Supplementary information

To the manuscript

Copper(I) halide cluster-based coordination polymers modulated by chiral ditopic dithiodianthranilide ligands: synthesis, crystal structure and photoluminescence

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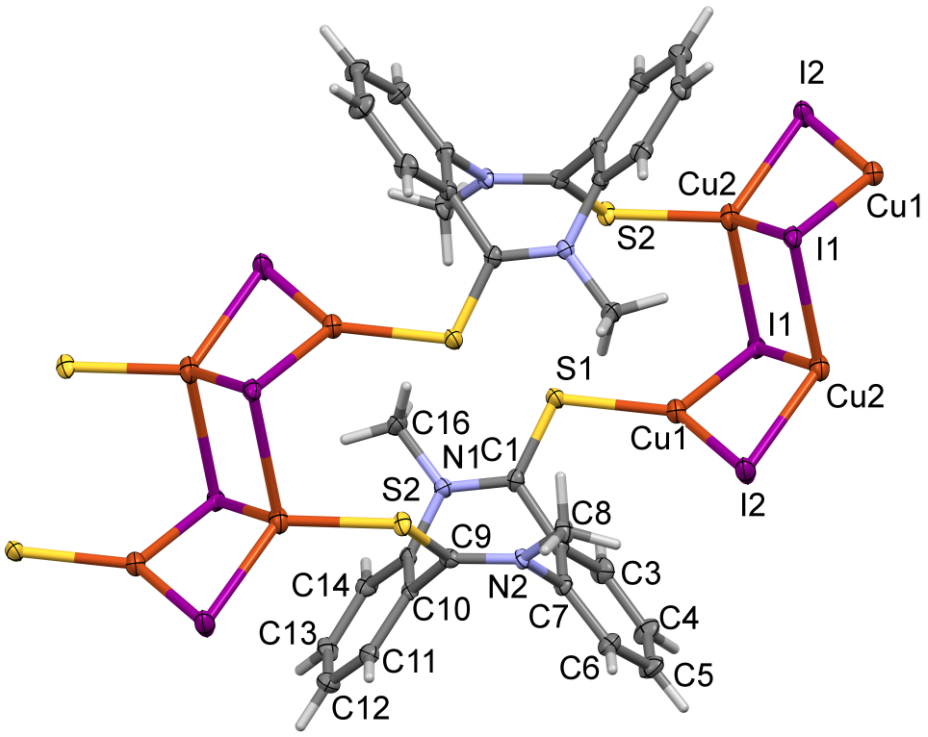

Figure S1. Molecular view and labeling scheme of the repeating unit of **$[Cu_2I_2(mdta)]_n$ (1)**. Hydrogen atoms not labelled, labels given for atoms of asymmetric unit and in some cases for symmetry equivalent (by symmetry centers) atoms.

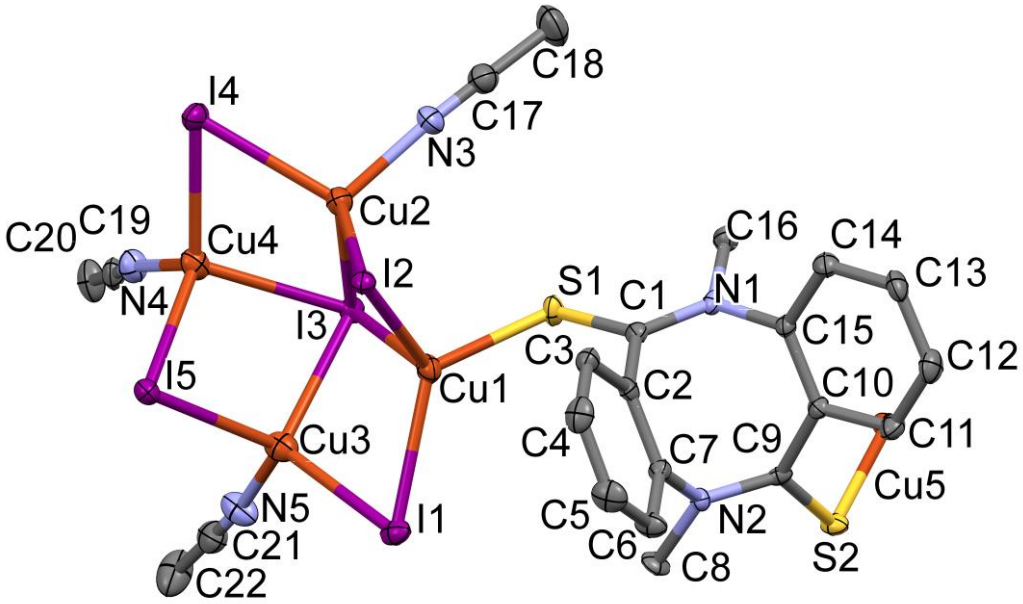

Figure S2. Molecular view and labeling scheme of the asymmetric unit of **$[Cu_5I_5\{(R)$-(−)-(mdta)$\}(MeCN)_3]_n$ (2)**. Hydrogen atoms omitted.

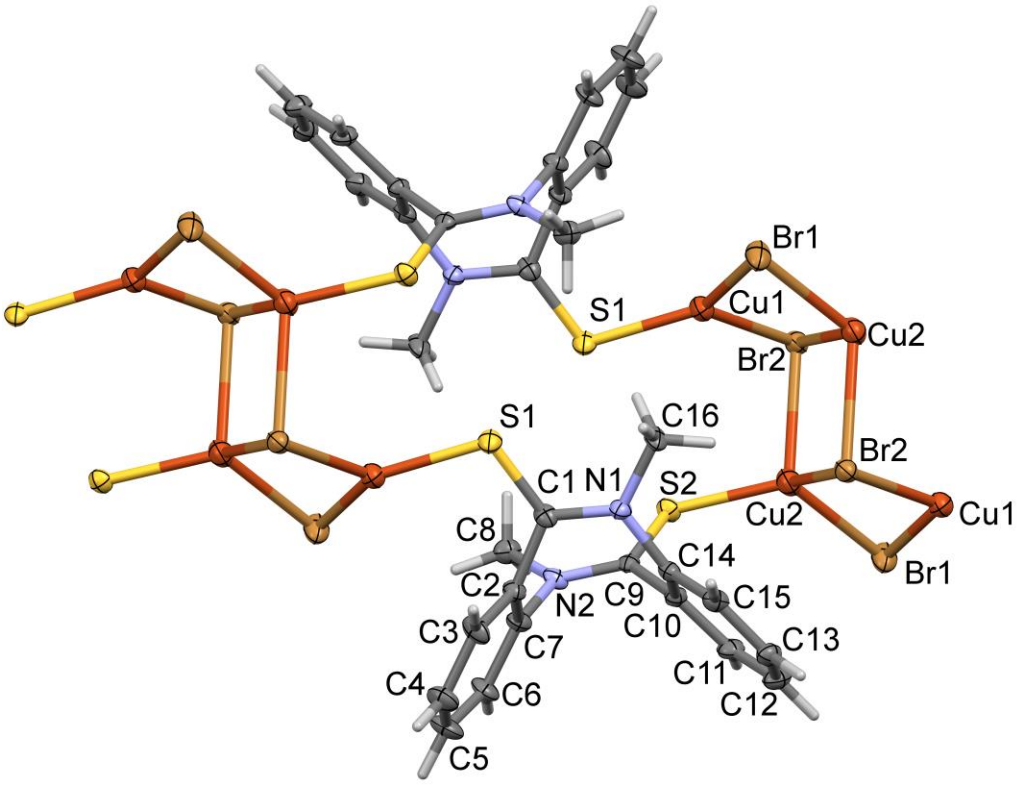

Figure S3. Molecular view of the repeating part and labeling scheme of the asymmetric unit of **$[Cu_2Br_2(mdta)]_n$ (3)**. Hydrogen atoms are not labelled. Some labels are doubled for equivalent atoms (by symmetry centers).

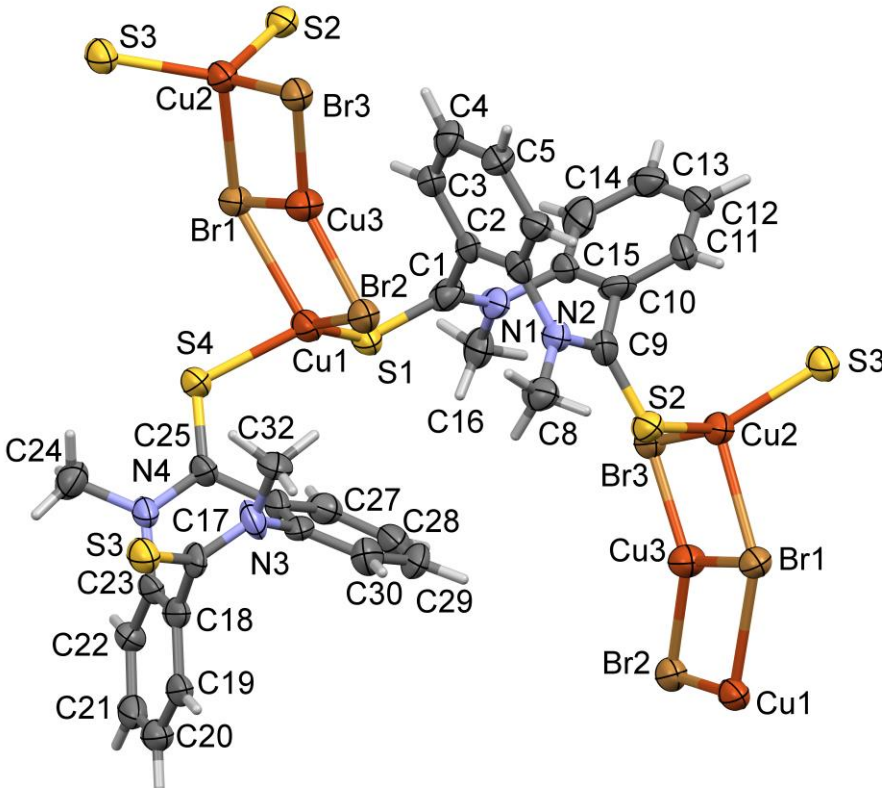

Figure S4. Molecular view and labeling scheme of the asymmetric unit of **$[Cu_3Br_3\{(R)\text{-}(-)\text{-}(mdta)\}_2(MeCN)]_n$ (4)**. Some labels are doubled for symmetry equivalent atoms (by a screw rotation).

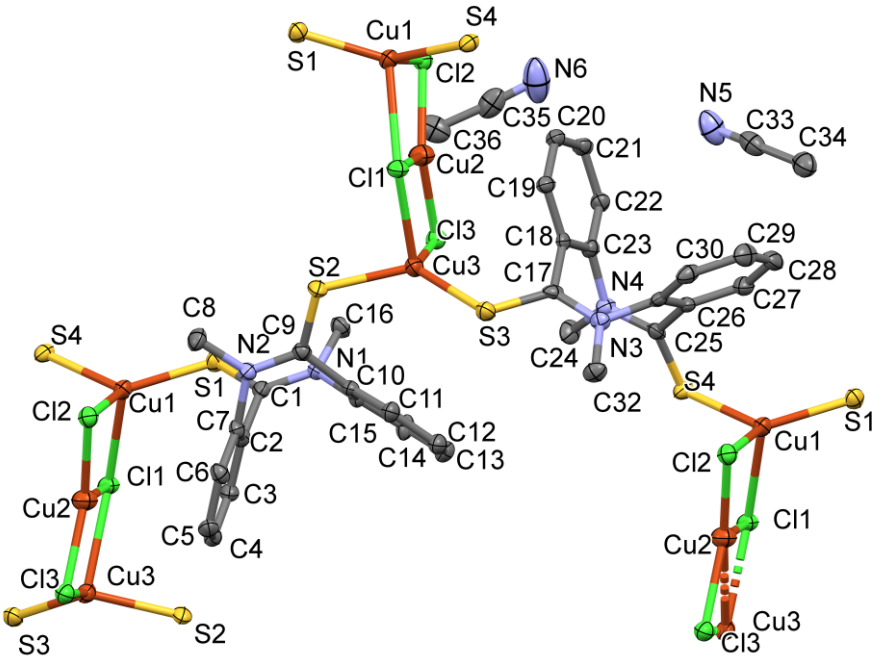

Figure S5. Molecular view and labeling scheme for the repeating part of structure **$[Cu_3Cl_3(mdta)_2(MeCN)_2]_n$ (5)**. Hydrogen atoms omitted. Some labels are doubled for symmetry equivalent atoms (by a screw rotation or translation). Solvent MeCN molecules are also shown for completeness.

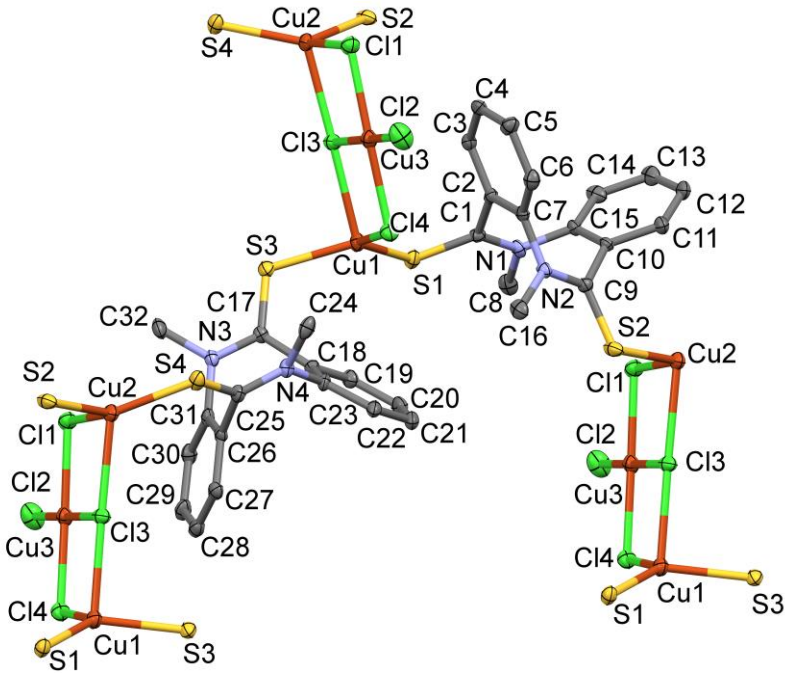

Figure S6. Molecular view and labeling scheme of the repeating unit of **$[Cu_3Cl_4\{(R)\text{-}(-)\text{-}(mdta)\}_2(MeCN)]_n$ (7)**. Hydrogen atoms omitted. Some labels are doubled for symmetry equivalent atoms (by a screw rotation or translation). Solvent MeCN molecule not drawn. Note topological similarity of **$[Cu_3Cl_3(mdta)_2(MeCN)_2]_n$ (5)** and **$[Cu_3Cl_4\{(R)\text{-}(-)\text{-}(mdta)\}_2(MeCN)]_n$ (7)** and additional Cl2 atom in the Cu_3Cl_4 clusters.

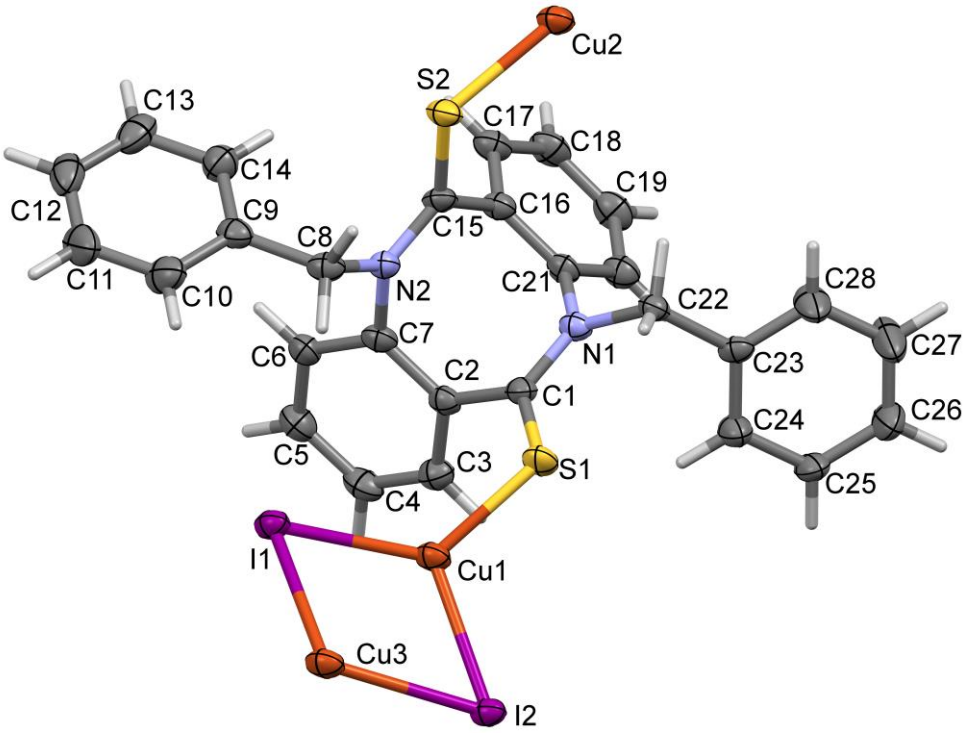

Figure S7. Molecular view and labeling scheme of the asymmetric unit of **$[Cu_2I_2(bdta)(MeCN)]_n$ (8)**. Hydrogen atoms not labelled.

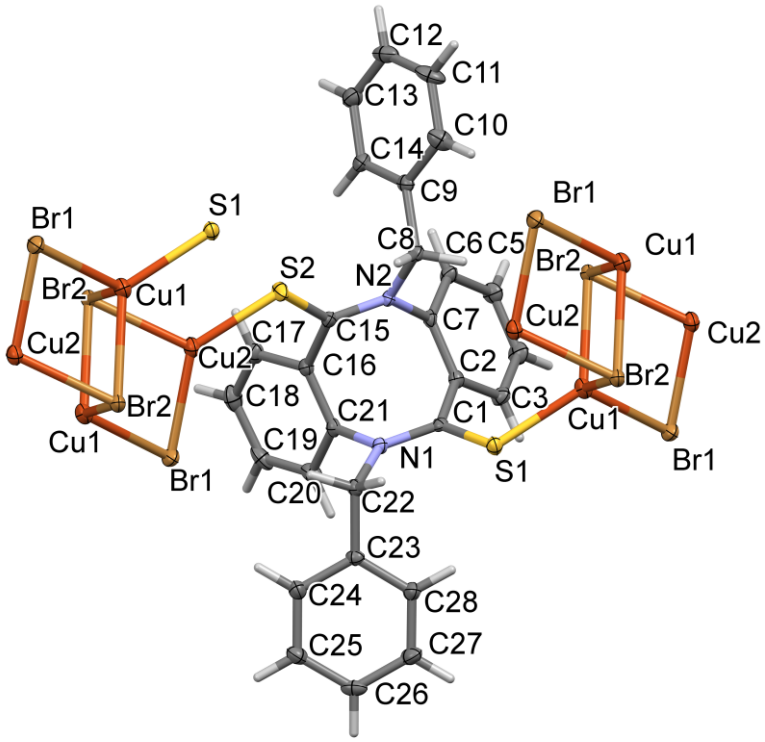

Figure S8. Molecular view of repeating part and labeling scheme of the asymmetric unit of **$[Cu_2Br_2(bdta)]_n$ (9)**. Hydrogen atoms not labelled. Some labels are doubled for symmetry equivalent atoms (by symmetry centers).

