cu5–Cu8–I7	56.18(2)	S2–C11–H11	107.9
Cu5–Cu8–Cu7	57.69(3)	C12–C11–S2	108.6(5)
Cu6–Cu8–I7	107.40(3)	C12–C11–H11	107.9
Cu6–Cu8–Cu5	62.98(3)	C16–C11–S2	112.4(5)
Cu6–Cu8–Cu7	60.55(3)	C16–C11–H11	107.9
Cu7–Cu8–I7	55.51(2)	C16–C11–C12	112.0(6)
S7–Cu8–I6	116.42(6)	C11–C12–H12A	109.5
S7–Cu8–I7	94.03(4)	C11–C12–H12B	109.5
S7–Cu8–I8	109.84(5)	C11–C12–C13	110.6(7)
S7–Cu8–Cu5	137.56(5)	H12A–C12–H12B	108.1
S7–Cu8–Cu6	157.78(5)	C13–C12–H12A	109.5
S7–Cu8–Cu7	132.89(6)	C13–C12–H12B	109.5
C7–S1–Cu1	100.0(2)	C12–C13–H13A	109.4

C12–C13–H13B	109.4	C33–C34–C35	110.1(6)
H13A–C13–H13B	108.0	H34A–C34–H34B	108.2
C14–C13–C12	111.3(7)	C35–C34–H34A	109.7
C14–C13–H13A	109.4	C35–C34–H34B	109.7
C14–C13–H13B	109.4	C34–C35–H35A	109.5
C13–C14–H14A	109.1	C34–C35–H35B	109.5
C13–C14–H14B	109.1	H35A–C35–H35B	108.1
H14A–C14–H14B	107.8	C36–C35–C34	110.8(7)
C15–C14–C13	112.7(8)	C36–C35–H35A	109.5
C15–C14–H14A	109.1	C36–C35–H35B	109.5
C15–C14–H14B	109.1	C35–C36–H36A	109.2
C14–C15–H15A	109.3	C35–C36–H36B	109.2
C14–C15–H15B	109.3	C35–C36–C37	112.0(8)
C14–C15–C16	111.8(8)	H36A–C36–H36B	107.9
H15A–C15–H15B	107.9	C37–C36–H36A	109.2
C16–C15–H15A	109.3	C37–C36–H36B	109.2
C16–C15–H15B	109.3	C36–C37–H37A	109.6
C11–C16–C15	108.9(7)	C36–C37–H37B	109.6
C11–C16–H16A	109.9	C36–C37–C38	110.2(8)
C11–C16–H16B	109.9	H37A–C37–H37B	108.1
C15–C16–H16A	109.9	C38–C37–H37A	109.6
C15–C16–H16B	109.9	C38–C37–H37B	109.6
H16A–C16–H16B	108.3	C33–C38–C37	109.2(6)
S3–C23–H23A	109.1	C33–C38–H38A	109.8
S3–C23–H23B	109.1	C33–C38–H38B	109.8
H23A–C23–H23B	107.8	C37–C38–H38A	109.8
C24–C23–S3	112.4(5)	C37–C38–H38B	109.8
C24–C23–H23A	109.1	H38A–C38–H38B	108.3
C24–C23–H23B	109.1	S5–C39–H39A	109.6
C25–C24–C23	176.1(7)	S5–C39–H39B	109.6
C24–C25–C26	177.2(7)	H39A–C39–H39B	108.1
S4–C26–H26A	108.8	C40–C39–S5	110.5(5)
S4–C26–H26B	108.8	C40–C39–H39A	109.6
C25–C26–S4	113.6(5)	C40–C39–H39B	109.6
C25–C26–H26A	108.8	C41–C40–C39	174.9(9)
C25–C26–H26B	108.8	C40–C41–C42	175.8(9)
H26A–C26–H26B	107.7	S6–C42–H42A	109.2
S4–C27–H27	105.3	S6–C42–H42B	109.2
S4–C27–H27A	100.8	C41–C42–S6	112.0(5)
C28A–C27–S4	116.5(7)	C41–C42–H42A	109.2
C28A–C27–H27	105.3	C41–C42–H42B	109.2
C28A–C27–C32A	112.2(8)	H42A–C42–H42B	107.9
C32A–C27–S4	111.2(7)	S6–C43–H43	106.0
C32A–C27–H27	105.3	C44–C43–S6	112.1(6)
C28B–C27–S4	104.0(12)	C44–C43–H43	106.0
C28B–C27–H27A	100.8	C48–C43–S6	114.5(5)
C32B–C27–S4	125.0(11)	C48–C43–H43	106.0
C32B–C27–H27A	100.8	C48–C43–C44	111.4(7)
C32B–C27–C28B	120.5(16)	C43–C44–H44A	109.7
S5–C33–H33	107.7	C43–C44–H44B	109.7
C34–C33–S5	108.5(4)	C43–C44–C45	109.8(8)
C34–C33–H33	107.7	H44A–C44–H44B	108.2
C38–C33–S5	112.8(4)	C45–C44–H44A	109.7
C38–C33–H33	107.7	C45–C44–H44B	109.7
C38–C33–C34	112.1(6)	C44–C45–H45A	109.3
C33–C34–H34A	109.7	C44–C45–H45B	109.3
C33–C34–H34B	109.7	H45A–C45–H45B	108.0

C46–C45–C44	111.6(8)	C5A–C4A–H4AA	109.5
C46–C45–H45A	109.3	C5A–C4A–H4AB	109.5
C46–C45–H45B	109.3	C4A–C5A–H5AA	109.0
C45–C46–H46A	109.3	C4A–C5A–H5AB	109.0
C45–C46–H46B	109.3	C4A–C5A–C6A	112.9(10)
H46A–C46–H46B	107.9	H5AA–C5A–H5AB	107.8
C47–C46–C45	111.8(7)	C6A–C5A–H5AA	109.0
C47–C46–H46A	109.3	C6A–C5A–H5AB	109.0
C47–C46–H46B	109.3	C1A–C6A–C5A	111.2(11)
C46–C47–H47A	109.8	C1A–C6A–H6AA	109.4
C46–C47–H47B	109.8	C1A–C6A–H6AB	109.4
C46–C47–C48	109.2(8)	C5A–C6A–H6AA	109.4
H47A–C47–H47B	108.3	C5A–C6A–H6AB	109.4
C48–C47–H47A	109.8	H6AA–C6A–H6AB	108.0
C48–C47–H47B	109.8	S3–C17A–H17A	108.1
C43–C48–C47	112.2(6)	C18A–C17A–S3	115.2(6)
C43–C48–H48A	109.2	C18A–C17A–H17A	108.1
C43–C48–H48B	109.2	C22A–C17A–S3	106.3(8)
C47–C48–H48A	109.2	C22A–C17A–H17A	108.1
C47–C48–H48B	109.2	C22A–C17A–C18A	110.7(9)
H48A–C48–H48B	107.9	C17A–C18A–H18A	109.4
S7–C55–H55A	108.8	C17A–C18A–H18B	109.4
S7–C55–H55B	108.8	H18A–C18A–H18B	108.0
H55A–C55–H55B	107.7	C19A–C18A–C17A	111.3(8)
C56–C55–S7	113.7(5)	C19A–C18A–H18A	109.4
C56–C55–H55A	108.8	C19A–C18A–H18B	109.4
C56–C55–H55B	108.8	C18A–C19A–H19A	109.3
C57–C56–C55	176.5(7)	C18A–C19A–H19B	109.3
C56–C57–C58	176.9(7)	H19A–C19A–H19B	108.0
S8–C58–H58A	109.0	C20A–C19A–C18A	111.6(11)
S8–C58–H58B	109.0	C20A–C19A–H19A	109.3
C57–C58–S8	113.0(5)	C20A–C19A–H19B	109.3
C57–C58–H58A	109.0	C19A–C20A–H20A	109.0
C57–C58–H58B	109.0	C19A–C20A–H20B	109.0
H58A–C58–H58B	107.8	H20A–C20A–H20B	107.8
S1–C1A–H1A	108.9	C21A–C20A–C19A	112.9(12)
C2A–C1A–S1	108.3(6)	C21A–C20A–H20A	109.0
C2A–C1A–H1A	108.9	C21A–C20A–H20B	109.0
C6A–C1A–S1	110.2(8)	C20A–C21A–H21A	110.0
C6A–C1A–H1A	108.9	C20A–C21A–H21B	110.0
C6A–C1A–C2A	111.7(8)	C20A–C21A–C22A	108.6(11)
C1A–C2A–H2AA	109.6	H21A–C21A–H21B	108.3
C1A–C2A–H2AB	109.6	C22A–C21A–H21A	110.0
H2AA–C2A–H2AB	108.1	C22A–C21A–H21B	110.0
C3A–C2A–C1A	110.3(12)	C17A–C22A–C21A	113.0(10)
C3A–C2A–H2AA	109.6	C17A–C22A–H22A	109.0
C3A–C2A–H2AB	109.6	C17A–C22A–H22B	109.0
C2A–C3A–H3AA	109.2	C21A–C22A–H22A	109.0
C2A–C3A–H3AB	109.2	C21A–C22A–H22B	109.0
C2A–C3A–C4A	111.9(15)	H22A–C22A–H22B	107.8
H3AA–C3A–H3AB	107.9	C27–C28A–H28A	109.0
C4A–C3A–H3AA	109.2	C27–C28A–H28B	109.0
C4A–C3A–H3AB	109.2	C27–C28A–C29A	112.9(10)
C3A–C4A–H4AA	109.5	H28A–C28A–H28B	107.8
C3A–C4A–H4AB	109.5	C29A–C28A–H28A	109.0
H4AA–C4A–H4AB	108.1	C29A–C28A–H28B	109.0
C5A–C4A–C3A	110.6(13)	C28A–C29A–H29A	108.3

C28A–C29A–H29B	108.3
H29A–C29A–H29B	107.4
C30A–C29A–C28A	116.0(12)
C30A–C29A–H29A	108.3
C30A–C29A–H29B	108.3
C29A–C30A–H30A	108.8
C29A–C30A–H30B	108.8
C29A–C30A–C31A	113.7(11)
H30A–C30A–H30B	107.7
C31A–C30A–H30A	108.8
C31A–C30A–H30B	108.8
C30A–C31A–H31A	109.8
C30A–C31A–H31B	109.8
H31A–C31A–H31B	108.2
C32A–C31A–C30A	109.5(13)
C32A–C31A–H31A	109.8
C32A–C31A–H31B	109.8
C27–C32A–H32A	109.3
C27–C32A–H32B	109.3
C31A–C32A–C27	111.7(12)
C31A–C32A–H32A	109.3
C31A–C32A–H32B	109.3
H32A–C32A–H32B	107.9
S7–C49A–H49A	107.8
C50A–C49A–S7	118.3(8)
C50A–C49A–H49A	107.8
C50A–C49A–C54A	110.8(12)
C54A–C49A–S7	104.0(10)
C54A–C49A–H49A	107.8
C49A–C50A–H50A	109.3
C49A–C50A–H50B	109.3
C49A–C50A–C51A	111.4(10)
H50A–C50A–H50B	108.0
C51A–C50A–H50A	109.3
C51A–C50A–H50B	109.3
C50A–C51A–H51A	109.3
C50A–C51A–H51B	109.3
H51A–C51A–H51B	107.9
C52A–C51A–C50A	111.8(13)
C52A–C51A–H51A	109.3
C52A–C51A–H51B	109.3
C51A–C52A–H52A	108.5
C51A–C52A–H52B	108.5
H52A–C52A–H52B	107.5
C53A–C52A–C51A	115.0(12)
C53A–C52A–H52A	108.5
C53A–C52A–H52B	108.5
C52A–C53A–H53A	109.6
C52A–C53A–H53B	109.6
C52A–C53A–C54A	110.4(15)
H53A–C53A–H53B	108.1
C54A–C53A–H53A	109.6
C54A–C53A–H53B	109.6
C49A–C54A–C53A	111.7(14)
C49A–C54A–H54A	109.3
C49A–C54A–H54B	109.3
C53A–C54A–H54A	109.3
C53A–C54A–H54B	109.3
H54A–C54A–H54B	107.9
S8–C59A–H59A	105.8
C60A–C59A–S8	112.4(8)
C60A–C59A–H59A	105.8
C60A–C59A–C64A	112.2(9)
C64A–C59A–S8	113.8(7)
C64A–C59A–H59A	105.8
C59A–C60A–H60A	109.6
C59A–C60A–H60B	109.6
C59A–C60A–C61A	110.2(10)
H60A–C60A–H60B	108.1
C61A–C60A–H60A	109.6
C61A–C60A–H60B	109.6
C60A–C61A–H61A	108.9
C60A–C61A–H61B	108.9
H61A–C61A–H61B	107.7
C62A–C61A–C60A	113.5(11)
C62A–C61A–H61A	108.9
C62A–C61A–H61B	108.9
C61A–C62A–H62A	108.9
C61A–C62A–H62B	108.9
C61A–C62A–C63A	113.5(12)
H62A–C62A–H62B	107.7
C63A–C62A–H62A	108.9
C63A–C62A–H62B	108.9
C62A–C63A–H63A	109.3
C62A–C63A–H63B	109.3
C62A–C63A–C64A	111.4(12)
H63A–C63A–H63B	108.0
C64A–C63A–H63A	109.3
C64A–C63A–H63B	109.3
C59A–C64A–C63A	111.4(11)
C59A–C64A–H64A	109.3
C59A–C64A–H64B	109.3
C63A–C64A–H64A	109.3
C63A–C64A–H64B	109.3
H64A–C64A–H64B	108.0
S1–C1B–H1B	106.8
C2B–C1B–S1	110.7(13)
C2B–C1B–H1B	106.8
C6B–C1B–S1	114.1(13)
C6B–C1B–H1B	106.8
C6B–C1B–C2B	111.2(16)
C1B–C2B–H2BA	108.9
C1B–C2B–H2BB	108.9
C1B–C2B–C3B	114(2)
H2BA–C2B–H2BB	107.7
C3B–C2B–H2BA	108.9
C3B–C2B–H2BB	108.9
C2B–C3B–H3BA	109.5
C2B–C3B–H3BB	109.5
H3BA–C3B–H3BB	108.1
C4B–C3B–C2B	111(3)
C4B–C3B–H3BA	109.5
C4B–C3B–H3BB	109.5
C3B–C4B–H4BA	109.0

C3B–C4B–H4BB	109.0	C29B–C28B–H28C	109.1
H4BA–C4B–H4BB	107.8	C29B–C28B–H28D	109.1
C5B–C4B–C3B	113(3)	C28B–C29B–H29C	109.6
C5B–C4B–H4BA	109.0	C28B–C29B–H29D	109.6
C5B–C4B–H4BB	109.0	H29C–C29B–H29D	108.1
C4B–C5B–H5BA	109.4	C30B–C29B–C28B	110(3)
C4B–C5B–H5BB	109.4	C30B–C29B–H29C	109.6
C4B–C5B–C6B	111(2)	C30B–C29B–H29D	109.6
H5BA–C5B–H5BB	108.0	C29B–C30B–H30C	109.2
C6B–C5B–H5BA	109.4	C29B–C30B–H30D	109.2
C6B–C5B–H5BB	109.4	H30C–C30B–H30D	107.9
C1B–C6B–C5B	113.6(18)	C31B–C30B–C29B	112(3)
C1B–C6B–H6BA	108.9	C31B–C30B–H30C	109.2
C1B–C6B–H6BB	108.9	C31B–C30B–H30D	109.2
C5B–C6B–H6BA	108.9	C30B–C31B–H31C	110.3
C5B–C6B–H6BB	108.9	C30B–C31B–H31D	110.3
H6BA–C6B–H6BB	107.7	C30B–C31B–C32B	107(3)
S3–C17B–H17B	107.1	H31C–C31B–H31D	108.5
C18B–C17B–S3	112.7(15)	C32B–C31B–H31C	110.3
C18B–C17B–H17B	107.1	C32B–C31B–H31D	110.3
C18B–C17B–C22B	117.3(16)	C27–C32B–C31B	111(2)
C22B–C17B–S3	105.0(12)	C27–C32B–H32C	109.4
C22B–C17B–H17B	107.1	C27–C32B–H32D	109.4
C17B–C18B–H18C	108.8	C31B–C32B–H32C	109.4
C17B–C18B–H18D	108.8	C31B–C32B–H32D	109.4
C17B–C18B–C19B	114(2)	H32C–C32B–H32D	108.0
H18C–C18B–H18D	107.7	S7–C49B–H49B	107.9
C19B–C18B–H18C	108.8	C50B–C49B–S7	112.2(14)
C19B–C18B–H18D	108.8	C50B–C49B–H49B	107.9
C18B–C19B–H19C	109.2	C50B–C49B–C54B	112.6(14)
C18B–C19B–H19D	109.2	C54B–C49B–S7	108.3(11)
C18B–C19B–C20B	112(2)	C54B–C49B–H49B	107.9
H19C–C19B–H19D	107.9	C49B–C50B–H50C	109.5
C20B–C19B–H19C	109.2	C49B–C50B–H50D	109.5
C20B–C19B–H19D	109.2	C49B–C50B–C51B	110.6(19)
C19B–C20B–H20C	108.8	H50C–C50B–H50D	108.1
C19B–C20B–H20D	108.8	C51B–C50B–H50C	109.5
H20C–C20B–H20D	107.7	C51B–C50B–H50D	109.5
C21B–C20B–C19B	114(3)	C50B–C51B–H51C	110.5
C21B–C20B–H20C	108.8	C50B–C51B–H51D	110.5
C21B–C20B–H20D	108.8	C50B–C51B–C52B	106.2(19)
C20B–C21B–H21C	108.0	H51C–C51B–H51D	108.7
C20B–C21B–H21D	108.0	C52B–C51B–H51C	110.5
C20B–C21B–C22B	117(2)	C52B–C51B–H51D	110.5
H21C–C21B–H21D	107.3	C51B–C52B–H52C	110.6
C22B–C21B–H21C	108.0	C51B–C52B–H52D	110.6
C22B–C21B–H21D	108.0	H52C–C52B–H52D	108.8
C17B–C22B–H22C	110.1	C53B–C52B–C51B	105.5(19)
C17B–C22B–H22D	110.1	C53B–C52B–H52C	110.6
C21B–C22B–C17B	107.9(17)	C53B–C52B–H52D	110.6
C21B–C22B–H22C	110.1	C52B–C53B–H53C	109.0
C21B–C22B–H22D	110.1	C52B–C53B–H53D	109.0
H22C–C22B–H22D	108.4	C52B–C53B–C54B	113.0(18)
C27–C28B–H28C	109.1	H53C–C53B–H53D	107.8
C27–C28B–H28D	109.1	C54B–C53B–H53C	109.0
H28C–C28B–H28D	107.9	C54B–C53B–H53D	109.0
C29B–C28B–C27	112(2)	C49B–C54B–H54C	109.7

C49B–C54B–H54D	109.7	C62B–C61B–H61D	109.4
C53B–C54B–C49B	109.9(13)	C61B–C62B–H62C	109.2
C53B–C54B–H54C	109.7	C61B–C62B–H62D	109.2
C53B–C54B–H54D	109.7	C61B–C62B–C63B	112(2)
H54C–C54B–H54D	108.2	H62C–C62B–H62D	107.9
S8–C59B–H59B	109.5	C63B–C62B–H62C	109.2
C60B–C59B–S8	103.2(14)	C63B–C62B–H62D	109.2
C60B–C59B–H59B	109.5	C62B–C63B–H63C	110.0
C64B–C59B–S8	113.6(18)	C62B–C63B–H63D	110.0
C64B–C59B–H59B	109.5	C62B–C63B–C64B	108(2)
C64B–C59B–C60B	111(2)	H63C–C63B–H63D	108.4
C59B–C60B–H60C	109.4	C64B–C63B–H63C	110.0
C59B–C60B–H60D	109.4	C64B–C63B–H63D	110.0
H60C–C60B–H60D	108.0	C59B–C64B–C63B	114(3)
C61B–C60B–C59B	111.1(19)	C59B–C64B–H64C	108.7
C61B–C60B–H60C	109.4	C59B–C64B–H64D	108.7
C61B–C60B–H60D	109.4	C63B–C64B–H64C	108.7
C60B–C61B–H61C	109.4	C63B–C64B–H64D	108.7
C60B–C61B–H61D	109.4	H64C–C64B–H64D	107.6
H61C–C61B–H61D	108.0		
C62B–C61B–C60B	111(2)		
C62B–C61B–H61C	109.4		

Symmetry transformations used to generate equivalent atoms:
#1: -1+X, -1+Y, -1+Z; #2: 1+X, +Y, +Z; #3: -1+X, +Y, +Z; #4: 1+X, 1+Y, 1+Z;

Table S18. Torsion angles for CP1_250K

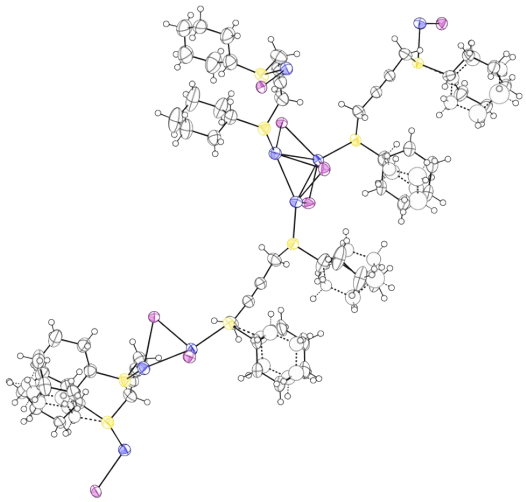
Atom–Atom–Atom–Atom	Torsion Angle [°]		
Cu1–S1–C7–C8	−156.1(5)	S1–C1B–C2B–C3B	−179(2)
Cu1–S1–C1B–C2B	−50.0(16)	S1–C1B–C6B–C5B	178.6(14)
Cu1–S1–C1B–C6B	−176.4(12)	S2–C11–C12–C13	−178.4(6)
Cu2$^{\#1}$–S8–C58–C57	159.3(5)	S2–C11–C16–C15	−178.7(7)
Cu2$^{\#1}$–S8–C59A–C60A	177.0(8)	S3–C17A–C18A–C19A	−174.7(8)
Cu2$^{\#1}$–S8–C59A–C64A	47.9(10)	S3–C17A–C22A–C21A	−179.2(10)
Cu2$^{\#1}$–S8–C59B–C60B	−97.3(14)	S3–C17B–C18B–C19B	172.6(17)
Cu2$^{\#1}$–S8–C59B–C64B	23(2)	S3–C17B–C22B–C21B	−174.5(16)
Cu3$^{\#2}$–S2–C10–C9	161.0(5)	S4–C27–C28A–C29A	−179.7(10)
Cu3$^{\#2}$–S2–C11–C12	−89.6(5)	S4–C27–C32A–C31A	−173.5(12)
Cu3$^{\#2}$–S2–C11–C16	34.9(6)	S4–C27–C28B–C29B	176(2)
Cu4–S3–C23–C24	150.1(5)	S4–C27–C32B–C31B	−175.1(17)
Cu4–S3–C17A–C18A	29.2(9)	S5–C33–C34–C35	177.8(5)
Cu4–S3–C17A–C22A	−93.9(8)	S5–C33–C38–C37	−179.9(7)
Cu5–S5–C33–C34	84.7(5)	S6–C43–C44–C45	174.6(6)
Cu5–S5–C33–C38	−40.2(6)	S6–C43–C48–C47	−174.5(6)
Cu5–S5–C39–C40	−172.1(5)	S7–C49A–C50A–C51A	176.3(11)
Cu6–S4–C26–C25	−164.8(5)	S7–C49A–C54A–C53A	174.9(16)
Cu6–S4–C27–C28A	176.5(8)	S7–C49B–C50B–C51B	−179.7(15)
Cu6–S4–C27–C32A	46.2(10)	S7–C49B–C54B–C53B	177.4(12)
Cu6–S4–C27–C28B	101.2(14)	S8–C59A–C60A–C61A	178.2(10)
Cu6–S4–C27–C32B	−43.2(16)	S8–C59A–C64A–C63A	−177.2(10)
Cu7$^{\#2}$–S6–C42–C41	139.4(5)	S8–C59B–C60B–C61B	174.8(17)
Cu7$^{\#2}$–S6–C43–C44	173.8(5)	S8–C59B–C64B–C63B	−169.5(18)
Cu7$^{\#2}$–S6–C43–C48	45.7(6)	C7–S1–C1B–C2B	67.4(15)
Cu8–S7–C55–C56	−158.5(5)	C7–S1–C1B–C6B	−59.0(15)
Cu8–S7–C49A–C50A	−31.1(13)	C10–S2–C11–C12	158.2(5)
Cu8–S7–C49A–C54A	92.3(14)	C10–S2–C11–C16	−77.3(6)
S1–C1A–C2A–C3A	177.1(10)	C11–S2–C10–C9	−79.1(6)
S1–C1A–C6A–C5A	−173.4(9)	C11–C12–C13–C14	−54.4(11)
		C12–C11–C16–C15	−56.1(9)
		C12–C13–C14–C15	54.8(13)

C13–C14–C15–C16	−55.3(13)
C14–C15–C16–C11	55.2(11)
C16–C11–C12–C13	56.9(8)
C23–S3–C17A–C18A	−76.4(8)
C23–S3–C17A–C22A	160.5(8)
C26–S4–C27–C28A	−76.7(9)
C26–S4–C27–C32A	153.1(10)
C26–S4–C27–C28B	−151.9(14)
C26–S4–C27–C32B	63.7(16)
C27–S4–C26–C25	81.7(6)
C27–C28A–C29A–C30A	49(2)
C27–C28B–C29B–C30B	39(4)
C33–S5–C39–C40	68.8(6)
C33–C34–C35–C36	55.7(10)
C34–C33–C38–C37	57.2(10)
C34–C35–C36–C37	−57.1(12)
C35–C36–C37–C38	57.5(12)
C36–C37–C38–C33	−56.4(12)
C38–C33–C34–C35	−57.0(8)
C39–S5–C33–C34	−164.5(5)
C39–S5–C33–C38	70.7(6)
C42–S6–C43–C44	61.0(7)
C42–S6–C43–C48	−67.1(6)
C43–S6–C42–C41	−103.5(6)
C43–C44–C45–C46	55.5(11)
C44–C43–C48–C47	57.0(10)
C44–C45–C46–C47	−56.8(13)
C45–C46–C47–C48	55.5(11)
C46–C47–C48–C43	−56.0(9)
C48–C43–C44–C45	−55.6(10)
C55–S7–C49A–C50A	71.8(11)
C55–S7–C49A–C54A	−164.8(14)
C58–S8–C59A–C60A	65.1(9)
C58–S8–C59A–C64A	−63.9(10)
C58–S8–C59B–C60B	157.4(15)
C58–S8–C59B–C64B	−82(2)
C1A–S1–C7–C8	93.1(6)
C1A–C2A–C3A–C4A	−57.2(18)
C2A–C1A–C6A–C5A	−52.9(14)
C2A–C3A–C4A–C5A	56(2)
C3A–C4A–C5A–C6A	−54(2)
C4A–C5A–C6A–C1A	52.5(17)
C6A–C1A–C2A–C3A	55.6(14)
C17A–S3–C23–C24	−91.4(6)
C17A–C18A–C19A–C20A	54.5(15)
C18A–C17A–C22A–C21A	54.9(15)
C18A–C19A–C20A–C21A	−56.7(18)
C19A–C20A–C21A–C22A	55.1(18)
C20A–C21A–C22A–C17A	−55.0(17)
C22A–C17A–C18A–C19A	−53.9(14)
C28A–C27–C32A–C31A	54.0(19)
C28A–C29A–C30A–C31A	−50(3)
C29A–C30A–C31A–C32A	51(3)
C30A–C31A–C32A–C27	−53(2)
C32A–C27–C28A–C29A	−49.9(17)
C49A–S7–C55–C56	84.4(6)
C49A–C50A–C51A–C52A	−51.8(19)
C50A–C49A–C54A–C53A	−57(2)
C50A–C51A–C52A–C53A	51(3)
C51A–C52A–C53A–C54A	−51(3)
C52A–C53A–C54A–C49A	54(3)
C54A–C49A–C50A–C51A	56.4(19)
C59A–S8–C58–C57	−87.1(6)
C59A–C60A–C61A–C62A	52.2(18)
C60A–C59A–C64A–C63A	53.6(16)
C60A–C61A–C62A–C63A	−54(2)
C61A–C62A–C63A–C64A	54(2)
C62A–C63A–C64A–C59A	−53(2)
C64A–C59A–C60A–C61A	−51.9(15)
C1B–S1–C7–C8	79.9(8)
C1B–C2B–C3B–C4B	51(4)
C2B–C1B–C6B–C5B	52(2)
C2B–C3B–C4B–C5B	−53(4)
C3B–C4B–C5B–C6B	54(3)
C4B–C5B–C6B–C1B	−54(3)
C6B–C1B–C2B–C3B	−51(3)
C17B–S3–C23–C24	−95.3(7)
C17B–C18B–C19B–C20B	−47(3)
C18B–C17B–C22B–C21B	−48(3)
C18B–C19B–C20B–C21B	46(4)
C19B–C20B–C21B–C22B	−49(4)
C20B–C21B–C22B–C17B	47(3)
C22B–C17B–C18B–C19B	50(3)
C28B–C27–C32B–C31B	46(3)
C28B–C29B–C30B–C31B	−58(5)
C29B–C30B–C31B–C32B	65(5)
C30B–C31B–C32B–C27	−58(4)
C32B–C27–C28B–C29B	−38(3)
C49B–S7–C55–C56	85.4(7)
C49B–C50B–C51B–C52B	61(3)
C50B–C49B–C54B–C53B	53(2)
C50B–C51B–C52B–C53B	−63(3)
C51B–C52B–C53B–C54B	63(2)
C52B–C53B–C54B–C49B	−58(2)
C54B–C49B–C50B–C51B	−57(2)
C59B–S8–C58–C57	−79.2(8)
C59B–C60B–C61B–C62B	−55(3)
C60B–C59B–C64B–C63B	−54(3)
C60B–C61B–C62B–C63B	58(3)
C61B–C62B–C63B–C64B	−56(3)
C62B–C63B–C64B–C59B	55(3)
C64B–C59B–C60B–C61B	53(3)

Symmetry transformations used to generate equivalent atoms:
#1: 1+X, 1+Y, 1+Z; #2: -1+X, +Y, +Z;

Crystal structure of CP1_300K

Crystal Data and Experimental



Experimental: The data for CP1_300K were collected from a shock-cooled single crystal at 300.0(1) K on a Bruker D8 VENTURE area detector four-circle diffractometer with a X-ray tube using a graphite as monochromator and a CPAD PHOTON II area detector detector. The diffractometer was equipped with an Oxford Cryostream 800 low temperature device and used Mo K_{α} radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.38A and a multi-scan absorption correction using SADABS 2016/2 was applied. [1,2] The structure was solved by direct methods with XT and refined by full-matrix least-squares methods against F^2 using SHELXL.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters, excepted minor disordered parts. For each compound, some disorders were found in the crystal structure and some geometric parameters of disordered components in each group were restrained by using RIGU or DFIX restraints. For more detail see the .res file included in the cif files.The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[5] CCDC 2326653 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures. This report and the CIF file were generated using FinalCif.[6]

Table S19. Crystal data and structure refinement for CP1_300K

Internal Reference	CP1_300K
CCDC number	2326653
Empirical formula	$C_{64}H_{104}Cu_8I_8S_8$
Formula weight	2653.47
Temperature [K]	300.0(1)
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	11.9606(16)
b [Å]	19.095(3)
c [Å]	21.026(3)
α [°]	96.658(4)
β [°]	105.219(4)
γ [°]	105.342(4)
Volume [Å^3]	4378.9(10)
Z	2
ρ_{calc} [gcm^{-3}]	2.012
μ [mm^{-1}]	4.948
F(000)	2544
Crystal size [mm^3]	0.084×0.143×0.168
Crystal colour	clear light colourless
Crystal shape	block
Radiation	Mo K_{α} (λ=0.71073 Å)
2θ range [°]	2.05 to 50.00 (0.84 Å)
Index ranges	−14 ≤ h ≤ 14 −22 ≤ k ≤ 22 −24 ≤ l ≤ 24
Reflections collected	100554
Independent reflections	15416 R_{int} = 0.0941 R_{sigma} = 0.0442
Completeness to θ = 24.999°	99.9 %
Data / Restraints / Parameters	15416 / 675 / 910
Goodness-of-fit on F^2	1.040
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0573 wR_2 = 0.1493
Final *R* indexes [all data]	R_1 = 0.0825 wR_2 = 0.1673
Largest peak/hole [eÅ^{-3}]	2.06/−0.63

Table S20. Bond lengths and angles for CP1_300K

Atom–Atom	Length [Å]
I1–Cu1	2.6345(16)
I1–Cu6$^{\#1}$	2.6830(15)
I1–Cu7$^{\#1}$	2.7754(15)
I2–Cu2	2.6433(15)
I2–Cu3	2.6908(17)
I2–Cu5$^{\#2}$	2.7023(15)
I3–Cu2	2.6962(16)
I3–Cu3	2.6252(17)
I3–Cu4	2.7715(15)
I4–Cu2	2.6953(14)
I4–Cu4	2.6851(15)
I4–Cu5$^{\#2}$	2.6997(15)
I5–Cu3$^{\#3}$	2.8200(15)
I5–Cu4$^{\#3}$	2.6203(15)
I5–Cu5	2.6153(15)
I6–Cu6	2.7043(14)
I6–Cu7	2.6717(15)
I6–Cu8$^{\#3}$	2.7181(14)
I7–Cu1$^{\#4}$	2.6827(16)
I7–Cu6	2.6435(15)
I7–Cu8$^{\#3}$	2.7404(15)
I8–Cu1$^{\#5}$	2.7942(15)
I8–Cu7$^{\#2}$	2.6317(15)
I8–Cu8	2.5992(14)
Cu1–Cu6$^{\#1}$	2.7191(17)
Cu1–Cu7$^{\#1}$	2.7704(19)
Cu1–Cu8$^{\#6}$	2.8087(18)
Cu1–S1	2.304(3)
Cu2–Cu3	2.7150(17)
Cu2–Cu4	2.8557(17)
Cu2–Cu5$^{\#2}$	2.7818(18)
Cu2–S2	2.312(3)
Cu3–Cu4	2.7613(18)
Cu3–Cu5$^{\#2}$	2.8127(19)
Cu3–S3	2.302(3)
Cu4–Cu5$^{\#2}$	2.674(2)
Cu4–S5	2.291(3)
Cu5–S6	2.295(3)
Cu6–Cu7	2.8489(17)
Cu6–Cu8$^{\#3}$	2.7563(17)
Cu6–S4	2.313(3)
Cu7–Cu8$^{\#3}$	2.6377(19)
Cu7–S7	2.294(3)
Cu8–S8	2.289(3)
S1–C1	1.856(16)
S1–C1A	1.90(4)
S1–C7	1.826(12)
S2–C10	1.807(13)
S2–C11	1.784(12)
S3–C33	1.816(12)
S3–C39	1.812(13)
S4–C42	1.801(12)
S4–C43	1.85(2)
S4–C43A	1.80(3)
S5–C17	1.810(11)
S5–C23	1.801(12)
S6–C26	1.813(13)
S6–C27	1.744(13)
S7–C49	1.822(11)
S7–C55	1.794(12)
S8–C58	1.791(10)
S8–C59	1.94(2)
S8–C59A	1.73(3)
C1–H1	0.9800
C1–C2	1.501(5)
C1–C6	1.501(5)
C1A–H1A	0.9800
C1A–C2A	1.500(5)
C1A–C6A	1.502(5)
C2–H2A	0.9700
C2–H2B	0.9700
C2–C3	1.500(5)
C2A–H2AA	0.9700
C2A–H2AB	0.9700
C2A–C3A	1.499(5)
C3–H3A	0.9700
C3–H3B	0.9700
C3–C4	1.498(5)
C3A–H3AA	0.9700
C3A–H3AB	0.9700
C3A–C4A	1.500(5)
C4–H4A	0.9700
C4–H4B	0.9700
C4–C5	1.497(5)
C4A–H4AA	0.9700
C4A–H4AB	0.9700
C4A–C5A	1.500(5)
C5–H5A	0.9700
C5–H5B	0.9700
C5–C6	1.501(5)
C5A–H5AA	0.9700
C5A–H5AB	0.9700
C5A–C6A	1.499(5)
C6–H6A	0.9700
C6–H6B	0.9700
C6A–H6AA	0.9700
C6A–H6AB	0.9700
C7–H7A	0.9700
C7–H7B	0.9700
C7–C8	1.475(14)
C8–C9	1.172(13)
C9–C10	1.450(14)
C10–H10A	0.9700
C10–H10B	0.9700
C11–H11	0.9800
C11–H11A	0.9800
C11–C12	1.500(5)
C11–C12A	1.499(5)
C11–C16	1.493(5)