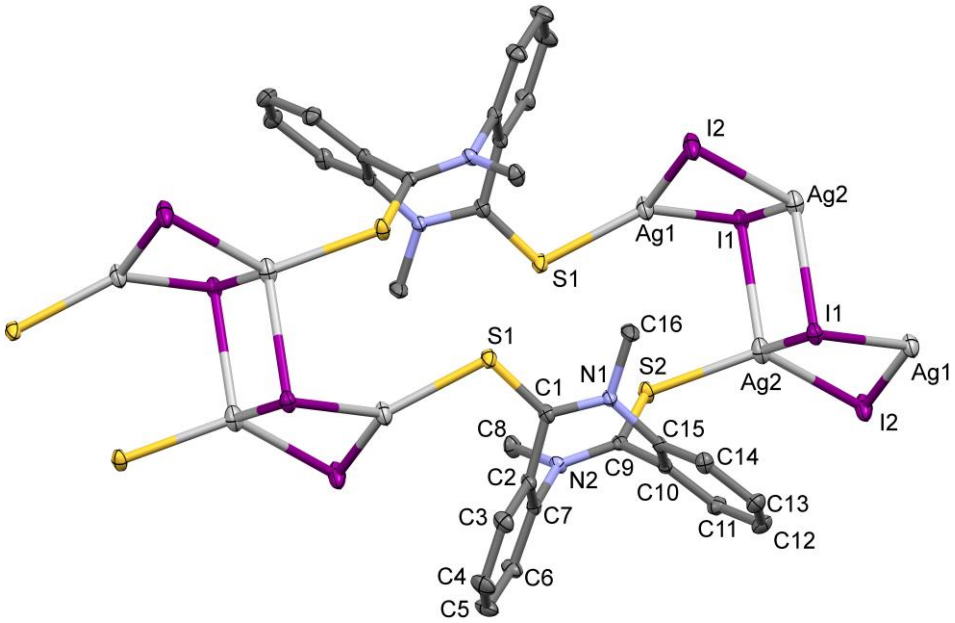

Figure S9. Molecular view of the repeating part and labeling scheme of the asymmetric unit of **$[Ag_2I_2(mdta)]_n$ (10)**. Hydrogen atoms not shown. Some labels are doubled for symmetry equivalent atoms (by the symmetry centers).

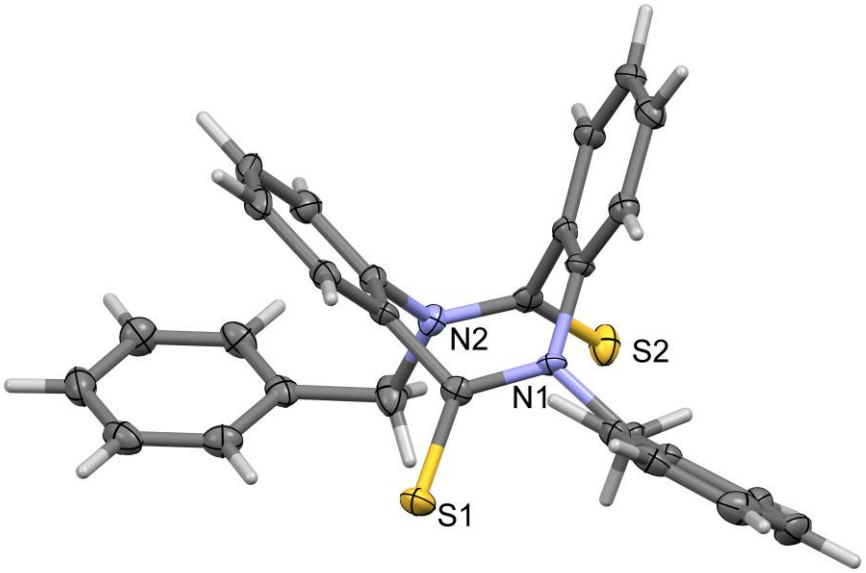

Figure S10. Molecular view of **5,11-Dibenzyldibenzo[*b*,*f*][1,5]diazocine-6,12(5*H*,11*H*)-dithione (bdta)**. Displacement ellipsoids drawn at 50% probability level. Only the most important atoms are labelled.

Table S1.

Crystal data, data collection and structure refinement details

	1	**2**	**3**	**4**
Crystal data				
Chemical formula	$C_{16}H_{14}Cu_2I_2N_2S_2$	$C_{22}H_{23}Cu_5I_5N_5S_2$	$C_{16}H_{14}Br_2Cu_2N_2S_2$	$C_{32}H_{28}Br_3Cu_3N_4S_4 \cdot C_2H_3N$
CCDC code	2013594	2013595	2013596	2013597
M_r	679.29	1373.77	585.31	1068.23
Crystal system, space group	Monoclinic, $P2_1/n$	Orthorhombic, $P2_12_12_1$	Monoclinic, $P2_1/n$	Monoclinic, $P2_1$
Temperature (K)	120	120	120	120
a, *b*, *c* (Å)	13.353 (3), 10.6593 (16), 13.978 (3)	10.3178 (4), 15.5879 (11), 21.9885 (8)	13.306 (3), 10.4481 (12), 13.639 (3)	8.7415 (4), 17.1309 (8), 13.1531 (6)
α, β, γ (°)	90, 101.058 (16), 90	90, 90, 90	90, 99.860 (15), 90	90, 95.007 (3), 90
V ($Å^3$)	1952.6 (6)	3536.5 (3)	1868.1 (6)	1962.16 (16)
Z	4	4	4	2
Radiation type	Mo *K*α	Mo *K*α	Mo *K*α	Mo *K*α
μ (mm^{-1})	5.56	7.46	6.78	4.91
Crystal size (mm)	0.48 × 0.05 × 0.02	0.22 × 0.08 × 0.06	0.45 × 0.31 × 0.28	0.41 × 0.08 × 0.05
Data collection				
Diffractometer	STOE *IPDS* 2T	STOE *IPDS* 2T	STOE *IPDS* 2T	STOE *IPDS* 2T
Absorption correction	Integration STOE *X-RED32*, absorption correction by Gaussian integration, analogous to P. Coppens, "The Evaluation of Absorption and Extinction in Single-Crystal Structure Analysis", published in F. R. Ahmed (Editor), "Crystallographic Computing", Munksgaard, Copenhagen (1970), 255 - 270	Integration STOE *X-RED32*, absorption correction by Gaussian integration, analogous to P. Coppens, "The Evaluation of Absorption and Extinction in Single-Crystal Structure Analysis", published in F. R. Ahmed (Editor), "Crystallographic Computing", Munksgaard, Copenhagen (1970), 255 - 270	Integration STOE *X-RED32*, absorption correction by Gaussian integration, analogous to P. Coppens, "The Evaluation of Absorption and Extinction in Single-Crystal Structure Analysis", published in F. R. Ahmed (Editor), "Crystallographic Computing", Munksgaard, Copenhagen (1970), 255 - 270	Integration STOE *X-RED32*, absorption correction by Gaussian integration, analogous to P. Coppens, "The Evaluation of Absorption and Extinction in Single-Crystal Structure Analysis", published in F. R. Ahmed (Editor), "Crystallographic Computing", Munksgaard, Copenhagen (1970), 255 - 270
T_{min}, T_{max}	0.251, 0.797	0.258, 0.501	0.099, 0.207	0.187, 0.535
No. of measured, independent and	25748, 5272, 4599	20418, 9471, 8678	24955, 5043, 4157	19182, 7709, 5814

observed [$I > 2\sigma(I)$] reflections				
R_{int}	0.051	0.028	0.085	0.086
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.688	0.687	0.688	0.617
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.110, 1.00	0.025, 0.057, 1.07	0.053, 0.147, 1.06	0.105, 0.293, 1.03
No. of reflections	5272	9471	5043	7709
No. of parameters	219	357	219	447
No. of restraints	0	0	0	1
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
	$w = 1/[\sigma^2(F_o^2) + (0.0881P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0323P)^2 + 0.3461P]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.1022P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.1897P)^2 + 10.6517P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	2.95, -1.56	0.59, -0.64	1.49, -1.32	4.18, -1.42
Absolute structure	–	Flack x determined using 3585 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).	–	Classical Flack method preferred over Parsons because s.u. lower.
Absolute structure parameter	–	0.000 (16)	–	0.00 (3)

	5	**7**	**8**	**9**
Crystal data				
Chemical formula	$C_{32}H_{28}Cl_3Cu_3N_4S_4 \cdot 2(C_2H_3N)$	$C_{32}H_{28}Cl_4Cu_3N_4S_4 \cdot C_2H_3N$	$C_{28}H_{22}Cu_2I_2N_2S_2$	$C_{28}H_{22}Br_2Cu_2N_2S_2$
CCDC code	2013598	2013599	2013600	2013601
M_r	975.90	970.30	831.47	737.49
Crystal system, space group	Monoclinic, $P2_1$	Monoclinic, $P2_1$	Monoclinic, $I2/a$	Triclinic, $P\bar{1}$
Temperature (K)	120	120	120	120
a, b, c (Å)	8.8353 (2), 16.7129 (5), 13.6256 (4)	8.7179 (9), 16.8411 (17), 12.8872 (13)	19.2485 (11), 16.5225 (8), 21.3838 (11)	10.6426 (12), 11.6334 (14), 12.1551 (15)
α, β, γ (°)	90, 99.427 (2), 90	90, 94.018 (8), 90	90, 114.655 (4),	108.021 (9),

			90	107.195 (9), 98.463 (9)
V (Å^3)	1984.83 (10)	1887.4 (3)	6180.8 (6)	1319.1 (3)
Z	2	2	8	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	2.04	2.21	3.53	4.82
Crystal size (mm)	0.29 × 0.11 × 0.03	0.41 × 0.32 × 0.16	0.45 × 0.23 × 0.19	0.16 × 0.09 × 0.08
Data collection				
Diffractometer	STOE *IPDS* 2T	STOE *IPDS* 2T	STOE *IPDS* 2T	STOE *IPDS* 2T
Absorption correction	Integration STOE *X-RED32*, absorption correction by Gaussian integration, analogous to P. Coppens, "The Evaluation of Absorption and Extinction in Single-Crystal Structure Analysis", published in F. R. Ahmed (Editor), "Crystallographic Computing", Munksgaard, Copenhagen (1970), 255 - 270	Multi-scan STOE *X-RED32*, absorption correction by Gaussian integration, analogous to P. Coppens, "The Evaluation of Absorption and Extinction in Single-Crystal Structure Analysis", published in F. R. Ahmed (Editor), "Crystallographic Computing", Munksgaard, Copenhagen (1970), 255 - 270	Integration STOE *X-RED32*, absorption correction by Gaussian integration, analogous to P. Coppens, "The Evaluation of Absorption and Extinction in Single-Crystal Structure Analysis", published in F. R. Ahmed (Editor), "Crystallographic Computing", Munksgaard, Copenhagen (1970), 255 - 270	Multi-scan STOE LANA, absorption correction by scaling of reflection intensities. J. Koziskova, F. Hahn, J. Richter, J. Kozisek, "Comparison of different absorption corrections on the model structure of tetrakis(μ_2-acetato)- diaqua-di-copper(II)", Acta Chimica Slovaca, vol. 9, no. 2, 2016, pp. 136 - 140. Afterwards a spherical absorption correction was performed within STOE LANA.
T_{min}, T_{max}	0.656, 0.906	0.105, 0.505	0.175, 0.406	0.293, 0.701
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10633, 10633, 8879	26594, 10114, 9422	42187, 8343, 7370	12200, 6508, 5508
R_{int}	0 (affected by twinning)	0.033	0.060	0.035
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.688	0.687	0.688	0.686
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.055, 0.165, 1.03	0.039, 0.102, 1.06	0.056, 0.159, 1.09	0.031, 0.082, 1.03
No. of reflections	10633	10114	8343	6508

No. of parameters	476	456	326	325
No. of restraints	1	1	0	0
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
	$w = 1/[\sigma^2(F_o^2) + (0.1092P)^2 + 2.1782P]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0651P)^2 + 1.3569P]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0937P)^2 + 44.3932P]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0535P)^2 + 0.0582P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	1.03, -1.20	1.32, -0.81	2.12, -3.30	0.85, -0.83
Absolute structure	Flack x determined using 3638 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).	Classical Flack method preferred over Parsons because s.u. lower.	–	–
Absolute structure parameter	0.016 (12)	0.003 (11)	–	–

	10	**bdta**
Crystal data		
Chemical formula	$C_{16}H_{14}Ag_2I_2N_2S_2$	$C_{28}H_{22}N_2S_2$
CCDC code	2013602	2013603
M_r	767.95	450.59
Crystal system, space group	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/c$
Temperature (K)	120	120
a, *b*, *c* (Å)	13.3327 (8), 11.2308 (4), 13.8158 (8)	9.3720 (3), 14.5073 (9), 16.6745 (7)
α, β, γ (°)	90, 101.542 (5), 90	90, 98.533 (3), 90
V (Å^3)	2026.90 (19)	2242.01 (18)
Z	4	4
Radiation type	Mo *K*α	Mo *K*α
μ (mm^{-1})	5.19	0.26
Crystal size (mm)	0.22 × 0.17 × 0.05	0.41 × 0.35 × 0.22
Data collection		
Diffractometer	STOE *IPDS* 2T	STOE *IPDS* 2T
Absorption correction	Integration STOE *X-RED32*, absorption correction by Gaussian	none

	integration, analogous to P. Coppens, "The Evaluation of Absorption and Extinction in Single-Crystal Structure Analysis", published in F. R. Ahmed (Editor), "Crystallographic Computing", Munksgaard, Copenhagen (1970), 255 - 270	
T_{min}, T_{max}	0.288, 0.832	–
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	24114, 5461, 4861	20437, 4270, 3451
R_{int}	0.020	0.111
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.686	0.617
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.019, 0.048, 1.07	0.055, 0.154, 1.15
No. of reflections	5461	4270
No. of parameters	219	289
No. of restraints	0	0
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
	$w = 1/[\sigma^2(F_o^2) + (0.0267P)^2 + 1.616P]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0235P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	1.15, -1.27	0.53, -0.36
Absolute structure	–	–
Absolute structure parameter	–	–

Computer programs: *X-AREA* WinXpose 2.0.22.0 (STOE, 2016), *X-AREA* Recipe 1.33.0.0 (STOE, 2015), *X-AREA* Integrate 1.72.0.0 (STOE, 2018) *X-AREA X-RED32* 1.63.4.0 (STOE, 2017), *X-AREA* Integrate 1.72.0.0 (STOE, 2018) *X-AREA* LANA 1.71.6.0 (STOE, 2017), ShelXT (Sheldrick, 2015), SHELXT 2018/2 (Sheldrick, 2018), *SHELXL* (Sheldrick, 2015), Olex2 (Dolomanov *et al.*, 2009).

Document origin: *publCIF* [Westrip, S. P. (2010). *J. Apply. Cryst.*, **43**, 920–925].

Computing details

For all compounds, data collection: *X-AREA* WinXpose 2.0.22.0 (STOE, 2016); cell refinement: *X-AREA* Recipe 1.33.0.0 (STOE, 2015). Data reduction: *X-AREA* Integrate 1.72.0.0 (STOE, 2018) *X-AREA X-RED32* 1.63.4.0 (STOE, 2017) for (1), (2), (3), (4), (5), (7), (8), (10), bdta; *X-AREA* Integrate 1.72.0.0 (STOE, 2018) *X-AREA* LANA 1.71.6.0 (STOE, 2017) for (9). Program(s) used to solve structure: ShelXT (Sheldrick, 2015) for (1), (2), (4), (5), (7), (8), (9), (10), bdta; SHELXT 2018/2 (Sheldrick, 2018) for (3). For all compounds, program(s) used to refine structure: *SHELXL* (Sheldrick, 2015); molecular graphics: Olex2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: Olex2 (Dolomanov *et al.*, 2009).