C11–C16A	1.496(5)	C28–H28B	0.9700
C12–H12A	0.9700	C28–C29	1.504(5)
C12–H12B	0.9700	C29–H29A	0.9700
C12–C13	1.501(5)	C29–H29B	0.9700
C12A–H12C	0.9700	C29–C30	1.498(5)
C12A–H12D	0.9700	C30–H30A	0.9700
C12A–C13A	1.499(5)	C30–H30B	0.9700
C13–H13A	0.9700	C30–C31	1.500(5)
C13–H13B	0.9700	C31–H31A	0.9700
C13–C14	1.499(5)	C31–H31B	0.9700
C13A–H13C	0.9700	C31–C32	1.502(5)
C13A–H13D	0.9700	C32–H32A	0.9700
C13A–C14A	1.500(5)	C32–H32B	0.9700
C14–H14A	0.9700	C33–H33	0.9800
C14–H14B	0.9700	C33–H33A	0.9800
C14–C15	1.496(5)	C33–C34	1.493(5)
C14A–H14C	0.9700	C33–C34A	1.501(5)
C14A–H14D	0.9700	C33–C38	1.501(5)
C14A–C15A	1.499(5)	C33–C38A	1.497(5)
C15–H15A	0.9700	C34–H34A	0.9700
C15–H15B	0.9700	C34–H34B	0.9700
C15–C16	1.499(5)	C34–C35	1.502(5)
C15A–H15C	0.9700	C34A–H34C	0.9700
C15A–H15D	0.9700	C34A–H34D	0.9700
C15A–C16A	1.501(5)	C34A–C35A	1.500(5)
C16–H16A	0.9700	C35–H35A	0.9700
C16–H16B	0.9700	C35–H35B	0.9700
C16A–H16C	0.9700	C35–C36	1.499(5)
C16A–H16D	0.9700	C35A–H35C	0.9700
C17–H17	0.9800	C35A–H35D	0.9700
C17–C18	1.500(5)	C35A–C36A	1.499(5)
C17–C22	1.499(5)	C36–H36A	0.9700
C18–H18A	0.9700	C36–H36B	0.9700
C18–H18B	0.9700	C36–C37	1.496(5)
C18–C19	1.504(5)	C36A–H36C	0.9700
C19–H19A	0.9700	C36A–H36D	0.9700
C19–H19B	0.9700	C36A–C37A	1.499(5)
C19–C20	1.498(5)	C37–H37A	0.9700
C20–H20A	0.9700	C37–H37B	0.9700
C20–H20B	0.9700	C37–C38	1.502(5)
C20–C21	1.498(5)	C37A–H37C	0.9700
C21–H21A	0.9700	C37A–H37D	0.9700
C21–H21B	0.9700	C37A–C38A	1.500(5)
C21–C22	1.500(5)	C38–H38A	0.9700
C22–H22A	0.9700	C38–H38B	0.9700
C22–H22B	0.9700	C38A–H38C	0.9700
C23–H23A	0.9700	C38A–H38D	0.9700
C23–H23B	0.9700	C39–H39A	0.9700
C23–C24	1.482(16)	C39–H39B	0.9700
C24–C25	1.192(15)	C39–C40	1.468(14)
C25–C26	1.442(17)	C40–C41	1.165(13)
C26–H26A	0.9700	C41–C42	1.467(14)
C26–H26B	0.9700	C42–H42A	0.9700
C27–H27	0.9800	C42–H42B	0.9700
C27–C28	1.498(5)	C43–H43	0.9800
C27–C32	1.495(5)	C43–C44	1.501(5)
C28–H28A	0.9700	C43–C48	1.499(5)

C43A–H43A	0.9800
C43A–C44A	1.499(5)
C43A–C48A	1.500(5)
C44–H44A	0.9700
C44–H44B	0.9700
C44–C45	1.502(5)
C44A–H44C	0.9700
C44A–H44D	0.9700
C44A–C45A	1.500(5)
C45–H45A	0.9700
C45–H45B	0.9700
C45–C46	1.498(5)
C45A–H45C	0.9700
C45A–H45D	0.9700
C45A–C46A	1.499(5)
C46–H46A	0.9700
C46–H46B	0.9700
C46–C47	1.498(5)
C46A–H46C	0.9700
C46A–H46D	0.9700
C46A–C47A	1.499(5)
C47–H47A	0.9700
C47–H47B	0.9700
C47–C48	1.499(5)
C47A–H47C	0.9700
C47A–H47D	0.9700
C47A–C48A	1.501(5)
C48–H48A	0.9700
C48–H48B	0.9700
C48A–H48C	0.9700
C48A–H48D	0.9700
C49–H49	0.9800
C49–C50	1.501(5)
C49–C54	1.501(5)
C50–H50A	0.9700
C50–H50B	0.9700
C50–C51	1.506(5)
C51–H51A	0.9700
C51–H51B	0.9700
C51–C52	1.498(5)
C52–H52A	0.9700
C52–H52B	0.9700
C52–C53	1.499(5)
C53–H53A	0.9700
C53–H53B	0.9700
C53–C54	1.500(5)
C54–H54A	0.9700
C54–H54B	0.9700
C55–H55A	0.9700
C55–H55B	0.9700
C55–C56	1.493(16)
C56–C57	1.171(14)
C57–C58	1.458(15)
C58–H58A	0.9700
C58–H58B	0.9700
C59–H59	0.9800
C59–C60	1.500(5)
C59–C64	1.501(5)
C59A–H59A	0.9800
C59A–C60A	1.500(5)
C59A–C64A	1.500(5)
C60–H60A	0.9700
C60–H60B	0.9700
C60–C61	1.501(5)
C60A–H60C	0.9700
C60A–H60D	0.9700
C60A–C61A	1.501(5)
C61–H61A	0.9700
C61–H61B	0.9700
C61–C62	1.499(5)
C61A–H61C	0.9700
C61A–H61D	0.9700
C61A–C62A	1.500(5)
C62–H62A	0.9700
C62–H62B	0.9700
C62–C63	1.500(5)
C62A–H62C	0.9700
C62A–H62D	0.9700
C62A–C63A	1.36(6)
C63–H63A	0.9700
C63–H63B	0.9700
C63–C64	1.501(5)
C63A–H63C	0.9700
C63A–H63D	0.9700
C63A–C64A	1.500(5)
C64–H64A	0.9700
C64–H64B	0.9700
C64A–H64C	0.9700
C64A–H64D	0.9700

Atom–Atom–Atom	**Angle [°]**
Cu1–I1–Cu6$^{\#1}$	61.50(4)
Cu1–I1–Cu7$^{\#1}$	61.54(4)
Cu6$^{\#1}$–I1–Cu7$^{\#1}$	62.90(4)
Cu2–I2–Cu3	61.19(4)
Cu2–I2–Cu5$^{\#2}$	62.71(4)
Cu3–I2–Cu5$^{\#2}$	62.87(4)
Cu2–I3–Cu4	62.95(4)
Cu3–I3–Cu2	61.34(4)
Cu3–I3–Cu4	61.48(4)
Cu2–I4–Cu5$^{\#2}$	62.08(4)
Cu4–I4–Cu2	64.11(4)
Cu4–I4–Cu5$^{\#2}$	59.56(4)
Cu4$^{\#3}$–I5–Cu3$^{\#3}$	60.87(4)
Cu5–I5–Cu3$^{\#3}$	62.19(4)
Cu5–I5–Cu4$^{\#3}$	61.44(4)
Cu6–I6–Cu8$^{\#3}$	61.10(4)
Cu7–I6–Cu6	64.00(4)
Cu7–I6–Cu8$^{\#3}$	58.59(4)
Cu1$^{\#4}$–I7–Cu8$^{\#3}$	62.37(4)
Cu6–I7–Cu1$^{\#4}$	61.39(4)
Cu6–I7–Cu8$^{\#3}$	61.56(4)
Cu7$^{\#2}$–I8–Cu1$^{\#5}$	61.32(4)
Cu8–I8–Cu1$^{\#5}$	62.64(4)

Cu8–I8–Cu7$^{\#2}$	60.56(4)
I1–Cu1–I7$^{\#1}$	113.29(5)
I1–Cu1–I8$^{\#6}$	113.06(5)
I1–Cu1–Cu6$^{\#1}$	60.13(4)
I1–Cu1–Cu7$^{\#1}$	61.73(4)
I1–Cu1–Cu8$^{\#6}$	107.19(5)
I7$^{\#1}$–Cu1–I8$^{\#6}$	107.66(5)
I7$^{\#1}$–Cu1–Cu6$^{\#1}$	58.60(4)
I7$^{\#1}$–Cu1–Cu7$^{\#1}$	107.84(5)
I7$^{\#1}$–Cu1–Cu8$^{\#6}$	59.82(4)
I8$^{\#6}$–Cu1–Cu8$^{\#6}$	55.28(4)
Cu6$^{\#1}$–Cu1–I8$^{\#6}$	107.15(5)
Cu6$^{\#1}$–Cu1–Cu7$^{\#1}$	62.52(5)
Cu6$^{\#1}$–Cu1–Cu8$^{\#6}$	59.79(4)
Cu7$^{\#1}$–Cu1–I8$^{\#6}$	56.45(4)
Cu7$^{\#1}$–Cu1–Cu8$^{\#6}$	56.43(5)
S1–Cu1–I1	116.27(10)
S1–Cu1–I7$^{\#1}$	110.18(10)
S1–Cu1–I8$^{\#6}$	94.70(8)
S1–Cu1–Cu6$^{\#1}$	157.51(9)
S1–Cu1–Cu7$^{\#1}$	137.91(9)
S1–Cu1–Cu8$^{\#6}$	134.72(10)
I2–Cu2–I3	113.27(5)
I2–Cu2–I4	112.34(5)
I2–Cu2–Cu3	60.27(4)
I2–Cu2–Cu4	106.24(5)
I2–Cu2–Cu5$^{\#2}$	59.69(4)
I3–Cu2–Cu3	58.04(5)
I3–Cu2–Cu4	59.81(4)
I3–Cu2–Cu5$^{\#2}$	107.27(5)
I4–Cu2–I3	109.59(5)
I4–Cu2–Cu3	109.33(5)
I4–Cu2–Cu4	57.77(4)
I4–Cu2–Cu5$^{\#2}$	59.04(4)
Cu3–Cu2–Cu4	59.37(5)
Cu3–Cu2–Cu5$^{\#2}$	61.54(5)
Cu5$^{\#2}$–Cu2–Cu4	56.62(5)
S2–Cu2–I2	109.71(9)
S2–Cu2–I3	109.36(9)
S2–Cu2–I4	101.95(8)
S2–Cu2–Cu3	148.63(9)
S2–Cu2–Cu4	143.55(9)
S2–Cu2–Cu5$^{\#2}$	142.82(10)
I2–Cu3–I5$^{\#2}$	107.28(5)
I2–Cu3–Cu2	58.54(4)
I2–Cu3–Cu4	107.62(5)
I2–Cu3–Cu5$^{\#2}$	58.77(4)
I3–Cu3–I2	114.04(5)
I3–Cu3–I5$^{\#2}$	112.57(5)
I3–Cu3–Cu2	60.62(4)
I3–Cu3–Cu4	61.87(5)
I3–Cu3–Cu5$^{\#2}$	108.38(5)
Cu2–Cu3–I5$^{\#2}$	107.14(5)
Cu2–Cu3–Cu4	62.85(5)
Cu2–Cu3–Cu5$^{\#2}$	60.40(5)
Cu4–Cu3–I5$^{\#2}$	55.99(4)
Cu4–Cu3–Cu5$^{\#2}$	57.33(5)
Cu5$^{\#2}$–Cu3–I5$^{\#2}$	55.33(4)
S3–Cu3–I2	110.13(10)
S3–Cu3–I3	116.45(10)
S3–Cu3–I5$^{\#2}$	94.43(8)
S3–Cu3–Cu2	157.70(9)
S3–Cu3–Cu4	137.67(9)
S3–Cu3–Cu5$^{\#2}$	133.35(10)
I3–Cu4–Cu2	57.23(4)
I4–Cu4–I3	107.66(5)
I4–Cu4–Cu2	58.12(4)
I4–Cu4–Cu3	108.26(5)
I5$^{\#2}$–Cu4–I3	114.32(5)
I5$^{\#2}$–Cu4–I4	113.90(6)
I5$^{\#2}$–Cu4–Cu2	108.77(5)
I5$^{\#2}$–Cu4–Cu3	63.14(4)
I5$^{\#2}$–Cu4–Cu5$^{\#2}$	59.19(4)
Cu3–Cu4–I3	56.65(4)
Cu3–Cu4–Cu2	57.78(4)
Cu5$^{\#2}$–Cu4–I3	108.19(5)
Cu5$^{\#2}$–Cu4–I4	60.49(4)
Cu5$^{\#2}$–Cu4–Cu2	60.30(5)
Cu5$^{\#2}$–Cu4–Cu3	62.30(5)
S5–Cu4–I3	97.72(9)
S5–Cu4–I4	110.59(9)
S5–Cu4–I5$^{\#2}$	111.47(9)
S5–Cu4–Cu2	138.88(10)
S5–Cu4–Cu3	138.64(10)
S5–Cu4–Cu5$^{\#2}$	154.04(10)
I2$^{\#3}$–Cu5–Cu2$^{\#3}$	57.61(4)
I2$^{\#3}$–Cu5–Cu3$^{\#3}$	58.37(4)
I4$^{\#3}$–Cu5–I2$^{\#3}$	110.37(5)
I4$^{\#3}$–Cu5–Cu2$^{\#3}$	58.89(4)
I4$^{\#3}$–Cu5–Cu3$^{\#3}$	106.38(6)
I5–Cu5–I2$^{\#3}$	113.16(5)
I5–Cu5–I4$^{\#3}$	113.58(6)
I5–Cu5–Cu2$^{\#3}$	111.18(6)
I5–Cu5–Cu3$^{\#3}$	62.48(4)
I5–Cu5–Cu4$^{\#3}$	59.37(4)
Cu2$^{\#3}$–Cu5–Cu3$^{\#3}$	58.06(4)
Cu4$^{\#3}$–Cu5–I2$^{\#3}$	109.86(6)
Cu4$^{\#3}$–Cu5–I4$^{\#3}$	59.95(4)
Cu4$^{\#3}$–Cu5–Cu2$^{\#3}$	63.09(5)
Cu4$^{\#3}$–Cu5–Cu3$^{\#3}$	60.37(5)
S6–Cu5–I2$^{\#3}$	97.47(10)
S6–Cu5–I4$^{\#3}$	111.86(10)
S6–Cu5–I5	109.32(9)
S6–Cu5–Cu2$^{\#3}$	138.35(10)
S6–Cu5–Cu3$^{\#3}$	140.28(10)
S6–Cu5–Cu4$^{\#3}$	152.66(11)
I1$^{\#4}$–Cu6–I6	108.83(5)
I1$^{\#4}$–Cu6–Cu1$^{\#4}$	58.38(4)
I1$^{\#4}$–Cu6–Cu7	60.14(4)
I1$^{\#4}$–Cu6–Cu8$^{\#3}$	107.34(5)
I6–Cu6–Cu1$^{\#4}$	109.93(5)
I6–Cu6–Cu7	57.45(4)
I6–Cu6–Cu8$^{\#3}$	59.70(4)
I7–Cu6–I1$^{\#4}$	112.99(5)

I7–Cu6–I6	114.44(5)	C7–S1–Cu1	102.6(4)
I7–Cu6–Cu1$^{\#4}$	60.01(4)	C7–S1–C1	93.0(7)
I7–Cu6–Cu7	106.67(5)	C7–S1–C1A	118.7(12)
I7–Cu6–Cu8$^{\#3}$	60.95(4)	C10–S2–Cu2	102.1(4)
Cu1$^{\#4}$–Cu6–Cu7	59.62(5)	C11–S2–Cu2	110.0(4)
Cu1$^{\#4}$–Cu6–Cu8$^{\#3}$	61.72(5)	C11–S2–C10	101.3(7)
Cu8$^{\#3}$–Cu6–Cu7	56.12(5)	C33–S3–Cu3	114.0(5)
S4–Cu6–I1$^{\#4}$	113.94(9)	C39–S3–Cu3	100.8(4)
S4–Cu6–I6	100.71(8)	C39–S3–C33	98.5(7)
S4–Cu6–I7	105.37(9)	C42–S4–Cu6	103.2(4)
S4–Cu6–Cu1$^{\#4}$	149.28(9)	C42–S4–C43	110.7(10)
S4–Cu6–Cu7	146.73(9)	C42–S4–C43A	93.1(10)
S4–Cu6–Cu8$^{\#3}$	138.38(9)	C43–S4–Cu6	107.0(5)
I1$^{\#4}$–Cu7–Cu6	56.97(4)	C43A–S4–Cu6	120.8(11)
I6–Cu7–I1$^{\#4}$	107.07(5)	C17–S5–Cu4	116.0(4)
I6–Cu7–Cu1$^{\#4}$	109.36(5)	C23–S5–Cu4	103.6(4)
I6–Cu7–Cu6	58.56(4)	C23–S5–C17	101.4(6)
I8$^{\#3}$–Cu7–I1$^{\#4}$	113.76(5)	C26–S6–Cu5	103.3(5)
I8$^{\#3}$–Cu7–I6	115.19(5)	C27–S6–Cu5	111.3(4)
I8$^{\#3}$–Cu7–Cu1$^{\#4}$	62.23(4)	C27–S6–C26	108.9(7)
I8$^{\#3}$–Cu7–Cu6	108.03(5)	C49–S7–Cu7	115.5(4)
I8$^{\#3}$–Cu7–Cu8$^{\#3}$	59.11(4)	C55–S7–Cu7	103.9(4)
Cu1$^{\#4}$–Cu7–I1$^{\#4}$	56.73(4)	C55–S7–C49	100.9(6)
Cu1$^{\#4}$–Cu7–Cu6	57.86(4)	C58–S8–Cu8	100.5(4)
Cu8$^{\#3}$–Cu7–I1$^{\#4}$	108.08(5)	C58–S8–C59	93.5(6)
Cu8$^{\#3}$–Cu7–I6	61.58(4)	C59–S8–Cu8	109.2(5)
Cu8$^{\#3}$–Cu7–Cu1$^{\#4}$	62.52(5)	C59A–S8–Cu8	113.0(8)
Cu8$^{\#3}$–Cu7–Cu6	60.17(5)	C59A–S8–C58	118.9(11)
S7–Cu7–I1$^{\#4}$	98.19(9)	S1–C1–H1	107.2
S7–Cu7–I6	112.62(10)	C2–C1–S1	107.1(12)
S7–Cu7–I8$^{\#3}$	108.79(9)	C2–C1–H1	107.2
S7–Cu7–Cu1$^{\#4}$	136.08(10)	C2–C1–C6	111.8(15)
S7–Cu7–Cu6	141.74(10)	C6–C1–S1	115.8(10)
S7–Cu7–Cu8$^{\#3}$	153.68(10)	C6–C1–H1	107.2
I6$^{\#2}$–Cu8–I7$^{\#2}$	110.92(5)	S1–C1A–H1A	108.3
I6$^{\#2}$–Cu8–Cu1$^{\#5}$	106.92(5)	C2A–C1A–S1	111(2)
I6$^{\#2}$–Cu8–Cu6$^{\#2}$	59.20(4)	C2A–C1A–H1A	108.3
I7$^{\#2}$–Cu8–Cu1$^{\#5}$	57.80(4)	C2A–C1A–C6A	116(3)
I7$^{\#2}$–Cu8–Cu6$^{\#2}$	57.49(4)	C6A–C1A–S1	104(2)
I8–Cu8–I6$^{\#2}$	114.70(5)	C6A–C1A–H1A	108.3
I8–Cu8–I7$^{\#2}$	111.78(5)	C1–C2–H2A	108.7
I8–Cu8–Cu1$^{\#5}$	62.08(4)	C1–C2–H2B	108.7
I8–Cu8–Cu6$^{\#2}$	111.84(5)	H2A–C2–H2B	107.6
I8–Cu8–Cu7$^{\#2}$	60.33(4)	C3–C2–C1	114.3(15)
Cu6$^{\#2}$–Cu8–Cu1$^{\#5}$	58.49(4)	C3–C2–H2A	108.7
Cu7$^{\#2}$–Cu8–I6$^{\#2}$	59.83(4)	C3–C2–H2B	108.7
Cu7$^{\#2}$–Cu8–I7$^{\#2}$	110.06(5)	C1A–C2A–H2AA	109.2
Cu7$^{\#2}$–Cu8–Cu1$^{\#5}$	61.06(5)	C1A–C2A–H2AB	109.2
Cu7$^{\#2}$–Cu8–Cu6$^{\#2}$	63.72(5)	C1A–C2A–C3A	112(3)
S8–Cu8–I6$^{\#2}$	108.56(9)	H2AA–C2A–H2AB	107.9
S8–Cu8–I7$^{\#2}$	96.52(9)	C3A–C2A–H2AA	109.2
S8–Cu8–I8	112.90(8)	C3A–C2A–H2AB	109.2
S8–Cu8–Cu1$^{\#5}$	142.00(10)	C2–C3–H3A	109.6
S8–Cu8–Cu6$^{\#2}$	134.20(9)	C2–C3–H3B	109.6
S8–Cu8–Cu7$^{\#2}$	153.27(10)	H3A–C3–H3B	108.1
C1–S1–Cu1	116.1(5)	C4–C3–C2	110.4(17)
C1A–S1–Cu1	105.8(7)	C4–C3–H3A	109.6

C4–C3–H3B	109.6
C2A–C3A–H3AA	110.8
C2A–C3A–H3AB	110.8
C2A–C3A–C4A	105(4)
H3AA–C3A–H3AB	108.9
C4A–C3A–H3AA	110.8
C4A–C3A–H3AB	110.8
C3–C4–H4A	108.6
C3–C4–H4B	108.6
H4A–C4–H4B	107.6
C5–C4–C3	114.7(17)
C5–C4–H4A	108.6
C5–C4–H4B	108.6
C3A–C4A–H4AA	107.2
C3A–C4A–H4AB	107.2
H4AA–C4A–H4AB	106.8
C5A–C4A–C3A	121(5)
C5A–C4A–H4AA	107.2
C5A–C4A–H4AB	107.2
C4–C5–H5A	108.5
C4–C5–H5B	108.5
C4–C5–C6	115.0(16)
H5A–C5–H5B	107.5
C6–C5–H5A	108.5
C6–C5–H5B	108.5
C4A–C5A–H5AA	108.3
C4A–C5A–H5AB	108.3
H5AA–C5A–H5AB	107.4
C6A–C5A–C4A	116(5)
C6A–C5A–H5AA	108.3
C6A–C5A–H5AB	108.3
C1–C6–H6A	109.5
C1–C6–H6B	109.5
C5–C6–C1	110.7(14)
C5–C6–H6A	109.5
C5–C6–H6B	109.5
H6A–C6–H6B	108.1
C1A–C6A–H6AA	110.0
C1A–C6A–H6AB	110.0
C5A–C6A–C1A	108(3)
C5A–C6A–H6AA	110.0
C5A–C6A–H6AB	110.0
H6AA–C6A–H6AB	108.4
S1–C7–H7A	109.3
S1–C7–H7B	109.3
H7A–C7–H7B	108.0
C8–C7–S1	111.5(8)
C8–C7–H7A	109.3
C8–C7–H7B	109.3
C9–C8–C7	177.4(12)
C8–C9–C10	177.2(12)
S2–C10–H10A	109.0
S2–C10–H10B	109.0
C9–C10–S2	113.1(9)
C9–C10–H10A	109.0
C9–C10–H10B	109.0
H10A–C10–H10B	107.8
S2–C11–H11	104.4
S2–C11–H11A	98.5
C12–C11–S2	115.1(10)
C12–C11–H11	104.4
C12A–C11–S2	104.9(16)
C12A–C11–H11A	98.5
C16–C11–S2	116.1(10)
C16–C11–H11	104.4
C16–C11–C12	110.9(14)
C16A–C11–S2	124.9(15)
C16A–C11–H11A	98.5
C16A–C11–C12A	124(2)
C11–C12–H12A	108.8
C11–C12–H12B	108.8
C11–C12–C13	113.8(17)
H12A–C12–H12B	107.7
C13–C12–H12A	108.8
C13–C12–H12B	108.8
C11–C12A–H12C	109.4
C11–C12A–H12D	109.4
C11–C12A–C13A	111(3)
H12C–C12A–H12D	108.0
C13A–C12A–H12C	109.4
C13A–C12A–H12D	109.4
C12–C13–H13A	110.5
C12–C13–H13B	110.5
H13A–C13–H13B	108.7
C14–C13–C12	106.1(16)
C14–C13–H13A	110.5
C14–C13–H13B	110.5
C12A–C13A–H13C	108.6
C12A–C13A–H13D	108.6
C12A–C13A–C14A	114(4)
H13C–C13A–H13D	107.6
C14A–C13A–H13C	108.6
C14A–C13A–H13D	108.6
C13–C14–H14A	109.2
C13–C14–H14B	109.2
H14A–C14–H14B	107.9
C15–C14–C13	112(2)
C15–C14–H14A	109.2
C15–C14–H14B	109.2
C13A–C14A–H14C	111.7
C13A–C14A–H14D	111.7
H14C–C14A–H14D	109.5
C15A–C14A–C13A	100(4)
C15A–C14A–H14C	111.7
C15A–C14A–H14D	111.7
C14–C15–H15A	109.3
C14–C15–H15B	109.3
C14–C15–C16	111.6(19)
H15A–C15–H15B	108.0
C16–C15–H15A	109.3
C16–C15–H15B	109.3
C14A–C15A–H15C	110.2
C14A–C15A–H15D	110.2
C14A–C15A–C16A	107(5)

H15C–C15A–H15D	108.5	C25–C24–C23	175.8(16)
C16A–C15A–H15C	110.2	C24–C25–C26	174.4(16)
C16A–C15A–H15D	110.2	S6–C26–H26A	109.2
C11–C16–C15	112.4(14)	S6–C26–H26B	109.2
C11–C16–H16A	109.1	C25–C26–S6	112.0(9)
C11–C16–H16B	109.1	C25–C26–H26A	109.2
C15–C16–H16A	109.1	C25–C26–H26B	109.2
C15–C16–H16B	109.1	H26A–C26–H26B	107.9
H16A–C16–H16B	107.9	S6–C27–H27	104.2
C11–C16A–C15A	99(3)	C28–C27–S6	115.5(10)
C11–C16A–H16C	112.0	C28–C27–H27	104.2
C11–C16A–H16D	112.0	C32–C27–S6	118.4(9)
C15A–C16A–H16C	112.0	C32–C27–H27	104.2
C15A–C16A–H16D	112.0	C32–C27–C28	108.6(12)
H16C–C16A–H16D	109.7	C27–C28–H28A	109.0
S5–C17–H17	107.2	C27–C28–H28B	109.0
C18–C17–S5	113.1(7)	C27–C28–C29	112.9(13)
C18–C17–H17	107.2	H28A–C28–H28B	107.8
C22–C17–S5	108.3(7)	C29–C28–H28A	109.0
C22–C17–H17	107.2	C29–C28–H28B	109.0
C22–C17–C18	113.5(11)	C28–C29–H29A	109.3
C17–C18–H18A	109.9	C28–C29–H29B	109.3
C17–C18–H18B	109.9	H29A–C29–H29B	108.0
C17–C18–C19	108.9(10)	C30–C29–C28	111.6(14)
H18A–C18–H18B	108.3	C30–C29–H29A	109.3
C19–C18–H18A	109.9	C30–C29–H29B	109.3
C19–C18–H18B	109.9	C29–C30–H30A	109.2
C18–C19–H19A	109.0	C29–C30–H30B	109.2
C18–C19–H19B	109.0	C29–C30–C31	112.0(13)
H19A–C19–H19B	107.8	H30A–C30–H30B	107.9
C20–C19–C18	112.9(14)	C31–C30–H30A	109.2
C20–C19–H19A	109.0	C31–C30–H30B	109.2
C20–C19–H19B	109.0	C30–C31–H31A	109.9
C19–C20–H20A	109.6	C30–C31–H31B	109.9
C19–C20–H20B	109.6	C30–C31–C32	108.8(12)
C19–C20–C21	110.5(14)	H31A–C31–H31B	108.3
H20A–C20–H20B	108.1	C32–C31–H31A	109.9
C21–C20–H20A	109.6	C32–C31–H31B	109.9
C21–C20–H20B	109.6	C27–C32–C31	116.6(12)
C20–C21–H21A	109.1	C27–C32–H32A	108.2
C20–C21–H21B	109.1	C27–C32–H32B	108.2
C20–C21–C22	112.7(12)	C31–C32–H32A	108.2
H21A–C21–H21B	107.8	C31–C32–H32B	108.2
C22–C21–H21A	109.1	H32A–C32–H32B	107.3
C22–C21–H21B	109.1	S3–C33–H33	105.2
C17–C22–C21	110.5(10)	S3–C33–H33A	97.7
C17–C22–H22A	109.6	C34–C33–S3	108.2(10)
C17–C22–H22B	109.6	C34–C33–H33	105.2
C21–C22–H22A	109.6	C34–C33–C38	114.4(14)
C21–C22–H22B	109.6	C34A–C33–S3	118.8(16)
H22A–C22–H22B	108.1	C34A–C33–H33A	97.7
S5–C23–H23A	109.6	C38–C33–S3	117.5(8)
S5–C23–H23B	109.6	C38–C33–H33	105.2
H23A–C23–H23B	108.1	C38A–C33–S3	116.7(11)
C24–C23–S5	110.4(9)	C38A–C33–H33A	97.7
C24–C23–H23A	109.6	C38A–C33–C34A	119.3(17)
C24–C23–H23B	109.6	C33–C34–H34A	110.3

C33–C34–H34B	110.3
C33–C34–C35	107.0(15)
H34A–C34–H34B	108.6
C35–C34–H34A	110.3
C35–C34–H34B	110.3
C33–C34A–H34C	107.2
C33–C34A–H34D	107.2
H34C–C34A–H34D	106.8
C35A–C34A–C33	120(2)
C35A–C34A–H34C	107.2
C35A–C34A–H34D	107.2
C34–C35–H35A	108.4
C34–C35–H35B	108.4
H35A–C35–H35B	107.4
C36–C35–C34	115.7(18)
C36–C35–H35A	108.4
C36–C35–H35B	108.4
C34A–C35A–H35C	108.2
C34A–C35A–H35D	108.2
H35C–C35A–H35D	107.4
C36A–C35A–C34A	116(4)
C36A–C35A–H35C	108.2
C36A–C35A–H35D	108.2
C35–C36–H36A	107.9
C35–C36–H36B	107.9
H36A–C36–H36B	107.2
C37–C36–C35	117.5(17)
C37–C36–H36A	107.9
C37–C36–H36B	107.9
C35A–C36A–H36C	109.5
C35A–C36A–H36D	109.5
H36C–C36A–H36D	108.1
C37A–C36A–C35A	111(4)
C37A–C36A–H36C	109.5
C37A–C36A–H36D	109.5
C36–C37–H37A	108.2
C36–C37–H37B	108.2
C36–C37–C38	116.2(16)
H37A–C37–H37B	107.4
C38–C37–H37A	108.2
C38–C37–H37B	108.2
C36A–C37A–H37C	108.5
C36A–C37A–H37D	108.5
C36A–C37A–C38A	115(4)
H37C–C37A–H37D	107.5
C38A–C37A–H37C	108.5
C38A–C37A–H37D	108.5
C33–C38–C37	113.0(13)
C33–C38–H38A	109.0
C33–C38–H38B	109.0
C37–C38–H38A	109.0
C37–C38–H38B	109.0
H38A–C38–H38B	107.8
C33–C38A–C37A	113(2)
C33–C38A–H38C	109.0
C33–C38A–H38D	109.0
C37A–C38A–H38C	109.0
C37A–C38A–H38D	109.0
H38C–C38A–H38D	107.8
S3–C39–H39A	108.9
S3–C39–H39B	108.9
H39A–C39–H39B	107.7
C40–C39–S3	113.4(9)
C40–C39–H39A	108.9
C40–C39–H39B	108.9
C41–C40–C39	176.7(12)
C40–C41–C42	175.5(12)
S4–C42–H42A	109.1
S4–C42–H42B	109.1
C41–C42–S4	112.5(9)
C41–C42–H42A	109.1
C41–C42–H42B	109.1
H42A–C42–H42B	107.8
S4–C43–H43	104.9
C44–C43–S4	112.1(14)
C44–C43–H43	104.9
C48–C43–S4	115.3(13)
C48–C43–H43	104.9
C48–C43–C44	113.4(17)
S4–C43A–H43A	107.2
C44A–C43A–S4	114(2)
C44A–C43A–H43A	107.2
C44A–C43A–C48A	110(3)
C48A–C43A–S4	110(2)
C48A–C43A–H43A	107.2
C43–C44–H44A	109.3
C43–C44–H44B	109.3
C43–C44–C45	111.7(15)
H44A–C44–H44B	108.0
C45–C44–H44A	109.3
C45–C44–H44B	109.3
C43A–C44A–H44C	109.2
C43A–C44A–H44D	109.2
C43A–C44A–C45A	112(3)
H44C–C44A–H44D	107.9
C45A–C44A–H44C	109.2
C45A–C44A–H44D	109.2
C44–C45–H45A	109.4
C44–C45–H45B	109.4
H45A–C45–H45B	108.0
C46–C45–C44	111.1(19)
C46–C45–H45A	109.4
C46–C45–H45B	109.4
C44A–C45A–H45C	108.2
C44A–C45A–H45D	108.2
H45C–C45A–H45D	107.3
C46A–C45A–C44A	116(3)
C46A–C45A–H45C	108.2
C46A–C45A–H45D	108.2
C45–C46–H46A	109.0
C45–C46–H46B	109.0
C45–C46–C47	113(2)
H46A–C46–H46B	107.8
C47–C46–H46A	109.0

C47–C46–H46B	109.0	C52–C53–C54	112.0(12)
C45A–C46A–H46C	110.1	H53A–C53–H53B	107.9
C45A–C46A–H46D	110.1	C54–C53–H53A	109.2
H46C–C46A–H46D	108.4	C54–C53–H53B	109.2
C47A–C46A–C45A	108(3)	C49–C54–H54A	109.1
C47A–C46A–H46C	110.1	C49–C54–H54B	109.1
C47A–C46A–H46D	110.1	C53–C54–C49	112.5(10)
C46–C47–H47A	109.7	C53–C54–H54A	109.1
C46–C47–H47B	109.7	C53–C54–H54B	109.1
C46–C47–C48	109.9(18)	H54A–C54–H54B	107.8
H47A–C47–H47B	108.2	S7–C55–H55A	109.6
C48–C47–H47A	109.7	S7–C55–H55B	109.6
C48–C47–H47B	109.7	H55A–C55–H55B	108.2
C46A–C47A–H47C	109.9	C56–C55–S7	110.1(8)
C46A–C47A–H47D	109.9	C56–C55–H55A	109.6
C46A–C47A–C48A	109(3)	C56–C55–H55B	109.6
H47C–C47A–H47D	108.3	C57–C56–C55	172.8(14)
C48A–C47A–H47C	109.9	C56–C57–C58	174.5(13)
C48A–C47A–H47D	109.9	S8–C58–H58A	109.0
C43–C48–C47	112.8(19)	S8–C58–H58B	109.0
C43–C48–H48A	109.0	C57–C58–S8	112.8(8)
C43–C48–H48B	109.0	C57–C58–H58A	109.0
C47–C48–H48A	109.0	C57–C58–H58B	109.0
C47–C48–H48B	109.0	H58A–C58–H58B	107.8
H48A–C48–H48B	107.8	S8–C59–H59	108.6
C43A–C48A–C47A	117(3)	C60–C59–S8	109.5(13)
C43A–C48A–H48C	108.1	C60–C59–H59	108.6
C43A–C48A–H48D	108.1	C60–C59–C64	113.4(14)
C47A–C48A–H48C	108.1	C64–C59–S8	108.1(12)
C47A–C48A–H48D	108.1	C64–C59–H59	108.6
H48C–C48A–H48D	107.3	S8–C59A–H59A	106.7
S7–C49–H49	107.6	C60A–C59A–S8	112.9(19)
C50–C49–S7	113.6(7)	C60A–C59A–H59A	106.7
C50–C49–H49	107.6	C64A–C59A–S8	116.8(18)
C54–C49–S7	109.0(7)	C64A–C59A–H59A	106.7
C54–C49–H49	107.6	C64A–C59A–C60A	106(2)
C54–C49–C50	111.1(10)	C59–C60–H60A	109.8
C49–C50–H50A	109.2	C59–C60–H60B	109.8
C49–C50–H50B	109.2	C59–C60–C61	109.4(16)
C49–C50–C51	112.0(10)	H60A–C60–H60B	108.2
H50A–C50–H50B	107.9	C61–C60–H60A	109.8
C51–C50–H50A	109.2	C61–C60–H60B	109.8
C51–C50–H50B	109.2	C59A–C60A–H60C	108.7
C50–C51–H51A	109.7	C59A–C60A–H60D	108.7
C50–C51–H51B	109.7	C59A–C60A–C61A	114(3)
H51A–C51–H51B	108.2	H60C–C60A–H60D	107.6
C52–C51–C50	110.0(12)	C61A–C60A–H60C	108.7
C52–C51–H51A	109.7	C61A–C60A–H60D	108.7
C52–C51–H51B	109.7	C60–C61–H61A	108.0
C51–C52–H52A	108.7	C60–C61–H61B	108.0
C51–C52–H52B	108.7	H61A–C61–H61B	107.2
C51–C52–C53	114.3(14)	C62–C61–C60	117.4(18)
H52A–C52–H52B	107.6	C62–C61–H61A	108.0
C53–C52–H52A	108.7	C62–C61–H61B	108.0
C53–C52–H52B	108.7	C60A–C61A–H61C	109.4
C52–C53–H53A	109.2	C60A–C61A–H61D	109.4
C52–C53–H53B	109.2	H61C–C61A–H61D	108.0