Crystal data for **$[Cu_2I_2(mdta)]_n$ (1)**

$C_{16}H_{14}Cu_2I_2N_2S_2$	$F(000) = 1280$
$M_r = 679.29$	$D_x = 2.311$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 13.353$ (3) Å	Cell parameters from 35699 reflections
$b = 10.6593$ (16) Å	$\theta = 2.4$–$29.7°$
$c = 13.978$ (3) Å	$\mu = 5.56$ mm^{-1}
$\beta = 101.058$ (16)°	$T = 120$ K
$V = 1952.6$ (6) Å^3	Plate, yellow
$Z = 4$	0.48 × 0.05 × 0.02 mm

Data collection

STOE IPDS 2T diffractometer	5272 independent reflections
Radiation source: GeniX Mo, 0.05 x 0.05 mm2 microfocus	4599 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	$R_{int} = 0.051$
rotation method, ω scans	$\theta_{max} = 29.3°$, $\theta_{min} = 2.4°$
Absorption correction: integration STOE *X-RED32*, absorption correction by Gaussian integration, analogous to P. Coppens, "The Evaluation of Absorption and Extinction in Single-Crystal Structure Analysis", published in F. R. Ahmed (Editor), "Crystallographic Computing", Munksgaard, Copenhagen (1970), 255 - 270	$h = -18 \rightarrow 18$
$T_{min} = 0.251$, $T_{max} = 0.797$	$k = -14 \rightarrow 14$
25748 measured reflections	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods

Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.042$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.110$	H-atom parameters constrained
$S = 1.00$	$w = 1/[\sigma^2(F_o^2) + (0.0881P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
5272 reflections	$(\Delta/\sigma)_{max} = 0.005$
219 parameters	$\Delta\rangle_{max} = 2.95$ e Å^{-3}
0 restraints	$\Delta\rangle_{min} = -1.56$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for **$[Cu_2I_2(mdta)]_n$ (1)**

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.12698 (2)	0.99084 (2)	0.61842 (2)	0.01609 (9)
I2	0.15630 (2)	0.82912 (2)	0.34273 (2)	0.02588 (9)
Cu1	0.13278 (4)	0.79052 (4)	0.51552 (3)	0.01930 (12)
Cu2	0.08335 (4)	0.02447 (4)	0.42459 (4)	0.02125 (12)
S1	0.10328 (7)	0.60986 (8)	0.58649 (7)	0.01732 (18)
S2	0.09882 (6)	0.21179 (8)	0.34880 (6)	0.01568 (17)
N1	0.1913 (2)	0.3877 (3)	0.6037 (2)	0.0138 (5)
N2	0.2082 (2)	0.4196 (3)	0.3782 (2)	0.0123 (5)
C1	0.1931 (3)	0.5047 (3)	0.5714 (2)	0.0140 (6)
C2	0.2788 (3)	0.5428 (3)	0.5245 (2)	0.0138 (6)
C3	0.3523 (3)	0.6252 (3)	0.5737 (3)	0.0200 (7)
H3	0.348000	0.653621	0.637153	0.024*
C4	0.4315 (3)	0.6656 (4)	0.5301 (3)	0.0232 (8)
H4	0.482768	0.719322	0.564597	0.028*
C5	0.4359 (3)	0.6274 (4)	0.4363 (3)	0.0224 (7)
H5	0.488500	0.658313	0.405617	0.027*
C6	0.3640 (3)	0.5446 (4)	0.3867 (3)	0.0183 (7)
H6	0.367839	0.517740	0.322740	0.022*
C7	0.2866 (3)	0.5014 (3)	0.4317 (3)	0.0133 (6)
C8	0.1421 (3)	0.4727 (3)	0.2912 (3)	0.0176 (7)
H8A	0.074504	0.490221	0.305700	0.026*

H8B	0.135549	0.412421	0.237433	0.026*
H8C	0.172204	0.550662	0.272675	0.026*
C9	0.1935 (2)	0.3034 (3)	0.4072 (2)	0.0117 (6)
C10	0.2659 (2)	0.2530 (3)	0.4931 (2)	0.0114 (6)
C11	0.3302 (3)	0.1543 (3)	0.4802 (3)	0.0163 (6)
H11	0.330761	0.123136	0.416652	0.020*
C12	0.3934 (3)	0.1014 (3)	0.5604 (3)	0.0186 (7)
H12	0.437265	0.034086	0.551197	0.022*
C13	0.3936 (3)	0.1455 (3)	0.6539 (3)	0.0181 (7)
H13	0.438160	0.109582	0.708085	0.022*
C14	0.3286 (2)	0.2419 (3)	0.6679 (2)	0.0161 (6)
H14	0.327284	0.271164	0.731846	0.019*
C15	0.2652 (2)	0.2959 (3)	0.5877 (2)	0.0124 (6)
C16	0.1135 (3)	0.3485 (4)	0.6581 (3)	0.0199 (7)
H16A	0.121911	0.395757	0.719255	0.030*
H16B	0.120906	0.258601	0.672516	0.030*
H16C	0.045638	0.364764	0.619049	0.030*

Atomic displacement parameters (Å^2) for **$[Cu_2I_2(mdta)]_n$ (1)**

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01571 (13)	0.01177 (13)	0.01991 (14)	-0.00209 (7)	0.00117 (9)	0.00088 (8)
I2	0.03855 (17)	0.01550 (15)	0.02838 (15)	0.00570 (9)	0.01843 (12)	0.00584 (9)
Cu1	0.0212 (2)	0.0140 (2)	0.0235 (2)	0.00038 (16)	0.00610 (18)	0.00289 (17)
Cu2	0.0246 (3)	0.0139 (2)	0.0243 (2)	-0.00224 (17)	0.00252 (19)	0.00209 (17)
S1	0.0214 (4)	0.0121 (4)	0.0205 (4)	0.0028 (3)	0.0091 (3)	0.0016 (3)
S2	0.0142 (4)	0.0123 (4)	0.0180 (4)	-0.0028 (3)	-0.0034 (3)	0.0004 (3)
N1	0.0146 (13)	0.0118 (13)	0.0152 (12)	-0.0002 (10)	0.0035 (10)	-0.0010 (10)
N2	0.0120 (12)	0.0100 (12)	0.0138 (12)	-0.0009 (9)	-0.0004 (10)	-0.0005 (10)
C1	0.0172 (16)	0.0124 (15)	0.0120 (14)	-0.0025 (11)	0.0022 (12)	-0.0012 (11)
C2	0.0159 (15)	0.0113 (15)	0.0146 (14)	0.0003 (12)	0.0038 (12)	0.0021 (12)
C3	0.0212 (17)	0.0182 (17)	0.0195 (16)	-0.0037 (13)	0.0012 (14)	-0.0061 (14)
C4	0.0193 (18)	0.0245 (19)	0.0255 (19)	-0.0089 (14)	0.0034 (14)	-0.0037 (15)
C5	0.0180 (17)	0.0223 (18)	0.0288 (19)	-0.0079 (14)	0.0090 (14)	-0.0046 (15)
C6	0.0159 (16)	0.0206 (18)	0.0192 (16)	-0.0038 (13)	0.0053 (13)	0.0013 (14)
C7	0.0123 (15)	0.0120 (15)	0.0144 (15)	-0.0029 (10)	-0.0003 (12)	-0.0005 (11)
C8	0.0183 (16)	0.0153 (16)	0.0164 (15)	0.0006 (12)	-0.0038 (13)	0.0045 (13)
C9	0.0110 (14)	0.0126 (14)	0.0105 (13)	-0.0003 (11)	-0.0004 (11)	-0.0027 (11)
C10	0.0094 (13)	0.0102 (14)	0.0136 (14)	-0.0011 (11)	-0.0007 (11)	-0.0005 (12)
C11	0.0149 (15)	0.0146 (16)	0.0196 (16)	-0.0010 (12)	0.0036 (12)	-0.0007 (13)

C12	0.0156 (16)	0.0182 (17)	0.0220 (17)	0.0032 (12)	0.0031 (13)	0.0019 (14)
C13	0.0156 (16)	0.0159 (16)	0.0199 (16)	0.0017 (12)	-0.0037 (13)	0.0035 (13)
C14	0.0130 (15)	0.0191 (17)	0.0150 (15)	-0.0024 (12)	-0.0004 (12)	0.0003 (13)
C15	0.0130 (14)	0.0084 (14)	0.0156 (14)	-0.0003 (11)	0.0021 (11)	-0.0006 (12)
C16	0.0228 (18)	0.0169 (17)	0.0229 (17)	0.0003 (13)	0.0121 (14)	0.0026 (14)

Geometric parameters (Å, º) for **$[Cu_2I_2(mdta)]_n$ (1)**

I1—Cu1	2.5840 (6)	C4—C5	1.384 (5)
I1—Cu2^{i}	2.7620 (8)	C5—H5	0.9500
I1—Cu2^{ii}	2.6838 (8)	C5—C6	1.388 (5)
I2—Cu1	2.5283 (7)	C6—H6	0.9500
I2—Cu2^{ii}	2.6498 (6)	C6—C7	1.387 (5)
Cu1—Cu2^{ii}	2.8192 (7)	C8—H8A	0.9800
Cu1—S1	2.2357 (10)	C8—H8B	0.9800
Cu2—S2	2.2881 (10)	C8—H8C	0.9800
S1—C1	1.685 (4)	C9—C10	1.490 (4)
S2—C9	1.680 (3)	C10—C11	1.391 (5)
N1—C1	1.328 (4)	C10—C15	1.401 (4)
N1—C15	1.437 (4)	C11—H11	0.9500
N1—C16	1.462 (4)	C11—C12	1.387 (5)
N2—C7	1.454 (4)	C12—H12	0.9500
N2—C8	1.471 (4)	C12—C13	1.389 (5)
N2—C9	1.330 (4)	C13—H13	0.9500
C1—C2	1.480 (5)	C13—C14	1.382 (5)
C2—C3	1.396 (5)	C14—H14	0.9500
C2—C7	1.393 (5)	C14—C15	1.393 (4)
C3—H3	0.9500	C16—H16A	0.9800
C3—C4	1.387 (5)	C16—H16B	0.9800
C4—H4	0.9500	C16—H16C	0.9800
Cu1—I1—Cu2^{ii}	64.678 (17)	C4—C5—C6	120.6 (3)
Cu1—I1—Cu2^{i}	88.154 (18)	C6—C5—H5	119.7
Cu2^{ii}—I1—Cu2^{i}	76.90 (2)	C5—C6—H6	120.4
Cu1—I2—Cu2^{ii}	65.925 (18)	C5—C6—C7	119.3 (3)
I1—Cu1—Cu2^{ii}	59.37 (2)	C7—C6—H6	120.4
I2—Cu1—I1	114.82 (2)	C2—C7—N2	119.6 (3)
I2—Cu1—Cu2^{ii}	59.110 (16)	C6—C7—N2	119.5 (3)
S1—Cu1—I1	115.98 (3)	C6—C7—C2	120.8 (3)
S1—Cu1—I2	128.97 (3)	N2—C8—H8A	109.5
S1—Cu1—Cu2^{ii}	156.36 (3)	N2—C8—H8B	109.5

I1^{iii}—Cu2—I1^{i}	103.10 (2)	N2—C8—H8C	109.5
I1^{iii}—Cu2—Cu1^{iii}	55.946 (15)	H8A—C8—H8B	109.5
I1^{i}—Cu2—Cu1^{iii}	100.73 (2)	H8A—C8—H8C	109.5
I2^{iii}—Cu2—I1^{i}	107.59 (2)	H8B—C8—H8C	109.5
I2^{iii}—Cu2—I1^{iii}	107.72 (2)	N2—C9—S2	122.3 (2)
I2^{iii}—Cu2—Cu1^{iii}	54.965 (18)	N2—C9—C10	118.1 (3)
S2—Cu2—I1^{i}	97.42 (3)	C10—C9—S2	119.6 (2)
S2—Cu2—I1^{iii}	124.23 (3)	C11—C10—C9	119.3 (3)
S2—Cu2—I2^{iii}	114.36 (3)	C11—C10—C15	119.0 (3)
S2—Cu2—Cu1^{iii}	161.17 (3)	C15—C10—C9	121.5 (3)
C1—S1—Cu1	109.10 (12)	C10—C11—H11	120.1
C9—S2—Cu2	114.11 (12)	C12—C11—C10	119.9 (3)
C1—N1—C15	122.0 (3)	C12—C11—H11	120.1
C1—N1—C16	120.4 (3)	C11—C12—H12	119.6
C15—N1—C16	117.6 (3)	C11—C12—C13	120.9 (3)
C7—N2—C8	117.0 (3)	C13—C12—H12	119.6
C9—N2—C7	122.3 (3)	C12—C13—H13	120.1
C9—N2—C8	120.7 (3)	C14—C13—C12	119.8 (3)
N1—C1—S1	121.5 (3)	C14—C13—H13	120.1
N1—C1—C2	118.3 (3)	C13—C14—H14	120.2
C2—C1—S1	120.2 (2)	C13—C14—C15	119.6 (3)
C3—C2—C1	119.0 (3)	C15—C14—H14	120.2
C7—C2—C1	121.8 (3)	C10—C15—N1	119.9 (3)
C7—C2—C3	119.1 (3)	C14—C15—N1	119.1 (3)
C2—C3—H3	119.9	C14—C15—C10	120.8 (3)
C4—C3—C2	120.2 (3)	N1—C16—H16A	109.5
C4—C3—H3	119.9	N1—C16—H16B	109.5
C3—C4—H4	120.0	N1—C16—H16C	109.5
C5—C4—C3	119.9 (3)	H16A—C16—H16B	109.5
C5—C4—H4	120.0	H16A—C16—H16C	109.5
C4—C5—H5	119.7	H16B—C16—H16C	109.5
Cu1—S1—C1—N1	-177.6 (2)	C7—N2—C9—C10	-5.0 (5)
Cu1—S1—C1—C2	4.7 (3)	C7—C2—C3—C4	0.4 (5)
Cu2—S2—C9—N2	-174.2 (2)	C8—N2—C7—C2	111.5 (4)
Cu2—S2—C9—C10	7.4 (3)	C8—N2—C7—C6	-63.7 (4)
S1—C1—C2—C3	68.8 (4)	C8—N2—C9—S2	-1.2 (5)
S1—C1—C2—C7	-109.5 (3)	C8—N2—C9—C10	177.3 (3)
S2—C9—C10—C11	65.2 (4)	C9—N2—C7—C2	-66.4 (4)
S2—C9—C10—C15	-109.7 (3)	C9—N2—C7—C6	118.4 (4)

N1—C1—C2—C3	-109.0 (4)	C9—C10—C11—C12	-176.1 (3)
N1—C1—C2—C7	72.8 (4)	C9—C10—C15—N1	2.0 (5)
N2—C9—C10—C11	-113.3 (4)	C9—C10—C15—C14	175.7 (3)
N2—C9—C10—C15	71.8 (4)	C10—C11—C12—C13	0.1 (5)
C1—N1—C15—C10	-67.5 (4)	C11—C10—C15—N1	-172.9 (3)
C1—N1—C15—C14	118.7 (4)	C11—C10—C15—C14	0.8 (5)
C1—C2—C3—C4	-177.9 (3)	C11—C12—C13—C14	1.2 (5)
C1—C2—C7—N2	0.8 (5)	C12—C13—C14—C15	-1.4 (5)
C1—C2—C7—C6	175.9 (3)	C13—C14—C15—N1	174.2 (3)
C2—C3—C4—C5	2.2 (6)	C13—C14—C15—C10	0.5 (5)
C3—C2—C7—N2	-177.5 (3)	C15—N1—C1—S1	177.4 (2)
C3—C2—C7—C6	-2.3 (5)	C15—N1—C1—C2	-4.8 (5)
C3—C4—C5—C6	-2.8 (6)	C15—C10—C11—C12	-1.1 (5)
C4—C5—C6—C7	0.9 (6)	C16—N1—C1—S1	-3.2 (5)
C5—C6—C7—N2	176.9 (3)	C16—N1—C1—C2	174.6 (3)
C5—C6—C7—C2	1.7 (5)	C16—N1—C15—C10	113.1 (4)
C7—N2—C9—S2	176.6 (3)	C16—N1—C15—C14	-60.7 (4)

Symmetry codes: (i) -*x*, -*y*+1, -*z*+1; (ii) *x*, *y*+1, *z*; (iii) *x*, *y*-1, *z*.

Crystal data for **[Cu_5I_5{(*R*)-(−)-(mdta)}$(MeCN)_3$]$_n$ (2)**

$C_{22}H_{23}Cu_5I_5N_5S_2$	D_x = 2.580 Mg m^{-3}
M_r = 1373.77	Mo *K*α radiation, λ = 0.71073 Å
Orthorhombic, $P2_12_12_1$	Cell parameters from 8622 reflections
a = 10.3178 (4) Å	θ = 2.2–29.6°
b = 15.5879 (11) Å	μ = 7.46 mm^{-1}
c = 21.9885 (8) Å	*T* = 120 K
V = 3536.5 (3) Å^3	Prism, yellow
Z = 4	0.22 × 0.08 × 0.06 mm
F(000) = 2528	

Data collection

STOE IPDS 2T diffractometer	8678 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	R_{int} = 0.028
rotation method, ω scans	θ_{max} = 29.2°, θ_{min} = 2.3°
Absorption correction: integration STOE *X-RED32*, absorption correction by Gaussian integration, analogous to P. Coppens, "The Evaluation of Absorption and Extinction	*h* = -14→14

in Single-Crystal Structure Analysis", published in F. R. Ahmed (Editor), "Crystallographic Computing", Munksgaard, Copenhagen (1970), 255 - 270	
T_{min} = 0.258, T_{max} = 0.501	k = -17→21
20418 measured reflections	l = -27→30
9471 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.025	H-atom parameters constrained
$wR(F^2)$ = 0.057	$w = 1/[\sigma^2(F_o^2) + (0.0323P)^2 + 0.3461P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max}$ = 0.001
9471 reflections	$\Delta\rangle_{max}$ = 0.59 e Å^{-3}
357 parameters	$\Delta\rangle_{min}$ = -0.64 e Å^{-3}
0 restraints	Absolute structure: Flack x determined using 3585 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Primary atom site location: structure-invariant direct methods	Absolute structure parameter: 0.000 (16)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for **[Cu$_5$I$_5${(*R*)-(−)-(mdta)}(MeCN)$_3$]$_n$ (2)**

	x	y	z	U_{iso}*/U_{eq}
I1	0.59768 (4)	0.21758 (3)	0.26415 (2)	0.02147 (9)
I2	0.71918 (4)	0.49008 (2)	0.25937 (2)	0.01630 (8)
I3	0.56265 (4)	0.37499 (2)	0.42733 (2)	0.01720 (8)
I4	0.86535 (4)	0.57849 (3)	0.43598 (2)	0.02386 (9)
I5	0.94585 (4)	0.31576 (2)	0.36841 (2)	0.01848 (8)
Cu1	0.54781 (7)	0.37680 (5)	0.29914 (3)	0.02033 (15)
Cu2	0.66236 (8)	0.51822 (5)	0.37611 (4)	0.02271 (16)
Cu3	0.70471 (8)	0.25615 (5)	0.37001 (4)	0.02565 (17)