C62A–C61A–C60A	111(3)
C62A–C61A–H61C	109.4
C62A–C61A–H61D	109.4
C61–C62–H62A	109.6
C61–C62–H62B	109.6
C61–C62–C63	110(2)
H62A–C62–H62B	108.1
C63–C62–H62A	109.6
C63–C62–H62B	109.6
C61A–C62A–H62C	108.8
C61A–C62A–H62D	108.8
H62C–C62A–H62D	107.7
C63A–C62A–C61A	114(4)
C63A–C62A–H62C	108.8
C63A–C62A–H62D	108.8
C62–C63–H63A	109.3
C62–C63–H63B	109.3
C62–C63–C64	111.7(19)
H63A–C63–H63B	107.9
C64–C63–H63A	109.3
C64–C63–H63B	109.3
C62A–C63A–H63C	109.4
C62A–C63A–H63D	109.4
C62A–C63A–C64A	111(3)
H63C–C63A–H63D	108.0
C64A–C63A–H63C	109.4
C64A–C63A–H63D	109.4
C59–C64–H64A	109.3
C59–C64–H64B	109.3
C63–C64–C59	111.4(19)
C63–C64–H64A	109.3
C63–C64–H64B	109.3
H64A–C64–H64B	108.0
C59A–C64A–H64C	108.4
C59A–C64A–H64D	108.4
C63A–C64A–C59A	115(3)
C63A–C64A–H64C	108.4
C63A–C64A–H64D	108.4
H64C–C64A–H64D	107.5

Symmetry transformations used to generate equivalent atoms:
#1: -1+X, -1+Y, -1+Z; #2: 1+X, +Y, +Z; #3: -1+X, +Y, +Z; #4: 1+X, 1+Y, 1+Z; #5: 2+X, 1+Y, 1+Z; #6: -2+X, -1+Y, -1+Z;

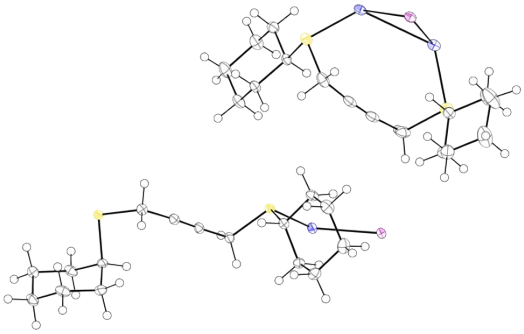
Table S21. Torsion angles for CP1_300K

Atom–Atom–Atom–Atom	Torsion Angle [°]
Cu1–S1–C1–C2	−94.1(15)
Cu1–S1–C1–C6	31.4(16)
Cu1–S1–C7–C8	149.4(7)
Cu2–S2–C10–C9	−164.2(8)
Cu2–S2–C11–C12	44.3(18)
Cu2–S2–C11–C12A	105.8(19)
Cu2–S2–C11–C16	176.3(13)
Cu2–S2–C11–C16A	−46(2)
Cu3–S3–C33–C34	88.1(13)
Cu3–S3–C33–C34A	3(2)
Cu3–S3–C33–C38	−43.2(17)
Cu3–S3–C33–C38A	156.9(15)
Cu3–S3–C39–C40	−157.6(8)
Cu4–S5–C17–C18	−40.6(11)
Cu4–S5–C17–C22	86.1(9)
Cu4–S5–C23–C24	−171.4(9)
Cu5–S6–C26–C25	142.3(10)
Cu5–S6–C27–C28	174.0(12)
Cu5–S6–C27–C32	42.8(14)
Cu6–S4–C42–C41	162.1(8)
Cu6–S4–C43–C44	176.0(17)
Cu6–S4–C43–C48	44(2)
Cu6–S4–C43A–C44A	32(3)
Cu6–S4–C43A–C48A	−93(3)
Cu7–S7–C49–C50	34.5(10)
Cu7–S7–C49–C54	−90.0(8)
Cu7–S7–C55–C56	162.6(8)
Cu8–S8–C58–C57	−153.3(8)
Cu8–S8–C59A–C60A	−53(3)
Cu8–S8–C59A–C64A	−176(2)
S1–C1–C2–C3	−176.4(18)
S1–C1–C6–C5	−175.3(14)
S1–C1A–C2A–C3A	−179(3)
S1–C1A–C6A–C5A	−172(3)
S2–C11–C12–C13	−170.2(18)
S2–C11–C12A–C13A	180(3)
S2–C11–C16–C15	176.5(17)
S2–C11–C16A–C15A	−168(2)
S3–C33–C34–C35	166.2(16)
S3–C33–C34A–C35A	153(3)
S3–C33–C38–C37	−178.6(15)
S3–C33–C38A–C37A	−172(2)
S4–C43–C44–C45	177(2)
S4–C43–C48–C47	−177.3(19)
S4–C43A–C44A–C45A	−169(3)
S4–C43A–C48A–C47A	177(3)
S5–C17–C18–C19	179.0(12)
S5–C17–C22–C21	179.1(10)
S6–C27–C28–C29	172.3(13)
S6–C27–C32–C31	−172.5(11)
S7–C49–C50–C51	−180.0(11)
S7–C49–C54–C53	179.8(10)
S8–C59–C60–C61	−171.3(16)
S8–C59–C64–C63	177.9(14)
S8–C59A–C60A–C61A	−180(2)
S8–C59A–C64A–C63A	180(2)
C1–S1–C7–C8	−93.1(9)
C1–C2–C3–C4	−52(3)
C1A–S1–C7–C8	−94.4(12)
C1A–C2A–C3A–C4A	−55(5)
C2–C1–C6–C5	−52(2)
C2–C3–C4–C5	47(3)
C2A–C1A–C6A–C5A	−49(5)
C2A–C3A–C4A–C5A	49(7)

C3–C4–C5–C6	−48(3)
C3A–C4A–C5A–C6A	−43(8)
C4–C5–C6–C1	49(3)
C4A–C5A–C6A–C1A	38(6)
C6–C1–C2–C3	56(3)
C6A–C1A–C2A–C3A	62(5)
C7–S1–C1–C2	160.3(16)
C7–S1–C1–C6	−74.2(15)
C10–S2–C11–C12	151.8(17)
C10–S2–C11–C12A	−146.8(19)
C10–S2–C11–C16	−76.2(15)
C10–S2–C11–C16A	61(2)
C11–S2–C10–C9	82.2(10)
C11–C12–C13–C14	−59(3)
C11–C12A–C13A–C14A	34(5)
C12–C11–C16–C15	−50(3)
C12–C13–C14–C15	59(4)
C12A–C11–C16A–C15A	45(4)
C12A–C13A–C14A–C15A	−59(6)
C13–C14–C15–C16	−58(4)
C13A–C14A–C15A–C16A	84(6)
C14–C15–C16–C11	51(3)
C14A–C15A–C16A–C11	−73(4)
C16–C11–C12–C13	55(3)
C16A–C11–C12A–C13A	−28(4)
C17–S5–C23–C24	68.0(11)
C17–C18–C19–C20	−56(2)
C18–C17–C22–C21	−54.4(16)
C18–C19–C20–C21	56(2)
C19–C20–C21–C22	−54(2)
C20–C21–C22–C17	53.1(19)
C22–C17–C18–C19	55.2(18)
C23–S5–C17–C18	70.7(12)
C23–S5–C17–C22	−162.5(9)
C26–S6–C27–C28	60.8(15)
C26–S6–C27–C32	−70.4(13)
C27–S6–C26–C25	−99.3(11)
C27–C28–C29–C30	55(2)
C28–C27–C32–C31	53.3(19)
C28–C29–C30–C31	−56(2)
C29–C30–C31–C32	53(2)
C30–C31–C32–C27	−54.2(19)
C32–C27–C28–C29	−52(2)
C33–S3–C39–C40	85.8(10)
C33–C34–C35–C36	52(3)
C33–C34A–C35A–C36A	−11(6)
C34–C33–C38–C37	53(2)
C34–C35–C36–C37	−38(4)
C34A–C33–C38A–C37A	−18(4)
C34A–C35A–C36A–C37A	39(7)
C35–C36–C37–C38	27(4)
C35A–C36A–C37A–C38A	−59(7)
C36–C37–C38–C33	−34(3)
C36A–C37A–C38A–C33	48(5)
C38–C33–C34–C35	−61(2)
C38A–C33–C34A–C35A	−1(5)
C39–S3–C33–C34	−165.9(13)
C39–S3–C33–C34A	109(2)
C39–S3–C33–C38	62.8(16)
C39–S3–C33–C38A	−97.2(16)
C42–S4–C43–C44	64(2)
C42–S4–C43–C48	−67(2)
C42–S4–C43A–C44A	−75(3)
C42–S4–C43A–C48A	160(3)
C43–S4–C42–C41	−83.7(10)
C43–C44–C45–C46	52(3)
C43A–S4–C42–C41	−75.3(14)
C43A–C44A–C45A–C46A	51(5)
C44–C43–C48–C47	52(3)
C44–C45–C46–C47	−56(4)
C44A–C43A–C48A–C47A	50(5)
C44A–C45A–C46A–C47A	−56(5)
C45–C46–C47–C48	56(4)
C45A–C46A–C47A–C48A	56(5)
C46–C47–C48–C43	−53(4)
C46A–C47A–C48A–C43A	−57(4)
C48–C43–C44–C45	−51(3)
C48A–C43A–C44A–C45A	−44(5)
C49–S7–C55–C56	−77.4(10)
C49–C50–C51–C52	55(2)
C50–C49–C54–C53	53.8(15)
C50–C51–C52–C53	−52(2)
C51–C52–C53–C54	50(2)
C52–C53–C54–C49	−50.4(19)
C54–C49–C50–C51	−56.6(16)
C55–S7–C49–C50	−76.7(10)
C55–S7–C49–C54	158.8(9)
C58–S8–C59A–C60A	65(3)
C58–S8–C59A–C64A	−59(3)
C59–S8–C58–C57	96.4(10)
C59–C60–C61–C62	49(3)
C59A–S8–C58–C57	82.9(12)
C59A–C60A–C61A–C62A	51(5)
C60–C59–C64–C63	56(3)
C60–C61–C62–C63	−50(3)
C60A–C59A–C64A–C63A	52(4)
C60A–C61A–C62A–C63A	−54(6)
C61–C62–C63–C64	52(3)
C61A–C62A–C63A–C64A	55(5)
C62–C63–C64–C59	−56(3)
C62A–C63A–C64A–C59A	−57(5)
C64–C59–C60–C61	−50(3)
C64A–C59A–C60A–C61A	−50(4)

Crystal structure of CP2D1_100K

Crystal Data and Experimental



Experimental: The data for CP2D1_100K were collected from a shock-cooled single crystal at 100.0(1) K on a Bruker D8 Venture four-circle diffractometer with a X-ray tube using a graphite as monochromator and a CPAD PHOTON II area detector detector. The diffractometer was equipped with an Oxford Cryostream 800 low temperature device and used Mo K_{α} radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.38A and a multi-scan absorption correction using SADABS 2016/2 was applied. [1,2] The structure was solved by direct methods with XT and refined by full-matrix least-squares methods against F^2 using SHELXL.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[5] CCDC 2326783 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures. This report and the CIF file were generated using FinalCif.[6]

Table S22. Crystal data and structure refinement for CP2D1_100K

Internal Reference	CP2D1_100K
CCDC number	2326783
Empirical formula	$C_{16}H_{26}CuIS_2$
Formula weight	472.93
Temperature [K]	100.0(1)
Crystal system	monoclinic
Space group (number)	$C2/c$ (15)
a [Å]	31.839(2)
b [Å]	10.1369(7)
c [Å]	22.8562(15)
α [°]	90
β [°]	96.789(2)
γ [°]	90
Volume [Å^3]	7325.0(9)
Z	16
ρ_{calc} [gcm^{-3}]	1.715
μ [mm^{-1}]	3.096
F(000)	3776
Crystal size [mm^3]	0.247×0.279×0.481
Crystal colour	clear light yellow
Crystal shape	block
Radiation	Mo K_{α} (λ=0.71073 Å)
2θ range [°]	5.64 to 55.00 (0.77 Å)
Index ranges	−41 ≤ h ≤ 41 −13 ≤ k ≤ 13 −29 ≤ l ≤ 29
Reflections collected	96786
Independent reflections	8412 R_{int} = 0.0284 R_{sigma} = 0.0127
Completeness to θ = 25.242°	99.8 %
Data / Restraints / Parameters	8412 / 0 / 362
Goodness-of-fit on F^2	1.169
Final R indexes [I≥2σ(I)]	R_1 = 0.0161 wR_2 = 0.0388
Final R indexes [all data]	R_1 = 0.0163 wR_2 = 0.0389
Largest peak/hole [eÅ^{-3}]	0.88/−0.52

Table S23. Bond lengths and angles for CP2D1_100K

Atom–Atom	Length [Å]
I1–Cu1	2.6302(3)
I1–Cu1$^{\#1}$	2.6631(3)
Cu1–Cu1$^{\#1}$	2.8535(4)
Cu1–S1$^{\#2}$	2.3424(4)
Cu1–S2	2.3175(4)
S1–C1	1.8382(16)
S1–C7	1.8243(16)
S2–C10	1.8209(16)
S2–C11	1.8314(16)
C1–H1	1.0000
C1–C2	1.528(2)
C1–C6	1.531(2)
C2–H2A	0.9900
C2–H2B	0.9900
C2–C3	1.526(2)
C3–H3A	0.9900
C3–H3B	0.9900
C3–C4	1.525(2)
C4–H4A	0.9900
C4–H4B	0.9900
C4–C5	1.526(2)
C5–H5A	0.9900
C5–H5B	0.9900
C5–C6	1.524(3)
C6–H6A	0.9900
C6–H6B	0.9900
C7–H7A	0.9900
C7–H7B	0.9900
C7–C8	1.459(2)
C8–C9	1.194(2)
C9–C10	1.461(2)
C10–H10A	0.9900
C10–H10B	0.9900
C11–H11	1.0000
C11–C12	1.525(2)
C11–C16	1.528(2)
C12–H12A	0.9900
C12–H12B	0.9900
C12–C13	1.530(2)
C13–H13A	0.9900
C13–H13B	0.9900
C13–C14	1.524(3)
C14–H14A	0.9900
C14–H14B	0.9900
C14–C15	1.528(3)
C15–H15A	0.9900
C15–H15B	0.9900
C15–C16	1.532(2)
C16–H16A	0.9900
C16–H16B	0.9900
I2–Cu2	2.6289(2)
I2–Cu3	2.6421(2)
Cu2–Cu3	2.9856(5)
Cu2–S3	2.3296(5)
Cu2–S3$^{\#3}$	2.3297(5)
Cu3–S4	2.3482(5)
Cu3–S4$^{\#3}$	2.3482(5)
S3–C17	1.8259(16)
S3–C23	1.8265(19)
S4–C26	1.8323(19)
S4–C27	1.8248(17)
C17–H17	1.0000
C17–C18	1.527(2)
C17–C22	1.527(2)
C18–H18A	0.9900
C18–H18B	0.9900
C18–C19	1.531(2)
C19–H19A	0.9900
C19–H19B	0.9900
C19–C20	1.526(2)
C20–H20A	0.9900
C20–H20B	0.9900
C20–C21	1.523(3)
C21–H21A	0.9900
C21–H21B	0.9900
C21–C22	1.528(2)
C22–H22A	0.9900
C22–H22B	0.9900
C23–H23A	0.9900
C23–H23B	0.9900
C23–C24	1.456(3)
C24–C25	1.188(3)
C25–C26	1.452(3)
C26–H26A	0.9900
C26–H26B	0.9900
C27–H27	1.0000
C27–C28	1.522(2)
C27–C32	1.526(2)
C28–H28A	0.9900
C28–H28B	0.9900
C28–C29	1.532(3)
C29–H29A	0.9900
C29–H29B	0.9900
C29–C30	1.519(3)
C30–H30A	0.9900
C30–H30B	0.9900
C30–C31	1.520(3)
C31–H31A	0.9900
C31–H31B	0.9900
C31–C32	1.524(3)
C32–H32A	0.9900
C32–H32B	0.9900

Atom–Atom–Atom	Angle [°]
Cu1–I1–Cu1$^{\#1}$	65.240(8)
I1–Cu1–I1$^{\#1}$	114.759(8)
I1$^{\#1}$–Cu1–Cu1$^{\#1}$	56.823(7)
I1–Cu1–Cu1$^{\#1}$	57.936(8)
S1$^{\#2}$–Cu1–I1	102.411(12)

S1$^{\#2}$–Cu1–I1$^{\#1}$	102.476(13)	S2–C10–H10B	109.2
S1$^{\#2}$–Cu1–Cu1$^{\#1}$	113.557(14)	C9–C10–S2	112.06(11)
S2–Cu1–I1$^{\#1}$	107.768(12)	C9–C10–H10A	109.2
S2–Cu1–I1	115.632(13)	C9–C10–H10B	109.2
S2–Cu1–Cu1$^{\#1}$	133.121(15)	H10A–C10–H10B	107.9
S2–Cu1–S1$^{\#2}$	113.039(15)	S2–C11–H11	108.6
C1–S1–Cu1$^{\#2}$	110.48(5)	C12–C11–S2	112.05(11)
C7–S1–Cu1$^{\#2}$	104.94(5)	C12–C11–H11	108.6
C7–S1–C1	100.83(8)	C12–C11–C16	112.19(13)
C10–S2–Cu1	104.54(5)	C16–C11–S2	106.81(10)
C10–S2–C11	100.18(7)	C16–C11–H11	108.6
C11–S2–Cu1	110.90(5)	C11–C12–H12A	109.3
S1–C1–H1	108.6	C11–C12–H12B	109.3
C2–C1–S1	108.38(11)	C11–C12–C13	111.52(13)
C2–C1–H1	108.6	H12A–C12–H12B	108.0
C2–C1–C6	111.08(13)	C13–C12–H12A	109.3
C6–C1–S1	111.43(12)	C13–C12–H12B	109.3
C6–C1–H1	108.6	C12–C13–H13A	109.4
C1–C2–H2A	109.1	C12–C13–H13B	109.4
C1–C2–H2B	109.1	H13A–C13–H13B	108.0
H2A–C2–H2B	107.8	C14–C13–C12	111.01(14)
C3–C2–C1	112.58(13)	C14–C13–H13A	109.4
C3–C2–H2A	109.1	C14–C13–H13B	109.4
C3–C2–H2B	109.1	C13–C14–H14A	109.5
C2–C3–H3A	109.4	C13–C14–H14B	109.5
C2–C3–H3B	109.4	C13–C14–C15	110.59(15)
H3A–C3–H3B	108.0	H14A–C14–H14B	108.1
C4–C3–C2	111.23(14)	C15–C14–H14A	109.5
C4–C3–H3A	109.4	C15–C14–H14B	109.5
C4–C3–H3B	109.4	C14–C15–H15A	109.4
C3–C4–H4A	109.4	C14–C15–H15B	109.4
C3–C4–H4B	109.4	C14–C15–C16	110.97(14)
C3–C4–C5	111.15(14)	H15A–C15–H15B	108.0
H4A–C4–H4B	108.0	C16–C15–H15A	109.4
C5–C4–H4A	109.4	C16–C15–H15B	109.4
C5–C4–H4B	109.4	C11–C16–C15	110.78(13)
C4–C5–H5A	109.4	C11–C16–H16A	109.5
C4–C5–H5B	109.4	C11–C16–H16B	109.5
H5A–C5–H5B	108.0	C15–C16–H16A	109.5
C6–C5–C4	110.96(14)	C15–C16–H16B	109.5
C6–C5–H5A	109.4	H16A–C16–H16B	108.1
C6–C5–H5B	109.4	Cu2–I2–Cu3	69.001(10)
C1–C6–H6A	109.1	I2$^{\#3}$–Cu2–I2	111.419(13)
C1–C6–H6B	109.1	I2$^{\#3}$–Cu2–Cu3	55.709(7)
C5–C6–C1	112.50(14)	I2–Cu2–Cu3	55.710(7)
C5–C6–H6A	109.1	S3$^{\#3}$–Cu2–I2$^{\#3}$	107.551(11)
C5–C6–H6B	109.1	S3–Cu2–I2$^{\#3}$	111.408(11)
H6A–C6–H6B	107.8	S3$^{\#3}$–Cu2–I2	111.407(11)
S1–C7–H7A	109.1	S3–Cu2–I2	107.554(11)
S1–C7–H7B	109.1	S3$^{\#3}$–Cu2–Cu3	126.269(13)
H7A–C7–H7B	107.8	S3–Cu2–Cu3	126.269(13)
C8–C7–S1	112.57(11)	S3–Cu2–S3$^{\#3}$	107.46(3)
C8–C7–H7A	109.1	I2$^{\#3}$–Cu3–I2	110.577(13)
C8–C7–H7B	109.1	I2$^{\#3}$–Cu3–Cu2	55.287(7)
C9–C8–C7	176.02(17)	I2–Cu3–Cu2	55.289(6)
C8–C9–C10	178.24(17)	S4$^{\#3}$–Cu3–I2$^{\#3}$	110.777(11)
S2–C10–H10A	109.2	S4–Cu3–I2$^{\#3}$	107.665(11)

S4$^{\#3}$–Cu3–I2	107.665(11)	C24–C23–S3	112.90(12)
S4–Cu3–I2	110.779(11)	C24–C23–H23A	109.0
S4–Cu3–Cu2	125.305(13)	C24–C23–H23B	109.0
S4$^{\#3}$–Cu3–Cu2	125.306(13)	C25–C24–C23	175.25(18)
S4$^{\#3}$–Cu3–S4	109.39(3)	C24–C25–C26	173.49(18)
C17–S3–Cu2	104.25(5)	S4–C26–H26A	109.3
C17–S3–C23	102.41(8)	S4–C26–H26B	109.3
C23–S3–Cu2	104.37(6)	C25–C26–S4	111.51(12)
C26–S4–Cu3	105.21(6)	C25–C26–H26A	109.3
C27–S4–Cu3	100.94(6)	C25–C26–H26B	109.3
C27–S4–C26	102.41(8)	H26A–C26–H26B	108.0
S3–C17–H17	108.6	S4–C27–H27	108.2
C18–C17–S3	106.92(11)	C28–C27–S4	114.64(13)
C18–C17–H17	108.6	C28–C27–H27	108.2
C22–C17–S3	112.71(11)	C28–C27–C32	110.96(15)
C22–C17–H17	108.6	C32–C27–S4	106.41(12)
C22–C17–C18	111.23(14)	C32–C27–H27	108.2
C17–C18–H18A	109.6	C27–C28–H28A	109.9
C17–C18–H18B	109.6	C27–C28–H28B	109.9
C17–C18–C19	110.18(14)	C27–C28–C29	109.07(16)
H18A–C18–H18B	108.1	H28A–C28–H28B	108.3
C19–C18–H18A	109.6	C29–C28–H28A	109.9
C19–C18–H18B	109.6	C29–C28–H28B	109.9
C18–C19–H19A	109.4	C28–C29–H29A	109.4
C18–C19–H19B	109.4	C28–C29–H29B	109.4
H19A–C19–H19B	108.0	H29A–C29–H29B	108.0
C20–C19–C18	111.34(15)	C30–C29–C28	111.16(16)
C20–C19–H19A	109.4	C30–C29–H29A	109.4
C20–C19–H19B	109.4	C30–C29–H29B	109.4
C19–C20–H20A	109.5	C29–C30–H30A	109.5
C19–C20–H20B	109.5	C29–C30–H30B	109.5
H20A–C20–H20B	108.0	C29–C30–C31	110.74(18)
C21–C20–C19	110.91(15)	H30A–C30–H30B	108.1
C21–C20–H20A	109.5	C31–C30–H30A	109.5
C21–C20–H20B	109.5	C31–C30–H30B	109.5
C20–C21–H21A	109.4	C30–C31–H31A	109.2
C20–C21–H21B	109.4	C30–C31–H31B	109.2
C20–C21–C22	111.23(15)	C30–C31–C32	112.1(2)
H21A–C21–H21B	108.0	H31A–C31–H31B	107.9
C22–C21–H21A	109.4	C32–C31–H31A	109.2
C22–C21–H21B	109.4	C32–C31–H31B	109.2
C17–C22–C21	109.91(13)	C27–C32–H32A	109.6
C17–C22–H22A	109.7	C27–C32–H32B	109.6
C17–C22–H22B	109.7	C31–C32–C27	110.48(16)
C21–C22–H22A	109.7	C31–C32–H32A	109.6
C21–C22–H22B	109.7	C31–C32–H32B	109.6
H22A–C22–H22B	108.2	H32A–C32–H32B	108.1
S3–C23–H23A	109.0		
S3–C23–H23B	109.0		
H23A–C23–H23B	107.8		

Symmetry transformations used to generate equivalent atoms:
#1: 0.5-X, 1.5-Y, 1-Z; #2: 0.5-X, 0.5-Y, 1-Z; #3: 1-X, +Y, 1.5-Z;

Table S24. Torsion angles for CP2D1_100K

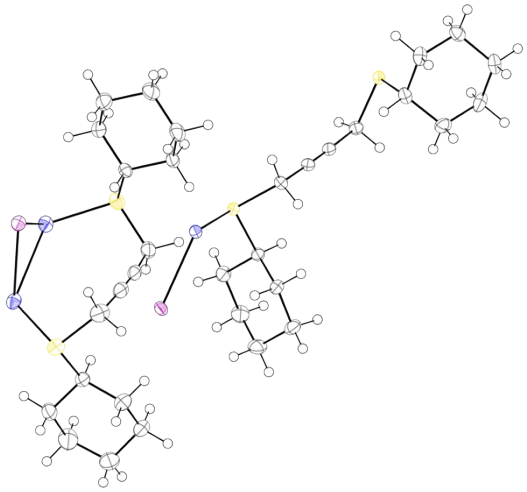
Atom–Atom–Atom–Atom	Torsion Angle [°]		
Cu1$^{\#1}$–S1–C1–C2	−59.69(11)	Cu1$^{\#1}$–S1–C7–C8	−60.57(12)
Cu1$^{\#1}$–S1–C1–C6	177.80(10)	Cu1–S2–C10–C9	−177.75(10)
		Cu1–S2–C11–C12	−40.57(12)
		Cu1–S2–C11–C16	82.66(11)

S1–C1–C2–C3	−70.43(15)
S1–C1–C6–C5	68.20(16)
S2–C11–C12–C13	173.70(11)
S2–C11–C16–C15	−177.06(12)
C1–S1–C7–C8	54.24(13)
C1–C2–C3–C4	−54.29(18)
C2–C1–C6–C5	−52.74(19)
C2–C3–C4–C5	55.84(19)
C3–C4–C5–C6	−56.17(19)
C4–C5–C6–C1	54.98(19)
C6–C1–C2–C3	52.30(18)
C7–S1–C1–C2	−170.27(11)
C7–S1–C1–C6	67.22(13)
C10–S2–C11–C12	69.40(12)
C10–S2–C11–C16	−167.37(11)
C11–S2–C10–C9	67.36(12)
C11–C12–C13–C14	−54.89(19)
C12–C11–C16–C15	−53.92(18)
C12–C13–C14–C15	57.04(19)
C13–C14–C15–C16	−57.80(19)
C14–C15–C16–C11	55.92(19)
C16–C11–C12–C13	53.56(18)
Cu2–S3–C17–C18	−68.90(11)
Cu2–S3–C17–C22	168.57(11)
Cu2–S3–C23–C24	−50.16(13)
Cu3–S4–C26–C25	−50.90(14)
Cu3–S4–C27–C28	160.32(12)
Cu3–S4–C27–C32	−76.63(13)
S3–C17–C18–C19	179.42(12)
S3–C17–C22–C21	177.74(12)
S4–C27–C28–C29	179.49(13)
S4–C27–C32–C31	177.61(17)
C17–S3–C23–C24	58.30(14)
C17–C18–C19–C20	55.8(2)
C18–C17–C22–C21	57.67(19)
C18–C19–C20–C21	−55.6(2)
C19–C20–C21–C22	56.2(2)
C20–C21–C22–C17	−57.00(19)
C22–C17–C18–C19	−57.14(19)
C23–S3–C17–C18	−177.45(12)
C23–S3–C17–C22	60.02(14)
C26–S4–C27–C28	51.89(15)
C26–S4–C27–C32	174.94(13)
C27–S4–C26–C25	54.25(15)
C27–C28–C29–C30	−58.7(2)
C28–C27–C32–C31	−57.1(2)
C28–C29–C30–C31	56.5(3)
C29–C30–C31–C32	−54.3(3)
C30–C31–C32–C27	54.5(3)
C32–C27–C28–C29	58.9(2)

Symmetry transformations used to generate equivalent atoms:
#1: 0.5-X, 0.5-Y, 1-Z;

Crystal structure of CP2D1_140K

Crystal Data and Experimental



Experimental: The data for CP2D1_140K were collected from a shock-cooled single crystal at 140.0(1) K on a Bruker D8 VENTURE area detector four-circle diffractometer with a X-ray tube using a graphite as monochromator and a CPAD PHOTON II area detector detector. The diffractometer was equipped with an Oxford Cryostream 800 low temperature device and used Mo K_{α} radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.38A and a multi-scan absorption correction using SADABS 2016/2 was applied. [1,2] The structure was solved by direct methods with XT and refined by full-matrix least-squares methods against F^2 using SHELXL.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[5] CCDC 2326502 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures. This report and the CIF file were generated using FinalCif.[6]

Table S25. Crystal data and structure refinement for CP2D1_140K

Internal Reference	CP2D1_140K
CCDC number	2326502
Empirical formula	$C_{16}H_{26}CuIS_2$
Formula weight	472.93
Temperature [K]	140.0(1)
Crystal system	monoclinic
Space group (number)	$C2/c$ (15)
a [Å]	31.853(2)
b [Å]	10.1612(6)
c [Å]	22.9100(14)
α [°]	90
β [°]	96.804(2)
γ [°]	90
Volume [Å^3]	7363.0(8)
Z	16
ρ_{calc} [gcm^{-3}]	1.707
μ [mm^{-1}]	3.080
$F(000)$	3776
Crystal size [mm^3]	0.247×0.279×0.481
Crystal colour	clear light yellow
Crystal shape	block
Radiation	Mo K_{α} (λ=0.71073 Å)
2θ range [°]	5.43 to 54.99 (0.77 Å)
Index ranges	−41 ≤ h ≤ 41 −13 ≤ k ≤ 13 −29 ≤ l ≤ 29
Reflections collected	85404
Independent reflections	8436 R_{int} = 0.0248 R_{sigma} = 0.0117
Completeness to θ = 25.242°	99.7 %
Data / Restraints / Parameters	8436 / 0 / 362
Goodness-of-fit on F^2	1.147
Final R indexes [I≥2σ(I)]	R_1 = 0.0162 wR_2 = 0.0390
Final R indexes [all data]	R_1 = 0.0165 wR_2 = 0.0391
Largest peak/hole [eÅ^{-3}]	0.64/−0.47

Table S26. Bond lengths and angles for CP2D1_140K

Atom–Atom	Length [Å]
I1–Cu1	2.6310(3)
I1–Cu1$^{\#1}$	2.6637(3)
Cu1–Cu1$^{\#1}$	2.8651(4)
Cu1–S1$^{\#2}$	2.3435(4)
Cu1–S2	2.3191(4)
S1–C1	1.8382(16)
S1–C7	1.8236(16)
S2–C10	1.8194(16)
S2–C11	1.8312(15)
C1–H1	1.0000
C1–C2	1.526(2)
C1–C6	1.529(2)
C2–H2A	0.9900
C2–H2B	0.9900
C2–C3	1.522(2)
C3–H3A	0.9900
C3–H3B	0.9900
C3–C4	1.520(2)
C4–H4A	0.9900
C4–H4B	0.9900
C4–C5	1.523(3)
C5–H5A	0.9900
C5–H5B	0.9900
C5–C6	1.520(3)
C6–H6A	0.9900
C6–H6B	0.9900
C7–H7A	0.9900
C7–H7B	0.9900
C7–C8	1.458(2)
C8–C9	1.193(2)
C9–C10	1.461(2)
C10–H10A	0.9900
C10–H10B	0.9900
C11–H11	1.0000
C11–C12	1.526(2)
C11–C16	1.524(2)
C12–H12A	0.9900
C12–H12B	0.9900
C12–C13	1.530(2)
C13–H13A	0.9900
C13–H13B	0.9900
C13–C14	1.522(3)
C14–H14A	0.9900
C14–H14B	0.9900
C14–C15	1.522(3)
C15–H15A	0.9900
C15–H15B	0.9900
C15–C16	1.531(2)
C16–H16A	0.9900
C16–H16B	0.9900
I2–Cu2	2.6292(2)
I2–Cu3	2.6418(2)
Cu2–Cu3	2.9828(5)
Cu2–S3$^{\#3}$	2.3312(5)
Cu2–S3	2.3312(5)
Cu3–S4$^{\#3}$	2.3505(5)
Cu3–S4	2.3505(5)
S3–C17	1.8247(16)
S3–C23	1.824(2)
S4–C26	1.831(2)
S4–C27	1.8232(17)
C17–H17	1.0000
C17–C18	1.526(2)
C17–C22	1.524(2)
C18–H18A	0.9900
C18–H18B	0.9900
C18–C19	1.529(3)
C19–H19A	0.9900
C19–H19B	0.9900
C19–C20	1.521(3)
C20–H20A	0.9900
C20–H20B	0.9900
C20–C21	1.521(3)
C21–H21A	0.9900
C21–H21B	0.9900
C21–C22	1.526(2)
C22–H22A	0.9900
C22–H22B	0.9900
C23–H23A	0.9900
C23–H23B	0.9900
C23–C24	1.455(3)
C24–C25	1.187(3)
C25–C26	1.450(3)
C26–H26A	0.9900
C26–H26B	0.9900
C27–H27	1.0000
C27–C28	1.520(2)
C27–C32	1.524(2)
C28–H28A	0.9900
C28–H28B	0.9900
C28–C29	1.529(3)
C29–H29A	0.9900
C29–H29B	0.9900
C29–C30	1.516(3)
C30–H30A	0.9900
C30–H30B	0.9900
C30–C31	1.517(4)
C31–H31A	0.9900
C31–H31B	0.9900
C31–C32	1.523(3)
C32–H32A	0.9900
C32–H32B	0.9900

Atom–Atom–Atom	Angle [°]
Cu1–I1–Cu1$^{\#1}$	65.516(8)
I1–Cu1–I1$^{\#1}$	114.485(8)
I1$^{\#1}$–Cu1–Cu1$^{\#1}$	56.692(7)
I1–Cu1–Cu1$^{\#1}$	57.793(8)
S1$^{\#2}$–Cu1–I1	102.520(12)

S1$^{\#2}$–Cu1–I1$^{\#1}$	102.447(12)
S1$^{\#2}$–Cu1–Cu1$^{\#1}$	113.544(14)
S2–Cu1–I1$^{\#1}$	107.843(12)
S2–Cu1–I1	115.759(13)
S2–Cu1–Cu1$^{\#1}$	133.155(14)
S2–Cu1–S1$^{\#2}$	113.007(15)
C1–S1–Cu1$^{\#2}$	110.60(6)
C7–S1–Cu1$^{\#2}$	105.03(5)
C7–S1–C1	100.81(8)
C10–S2–Cu1	104.56(5)
C10–S2–C11	100.27(7)
C11–S2–Cu1	110.94(5)
S1–C1–H1	108.7
C2–C1–S1	108.29(11)
C2–C1–H1	108.7
C2–C1–C6	110.94(13)
C6–C1–S1	111.53(12)
C6–C1–H1	108.7
C1–C2–H2A	109.1
C1–C2–H2B	109.1
H2A–C2–H2B	107.8
C3–C2–C1	112.70(14)
C3–C2–H2A	109.1
C3–C2–H2B	109.1
C2–C3–H3A	109.4
C2–C3–H3B	109.4
H3A–C3–H3B	108.0
C4–C3–C2	111.33(15)
C4–C3–H3A	109.4
C4–C3–H3B	109.4
C3–C4–H4A	109.4
C3–C4–H4B	109.4
C3–C4–C5	111.13(14)
H4A–C4–H4B	108.0
C5–C4–H4A	109.4
C5–C4–H4B	109.4
C4–C5–H5A	109.5
C4–C5–H5B	109.5
H5A–C5–H5B	108.1
C6–C5–C4	110.84(15)
C6–C5–H5A	109.5
C6–C5–H5B	109.5
C1–C6–H6A	109.1
C1–C6–H6B	109.1
C5–C6–C1	112.59(14)
C5–C6–H6A	109.1
C5–C6–H6B	109.1
H6A–C6–H6B	107.8
S1–C7–H7A	109.0
S1–C7–H7B	109.0
H7A–C7–H7B	107.8
C8–C7–S1	112.84(11)
C8–C7–H7A	109.0
C8–C7–H7B	109.0
C9–C8–C7	175.99(17)
C8–C9–C10	178.20(17)
S2–C10–H10A	109.2
S2–C10–H10B	109.2
C9–C10–S2	112.18(11)
C9–C10–H10A	109.2
C9–C10–H10B	109.2
H10A–C10–H10B	107.9
S2–C11–H11	108.6
C12–C11–S2	111.99(11)
C12–C11–H11	108.6
C16–C11–S2	106.89(10)
C16–C11–H11	108.6
C16–C11–C12	112.16(13)
C11–C12–H12A	109.3
C11–C12–H12B	109.3
C11–C12–C13	111.48(13)
H12A–C12–H12B	108.0
C13–C12–H12A	109.3
C13–C12–H12B	109.3
C12–C13–H13A	109.4
C12–C13–H13B	109.4
H13A–C13–H13B	108.0
C14–C13–C12	110.97(14)
C14–C13–H13A	109.4
C14–C13–H13B	109.4
C13–C14–H14A	109.5
C13–C14–H14B	109.5
H14A–C14–H14B	108.1
C15–C14–C13	110.70(15)
C15–C14–H14A	109.5
C15–C14–H14B	109.5
C14–C15–H15A	109.4
C14–C15–H15B	109.4
C14–C15–C16	111.02(15)
H15A–C15–H15B	108.0
C16–C15–H15A	109.4
C16–C15–H15B	109.4
C11–C16–C15	110.85(14)
C11–C16–H16A	109.5
C11–C16–H16B	109.5
C15–C16–H16A	109.5
C15–C16–H16B	109.5
H16A–C16–H16B	108.1
Cu2–I2–Cu3	68.927(9)
I2–Cu2–I2$^{\#3}$	111.472(13)
I2–Cu2–Cu3	55.736(7)
I2$^{\#3}$–Cu2–Cu3	55.736(6)
S3–Cu2–I2	111.352(11)
S3$^{\#3}$–Cu2–I2	107.540(11)
S3–Cu2–I2$^{\#3}$	107.542(11)
S3$^{\#3}$–Cu2–I2$^{\#3}$	111.354(11)
S3–Cu2–Cu3	126.229(13)
S3$^{\#3}$–Cu2–Cu3	126.229(13)
S3$^{\#3}$–Cu2–S3	107.54(3)
I2–Cu3–I2$^{\#3}$	110.674(13)
I2$^{\#3}$–Cu3–Cu2	55.338(7)
I2–Cu3–Cu2	55.337(6)
S4–Cu3–I2	107.759(11)
S4–Cu3–I2$^{\#3}$	110.730(11)

S4$^{\#3}$–Cu3–I2	110.728(11)	C24–C23–S3	113.08(13)
S4$^{\#3}$–Cu3–I2$^{\#3}$	107.760(12)	C24–C23–H23A	109.0
S4–Cu3–Cu2	125.403(13)	C24–C23–H23B	109.0
S4$^{\#3}$–Cu3–Cu2	125.402(13)	C25–C24–C23	175.20(18)
S4–Cu3–S4$^{\#3}$	109.20(3)	C24–C25–C26	173.56(19)
C17–S3–Cu2	104.36(5)	S4–C26–H26A	109.3
C23–S3–Cu2	104.37(6)	S4–C26–H26B	109.3
C23–S3–C17	102.39(8)	C25–C26–S4	111.65(12)
C26–S4–Cu3	105.00(6)	C25–C26–H26A	109.3
C27–S4–Cu3	101.16(6)	C25–C26–H26B	109.3
C27–S4–C26	102.41(9)	H26A–C26–H26B	108.0
S3–C17–H17	108.7	S4–C27–H27	108.2
C18–C17–S3	106.89(11)	C28–C27–S4	114.59(13)
C18–C17–H17	108.7	C28–C27–H27	108.2
C22–C17–S3	112.78(11)	C28–C27–C32	110.86(15)
C22–C17–H17	108.7	C32–C27–S4	106.48(12)
C22–C17–C18	111.08(14)	C32–C27–H27	108.2
C17–C18–H18A	109.6	C27–C28–H28A	109.9
C17–C18–H18B	109.6	C27–C28–H28B	109.9
C17–C18–C19	110.12(15)	C27–C28–C29	109.02(16)
H18A–C18–H18B	108.2	H28A–C28–H28B	108.3
C19–C18–H18A	109.6	C29–C28–H28A	109.9
C19–C18–H18B	109.6	C29–C28–H28B	109.9
C18–C19–H19A	109.4	C28–C29–H29A	109.4
C18–C19–H19B	109.4	C28–C29–H29B	109.4
H19A–C19–H19B	108.0	H29A–C29–H29B	108.0
C20–C19–C18	111.30(15)	C30–C29–C28	111.31(17)
C20–C19–H19A	109.4	C30–C29–H29A	109.4
C20–C19–H19B	109.4	C30–C29–H29B	109.4
C19–C20–H20A	109.4	C29–C30–H30A	109.5
C19–C20–H20B	109.4	C29–C30–H30B	109.5
H20A–C20–H20B	108.0	C29–C30–C31	110.77(19)
C21–C20–C19	110.98(16)	H30A–C30–H30B	108.1
C21–C20–H20A	109.4	C31–C30–H30A	109.5
C21–C20–H20B	109.4	C31–C30–H30B	109.5
C20–C21–H21A	109.4	C30–C31–H31A	109.2
C20–C21–H21B	109.4	C30–C31–H31B	109.2
C20–C21–C22	111.11(16)	C30–C31–C32	111.9(2)
H21A–C21–H21B	108.0	H31A–C31–H31B	107.9
C22–C21–H21A	109.4	C32–C31–H31A	109.2
C22–C21–H21B	109.4	C32–C31–H31B	109.2
C17–C22–C21	110.03(14)	C27–C32–H32A	109.5
C17–C22–H22A	109.7	C27–C32–H32B	109.5
C17–C22–H22B	109.7	C31–C32–C27	110.55(16)
C21–C22–H22A	109.7	C31–C32–H32A	109.5
C21–C22–H22B	109.7	C31–C32–H32B	109.5
H22A–C22–H22B	108.2	H32A–C32–H32B	108.1
S3–C23–H23A	109.0		
S3–C23–H23B	109.0		
H23A–C23–H23B	107.8		

Symmetry transformations used to generate equivalent atoms:
#1: 1.5-X, 1.5-Y, 1-Z; #2: 1.5-X, 0.5-Y, 1-Z; #3: 1-X, +Y, 0.5-Z;

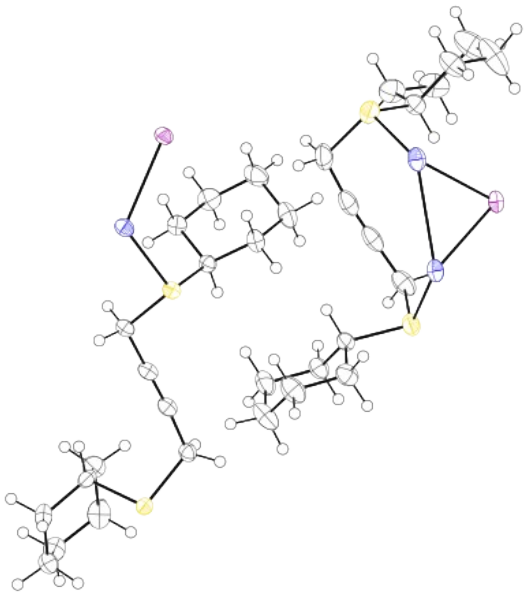
Table S27. Torsion angles for CP2D1_140K

Atom–Atom–Atom–Atom	Torsion Angle [°]		
Cu1$^{\#1}$–S1–C1–C2	−59.69(11)	Cu1$^{\#1}$–S1–C7–C8	−60.62(12)
Cu1$^{\#1}$–S1–C1–C6	177.95(10)	Cu1–S2–C10–C9	−177.51(10)
		Cu1–S2–C11–C12	−40.60(12)
		Cu1–S2–C11–C16	82.61(11)

S1–C1–C2–C3	−70.71(15)
S1–C1–C6–C5	68.11(17)
S2–C11–C12–C13	173.69(11)
S2–C11–C16–C15	−176.99(12)
C1–S1–C7–C8	54.35(13)
C1–C2–C3–C4	−54.11(19)
C2–C1–C6–C5	−52.71(19)
C2–C3–C4–C5	55.8(2)
C3–C4–C5–C6	−56.3(2)
C4–C5–C6–C1	55.2(2)
C6–C1–C2–C3	52.00(19)
C7–S1–C1–C2	−170.41(11)
C7–S1–C1–C6	67.24(13)
C10–S2–C11–C12	69.45(12)
C10–S2–C11–C16	−167.34(11)
C11–S2–C10–C9	67.50(12)
C11–C12–C13–C14	−54.75(19)
C12–C11–C16–C15	−53.88(19)
C12–C13–C14–C15	57.0(2)
C13–C14–C15–C16	−57.8(2)
C14–C15–C16–C11	55.9(2)
C16–C11–C12–C13	53.50(18)
Cu2–S3–C17–C18	−69.01(11)
Cu2–S3–C17–C22	168.63(11)
Cu2–S3–C23–C24	−50.07(14)
Cu3–S4–C26–C25	−51.02(14)
Cu3–S4–C27–C28	160.65(12)
Cu3–S4–C27–C32	−76.41(13)
S3–C17–C18–C19	179.38(12)
S3–C17–C22–C21	177.71(12)
S4–C27–C28–C29	179.43(13)
S4–C27–C32–C31	177.53(18)
C17–S3–C23–C24	58.50(14)
C17–C18–C19–C20	56.0(2)
C18–C17–C22–C21	57.73(19)
C18–C19–C20–C21	−55.8(2)
C19–C20–C21–C22	56.3(2)
C20–C21–C22–C17	−57.0(2)
C22–C17–C18–C19	−57.20(19)
C23–S3–C17–C18	−177.59(12)
C23–S3–C17–C22	60.05(14)
C26–S4–C27–C28	52.38(15)
C26–S4–C27–C32	175.32(14)
C27–S4–C26–C25	54.29(15)
C27–C28–C29–C30	−58.7(2)
C28–C27–C32–C31	−57.2(2)
C28–C29–C30–C31	56.5(3)
C29–C30–C31–C32	−54.3(3)
C30–C31–C32–C27	54.6(3)
C32–C27–C28–C29	58.9(2)

Symmetry transformations used to generate equivalent atoms:
#1: 1.5-X, 0.5-Y, 1-Z;

Crystal Data and Experimental



Experimental: The data for CP2D1_180K were collected from a shock-cooled single crystal at 180.0(1) K on a Bruker D8 Venture CMOS with Photon 2 four-circle diffractometer with a X-ray tube using a graphite as monochromator and a CPAD PHOTON II area detector detector. The diffractometer was equipped with an Oxford Cryostream 800 low temperature device and used Mo K_{α} radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.38A and a multi-scan absorption correction using SADABS 2016/2 was applied. [1,2] The structure was solved by direct methods with ShelXT and refined by full-matrix least-squares methods against F^2 using SHELXL.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[5] CCDC 2326503 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures. This report and the CIF file were generated using FinalCif.[6]

Table S28. Crystal data and structure refinement for CP2D1_180K

Internal Reference	CP2D1_180K
CCDC number	2326503
Empirical formula	$C_{16}H_{26}CuIS_2$
Formula weight	472.93
Temperature [K]	180.0(1)
Crystal system	monoclinic
Space group (number)	$C2/c$ (15)
a [Å]	31.8836(12)
b [Å]	10.1900(4)
c [Å]	22.9758(9)
α [°]	90
β [°]	96.8390(10)
γ [°]	90
Volume [Å^3]	7411.6(5)
Z	16
ρ_{calc} [gcm^{-3}]	1.695
μ [mm^{-1}]	3.060
F(000)	3776
Crystal size [mm^3]	0.247×0.279×0.481
Crystal colour	clear light yellow
Crystal shape	block
Radiation	Mo K_{α} (λ=0.71073 Å)
2θ range [°]	5.41 to 55.00 (0.77 Å)
Index ranges	−41 ≤ h ≤ 41 −13 ≤ k ≤ 13 −29 ≤ l ≤ 29
Reflections collected	85592
Independent reflections	8493 R_{int} = 0.0236 R_{sigma} = 0.0122
Completeness to θ = 25.242°	99.7 %
Data / Restraints / Parameters	8493 / 0 / 362
Goodness-of-fit on F^2	1.157
Final R indexes [I≥2σ(I)]	R_1 = 0.0165 wR_2 = 0.0401
Final R indexes [all data]	R_1 = 0.0169 wR_2 = 0.0403
Largest peak/hole [eÅ^{-3}]	0.60/−0.50

Table S29. Bond lengths and angles for CP2D1_180K

Atom–Atom	Length [Å]
I1–Cu1	2.6322(2)
I1–Cu1$^{\#1}$	2.6654(2)
Cu1–Cu1$^{\#1}$	2.8770(4)
Cu1–S1$^{\#2}$	2.3463(4)
Cu1–S2	2.3215(4)
S1–C1	1.8368(16)
S1–C7	1.8246(16)
S2–C10	1.8209(16)
S2–C11	1.8305(15)
C1–H1	1.0000
C1–C2	1.524(2)
C1–C6	1.526(3)
C2–H2A	0.9900
C2–H2B	0.9900
C2–C3	1.520(2)
C3–H3A	0.9900
C3–H3B	0.9900
C3–C4	1.517(3)
C4–H4A	0.9900
C4–H4B	0.9900
C4–C5	1.516(3)
C5–H5A	0.9900
C5–H5B	0.9900
C5–C6	1.520(3)
C6–H6A	0.9900
C6–H6B	0.9900
C7–H7A	0.9900
C7–H7B	0.9900
C7–C8	1.459(2)
C8–C9	1.192(2)
C9–C10	1.459(2)
C10–H10A	0.9900
C10–H10B	0.9900
C11–H11	1.0000
C11–C12	1.522(2)
C11–C16	1.523(2)
C12–H12A	0.9900
C12–H12B	0.9900
C12–C13	1.527(2)
C13–H13A	0.9900
C13–H13B	0.9900
C13–C14	1.518(3)
C14–H14A	0.9900
C14–H14B	0.9900
C14–C15	1.519(3)
C15–H15A	0.9900
C15–H15B	0.9900
C15–C16	1.532(2)
C16–H16A	0.9900
C16–H16B	0.9900
I2–Cu2	2.6305(2)
I2–Cu3	2.6424(2)
Cu2–Cu3	2.9769(5)
Cu2–S3$^{\#3}$	2.3345(5)
Cu2–S3	2.3345(5)
Cu3–S4$^{\#3}$	2.3527(5)
Cu3–S4	2.3527(5)
S3–C17	1.8250(16)
S3–C23	1.824(2)
S4–C26	1.831(2)
S4–C27	1.8262(18)
C17–H17	1.0000
C17–C18	1.522(2)
C17–C22	1.523(2)
C18–H18A	0.9900
C18–H18B	0.9900
C18–C19	1.529(3)
C19–H19A	0.9900
C19–H19B	0.9900
C19–C20	1.522(3)
C20–H20A	0.9900
C20–H20B	0.9900
C20–C21	1.517(3)
C21–H21A	0.9900
C21–H21B	0.9900
C21–C22	1.525(2)
C22–H22A	0.9900
C22–H22B	0.9900
C23–H23A	0.9900
C23–H23B	0.9900
C23–C24	1.453(3)
C24–C25	1.185(3)
C25–C26	1.448(3)
C26–H26A	0.9900
C26–H26B	0.9900
C27–H27	1.0000
C27–C28	1.519(2)
C27–C32	1.521(3)
C28–H28A	0.9900
C28–H28B	0.9900
C28–C29	1.529(3)
C29–H29A	0.9900
C29–H29B	0.9900
C29–C30	1.513(3)
C30–H30A	0.9900
C30–H30B	0.9900
C30–C31	1.511(4)
C31–H31A	0.9900
C31–H31B	0.9900
C31–C32	1.521(3)
C32–H32A	0.9900
C32–H32B	0.9900

Atom–Atom–Atom	Angle [°]
Cu1–I1–Cu1$^{\#1}$	65.784(8)
I1–Cu1–I1$^{\#1}$	114.215(8)
I1$^{\#1}$–Cu1–Cu1$^{\#1}$	56.553(7)
I1–Cu1–Cu1$^{\#1}$	57.663(7)
S1$^{\#2}$–Cu1–I1	102.679(11)

S1$^{\#2}$–Cu1–I1$^{\#1}$	102.418(12)	S2–C10–H10B	109.2
S1$^{\#2}$–Cu1–Cu1$^{\#1}$	113.581(14)	C9–C10–S2	112.18(11)
S2–Cu1–I1$^{\#1}$	107.939(12)	C9–C10–H10A	109.2
S2–Cu1–I1	115.828(12)	C9–C10–H10B	109.2
S2–Cu1–Cu1$^{\#1}$	133.150(14)	H10A–C10–H10B	107.9
S2–Cu1–S1$^{\#2}$	112.966(15)	S2–C11–H11	108.5
C1–S1–Cu1$^{\#2}$	110.75(6)	C12–C11–S2	112.14(11)
C7–S1–Cu1$^{\#2}$	105.18(5)	C12–C11–H11	108.5
C7–S1–C1	100.88(8)	C12–C11–C16	112.26(13)
C10–S2–Cu1	104.56(5)	C16–C11–S2	106.84(11)
C10–S2–C11	100.32(7)	C16–C11–H11	108.5
C11–S2–Cu1	110.95(5)	C11–C12–H12A	109.3
S1–C1–H1	108.6	C11–C12–H12B	109.3
C2–C1–S1	108.32(12)	C11–C12–C13	111.49(14)
C2–C1–H1	108.6	H12A–C12–H12B	108.0
C2–C1–C6	110.90(14)	C13–C12–H12A	109.3
C6–C1–S1	111.70(12)	C13–C12–H12B	109.3
C6–C1–H1	108.6	C12–C13–H13A	109.4
C1–C2–H2A	109.1	C12–C13–H13B	109.4
C1–C2–H2B	109.1	H13A–C13–H13B	108.0
H2A–C2–H2B	107.8	C14–C13–C12	111.16(15)
C3–C2–C1	112.67(14)	C14–C13–H13A	109.4
C3–C2–H2A	109.1	C14–C13–H13B	109.4
C3–C2–H2B	109.1	C13–C14–H14A	109.5
C2–C3–H3A	109.3	C13–C14–H14B	109.5
C2–C3–H3B	109.3	C13–C14–C15	110.83(16)
H3A–C3–H3B	108.0	H14A–C14–H14B	108.1
C4–C3–C2	111.45(16)	C15–C14–H14A	109.5
C4–C3–H3A	109.3	C15–C14–H14B	109.5
C4–C3–H3B	109.3	C14–C15–H15A	109.4
C3–C4–H4A	109.4	C14–C15–H15B	109.4
C3–C4–H4B	109.4	C14–C15–C16	111.10(15)
H4A–C4–H4B	108.0	H15A–C15–H15B	108.0
C5–C4–C3	111.10(14)	C16–C15–H15A	109.4
C5–C4–H4A	109.4	C16–C15–H15B	109.4
C5–C4–H4B	109.4	C11–C16–C15	110.85(14)
C4–C5–H5A	109.5	C11–C16–H16A	109.5
C4–C5–H5B	109.5	C11–C16–H16B	109.5
C4–C5–C6	110.89(16)	C15–C16–H16A	109.5
H5A–C5–H5B	108.0	C15–C16–H16B	109.5
C6–C5–H5A	109.5	H16A–C16–H16B	108.1
C6–C5–H5B	109.5	Cu2–I2–Cu3	68.745(9)
C1–C6–H6A	109.1	I2$^{\#3}$–Cu2–I2	111.635(13)
C1–C6–H6B	109.1	I2$^{\#3}$–Cu2–Cu3	55.818(6)
C5–C6–C1	112.58(15)	I2–Cu2–Cu3	55.818(6)
C5–C6–H6A	109.1	S3–Cu2–I2$^{\#3}$	111.315(11)
C5–C6–H6B	109.1	S3$^{\#3}$–Cu2–I2$^{\#3}$	107.462(11)
H6A–C6–H6B	107.8	S3–Cu2–I2	107.460(11)
S1–C7–H7A	109.0	S3$^{\#3}$–Cu2–I2	111.314(11)
S1–C7–H7B	109.0	S3–Cu2–Cu3	126.193(13)
H7A–C7–H7B	107.8	S3$^{\#3}$–Cu2–Cu3	126.194(14)
C8–C7–S1	112.84(11)	S3$^{\#3}$–Cu2–S3	107.61(3)
C8–C7–H7A	109.0	I2$^{\#3}$–Cu3–I2	110.874(13)
C8–C7–H7B	109.0	I2–Cu3–Cu2	55.437(7)
C9–C8–C7	176.23(17)	I2$^{\#3}$–Cu3–Cu2	55.436(6)
C8–C9–C10	178.20(17)	S4–Cu3–I2$^{\#3}$	107.741(12)
S2–C10–H10A	109.2	S4–Cu3–I2	110.774(11)

S4$^{\#3}$–Cu3–I2$^{\#3}$	110.775(11)
S4$^{\#3}$–Cu3–I2	107.741(12)
S4–Cu3–Cu2	125.532(14)
S4$^{\#3}$–Cu3–Cu2	125.533(14)
S4–Cu3–S4$^{\#3}$	108.94(3)
C17–S3–Cu2	104.45(5)
C23–S3–Cu2	104.40(6)
C23–S3–C17	102.37(9)
C26–S4–Cu3	104.93(7)
C27–S4–Cu3	101.37(6)
C27–S4–C26	102.37(9)
S3–C17–H17	108.6
C18–C17–S3	107.05(12)
C18–C17–H17	108.6
C18–C17–C22	111.06(14)
C22–C17–S3	112.78(12)
C22–C17–H17	108.6
C17–C18–H18A	109.6
C17–C18–H18B	109.6
C17–C18–C19	110.24(15)
H18A–C18–H18B	108.1
C19–C18–H18A	109.6
C19–C18–H18B	109.6
C18–C19–H19A	109.4
C18–C19–H19B	109.4
H19A–C19–H19B	108.0
C20–C19–C18	111.25(17)
C20–C19–H19A	109.4
C20–C19–H19B	109.4
C19–C20–H20A	109.4
C19–C20–H20B	109.4
H20A–C20–H20B	108.0
C21–C20–C19	110.96(17)
C21–C20–H20A	109.4
C21–C20–H20B	109.4
C20–C21–H21A	109.4
C20–C21–H21B	109.4
C20–C21–C22	111.13(17)
H21A–C21–H21B	108.0
C22–C21–H21A	109.4
C22–C21–H21B	109.4
C17–C22–C21	110.06(14)
C17–C22–H22A	109.6
C17–C22–H22B	109.6
C21–C22–H22A	109.6
C21–C22–H22B	109.6
H22A–C22–H22B	108.2
S3–C23–H23A	108.9
S3–C23–H23B	108.9
H23A–C23–H23B	107.8
C24–C23–S3	113.20(13)
C24–C23–H23A	108.9
C24–C23–H23B	108.9
C25–C24–C23	175.09(19)
C24–C25–C26	173.73(19)
S4–C26–H26A	109.3
S4–C26–H26B	109.3
C25–C26–S4	111.78(13)
C25–C26–H26A	109.3
C25–C26–H26B	109.3
H26A–C26–H26B	107.9
S4–C27–H27	108.2
C28–C27–S4	114.60(13)
C28–C27–H27	108.2
C28–C27–C32	111.05(16)
C32–C27–S4	106.48(13)
C32–C27–H27	108.2
C27–C28–H28A	109.9
C27–C28–H28B	109.9
C27–C28–C29	109.05(17)
H28A–C28–H28B	108.3
C29–C28–H28A	109.9
C29–C28–H28B	109.9
C28–C29–H29A	109.3
C28–C29–H29B	109.3
H29A–C29–H29B	108.0
C30–C29–C28	111.47(19)
C30–C29–H29A	109.3
C30–C29–H29B	109.3
C29–C30–H30A	109.5
C29–C30–H30B	109.5
H30A–C30–H30B	108.1
C31–C30–C29	110.9(2)
C31–C30–H30A	109.5
C31–C30–H30B	109.5
C30–C31–H31A	109.1
C30–C31–H31B	109.1
C30–C31–C32	112.3(2)
H31A–C31–H31B	107.9
C32–C31–H31A	109.1
C32–C31–H31B	109.1
C27–C32–H32A	109.6
C27–C32–H32B	109.6
C31–C32–C27	110.38(17)
C31–C32–H32A	109.6
C31–C32–H32B	109.6
H32A–C32–H32B	108.1

Symmetry transformations used to generate equivalent atoms:
#1: -1.5-X, -0.5-Y, -1-Z; #2: -1.5-X, -1.5-Y, -1-Z; #3: -1-X, +Y, -0.5-Z;

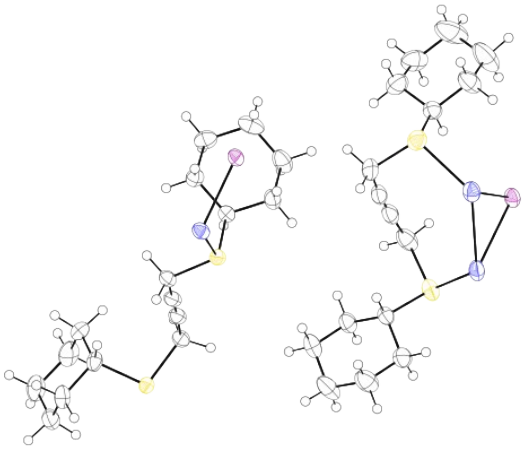
Table S30. Torsion angles for CP2D1_180K

Atom–Atom–Atom–Atom	Torsion Angle [°]
Cu1$^{\#1}$–S1–C1–C2	−59.46(11)
Cu1$^{\#1}$–S1–C1–C6	178.11(11)
Cu1$^{\#1}$–S1–C7–C8	−60.79(12)
Cu1–S2–C10–C9	−177.27(10)
Cu1–S2–C11–C12	−40.64(12)
Cu1–S2–C11–C16	82.76(11)

S1–C1–C2–C3	−71.05(16)
S1–C1–C6–C5	68.33(18)
S2–C11–C12–C13	173.65(12)
S2–C11–C16–C15	−176.95(13)
C1–S1–C7–C8	54.41(13)
C1–C2–C3–C4	−54.0(2)
C2–C1–C6–C5	−52.6(2)
C2–C3–C4–C5	55.9(2)
C3–C4–C5–C6	−56.4(2)
C4–C5–C6–C1	55.2(2)
C6–C1–C2–C3	51.87(19)
C7–S1–C1–C2	−170.43(11)
C7–S1–C1–C6	67.14(13)
C10–S2–C11–C12	69.45(12)
C10–S2–C11–C16	−167.16(11)
C11–S2–C10–C9	67.71(12)
C11–C12–C13–C14	−54.6(2)
C12–C11–C16–C15	−53.62(19)
C12–C13–C14–C15	56.8(2)
C13–C14–C15–C16	−57.4(2)
C14–C15–C16–C11	55.5(2)
C16–C11–C12–C13	53.35(18)
Cu2–S3–C17–C18	−68.98(12)
Cu2–S3–C17–C22	168.58(11)
Cu2–S3–C23–C24	−49.88(14)
Cu3–S4–C26–C25	−50.74(15)
Cu3–S4–C27–C28	160.65(13)
Cu3–S4–C27–C32	−76.16(14)
S3–C17–C18–C19	179.38(13)
S3–C17–C22–C21	177.82(13)
S4–C27–C28–C29	179.38(14)
S4–C27–C32–C31	177.6(2)
C17–S3–C23–C24	58.78(15)
C17–C18–C19–C20	55.9(2)
C18–C17–C22–C21	57.7(2)
C18–C19–C20–C21	−55.7(3)
C19–C20–C21–C22	56.3(2)
C20–C21–C22–C17	−57.1(2)
C22–C17–C18–C19	−57.1(2)
C23–S3–C17–C18	−177.61(12)
C23–S3–C17–C22	59.95(14)
C26–S4–C27–C28	52.40(16)
C26–S4–C27–C32	175.59(15)
C27–S4–C26–C25	54.76(16)
C27–C28–C29–C30	−58.2(3)
C28–C27–C32–C31	−57.1(3)
C28–C29–C30–C31	56.0(3)
C29–C30–C31–C32	−54.0(4)
C30–C31–C32–C27	54.5(3)
C32–C27–C28–C29	58.7(2)

Symmetry transformations used to generate equivalent atoms:
#1: -1.5-X, -1.5-Y, -1-Z;

Crystal Data and Experimental



Experimental: The data for CP2D1_220K were collected from a shock-cooled single crystal at 220.0(1) K on a Bruker D8 Venture CMOS with Photon 2 four-circle diffractometer with a X-ray tube using a graphite as monochromator and a CPAD PHOTON II area detector detector. The diffractometer was equipped with an Oxford Cryostream 800 low temperature device and used Mo K_{α} radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.38A and a multi-scan absorption correction using SADABS 2016/2 was applied. [1,2] The structure was solved by direct methods with ShelXT and refined by full-matrix least-squares methods against F^2 using SHELXL.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[5] CCDC 2326504 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures. This report and the CIF file were generated using FinalCif.[6]

Table S31. Crystal data and structure refinement for CP2D1_220K

Internal Reference	CP2D1_220K
CCDC number	2326504
Empirical formula	$C_{16}H_{26}CuIS_2$
Formula weight	472.93
Temperature [K]	220.0(1)
Crystal system	monoclinic
Space group (number)	$C2/c$ (15)
a [Å]	31.903(2)
b [Å]	10.2246(7)
c [Å]	23.0547(15)
α [°]	90
β [°]	96.911(2)
γ [°]	90
Volume [Å^3]	7465.8(9)
Z	16
ρ_{calc} [gcm^{-3}]	1.683
μ [mm^{-1}]	3.038
F(000)	3776
Crystal size [mm^3]	0.247×0.279×0.481
Crystal colour	clear light yellow
Crystal shape	block
Radiation	Mo K_{α} (λ=0.71073 Å)
2θ range [°]	5.39 to 55.00 (0.77 Å)
Index ranges	−41 ≤ h ≤ 41 −13 ≤ k ≤ 13 −29 ≤ l ≤ 29
Reflections collected	85128
Independent reflections	8547 R_{int} = 0.0225 R_{sigma} = 0.0128
Completeness to θ = 25.242°	99.6 %
Data / Restraints / Parameters	8547 / 0 / 363
Goodness-of-fit on F^2	1.163
Final R indexes [I≥2σ(I)]	R_1 = 0.0165 wR_2 = 0.0411
Final R indexes [all data]	R_1 = 0.0171 wR_2 = 0.0414
Largest peak/hole [eÅ^{-3}]	0.67/−0.42
Extinction coefficient	0.00022(2)

Table S32. Bond lengths and angles for CP2D1_220K

Atom–Atom	Length [Å]
I1–Cu1	2.6336(3)
I1–Cu1$^{\#1}$	2.6660(3)
Cu1–Cu1$^{\#1}$	2.8889(4)
Cu1–S1$^{\#2}$	2.3504(4)
Cu1–S2	2.3246(4)
S1–C1	1.8352(16)
S1–C7	1.8236(16)
S2–C10	1.8208(16)
S2–C11	1.8317(15)
C1–H1	0.9900
C1–C2	1.522(3)
C1–C6	1.524(3)
C2–H2A	0.9800
C2–H2B	0.9800
C2–C3	1.515(3)
C3–H3A	0.9800
C3–H3B	0.9800
C3–C4	1.511(3)
C4–H4A	0.9800
C4–H4B	0.9800
C4–C5	1.513(3)
C5–H5A	0.9800
C5–H5B	0.9800
C5–C6	1.520(3)
C6–H6A	0.9800
C6–H6B	0.9800
C7–H7A	0.9800
C7–H7B	0.9800
C7–C8	1.457(2)
C8–C9	1.192(2)
C9–C10	1.459(2)
C10–H10A	0.9800
C10–H10B	0.9800
C11–H11	0.9900
C11–C12	1.524(2)
C11–C16	1.521(2)
C12–H12A	0.9800
C12–H12B	0.9800
C12–C13	1.527(2)
C13–H13A	0.9800
C13–H13B	0.9800
C13–C14	1.516(3)
C14–H14A	0.9800
C14–H14B	0.9800
C14–C15	1.518(3)
C15–H15A	0.9800
C15–H15B	0.9800
C15–C16	1.529(3)
C16–H16A	0.9800
C16–H16B	0.9800
I2–Cu2	2.6316(3)
I2–Cu3	2.6429(3)
Cu2–Cu3	2.9712(5)
Cu2–S3	2.3386(5)
Cu2–S3$^{\#3}$	2.3386(5)
Cu3–S4	2.3561(5)
Cu3–S4$^{\#3}$	2.3560(5)
S3–C17	1.8243(17)
S3–C23	1.824(2)
S4–C26	1.830(2)
S4–C27	1.8266(19)
C17–H17	0.9900
C17–C18	1.520(3)
C17–C22	1.524(2)
C18–H18A	0.9800
C18–H18B	0.9800
C18–C19	1.529(3)
C19–H19A	0.9800
C19–H19B	0.9800
C19–C20	1.517(3)
C20–H20A	0.9800
C20–H20B	0.9800
C20–C21	1.512(3)
C21–H21A	0.9800
C21–H21B	0.9800
C21–C22	1.522(3)
C22–H22A	0.9800
C22–H22B	0.9800
C23–H23A	0.9800
C23–H23B	0.9800
C23–C24	1.455(3)
C24–C25	1.182(3)
C25–C26	1.445(3)
C26–H26A	0.9800
C26–H26B	0.9800
C27–H27	0.9900
C27–C28	1.516(3)
C27–C32	1.521(3)
C28–H28A	0.9800
C28–H28B	0.9800
C28–C29	1.527(3)
C29–H29A	0.9800
C29–H29B	0.9800
C29–C30	1.507(4)
C30–H30A	0.9800
C30–H30B	0.9800
C30–C31	1.504(4)
C31–H31A	0.9800
C31–H31B	0.9800
C31–C32	1.523(3)
C32–H32A	0.9800
C32–H32B	0.9800

Atom–Atom–Atom	Angle [°]
Cu1–I1–Cu1$^{\#1}$	66.063(9)
I1–Cu1–I1$^{\#1}$	113.937(8)
I1$^{\#1}$–Cu1–Cu1$^{\#1}$	56.429(7)
I1–Cu1–Cu1$^{\#1}$	57.508(8)
S1$^{\#2}$–Cu1–I1	102.854(12)