Cu4	0.82108 (8)	0.41564 (5)	0.44393 (3)	0.02331 (17)
Cu5	-0.20413 (7)	0.33294 (5)	0.26739 (3)	0.02026 (15)
S1	0.34593 (14)	0.43635 (11)	0.30651 (6)	0.0186 (3)
S2	-0.07396 (14)	0.26026 (9)	0.20079 (7)	0.0171 (3)
N1	0.1496 (4)	0.4811 (3)	0.2368 (2)	0.0137 (9)
N2	0.1736 (5)	0.2949 (3)	0.1842 (2)	0.0137 (9)
N3	0.5164 (6)	0.5995 (4)	0.3895 (3)	0.0252 (12)
N4	0.8406 (5)	0.3708 (4)	0.5278 (2)	0.0247 (12)
N5	0.7002 (6)	0.1590 (4)	0.4287 (3)	0.0291 (13)
C1	0.2664 (5)	0.4459 (4)	0.2406 (3)	0.0146 (10)
C2	0.3247 (5)	0.4147 (4)	0.1824 (2)	0.0146 (11)
C3	0.4276 (6)	0.4589 (4)	0.1551 (3)	0.0183 (12)
H3	0.460348	0.510001	0.172960	0.022*
C4	0.4811 (6)	0.4274 (5)	0.1019 (3)	0.0243 (14)
H4	0.549956	0.457778	0.082978	0.029*
C5	0.4365 (7)	0.3530 (4)	0.0761 (3)	0.0264 (14)
H5	0.476191	0.331549	0.040234	0.032*
C6	0.3332 (6)	0.3085 (4)	0.1023 (3)	0.0205 (12)
H6	0.300958	0.257562	0.084093	0.025*
C7	0.2783 (6)	0.3404 (4)	0.1556 (2)	0.0148 (10)
C8	0.2058 (6)	0.2118 (4)	0.2115 (3)	0.0188 (12)
H8A	0.147716	0.200725	0.245840	0.028*
H8B	0.295715	0.212767	0.225807	0.028*
H8C	0.195483	0.166487	0.180990	0.028*
C9	0.0516 (6)	0.3225 (4)	0.1803 (2)	0.0131 (10)
C10	0.0287 (5)	0.4096 (4)	0.1547 (2)	0.0133 (10)
C11	-0.0468 (6)	0.4158 (4)	0.1014 (3)	0.0194 (11)
H11	-0.081801	0.365422	0.083474	0.023*
C12	-0.0700 (6)	0.4947 (4)	0.0752 (3)	0.0229 (12)
H12	-0.120764	0.498629	0.039303	0.027*
C13	-0.0193 (6)	0.5681 (4)	0.1012 (3)	0.0211 (12)
H13	-0.033879	0.622154	0.082425	0.025*
C14	0.0522 (6)	0.5638 (4)	0.1543 (3)	0.0183 (11)
H14	0.083786	0.614743	0.172730	0.022*
C15	0.0779 (5)	0.4841 (4)	0.1805 (2)	0.0130 (10)
C16	0.0901 (6)	0.5224 (4)	0.2902 (3)	0.0194 (12)
H16A	0.073045	0.479154	0.321514	0.029*
H16B	0.008462	0.549723	0.278202	0.029*
H16C	0.149314	0.565976	0.306415	0.029*
C17	0.4278 (7)	0.6393 (4)	0.3998 (3)	0.0267 (14)

C18	0.3110 (8)	0.6897 (6)	0.4136 (4)	0.043 (2)
H18A	0.308117	0.740264	0.387122	0.064*
H18B	0.313215	0.708007	0.456175	0.064*
H18C	0.233890	0.654372	0.406518	0.064*
C19	0.8251 (6)	0.3390 (4)	0.5739 (3)	0.0230 (13)
C20	0.8007 (6)	0.3014 (5)	0.6333 (3)	0.0294 (15)
H20A	0.718558	0.269838	0.632347	0.044*
H20B	0.795759	0.346993	0.663861	0.044*
H20C	0.871319	0.261985	0.643656	0.044*
C21	0.7015 (7)	0.1098 (5)	0.4659 (3)	0.0294 (15)
C22	0.7066 (8)	0.0459 (6)	0.5148 (4)	0.042 (2)
H22A	0.761235	-0.002330	0.502164	0.063*
H22B	0.618862	0.025148	0.523481	0.063*
H22C	0.743124	0.072191	0.551498	0.063*

Atomic displacement parameters (Å^2) for **[Cu_5I_5{(*R*)-(−)-(mdta)}$(MeCN)_3]_n$ (2)**

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01729 (16)	0.02011 (19)	0.02700 (19)	-0.00484 (14)	0.00588 (15)	-0.00578 (16)
I2	0.01650 (17)	0.01407 (17)	0.01833 (16)	-0.00090 (13)	-0.00173 (14)	0.00114 (13)
I3	0.01749 (16)	0.02035 (18)	0.01376 (15)	0.00171 (14)	-0.00029 (14)	-0.00061 (14)
I4	0.0287 (2)	0.0207 (2)	0.02219 (18)	0.00027 (16)	-0.01072 (16)	-0.00106 (15)
I5	0.01735 (16)	0.01677 (17)	0.02134 (17)	0.00264 (14)	-0.00090 (15)	-0.00046 (14)
Cu1	0.0143 (3)	0.0216 (4)	0.0251 (4)	0.0011 (3)	0.0002 (3)	0.0017 (3)
Cu2	0.0235 (4)	0.0210 (4)	0.0237 (4)	0.0032 (3)	-0.0042 (3)	-0.0007 (3)
Cu3	0.0261 (4)	0.0224 (4)	0.0285 (4)	0.0001 (3)	0.0056 (3)	0.0032 (3)
Cu4	0.0278 (4)	0.0251 (4)	0.0171 (3)	0.0048 (3)	-0.0001 (3)	0.0026 (3)
Cu5	0.0182 (3)	0.0184 (4)	0.0242 (4)	0.0010 (3)	0.0056 (3)	-0.0001 (3)
S1	0.0149 (6)	0.0269 (8)	0.0140 (6)	0.0038 (6)	-0.0032 (5)	-0.0011 (6)
S2	0.0156 (6)	0.0127 (7)	0.0229 (7)	-0.0025 (5)	0.0055 (5)	-0.0016 (5)
N1	0.012 (2)	0.015 (2)	0.014 (2)	-0.0026 (18)	-0.0010 (18)	0.0011 (18)
N2	0.015 (2)	0.013 (2)	0.013 (2)	0.0009 (18)	-0.0028 (17)	0.0010 (17)
N3	0.026 (3)	0.019 (3)	0.030 (3)	0.006 (2)	-0.006 (2)	-0.001 (2)
N4	0.025 (3)	0.030 (3)	0.019 (2)	0.004 (2)	0.000 (2)	0.001 (2)
N5	0.028 (3)	0.024 (3)	0.035 (3)	0.003 (2)	0.012 (3)	0.008 (3)
C1	0.013 (2)	0.013 (3)	0.018 (2)	-0.001 (2)	-0.001 (2)	0.000 (2)
C2	0.015 (2)	0.015 (3)	0.014 (2)	0.004 (2)	-0.001 (2)	0.003 (2)
C3	0.016 (3)	0.020 (3)	0.018 (3)	-0.001 (2)	-0.003 (2)	-0.001 (2)
C4	0.019 (3)	0.032 (4)	0.023 (3)	-0.005 (3)	0.003 (2)	0.006 (3)
C5	0.027 (3)	0.029 (3)	0.023 (3)	0.001 (3)	0.011 (3)	-0.001 (3)
C6	0.023 (3)	0.018 (3)	0.021 (3)	0.001 (2)	0.006 (2)	-0.002 (2)

C7	0.013 (2)	0.015 (3)	0.016 (2)	-0.001 (2)	-0.001 (2)	0.000 (2)
C8	0.026 (3)	0.011 (3)	0.019 (3)	0.005 (2)	-0.002 (2)	0.006 (2)
C9	0.016 (2)	0.012 (2)	0.011 (2)	-0.003 (2)	0.003 (2)	-0.0031 (19)
C10	0.011 (2)	0.013 (3)	0.017 (2)	-0.0017 (19)	0.001 (2)	0.001 (2)
C11	0.019 (3)	0.017 (3)	0.022 (3)	-0.004 (2)	-0.004 (2)	0.001 (2)
C12	0.021 (3)	0.028 (3)	0.019 (3)	0.000 (3)	-0.006 (2)	0.006 (2)
C13	0.016 (3)	0.021 (3)	0.027 (3)	0.004 (2)	-0.003 (2)	0.008 (2)
C14	0.018 (3)	0.015 (3)	0.022 (3)	-0.002 (2)	-0.001 (2)	0.002 (2)
C15	0.012 (2)	0.013 (3)	0.014 (2)	0.000 (2)	-0.002 (2)	0.0013 (19)
C16	0.016 (3)	0.022 (3)	0.021 (3)	0.001 (2)	-0.001 (2)	-0.004 (2)
C17	0.031 (4)	0.023 (3)	0.026 (3)	0.001 (3)	-0.005 (3)	-0.001 (3)
C18	0.031 (4)	0.050 (5)	0.047 (5)	0.018 (4)	-0.003 (3)	-0.006 (4)
C19	0.018 (3)	0.029 (3)	0.022 (3)	0.005 (2)	-0.007 (2)	-0.001 (3)
C20	0.021 (3)	0.043 (4)	0.025 (3)	0.004 (3)	0.003 (3)	0.010 (3)
C21	0.022 (3)	0.028 (4)	0.038 (4)	-0.003 (3)	0.001 (3)	0.000 (3)
C22	0.039 (4)	0.048 (5)	0.040 (4)	-0.016 (4)	-0.010 (4)	0.020 (4)

Geometric parameters (Å, °) for **$[Cu_5I_5\{(R)$-(−)-(mdta)$\}(MeCN)_3]_n$ (2)**

I1—Cu1	2.6489 (9)	C2—C7	1.384 (8)
I1—Cu3	2.6454 (10)	C3—H3	0.9500
I1—Cu5^{i}	2.7240 (8)	C3—C4	1.384 (9)
I2—Cu1	2.6474 (9)	C4—H4	0.9500
I2—Cu2	2.6695 (9)	C4—C5	1.370 (10)
I2—Cu5^{i}	2.5801 (9)	C5—H5	0.9500
I3—Cu1	2.8231 (8)	C5—C6	1.395 (9)
I3—Cu2	2.7039 (9)	C6—H6	0.9500
I3—Cu3	2.6775 (9)	C6—C7	1.395 (8)
I3—Cu4	2.7648 (9)	C8—H8A	0.9800
I4—Cu2	2.6462 (9)	C8—H8B	0.9800
I4—Cu4	2.5853 (10)	C8—H8C	0.9800
I5—Cu3	2.6561 (9)	C9—C10	1.489 (8)
I5—Cu4	2.6151 (9)	C10—C11	1.410 (8)
I5—Cu5^{i}	2.7205 (9)	C10—C15	1.388 (8)
Cu1—Cu2	3.0201 (11)	C11—H11	0.9500
Cu1—Cu3	2.9302 (11)	C11—C12	1.379 (9)
Cu1—Cu5^{i}	2.7396 (11)	C12—H12	0.9500
Cu1—S1	2.2862 (17)	C12—C13	1.381 (9)
Cu2—Cu4	2.7317 (11)	C13—H13	0.9500
Cu2—N3	1.990 (6)	C13—C14	1.382 (8)
Cu3—Cu5^{i}	2.7219 (11)	C14—H14	0.9500

Cu3—N5	1.991 (6)	C14—C15	1.395 (8)
Cu4—N4	1.982 (5)	C16—H16A	0.9800
Cu5—S2	2.2873 (16)	C16—H16B	0.9800
S1—C1	1.672 (6)	C16—H16C	0.9800
S2—C9	1.680 (6)	C17—C18	1.469 (10)
N1—C1	1.327 (7)	C18—H18A	0.9800
N1—C15	1.443 (7)	C18—H18B	0.9800
N1—C16	1.473 (7)	C18—H18C	0.9800
N2—C7	1.437 (7)	C19—C20	1.453 (9)
N2—C8	1.464 (7)	C20—H20A	0.9800
N2—C9	1.333 (7)	C20—H20B	0.9800
N3—C17	1.129 (9)	C20—H20C	0.9800
N4—C19	1.139 (8)	C21—C22	1.466 (10)
N5—C21	1.122 (9)	C22—H22A	0.9800
C1—C2	1.496 (8)	C22—H22B	0.9800
C2—C3	1.400 (8)	C22—H22C	0.9800
Cu1—I1—Cu5^{i}	61.29 (2)	S2—Cu5—I5^{ii}	98.05 (5)
Cu3—I1—Cu1	67.21 (3)	S2—Cu5—Cu1^{ii}	146.65 (5)
Cu3—I1—Cu5^{i}	60.90 (3)	S2—Cu5—Cu3^{ii}	121.05 (5)
Cu1—I2—Cu2	69.22 (3)	C1—S1—Cu1	114.9 (2)
Cu5^{i}—I2—Cu1	63.19 (3)	C9—S2—Cu5	109.8 (2)
Cu5^{i}—I2—Cu2	99.07 (3)	C1—N1—C15	122.2 (5)
Cu2—I3—Cu1	66.20 (2)	C1—N1—C16	120.6 (5)
Cu2—I3—Cu4	59.92 (2)	C15—N1—C16	117.1 (5)
Cu3—I3—Cu1	64.31 (2)	C7—N2—C8	116.5 (5)
Cu3—I3—Cu2	99.61 (3)	C9—N2—C7	121.4 (5)
Cu3—I3—Cu4	72.11 (3)	C9—N2—C8	121.8 (5)
Cu4—I3—Cu1	100.48 (2)	C17—N3—Cu2	173.3 (6)
Cu4—I4—Cu2	62.94 (3)	C19—N4—Cu4	165.1 (6)
Cu3—I5—Cu5^{i}	60.82 (3)	C21—N5—Cu3	173.3 (6)
Cu4—I5—Cu3	74.86 (3)	N1—C1—S1	122.5 (4)
Cu4—I5—Cu5^{i}	100.36 (3)	N1—C1—C2	116.5 (5)
I1—Cu1—I3	105.67 (3)	C2—C1—S1	121.0 (4)
I1—Cu1—Cu2	140.41 (3)	C3—C2—C1	120.8 (5)
I1—Cu1—Cu3	56.34 (2)	C7—C2—C1	119.8 (5)
I1—Cu1—Cu5^{i}	60.70 (2)	C7—C2—C3	119.5 (5)
I2—Cu1—I1	113.53 (3)	C2—C3—H3	120.3
I2—Cu1—I3	107.47 (3)	C4—C3—C2	119.3 (6)
I2—Cu1—Cu2	55.73 (2)	C4—C3—H3	120.3

I2—Cu1—Cu3	103.58 (3)	C3—C4—H4	119.5
I2—Cu1—Cu5^{i}	57.20 (2)	C5—C4—C3	121.1 (6)
I3—Cu1—Cu2	55.00 (2)	C5—C4—H4	119.5
I3—Cu1—Cu3	55.43 (2)	C4—C5—H5	119.8
Cu3—Cu1—Cu2	87.38 (3)	C4—C5—C6	120.4 (6)
Cu5^{i}—Cu1—I3	101.61 (3)	C6—C5—H5	119.8
Cu5^{i}—Cu1—Cu2	87.67 (3)	C5—C6—H6	120.6
Cu5^{i}—Cu1—Cu3	57.26 (3)	C7—C6—C5	118.7 (6)
S1—Cu1—I1	125.31 (5)	C7—C6—H6	120.6
S1—Cu1—I2	111.17 (5)	C2—C7—N2	119.2 (5)
S1—Cu1—I3	89.01 (4)	C2—C7—C6	121.0 (5)
S1—Cu1—Cu2	91.17 (5)	C6—C7—N2	119.8 (5)
S1—Cu1—Cu3	136.57 (5)	N2—C8—H8A	109.5
S1—Cu1—Cu5^{i}	166.07 (6)	N2—C8—H8B	109.5
I2—Cu2—I3	110.39 (3)	N2—C8—H8C	109.5
I2—Cu2—Cu1	55.04 (2)	H8A—C8—H8B	109.5
I2—Cu2—Cu4	107.28 (3)	H8A—C8—H8C	109.5
I3—Cu2—Cu1	58.79 (2)	H8B—C8—H8C	109.5
I3—Cu2—Cu4	61.14 (3)	N2—C9—S2	121.6 (4)
I4—Cu2—I2	111.28 (3)	N2—C9—C10	118.0 (5)
I4—Cu2—I3	112.77 (3)	C10—C9—S2	120.4 (4)
I4—Cu2—Cu1	147.96 (3)	C11—C10—C9	117.7 (5)
I4—Cu2—Cu4	57.44 (3)	C15—C10—C9	123.3 (5)
Cu4—Cu2—Cu1	96.51 (3)	C15—C10—C11	119.0 (5)
N3—Cu2—I2	114.37 (16)	C10—C11—H11	119.9
N3—Cu2—I3	100.17 (17)	C12—C11—C10	120.2 (6)
N3—Cu2—I4	107.43 (16)	C12—C11—H11	119.9
N3—Cu2—Cu1	104.56 (17)	C11—C12—H12	120.0
N3—Cu2—Cu4	138.24 (16)	C11—C12—C13	120.0 (5)
I1—Cu3—I3	110.06 (3)	C13—C12—H12	120.0
I1—Cu3—I5	117.32 (3)	C12—C13—H13	119.7
I1—Cu3—Cu1	56.45 (2)	C12—C13—C14	120.7 (6)
I1—Cu3—Cu5^{i}	60.98 (3)	C14—C13—H13	119.7
I3—Cu3—Cu1	60.25 (2)	C13—C14—H14	120.2
I3—Cu3—Cu5^{i}	105.97 (3)	C13—C14—C15	119.6 (6)
I5—Cu3—I3	106.08 (3)	C15—C14—H14	120.2
I5—Cu3—Cu1	106.62 (3)	C10—C15—N1	120.8 (5)
I5—Cu3—Cu5^{i}	60.76 (3)	C10—C15—C14	120.4 (5)
Cu5^{i}—Cu3—Cu1	57.84 (3)	C14—C15—N1	118.8 (5)
N5—Cu3—I1	112.82 (19)	N1—C16—H16A	109.5

N5—Cu3—I3	102.03 (17)	N1—C16—H16B	109.5
N5—Cu3—I5	107.25 (18)	N1—C16—H16C	109.5
N5—Cu3—Cu1	145.12 (17)	H16A—C16—H16B	109.5
N5—Cu3—Cu5^{i}	151.67 (17)	H16A—C16—H16C	109.5
I4—Cu4—I3	112.74 (3)	H16B—C16—H16C	109.5
I4—Cu4—I5	117.04 (3)	N3—C17—C18	179.0 (8)
I4—Cu4—Cu2	59.62 (3)	C17—C18—H18A	109.5
I5—Cu4—I3	104.74 (3)	C17—C18—H18B	109.5
I5—Cu4—Cu2	107.28 (3)	C17—C18—H18C	109.5
Cu2—Cu4—I3	58.93 (3)	H18A—C18—H18B	109.5
N4—Cu4—I3	98.04 (17)	H18A—C18—H18C	109.5
N4—Cu4—I4	113.04 (18)	H18B—C18—H18C	109.5
N4—Cu4—I5	109.30 (17)	N4—C19—C20	177.3 (7)
N4—Cu4—Cu2	140.83 (16)	C19—C20—H20A	109.5
I1^{ii}—Cu5—Cu1^{ii}	58.00 (2)	C19—C20—H20B	109.5
I2^{ii}—Cu5—I1^{ii}	113.25 (3)	C19—C20—H20C	109.5
I2^{ii}—Cu5—I5^{ii}	108.89 (3)	H20A—C20—H20B	109.5
I2^{ii}—Cu5—Cu1^{ii}	59.60 (2)	H20A—C20—H20C	109.5
I2^{ii}—Cu5—Cu3^{ii}	111.61 (3)	H20B—C20—H20C	109.5
I5^{ii}—Cu5—I1^{ii}	112.54 (3)	N5—C21—C22	178.6 (8)
I5^{ii}—Cu5—Cu1^{ii}	110.36 (3)	C21—C22—H22A	109.5
I5^{ii}—Cu5—Cu3^{ii}	58.42 (3)	C21—C22—H22B	109.5
Cu3^{ii}—Cu5—I1^{ii}	58.13 (3)	C21—C22—H22C	109.5
Cu3^{ii}—Cu5—Cu1^{ii}	64.89 (3)	H22A—C22—H22B	109.5
S2—Cu5—I1^{ii}	95.57 (5)	H22A—C22—H22C	109.5
S2—Cu5—I2^{ii}	127.34 (5)	H22B—C22—H22C	109.5

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*-1, *y*, *z*.