$S1^{\#2}$–Cu1–$I1^{\#1}$	102.401(12)	S2–C10–H10B	109.1
$S1^{\#2}$–Cu1–$Cu1^{\#1}$	113.640(14)	C9–C10–S2	112.29(12)
S2–Cu1–$I1^{\#1}$	108.011(12)	C9–C10–H10A	109.1
S2–Cu1–I1	115.949(13)	C9–C10–H10B	109.1
S2–Cu1–$Cu1^{\#1}$	133.175(15)	H10A–C10–H10B	107.9
S2–Cu1–$S1^{\#2}$	112.870(15)	S2–C11–H11	108.5
C1–S1–$Cu1^{\#2}$	110.95(6)	C12–C11–S2	112.10(11)
C7–S1–$Cu1^{\#2}$	105.31(5)	C12–C11–H11	108.5
C7–S1–C1	100.90(8)	C16–C11–S2	106.88(11)
C10–S2–Cu1	104.64(5)	C16–C11–H11	108.5
C10–S2–C11	100.33(7)	C16–C11–C12	112.26(14)
C11–S2–Cu1	111.00(5)	C11–C12–H12A	109.3
S1–C1–H1	108.6	C11–C12–H12B	109.3
C2–C1–S1	108.40(12)	C11–C12–C13	111.41(14)
C2–C1–H1	108.6	H12A–C12–H12B	108.0
C2–C1–C6	110.80(14)	C13–C12–H12A	109.3
C6–C1–S1	111.90(13)	C13–C12–H12B	109.3
C6–C1–H1	108.6	C12–C13–H13A	109.4
C1–C2–H2A	109.1	C12–C13–H13B	109.4
C1–C2–H2B	109.1	H13A–C13–H13B	108.0
H2A–C2–H2B	107.8	C14–C13–C12	111.07(15)
C3–C2–C1	112.70(14)	C14–C13–H13A	109.4
C3–C2–H2A	109.1	C14–C13–H13B	109.4
C3–C2–H2B	109.1	C13–C14–H14A	109.5
C2–C3–H3A	109.3	C13–C14–H14B	109.5
C2–C3–H3B	109.3	C13–C14–C15	110.87(17)
H3A–C3–H3B	108.0	H14A–C14–H14B	108.1
C4–C3–C2	111.64(17)	C15–C14–H14A	109.5
C4–C3–H3A	109.3	C15–C14–H14B	109.5
C4–C3–H3B	109.3	C14–C15–H15A	109.4
C3–C4–H4A	109.4	C14–C15–H15B	109.4
C3–C4–H4B	109.4	C14–C15–C16	111.12(16)
C3–C4–C5	111.13(15)	H15A–C15–H15B	108.0
H4A–C4–H4B	108.0	C16–C15–H15A	109.4
C5–C4–H4A	109.4	C16–C15–H15B	109.4
C5–C4–H4B	109.4	C11–C16–C15	110.80(15)
C4–C5–H5A	109.5	C11–C16–H16A	109.5
C4–C5–H5B	109.5	C11–C16–H16B	109.5
C4–C5–C6	110.84(17)	C15–C16–H16A	109.5
H5A–C5–H5B	108.1	C15–C16–H16B	109.5
C6–C5–H5A	109.5	H16A–C16–H16B	108.1
C6–C5–H5B	109.5	Cu2–I2–Cu3	68.570(11)
C1–C6–H6A	109.1	I2–Cu2–$I2^{\#3}$	111.788(14)
C1–C6–H6B	109.1	I2–Cu2–Cu3	55.894(7)
C5–C6–C1	112.62(16)	$I2^{\#3}$–Cu2–Cu3	55.895(7)
C5–C6–H6A	109.1	$S3^{\#3}$–Cu2–I2	111.327(11)
C5–C6–H6B	109.1	S3–Cu2–I2	107.351(12)
H6A–C6–H6B	107.8	$S3^{\#3}$–Cu2–$I2^{\#3}$	107.349(12)
S1–C7–H7A	109.0	S3–Cu2–$I2^{\#3}$	111.325(12)
S1–C7–H7B	109.0	$S3^{\#3}$–Cu2–Cu3	126.171(14)
H7A–C7–H7B	107.8	S3–Cu2–Cu3	126.172(14)
C8–C7–S1	113.02(11)	S3–Cu2–$S3^{\#3}$	107.66(3)
C8–C7–H7A	109.0	I2–Cu3–$I2^{\#3}$	111.074(14)
C8–C7–H7B	109.0	$I2^{\#3}$–Cu3–Cu2	55.538(7)
C9–C8–C7	176.39(17)	I2–Cu3–Cu2	55.536(7)
C8–C9–C10	178.31(18)	$S4^{\#3}$–Cu3–I2	107.739(13)
S2–C10–H10A	109.1	$S4^{\#3}$–Cu3–$I2^{\#3}$	110.792(12)

S4–Cu3–I2	110.791(12)	C24–C23–S3	113.19(14)
S4–Cu3–I2$^{\#3}$	107.737(13)	C24–C23–H23A	108.9
S4$^{\#3}$–Cu3–Cu2	125.652(15)	C24–C23–H23B	108.9
S4–Cu3–Cu2	125.650(15)	C25–C24–C23	175.3(2)
S4$^{\#3}$–Cu3–S4	108.70(3)	C24–C25–C26	173.6(2)
C17–S3–Cu2	104.53(6)	S4–C26–H26A	109.2
C17–S3–C23	102.35(9)	S4–C26–H26B	109.2
C23–S3–Cu2	104.49(7)	C25–C26–S4	112.11(13)
C26–S4–Cu3	104.82(7)	C25–C26–H26A	109.2
C27–S4–Cu3	101.62(6)	C25–C26–H26B	109.2
C27–S4–C26	102.32(10)	H26A–C26–H26B	107.9
S3–C17–H17	108.6	S4–C27–H27	108.1
C18–C17–S3	107.07(12)	C28–C27–S4	114.76(15)
C18–C17–H17	108.6	C28–C27–H27	108.1
C18–C17–C22	111.06(15)	C28–C27–C32	110.98(17)
C22–C17–S3	112.75(12)	C32–C27–S4	106.62(13)
C22–C17–H17	108.6	C32–C27–H27	108.1
C17–C18–H18A	109.6	C27–C28–H28A	109.8
C17–C18–H18B	109.6	C27–C28–H28B	109.8
C17–C18–C19	110.22(16)	C27–C28–C29	109.23(19)
H18A–C18–H18B	108.1	H28A–C28–H28B	108.3
C19–C18–H18A	109.6	C29–C28–H28A	109.8
C19–C18–H18B	109.6	C29–C28–H28B	109.8
C18–C19–H19A	109.4	C28–C29–H29A	109.3
C18–C19–H19B	109.4	C28–C29–H29B	109.3
H19A–C19–H19B	108.0	H29A–C29–H29B	107.9
C20–C19–C18	111.18(18)	C30–C29–C28	111.7(2)
C20–C19–H19A	109.4	C30–C29–H29A	109.3
C20–C19–H19B	109.4	C30–C29–H29B	109.3
C19–C20–H20A	109.4	C29–C30–H30A	109.5
C19–C20–H20B	109.4	C29–C30–H30B	109.5
H20A–C20–H20B	108.0	H30A–C30–H30B	108.1
C21–C20–C19	111.26(18)	C31–C30–C29	110.8(2)
C21–C20–H20A	109.4	C31–C30–H30A	109.5
C21–C20–H20B	109.4	C31–C30–H30B	109.5
C20–C21–H21A	109.4	C30–C31–H31A	109.1
C20–C21–H21B	109.4	C30–C31–H31B	109.1
C20–C21–C22	111.23(18)	C30–C31–C32	112.5(3)
H21A–C21–H21B	108.0	H31A–C31–H31B	107.8
C22–C21–H21A	109.4	C32–C31–H31A	109.1
C22–C21–H21B	109.4	C32–C31–H31B	109.1
C17–C22–H22A	109.7	C27–C32–C31	110.14(19)
C17–C22–H22B	109.7	C27–C32–H32A	109.6
C21–C22–C17	110.02(15)	C27–C32–H32B	109.6
C21–C22–H22A	109.7	C31–C32–H32A	109.6
C21–C22–H22B	109.7	C31–C32–H32B	109.6
H22A–C22–H22B	108.2	H32A–C32–H32B	108.1
S3–C23–H23A	108.9		
S3–C23–H23B	108.9		
H23A–C23–H23B	107.8		

Symmetry transformations used to generate equivalent atoms:
#1: 0.5-X, 1.5-Y, 1-Z; #2: 0.5-X, 0.5-Y, 1-Z; #3: 1-X, +Y, 1.5-Z;

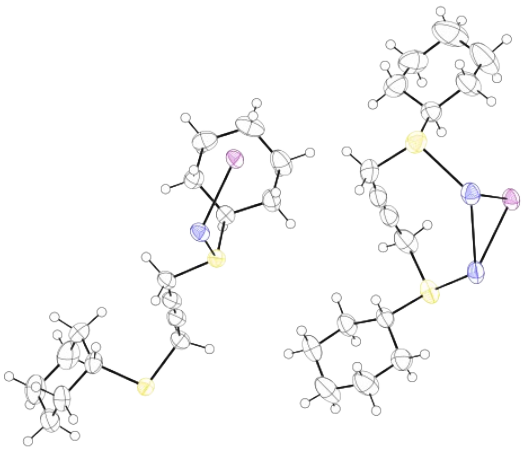
Table S33. Torsion angles for CP2D1_220K

Atom–Atom–Atom–Atom	Torsion Angle [°]		
Cu1$^{\#1}$–S1–C1–C2	−59.25(12)	Cu1$^{\#1}$–S1–C7–C8	−60.96(12)
Cu1$^{\#1}$–S1–C1–C6	178.27(11)	Cu1–S2–C10–C9	−176.90(10)
		Cu1–S2–C11–C12	−40.65(12)
		Cu1–S2–C11–C16	82.76(11)

S1–C1–C2–C3	−71.38(17)
S1–C1–C6–C5	68.57(19)
S2–C11–C12–C13	173.77(12)
S2–C11–C16–C15	−177.04(14)
C1–S1–C7–C8	54.52(13)
C1–C2–C3–C4	−54.0(2)
C2–C1–C6–C5	−52.5(2)
C2–C3–C4–C5	55.9(2)
C3–C4–C5–C6	−56.2(2)
C4–C5–C6–C1	55.2(2)
C6–C1–C2–C3	51.8(2)
C7–S1–C1–C2	−170.45(11)
C7–S1–C1–C6	67.06(14)
C10–S2–C11–C12	69.55(12)
C10–S2–C11–C16	−167.05(12)
C11–S2–C10–C9	68.00(13)
C11–C12–C13–C14	−54.6(2)
C12–C11–C16–C15	−53.7(2)
C12–C13–C14–C15	56.9(2)
C13–C14–C15–C16	−57.5(2)
C14–C15–C16–C11	55.6(2)
C16–C11–C12–C13	53.44(19)
Cu2–S3–C17–C18	−69.02(12)
Cu2–S3–C17–C22	168.54(12)
Cu2–S3–C23–C24	−49.64(15)
Cu3–S4–C26–C25	−50.56(16)
Cu3–S4–C27–C28	160.74(14)
Cu3–S4–C27–C32	−75.96(15)
S3–C17–C18–C19	179.37(14)
S3–C17–C22–C21	177.77(14)
S4–C27–C28–C29	179.34(15)
S4–C27–C32–C31	177.4(2)
C17–S3–C23–C24	59.13(15)
C17–C18–C19–C20	55.8(3)
C18–C17–C22–C21	57.6(2)
C18–C19–C20–C21	−55.5(3)
C19–C20–C21–C22	56.1(3)
C20–C21–C22–C17	−56.8(2)
C22–C17–C18–C19	−57.1(2)
C23–S3–C17–C18	−177.76(13)
C23–S3–C17–C22	59.79(15)
C26–S4–C27–C28	52.54(17)
C26–S4–C27–C32	175.84(16)
C27–S4–C26–C25	55.17(17)
C27–C28–C29–C30	−57.9(3)
C28–C27–C32–C31	−56.9(3)
C28–C29–C30–C31	55.8(4)
C29–C30–C31–C32	−54.2(4)
C30–C31–C32–C27	54.7(4)
C32–C27–C28–C29	58.4(2)

Symmetry transformations used to generate equivalent atoms:
#1: 0.5-X, 0.5-Y, 1-Z;

Crystal Data and Experimental



Experimental: The data for CP2D1_260K were collected from a shock-cooled single crystal at 260.0(1) K on a Bruker D8 Venture CMOS with Photon 2 four-circle diffractometer with a X-ray tube using a graphite as monochromator and a CPAD PHOTON II area detector detector. The diffractometer was equipped with an Oxford Cryostream 800 low temperature device and used Mo K_{α} radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.38A and a multi-scan absorption correction using SADABS 2016/2 was applied. [1,2] The structure was solved by direct methods with ShelXT and refined by full-matrix least-squares methods against F^2 using SHELXL.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[5] CCDC 2326505 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures. This report and the CIF file were generated using FinalCif.[6]

Table S34. Crystal data and structure refinement for CP2D1_260K

Internal Reference	CP2D1_260K
CCDC number	2326505
Empirical formula	$C_{16}H_{26}CuIS_2$
Formula weight	472.93
Temperature [K]	260.0(1)
Crystal system	monoclinic
Space group (number)	$C2/c$ (15)
a [Å]	31.932(2)
b [Å]	10.2558(7)
c [Å]	23.1217(16)
α [°]	90
β [°]	96.952(3)
γ [°]	90
Volume [Å^3]	7516.5(9)
Z	16
ρ_{calc} [gcm^{-3}]	1.672
μ [mm^{-1}]	3.017
F(000)	3776
Crystal size [mm^3]	0.247×0.279×0.481
Crystal colour	clear light yellow
Crystal shape	block
Radiation	Mo K_{α} (λ=0.71073 Å)
2θ range [°]	5.67 to 55.00 (0.77 Å)
Index ranges	−41 ≤ h ≤ 41 −13 ≤ k ≤ 13 −30 ≤ l ≤ 30
Reflections collected	67034
Independent reflections	8597 R_{int} = 0.0242 R_{sigma} = 0.0151
Completeness to θ = 25.242°	99.6 %
Data / Restraints / Parameters	8597 / 0 / 362
Goodness-of-fit on F^2	1.124
Final R indexes [I≥2σ(I)]	R_1 = 0.0177 wR_2 = 0.0432
Final R indexes [all data]	R_1 = 0.0189 wR_2 = 0.0438
Largest peak/hole [eÅ^{-3}]	0.59/−0.49

Table S35. Bond lengths and angles for CP2D1_260K

Atom–Atom	Length [Å]
I1–Cu1	2.6341(3)
I1–Cu1$^{\#1}$	2.6679(3)
Cu1–Cu1$^{\#1}$	2.9000(5)
Cu1–S1$^{\#2}$	2.3526(5)
Cu1–S2	2.3264(5)
S1–C1	1.8365(17)
S1–C7	1.8230(17)
S2–C10	1.8203(17)
S2–C11	1.8303(17)
C1–H1	0.9800
C1–C2	1.513(3)
C1–C6	1.523(3)
C2–H2A	0.9700
C2–H2B	0.9700
C2–C3	1.512(3)
C3–H3A	0.9700
C3–H3B	0.9700
C3–C4	1.503(3)
C4–H4A	0.9700
C4–H4B	0.9700
C4–C5	1.508(4)
C5–H5A	0.9700
C5–H5B	0.9700
C5–C6	1.518(4)
C6–H6A	0.9700
C6–H6B	0.9700
C7–H7A	0.9700
C7–H7B	0.9700
C7–C8	1.457(2)
C8–C9	1.190(3)
C9–C10	1.456(2)
C10–H10A	0.9700
C10–H10B	0.9700
C11–H11	0.9800
C11–C12	1.521(2)
C11–C16	1.519(2)
C12–H12A	0.9700
C12–H12B	0.9700
C12–C13	1.524(3)
C13–H13A	0.9700
C13–H13B	0.9700
C13–C14	1.512(3)
C14–H14A	0.9700
C14–H14B	0.9700
C14–C15	1.517(4)
C15–H15A	0.9700
C15–H15B	0.9700
C15–C16	1.527(3)
C16–H16A	0.9700
C16–H16B	0.9700
I2–Cu2	2.6321(3)
I2–Cu3	2.6426(3)
Cu2–Cu3	2.9628(6)
Cu2–S3	2.3421(5)
Cu2–S3$^{\#3}$	2.3421(5)
Cu3–S4	2.3586(6)
Cu3–S4$^{\#3}$	2.3586(6)
S3–C17	1.8246(18)
S3–C23	1.825(2)
S4–C26	1.829(2)
S4–C27	1.826(2)
C17–H17	0.9800
C17–C18	1.517(3)
C17–C22	1.524(2)
C18–H18A	0.9700
C18–H18B	0.9700
C18–C19	1.531(3)
C19–H19A	0.9700
C19–H19B	0.9700
C19–C20	1.511(3)
C20–H20A	0.9700
C20–H20B	0.9700
C20–C21	1.503(4)
C21–H21A	0.9700
C21–H21B	0.9700
C21–C22	1.520(3)
C22–H22A	0.9700
C22–H22B	0.9700
C23–H23A	0.9700
C23–H23B	0.9700
C23–C24	1.453(4)
C24–C25	1.179(4)
C25–C26	1.446(4)
C26–H26A	0.9700
C26–H26B	0.9700
C27–H27	0.9800
C27–C28	1.511(3)
C27–C32	1.517(3)
C28–H28A	0.9700
C28–H28B	0.9700
C28–C29	1.527(4)
C29–H29A	0.9700
C29–H29B	0.9700
C29–C30	1.510(4)
C30–H30A	0.9700
C30–H30B	0.9700
C30–C31	1.485(5)
C31–H31A	0.9700
C31–H31B	0.9700
C31–C32	1.526(4)
C32–H32A	0.9700
C32–H32B	0.9700

Atom–Atom–Atom	Angle [°]
Cu1–I1–Cu1$^{\#1}$	66.314(9)
I1–Cu1–I1$^{\#1}$	113.685(9)
I1$^{\#1}$–Cu1–Cu1$^{\#1}$	56.282(8)
I1–Cu1–Cu1$^{\#1}$	57.404(9)
S1$^{\#2}$–Cu1–I1	103.039(12)

S1$^{\#2}$–Cu1–I1$^{\#1}$	102.368(13)	S2–C10–H10B	109.1
S1$^{\#2}$–Cu1–Cu1$^{\#1}$	113.701(15)	C9–C10–S2	112.34(13)
S2–Cu1–I1$^{\#1}$	108.131(13)	C9–C10–H10A	109.1
S2–Cu1–I1	116.019(14)	C9–C10–H10B	109.1
S2–Cu1–Cu1$^{\#1}$	133.215(16)	H10A–C10–H10B	107.9
S2–Cu1–S1$^{\#2}$	112.757(16)	S2–C11–H11	108.4
C1–S1–Cu1$^{\#2}$	111.00(7)	C12–C11–S2	112.28(12)
C7–S1–Cu1$^{\#2}$	105.54(6)	C12–C11–H11	108.4
C7–S1–C1	101.11(9)	C16–C11–S2	106.86(12)
C10–S2–Cu1	104.70(6)	C16–C11–H11	108.4
C10–S2–C11	100.42(8)	C16–C11–C12	112.24(15)
C11–S2–Cu1	111.05(6)	C11–C12–H12A	109.3
S1–C1–H1	108.5	C11–C12–H12B	109.3
C2–C1–S1	108.71(13)	C11–C12–C13	111.56(16)
C2–C1–H1	108.5	H12A–C12–H12B	108.0
C2–C1–C6	110.86(16)	C13–C12–H12A	109.3
C6–C1–S1	111.81(14)	C13–C12–H12B	109.3
C6–C1–H1	108.5	C12–C13–H13A	109.4
C1–C2–H2A	109.1	C12–C13–H13B	109.4
C1–C2–H2B	109.1	H13A–C13–H13B	108.0
H2A–C2–H2B	107.8	C14–C13–C12	111.22(17)
C3–C2–C1	112.67(16)	C14–C13–H13A	109.4
C3–C2–H2A	109.1	C14–C13–H13B	109.4
C3–C2–H2B	109.1	C13–C14–H14A	109.4
C2–C3–H3A	109.2	C13–C14–H14B	109.4
C2–C3–H3B	109.2	C13–C14–C15	111.07(19)
H3A–C3–H3B	107.9	H14A–C14–H14B	108.0
C4–C3–C2	111.92(19)	C15–C14–H14A	109.4
C4–C3–H3A	109.2	C15–C14–H14B	109.4
C4–C3–H3B	109.2	C14–C15–H15A	109.4
C3–C4–H4A	109.4	C14–C15–H15B	109.4
C3–C4–H4B	109.4	C14–C15–C16	111.16(18)
C3–C4–C5	111.00(17)	H15A–C15–H15B	108.0
H4A–C4–H4B	108.0	C16–C15–H15A	109.4
C5–C4–H4A	109.4	C16–C15–H15B	109.4
C5–C4–H4B	109.4	C11–C16–C15	110.84(16)
C4–C5–H5A	109.5	C11–C16–H16A	109.5
C4–C5–H5B	109.5	C11–C16–H16B	109.5
C4–C5–C6	110.8(2)	C15–C16–H16A	109.5
H5A–C5–H5B	108.1	C15–C16–H16B	109.5
C6–C5–H5A	109.5	H16A–C16–H16B	108.1
C6–C5–H5B	109.5	Cu2–I2–Cu3	68.346(11)
C1–C6–H6A	109.1	I2–Cu2–I2$^{\#3}$	111.990(15)
C1–C6–H6B	109.1	I2–Cu2–Cu3	55.994(8)
C5–C6–C1	112.57(18)	I2$^{\#3}$–Cu2–Cu3	55.996(8)
C5–C6–H6A	109.1	S3$^{\#3}$–Cu2–I2	111.293(13)
C5–C6–H6B	109.1	S3–Cu2–I2	107.258(14)
H6A–C6–H6B	107.8	S3$^{\#3}$–Cu2–I2$^{\#3}$	107.257(14)
S1–C7–H7A	109.0	S3–Cu2–I2$^{\#3}$	111.295(13)
S1–C7–H7B	109.0	S3$^{\#3}$–Cu2–Cu3	126.149(16)
H7A–C7–H7B	107.8	S3–Cu2–Cu3	126.150(16)
C8–C7–S1	113.12(12)	S3–Cu2–S3$^{\#3}$	107.70(3)
C8–C7–H7A	109.0	I2–Cu3–I2$^{\#3}$	111.320(15)
C8–C7–H7B	109.0	I2$^{\#3}$–Cu3–Cu2	55.661(8)
C9–C8–C7	176.74(19)	I2–Cu3–Cu2	55.659(8)
C8–C9–C10	178.20(18)	S4$^{\#3}$–Cu3–I2	107.659(14)
S2–C10–H10A	109.1	S4$^{\#3}$–Cu3–I2$^{\#3}$	110.848(13)

S4–Cu3–I2	110.848(13)	C24–C23–S3	113.22(15)
S4–Cu3–I2$^{\#3}$	107.659(14)	C24–C23–H23A	108.9
S4$^{\#3}$–Cu3–Cu2	125.756(16)	C24–C23–H23B	108.9
S4–Cu3–Cu2	125.756(16)	C25–C24–C23	175.4(2)
S4$^{\#3}$–Cu3–S4	108.49(3)	C24–C25–C26	173.7(2)
C17–S3–Cu2	104.63(6)	S4–C26–H26A	109.2
C17–S3–C23	102.38(10)	S4–C26–H26B	109.2
C23–S3–Cu2	104.46(7)	C25–C26–S4	112.15(15)
C26–S4–Cu3	104.83(8)	C25–C26–H26A	109.2
C27–S4–Cu3	101.88(7)	C25–C26–H26B	109.2
C27–S4–C26	102.33(11)	H26A–C26–H26B	107.9
S3–C17–H17	108.6	S4–C27–H27	107.9
C18–C17–S3	107.06(13)	C28–C27–S4	114.83(16)
C18–C17–H17	108.6	C28–C27–H27	107.9
C18–C17–C22	111.12(16)	C28–C27–C32	111.21(19)
C22–C17–S3	112.78(13)	C32–C27–S4	106.77(15)
C22–C17–H17	108.6	C32–C27–H27	107.9
C17–C18–H18A	109.7	C27–C28–H28A	109.8
C17–C18–H18B	109.7	C27–C28–H28B	109.8
C17–C18–C19	109.99(18)	C27–C28–C29	109.2(2)
H18A–C18–H18B	108.2	H28A–C28–H28B	108.3
C19–C18–H18A	109.7	C29–C28–H28A	109.8
C19–C18–H18B	109.7	C29–C28–H28B	109.8
C18–C19–H19A	109.4	C28–C29–H29A	109.3
C18–C19–H19B	109.4	C28–C29–H29B	109.3
H19A–C19–H19B	108.0	H29A–C29–H29B	107.9
C20–C19–C18	111.3(2)	C30–C29–C28	111.7(2)
C20–C19–H19A	109.4	C30–C29–H29A	109.3
C20–C19–H19B	109.4	C30–C29–H29B	109.3
C19–C20–H20A	109.4	C29–C30–H30A	109.4
C19–C20–H20B	109.4	C29–C30–H30B	109.4
H20A–C20–H20B	108.0	H30A–C30–H30B	108.0
C21–C20–C19	111.3(2)	C31–C30–C29	111.2(3)
C21–C20–H20A	109.4	C31–C30–H30A	109.4
C21–C20–H20B	109.4	C31–C30–H30B	109.4
C20–C21–H21A	109.3	C30–C31–H31A	109.0
C20–C21–H21B	109.3	C30–C31–H31B	109.0
C20–C21–C22	111.5(2)	C30–C31–C32	112.9(3)
H21A–C21–H21B	108.0	H31A–C31–H31B	107.8
C22–C21–H21A	109.3	C32–C31–H31A	109.0
C22–C21–H21B	109.3	C32–C31–H31B	109.0
C17–C22–H22A	109.7	C27–C32–C31	110.2(2)
C17–C22–H22B	109.7	C27–C32–H32A	109.6
C21–C22–C17	109.95(17)	C27–C32–H32B	109.6
C21–C22–H22A	109.7	C31–C32–H32A	109.6
C21–C22–H22B	109.7	C31–C32–H32B	109.6
H22A–C22–H22B	108.2	H32A–C32–H32B	108.1
S3–C23–H23A	108.9		
S3–C23–H23B	108.9		
H23A–C23–H23B	107.7		

Symmetry transformations used to generate equivalent atoms:
#1: 0.5-X, 1.5-Y, 1-Z; #2: 0.5-X, 0.5-Y, 1-Z; #3: 1-X, +Y, 1.5-Z;

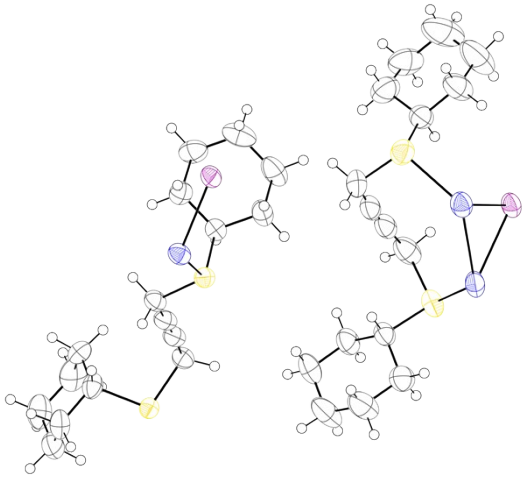
Table S36. Torsion angles for CP2D1_260K

Atom–Atom–Atom–Atom	Torsion Angle [°]		
Cu1$^{\#1}$–S1–C1–C2	−58.93(13)	Cu1$^{\#1}$–S1–C7–C8	−61.01(13)
Cu1$^{\#1}$–S1–C1–C6	178.35(13)	Cu1–S2–C10–C9	−176.71(11)
		Cu1–S2–C11–C12	−40.69(13)
		Cu1–S2–C11–C16	82.78(12)

S1–C1–C2–C3	−71.76(19)
S1–C1–C6–C5	69.1(2)
S2–C11–C12–C13	173.71(13)
S2–C11–C16–C15	−177.20(15)
C1–S1–C7–C8	54.69(14)
C1–C2–C3–C4	−54.0(2)
C2–C1–C6–C5	−52.4(2)
C2–C3–C4–C5	55.9(3)
C3–C4–C5–C6	−56.2(3)
C4–C5–C6–C1	55.1(3)
C6–C1–C2–C3	51.5(2)
C7–S1–C1–C2	−170.52(12)
C7–S1–C1–C6	66.76(15)
C10–S2–C11–C12	69.63(13)
C10–S2–C11–C16	−166.90(13)
C11–S2–C10–C9	68.09(14)
C11–C12–C13–C14	−54.3(2)
C12–C11–C16–C15	−53.7(2)
C12–C13–C14–C15	56.4(2)
C13–C14–C15–C16	−57.2(3)
C14–C15–C16–C11	55.4(3)
C16–C11–C12–C13	53.3(2)
Cu2–S3–C17–C18	−69.04(13)
Cu2–S3–C17–C22	168.44(13)
Cu2–S3–C23–C24	−49.56(16)
Cu3–S4–C26–C25	−50.36(18)
Cu3–S4–C27–C28	160.71(16)
Cu3–S4–C27–C32	−75.53(17)
S3–C17–C18–C19	179.45(16)
S3–C17–C22–C21	177.58(16)
S4–C27–C28–C29	179.51(17)
S4–C27–C32–C31	177.7(2)
C17–S3–C23–C24	59.33(17)
C17–C18–C19–C20	55.8(3)
C18–C17–C22–C21	57.4(2)
C18–C19–C20–C21	−55.5(3)
C19–C20–C21–C22	56.1(3)
C20–C21–C22–C17	−56.6(3)
C22–C17–C18–C19	−57.0(2)
C23–S3–C17–C18	−177.79(14)
C23–S3–C17–C22	59.69(16)
C26–S4–C27–C28	52.43(19)
C26–S4–C27–C32	176.19(17)
C27–S4–C26–C25	55.65(19)
C27–C28–C29–C30	−57.4(3)
C28–C27–C32–C31	−56.4(3)
C28–C29–C30–C31	55.3(4)
C29–C30–C31–C32	−53.6(5)
C30–C31–C32–C27	54.1(4)
C32–C27–C28–C29	58.1(3)

Symmetry transformations used to generate equivalent atoms:
#1: 0.5-X, 0.5-Y, 1-Z;

Crystal Data and Experimental



Experimental: The data for CP2D1_300k were collected from a shock-cooled single crystal at 300.0(1) K on a Bruker D8 Venture CMOS with Photon 2 four-circle diffractometer with a X-ray tube using a graphite as monochromator and a CPAD PHOTON II area detector detector. The diffractometer was equipped with an Oxford Cryostream 800 low temperature device and used Mo K_{α} radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.38A and a multi-scan absorption correction using SADABS 2016/2 was applied. [1,2] The structure was solved by direct methods with ShelXT and refined by full-matrix least-squares methods against F^2 using SHELXL.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters. For each compound, some disorders were found in the crystal structure and some geometric parameters of disordered components in each group were restrained by using DELU restraints. For more detail see the .res file included in the cif files.The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[5] CCDC 2326506 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures. This report and the CIF file were generated using FinalCif.[6]

Table S37. Crystal data and structure refinement for CP2D1_300k

Internal Reference	CP2D1_300k
CCDC number	2326506
Empirical formula	$C_{16}H_{26}CuIS_2$
Formula weight	472.93
Temperature [K]	300.0(1)
Crystal system	monoclinic
Space group (number)	$C2/c$ (15)
a [Å]	31.9681(8)
b [Å]	10.2932(2)
c [Å]	23.1990(7)
α [°]	90
β [°]	97.0950(10)
γ [°]	90
Volume [Å^3]	7575.3(3)
Z	16
ρ_{calc} [gcm^{-3}]	1.659
μ [mm^{-1}]	2.994
F(000)	3776
Crystal size [mm^3]	0.247×0.279×0.481
Crystal colour	clear light yellow
Crystal shape	block
Radiation	Mo K_{α} (λ=0.71073 Å)
2θ range [°]	5.52 to 55.00 (0.77 Å)
Index ranges	−41 ≤ h ≤ 41 −13 ≤ k ≤ 13 −30 ≤ l ≤ 30
Reflections collected	72825
Independent reflections	8681 R_{int} = 0.0514 R_{sigma} = 0.0252
Completeness to θ = 25.242°	99.7 %
Data / Restraints / Parameters	8681 / 12 / 362
Goodness-of-fit on F^2	1.041
Final R indexes [I≥2σ(I)]	R_1 = 0.0198 wR_2 = 0.0511
Final R indexes [all data]	R_1 = 0.0254 wR_2 = 0.0527
Largest peak/hole [eÅ^{-3}]	0.64/−0.32

Table S38. Bond lengths and angles for CP2D1_300k

Atom–Atom	Length [Å]
I1–Cu1	2.6348(3)
I1–Cu1$^{\#1}$	2.6683(3)
Cu1–Cu1$^{\#1}$	2.9112(5)
Cu1–S1$^{\#2}$	2.3577(5)
Cu1–S2	2.3298(5)
S1–C1	1.833(2)
S1–C7	1.825(2)
S2–C10	1.8189(19)
S2–C11	1.8320(18)
C1–H1	0.9800
C1–C2	1.504(3)
C1–C6	1.526(3)
C2–H2A	0.9700
C2–H2B	0.9700
C2–C3	1.506(3)
C3–H3A	0.9700
C3–H3B	0.9700
C3–C4	1.507(4)
C4–H4A	0.9700
C4–H4B	0.9700
C4–C5	1.496(4)
C5–H5A	0.9700
C5–H5B	0.9700
C5–C6	1.517(4)
C6–H6A	0.9700
C6–H6B	0.9700
C7–H7A	0.9700
C7–H7B	0.9700
C7–C8	1.457(3)
C8–C9	1.187(3)
C9–C10	1.456(3)
C10–H10A	0.9700
C10–H10B	0.9700
C11–H11	0.9800
C11–C12	1.513(3)
C11–C16	1.517(3)
C12–H12A	0.9700
C12–H12B	0.9700
C12–C13	1.525(3)
C13–H13A	0.9700
C13–H13B	0.9700
C13–C14	1.503(4)
C14–H14A	0.9700
C14–H14B	0.9700
C14–C15	1.517(4)
C15–H15A	0.9700
C15–H15B	0.9700
C15–C16	1.527(3)
C16–H16A	0.9700
C16–H16B	0.9700
I2–Cu2	2.6338(3)
I2–Cu3	2.6438(3)
Cu2–Cu3	2.9564(6)
Cu2–S3	2.3453(6)
Cu2–S3$^{\#3}$	2.3454(6)
Cu3–S4$^{\#3}$	2.3609(6)
Cu3–S4	2.3609(6)
S3–C17	1.824(2)
S3–C23	1.826(3)
S4–C26	1.825(3)
S4–C27	1.826(2)
C17–H17	0.9800
C17–C18	1.522(3)
C17–C22	1.518(3)
C18–H18A	0.9700
C18–H18B	0.9700
C18–C19	1.528(4)
C19–H19A	0.9700
C19–H19B	0.9700
C19–C20	1.503(4)
C20–H20A	0.9700
C20–H20B	0.9700
C20–C21	1.499(4)
C21–H21A	0.9700
C21–H21B	0.9700
C21–C22	1.515(3)
C22–H22A	0.9700
C22–H22B	0.9700
C23–H23A	0.9700
C23–H23B	0.9700
C23–C24	1.450(4)
C24–C25	1.176(4)
C25–C26	1.445(4)
C26–H26A	0.9700
C26–H26B	0.9700
C27–H27	0.9800
C27–C28	1.501(3)
C27–C32	1.514(3)
C28–H28A	0.9700
C28–H28B	0.9700
C28–C29	1.531(4)
C29–H29A	0.9700
C29–H29B	0.9700
C29–C30	1.508(5)
C30–H30A	0.9700
C30–H30B	0.9700
C30–C31	1.466(5)
C31–H31A	0.9700
C31–H31B	0.9700
C31–C32	1.527(4)
C32–H32A	0.9700
C32–H32B	0.9700

Atom–Atom–Atom	Angle [°]
Cu1–I1–Cu1$^{\#1}$	66.587(10)

I1–Cu1–I1$^{\#1}$	113.413(10)	C8–C7–H7B	108.9
I1$^{\#1}$–Cu1–Cu1$^{\#1}$	56.156(9)	C9–C8–C7	176.9(2)
I1–Cu1–Cu1$^{\#1}$	57.258(8)	C8–C9–C10	178.4(2)
S1$^{\#2}$–Cu1–I1	103.253(14)	S2–C10–H10A	109.1
S1$^{\#2}$–Cu1–I1$^{\#1}$	102.296(15)	S2–C10–H10B	109.1
S1$^{\#2}$–Cu1–Cu1$^{\#1}$	113.746(17)	C9–C10–S2	112.43(15)
S2–Cu1–I1$^{\#1}$	108.262(15)	C9–C10–H10A	109.1
S2–Cu1–I1	116.084(16)	C9–C10–H10B	109.1
S2–Cu1–Cu1$^{\#1}$	133.249(17)	H10A–C10–H10B	107.9
S2–Cu1–S1$^{\#2}$	112.666(18)	S2–C11–H11	108.3
C1–S1–Cu1$^{\#2}$	111.10(7)	C12–C11–S2	112.41(13)
C7–S1–Cu1$^{\#2}$	105.72(6)	C12–C11–H11	108.3
C7–S1–C1	101.26(10)	C12–C11–C16	112.34(18)
C10–S2–Cu1	104.74(7)	C16–C11–S2	106.92(13)
C10–S2–C11	100.40(9)	C16–C11–H11	108.3
C11–S2–Cu1	111.05(6)	C11–C12–H12A	109.3
S1–C1–H1	108.4	C11–C12–H12B	109.3
C2–C1–S1	109.02(15)	C11–C12–C13	111.70(18)
C2–C1–H1	108.4	H12A–C12–H12B	107.9
C2–C1–C6	110.65(18)	C13–C12–H12A	109.3
C6–C1–S1	111.85(17)	C13–C12–H12B	109.3
C6–C1–H1	108.4	C12–C13–H13A	109.4
C1–C2–H2A	109.0	C12–C13–H13B	109.4
C1–C2–H2B	109.0	H13A–C13–H13B	108.0
C1–C2–C3	112.85(19)	C14–C13–C12	111.03(19)
H2A–C2–H2B	107.8	C14–C13–H13A	109.4
C3–C2–H2A	109.0	C14–C13–H13B	109.4
C3–C2–H2B	109.0	C13–C14–H14A	109.4
C2–C3–H3A	109.3	C13–C14–H14B	109.4
C2–C3–H3B	109.3	C13–C14–C15	111.3(2)
C2–C3–C4	111.7(2)	H14A–C14–H14B	108.0
H3A–C3–H3B	107.9	C15–C14–H14A	109.4
C4–C3–H3A	109.3	C15–C14–H14B	109.4
C4–C3–H3B	109.3	C14–C15–H15A	109.5
C3–C4–H4A	109.5	C14–C15–H15B	109.5
C3–C4–H4B	109.5	C14–C15–C16	110.9(2)
H4A–C4–H4B	108.1	H15A–C15–H15B	108.0
C5–C4–C3	110.8(2)	C16–C15–H15A	109.5
C5–C4–H4A	109.5	C16–C15–H15B	109.5
C5–C4–H4B	109.5	C11–C16–C15	110.90(18)
C4–C5–H5A	109.5	C11–C16–H16A	109.5
C4–C5–H5B	109.5	C11–C16–H16B	109.5
C4–C5–C6	110.9(2)	C15–C16–H16A	109.5
H5A–C5–H5B	108.0	C15–C16–H16B	109.5
C6–C5–H5A	109.5	H16A–C16–H16B	108.0
C6–C5–H5B	109.5	Cu2–I2–Cu3	68.138(12)
C1–C6–H6A	109.1	I2$^{\#3}$–Cu2–I2	112.182(17)
C1–C6–H6B	109.1	I2$^{\#3}$–Cu2–Cu3	56.091(8)
C5–C6–C1	112.4(2)	I2–Cu2–Cu3	56.091(8)
C5–C6–H6A	109.1	S3$^{\#3}$–Cu2–I2$^{\#3}$	107.134(15)
C5–C6–H6B	109.1	S3–Cu2–I2$^{\#3}$	111.326(15)
H6A–C6–H6B	107.9	S3$^{\#3}$–Cu2–I2	111.327(14)
S1–C7–H7A	108.9	S3–Cu2–I2	107.137(15)
S1–C7–H7B	108.9	S3$^{\#3}$–Cu2–Cu3	126.158(18)
H7A–C7–H7B	107.7	S3–Cu2–Cu3	126.158(18)
C8–C7–S1	113.25(14)	S3–Cu2–S3$^{\#3}$	107.68(4)
C8–C7–H7A	108.9	I2$^{\#3}$–Cu3–I2	111.540(17)

I2–Cu3–Cu2	55.771(8)	S3–C23–H23B	108.9
I2$^{\#3}$–Cu3–Cu2	55.770(8)	H23A–C23–H23B	107.7
S4–Cu3–I2$^{\#3}$	107.642(16)	C24–C23–S3	113.35(17)
S4–Cu3–I2	110.844(15)	C24–C23–H23A	108.9
S4$^{\#3}$–Cu3–I2$^{\#3}$	110.846(15)	C24–C23–H23B	108.9
S4$^{\#3}$–Cu3–I2	107.638(16)	C25–C24–C23	175.7(2)
S4–Cu3–Cu2	125.850(18)	C24–C25–C26	173.5(3)
S4$^{\#3}$–Cu3–Cu2	125.850(18)	S4–C26–H26A	109.1
S4–Cu3–S4$^{\#3}$	108.30(4)	S4–C26–H26B	109.1
C17–S3–Cu2	104.76(7)	C25–C26–S4	112.42(17)
C17–S3–C23	102.26(11)	C25–C26–H26A	109.1
C23–S3–Cu2	104.53(9)	C25–C26–H26B	109.1
C26–S4–Cu3	104.68(9)	H26A–C26–H26B	107.9
C26–S4–C27	102.35(12)	S4–C27–H27	107.8
C27–S4–Cu3	102.36(8)	C28–C27–S4	115.1(2)
S3–C17–H17	108.5	C28–C27–H27	107.8
C18–C17–S3	107.27(16)	C28–C27–C32	111.1(2)
C18–C17–H17	108.5	C32–C27–S4	106.97(16)
C22–C17–S3	113.00(15)	C32–C27–H27	107.8
C22–C17–H17	108.5	C27–C28–H28A	109.8
C22–C17–C18	110.98(19)	C27–C28–H28B	109.8
C17–C18–H18A	109.7	C27–C28–C29	109.3(3)
C17–C18–H18B	109.7	H28A–C28–H28B	108.3
C17–C18–C19	109.7(2)	C29–C28–H28A	109.8
H18A–C18–H18B	108.2	C29–C28–H28B	109.8
C19–C18–H18A	109.7	C28–C29–H29A	109.3
C19–C18–H18B	109.7	C28–C29–H29B	109.3
C18–C19–H19A	109.4	H29A–C29–H29B	107.9
C18–C19–H19B	109.4	C30–C29–C28	111.7(3)
H19A–C19–H19B	108.0	C30–C29–H29A	109.3
C20–C19–C18	111.4(2)	C30–C29–H29B	109.3
C20–C19–H19A	109.4	C29–C30–H30A	109.2
C20–C19–H19B	109.4	C29–C30–H30B	109.2
C19–C20–H20A	109.3	H30A–C30–H30B	107.9
C19–C20–H20B	109.3	C31–C30–C29	112.1(3)
H20A–C20–H20B	108.0	C31–C30–H30A	109.2
C21–C20–C19	111.5(2)	C31–C30–H30B	109.2
C21–C20–H20A	109.3	C30–C31–H31A	109.0
C21–C20–H20B	109.3	C30–C31–H31B	109.0
C20–C21–H21A	109.4	C30–C31–C32	113.1(4)
C20–C21–H21B	109.4	H31A–C31–H31B	107.8
C20–C21–C22	111.3(2)	C32–C31–H31A	109.0
H21A–C21–H21B	108.0	C32–C31–H31B	109.0
C22–C21–H21A	109.4	C27–C32–C31	110.7(2)
C22–C21–H21B	109.4	C27–C32–H32A	109.5
C17–C22–H22A	109.6	C27–C32–H32B	109.5
C17–C22–H22B	109.6	C31–C32–H32A	109.5
C21–C22–C17	110.29(19)	C31–C32–H32B	109.5
C21–C22–H22A	109.6	H32A–C32–H32B	108.1
C21–C22–H22B	109.6		
H22A–C22–H22B	108.1		

Symmetry transformations used to generate equivalent atoms:
#1: 0.5-X, 1.5-Y, 1-Z; #2: 0.5-X, 0.5-Y, 1-Z; #3: 1-X, +Y, 1.5-Z;

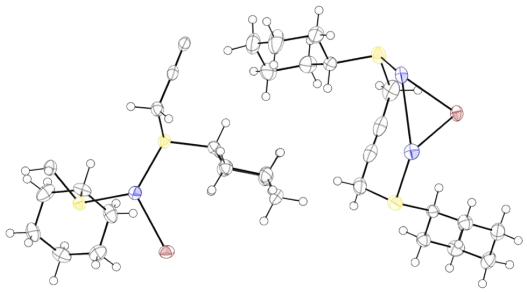
Table S39. Torsion angles for CP2D1_300k

Atom–Atom–Atom–Atom	Torsion Angle [°]		
		Cu1$^{\#1}$–S1–C1–C2	−58.78(15)
		Cu1$^{\#1}$–S1–C1–C6	178.54(15)

Cu1[#1]–S1–C7–C8	−61.27(15)
Cu1–S2–C10–C9	−176.19(12)
Cu1–S2–C11–C12	−40.67(15)
Cu1–S2–C11–C16	83.05(15)
S1–C1–C2–C3	−71.6(2)
S1–C1–C6–C5	69.4(3)
S2–C11–C12–C13	173.94(15)
S2–C11–C16–C15	−177.35(18)
C1–S1–C7–C8	54.67(16)
C1–C2–C3–C4	−54.4(3)
C2–C1–C6–C5	−52.3(3)
C2–C3–C4–C5	56.2(3)
C3–C4–C5–C6	−56.5(3)
C4–C5–C6–C1	55.3(3)
C6–C1–C2–C3	51.8(3)
C7–S1–C1–C2	−170.67(14)
C7–S1–C1–C6	66.64(18)
C10–S2–C11–C12	69.68(16)
C10–S2–C11–C16	−166.59(15)
C11–S2–C10–C9	68.59(15)
C11–C12–C13–C14	−54.4(3)
C12–C11–C16–C15	−53.6(3)
C12–C13–C14–C15	56.4(3)
C13–C14–C15–C16	−57.1(3)
C14–C15–C16–C11	55.1(3)
C16–C11–C12–C13	53.3(2)
Cu2–S3–C17–C18	−68.99(16)
Cu2–S3–C17–C22	168.37(15)
Cu2–S3–C23–C24	−48.9(2)
Cu3–S4–C26–C25	−50.4(2)
Cu3–S4–C27–C28	160.87(18)
Cu3–S4–C27–C32	−75.12(19)
S3–C17–C18–C19	179.29(18)
S3–C17–C22–C21	177.89(18)
S4–C27–C28–C29	179.82(19)
S4–C27–C32–C31	177.6(3)
C17–S3–C23–C24	60.1(2)
C17–C18–C19–C20	55.9(3)
C18–C17–C22–C21	57.3(3)
C18–C19–C20–C21	−55.9(4)
C19–C20–C21–C22	56.0(4)
C20–C21–C22–C17	−56.5(3)
C22–C17–C18–C19	−56.8(3)
C23–S3–C17–C18	−177.82(16)
C23–S3–C17–C22	59.53(19)
C26–S4–C27–C28	52.6(2)
C26–S4–C27–C32	176.6(2)
C27–S4–C26–C25	56.1(2)
C27–C28–C29–C30	−56.8(4)
C28–C27–C32–C31	−56.0(4)
C28–C29–C30–C31	54.3(5)
C29–C30–C31–C32	−52.2(5)
C30–C31–C32–C27	52.9(5)
C32–C27–C28–C29	58.0(3)

Symmetry transformations used to generate equivalent atoms:
#1: 0.5-X, 0.5-Y, 1-Z;

Crystal Data and Experimental



Experimental: The data for CP3D2 were collected from a shock-cooled single crystal at 150.0(1) K on a Xcalibur, Sapphire3 four-circle diffractometer with a X-ray tube using a graphite as monochromator and a CCD area detector detector. The diffractometer used MoK_α radiation (λ = 0.71073 Å). All data were integrated with Crysalis and a multi-scan absorption correction using SCALE3 ABSPACK was applied.[7] The structure was solved by direct methods with SHELXS97 and refined by full-matrix least-squares methods against F^2 using SHELXL.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[5] CCDC 2326258 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures. This report and the CIF file were generated using FinalCif.[6]

Table S40. Crystal data and structure refinement for CP3D2

Internal Reference	CP3D2
CCDC number	2326258
Empirical formula	$C_{16}H_{26}BrCuS_2$
Formula weight	425.94
Temperature [K]	150.0(1)
Crystal system	monoclinic
Space group (number)	$C2/c$ (15)
a [Å]	31.366(2)
b [Å]	10.0042(7)
c [Å]	22.8146(17)
α [°]	90
β [°]	96.959(8)
γ [°]	90
Volume [Å^3]	7106.2(9)
Z	16
ρ_{calc} [gcm^{-3}]	1.592
μ [mm^{-1}]	3.703
F(000)	3488
Crystal size [mm^3]	0.1×0.2×0.2
Crystal colour	clear light colourless
Crystal shape	block
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	4.28 to 50.00 (0.84 Å)
Index ranges	−36 ≤ h ≤ 36 −11 ≤ k ≤ 11 −27 ≤ l ≤ 17
Reflections collected	18548
Independent reflections	6118 R_{int} = 0.0301 R_{sigma} = 0.0556
Completeness to θ = 25.000°	97.7 %
Data / Restraints / Parameters	6118 / 0 / 362
Goodness-of-fit on F^2	0.890
Final R indexes [I≥2σ(I)]	R_1 = 0.0301 wR_2 = 0.0636
Final R indexes [all data]	R_1 = 0.0483 wR_2 = 0.0653
Largest peak/hole [eÅ^{-3}]	1.22/−0.67

Table S41. Bond lengths and angles for CP3D2

Atom–Atom	Length [Å]
Cu2–Cu3	2.9438(9)
Cu2–Br2$^{\#1}$	2.4761(5)
Cu2–Br2	2.4761(5)
Cu2–S3$^{\#1}$	2.3009(10)
Cu2–S3	2.3009(10)
Cu3–Br2	2.4874(5)
Cu3–Br2$^{\#1}$	2.4873(5)
Cu3–S4	2.3270(10)
Cu3–S4$^{\#1}$	2.3269(10)
Br1–Cu1	2.4527(5)
Br1–Cu1$^{\#2}$	2.5282(6)
Cu1–Cu1$^{\#2}$	2.8624(9)
Cu1–S1	2.2843(10)
Cu1–S2	2.3229(10)
S1–C1	1.833(3)
S1–C7	1.809(3)
S2–C10	1.806(3)
S2–C11	1.826(3)
S3–C17	1.820(3)
S3–C23	1.810(4)
S4–C27	1.817(3)
S4–C26	1.813(4)
C19–H19A	0.9900
C19–H19B	0.9900
C19–C18	1.512(5)
C19–C20	1.512(5)
C10–H10A	0.9900
C10–H10B	0.9900
C10–C9$^{\#3}$	1.455(5)
C17–H17	1.0000
C17–C18	1.508(5)
C17–C22	1.518(5)
C6–H6A	0.9900
C6–H6B	0.9900
C6–C5	1.513(4)
C6–C1	1.516(5)
C2–H2A	0.9900
C2–H2B	0.9900
C2–C1	1.505(5)
C2–C3	1.519(5)
C5–H5A	0.9900
C5–H5B	0.9900
C5–C4	1.511(5)
C27–H27	1.0000
C27–C32	1.509(5)
C27–C28	1.518(5)
C9–C8	1.182(4)
C1–H1	1.0000
C7–H7A	0.9900
C7–H7B	0.9900
C7–C8	1.465(5)
C12–H12A	0.9900
C12–H12B	0.9900
C12–C11	1.518(5)
C12–C13	1.511(5)
C18–H18A	0.9900
C18–H18B	0.9900
C25–C24	1.170(5)
C25–C26	1.445(6)
C32–H32A	0.9900
C32–H32B	0.9900
C32–C31	1.516(5)
C20–H20A	0.9900
C20–H20B	0.9900
C20–C21	1.505(5)
C31–H31A	0.9900
C31–H31B	0.9900
C31–C30	1.506(5)
C24–C23	1.461(6)
C23–H23A	0.9900
C23–H23B	0.9900
C4–H4A	0.9900
C4–H4B	0.9900
C4–C3	1.516(5)
C3–H3A	0.9900
C3–H3B	0.9900
C15–H15A	0.9900
C15–H15B	0.9900
C15–C14	1.499(5)
C15–C16	1.519(5)
C14–H14A	0.9900
C14–H14B	0.9900
C14–C13	1.510(5)
C28–H28A	0.9900
C28–H28B	0.9900
C28–C29	1.518(5)
C30–H30A	0.9900
C30–H30B	0.9900
C30–C29	1.502(6)
C11–H11	1.0000
C11–C16	1.511(5)
C22–H22A	0.9900
C22–H22B	0.9900
C22–C21	1.531(5)
C29–H29A	0.9900
C29–H29B	0.9900
C26–H26A	0.9900
C26–H26B	0.9900
C16–H16A	0.9900
C16–H16B	0.9900
C13–H13A	0.9900
C13–H13B	0.9900
C21–H21A	0.9900
C21–H21B	0.9900

Atom–Atom–Atom	Angle [°]
Br2–Cu2–Cu3	53.799(14)
Br2$^{\#1}$–Cu2–Cu3	53.797(14)
Br2$^{\#1}$–Cu2–Br2	107.60(3)

S3–Cu2–Cu3	125.91(3)	C22–C17–S3	106.8(2)
S3$^{\#1}$–Cu2–Cu3	125.91(3)	C22–C17–H17	108.6
S3$^{\#1}$–Cu2–Br2	108.29(2)	H6A–C6–H6B	108.0
S3–Cu2–Br2	112.28(2)	C5–C6–H6A	109.4
S3–Cu2–Br2$^{\#1}$	108.29(2)	C5–C6–H6B	109.4
S3$^{\#1}$–Cu2–Br2$^{\#1}$	112.27(2)	C5–C6–C1	111.3(3)
S3$^{\#1}$–Cu2–S3	108.17(6)	C1–C6–H6A	109.4
Br2–Cu3–Cu2	53.447(14)	C1–C6–H6B	109.4
Br2$^{\#1}$–Cu3–Cu2	53.446(14)	H2A–C2–H2B	108.0
Br2$^{\#1}$–Cu3–Br2	106.89(3)	C1–C2–H2A	109.4
S4$^{\#1}$–Cu3–Cu2	126.34(3)	C1–C2–H2B	109.4
S4–Cu3–Cu2	126.34(3)	C1–C2–C3	111.2(3)
S4$^{\#1}$–Cu3–Br2	111.58(2)	C3–C2–H2A	109.4
S4$^{\#1}$–Cu3–Br2$^{\#1}$	109.76(3)	C3–C2–H2B	109.4
S4–Cu3–Br2$^{\#1}$	111.58(2)	C6–C5–H5A	109.4
S4–Cu3–Br2	109.76(3)	C6–C5–H5B	109.4
S4$^{\#1}$–Cu3–S4	107.32(6)	H5A–C5–H5B	108.0
Cu2–Br2–Cu3	72.75(2)	C4–C5–C6	111.2(3)
Cu1–Br1–Cu1$^{\#2}$	70.134(19)	C4–C5–H5A	109.4
Br1–Cu1–Br1$^{\#2}$	109.867(19)	C4–C5–H5B	109.4
Br1–Cu1–Cu1$^{\#2}$	56.170(17)	S4–C27–H27	108.1
Br1$^{\#2}$–Cu1–Cu1$^{\#2}$	53.697(17)	C32–C27–S4	114.5(3)
S1–Cu1–Br1	118.13(3)	C32–C27–H27	108.1
S1–Cu1–Br1$^{\#2}$	108.43(3)	C32–C27–C28	110.6(3)
S1–Cu1–Cu1$^{\#2}$	133.09(3)	C28–C27–S4	107.1(2)
S1–Cu1–S2	114.12(3)	C28–C27–H27	108.1
S2–Cu1–Br1$^{\#2}$	101.72(3)	C8–C9–C10$^{\#3}$	175.9(4)
S2–Cu1–Br1	103.30(3)	S1–C1–H1	108.5
S2–Cu1–Cu1$^{\#2}$	112.12(3)	C6–C1–S1	112.4(2)
C1–S1–Cu1	110.53(11)	C6–C1–H1	108.5
C7–S1–Cu1	103.76(11)	C2–C1–S1	106.6(2)
C7–S1–C1	100.86(16)	C2–C1–C6	112.3(3)
C10–S2–Cu1	103.65(12)	C2–C1–H1	108.5
C10–S2–C11	101.02(16)	S1–C7–H7A	109.2
C11–S2–Cu1	110.07(12)	S1–C7–H7B	109.2
C17–S3–Cu2	105.38(11)	H7A–C7–H7B	107.9
C23–S3–Cu2	104.26(12)	C8–C7–S1	112.0(2)
C23–S3–C17	102.18(17)	C8–C7–H7A	109.2
C27–S4–Cu3	100.13(12)	C8–C7–H7B	109.2
C26–S4–Cu3	104.62(13)	H12A–C12–H12B	107.8
C26–S4–C27	102.08(17)	C11–C12–H12A	109.0
H19A–C19–H19B	108.0	C11–C12–H12B	109.0
C18–C19–H19A	109.4	C13–C12–H12A	109.0
C18–C19–H19B	109.4	C13–C12–H12B	109.0
C20–C19–H19A	109.4	C13–C12–C11	112.8(3)
C20–C19–H19B	109.4	C19–C18–H18A	109.4
C20–C19–C18	111.3(3)	C19–C18–H18B	109.4
S2–C10–H10A	108.8	C17–C18–C19	111.1(3)
S2–C10–H10B	108.8	C17–C18–H18A	109.4
H10A–C10–H10B	107.7	C17–C18–H18B	109.4
C9$^{\#3}$–C10–S2	113.7(2)	H18A–C18–H18B	108.0
C9$^{\#3}$–C10–H10A	108.8	C24–C25–C26	171.4(4)
C9$^{\#3}$–C10–H10B	108.8	C27–C32–H32A	109.7
S3–C17–H17	108.6	C27–C32–H32B	109.7
C18–C17–S3	112.1(2)	C27–C32–C31	109.9(3)
C18–C17–H17	108.6	H32A–C32–H32B	108.2
C18–C17–C22	112.0(3)	C31–C32–H32A	109.7

C31–C32–H32B	109.7
C19–C20–H20A	109.5
C19–C20–H20B	109.5
H20A–C20–H20B	108.1
C21–C20–C19	110.7(3)
C21–C20–H20A	109.5
C21–C20–H20B	109.5
C32–C31–H31A	109.3
C32–C31–H31B	109.3
H31A–C31–H31B	107.9
C30–C31–C32	111.7(3)
C30–C31–H31A	109.3
C30–C31–H31B	109.3
C25–C24–C23	176.0(4)
S3–C23–H23A	108.9
S3–C23–H23B	108.9
C24–C23–S3	113.2(3)
C24–C23–H23A	108.9
C24–C23–H23B	108.9
H23A–C23–H23B	107.8
C5–C4–H4A	109.5
C5–C4–H4B	109.5
C5–C4–C3	110.7(3)
H4A–C4–H4B	108.1
C3–C4–H4A	109.5
C3–C4–H4B	109.5
C2–C3–H3A	109.6
C2–C3–H3B	109.6
C4–C3–C2	110.5(3)
C4–C3–H3A	109.6
C4–C3–H3B	109.6
H3A–C3–H3B	108.1
H15A–C15–H15B	108.0
C14–C15–H15A	109.4
C14–C15–H15B	109.4
C14–C15–C16	111.1(3)
C16–C15–H15A	109.4
C16–C15–H15B	109.4
C15–C14–H14A	109.3
C15–C14–H14B	109.3
C15–C14–C13	111.7(3)
H14A–C14–H14B	107.9
C13–C14–H14A	109.3
C13–C14–H14B	109.3
C27–C28–H28A	109.6
C27–C28–H28B	109.6
C27–C28–C29	110.1(3)
H28A–C28–H28B	108.2
C29–C28–H28A	109.6
C29–C28–H28B	109.6
C31–C30–H30A	109.4
C31–C30–H30B	109.4
H30A–C30–H30B	108.0
C29–C30–C31	111.0(3)
C29–C30–H30A	109.4
C29–C30–H30B	109.4
S2–C11–H11	108.8
C12–C11–S2	111.9(3)
C12–C11–H11	108.8
C16–C11–S2	108.1(2)
C16–C11–C12	110.4(3)
C16–C11–H11	108.8
C17–C22–H22A	109.7
C17–C22–H22B	109.7
C17–C22–C21	110.0(3)
H22A–C22–H22B	108.2
C21–C22–H22A	109.7
C21–C22–H22B	109.7
C28–C29–H29A	109.1
C28–C29–H29B	109.1
C30–C29–C28	112.3(4)
C30–C29–H29A	109.1
C30–C29–H29B	109.1
H29A–C29–H29B	107.9
S4–C26–H26A	109.3
S4–C26–H26B	109.3
C25–C26–S4	111.8(3)
C25–C26–H26A	109.3
C25–C26–H26B	109.3
H26A–C26–H26B	107.9
C15–C16–H16A	109.0
C15–C16–H16B	109.0
C11–C16–C15	113.0(3)
C11–C16–H16A	109.0
C11–C16–H16B	109.0
H16A–C16–H16B	107.8
C12–C13–H13A	109.6
C12–C13–H13B	109.6
C14–C13–C12	110.3(3)
C14–C13–H13A	109.6
C14–C13–H13B	109.6
H13A–C13–H13B	108.1
C9–C8–C7	176.8(4)
C20–C21–C22	111.8(3)
C20–C21–H21A	109.3
C20–C21–H21B	109.3
C22–C21–H21A	109.3
C22–C21–H21B	109.3
H21A–C21–H21B	107.9

Symmetry transformations used to generate equivalent atoms:
#1: 1-X, +Y, 1.5-Z; #2: 1.5-X, 1.5-Y, 1-Z; #3: 1.5-X, 0.5-Y, 1-Z;

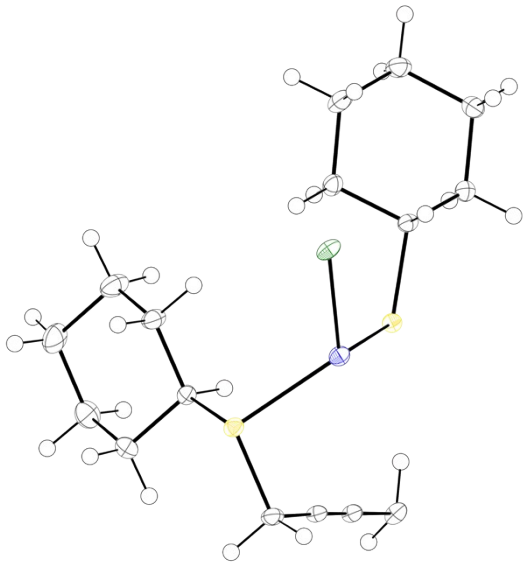
Table S42. Torsion angles for CP3D2

Atom–Atom–Atom–Atom	Torsion Angle [°]
Cu2–S3–C17–C18	−169.9(2)
Cu2–S3–C17–C22	67.1(2)
Cu2–S3–C23–C24	50.3(3)
Cu3–S4–C27–C32	−162.9(2)

Cu3–S4–C27–C28	74.0(3)
Cu3–S4–C26–C25	51.5(3)
Cu1–S1–C1–C6	−42.0(3)
Cu1–S1–C1–C2	81.5(2)
Cu1–S1–C7–C8	−176.8(2)
Cu1–S2–C10–C9$^{\#1}$	61.0(3)
Cu1–S2–C11–C12	−175.3(2)
Cu1–S2–C11–C16	62.9(2)
S2–C11–C16–C15	70.6(4)
S3–C17–C18–C19	−175.6(2)
S3–C17–C22–C21	177.8(2)
S4–C27–C32–C31	−179.6(2)
S4–C27–C28–C29	−177.3(3)
C19–C20–C21–C22	56.4(4)
C10–S2–C11–C12	−66.2(3)
C10–S2–C11–C16	172.0(2)
C17–S3–C23–C24	−59.2(3)
C17–C22–C21–C20	−55.3(4)
C6–C5–C4–C3	57.1(4)
C5–C6–C1–S1	173.5(2)
C5–C6–C1–C2	53.3(4)
C5–C4–C3–C2	−57.6(4)
C27–S4–C26–C25	−52.5(3)
C27–C32–C31–C30	57.2(4)
C27–C28–C29–C30	−55.1(5)
C1–S1–C7–C8	68.7(3)
C1–C6–C5–C4	−54.5(4)
C1–C2–C3–C4	56.1(4)
C7–S1–C1–C6	67.3(3)
C7–S1–C1–C2	−169.2(2)
C12–C11–C16–C15	−52.1(4)
C18–C19–C20–C21	−56.4(4)
C18–C17–C22–C21	54.7(4)
C32–C27–C28–C29	57.4(5)
C32–C31–C30–C29	−54.8(5)
C20–C19–C18–C17	55.9(4)
C31–C30–C29–C28	53.9(5)
C23–S3–C17–C18	−61.2(3)
C23–S3–C17–C22	175.8(2)
C3–C2–C1–S1	−177.7(3)
C3–C2–C1–C6	−54.2(4)
C15–C14–C13–C12	56.5(4)
C14–C15–C16–C11	53.8(4)
C28–C27–C32–C31	−58.4(4)
C11–S2–C10–C9$^{\#1}$	−53.1(3)
C11–C12–C13–C14	−55.6(4)
C22–C17–C18–C19	−55.6(4)
C26–S4–C27–C32	−55.5(3)
C26–S4–C27–C28	−178.5(3)
C16–C15–C14–C13	−55.6(4)
C13–C12–C11–S2	−67.1(4)
C13–C12–C11–C16	53.3(4)

Symmetry transformations used to generate equivalent atoms:
#1: 1.5-X, 0.5-Y, 1-Z;

Crystal Data and Experimental



Experimental: The material was recrystallised from a mixture of acetonitrile and methanol by slow evaporation. The data for CP4 were collected from a shock-cooled single crystal at 115.0(1) K on a Nonius Kappa Apex II \k-geometry diffractometer with a X-ray tube using a graphite as monochromator and an APEX2 detector. The diffractometer was equipped with an Oxford Cryostream 600 low temperature device and used Mo K_{α} radiation (λ = 0.71073 Å). All data were integrated with SAINT (2013). and a multi-scan absorption correction using SADABS 2012/1 was applied. [1,2] The structure was solved by direct methods with SUPERFLIP,[8] and refined by full-matrix least-squares methods against F^2 using SHELXL.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[5] CCDC 2326259 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures. This report and the CIF file were generated using FinalCif.[6]

Table S43. Crystal data and structure refinement for CP4

Internal Reference	CP4
CCDC number	2326259
Empirical formula	$C_{16}H_{26}ClCuS_2$
Formula weight	381.48
Temperature [K]	115.0(1)
Crystal system	monoclinic
Space group (number)	$P2_1/c$ (14)
a [Å]	11.3631(5)
b [Å]	9.2959(4)
c [Å]	17.5929(7)
α [°]	90
β [°]	107.3267(13)
γ [°]	90
Volume [Å^3]	1774.01(13)
Z	4
ρ_{calc} [gcm^{-3}]	1.428
μ [mm^{-1}]	1.606
F(000)	800
Crystal size [mm^3]	0.15×0.2×0.25
Crystal colour	clear light colourless
Crystal shape	prism
Radiation	Mo K_{α} (λ=0.71073 Å)
2θ range [°]	5.77 to 55.00 (0.77 Å)
Index ranges	−14 ≤ h ≤ 14 −12 ≤ k ≤ 12 −16 ≤ l ≤ 22
Reflections collected	33599
Independent reflections	4063 R_{int} = 0.0343 R_{sigma} = 0.0192
Completeness to θ = 26.000°	99.9 %
Data / Restraints / Parameters	4063 / 0 / 181
Goodness-of-fit on F^2	1.046
Final R indexes [I≥2σ(I)]	R_1 = 0.0196 wR_2 = 0.0445
Final R indexes [all data]	R_1 = 0.0265 wR_2 = 0.0472
Largest peak/hole [eÅ^{-3}]	0.31/−0.23

Table S44. Bond lengths and angles for CP4

Atom–Atom	Length [Å]
Cu1–Cu1$^{\#1}$	2.7766(3)
Cu1–Cl1$^{\#1}$	2.3785(4)
Cu1–Cl1	2.3387(4)
Cu1–S1	2.3148(4)
Cu1–S2	2.2973(4)
S1–C11	1.8332(13)
S1–C1$^{\#2}$	1.8293(14)
S2–C5	1.8236(14)
S2–C4	1.8281(14)
C8–H8A	0.9900
C8–H8B	0.9900
C8–C9	1.526(2)
C8–C7	1.523(2)
C9–H9A	0.9900
C9–H9B	0.9900
C9–C10	1.528(2)
C5–H5	1.0000
C5–C6	1.5220(19)
C5–C10	1.5282(18)
C6–H6A	0.9900
C6–H6B	0.9900
C6–C7	1.532(2)
C12–H12A	0.9900
C12–H12B	0.9900
C12–C13	1.5348(19)
C12–C11	1.5245(18)
C10–H10A	0.9900
C10–H10B	0.9900
C13–H13A	0.9900
C13–H13B	0.9900
C13–C14	1.527(2)
C7–H7A	0.9900
C7–H7B	0.9900
C16–H16A	0.9900
C16–H16B	0.9900
C16–C11	1.5283(18)
C16–C15	1.530(2)
C11–H11	1.0000
C15–H15A	0.9900
C15–H15B	0.9900
C15–C14	1.524(2)
C14–H14A	0.9900
C14–H14B	0.9900
C4–H4A	0.9900
C4–H4B	0.9900
C4–C3	1.4603(19)
C2–C3	1.191(2)
C2–C1	1.4646(19)
C1–H1A	0.9900
C1–H1B	0.9900

Atom–Atom–Atom	Angle [°]
Cl1–Cu1–Cu1$^{\#1}$	54.612(10)
Cl1$^{\#1}$–Cu1–Cu1$^{\#1}$	53.279(10)
Cl1–Cu1–Cl1$^{\#1}$	107.892(11)
S1–Cu1–Cu1$^{\#1}$	121.449(13)
S1–Cu1–Cl1$^{\#1}$	106.991(13)
S1–Cu1–Cl1	108.796(13)
S2–Cu1–Cu1$^{\#1}$	121.849(13)
S2–Cu1–Cl1	114.721(14)
S2–Cu1–Cl1$^{\#1}$	101.817(13)
S2–Cu1–S1	115.850(14)
Cu1–Cl1–Cu1$^{\#1}$	72.109(11)
C11–S1–Cu1	102.35(4)
C1$^{\#2}$–S1–Cu1	100.61(5)
C1$^{\#2}$–S1–C11	103.27(6)
C5–S2–Cu1	104.49(4)
C5–S2–C4	102.96(6)
C4–S2–Cu1	101.06(5)
H8A–C8–H8B	108.0
C9–C8–H8A	109.4
C9–C8–H8B	109.4
C7–C8–H8A	109.4
C7–C8–H8B	109.4
C7–C8–C9	111.12(13)
C8–C9–H9A	109.4
C8–C9–H9B	109.4
C8–C9–C10	111.10(13)
H9A–C9–H9B	108.0
C10–C9–H9A	109.4
C10–C9–H9B	109.4
S2–C5–H5	108.8
C6–C5–S2	113.47(10)
C6–C5–H5	108.8
C6–C5–C10	110.70(11)
C10–C5–S2	106.21(9)
C10–C5–H5	108.8
C5–C6–H6A	109.7
C5–C6–H6B	109.7
C5–C6–C7	110.00(12)
H6A–C6–H6B	108.2
C7–C6–H6A	109.7
C7–C6–H6B	109.7
H12A–C12–H12B	108.2
C13–C12–H12A	109.7
C13–C12–H12B	109.7
C11–C12–H12A	109.7
C11–C12–H12B	109.7
C11–C12–C13	109.79(11)
C9–C10–H10A	109.5
C9–C10–H10B	109.5
C5–C10–C9	110.61(12)
C5–C10–H10A	109.5
C5–C10–H10B	109.5
H10A–C10–H10B	108.1
C12–C13–H13A	109.4
C12–C13–H13B	109.4
H13A–C13–H13B	108.0
C14–C13–C12	111.25(12)

C14–C13–H13A	109.4
C14–C13–H13B	109.4
C8–C7–C6	111.41(13)
C8–C7–H7A	109.3
C8–C7–H7B	109.3
C6–C7–H7A	109.3
C6–C7–H7B	109.3
H7A–C7–H7B	108.0
H16A–C16–H16B	108.2
C11–C16–H16A	109.6
C11–C16–H16B	109.6
C11–C16–C15	110.11(11)
C15–C16–H16A	109.6
C15–C16–H16B	109.6
S1–C11–H11	108.6
C12–C11–S1	113.61(9)
C12–C11–C16	110.65(11)
C12–C11–H11	108.6
C16–C11–S1	106.60(9)
C16–C11–H11	108.6
C16–C15–H15A	109.3
C16–C15–H15B	109.3
H15A–C15–H15B	108.0
C14–C15–C16	111.46(12)
C14–C15–H15A	109.3
C14–C15–H15B	109.3
C13–C14–H14A	109.4
C13–C14–H14B	109.4
C15–C14–C13	111.05(12)
C15–C14–H14A	109.4
C15–C14–H14B	109.4
H14A–C14–H14B	108.0
S2–C4–H4A	108.7
S2–C4–H4B	108.7
H4A–C4–H4B	107.6
C3–C4–S2	114.44(9)
C3–C4–H4A	108.7
C3–C4–H4B	108.7
C3–C2–C1	179.64(14)
C2–C3–C4	178.09(15)
$S1^{\#2}$–C1–H1A	108.8
$S1^{\#2}$–C1–H1B	108.8
C2–C1–$S1^{\#2}$	113.92(10)
C2–C1–H1A	108.8
C2–C1–H1B	108.8
H1A–C1–H1B	107.7

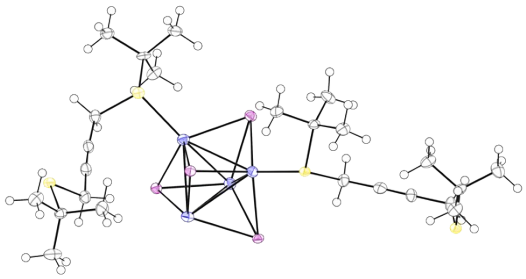
Symmetry transformations used to generate equivalent atoms:
#1: -X, -Y, 1-Z; #2: -X, 1-Y, 1-Z;

Table S45. Torsion angles for CP4

Atom–Atom–Atom–Atom	Torsion Angle [°]
Cu1–S1–C11–C12	160.24(9)
Cu1–S1–C11–C16	−77.62(9)
Cu1–S2–C5–C6	164.27(9)
Cu1–S2–C5–C10	−73.90(9)
Cu1–S2–C4–C3	−55.40(11)
S2–C5–C6–C7	177.19(10)
S2–C5–C10–C9	178.53(10)
C8–C9–C10–C5	56.08(17)
C9–C8–C7–C6	55.45(19)
C5–S2–C4–C3	52.45(12)
C5–C6–C7–C8	−56.83(17)
C6–C5–C10–C9	−57.88(16)
C12–C13–C14–C15	55.26(16)
C10–C5–C6–C7	57.89(16)
C13–C12–C11–S1	178.55(9)
C13–C12–C11–C16	58.68(15)
C7–C8–C9–C10	−54.91(19)
C16–C15–C14–C13	−54.93(16)
C11–C12–C13–C14	−57.04(15)
C11–C16–C15–C14	56.35(16)
C15–C16–C11–S1	177.60(9)
C15–C16–C11–C12	−58.41(15)
C4–S2–C5–C6	59.03(11)
C4–S2–C5–C10	−179.14(9)
$C1^{\#1}$–S1–C11–C12	56.04(11)
$C1^{\#1}$–S1–C11–C16	178.18(9)

Symmetry transformations used to generate equivalent atoms:
#1: -X, 1-Y, 1-Z;

Crystal Data and Experimental



Experimental: The data for CP5 were collected from a shock-cooled single crystal at 100.0(1) K on a Bruker D8 VENTURE four-circle diffractometer with a X-ray tube using a graphite as monochromator and a CPAD PHOTON II area detector detector. The diffractometer used Mo K_{α} radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.38A and a multi-scan absorption correction using SADABS 2016/2 was applied. [1,2] The structure was solved by direct methods with XT and refined by full-matrix least-squares methods against F^2 using SHELXL.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[5] CCDC 2326261 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures. This report and the CIF file were generated using FinalCif.[6]

Table S46. Crystal data and structure refinement for CP5

Internal Reference	CP5
CCDC number	2326261
Empirical formula	$C_{24}H_{44}Cu_4I_4S_4$
Formula weight	1222.59
Temperature [K]	100.0(1)
Crystal system	orthorhombic
Space group (number)	$P2_12_12_1$ (19)
a [Å]	9.9428(8)
b [Å]	18.9973(17)
c [Å]	19.2437(15)
α [°]	90
β [°]	90
γ [°]	90
Volume [Å^3]	3634.9(5)
Z	4
ρ_{calc} [gcm^{-3}]	2.234
μ [mm^{-1}]	5.950
F(000)	2320
Crystal size [mm^3]	0.081×0.109×0.139
Crystal colour	clear light colourless
Crystal shape	block
Radiation	Mo K_{α} (λ=0.71073 Å)
2θ range [°]	4.29 to 55.00 (0.77 Å)
Index ranges	−12 ≤ h ≤ 12 −24 ≤ k ≤ 24 −25 ≤ l ≤ 23
Reflections collected	32078
Independent reflections	8319 R_{int} = 0.0437 R_{sigma} = 0.0395
Completeness to θ = 25.242°	99.9 %
Data / Restraints / Parameters	8319 / 0 / 338
Goodness-of-fit on F^2	1.064
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0296 wR_2 = 0.0720
Final *R* indexes [all data]	R_1 = 0.0314 wR_2 = 0.0732
Largest peak/hole [eÅ^{-3}]	2.08/−1.36
Flack X parameter	-0.02(2)

Refinement details for CP5

Refined as a 2-component inversion twin.