Crystal data for **[Cu_2Br_2(mdta)]$_n$ (3)**

$C_{16}H_{14}Br_2Cu_2N_2S_2$	F(000) = 1136
M_r = 585.31	D_x = 2.081 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, λ = 0.71073 Å
a = 13.306 (3) Å	Cell parameters from 26739 reflections
b = 10.4481 (12) Å	θ = 2.0–29.7°
c = 13.639 (3) Å	μ = 6.78 mm^{-1}
β = 99.860 (15)°	T = 120 K
V = 1868.1 (6) Å^3	Prism, yellow
Z = 4	0.45 × 0.31 × 0.28 mm

Data collection

STOE IPDS 2T diffractometer	5043 independent reflections
Radiation source: GeniX Mo, 0.05 x 0.05 mm2 microfocus	4157 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	$R_{int} = 0.085$
rotation method, ω scans	$\theta_{max} = 29.3°$, $\theta_{min} = 2.0°$
Absorption correction: integration STOE *X-RED32*, absorption correction by Gaussian integration, analogous to P. Coppens, "The Evaluation of Absorption and Extinction in Single-Crystal Structure Analysis", published in F. R. Ahmed (Editor), "Crystallographic Computing", Munksgaard, Copenhagen (1970), 255 - 270	$h = -18 \rightarrow 18$
$T_{min} = 0.099$, $T_{max} = 0.207$	$k = -14 \rightarrow 14$
24955 measured reflections	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	Primary atom site location: dual
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.053$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.147$	H-atom parameters constrained
$S = 1.06$	$w = 1/[\sigma^2(F_o^2) + (0.1022P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
5043 reflections	$(\Delta/\sigma)_{max} = 0.001$
219 parameters	$\Delta\rangle_{max} = 1.49$ e Å^{-3}
0 restraints	$\Delta\rangle_{min} = -1.32$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for **$[Cu_2Br_2(mdta)]_n$ (3)**

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.84996 (4)	0.16475 (4)	0.65221 (3)	0.03039 (14)
Br2	0.88057 (3)	0.01037 (4)	0.39356 (3)	0.02060 (12)

Cu1	0.87147 (4)	0.20853 (5)	0.48670 (4)	0.02396 (15)
Cu2	0.92234 (4)	0.97163 (5)	0.58141 (4)	0.02592 (15)
S1	0.90198 (8)	0.38935 (9)	0.41274 (8)	0.0206 (2)
S2	0.90186 (8)	0.78656 (9)	0.65983 (7)	0.0187 (2)
N1	0.8140 (3)	0.6157 (3)	0.3972 (2)	0.0168 (6)
N2	0.7902 (3)	0.5778 (3)	0.6253 (2)	0.0165 (6)
C1	0.8107 (3)	0.4946 (3)	0.4285 (3)	0.0172 (7)
C2	0.7224 (3)	0.4564 (3)	0.4746 (3)	0.0177 (7)
C3	0.6494 (3)	0.3734 (4)	0.4229 (3)	0.0237 (8)
H3	0.655103	0.345934	0.357639	0.028*
C4	0.5685 (4)	0.3310 (4)	0.4670 (4)	0.0282 (9)
H4	0.518446	0.275498	0.431629	0.034*
C5	0.5613 (4)	0.3697 (5)	0.5621 (4)	0.0298 (9)
H5	0.506974	0.338777	0.592600	0.036*
C6	0.6324 (3)	0.4533 (4)	0.6141 (3)	0.0225 (8)
H6	0.626432	0.480407	0.679365	0.027*
C7	0.7119 (3)	0.4966 (3)	0.5699 (3)	0.0175 (7)
C8	0.8525 (3)	0.5210 (4)	0.7133 (3)	0.0215 (8)
H8A	0.827627	0.434534	0.723591	0.032*
H8B	0.847939	0.573808	0.771745	0.032*
H8C	0.923692	0.516470	0.703549	0.032*
C9	0.8071 (3)	0.6972 (3)	0.5976 (3)	0.0144 (7)
C10	0.7371 (3)	0.7524 (3)	0.5106 (3)	0.0152 (7)
C11	0.6748 (3)	0.8551 (4)	0.5252 (3)	0.0207 (8)
H11	0.675408	0.887348	0.590394	0.025*
C12	0.6119 (3)	0.9107 (4)	0.4449 (3)	0.0228 (8)
H12	0.568518	0.979805	0.455156	0.027*
C13	0.6126 (3)	0.8650 (4)	0.3495 (3)	0.0210 (8)
H13	0.568953	0.902722	0.294704	0.025*
C14	0.7395 (3)	0.7094 (3)	0.4150 (3)	0.0162 (7)
C15	0.6765 (3)	0.7646 (4)	0.3332 (3)	0.0194 (7)
H15	0.677328	0.734090	0.267729	0.023*
C16	0.8948 (4)	0.6584 (4)	0.3442 (3)	0.0230 (8)
H16A	0.961505	0.637294	0.383508	0.034*
H16B	0.889825	0.751234	0.334082	0.034*
H16C	0.887230	0.615385	0.279507	0.034*

Atomic displacement parameters (Å^2) for **$[Cu_2Br_2(mdta)]_n$ (3)**

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0427 (3)	0.0233 (2)	0.0310 (3)	0.00437 (17)	0.0229 (2)	0.00433 (15)

Br2	0.0203 (2)	0.0197 (2)	0.0226 (2)	-0.00238 (13)	0.00613 (16)	0.00013 (13)
Cu1	0.0249 (3)	0.0213 (3)	0.0272 (3)	0.00055 (19)	0.0088 (2)	0.00380 (19)
Cu2	0.0281 (3)	0.0223 (3)	0.0284 (3)	-0.0033 (2)	0.0078 (2)	0.00169 (19)
S1	0.0246 (5)	0.0194 (4)	0.0203 (5)	0.0029 (4)	0.0114 (4)	0.0011 (3)
S2	0.0182 (5)	0.0194 (4)	0.0177 (5)	-0.0026 (3)	0.0012 (4)	-0.0002 (3)
N1	0.0166 (16)	0.0182 (14)	0.0171 (15)	0.0015 (12)	0.0067 (12)	0.0024 (11)
N2	0.0165 (15)	0.0225 (15)	0.0109 (14)	-0.0041 (12)	0.0034 (12)	0.0017 (11)
C1	0.022 (2)	0.0175 (15)	0.0129 (17)	-0.0026 (13)	0.0061 (15)	-0.0028 (12)
C2	0.0192 (19)	0.0184 (16)	0.0173 (18)	-0.0009 (13)	0.0082 (15)	0.0010 (13)
C3	0.028 (2)	0.0236 (17)	0.021 (2)	-0.0105 (16)	0.0070 (17)	-0.0056 (15)
C4	0.022 (2)	0.031 (2)	0.032 (2)	-0.0102 (17)	0.0053 (18)	-0.0040 (17)
C5	0.022 (2)	0.038 (2)	0.032 (2)	-0.0116 (18)	0.0135 (18)	0.0001 (18)
C6	0.022 (2)	0.0277 (19)	0.0201 (19)	-0.0072 (15)	0.0106 (16)	0.0027 (15)
C7	0.0159 (18)	0.0216 (16)	0.0155 (17)	-0.0022 (13)	0.0041 (14)	0.0008 (13)
C8	0.020 (2)	0.0280 (18)	0.0157 (18)	0.0021 (15)	0.0021 (15)	0.0017 (14)
C9	0.0148 (17)	0.0159 (14)	0.0140 (16)	0.0025 (12)	0.0070 (13)	0.0002 (12)
C10	0.0143 (17)	0.0172 (15)	0.0142 (17)	0.0010 (12)	0.0026 (13)	0.0008 (12)
C11	0.0180 (19)	0.0252 (18)	0.0208 (19)	0.0022 (14)	0.0088 (15)	-0.0009 (14)
C12	0.0183 (19)	0.030 (2)	0.021 (2)	0.0055 (15)	0.0068 (16)	0.0033 (15)
C13	0.0165 (19)	0.0260 (18)	0.0205 (19)	0.0031 (15)	0.0028 (15)	0.0063 (15)
C14	0.0151 (17)	0.0181 (16)	0.0163 (18)	-0.0028 (13)	0.0054 (14)	-0.0011 (13)
C15	0.0161 (18)	0.0259 (18)	0.0160 (18)	-0.0006 (14)	0.0025 (15)	0.0019 (14)
C16	0.030 (2)	0.0180 (16)	0.026 (2)	0.0005 (15)	0.0187 (18)	0.0032 (14)

Geometric parameters (Å, °) for **$[Cu_2Br_2(mdta)]_n$ (3)**

Br1—Cu1	2.3682 (8)	N2—C9	1.334 (4)
Br1—Cu2^{i}	2.4998 (7)	C1—C2	1.480 (5)
Br2—Cu1	2.4428 (7)	C2—C3	1.400 (5)
Br2—Cu2^{i}	2.5592 (8)	C2—C7	1.395 (5)
Br2—Cu2^{ii}	2.5927 (9)	C3—C4	1.393 (6)
Cu1—Cu2^{i}	2.8202 (8)	C4—C5	1.378 (7)
Cu1—S1	2.2118 (11)	C5—C6	1.390 (6)
Cu2—S2	2.2488 (11)	C6—C7	1.380 (5)
S1—C1	1.679 (4)	C9—C10	1.493 (5)
S2—C9	1.678 (4)	C10—C11	1.390 (5)
N1—C1	1.338 (5)	C10—C14	1.385 (5)
N1—C14	1.444 (5)	C11—C12	1.387 (6)
N1—C16	1.464 (5)	C12—C13	1.387 (6)
N2—C7	1.451 (5)	C13—C15	1.392 (6)
N2—C8	1.463 (5)	C14—C15	1.400 (5)

Cu1—Br1—Cu2^{i}	70.75 (2)	C9—N2—C8	120.8 (3)
Cu1—Br2—Cu2^{i}	68.59 (2)	N1—C1—S1	121.0 (3)
Cu1—Br2—Cu2^{ii}	90.52 (2)	N1—C1—C2	117.6 (3)
Cu2^{i}—Br2—Cu2^{ii}	80.70 (3)	C2—C1—S1	121.4 (3)
Br1—Cu1—Br2	110.91 (2)	C3—C2—C1	119.1 (4)
Br1—Cu1—Cu2^{i}	56.81 (2)	C7—C2—C1	121.9 (4)
Br2—Cu1—Cu2^{i}	57.66 (2)	C7—C2—C3	119.0 (4)
S1—Cu1—Br1	131.40 (4)	C4—C3—C2	120.0 (4)
S1—Cu1—Br2	117.22 (4)	C5—C4—C3	119.8 (4)
S1—Cu1—Cu2^{i}	155.53 (4)	C4—C5—C6	120.9 (4)
Br1^{iii}—Cu2—Br2^{ii}	109.78 (3)	C7—C6—C5	119.2 (4)
Br1^{iii}—Cu2—Br2^{iii}	103.13 (3)	C2—C7—N2	118.9 (3)
Br1^{iii}—Cu2—Cu1^{iii}	52.44 (2)	C6—C7—N2	119.9 (4)
Br2^{iii}—Cu2—Br2^{ii}	99.30 (3)	C6—C7—C2	121.0 (4)
Br2^{iii}—Cu2—Cu1^{iii}	53.751 (18)	N2—C9—S2	121.7 (3)
Br2^{ii}—Cu2—Cu1^{iii}	98.90 (2)	N2—C9—C10	118.2 (3)
S2—Cu2—Br1^{iii}	115.10 (4)	C10—C9—S2	120.0 (3)
S2—Cu2—Br2^{iii}	126.08 (3)	C11—C10—C9	119.4 (3)
S2—Cu2—Br2^{ii}	101.65 (3)	C14—C10—C9	120.7 (3)
S2—Cu2—Cu1^{iii}	158.97 (4)	C14—C10—C11	119.7 (4)
C1—S1—Cu1	107.94 (14)	C12—C11—C10	120.3 (4)
C9—S2—Cu2	112.32 (13)	C13—C12—C11	119.8 (4)
C1—N1—C14	121.8 (3)	C12—C13—C15	120.8 (4)
C1—N1—C16	120.9 (3)	C10—C14—N1	120.4 (3)
C14—N1—C16	117.4 (3)	C10—C14—C15	120.7 (4)
C7—N2—C8	116.5 (3)	C15—C14—N1	118.7 (3)
C9—N2—C7	122.7 (3)	C13—C15—C14	118.8 (4)

Symmetry codes: (i) *x*, *y*-1, *z*; (ii) -*x*+2, -*y*+1, -*z*+1; (iii) *x*, *y*+1, *z*.

Crystal data for **[Cu_3Br_3{(*R*)-(−)-(mdta)}$_2$(MeCN)]$_n$ (4)**

$C_{32}H_{28}Br_3Cu_3N_4S_4 \cdot C_2H_3N$	$F(000)$ = 1052
M_r = 1068.23	D_x = 1.808 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation, λ = 0.71073 Å
a = 8.7415 (4) Å	Cell parameters from 22871 reflections
b = 17.1309 (8) Å	θ = 2.0–29.4°
c = 13.1531 (6) Å	μ = 4.91 mm^{-1}
β = 95.007 (3)°	T = 120 K

V = 1962.16 (16) Å^3	Block, yellow
Z = 2	0.41 × 0.08 × 0.05 mm

Data collection

STOE IPDS 2T diffractometer	7709 independent reflections
Radiation source: GeniX Mo, 0.05 x 0.05 mm2 microfocus	5814 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	R_{int} = 0.086
rotation method, ω scans	θ_{max} = 26.0°, θ_{min} = 2.0°
Absorption correction: integration STOE *X-RED32*, absorption correction by Gaussian integration, analogous to P. Coppens, "The Evaluation of Absorption and Extinction in Single-Crystal Structure Analysis", published in F. R. Ahmed (Editor), "Crystallographic Computing", Munksgaard, Copenhagen (1970), 255 - 270	h = -10→10
T_{min} = 0.187, T_{max} = 0.535	k = -21→21
19182 measured reflections	l = -16→16

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.105	H-atom parameters constrained
$wR(F^2)$ = 0.293	$w = 1/[\sigma^2(F_o^2) + (0.1897P)^2 + 10.6517P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max} < 0.001$
7709 reflections	$\Delta\rangle_{max}$ = 4.18 e Å^{-3}
447 parameters	$\Delta\rangle_{min}$ = -1.42 e Å^{-3}
1 restraint	Absolute structure: Classical Flack method preferred over Parsons because s.u. lower.
Primary atom site location: structure-invariant direct methods	Absolute structure parameter: 0.00 (3)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for **[Cu_3Br_3{(*R*)-(−)-(mdta)}$_2$(MeCN)]$_n$ (4)**

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.0953 (3)	0.29999 (14)	0.31854 (19)	0.0490 (5)
Br2	0.4311 (3)	0.42516 (12)	0.19249 (19)	0.0531 (7)
Br3	0.3912 (3)	0.17470 (12)	0.16822 (19)	0.0516 (6)
Cu1	0.2182 (3)	0.44158 (16)	0.3014 (2)	0.0535 (8)
Cu2	-0.1594 (3)	0.65741 (15)	-0.2625 (2)	0.0509 (8)
Cu3	0.3218 (4)	0.3013 (2)	0.2221 (3)	0.0583 (8)
S1	0.2403 (7)	0.4822 (3)	0.4648 (5)	0.0526 (15)
S2	0.7912 (7)	0.6261 (3)	0.5684 (5)	0.0519 (14)
S3	0.0618 (7)	0.6102 (4)	-0.1838 (5)	0.0540 (15)
S4	-0.0030 (7)	0.4774 (3)	0.2054 (5)	0.0500 (14)
N1	0.450 (2)	0.4798 (11)	0.6223 (15)	0.054 (5)
N2	0.692 (2)	0.5036 (11)	0.4590 (16)	0.050 (5)
N3	0.211 (2)	0.6076 (12)	-0.0011 (15)	0.050 (5)
N4	-0.102 (2)	0.5966 (10)	0.0895 (15)	0.045 (4)
C1	0.406 (3)	0.4532 (13)	0.5288 (17)	0.047 (5)
C2	0.510 (2)	0.3992 (12)	0.4814 (16)	0.041 (5)
C3	0.466 (2)	0.3210 (12)	0.4646 (18)	0.045 (5)
H3	0.372224	0.302545	0.486742	0.054*
C4	0.559 (3)	0.2716 (14)	0.4165 (18)	0.051 (6)
H4	0.530606	0.218243	0.409382	0.061*
C5	0.692 (3)	0.2961 (14)	0.378 (2)	0.054 (6)
H5	0.751131	0.260662	0.341818	0.065*
C6	0.742 (3)	0.3747 (13)	0.3928 (19)	0.053 (6)
H6	0.835094	0.393253	0.369072	0.064*
C7	0.646 (2)	0.4227 (13)	0.4444 (16)	0.044 (5)
C8	0.694 (3)	0.5527 (13)	0.3644 (18)	0.052 (6)
H8A	0.615890	0.593827	0.365670	0.078*
H8B	0.670529	0.519792	0.304053	0.078*
H8C	0.795161	0.576420	0.361833	0.078*
C9	0.736 (2)	0.5336 (13)	0.5525 (18)	0.046 (5)
C10	0.733 (3)	0.4815 (12)	0.6413 (19)	0.053 (6)
C11	0.870 (2)	0.4572 (14)	0.6942 (19)	0.050 (5)
H11	0.964438	0.471075	0.669029	0.060*
C12	0.870 (3)	0.4152 (13)	0.779 (2)	0.055 (6)
H12	0.965389	0.401159	0.815249	0.066*
C13	0.734 (3)	0.3918 (13)	0.816 (2)	0.064 (8)

H13	0.734997	0.360482	0.875368	0.076*
C14	0.591 (3)	0.4149 (16)	0.764 (2)	0.061 (6)
H14	0.496456	0.401763	0.789276	0.073*
C15	0.596 (3)	0.4570 (12)	0.6746 (18)	0.048 (5)
C16	0.356 (3)	0.5322 (16)	0.6746 (19)	0.057 (6)
H16A	0.265843	0.503951	0.695215	0.086*
H16B	0.321760	0.575239	0.629088	0.086*
H16C	0.414817	0.553022	0.735335	0.086*
C17	0.096 (2)	0.6365 (12)	-0.0610 (16)	0.042 (5)
C18	-0.001 (3)	0.6965 (12)	-0.0173 (17)	0.048 (6)
C19	-0.005 (3)	0.7759 (13)	-0.0522 (18)	0.048 (5)
H19	0.060331	0.792918	-0.101786	0.058*
C20	-0.106 (3)	0.8267 (13)	-0.0125 (18)	0.049 (5)
H20	-0.108157	0.879234	-0.035824	0.058*
C21	-0.201 (3)	0.8061 (15)	0.057 (2)	0.056 (6)
H21	-0.269935	0.843333	0.081132	0.067*
C22	-0.198 (2)	0.7302 (11)	0.0952 (18)	0.042 (5)
H22	-0.262504	0.715460	0.146545	0.050*
C23	-0.100 (3)	0.6764 (12)	0.0565 (17)	0.046 (5)
C24	-0.239 (3)	0.5494 (15)	0.058 (2)	0.053 (6)
H24A	-0.299119	0.574941	0.001288	0.079*
H24B	-0.302722	0.544426	0.116050	0.079*
H24C	-0.207804	0.497377	0.037297	0.079*
C25	0.010 (3)	0.5670 (12)	0.1544 (17)	0.045 (5)
C26	0.152 (3)	0.6156 (12)	0.1768 (19)	0.050 (6)
C27	0.191 (3)	0.6384 (13)	0.2790 (18)	0.048 (5)
H27	0.129562	0.623470	0.331756	0.057*
C28	0.325 (3)	0.6842 (15)	0.300 (2)	0.063 (7)
H28	0.349189	0.703432	0.367382	0.075*
C29	0.416 (3)	0.7005 (15)	0.229 (3)	0.064 (8)
H29	0.508607	0.728172	0.246244	0.077*
C30	0.377 (3)	0.6770 (16)	0.124 (2)	0.060 (6)
H30	0.441004	0.689578	0.071677	0.072*
C31	0.243 (2)	0.6355 (11)	0.1048 (19)	0.045 (5)
C32	0.313 (3)	0.5476 (13)	-0.039 (2)	0.054 (6)
H32A	0.376585	0.570923	-0.088282	0.081*
H32B	0.250825	0.505450	-0.071091	0.081*
H32C	0.379249	0.526560	0.018932	0.081*
N5	0.257 (3)	0.3239 (17)	0.692 (2)	0.084 (8)
C33	0.145 (3)	0.3089 (16)	0.643 (2)	0.055 (6)

C34	0.004 (3)	0.2896 (18)	0.583 (2)	0.064 (7)
H34A	-0.016827	0.328582	0.529143	0.096*
H34B	-0.081226	0.289385	0.627288	0.096*
H34C	0.012860	0.237909	0.552567	0.096*

Atomic displacement parameters (Å^2) for **[Cu_3Br_3{(*R*)-(−)-(mdta)}$_2$(MeCN)]$_n$ (4)**

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0513 (12)	0.0333 (9)	0.0592 (13)	0.0013 (8)	-0.0126 (9)	0.0014 (9)
Br2	0.0534 (13)	0.0414 (13)	0.0602 (14)	-0.0027 (9)	-0.0190 (11)	0.0038 (10)
Br3	0.0521 (13)	0.0386 (12)	0.0600 (14)	0.0017 (9)	-0.0176 (11)	-0.0017 (9)
Cu1	0.0582 (16)	0.0376 (15)	0.0595 (17)	0.0034 (12)	-0.0254 (13)	0.0006 (12)
Cu2	0.0540 (16)	0.0370 (15)	0.0572 (17)	-0.0008 (12)	-0.0203 (13)	-0.0019 (12)
Cu3	0.0626 (18)	0.0376 (13)	0.072 (2)	0.0006 (13)	-0.0120 (14)	0.0017 (14)
S1	0.051 (3)	0.042 (3)	0.060 (4)	0.008 (2)	-0.022 (3)	-0.006 (3)
S2	0.061 (3)	0.033 (3)	0.057 (3)	-0.003 (2)	-0.022 (3)	-0.001 (2)
S3	0.057 (3)	0.045 (3)	0.055 (4)	0.005 (2)	-0.022 (3)	-0.004 (3)
S4	0.051 (3)	0.036 (3)	0.059 (3)	-0.001 (2)	-0.022 (3)	0.007 (2)
N1	0.066 (12)	0.032 (9)	0.056 (12)	-0.001 (8)	-0.035 (9)	-0.010 (8)
N2	0.050 (10)	0.035 (9)	0.061 (12)	-0.001 (7)	-0.024 (9)	-0.004 (8)
N3	0.031 (9)	0.060 (12)	0.055 (12)	0.011 (8)	-0.015 (8)	0.000 (9)
N4	0.040 (9)	0.033 (9)	0.059 (11)	0.005 (7)	-0.023 (8)	-0.008 (8)
C1	0.064 (14)	0.037 (11)	0.038 (11)	-0.011 (10)	-0.009 (10)	-0.004 (9)
C2	0.043 (11)	0.037 (10)	0.038 (11)	-0.005 (8)	-0.022 (9)	0.005 (8)
C3	0.036 (10)	0.036 (11)	0.059 (13)	-0.003 (8)	-0.014 (9)	0.007 (9)
C4	0.055 (13)	0.044 (12)	0.049 (13)	-0.013 (10)	-0.020 (10)	-0.004 (10)
C5	0.052 (13)	0.033 (10)	0.075 (16)	0.000 (10)	-0.018 (11)	-0.005 (11)
C6	0.062 (14)	0.034 (11)	0.059 (14)	0.001 (10)	-0.023 (11)	0.005 (10)
C7	0.041 (11)	0.045 (11)	0.041 (11)	-0.002 (9)	-0.018 (8)	0.010 (9)
C8	0.073 (15)	0.037 (11)	0.043 (12)	-0.001 (10)	-0.017 (11)	-0.005 (9)
C9	0.030 (10)	0.048 (12)	0.058 (13)	-0.004 (9)	-0.010 (9)	0.007 (10)
C10	0.074 (16)	0.026 (10)	0.055 (14)	-0.010 (10)	-0.019 (11)	0.014 (9)
C11	0.033 (10)	0.048 (13)	0.064 (15)	0.005 (9)	-0.017 (10)	-0.003 (11)
C12	0.053 (13)	0.036 (11)	0.070 (16)	0.004 (10)	-0.028 (11)	0.005 (11)
C13	0.10 (2)	0.033 (11)	0.056 (15)	-0.008 (12)	-0.037 (14)	0.006 (10)
C14	0.064 (15)	0.057 (15)	0.057 (15)	-0.006 (12)	-0.017 (12)	-0.021 (12)
C15	0.053 (12)	0.031 (10)	0.054 (13)	0.000 (9)	-0.030 (10)	0.000 (9)
C16	0.054 (13)	0.057 (15)	0.056 (14)	-0.008 (11)	-0.019 (11)	-0.012 (11)
C17	0.042 (11)	0.041 (11)	0.038 (11)	-0.001 (8)	-0.022 (8)	-0.010 (8)
C18	0.055 (13)	0.034 (10)	0.049 (13)	-0.003 (9)	-0.031 (10)	-0.001 (9)
C19	0.048 (12)	0.038 (11)	0.053 (13)	-0.003 (9)	-0.026 (10)	0.003 (10)

C20	0.056 (13)	0.036 (11)	0.050 (13)	0.000 (10)	-0.018 (10)	0.000 (9)
C21	0.050 (13)	0.040 (11)	0.073 (16)	0.004 (10)	-0.027 (11)	-0.012 (12)
C22	0.034 (10)	0.032 (10)	0.059 (13)	0.003 (7)	-0.004 (9)	0.003 (9)
C23	0.048 (12)	0.034 (10)	0.048 (12)	0.002 (9)	-0.029 (10)	0.005 (9)
C24	0.055 (13)	0.049 (13)	0.053 (13)	-0.017 (10)	-0.007 (11)	-0.003 (10)
C25	0.049 (12)	0.037 (11)	0.046 (12)	0.001 (9)	-0.023 (9)	0.005 (9)
C26	0.045 (12)	0.031 (10)	0.067 (15)	0.000 (9)	-0.031 (11)	-0.003 (10)
C27	0.054 (13)	0.038 (12)	0.049 (13)	0.007 (9)	-0.004 (10)	0.002 (9)
C28	0.058 (15)	0.041 (13)	0.083 (19)	0.008 (11)	-0.031 (14)	0.003 (13)
C29	0.056 (15)	0.040 (13)	0.09 (2)	-0.007 (11)	-0.034 (15)	-0.011 (13)
C30	0.041 (12)	0.054 (14)	0.081 (18)	-0.003 (10)	-0.011 (11)	0.010 (13)
C31	0.042 (11)	0.020 (9)	0.068 (15)	0.001 (7)	-0.017 (10)	-0.003 (9)
C32	0.050 (13)	0.029 (10)	0.080 (17)	0.010 (9)	-0.014 (11)	-0.001 (10)
N5	0.059 (14)	0.083 (19)	0.10 (2)	-0.009 (12)	-0.031 (13)	0.021 (15)
C33	0.052 (14)	0.047 (13)	0.066 (16)	-0.005 (11)	0.003 (12)	0.007 (12)
C34	0.065 (16)	0.069 (18)	0.057 (16)	0.006 (13)	-0.005 (12)	0.000 (13)

Geometric parameters (Å, °) for **$[Cu_3Br_3\{(R)$-(−)-(mdta)$\}_2(MeCN)]_n$ (4)**

Br1—Cu1	2.670 (4)	C2—C3	1.40 (3)
Br1—Cu2^{i}	2.626 (4)	C2—C7	1.38 (3)
Br1—Cu3	2.443 (4)	C3—C4	1.37 (3)
Br2—Cu1	2.462 (4)	C4—C5	1.38 (4)
Br2—Cu3	2.373 (4)	C5—C6	1.42 (3)
Br3—Cu2^{i}	2.484 (4)	C6—C7	1.40 (4)
Br3—Cu3	2.377 (4)	C9—C10	1.47 (3)
Cu1—Cu3	2.802 (5)	C10—C11	1.39 (3)
Cu1—S1	2.250 (7)	C10—C15	1.38 (4)
Cu1—S4	2.299 (6)	C11—C12	1.33 (4)
Cu2—Cu3^{ii}	2.916 (4)	C12—C13	1.38 (4)
Cu2—S2^{iii}	2.292 (7)	C13—C14	1.42 (4)
Cu2—S3	2.262 (6)	C14—C15	1.38 (4)
S1—C1	1.68 (2)	C17—C18	1.48 (3)
S2—C9	1.67 (2)	C18—C19	1.43 (3)
S3—C17	1.68 (2)	C18—C23	1.40 (4)
S4—C25	1.68 (2)	C19—C20	1.37 (3)
N1—C1	1.34 (3)	C20—C21	1.34 (4)
N1—C15	1.45 (3)	C21—C22	1.39 (3)
N1—C16	1.43 (3)	C22—C23	1.39 (3)
N2—C7	1.45 (3)	C25—C26	1.50 (3)
N2—C8	1.50 (3)	C26—C27	1.41 (3)

N2—C9	1.36 (3)	C26—C31	1.33 (3)
N3—C17	1.32 (3)	C27—C28	1.41 (4)
N3—C31	1.48 (3)	C28—C29	1.31 (4)
N3—C32	1.47 (3)	C29—C30	1.44 (4)
N4—C23	1.44 (3)	C30—C31	1.37 (3)
N4—C24	1.48 (3)	N5—C33	1.15 (3)
N4—C25	1.34 (3)	C33—C34	1.45 (4)
C1—C2	1.47 (3)		
Cu2^{i}—Br1—Cu1	136.38 (14)	N1—C1—C2	117 (2)
Cu3—Br1—Cu1	66.27 (12)	C2—C1—S1	120.6 (15)
Cu3—Br1—Cu2^{i}	70.14 (12)	C3—C2—C1	120 (2)
Cu3—Br2—Cu1	70.79 (13)	C7—C2—C1	123.2 (19)
Cu3—Br3—Cu2^{i}	73.69 (13)	C7—C2—C3	117 (2)
Br1—Cu1—Cu3	52.97 (10)	C4—C3—C2	120 (2)
Br2—Cu1—Br1	105.99 (13)	C3—C4—C5	123 (2)
Br2—Cu1—Cu3	53.13 (11)	C4—C5—C6	120 (2)
S1—Cu1—Br1	101.7 (2)	C7—C6—C5	116 (2)
S1—Cu1—Br2	125.8 (2)	C2—C7—N2	118 (2)
S1—Cu1—Cu3	128.1 (2)	C2—C7—C6	125 (2)
S1—Cu1—S4	116.1 (3)	C6—C7—N2	117 (2)
S4—Cu1—Br1	87.91 (18)	N2—C9—S2	122.0 (17)
S4—Cu1—Br2	110.7 (2)	N2—C9—C10	118 (2)
S4—Cu1—Cu3	108.0 (2)	C10—C9—S2	120.1 (18)
Br1^{ii}—Cu2—Cu3^{ii}	51.99 (10)	C11—C10—C9	120 (2)
Br3^{ii}—Cu2—Br1^{ii}	103.45 (13)	C15—C10—C9	121 (2)
Br3^{ii}—Cu2—Cu3^{ii}	51.47 (10)	C15—C10—C11	119 (2)
S2^{iii}—Cu2—Br1^{ii}	88.37 (18)	C12—C11—C10	122 (2)
S2^{iii}—Cu2—Br3^{ii}	114.8 (2)	C11—C12—C13	120 (2)
S2^{iii}—Cu2—Cu3^{ii}	108.71 (19)	C12—C13—C14	120 (2)
S3—Cu2—Br1^{ii}	105.5 (2)	C15—C14—C13	118 (3)
S3—Cu2—Br3^{ii}	121.1 (2)	C10—C15—N1	121 (2)
S3—Cu2—Cu3^{ii}	129.0 (2)	C14—C15—N1	117 (2)
S3—Cu2—S2^{iii}	116.2 (3)	C14—C15—C10	121 (2)
Br1—Cu3—Cu1	60.76 (12)	N3—C17—S3	122.5 (17)
Br1—Cu3—Cu2^{i}	57.87 (11)	N3—C17—C18	117.6 (18)
Br2—Cu3—Br1	116.72 (16)	C18—C17—S3	119.9 (14)
Br2—Cu3—Br3	130.53 (17)	C19—C18—C17	122 (2)
Br2—Cu3—Cu1	56.09 (12)	C23—C18—C17	121 (2)
Br2—Cu3—Cu2^{i}	174.25 (17)	C23—C18—C19	117 (2)

Br3—Cu3—Br1	112.72 (15)	C20—C19—C18	119 (2)
Br3—Cu3—Cu1	173.23 (18)	C21—C20—C19	123 (2)
Br3—Cu3—Cu2^{i}	54.84 (11)	C20—C21—C22	120 (2)
Cu1—Cu3—Cu2^{i}	118.61 (15)	C23—C22—C21	119 (2)
C1—S1—Cu1	112.6 (8)	C18—C23—N4	118 (2)
C9—S2—Cu2^{iv}	111.9 (9)	C22—C23—N4	120 (2)
C17—S3—Cu2	114.8 (8)	C22—C23—C18	122 (2)
C25—S4—Cu1	112.3 (8)	N4—C25—S4	121.7 (17)
C1—N1—C15	121 (2)	N4—C25—C26	117.5 (19)
C1—N1—C16	121 (2)	C26—C25—S4	120.8 (15)
C16—N1—C15	117.5 (18)	C27—C26—C25	118 (2)
C7—N2—C8	116.6 (18)	C31—C26—C25	122 (2)
C9—N2—C7	122.2 (19)	C31—C26—C27	120 (2)
C9—N2—C8	121.2 (18)	C26—C27—C28	118 (2)
C17—N3—C31	120.9 (18)	C29—C28—C27	121 (3)
C17—N3—C32	120.9 (19)	C28—C29—C30	121 (2)
C32—N3—C31	118.1 (17)	C31—C30—C29	116 (3)
C23—N4—C24	118.1 (17)	C26—C31—N3	120.8 (18)
C25—N4—C23	121.5 (17)	C26—C31—C30	124 (2)
C25—N4—C24	120.1 (19)	C30—C31—N3	116 (2)
N1—C1—S1	121.9 (19)	N5—C33—C34	179 (3)
Cu1—S1—C1—N1	170.9 (17)	C11—C10—C15—C14	6 (4)
Cu1—S1—C1—C2	-7 (2)	C11—C12—C13—C14	-2 (4)
Cu1—S4—C25—N4	174.9 (18)	C12—C13—C14—C15	3 (4)
Cu1—S4—C25—C26	-3 (2)	C13—C14—C15—N1	180 (2)
Cu2^{iv}—S2—C9—N2	176.2 (16)	C13—C14—C15—C10	-5 (4)
Cu2^{iv}—S2—C9—C10	-4 (2)	C15—N1—C1—S1	-177.3 (17)
Cu2—S3—C17—N3	172.7 (17)	C15—N1—C1—C2	0 (3)
Cu2—S3—C17—C18	-10 (2)	C15—C10—C11—C12	-4 (4)
S1—C1—C2—C3	-70 (2)	C16—N1—C1—S1	3 (3)
S1—C1—C2—C7	105 (2)	C16—N1—C1—C2	-180 (2)
S2—C9—C10—C11	-70 (3)	C16—N1—C15—C10	-111 (3)
S2—C9—C10—C15	109 (2)	C16—N1—C15—C14	64 (3)
S3—C17—C18—C19	-65 (3)	C17—N3—C31—C26	73 (3)
S3—C17—C18—C23	112 (2)	C17—N3—C31—C30	-112 (2)
S4—C25—C26—C27	-63 (3)	C17—C18—C19—C20	175.8 (18)
S4—C25—C26—C31	115 (2)	C17—C18—C23—N4	1 (3)
N1—C1—C2—C3	112 (2)	C17—C18—C23—C22	-176.7 (18)
N1—C1—C2—C7	-73 (3)	C18—C19—C20—C21	0 (3)

N2—C9—C10—C11	110 (2)	C19—C18—C23—N4	177.5 (16)
N2—C9—C10—C15	-71 (3)	C19—C18—C23—C22	0 (3)
N3—C17—C18—C19	113 (2)	C19—C20—C21—C22	2 (3)
N3—C17—C18—C23	-70 (3)	C20—C21—C22—C23	-2 (3)
N4—C25—C26—C27	120 (2)	C21—C22—C23—N4	-176.0 (18)
N4—C25—C26—C31	-62 (3)	C21—C22—C23—C18	2 (3)
C1—N1—C15—C10	69 (3)	C23—N4—C25—S4	171.8 (18)
C1—N1—C15—C14	-116 (3)	C23—N4—C25—C26	-11 (3)
C1—C2—C3—C4	177.0 (19)	C23—C18—C19—C20	-1 (3)
C1—C2—C7—N2	4 (3)	C24—N4—C23—C18	-109 (2)
C1—C2—C7—C6	-175 (2)	C24—N4—C23—C22	68 (3)
C2—C3—C4—C5	-4 (3)	C24—N4—C25—S4	-2 (3)
C3—C2—C7—N2	178.9 (18)	C24—N4—C25—C26	175 (2)
C3—C2—C7—C6	0 (3)	C25—N4—C23—C18	77 (3)
C3—C4—C5—C6	3 (4)	C25—N4—C23—C22	-106 (3)
C4—C5—C6—C7	-2 (3)	C25—C26—C27—C28	180 (2)
C5—C6—C7—N2	-179.0 (19)	C25—C26—C31—N3	-2 (3)
C5—C6—C7—C2	0 (3)	C25—C26—C31—C30	-177 (2)
C7—N2—C9—S2	179.2 (16)	C26—C27—C28—C29	-5 (4)
C7—N2—C9—C10	-1 (3)	C27—C26—C31—N3	175.5 (18)
C7—C2—C3—C4	2 (3)	C27—C26—C31—C30	1 (3)
C8—N2—C7—C2	-113 (2)	C27—C28—C29—C30	4 (4)
C8—N2—C7—C6	66 (3)	C28—C29—C30—C31	-2 (4)
C8—N2—C9—S2	1 (3)	C29—C30—C31—N3	-176 (2)
C8—N2—C9—C10	-179 (2)	C29—C30—C31—C26	-1 (3)
C9—N2—C7—C2	68 (3)	C31—N3—C17—S3	176.5 (17)
C9—N2—C7—C6	-113 (3)	C31—N3—C17—C18	-1 (3)
C9—C10—C11—C12	175 (2)	C31—C26—C27—C28	2 (3)
C9—C10—C15—N1	2 (4)	C32—N3—C17—S3	-2 (3)
C9—C10—C15—C14	-173 (2)	C32—N3—C17—C18	180 (2)
C10—C11—C12—C13	2 (4)	C32—N3—C31—C26	-108 (2)
C11—C10—C15—N1	-180 (2)	C32—N3—C31—C30	67 (3)

Symmetry codes: (i) -*x*, *y*-1/2, -*z*; (ii) -*x*, *y*+1/2, -*z*; (iii) *x*-1, *y*, *z*-1; (iv) *x*+1, *y*, *z*+1.