Table S47. Bond lengths and angles for CP5

Atom–Atom	Length [Å]
I1–Cu1	2.7199(10)
I1–Cu3	2.6434(10)
I1–Cu4	2.6435(10)
I2–Cu2	2.6679(10)
I2–Cu3	2.6971(10)
I2–Cu4	2.6914(10)
I3–Cu1	2.6628(10)
I3–Cu2	2.6470(10)
I3–Cu3	2.7202(10)
I4–Cu1	2.6910(10)
I4–Cu2	2.6621(10)
I4–Cu4	2.6764(10)
Cu1–Cu2	2.8905(12)
Cu1–Cu3	2.9060(13)
Cu1–Cu4	2.7715(13)
Cu1–S2	2.3239(19)
Cu2–Cu3	2.9039(12)
Cu2–Cu4	2.8927(12)
Cu2–S3	2.3216(18)
Cu3–Cu4	2.8512(12)
Cu3–S1$^{\#1}$	2.330(2)
Cu4–S4$^{\#2}$	2.3311(19)
S1–C1	1.857(7)
S1–C5	1.839(7)
S2–C8	1.824(7)
S2–C9	1.862(7)
S3–C13	1.861(7)
S3–C17	1.837(7)
S4–C20	1.836(7)
S4–C21	1.860(7)
C1–C2	1.525(10)
C1–C3	1.521(10)
C1–C4	1.531(10)
C2–H2A	0.9800
C2–H2B	0.9800
C2–H2C	0.9800
C3–H3A	0.9800
C3–H3B	0.9800
C3–H3C	0.9800
C4–H4A	0.9800
C4–H4B	0.9800
C4–H4C	0.9800
C5–H5A	0.9900
C5–H5B	0.9900
C5–C6	1.476(10)
C6–C7	1.176(11)
C7–C8	1.461(10)
C8–H8A	0.9900
C8–H8B	0.9900
C9–C10	1.511(10)
C9–C11	1.531(10)
C9–C12	1.531(10)
C10–H10A	0.9800
C10–H10B	0.9800
C10–H10C	0.9800
C11–H11A	0.9800
C11–H11B	0.9800
C11–H11C	0.9800
C12–H12A	0.9800
C12–H12B	0.9800
C12–H12C	0.9800
C13–C14	1.532(10)
C13–C15	1.514(10)
C13–C16	1.515(10)
C14–H14A	0.9800
C14–H14B	0.9800
C14–H14C	0.9800
C15–H15A	0.9800
C15–H15B	0.9800
C15–H15C	0.9800
C16–H16A	0.9800
C16–H16B	0.9800
C16–H16C	0.9800
C17–H17A	0.9900
C17–H17B	0.9900
C17–C18	1.463(10)
C18–C19	1.192(10)
C19–C20	1.477(9)
C20–H20A	0.9900
C20–H20B	0.9900
C21–C22	1.525(10)
C21–C23	1.522(10)
C21–C24	1.520(10)
C22–H22A	0.9800
C22–H22B	0.9800
C22–H22C	0.9800
C23–H23A	0.9800
C23–H23B	0.9800
C23–H23C	0.9800
C24–H24A	0.9800
C24–H24B	0.9800
C24–H24C	0.9800

Atom–Atom–Atom	Angle [°]
Cu3–I1–Cu1	65.60(3)
Cu3–I1–Cu4	65.27(3)
Cu4–I1–Cu1	62.21(3)
Cu2–I2–Cu3	65.54(3)
Cu2–I2–Cu4	65.33(3)
Cu4–I2–Cu3	63.89(3)
Cu1–I3–Cu3	65.33(3)

Cu2–I3–Cu1	65.96(3)	I3–Cu3–Cu2	56.04(3)
Cu2–I3–Cu3	65.49(3)	I3–Cu3–Cu4	103.60(4)
Cu2–I4–Cu1	65.36(3)	Cu2–Cu3–Cu1	59.67(3)
Cu2–I4–Cu4	65.62(3)	Cu4–Cu3–Cu1	57.55(3)
Cu4–I4–Cu1	62.18(3)	Cu4–Cu3–Cu2	60.34(3)
I1–Cu1–Cu2	106.23(4)	S1$^{\#1}$–Cu3–I1	115.00(6)
I1–Cu1–Cu3	55.93(3)	S1$^{\#1}$–Cu3–I2	105.95(5)
I1–Cu1–Cu4	57.54(3)	S1$^{\#1}$–Cu3–I3	107.25(6)
I3–Cu1–I1	109.07(3)	S1$^{\#1}$–Cu3–Cu1	149.14(6)
I3–Cu1–I4	108.13(3)	S1$^{\#1}$–Cu3–Cu2	137.06(6)
I3–Cu1–Cu2	56.75(3)	S1$^{\#1}$–Cu3–Cu4	148.70(6)
I3–Cu1–Cu3	58.29(3)	I1–Cu4–I2	109.97(3)
I3–Cu1–Cu4	107.36(4)	I1–Cu4–I4	115.60(3)
I4–Cu1–I1	112.60(3)	I1–Cu4–Cu1	60.25(3)
I4–Cu1–Cu2	56.84(3)	I1–Cu4–Cu2	108.26(3)
I4–Cu1–Cu3	106.29(3)	I1–Cu4–Cu3	57.36(3)
I4–Cu1–Cu4	58.65(3)	I2–Cu4–Cu1	108.27(4)
Cu2–Cu1–Cu3	60.13(3)	I2–Cu4–Cu2	56.94(3)
Cu4–Cu1–Cu2	61.40(3)	I2–Cu4–Cu3	58.15(3)
Cu4–Cu1–Cu3	60.23(3)	I4–Cu4–I2	107.54(3)
S2–Cu1–I1	106.64(5)	I4–Cu4–Cu1	59.17(3)
S2–Cu1–I3	115.36(6)	I4–Cu4–Cu2	56.95(3)
S2–Cu1–I4	105.10(5)	I4–Cu4–Cu3	108.25(4)
S2–Cu1–Cu2	146.76(6)	Cu1–Cu4–Cu2	61.33(3)
S2–Cu1–Cu3	148.23(6)	Cu1–Cu4–Cu3	62.22(3)
S2–Cu1–Cu4	137.27(6)	Cu3–Cu4–Cu2	60.73(3)
I2–Cu2–Cu1	105.53(3)	S4$^{\#2}$–Cu4–I1	110.65(5)
I2–Cu2–Cu3	57.71(3)	S4$^{\#2}$–Cu4–I2	114.21(5)
I2–Cu2–Cu4	57.73(3)	S4$^{\#2}$–Cu4–I4	98.57(5)
I3–Cu2–I2	112.16(3)	S4$^{\#2}$–Cu4–Cu1	136.57(6)
I3–Cu2–I4	109.47(3)	S4$^{\#2}$–Cu4–Cu2	140.37(6)
I3–Cu2–Cu1	57.28(3)	S4$^{\#2}$–Cu4–Cu3	153.18(6)
I3–Cu2–Cu3	58.47(3)	C1–S1–Cu3$^{\#3}$	111.3(2)
I3–Cu2–Cu4	104.38(3)	C5–S1–Cu3$^{\#3}$	102.1(3)
I4–Cu2–I2	108.65(3)	C5–S1–C1	102.0(3)
I4–Cu2–Cu1	57.80(3)	C8–S2–Cu1	103.2(2)
I4–Cu2–Cu3	107.12(3)	C8–S2–C9	103.6(3)
I4–Cu2–Cu4	57.43(3)	C9–S2–Cu1	111.1(2)
Cu1–Cu2–Cu3	60.20(3)	C13–S3–Cu2	112.2(2)
Cu1–Cu2–Cu4	57.27(3)	C17–S3–Cu2	103.5(2)
Cu4–Cu2–Cu3	58.93(3)	C17–S3–C13	105.7(3)
S3–Cu2–I2	101.96(5)	C20–S4–Cu4$^{\#4}$	104.2(2)
S3–Cu2–I3	113.91(5)	C20–S4–C21	104.4(3)
S3–Cu2–I4	110.40(5)	C21–S4–Cu4$^{\#4}$	112.2(2)
S3–Cu2–Cu1	152.37(6)	C2–C1–S1	104.5(5)
S3–Cu2–Cu3	141.66(6)	C2–C1–C4	109.6(6)
S3–Cu2–Cu4	141.49(6)	C3–C1–S1	111.2(5)
I1–Cu3–I2	109.80(3)	C3–C1–C2	111.0(6)
I1–Cu3–I3	109.64(3)	C3–C1–C4	110.0(6)
I1–Cu3–Cu1	58.47(3)	C4–C1–S1	110.4(5)
I1–Cu3–Cu2	107.93(4)	C1–C2–H2A	109.5
I1–Cu3–Cu4	57.37(3)	C1–C2–H2B	109.5
I2–Cu3–I3	109.00(3)	C1–C2–H2C	109.5
I2–Cu3–Cu1	104.35(3)	H2A–C2–H2B	109.5
I2–Cu3–Cu2	56.75(3)	H2A–C2–H2C	109.5
I2–Cu3–Cu4	57.96(3)	H2B–C2–H2C	109.5
I3–Cu3–Cu1	56.38(3)	C1–C3–H3A	109.5

C1–C3–H3B	109.5
C1–C3–H3C	109.5
H3A–C3–H3B	109.5
H3A–C3–H3C	109.5
H3B–C3–H3C	109.5
C1–C4–H4A	109.5
C1–C4–H4B	109.5
C1–C4–H4C	109.5
H4A–C4–H4B	109.5
H4A–C4–H4C	109.5
H4B–C4–H4C	109.5
S1–C5–H5A	109.8
S1–C5–H5B	109.8
H5A–C5–H5B	108.3
C6–C5–S1	109.3(5)
C6–C5–H5A	109.8
C6–C5–H5B	109.8
C7–C6–C5	176.0(8)
C6–C7–C8	174.2(8)
S2–C8–H8A	110.1
S2–C8–H8B	110.1
C7–C8–S2	107.8(5)
C7–C8–H8A	110.1
C7–C8–H8B	110.1
H8A–C8–H8B	108.5
C10–C9–S2	110.5(5)
C10–C9–C11	111.6(6)
C10–C9–C12	111.7(6)
C11–C9–S2	103.7(5)
C12–C9–S2	109.0(5)
C12–C9–C11	110.1(6)
C9–C10–H10A	109.5
C9–C10–H10B	109.5
C9–C10–H10C	109.5
H10A–C10–H10B	109.5
H10A–C10–H10C	109.5
H10B–C10–H10C	109.5
C9–C11–H11A	109.5
C9–C11–H11B	109.5
C9–C11–H11C	109.5
H11A–C11–H11B	109.5
H11A–C11–H11C	109.5
H11B–C11–H11C	109.5
C9–C12–H12A	109.5
C9–C12–H12B	109.5
C9–C12–H12C	109.5
H12A–C12–H12B	109.5
H12A–C12–H12C	109.5
H12B–C12–H12C	109.5
C14–C13–S3	107.7(5)
C15–C13–S3	111.4(5)
C15–C13–C14	110.6(6)
C15–C13–C16	110.9(6)
C16–C13–S3	105.2(5)
C16–C13–C14	110.9(6)
C13–C14–H14A	109.5
C13–C14–H14B	109.5
C13–C14–H14C	109.5
H14A–C14–H14B	109.5
H14A–C14–H14C	109.5
H14B–C14–H14C	109.5
C13–C15–H15A	109.5
C13–C15–H15B	109.5
C13–C15–H15C	109.5
H15A–C15–H15B	109.5
H15A–C15–H15C	109.5
H15B–C15–H15C	109.5
C13–C16–H16A	109.5
C13–C16–H16B	109.5
C13–C16–H16C	109.5
H16A–C16–H16B	109.5
H16A–C16–H16C	109.5
H16B–C16–H16C	109.5
S3–C17–H17A	108.1
S3–C17–H17B	108.1
H17A–C17–H17B	107.3
C18–C17–S3	116.8(5)
C18–C17–H17A	108.1
C18–C17–H17B	108.1
C19–C18–C17	173.1(8)
C18–C19–C20	177.1(8)
S4–C20–H20A	108.6
S4–C20–H20B	108.6
C19–C20–S4	114.5(5)
C19–C20–H20A	108.6
C19–C20–H20B	108.6
H20A–C20–H20B	107.6
C22–C21–S4	108.9(5)
C23–C21–S4	103.6(5)
C23–C21–C22	110.5(6)
C24–C21–S4	111.2(5)
C24–C21–C22	110.9(6)
C24–C21–C23	111.4(6)
C21–C22–H22A	109.5
C21–C22–H22B	109.5
C21–C22–H22C	109.5
H22A–C22–H22B	109.5
H22A–C22–H22C	109.5
H22B–C22–H22C	109.5
C21–C23–H23A	109.5
C21–C23–H23B	109.5
C21–C23–H23C	109.5
H23A–C23–H23B	109.5
H23A–C23–H23C	109.5
H23B–C23–H23C	109.5
C21–C24–H24A	109.5
C21–C24–H24B	109.5
C21–C24–H24C	109.5
H24A–C24–H24B	109.5
H24A–C24–H24C	109.5
H24B–C24–H24C	109.5

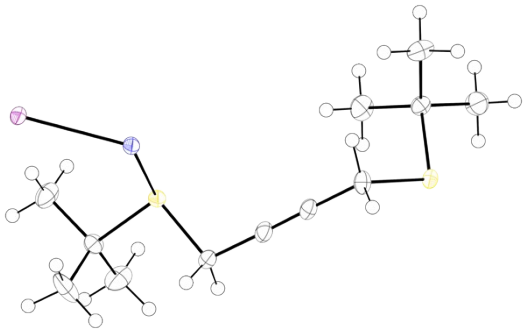
Symmetry transformations used to generate equivalent atoms:
#1: 1-X, 0.5+Y, 1.5-Z; #2: -X, -0.5+Y, 1.5-Z; #3: 1-X, -0.5+Y, 1.5-Z; #4: -X, 0.5+Y, 1.5-Z;

Table S48. Torsion angles for CP5

Atom–Atom–Atom–Atom	Torsion Angle [°]
Cu1–S2–C8–C7	64.1(5)
Cu1–S2–C9–C10	38.4(6)
Cu1–S2–C9–C11	−81.3(5)
Cu1–S2–C9–C12	161.4(4)
Cu2–S3–C13–C14	167.2(4)
Cu2–S3–C13–C15	−71.3(5)
Cu2–S3–C13–C16	48.9(5)
Cu2–S3–C17–C18	−170.3(5)
Cu3$^{\#1}$–S1–C1–C2	−79.3(5)
Cu3$^{\#1}$–S1–C1–C3	40.5(6)
Cu3$^{\#1}$–S1–C1–C4	162.9(5)
Cu3$^{\#1}$–S1–C5–C6	78.2(5)
Cu4$^{\#2}$–S4–C20–C19	153.5(5)
Cu4$^{\#2}$–S4–C21–C22	161.7(4)
Cu4$^{\#2}$–S4–C21–C23	−80.6(5)
Cu4$^{\#2}$–S4–C21–C24	39.2(6)
C1–S1–C5–C6	−166.6(5)
C5–S1–C1–C2	172.5(5)
C5–S1–C1–C3	−67.6(6)
C5–S1–C1–C4	54.7(6)
C8–S2–C9–C10	−71.8(6)
C8–S2–C9–C11	168.5(5)
C8–S2–C9–C12	51.2(6)
C9–S2–C8–C7	−179.9(5)
C13–S3–C17–C18	71.5(6)
C17–S3–C13–C14	−80.6(6)
C17–S3–C13–C15	40.9(6)
C17–S3–C13–C16	161.1(5)
C20–S4–C21–C22	49.5(6)
C20–S4–C21–C23	167.2(5)
C20–S4–C21–C24	−73.0(6)
C21–S4–C20–C19	−88.7(6)

Symmetry transformations used to generate equivalent atoms:
#1: 1-X, -0.5+Y, 1.5-Z; #2: -X, 0.5+Y, 1.5-Z;

Crystal Data and Experimental



Experimental: The data for CP6 were collected from a shock-cooled single crystal at 100.0(1) K on a Bruker D8 Venture four-circle diffractometer with a X-ray tube using a graphite as monochromator and a CPAD PHOTON II area detector detector. The diffractometer was equipped with an Oxford Cryostream 800 low temperature device and used Mo K_{α} radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.38A and a multi-scan absorption correction using SADABS 2016/2 was applied. [1,2] The structure was solved by direct methods with XT and refined by full-matrix least-squares methods against F^2 using SHELXL.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[5] CCDC 2326262 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures. This report and the CIF file were generated using FinalCif.[6]

Table S49. Crystal data and structure refinement for CP6

Internal Reference	CP6
CCDC number	2326262
Empirical formula	$C_{12}H_{22}CuIS_2$
Formula weight	420.85
Temperature [K]	100.0(1)
Crystal system	monoclinic
Space group (number)	$P2_1/c$ (14)
a [Å]	11.4251(3)
b [Å]	16.2605(4)
c [Å]	8.8793(2)
α [°]	90
β [°]	99.6380(10)
γ [°]	90
Volume [Å^3]	1626.29(7)
Z	4
ρ_{calc} [gcm^{-3}]	1.719
μ [mm^{-1}]	3.474
F(000)	832
Crystal size [mm^3]	0.073×0.172×0.268
Crystal colour	clear light colourless
Crystal shape	plate
Radiation	Mo K_{α} (λ=0.71073 Å)
2θ range [°]	4.40 to 54.99 (0.77 Å)
Index ranges	−14 ≤ h ≤ 14 −21 ≤ k ≤ 20 −11 ≤ l ≤ 11
Reflections collected	25701
Independent reflections	3733 R_{int} = 0.0252 R_{sigma} = 0.0155
Completeness to θ = 25.242°	99.9 %
Data / Restraints / Parameters	3733 / 0 / 151
Goodness-of-fit on F^2	1.079
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0176 wR_2 = 0.0430
Final *R* indexes [all data]	R_1 = 0.0190 wR_2 = 0.0438
Largest peak/hole [eÅ^{-3}]	1.29/−0.39

Table S50. Bond lengths and angles for CP6

Atom–Atom	Length [Å]
I1–Cu1	2.6025(3)
I1–Cu1$^{\#1}$	2.7143(3)
Cu1–S1	2.3340(5)
Cu1–S2$^{\#2}$	2.3480(5)
S1–C1	1.849(2)
S1–C5	1.825(2)
S2–C8	1.820(2)
S2–C9	1.856(2)
C1–C2	1.514(3)
C1–C3	1.523(3)
C1–C4	1.525(3)
C2–H2A	0.9800
C2–H2B	0.9800
C2–H2C	0.9800
C3–H3A	0.9800
C3–H3B	0.9800
C3–H3C	0.9800
C4–H4A	0.9800
C4–H4B	0.9800
C4–H4C	0.9800
C5–H5A	0.9900
C5–H5B	0.9900
C5–C6	1.456(3)
C6–C7	1.187(3)
C7–C8	1.458(3)
C8–H8A	0.9900
C8–H8B	0.9900
C9–C10	1.521(3)
C9–C11	1.523(3)
C9–C12	1.524(3)
C10–H10A	0.9800
C10–H10B	0.9800
C10–H10C	0.9800
C11–H11A	0.9800
C11–H11B	0.9800
C11–H11C	0.9800
C12–H12A	0.9800
C12–H12B	0.9800
C12–H12C	0.9800

Atom–Atom–Atom	Angle [°]
Cu1–I1–Cu1$^{\#1}$	79.831(8)
I1–Cu1–I1$^{\#1}$	100.169(8)
S1–Cu1–I1$^{\#1}$	111.540(15)
S1–Cu1–I1	122.422(15)
S1–Cu1–S2$^{\#2}$	97.433(18)
S2$^{\#2}$–Cu1–I1$^{\#1}$	103.435(14)
S2$^{\#2}$–Cu1–I1	120.763(14)
C1–S1–Cu1	114.93(7)
C5–S1–Cu1	102.01(7)
C5–S1–C1	101.68(9)
C8–S2–Cu1$^{\#3}$	106.87(7)
C8–S2–C9	104.15(9)
C9–S2–Cu1$^{\#3}$	113.96(6)
C2–C1–S1	110.96(14)
C2–C1–C3	111.14(19)
C2–C1–C4	111.53(19)
C3–C1–S1	104.09(14)
C3–C1–C4	110.06(17)
C4–C1–S1	108.79(15)
C1–C2–H2A	109.5
C1–C2–H2B	109.5
C1–C2–H2C	109.5
H2A–C2–H2B	109.5
H2A–C2–H2C	109.5
H2B–C2–H2C	109.5
C1–C3–H3A	109.5
C1–C3–H3B	109.5
C1–C3–H3C	109.5
H3A–C3–H3B	109.5
H3A–C3–H3C	109.5
H3B–C3–H3C	109.5
C1–C4–H4A	109.5
C1–C4–H4B	109.5
C1–C4–H4C	109.5
H4A–C4–H4B	109.5
H4A–C4–H4C	109.5
H4B–C4–H4C	109.5
S1–C5–H5A	109.7
S1–C5–H5B	109.7
H5A–C5–H5B	108.2
C6–C5–S1	109.63(14)
C6–C5–H5A	109.7
C6–C5–H5B	109.7
C7–C6–C5	177.2(2)
C6–C7–C8	177.5(2)
S2–C8–H8A	108.8
S2–C8–H8B	108.8
C7–C8–S2	113.79(14)
C7–C8–H8A	108.8
C7–C8–H8B	108.8
H8A–C8–H8B	107.7
C10–C9–S2	111.23(14)
C10–C9–C11	110.86(17)
C10–C9–C12	110.53(18)
C11–C9–S2	109.58(14)
C11–C9–C12	110.53(18)
C12–C9–S2	103.92(14)
C9–C10–H10A	109.5
C9–C10–H10B	109.5
C9–C10–H10C	109.5
H10A–C10–H10B	109.5
H10A–C10–H10C	109.5
H10B–C10–H10C	109.5
C9–C11–H11A	109.5
C9–C11–H11B	109.5
C9–C11–H11C	109.5
H11A–C11–H11B	109.5
H11A–C11–H11C	109.5

H11B–C11–H11C	109.5
C9–C12–H12A	109.5
C9–C12–H12B	109.5
C9–C12–H12C	109.5
H12A–C12–H12B	109.5
H12A–C12–H12C	109.5
H12B–C12–H12C	109.5

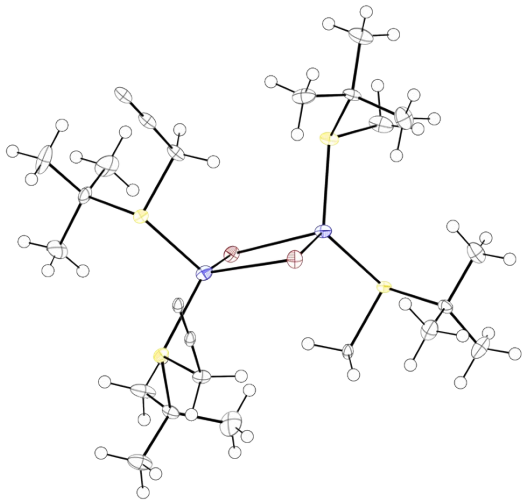
Symmetry transformations used to generate equivalent atoms:
#1: -X, 1-Y, 1-Z; #2: +X, 1.5-Y, -0.5+Z; #3: +X, 1.5-Y, 0.5+Z;

Table S51. Torsion angles for CP6

Atom–Atom–Atom–Atom	Torsion Angle [°]
Cu1–S1–C1–C2	−53.82(17)
Cu1–S1–C1–C3	65.80(15)
Cu1–S1–C1–C4	−176.88(13)
Cu1–S1–C5–C6	−66.17(14)
Cu1$^{\#1}$–S2–C8–C7	−153.53(13)
Cu1$^{\#1}$–S2–C9–C10	−54.08(16)
Cu1$^{\#1}$–S2–C9–C11	−177.01(12)
Cu1$^{\#1}$–S2–C9–C12	64.86(15)
C1–S1–C5–C6	174.89(14)
C5–S1–C1–C2	55.47(18)
C5–S1–C1–C3	175.10(14)
C5–S1–C1–C4	−67.59(16)
C8–S2–C9–C10	61.99(16)
C8–S2–C9–C11	−60.93(16)
C8–S2–C9–C12	−179.07(14)
C9–S2–C8–C7	85.53(16)

Symmetry transformations used to generate equivalent atoms:
#1: +X, 1.5-Y, 0.5+Z;

Crystal Data and Experimental



Experimental: The data for CP7 were collected from a shock-cooled single crystal at 115.00 K on a Nonius Kappa Apex II \k-geometry diffractometer with a X-ray tube using a graphite as monochromator and an APEX2 detector. The diffractometer was equipped with an Oxford Cryostream 600 low temperature device and used Mo K_{α} radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.27B and a multi-scan absorption correction using SADABS unknown version was applied. [1,2] The structure was solved by direct methods with SHELXS, and refined by full-matrix least-squares methods against F^2 using SHELXL.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[5] CCDC 2326263 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures. This report and the CIF file were generated using FinalCif.[6]

Table S52. Crystal data and structure refinement for CP7

Internal Reference	CP7
CCDC number	2326263
Empirical formula	$C_{24}H_{44}Br_2Cu_2S_4$
Formula weight	747.73
Temperature [K]	115.00
Crystal system	monoclinic
Space group (number)	$P2_1$ (4)
a [Å]	8.7637(14)
b [Å]	15.977(2)
c [Å]	11.262(2)
α [°]	90
β [°]	97.425(5)
γ [°]	90
Volume [Å^3]	1563.7(4)
Z	2
ρ_{calc} [gcm^{-3}]	1.588
μ [mm^{-1}]	4.194
F(000)	760
Crystal size [mm^3]	0.05×0.1×0.1
Crystal colour	clear light colourless
Crystal shape	needle
Radiation	Mo K_{α} (λ=0.71073 Å)
2θ range [°]	4.69 to 55.06 (0.77 Å)
Index ranges	−11 ≤ h ≤ 10 −20 ≤ k ≤ 19 −12 ≤ l ≤ 14
Reflections collected	11046
Independent reflections	6598 R_{int} = 0.0465 R_{sigma} = 0.1257
Completeness to θ = 25.242°	99.6 %
Data / Restraints / Parameters	6598 / 1 / 278
Goodness-of-fit on F^2	0.974
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0538 wR_2 = 0.0609
Final *R* indexes [all data]	R_1 = 0.0964 wR_2 = 0.0694
Largest peak/hole [eÅ^{-3}]	0.75/−0.77
Flack X parameter	0.437(14)

Refinement details for CP7

Refined as a 2-component inversion twin.

Table S53. Bond lengths and angles for CP7

Atom–Atom	Length [Å]
Br1–Cu1	2.5273(19)
Br1–Cu2	2.4573(16)
Br2–Cu1	2.4410(15)
Br2–Cu2	2.6106(19)
Cu1–S1	2.330(3)
Cu1–S2	2.341(3)
Cu2–S3	2.295(2)
Cu2–S4	2.319(3)
S1–C1	1.842(9)
S1–C5	1.834(8)
S2–C8	1.846(12)
S2–C12	1.821(10)
S3–C15	1.812(9)
S3–C16	1.844(10)
S4–C20	1.818(10)
S4–C21	1.848(12)
C1–C2	1.529(11)
C1–C3	1.515(15)
C1–C4	1.506(14)
C2–H2A	0.9800
C2–H2B	0.9800
C2–H2C	0.9800
C3–H3A	0.9800
C3–H3B	0.9800
C3–H3C	0.9800
C4–H4A	0.9800
C4–H4B	0.9800
C4–H4C	0.9800
C5–H5A	0.9900
C5–H5B	0.9900
C5–C6	1.450(11)
C6–C7	1.187(11)
C7–C20$^{\#1}$	1.452(12)
C8–C9	1.536(14)
C8–C10	1.528(15)
C8–C11	1.522(14)
C9–H9A	0.9800
C9–H9B	0.9800
C9–H9C	0.9800
C10–H10A	0.9800
C10–H10B	0.9800
C10–H10C	0.9800
C11–H11A	0.9800
C11–H11B	0.9800
C11–H11C	0.9800
C12–H12A	0.9900
C12–H12B	0.9900
C12–C13	1.481(13)
C13–C14	1.159(11)
C14–C15$^{\#2}$	1.471(11)
C15–H15A	0.9900
C15–H15B	0.9900
C16–C17	1.546(16)
C16–C18	1.519(12)
C16–C19	1.528(13)
C17–H17A	0.9800
C17–H17B	0.9800
C17–H17C	0.9800
C18–H18A	0.9800
C18–H18B	0.9800
C18–H18C	0.9800
C19–H19A	0.9800
C19–H19B	0.9800
C19–H19C	0.9800
C20–H20A	0.9900
C20–H20B	0.9900
C21–C22	1.520(13)
C21–C23	1.525(13)
C21–C24	1.517(13)
C22–H22A	0.9800
C22–H22B	0.9800
C22–H22C	0.9800
C23–H23A	0.9800
C23–H23B	0.9800
C23–H23C	0.9800
C24–H24A	0.9800
C24–H24B	0.9800
C24–H24C	0.9800

Atom–Atom–Atom	Angle [°]
Cu2–Br1–Cu1	81.46(6)
Cu1–Br2–Cu2	80.09(5)
Br2–Cu1–Br1	100.37(6)
S1–Cu1–Br1	112.85(8)
S1–Cu1–Br2	121.56(7)
S1–Cu1–S2	95.09(9)
S2–Cu1–Br1	106.13(9)
S2–Cu1–Br2	120.61(9)
Br1–Cu2–Br2	97.68(6)
S3–Cu2–Br1	117.50(8)
S3–Cu2–Br2	100.04(9)
S3–Cu2–S4	115.95(10)
S4–Cu2–Br1	118.56(9)
S4–Cu2–Br2	100.78(9)
C1–S1–Cu1	114.8(3)
C5–S1–Cu1	101.7(3)
C5–S1–C1	103.3(4)
C8–S2–Cu1	111.2(3)
C12–S2–Cu1	107.7(3)
C12–S2–C8	105.2(5)
C15–S3–Cu2	111.4(3)

C15–S3–C16	101.4(4)	C8–C11–H11C	109.5
C16–S3–Cu2	116.6(3)	H11A–C11–H11B	109.5
C20–S4–Cu2	104.9(3)	H11A–C11–H11C	109.5
C20–S4–C21	103.9(5)	H11B–C11–H11C	109.5
C21–S4–Cu2	113.7(3)	S2–C12–H12A	108.9
C2–C1–S1	108.4(6)	S2–C12–H12B	108.9
C3–C1–S1	103.3(7)	H12A–C12–H12B	107.7
C3–C1–C2	109.4(9)	C13–C12–S2	113.5(7)
C4–C1–S1	111.1(7)	C13–C12–H12A	108.9
C4–C1–C2	111.9(9)	C13–C12–H12B	108.9
C4–C1–C3	112.3(8)	C14–C13–C12	177.5(11)
C1–C2–H2A	109.5	C13–C14–C15$^{\#2}$	177.2(11)
C1–C2–H2B	109.5	S3–C15–H15A	109.2
C1–C2–H2C	109.5	S3–C15–H15B	109.2
H2A–C2–H2B	109.5	C14$^{\#3}$–C15–S3	111.9(7)
H2A–C2–H2C	109.5	C14$^{\#3}$–C15–H15A	109.2
H2B–C2–H2C	109.5	C14$^{\#3}$–C15–H15B	109.2
C1–C3–H3A	109.5	H15A–C15–H15B	107.9
C1–C3–H3B	109.5	C17–C16–S3	111.3(7)
C1–C3–H3C	109.5	C18–C16–S3	110.6(7)
H3A–C3–H3B	109.5	C18–C16–C17	111.6(9)
H3A–C3–H3C	109.5	C18–C16–C19	109.7(8)
H3B–C3–H3C	109.5	C19–C16–S3	103.9(7)
C1–C4–H4A	109.5	C19–C16–C17	109.4(8)
C1–C4–H4B	109.5	C16–C17–H17A	109.5
C1–C4–H4C	109.5	C16–C17–H17B	109.5
H4A–C4–H4B	109.5	C16–C17–H17C	109.5
H4A–C4–H4C	109.5	H17A–C17–H17B	109.5
H4B–C4–H4C	109.5	H17A–C17–H17C	109.5
S1–C5–H5A	110.1	H17B–C17–H17C	109.5
S1–C5–H5B	110.1	C16–C18–H18A	109.5
H5A–C5–H5B	108.4	C16–C18–H18B	109.5
C6–C5–S1	107.9(6)	C16–C18–H18C	109.5
C6–C5–H5A	110.1	H18A–C18–H18B	109.5
C6–C5–H5B	110.1	H18A–C18–H18C	109.5
C7–C6–C5	174.3(9)	H18B–C18–H18C	109.5
C6–C7–C20$^{\#1}$	177.2(10)	C16–C19–H19A	109.5
C9–C8–S2	104.4(7)	C16–C19–H19B	109.5
C10–C8–S2	109.2(8)	C16–C19–H19C	109.5
C10–C8–C9	109.8(10)	H19A–C19–H19B	109.5
C11–C8–S2	111.8(8)	H19A–C19–H19C	109.5
C11–C8–C9	109.6(9)	H19B–C19–H19C	109.5
C11–C8–C10	111.7(10)	S4–C20–H20A	108.6
C8–C9–H9A	109.5	S4–C20–H20B	108.6
C8–C9–H9B	109.5	C7$^{\#4}$–C20–S4	114.5(6)
C8–C9–H9C	109.5	C7$^{\#4}$–C20–H20A	108.6
H9A–C9–H9B	109.5	C7$^{\#4}$–C20–H20B	108.6
H9A–C9–H9C	109.5	H20A–C20–H20B	107.6
H9B–C9–H9C	109.5	C22–C21–S4	110.8(8)
C8–C10–H10A	109.5	C22–C21–C23	110.2(9)
C8–C10–H10B	109.5	C23–C21–S4	111.3(8)
C8–C10–H10C	109.5	C24–C21–S4	103.7(7)
H10A–C10–H10B	109.5	C24–C21–C22	110.3(10)
H10A–C10–H10C	109.5	C24–C21–C23	110.4(9)
H10B–C10–H10C	109.5	C21–C22–H22A	109.5
C8–C11–H11A	109.5	C21–C22–H22B	109.5
C8–C11–H11B	109.5	C21–C22–H22C	109.5