Crystal data for **$[Cu_3Cl_3(mdta)_2(MeCN)_2]_n$ (5)**

$C_{32}H_{28}Cl_3Cu_3N_4S_4 \cdot 2(C_2H_3N)$	$F(000) = 988$
$M_r = 975.90$	$D_x = 1.633$ Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

a = 8.8353 (2) Å	Cell parameters from 28217 reflections
1b = 16.7129 (5) Å	θ = 0.6–29.6°
c = 13.6256 (4) Å	μ = 2.04 mm^{-1}
β = 99.427 (2)°	T = 120 K
V = 1984.83 (10) $Å^3$	Block, pale green
Z = 2	0.29 × 0.11 × 0.03 mm

Data collection

STOE IPDS 2T diffractometer	10633 independent reflections
Radiation source: GeniX Mo, 0.05 x 0.05 mm2 microfocus	8879 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	θ_{max} = 29.3°, θ_{min} = 2.3°
rotation method, ω scans	h = -12→11
Absorption correction: integration STOE *X-RED32*, absorption correction by Gaussian integration, analogous to P. Coppens, "The Evaluation of Absorption and Extinction in Single-Crystal Structure Analysis", published in F. R. Ahmed (Editor), "Crystallographic Computing", Munksgaard, Copenhagen (1970), 255 - 270	k = -22→22
T_{min} = 0.656, T_{max} = 0.906	l = -6→18
10633 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.055	H-atom parameters constrained
$wR(F^2)$ = 0.165	$w = 1/[\sigma^2(F_o^2) + (0.1092P)^2 + 2.1782P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max} < 0.001$
10633 reflections	$\Delta\rangle_{max}$ = 1.03 e $Å^{-3}$
476 parameters	$\Delta\rangle_{min}$ = -1.20 e $Å^{-3}$
1 restraint	Absolute structure: Flack x determined using 3638 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Primary atom site location: structure-invariant direct methods	Absolute structure parameter: 0.016 (12)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.
Refinement. Refined as a 2-component twin.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for **$[Cu_3Cl_3(mdta)_2(MeCN)_2]_n$ (5)**

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.17673 (11)	0.58321 (6)	-0.17927 (7)	0.0244 (2)
Cu2	0.27361 (13)	0.72633 (7)	-0.26127 (9)	0.0321 (3)
Cu3	0.87602 (12)	0.36836 (6)	0.22719 (7)	0.0257 (2)
Cl1	0.0580 (2)	0.72543 (12)	-0.18053 (15)	0.0234 (3)
Cl2	0.3708 (2)	0.60298 (12)	-0.27534 (14)	0.0241 (4)
Cl3	0.3426 (2)	0.84948 (12)	-0.30399 (15)	0.0260 (4)
S1	0.2243 (2)	0.54489 (12)	-0.01977 (14)	0.0236 (4)
S2	0.8123 (2)	0.39886 (11)	0.06217 (14)	0.0241 (4)
S3	1.0873 (2)	0.41569 (12)	0.32358 (15)	0.0247 (4)
S4	0.9629 (2)	0.54654 (12)	0.71167 (14)	0.0222 (4)
N1	0.4625 (7)	0.5428 (4)	0.1247 (5)	0.0199 (12)
N2	0.6757 (7)	0.5217 (4)	-0.0383 (5)	0.0194 (12)
N3	1.2032 (7)	0.4253 (4)	0.5142 (5)	0.0206 (12)
N4	0.8910 (7)	0.4324 (4)	0.5782 (5)	0.0196 (12)
C1	0.4026 (9)	0.5713 (4)	0.0348 (5)	0.0199 (14)
C2	0.4958 (9)	0.6292 (5)	-0.0140 (5)	0.0203 (14)
C3	0.4488 (9)	0.7087 (4)	-0.0266 (6)	0.0218 (14)
H3	0.356650	0.725698	-0.005495	0.026*
C4	0.5364 (9)	0.7627 (5)	-0.0696 (6)	0.0216 (14)
H4	0.504888	0.816980	-0.077247	0.026*
C5	0.6701 (9)	0.7382 (5)	-0.1017 (6)	0.0240 (15)
H5	0.730550	0.775528	-0.130899	0.029*
C6	0.7149 (9)	0.6588 (5)	-0.0908 (6)	0.0223 (14)
H6	0.805367	0.641366	-0.113663	0.027*
C7	0.6285 (9)	0.6050 (5)	-0.0468 (5)	0.0199 (14)
C8	0.6623 (10)	0.4758 (5)	-0.1304 (6)	0.0273 (17)
H8A	0.595090	0.504224	-0.183443	0.041*
H8B	0.618606	0.423045	-0.120502	0.041*
H8C	0.764031	0.469200	-0.149056	0.041*

C9	0.7387 (8)	0.4920 (5)	0.0491 (6)	0.0200 (14)
C10	0.7464 (8)	0.5441 (4)	0.1384 (5)	0.0187 (13)
C11	0.8895 (9)	0.5675 (5)	0.1891 (6)	0.0253 (16)
H11	0.979802	0.551852	0.164695	0.030*
C12	0.9015 (10)	0.6134 (5)	0.2745 (6)	0.0256 (16)
H12	0.999468	0.629585	0.308149	0.031*
C13	0.7707 (11)	0.6356 (5)	0.3106 (6)	0.0297 (18)
H13	0.779298	0.667331	0.369058	0.036*
C14	0.6254 (9)	0.6121 (5)	0.2623 (6)	0.0248 (16)
H14	0.535769	0.624925	0.289138	0.030*
C15	0.6158 (8)	0.5691 (4)	0.1733 (5)	0.0197 (14)
C16	0.3766 (10)	0.4910 (5)	0.1819 (6)	0.0253 (16)
H16A	0.307233	0.523524	0.214657	0.038*
H16B	0.448102	0.462145	0.232197	0.038*
H16C	0.316628	0.452503	0.137106	0.038*
C17	1.0980 (8)	0.3912 (4)	0.4447 (6)	0.0199 (14)
C18	0.9969 (9)	0.3302 (4)	0.4782 (5)	0.0196 (14)
C19	0.9944 (9)	0.2511 (4)	0.4438 (6)	0.0214 (14)
H19	1.059203	0.235816	0.397821	0.026*
C20	0.8988 (9)	0.1952 (5)	0.4761 (6)	0.0232 (15)
H20	0.897896	0.141791	0.452135	0.028*
C21	0.8042 (9)	0.2165 (5)	0.5431 (6)	0.0240 (15)
H21	0.739346	0.177529	0.565490	0.029*
C22	0.8037 (9)	0.2944 (5)	0.5777 (6)	0.0227 (15)
H22	0.737988	0.309096	0.623320	0.027*
C23	0.8990 (8)	0.3504 (4)	0.5455 (6)	0.0202 (14)
C24	0.7513 (10)	0.4775 (6)	0.5379 (7)	0.0294 (18)
H24A	0.704780	0.454312	0.473944	0.044*
H24B	0.778059	0.533513	0.528202	0.044*
H24C	0.678204	0.474609	0.584637	0.044*
C25	0.9927 (9)	0.4607 (4)	0.6540 (6)	0.0205 (14)
C26	1.1349 (9)	0.4130 (4)	0.6835 (6)	0.0204 (14)
C27	1.1759 (11)	0.3866 (5)	0.7801 (6)	0.0292 (17)
H27	1.112151	0.399616	0.827595	0.035*
C28	1.3064 (11)	0.3418 (5)	0.8099 (7)	0.0327 (19)
H28	1.330528	0.323261	0.876527	0.039*
C29	1.4019 (10)	0.3243 (6)	0.7421 (7)	0.033 (2)
H29	1.492366	0.293768	0.762239	0.040*
C30	1.3662 (9)	0.3510 (5)	0.6444 (7)	0.0271 (17)
H30	1.431853	0.339138	0.597597	0.033*

C31	1.2325 (9)	0.3956 (5)	0.6160 (6)	0.0243 (16)
C32	1.3088 (9)	0.4869 (5)	0.4886 (6)	0.0254 (16)
H32A	1.383610	0.462264	0.452108	0.038*
H32B	1.362714	0.511691	0.549590	0.038*
H32C	1.250510	0.527827	0.446836	0.038*
N5	0.7359 (10)	0.2025 (7)	0.7910 (7)	0.048 (2)
C33	0.8427 (11)	0.2177 (6)	0.8471 (7)	0.0341 (19)
C34	0.9731 (12)	0.2385 (6)	0.9209 (7)	0.038 (2)
H34A	1.067833	0.227154	0.894797	0.056*
H34B	0.971188	0.206899	0.981257	0.056*
H34C	0.968870	0.295566	0.936688	0.056*
N6	0.4458 (13)	0.1523 (10)	0.5172 (8)	0.070 (4)
C35	0.4021 (11)	0.1854 (7)	0.4439 (8)	0.038 (2)
C36	0.3511 (12)	0.2226 (7)	0.3485 (9)	0.042 (2)
H36A	0.431504	0.217785	0.307179	0.063*
H36B	0.329311	0.279265	0.358250	0.063*
H36C	0.257719	0.195885	0.315463	0.063*

Atomic displacement parameters (Å^2) for **$[Cu_3Cl_3(mdta)_2(MeCN)_2]_n$ (5)**

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0258 (5)	0.0236 (5)	0.0220 (4)	-0.0045 (4)	-0.0015 (4)	-0.0003 (4)
Cu2	0.0330 (6)	0.0237 (5)	0.0393 (6)	-0.0005 (4)	0.0052 (5)	0.0005 (4)
Cu3	0.0287 (5)	0.0219 (5)	0.0239 (5)	-0.0019 (4)	-0.0031 (4)	0.0039 (4)
Cl1	0.0259 (8)	0.0170 (7)	0.0273 (9)	-0.0010 (7)	0.0041 (7)	-0.0007 (6)
Cl2	0.0231 (8)	0.0236 (9)	0.0245 (8)	0.0005 (7)	0.0009 (7)	0.0009 (7)
Cl3	0.0260 (9)	0.0220 (9)	0.0275 (9)	-0.0017 (7)	-0.0028 (7)	0.0012 (7)
S1	0.0201 (8)	0.0265 (9)	0.0227 (8)	-0.0053 (7)	-0.0005 (7)	0.0017 (7)
S2	0.0322 (10)	0.0161 (8)	0.0223 (8)	0.0056 (7)	-0.0006 (7)	0.0010 (7)
S3	0.0261 (9)	0.0224 (9)	0.0241 (9)	-0.0043 (7)	-0.0001 (7)	0.0044 (7)
S4	0.0203 (8)	0.0192 (8)	0.0257 (8)	-0.0003 (7)	-0.0005 (7)	-0.0047 (7)
N1	0.022 (3)	0.017 (3)	0.020 (3)	-0.001 (2)	0.000 (2)	0.002 (2)
N2	0.019 (3)	0.018 (3)	0.020 (3)	0.002 (2)	0.001 (2)	0.000 (2)
N3	0.019 (3)	0.022 (3)	0.021 (3)	-0.001 (2)	0.004 (2)	0.001 (2)
N4	0.016 (3)	0.017 (3)	0.025 (3)	0.002 (2)	0.000 (2)	-0.001 (2)
C1	0.024 (3)	0.018 (3)	0.017 (3)	0.001 (3)	0.000 (3)	-0.002 (3)
C2	0.022 (3)	0.021 (3)	0.016 (3)	-0.004 (3)	-0.002 (3)	0.000 (3)
C3	0.027 (4)	0.017 (3)	0.020 (3)	0.001 (3)	0.001 (3)	0.000 (3)
C4	0.023 (3)	0.017 (3)	0.022 (3)	-0.003 (3)	-0.003 (3)	0.000 (3)
C5	0.027 (4)	0.021 (4)	0.023 (4)	-0.008 (3)	0.001 (3)	0.001 (3)
C6	0.019 (3)	0.025 (4)	0.022 (3)	0.001 (3)	0.001 (3)	0.005 (3)

C7	0.021 (3)	0.018 (3)	0.019 (3)	0.002 (3)	-0.005 (3)	0.002 (3)
C8	0.031 (4)	0.029 (4)	0.021 (4)	0.003 (3)	0.000 (3)	-0.007 (3)
C9	0.019 (3)	0.019 (3)	0.022 (3)	-0.002 (3)	0.002 (3)	0.002 (3)
C10	0.023 (3)	0.012 (3)	0.020 (3)	0.000 (3)	0.000 (3)	0.002 (3)
C11	0.025 (4)	0.024 (4)	0.024 (4)	-0.003 (3)	-0.005 (3)	0.001 (3)
C12	0.027 (4)	0.022 (3)	0.024 (4)	-0.001 (3)	-0.005 (3)	0.000 (3)
C13	0.038 (5)	0.024 (4)	0.024 (4)	-0.004 (3)	-0.005 (3)	-0.004 (3)
C14	0.021 (3)	0.035 (4)	0.019 (3)	0.003 (3)	0.004 (3)	-0.005 (3)
C15	0.022 (3)	0.020 (3)	0.015 (3)	0.000 (3)	-0.002 (3)	0.001 (3)
C16	0.025 (4)	0.027 (4)	0.023 (4)	-0.003 (3)	0.003 (3)	0.007 (3)
C17	0.016 (3)	0.011 (3)	0.030 (4)	0.001 (2)	-0.002 (3)	0.003 (3)
C18	0.021 (3)	0.018 (3)	0.016 (3)	0.000 (3)	-0.006 (3)	0.002 (3)
C19	0.022 (3)	0.016 (3)	0.025 (3)	-0.001 (3)	-0.003 (3)	0.000 (3)
C20	0.025 (4)	0.018 (3)	0.024 (3)	-0.003 (3)	-0.002 (3)	0.000 (3)
C21	0.022 (3)	0.019 (4)	0.029 (4)	-0.006 (3)	-0.004 (3)	0.003 (3)
C22	0.022 (3)	0.023 (4)	0.022 (3)	-0.004 (3)	0.001 (3)	0.002 (3)
C23	0.018 (3)	0.018 (3)	0.023 (3)	-0.002 (3)	-0.004 (3)	0.000 (3)
C24	0.022 (4)	0.030 (4)	0.033 (4)	0.010 (3)	-0.008 (3)	-0.002 (3)
C25	0.022 (3)	0.017 (3)	0.022 (3)	-0.001 (3)	0.002 (3)	0.006 (3)
C26	0.023 (3)	0.012 (3)	0.024 (3)	-0.001 (3)	-0.002 (3)	0.000 (3)
C27	0.035 (4)	0.019 (4)	0.030 (4)	0.000 (3)	-0.005 (3)	0.000 (3)
C28	0.038 (5)	0.022 (4)	0.033 (4)	-0.003 (3)	-0.010 (4)	0.008 (3)
C29	0.023 (4)	0.028 (4)	0.043 (5)	0.003 (3)	-0.013 (4)	0.002 (4)
C30	0.019 (3)	0.021 (4)	0.037 (4)	0.001 (3)	-0.006 (3)	-0.006 (3)
C31	0.027 (4)	0.013 (3)	0.028 (4)	-0.002 (3)	-0.009 (3)	-0.005 (3)
C32	0.022 (3)	0.026 (4)	0.030 (4)	-0.006 (3)	0.008 (3)	-0.002 (3)
N5	0.029 (4)	0.068 (7)	0.047 (5)	0.006 (4)	0.003 (4)	0.019 (5)
C33	0.038 (5)	0.031 (4)	0.036 (5)	0.008 (4)	0.013 (4)	0.010 (4)
C34	0.047 (6)	0.034 (5)	0.032 (5)	0.005 (4)	0.010 (4)	0.001 (4)
N6	0.044 (5)	0.123 (12)	0.041 (5)	-0.017 (7)	0.005 (5)	0.015 (7)
C35	0.024 (4)	0.052 (6)	0.040 (5)	-0.007 (4)	0.011 (4)	-0.013 (5)
C36	0.032 (5)	0.041 (5)	0.056 (6)	0.007 (4)	0.017 (4)	0.009 (5)

Geometric parameters (Å, º) for **$[Cu_3Cl_3(mdta)_2(MeCN)_2]_n$ (5)**

Cu1—Cu2	2.8312 (15)	C12—H12	0.9500
Cu1—Cl1	2.597 (2)	C12—C13	1.379 (13)
Cu1—Cl2	2.345 (2)	C13—H13	0.9500
Cu1—S1	2.238 (2)	C13—C14	1.399 (11)
Cu1—S4^{i}	2.288 (2)	C14—H14	0.9500
Cu2—Cu3^{ii}	2.7927 (15)	C14—C15	1.400 (10)