H22A–C22–H22B	109.5
H22A–C22–H22C	109.5
H22B–C22–H22C	109.5
C21–C23–H23A	109.5
C21–C23–H23B	109.5
C21–C23–H23C	109.5
H23A–C23–H23B	109.5
H23A–C23–H23C	109.5
H23B–C23–H23C	109.5
C21–C24–H24A	109.5
C21–C24–H24B	109.5
C21–C24–H24C	109.5
H24A–C24–H24B	109.5
H24A–C24–H24C	109.5
H24B–C24–H24C	109.5

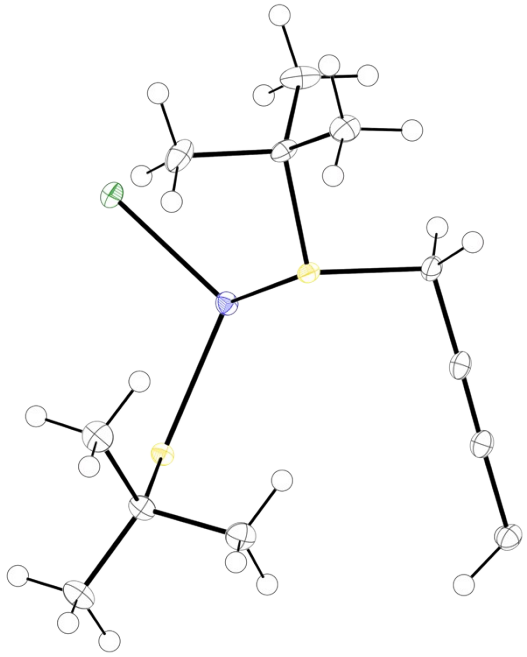
Symmetry transformations used to generate equivalent atoms:
#1: 1-X, 0.5+Y, 1-Z; #2: 2-X, 0.5+Y, 1-Z; #3: 2-X, -0.5+Y, 1-Z;
#4: 1-X, -0.5+Y, 1-Z;

Table S54. Torsion angles for CP7

Atom–Atom–Atom–Atom	Torsion Angle [°]
Cu1–S1–C1–C2	−179.7(6)
Cu1–S1–C1–C3	−63.7(8)
Cu1–S1–C1–C4	56.9(8)
Cu1–S1–C5–C6	69.3(6)
Cu1–S2–C8–C9	61.2(7)
Cu1–S2–C8–C10	178.6(7)
Cu1–S2–C8–C11	−57.2(8)
Cu1–S2–C12–C13	−161.9(7)
Cu2–S3–C15–C14$^{\#1}$	47.7(8)
Cu2–S3–C16–C17	48.1(8)
Cu2–S3–C16–C18	172.8(6)
Cu2–S3–C16–C19	−69.5(7)
Cu2–S4–C20–C7$^{\#2}$	152.3(7)
Cu2–S4–C21–C22	174.0(7)
Cu2–S4–C21–C23	51.0(8)
Cu2–S4–C21–C24	−67.7(7)
C1–S1–C5–C6	−171.4(7)
C5–S1–C1–C2	70.4(8)
C5–S1–C1–C3	−173.6(7)
C5–S1–C1–C4	−53.0(8)
C8–S2–C12–C13	79.3(8)
C12–S2–C8–C9	177.6(7)
C12–S2–C8–C10	−65.0(9)
C12–S2–C8–C11	59.1(9)
C15–S3–C16–C17	−73.0(8)
C15–S3–C16–C18	51.7(8)
C15–S3–C16–C19	169.3(6)
C16–S3–C15–C14$^{\#1}$	172.4(7)
C20–S4–C21–C22	60.6(9)
C20–S4–C21–C23	−62.4(8)
C20–S4–C21–C24	178.9(6)
C21–S4–C20–C7$^{\#2}$	−88.1(8)

Symmetry transformations used to generate equivalent atoms:
#1: 2-X, -0.5+Y, 1-Z; #2: 1-X, -0.5+Y, 1-Z;

Crystal Data and Experimental



Experimental: The material was recrystallised from acetonitrile by slow evaporation. The data for CP8 were collected from a shock-cooled single crystal at 100.0(1) K on a Bruker D8 VENTURE \k-geometry diffractometer with a X-ray tube using a graphite as monochromator and a Photon 100 detector. The diffractometer was equipped with an Oxford Cryostream 800 low temperature device and used Mo K_{α} radiation (λ = 0.71073 Å). All data were integrated with SAINT v8.34A and a numerical absorption correction using SADABS 2012/1 was applied. [1,2] The structure was solved by direct methods with SUPERFLIP[8] and refined by full-matrix least-squares methods against F^2 using SHELXL.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[5] CCDC 2326264 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures. This report and the CIF file were generated using FinalCif.[6]

Table S55. Crystal data and structure refinement for CP8

Internal Reference	CP8
CCDC number	2326264
Empirical formula	$C_{12}H_{22}ClCuS_2$
Formula weight	329.40
Temperature [K]	100.0(1)
Crystal system	monoclinic
Space group (number)	$P2_1/c$ (14)
a [Å]	12.0784(5)
b [Å]	9.6471(4)
c [Å]	13.6377(5)
α [°]	90
β [°]	107.3257(12)
γ [°]	90
Volume [Å^3]	1516.98(11)
Z	4
ρ_{calc} [gcm^{-3}]	1.442
μ [mm^{-1}]	1.865
F(000)	688
Crystal size [mm^3]	0.16×0.18×0.32
Crystal colour	clear light colourless
Crystal shape	prism
Radiation	Mo K_{α} (λ=0.71073 Å)
2θ range [°]	5.79 to 55.04 (0.77 Å)
Index ranges	−15 ≤ h ≤ 15 −12 ≤ k ≤ 12 −17 ≤ l ≤ 17
Reflections collected	43880
Independent reflections	3493 R_{int} = 0.0497 R_{sigma} = 0.0189
Completeness to θ = 26.000°	99.9 %
Data / Restraints / Parameters	3493 / 0 / 151
Goodness-of-fit on F^2	1.077
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0208 wR_2 = 0.0441
Final *R* indexes [all data]	R_1 = 0.0290 wR_2 = 0.0470
Largest peak/hole [eÅ^{-3}]	0.35/−0.25

Table S56. Bond lengths and angles for CP8

Atom–Atom	Length [Å]
C1–H1A	0.9900
C1–H1B	0.9900
C1–C2	1.463(2)
C1–S2$^{\#1}$	1.8329(15)
C2–C3	1.193(2)
C3–C4	1.462(2)
C4–H4A	0.9900
C4–H4B	0.9900
C4–S1	1.8280(15)
C5–C6	1.521(2)
C5–C7	1.529(2)
C5–C8	1.529(2)
C5–S1	1.8551(15)
C6–H6A	0.9800
C6–H6B	0.9800
C6–H6C	0.9800
C7–H7A	0.9800
C7–H7B	0.9800
C7–H7C	0.9800
C8–H8A	0.9800
C8–H8B	0.9800
C8–H8C	0.9800
C9–C10	1.527(2)
C9–C11	1.524(2)
C9–C12	1.528(2)
C9–S2	1.8564(15)
C10–H10A	0.9800
C10–H10B	0.9800
C10–H10C	0.9800
C11–H11A	0.9800
C11–H11B	0.9800
C11–H11C	0.9800
C12–H12A	0.9800
C12–H12B	0.9800
C12–H12C	0.9800
S1–Cu1	2.2858(4)
S2–Cu1	2.3202(4)
Cl1–Cu1	2.3526(4)
Cl1–Cu1$^{\#2}$	2.4187(4)

Atom–Atom–Atom	Angle [°]
H1A–C1–H1B	107.7
C2–C1–H1A	108.8
C2–C1–H1B	108.8
C2–C1–S2$^{\#1}$	113.86(11)
S2$^{\#1}$–C1–H1A	108.8
S2$^{\#1}$–C1–H1B	108.8
C3–C2–C1	174.91(16)
C2–C3–C4	177.12(16)
C3–C4–H4A	110.2
C3–C4–H4B	110.2
C3–C4–S1	107.47(10)
H4A–C4–H4B	108.5
S1–C4–H4A	110.2
S1–C4–H4B	110.2
C6–C5–C7	110.52(13)
C6–C5–C8	111.53(13)
C6–C5–S1	111.31(10)
C7–C5–C8	110.16(12)
C7–C5–S1	110.14(10)
C8–C5–S1	102.96(10)
C5–C6–H6A	109.5
C5–C6–H6B	109.5
C5–C6–H6C	109.5
H6A–C6–H6B	109.5
H6A–C6–H6C	109.5
H6B–C6–H6C	109.5
C5–C7–H7A	109.5
C5–C7–H7B	109.5
C5–C7–H7C	109.5
H7A–C7–H7B	109.5
H7A–C7–H7C	109.5
H7B–C7–H7C	109.5
C5–C8–H8A	109.5
C5–C8–H8B	109.5
C5–C8–H8C	109.5
H8A–C8–H8B	109.5
H8A–C8–H8C	109.5
H8B–C8–H8C	109.5
C10–C9–C12	110.08(13)
C10–C9–S2	111.40(11)
C11–C9–C10	110.25(12)
C11–C9–C12	110.66(13)
C11–C9–S2	109.52(10)
C12–C9–S2	104.81(10)
C9–C10–H10A	109.5
C9–C10–H10B	109.5
C9–C10–H10C	109.5
H10A–C10–H10B	109.5
H10A–C10–H10C	109.5
H10B–C10–H10C	109.5
C9–C11–H11A	109.5
C9–C11–H11B	109.5
C9–C11–H11C	109.5
H11A–C11–H11B	109.5
H11A–C11–H11C	109.5
H11B–C11–H11C	109.5
C9–C12–H12A	109.5
C9–C12–H12B	109.5
C9–C12–H12C	109.5
H12A–C12–H12B	109.5
H12A–C12–H12C	109.5
H12B–C12–H12C	109.5
C4–S1–C5	104.48(7)
C4–S1–Cu1	103.04(5)
C5–S1–Cu1	110.86(5)
C1$^{\#2}$–S2–C9	102.74(7)
C1$^{\#2}$–S2–Cu1	103.89(5)
C9–S2–Cu1	111.30(5)

Cu1–Cl1–Cu1$^{\#3}$	84.002(13)
S1–Cu1–S2	115.936(15)
S1–Cu1–Cl1$^{\#3}$	108.905(14)
S1–Cu1–Cl1	119.605(14)
S2–Cu1–Cl1	107.532(14)
S2–Cu1–Cl1$^{\#3}$	106.340(14)
Cl1–Cu1–Cl1$^{\#3}$	95.998(13)

Symmetry transformations used to generate equivalent atoms:
#1: +X, -0.5-Y, 0.5+Z; #2: +X, -0.5-Y, -0.5+Z; #3: 1-X, -Y, 1-Z;

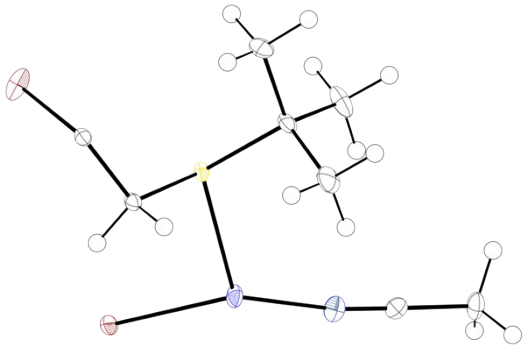
Table S57. Torsion angles for CP8

Atom–Atom–Atom–Atom	Torsion Angle [°]
C3–C4–S1–C5	172.29(10)
C3–C4–S1–Cu1	−71.78(10)
C6–C5–S1–C4	57.86(12)
C6–C5–S1–Cu1	−52.49(12)
C7–C5–S1–C4	−65.09(12)
C7–C5–S1–Cu1	−175.44(9)
C8–C5–S1–C4	177.46(10)
C8–C5–S1–Cu1	67.11(10)
C10–C9–S2–C1$^{\#1}$	−66.62(12)
C10–C9–S2–Cu1	44.01(11)
C11–C9–S2–C1$^{\#1}$	55.62(12)
C11–C9–S2–Cu1	166.25(9)
C12–C9–S2–C1$^{\#1}$	174.36(10)
C12–C9–S2–Cu1	−75.00(10)

Symmetry transformations used to generate equivalent atoms:
#1: +X, -0.5-Y, -0.5+Z;

Crystal structure of CP9

Crystal Data and Experimental



Experimental: The data for CP9 were collected from a shock-cooled single crystal at 100.0(1) K on a Bruker D8 VENTURE area detector four-circle diffractometer with a X-ray tube using a graphite as monochromator and a CPAD PHOTON II area detector detector. The diffractometer used Mo K_{α} radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.38A and a multi-scan absorption correction using SADABS 2016/2 was applied. [1,2] The structure was solved by direct methods with XT and refined by full-matrix least-squares methods against F^2 using SHELXL.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[5] CCDC 2326265 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures. This report and the CIF file were generated using FinalCif.[6]

Table S58. Crystal data and structure refinement for CP9

Internal Reference	CP9
CCDC number	2326265
Empirical formula	$C_8H_{14}Br_2CuNS$
Formula weight	379.62
Temperature [K]	100.0(1)
Crystal system	monoclinic
Space group (number)	$P2_1/n$ (14)
a [Å]	8.1661(4)
b [Å]	10.2416(5)
c [Å]	15.1301(6)
α [°]	90
β [°]	98.034(2)
γ [°]	90
Volume [Å^3]	1252.97(10)
Z	4
ρ_{calc} [gcm^{-3}]	2.012
μ [mm^{-1}]	8.247
F(000)	736
Crystal size [mm^3]	0.192×0.334×0.436
Crystal colour	clear light colourless
Crystal shape	block
Radiation	Mo K_{α} (λ=0.71073 Å)
2θ range [°]	4.82 to 55.00 (0.77 Å)
Index ranges	−9 ≤ h ≤ 10 −10 ≤ k ≤ 13 −19 ≤ l ≤ 19
Reflections collected	10454
Independent reflections	2860 R_{int} = 0.0354 R_{sigma} = 0.0369
Completeness to θ = 25.242°	99.6 %
Data / Restraints / Parameters	2860 / 0 / 122
Goodness-of-fit on F^2	1.062
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0258 wR_2 = 0.0554
Final *R* indexes [all data]	R_1 = 0.0308 wR_2 = 0.0576
Largest peak/hole [eÅ^{-3}]	0.54/−0.91

Table S59. Bond lengths and angles for CP9

Atom–Atom	Length [Å]
Br1–Cu1	2.4888(4)
Br1–Cu1$^{\#1}$	2.5469(4)
Br2–C8	1.912(2)
Cu1–Cu1$^{\#1}$	3.0534(7)
Cu1–S1	2.3112(7)
Cu1–N1	1.950(2)
S1–C3	1.851(2)
S1–C7	1.815(3)
N1–C2	1.140(3)
C1–H1A	0.9800
C1–H1B	0.9800
C1–H1C	0.9800
C1–C2	1.455(3)
C3–C4	1.529(4)
C3–C5	1.517(4)
C3–C6	1.521(4)
C4–H4A	0.9800
C4–H4B	0.9800
C4–H4C	0.9800
C5–H5A	0.9800
C5–H5B	0.9800
C5–H5C	0.9800
C6–H6A	0.9800
C6–H6B	0.9800
C6–H6C	0.9800
C7–H7A	0.9900
C7–H7B	0.9900
C7–C8	1.496(4)
C8–C8$^{\#2}$	1.331(5)

Atom–Atom–Atom	Angle [°]
Cu1–Br1–Cu1$^{\#1}$	74.643(14)
Br1–Cu1–Br1$^{\#1}$	105.358(14)
Br1–Cu1–Cu1$^{\#1}$	53.545(11)
Br1$^{\#1}$–Cu1–Cu1$^{\#1}$	51.813(11)
S1–Cu1–Br1$^{\#1}$	106.83(2)
S1–Cu1–Br1	98.269(19)
S1–Cu1–Cu1$^{\#1}$	111.02(2)
N1–Cu1–Br1	117.45(7)
N1–Cu1–Br1$^{\#1}$	108.95(7)
N1–Cu1–Cu1$^{\#1}$	130.28(8)
N1–Cu1–S1	118.67(8)
C3–S1–Cu1	111.46(9)
C7–S1–Cu1	98.55(9)
C7–S1–C3	107.05(12)
C2–N1–Cu1	170.8(2)
H1A–C1–H1B	109.5
H1A–C1–H1C	109.5
H1B–C1–H1C	109.5
C2–C1–H1A	109.5
C2–C1–H1B	109.5
C2–C1–H1C	109.5
N1–C2–C1	179.0(3)
C4–C3–S1	102.74(18)
C5–C3–S1	111.38(18)
C5–C3–C4	111.2(2)
C5–C3–C6	110.6(2)
C6–C3–S1	110.88(18)
C6–C3–C4	109.9(2)
C3–C4–H4A	109.5
C3–C4–H4B	109.5
C3–C4–H4C	109.5
H4A–C4–H4B	109.5
H4A–C4–H4C	109.5
H4B–C4–H4C	109.5
C3–C5–H5A	109.5
C3–C5–H5B	109.5
C3–C5–H5C	109.5
H5A–C5–H5B	109.5
H5A–C5–H5C	109.5
H5B–C5–H5C	109.5
C3–C6–H6A	109.5
C3–C6–H6B	109.5
C3–C6–H6C	109.5
H6A–C6–H6B	109.5
H6A–C6–H6C	109.5
H6B–C6–H6C	109.5
S1–C7–H7A	108.3
S1–C7–H7B	108.3
H7A–C7–H7B	107.4
C8–C7–S1	116.02(18)
C8–C7–H7A	108.3
C8–C7–H7B	108.3
C7–C8–Br2	113.09(18)
C8$^{\#2}$–C8–Br2	118.0(3)
C8$^{\#2}$–C8–C7	128.8(3)

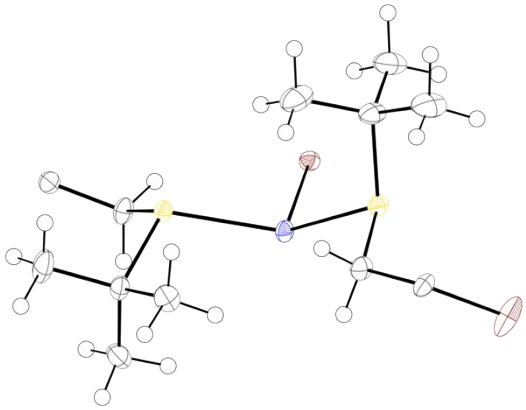
Symmetry transformations used to generate equivalent atoms:
#1: -X, 1-Y, 1-Z; #2: -X, 2-Y, 1-Z;

Table S60. Torsion angles for CP9

Atom–Atom–Atom–Atom	Torsion Angle [°]
Cu1–S1–C3–C4	72.23(19)
Cu1–S1–C3–C5	−46.9(2)
Cu1–S1–C3–C6	−170.42(17)
Cu1–S1–C7–C8	−166.95(16)
S1–C7–C8–Br2	59.1(2)
S1–C7–C8–C8$^{\#1}$	−124.8(3)
C3–S1–C7–C8	77.4(2)
C7–S1–C3–C4	178.94(19)
C7–S1–C3–C5	59.9(2)
C7–S1–C3–C6	−63.7(2)

Symmetry transformations used to generate equivalent atoms:
#1: -X, 2-Y, 1-Z;

Crystal Data and Experimental



Experimental: The data for CP10 were collected from a shock-cooled single crystal at 100.0(1) K on a Bruker D8 VENTURE area detector four-circle diffractometer with a X-ray tube using a graphite as monochromator and a CPAD PHOTON II area detector detector. The diffractometer was equipped with an Oxford Cryostream 800 low temperature device and used Mo K_{α} radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.40B and a multi-scan absorption correction using SADABS 2016/2 was applied. [1,2] The structure was solved by direct methods with XT and refined by full-matrix least-squares methods against F^2 using SHELXL.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[5] CCDC 2326266 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures. This report and the CIF file were generated using FinalCif.[6]

Table S61. Crystal data and structure refinement for CP10

Internal Reference	CP10
CCDC number	2326266
Empirical formula	$C_{12}H_{22}Br_2CuS_2$
Formula weight	453.77
Temperature [K]	100.0(1)
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	9.1382(11)
b [Å]	9.9911(8)
c [Å]	11.2700(10)
α [°]	65.156(4)
β [°]	70.131(4)
γ [°]	84.401(5)
Volume [Å^3]	876.92(15)
Z	2
ρ_{calc} [gcm^{-3}]	1.719
μ [mm^{-1}]	6.020
F(000)	450
Crystal size [mm^3]	0.138×0.263×0.508
Crystal colour	clear light colourless
Crystal shape	plate
Radiation	Mo K_{α} (λ=0.71073 Å)
2θ range [°]	4.22 to 55.00 (0.77 Å)
Index ranges	$-11 \le h \le 11$ $-12 \le k \le 12$ $-14 \le l \le 14$
Reflections collected	33300
Independent reflections	4027 R_{int} = 0.0286 R_{sigma} = 0.0154
Completeness to θ = 25.242°	99.9 %
Data / Restraints / Parameters	4027 / 0 / 160
Goodness-of-fit on F^2	1.048
Final *R* indexes [$I \ge 2\sigma(I)$]	R_1 = 0.0197 wR_2 = 0.0470
Final *R* indexes [all data]	R_1 = 0.0216 wR_2 = 0.0479
Largest peak/hole [eÅ^{-3}]	1.50/−0.80

Table S62. Bond lengths and angles for CP10

Atom–Atom	Length [Å]
Br1–C6	1.9041(19)
Br2–Cu1	2.4692(4)
Br2–Cu1$^{\#1}$	2.5405(4)
Cu1–Cu1$^{\#1}$	2.8474(5)
Cu1–S1	2.3225(5)
Cu1–S2	2.2924(5)
S1–C1	1.850(2)
S1–C5	1.817(2)
S2–C7	1.855(2)
S2–C11	1.8301(19)
C1–C2	1.525(3)
C1–C3	1.527(3)
C1–C4	1.528(3)
C2–H2A	0.9800
C2–H2B	0.9800
C2–H2C	0.9800
C3–H3A	0.9800
C3–H3B	0.9800
C3–H3C	0.9800
C4–H4A	0.9800
C4–H4B	0.9800
C4–H4C	0.9800
C5–H5A	0.9900
C5–H5B	0.9900
C5–C6	1.495(3)
C6–C6$^{\#2}$	1.329(4)
C7–C8	1.528(3)
C7–C9	1.529(3)
C7–C10	1.521(3)
C8–H8A	0.9800
C8–H8B	0.9800
C8–H8C	0.9800
C9–H9A	0.9800
C9–H9B	0.9800
C9–H9C	0.9800
C10–H10A	0.9800
C10–H10B	0.9800
C10–H10C	0.9800
C11–H11A	0.9900
C11–H11B	0.9900
C11–C12	1.466(3)
C12–C12$^{\#3}$	1.192(4)

Atom–Atom–Atom	Angle [°]
Cu1–Br2–Cu1$^{\#1}$	69.258(12)
Br2–Cu1–Br2$^{\#1}$	110.741(12)
Br2–Cu1–Cu1$^{\#1}$	56.551(11)
Br2$^{\#1}$–Cu1–Cu1$^{\#1}$	54.190(11)
S1–Cu1–Br2$^{\#1}$	93.070(15)
S1–Cu1–Br2	106.402(16)
S1–Cu1–Cu1$^{\#1}$	107.015(17)
S2–Cu1–Br2	102.124(16)
S2–Cu1–Br2$^{\#1}$	116.851(16)
S2–Cu1–Cu1$^{\#1}$	125.813(18)
S2–Cu1–S1	127.17(2)
C1–S1–Cu1	113.79(7)
C5–S1–Cu1	102.63(6)
C5–S1–C1	105.99(10)
C7–S2–Cu1	111.40(6)
C11–S2–Cu1	105.48(6)
C11–S2–C7	105.47(9)
C2–C1–S1	111.15(15)
C2–C1–C3	110.87(19)
C2–C1–C4	110.8(2)
C3–C1–S1	103.42(15)
C3–C1–C4	110.4(2)
C4–C1–S1	109.97(15)
C1–C2–H2A	109.5
C1–C2–H2B	109.5
C1–C2–H2C	109.5
H2A–C2–H2B	109.5
H2A–C2–H2C	109.5
H2B–C2–H2C	109.5
C1–C3–H3A	109.5
C1–C3–H3B	109.5
C1–C3–H3C	109.5
H3A–C3–H3B	109.5
H3A–C3–H3C	109.5
H3B–C3–H3C	109.5
C1–C4–H4A	109.5
C1–C4–H4B	109.5
C1–C4–H4C	109.5
H4A–C4–H4B	109.5
H4A–C4–H4C	109.5
H4B–C4–H4C	109.5
S1–C5–H5A	108.1
S1–C5–H5B	108.1
H5A–C5–H5B	107.3
C6–C5–S1	116.85(15)
C6–C5–H5A	108.1
C6–C5–H5B	108.1
C5–C6–Br1	113.19(14)
C6$^{\#2}$–C6–Br1	118.3(2)
C6$^{\#2}$–C6–C5	128.3(2)
C8–C7–S2	109.55(14)
C8–C7–C9	109.86(17)
C9–C7–S2	103.68(13)
C10–C7–S2	111.46(14)
C10–C7–C8	111.09(18)
C10–C7–C9	110.96(17)
C7–C8–H8A	109.5
C7–C8–H8B	109.5
C7–C8–H8C	109.5
H8A–C8–H8B	109.5
H8A–C8–H8C	109.5
H8B–C8–H8C	109.5
C7–C9–H9A	109.5
C7–C9–H9B	109.5
C7–C9–H9C	109.5

H9A–C9–H9B	109.5
H9A–C9–H9C	109.5
H9B–C9–H9C	109.5
C7–C10–H10A	109.5
C7–C10–H10B	109.5
C7–C10–H10C	109.5
H10A–C10–H10B	109.5
H10A–C10–H10C	109.5
H10B–C10–H10C	109.5
S2–C11–H11A	108.6
S2–C11–H11B	108.6
H11A–C11–H11B	107.6
C12–C11–S2	114.54(14)
C12–C11–H11A	108.6
C12–C11–H11B	108.6
C12$^{\#3}$–C12–C11	178.0(3)

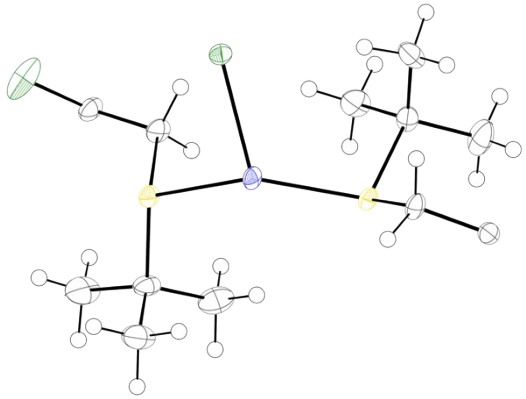
Symmetry transformations used to generate equivalent atoms:
#1: 1-X, 1-Y, 1-Z; #2: -X, 1-Y, 2-Z; #3: 1-X, 2-Y, -Z;

Table S63. Torsion angles for CP10

Atom–Atom–Atom–Atom	Torsion Angle [°]
Cu1–S1–C1–C2	48.80(17)
Cu1–S1–C1–C3	−70.22(15)
Cu1–S1–C1–C4	171.84(16)
Cu1–S1–C5–C6	159.03(13)
Cu1–S2–C7–C8	169.48(13)
Cu1–S2–C7–C9	52.25(14)
Cu1–S2–C7–C10	−67.17(14)
Cu1–S2–C11–C12	−166.58(13)
S1–C5–C6–Br1	−52.91(18)
S1–C5–C6–C6$^{\#1}$	132.3(3)
C1–S1–C5–C6	−81.35(16)
C5–S1–C1–C2	−63.22(17)
C5–S1–C1–C3	177.76(14)
C5–S1–C1–C4	59.8(2)
C7–S2–C11–C12	75.42(16)
C11–S2–C7–C8	−76.57(16)
C11–S2–C7–C9	166.20(13)
C11–S2–C7–C10	46.78(16)

Symmetry transformations used to generate equivalent atoms:
#1: -X, 1-Y, 2-Z;

Crystal Data and Experimental



Experimental: The data for CP11 were collected from a shock-cooled single crystal at 115.0(1) K on a Nonius Kappa Apex II \k-geometry diffractometer with a X-ray tube using a graphite as monochromator and an APEX2 detector. The diffractometer was equipped with an Oxford Cryostream 600 low temperature device and used Mo $K_{\alpha 1}$ radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.27B and a multi-scan absorption correction using SADABS unknown version was applied. [1,2] The structure was solved by direct methods with SHELXS-97, and refined by full-matrix least-squares methods against F^2 using SHELXL.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[5] CCDC 2326267 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures. This report and the CIF file were generated using FinalCif.[6]

Table S64. Crystal data and structure refinement for CP11

Internal Reference	CP11
CCDC number	2326267
Empirical formula	$C_{12}H_{22}Cl_2CuS_2$
Formula weight	364.85
Temperature [K]	115.0(1)
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	8.7545(14)
b [Å]	10.0042(15)
c [Å]	11.2498(15)
α [°]	64.220(6)
β [°]	70.764(6)
γ [°]	82.779(7)
Volume [Å^3]	837.5(2)
Z	2
ρ_{calc} [gcm^{-3}]	1.447
μ [mm^{-1}]	1.851
F(000)	378
Crystal size [mm^3]	0.1×0.15×0.2
Crystal colour	clear light colourless
Crystal shape	prism
Radiation	Mo $K_{\alpha 1}$ (λ=0.71073 Å)
2θ range [°]	6.62 to 55.35 (0.77 Å)
Index ranges	−11 ≤ h ≤ 11 −13 ≤ k ≤ 12 −14 ≤ l ≤ 14
Reflections collected	27840
Independent reflections	3875 R_{int} = 0.0413 R_{sigma} = 0.0261
Completeness to θ = 25.242°	99.8 %
Data / Restraints / Parameters	3875 / 0 / 160
Goodness-of-fit on F^2	1.063
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0256 wR_2 = 0.0638
Final *R* indexes [all data]	R_1 = 0.0338 wR_2 = 0.0673
Largest peak/hole [eÅ^{-3}]	0.43/−0.74

Table S65. Bond lengths and angles for CP11

Atom–Atom	Length [Å]
S1–Cu2	2.2767(6)
S1–C5	1.8238(19)
S1–C4	1.856(2)
Cu2–Cu2$^{\#1}$	2.8392(6)
Cu2–Cl2$^{\#1}$	2.3459(6)
Cu2–Cl2	2.4290(6)
Cu2–S2	2.3096(6)
S2–C7	1.815(2)
S2–C9	1.852(2)
C5–H5A	0.9900
C5–H5B	0.9900
C5–C6	1.462(3)
C6–C6$^{\#2}$	1.190(4)
C7–H7A	0.9900
C7–H7B	0.9900
C7–C8	1.493(3)
C8–C8$^{\#3}$	1.312(4)
C8–Cl1	1.751(2)
C9–C12	1.520(3)
C9–C11	1.524(3)
C9–C10	1.515(3)
C12–H12A	0.9800
C12–H12B	0.9800
C12–H12C	0.9800
C11–H11A	0.9800
C11–H11B	0.9800
C11–H11C	0.9800
C10–H10A	0.9800
C10–H10B	0.9800
C10–H10C	0.9800
C4–C3	1.518(3)
C4–C2	1.525(3)
C4–C1	1.519(3)
C3–H3A	0.9800
C3–H3B	0.9800
C3–H3C	0.9800
C2–H2A	0.9800
C2–H2B	0.9800
C2–H2C	0.9800
C1–H1A	0.9800
C1–H1B	0.9800
C1–H1C	0.9800

Atom–Atom–Atom	Angle [°]
C5–S1–Cu2	103.94(7)
C5–S1–C4	105.18(9)
C4–S1–Cu2	110.69(7)
S1–Cu2–Cu2$^{\#1}$	124.538(19)
S1–Cu2–Cl2	116.54(2)
S1–Cu2–Cl2$^{\#1}$	102.91(2)
S1–Cu2–S2	128.70(2)
Cl2–Cu2–Cu2$^{\#1}$	52.178(16)
Cl2$^{\#1}$–Cu2–Cu2$^{\#1}$	54.878(15)
Cl2$^{\#1}$–Cu2–Cl2	107.056(18)
S2–Cu2–Cu2$^{\#1}$	106.751(18)
S2–Cu2–Cl2$^{\#1}$	107.65(2)
S2–Cu2–Cl2	92.521(19)
Cu2$^{\#1}$–Cl2–Cu2	72.945(18)
C7–S2–Cu2	102.55(6)
C7–S2–C9	106.31(10)
C9–S2–Cu2	112.79(7)
S1–C5–H5A	108.7
S1–C5–H5B	108.7
H5A–C5–H5B	107.6
C6–C5–S1	114.42(14)
C6–C5–H5A	108.7
C6–C5–H5B	108.7
C6$^{\#2}$–C6–C5	178.6(3)
S2–C7–H7A	108.2
S2–C7–H7B	108.2
H7A–C7–H7B	107.3
C8–C7–S2	116.37(15)
C8–C7–H7A	108.2
C8–C7–H7B	108.2
C7–C8–Cl1	113.45(15)
C8$^{\#3}$–C8–C7	128.6(3)
C8$^{\#3}$–C8–Cl1	117.8(2)
C12–C9–S2	110.15(15)
C12–C9–C11	110.6(2)
C11–C9–S2	103.12(14)
C10–C9–S2	111.13(15)
C10–C9–C12	110.9(2)
C10–C9–C11	110.70(18)
C9–C12–H12A	109.5
C9–C12–H12B	109.5
C9–C12–H12C	109.5
H12A–C12–H12B	109.5
H12A–C12–H12C	109.5
H12B–C12–H12C	109.5
C9–C11–H11A	109.5
C9–C11–H11B	109.5
C9–C11–H11C	109.5
H11A–C11–H11B	109.5
H11A–C11–H11C	109.5
H11B–C11–H11C	109.5
C9–C10–H10A	109.5
C9–C10–H10B	109.5
C9–C10–H10C	109.5
H10A–C10–H10B	109.5
H10A–C10–H10C	109.5
H10B–C10–H10C	109.5
C3–C4–S1	111.74(14)
C3–C4–C2	110.55(17)
C3–C4–C1	111.21(19)
C2–C4–S1	103.75(14)
C1–C4–S1	109.45(15)
C1–C4–C2	109.89(18)
C4–C3–H3A	109.5
C4–C3–H3B	109.5

C4–C3–H3C	109.5
H3A–C3–H3B	109.5
H3A–C3–H3C	109.5
H3B–C3–H3C	109.5
C4–C2–H2A	109.5
C4–C2–H2B	109.5
C4–C2–H2C	109.5
H2A–C2–H2B	109.5
H2A–C2–H2C	109.5
H2B–C2–H2C	109.5
C4–C1–H1A	109.5
C4–C1–H1B	109.5
C4–C1–H1C	109.5
H1A–C1–H1B	109.5
H1A–C1–H1C	109.5
H1B–C1–H1C	109.5

Symmetry transformations used to generate equivalent atoms:
#1: 1-X, 2-Y, 1-Z; #2: 1-X, 1-Y, 2-Z; #3: 2-X, 2-Y, -Z;

Table S66. Torsion angles for CP11

Atom–Atom–Atom–Atom	Torsion Angle [°]
Cu2–S1–C5–C6	169.16(13)
Cu2–S1–C4–C3	64.10(15)
Cu2–S1–C4–C2	−55.02(15)
Cu2–S1–C4–C1	−172.27(14)
Cu2–S2–C7–C8	−158.68(14)
Cu2–S2–C9–C12	−172.87(17)
Cu2–S2–C9–C11	69.08(15)
Cu2–S2–C9–C10	−49.55(17)
S2–C7–C8–C8[#1]	−129.9(3)
S2–C7–C8–Cl1	54.12(19)
C5–S1–C4–C3	−47.57(16)
C5–S1–C4–C2	−166.69(14)
C5–S1–C4–C1	76.06(17)
C7–S2–C9–C12	−61.2(2)
C7–S2–C9–C11	−179.29(14)
C7–S2–C9–C10	62.08(17)
C9–S2–C7–C8	82.72(17)
C4–S1–C5–C6	−74.45(17)

Symmetry transformations used to generate equivalent atoms:
#1: 2-X, 2-Y, -Z;

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