Cu2—Cl1	2.351 (2)	C16—H16A	0.9800
Cu2—Cl2	2.254 (2)	C16—H16B	0.9800
Cu2—Cl3	2.250 (2)	C16—H16C	0.9800
Cu3—Cl1^{iii}	2.564 (2)	C17—C18	1.476 (10)
Cu3—Cl3^{iii}	2.364 (2)	C18—C19	1.403 (10)
Cu3—S2	2.284 (2)	C18—C23	1.400 (11)
Cu3—S3	2.243 (2)	C19—H19	0.9500
S1—C1	1.687 (8)	C19—C20	1.379 (11)
S2—C9	1.685 (8)	C20—H20	0.9500
S3—C17	1.688 (8)	C20—C21	1.381 (12)
S4—C25	1.677 (8)	C21—H21	0.9500
N1—C1	1.339 (9)	C21—C22	1.385 (11)
N1—C15	1.474 (9)	C22—H22	0.9500
N1—C16	1.458 (10)	C22—C23	1.379 (10)
N2—C7	1.452 (10)	C24—H24A	0.9800
N2—C8	1.460 (10)	C24—H24B	0.9800
N2—C9	1.325 (10)	C24—H24C	0.9800
N3—C17	1.341 (10)	C25—C26	1.487 (10)
N3—C31	1.456 (10)	C26—C27	1.380 (11)
N3—C32	1.470 (10)	C26—C31	1.390 (12)
N4—C23	1.446 (9)	C27—H27	0.9500
N4—C24	1.474 (9)	C27—C28	1.379 (13)
N4—C25	1.339 (10)	C28—H28	0.9500
C1—C2	1.496 (11)	C28—C29	1.381 (15)
C2—C3	1.394 (10)	C29—H29	0.9500
C2—C7	1.383 (11)	C29—C30	1.391 (13)
C3—H3	0.9500	C30—H30	0.9500
C3—C4	1.380 (11)	C30—C31	1.397 (11)
C4—H4	0.9500	C32—H32A	0.9800
C4—C5	1.387 (12)	C32—H32B	0.9800
C5—H5	0.9500	C32—H32C	0.9800
C5—C6	1.386 (11)	N5—C33	1.141 (14)
C6—H6	0.9500	C33—C34	1.442 (15)
C6—C7	1.377 (11)	C34—H34A	0.9800
C8—H8A	0.9800	C34—H34B	0.9800
C8—H8B	0.9800	C34—H34C	0.9800
C8—H8C	0.9800	N6—C35	1.152 (16)
C9—C10	1.488 (10)	C35—C36	1.444 (16)
C10—C11	1.394 (10)	C36—H36A	0.9800
C10—C15	1.383 (11)	C36—H36B	0.9800

C11—H11	0.9500	C36—H36C	0.9800
C11—C12	1.383 (11)		
Cl1—Cu1—Cu2	51.11 (5)	C11—C12—H12	120.1
Cl2—Cu1—Cu2	50.56 (6)	C13—C12—C11	119.7 (8)
Cl2—Cu1—Cl1	101.48 (7)	C13—C12—H12	120.1
S1—Cu1—Cu2	127.16 (7)	C12—C13—H13	119.5
S1—Cu1—Cl1	106.24 (8)	C12—C13—C14	121.0 (8)
S1—Cu1—Cl2	122.96 (8)	C14—C13—H13	119.5
S1—Cu1—S4^{i}	123.91 (8)	C13—C14—H14	120.9
S4^{i}—Cu1—Cu2	103.94 (7)	C13—C14—C15	118.2 (7)
S4^{i}—Cu1—Cl1	87.20 (7)	C15—C14—H14	120.9
S4^{i}—Cu1—Cl2	106.07 (8)	C10—C15—N1	120.8 (6)
Cu3^{ii}—Cu2—Cu1	118.07 (5)	C10—C15—C14	121.2 (7)
Cl1—Cu2—Cu1	59.29 (6)	C14—C15—N1	117.6 (7)
Cl1—Cu2—Cu3^{ii}	59.05 (6)	N1—C16—H16A	109.5
Cl2—Cu2—Cu1	53.47 (6)	N1—C16—H16B	109.5
Cl2—Cu2—Cu3^{ii}	171.54 (8)	N1—C16—H16C	109.5
Cl2—Cu2—Cl1	112.54 (8)	H16A—C16—H16B	109.5
Cl3—Cu2—Cu1	170.79 (8)	H16A—C16—H16C	109.5
Cl3—Cu2—Cu3^{ii}	54.63 (6)	H16B—C16—H16C	109.5
Cl3—Cu2—Cl1	113.67 (8)	N3—C17—S3	120.6 (6)
Cl3—Cu2—Cl2	133.76 (9)	N3—C17—C18	117.4 (7)
Cl1^{iii}—Cu3—Cu2^{iii}	51.86 (5)	C18—C17—S3	122.0 (5)
Cl3^{iii}—Cu3—Cu2^{iii}	50.91 (6)	C19—C18—C17	121.7 (7)
Cl3^{iii}—Cu3—Cl1^{iii}	102.77 (7)	C23—C18—C17	120.4 (7)
S2—Cu3—Cu2^{iii}	107.83 (7)	C23—C18—C19	117.9 (7)
S2—Cu3—Cl1^{iii}	89.61 (7)	C18—C19—H19	119.7
S2—Cu3—Cl3^{iii}	112.21 (8)	C20—C19—C18	120.6 (8)
S3—Cu3—Cu2^{iii}	125.00 (7)	C20—C19—H19	119.7
S3—Cu3—Cl1^{iii}	105.81 (8)	C19—C20—H20	119.8
S3—Cu3—Cl3^{iii}	116.73 (8)	C19—C20—C21	120.4 (8)
S3—Cu3—S2	123.02 (9)	C21—C20—H20	119.8
Cu2—Cl1—Cu1	69.60 (6)	C20—C21—H21	119.9
Cu2—Cl1—Cu3^{ii}	69.10 (6)	C20—C21—C22	120.2 (7)
Cu3^{ii}—Cl1—Cu1	138.27 (8)	C22—C21—H21	119.9
Cu2—Cl2—Cu1	75.97 (7)	C21—C22—H22	120.2
Cu2—Cl3—Cu3^{ii}	74.46 (7)	C23—C22—C21	119.6 (8)
C1—S1—Cu1	111.5 (3)	C23—C22—H22	120.2
C9—S2—Cu3	109.8 (3)	C18—C23—N4	119.8 (7)

C17—S3—Cu3	113.3 (3)	C22—C23—N4	118.8 (7)
C25—S4—Cu1^{iv}	110.9 (3)	C22—C23—C18	121.3 (7)
C1—N1—C15	120.1 (6)	N4—C24—H24A	109.5
C1—N1—C16	122.4 (6)	N4—C24—H24B	109.5
C16—N1—C15	117.3 (6)	N4—C24—H24C	109.5
C7—N2—C8	116.9 (6)	H24A—C24—H24B	109.5
C9—N2—C7	120.3 (6)	H24A—C24—H24C	109.5
C9—N2—C8	122.6 (7)	H24B—C24—H24C	109.5
C17—N3—C31	121.5 (6)	N4—C25—S4	121.8 (6)
C17—N3—C32	121.6 (7)	N4—C25—C26	116.7 (7)
C31—N3—C32	116.4 (6)	C26—C25—S4	121.5 (6)
C23—N4—C24	116.7 (6)	C27—C26—C25	120.5 (8)
C25—N4—C23	120.8 (6)	C27—C26—C31	118.0 (7)
C25—N4—C24	121.4 (7)	C31—C26—C25	121.5 (7)
N1—C1—S1	120.7 (6)	C26—C27—H27	119.0
N1—C1—C2	118.2 (7)	C28—C27—C26	122.0 (9)
C2—C1—S1	121.0 (5)	C28—C27—H27	119.0
C3—C2—C1	119.8 (7)	C27—C28—H28	120.3
C7—C2—C1	120.8 (7)	C27—C28—C29	119.4 (8)
C7—C2—C3	119.4 (7)	C29—C28—H28	120.3
C2—C3—H3	120.0	C28—C29—H29	119.8
C4—C3—C2	119.9 (8)	C28—C29—C30	120.3 (8)
C4—C3—H3	120.0	C30—C29—H29	119.8
C3—C4—H4	119.8	C29—C30—H30	120.5
C3—C4—C5	120.5 (7)	C29—C30—C31	119.0 (9)
C5—C4—H4	119.8	C31—C30—H30	120.5
C4—C5—H5	120.3	C26—C31—N3	121.7 (7)
C6—C5—C4	119.4 (7)	C26—C31—C30	121.2 (8)
C6—C5—H5	120.3	C30—C31—N3	117.1 (8)
C5—C6—H6	119.9	N3—C32—H32A	109.5
C7—C6—C5	120.2 (7)	N3—C32—H32B	109.5
C7—C6—H6	119.9	N3—C32—H32C	109.5
C2—C7—N2	120.1 (7)	H32A—C32—H32B	109.5
C6—C7—N2	119.2 (7)	H32A—C32—H32C	109.5
C6—C7—C2	120.6 (7)	H32B—C32—H32C	109.5
N2—C8—H8A	109.5	N5—C33—C34	177.4 (11)
N2—C8—H8B	109.5	C33—C34—H34A	109.5
N2—C8—H8C	109.5	C33—C34—H34B	109.5
H8A—C8—H8B	109.5	C33—C34—H34C	109.5
H8A—C8—H8C	109.5	H34A—C34—H34B	109.5

H8B—C8—H8C	109.5	H34A—C34—H34C	109.5
N2—C9—S2	122.6 (6)	H34B—C34—H34C	109.5
N2—C9—C10	118.1 (7)	N6—C35—C36	176.2 (13)
C10—C9—S2	119.2 (5)	C35—C36—H36A	109.5
C11—C10—C9	119.1 (7)	C35—C36—H36B	109.5
C15—C10—C9	122.0 (6)	C35—C36—H36C	109.5
C15—C10—C11	119.0 (7)	H36A—C36—H36B	109.5
C10—C11—H11	119.6	H36A—C36—H36C	109.5
C12—C11—C10	120.8 (8)	H36B—C36—H36C	109.5
C12—C11—H11	119.6		
Cu1—S1—C1—N1	-169.0 (5)	C11—C10—C15—C14	-5.0 (11)
Cu1—S1—C1—C2	13.1 (7)	C11—C12—C13—C14	0.3 (13)
Cu1^{iv}—S4—C25—N4	-171.8 (6)	C12—C13—C14—C15	-3.4 (13)
Cu1^{iv}—S4—C25—C26	7.2 (7)	C13—C14—C15—N1	178.3 (7)
Cu3—S2—C9—N2	-171.9 (6)	C13—C14—C15—C10	5.8 (12)
Cu3—S2—C9—C10	9.1 (7)	C15—N1—C1—S1	-177.4 (5)
Cu3—S3—C17—N3	-169.1 (5)	C15—N1—C1—C2	0.6 (10)
Cu3—S3—C17—C18	12.8 (7)	C15—C10—C11—C12	1.7 (11)
S1—C1—C2—C3	66.4 (9)	C16—N1—C1—S1	-2.8 (10)
S1—C1—C2—C7	-113.8 (7)	C16—N1—C1—C2	175.2 (7)
S2—C9—C10—C11	64.2 (9)	C16—N1—C15—C10	113.6 (8)
S2—C9—C10—C15	-115.1 (7)	C16—N1—C15—C14	-58.9 (10)
S3—C17—C18—C19	59.0 (9)	C17—N3—C31—C26	-77.9 (10)
S3—C17—C18—C23	-120.5 (7)	C17—N3—C31—C30	104.3 (9)
S4—C25—C26—C27	56.8 (10)	C17—C18—C19—C20	-179.9 (7)
S4—C25—C26—C31	-121.4 (7)	C17—C18—C23—N4	3.3 (10)
N1—C1—C2—C3	-111.5 (8)	C17—C18—C23—C22	-180.0 (7)
N1—C1—C2—C7	68.2 (10)	C18—C19—C20—C21	-0.1 (11)
N2—C9—C10—C11	-114.9 (8)	C19—C18—C23—N4	-176.3 (6)
N2—C9—C10—C15	65.9 (10)	C19—C18—C23—C22	0.5 (10)
N3—C17—C18—C19	-119.0 (8)	C19—C20—C21—C22	0.6 (11)
N3—C17—C18—C23	61.4 (9)	C20—C21—C22—C23	-0.5 (12)
N4—C25—C26—C27	-124.1 (8)	C21—C22—C23—N4	176.8 (7)
N4—C25—C26—C31	57.7 (10)	C21—C22—C23—C18	0.0 (11)
C1—N1—C15—C10	-71.5 (9)	C23—N4—C25—S4	-164.8 (6)
C1—N1—C15—C14	116.0 (8)	C23—N4—C25—C26	16.2 (11)
C1—C2—C3—C4	178.5 (6)	C23—C18—C19—C20	-0.4 (10)
C1—C2—C7—N2	2.8 (11)	C24—N4—C23—C18	106.9 (8)
C1—C2—C7—C6	-179.2 (7)	C24—N4—C23—C22	-69.9 (10)

C2—C3—C4—C5	0.8 (11)	C24—N4—C25—S4	3.5 (11)
C3—C2—C7—N2	-177.4 (6)	C24—N4—C25—C26	-175.6 (7)
C3—C2—C7—C6	0.6 (11)	C25—N4—C23—C18	-84.3 (9)
C3—C4—C5—C6	0.4 (11)	C25—N4—C23—C22	98.9 (9)
C4—C5—C6—C7	-1.1 (12)	C25—C26—C27—C28	179.6 (8)
C5—C6—C7—N2	178.6 (7)	C25—C26—C31—N3	2.1 (11)
C5—C6—C7—C2	0.6 (11)	C25—C26—C31—C30	179.8 (7)
C7—N2—C9—S2	-173.6 (6)	C26—C27—C28—C29	1.6 (13)
C7—N2—C9—C10	5.4 (10)	C27—C26—C31—N3	-176.2 (7)
C7—C2—C3—C4	-1.3 (11)	C27—C26—C31—C30	1.5 (11)
C8—N2—C7—C2	109.0 (8)	C27—C28—C29—C30	-0.4 (13)
C8—N2—C7—C6	-69.0 (9)	C28—C29—C30—C31	-0.2 (13)
C8—N2—C9—S2	1.1 (11)	C29—C30—C31—N3	177.4 (7)
C8—N2—C9—C10	-179.9 (7)	C29—C30—C31—C26	-0.4 (12)
C9—N2—C7—C2	-76.1 (9)	C31—N3—C17—S3	-169.2 (6)
C9—N2—C7—C6	106.0 (9)	C31—N3—C17—C18	8.9 (11)
C9—C10—C11—C12	-177.6 (7)	C31—C26—C27—C28	-2.1 (12)
C9—C10—C15—N1	2.0 (11)	C32—N3—C17—S3	2.2 (10)
C9—C10—C15—C14	174.3 (7)	C32—N3—C17—C18	-179.7 (7)
C10—C11—C12—C13	0.6 (12)	C32—N3—C31—C26	110.2 (8)
C11—C10—C15—N1	-177.3 (7)	C32—N3—C31—C30	-67.6 (9)

Symmetry codes: (i) *x*-1, *y*, *z*-1; (ii) -*x*+1, *y*+1/2, -*z*; (iii) -*x*+1, *y*-1/2, -*z*; (iv) *x*+1, *y*, *z*+1.

Crystal data for **[Cu_3Cl_4{(*R*)-(−)-(mdta)}$_2$(MeCN)]$_n$ (7)**

$C_{32}H_{28}Cl_4Cu_3N_4S_4 \cdot C_2H_3N$	$F(000)$ = 978
M_r = 970.30	D_x = 1.707 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation, λ = 0.71073 Å
a = 8.7179 (9) Å	Cell parameters from 885 reflections
b = 16.8411 (17) Å	θ = 2.4–29.0°
c = 12.8872 (13) Å	μ = 2.21 mm^{-1}
β = 94.018 (8)°	T = 120 K
V = 1887.4 (3) Å^3	Prism, black
Z = 2	0.41 × 0.32 × 0.16 mm

Data collection

STOE IPDS 2T diffractometer	10114 independent reflections
Radiation source: GeniX Mo, 0.05 x 0.05 mm2	9422 reflections with $I > 2\sigma(I)$

microfocus	
Detector resolution: 6.67 pixels mm^{-1}	R_{int} = 0.033
rotation method, ω scans	θ_{max} = 29.2°, θ_{min} = 2.0°
Absorption correction: multi-scan STOE *X-RED32*, absorption correction by Gaussian integration, analogous to P. Coppens, "The Evaluation of Absorption and Extinction in Single-Crystal Structure Analysis", published in F. R. Ahmed (Editor), "Crystallographic Computing", Munksgaard, Copenhagen (1970), 255 - 270	h = -11→11
T_{min} = 0.105, T_{max} = 0.505	k = -23→23
26594 measured reflections	l = -17→17

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.039	H-atom parameters constrained
$wR(F^2)$ = 0.102	$w = 1/[\sigma^2(F_o^2) + (0.0651P)^2 + 1.3569P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max} < 0.001$
10114 reflections	$\Delta\rangle_{max}$ = 1.32 e $Å^{-3}$
456 parameters	$\Delta\rangle_{min}$ = -0.81 e $Å^{-3}$
1 restraint	Absolute structure: Classical Flack method preferred over Parsons because s.u. lower.
Primary atom site location: dual	Absolute structure parameter: 0.003 (11)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$) for **$[Cu_3Cl_4\{(R)\text{-}(-)\text{-}(mdta)\}_2(MeCN)]_n$ (7)**

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.21467 (7)	0.44867 (4)	0.30693 (4)	0.01915 (13)
Cu2	-0.14244 (7)	0.65765 (3)	-0.26056 (4)	0.02029 (13)
Cu3	0.39761 (7)	0.30104 (4)	0.18048 (5)	0.01905 (13)
Cl1	0.36926 (14)	0.16587 (7)	0.17133 (9)	0.0223 (2)
Cl2	0.59563 (16)	0.29878 (10)	0.08038 (11)	0.0340 (3)

Cl3	0.18425 (14)	0.30307 (7)	0.28088 (9)	0.0195 (2)
Cl4	0.42031 (13)	0.43569 (7)	0.20108 (9)	0.0215 (2)
S1	0.24272 (13)	0.48113 (8)	0.47447 (9)	0.0192 (2)
S2	0.80510 (16)	0.63139 (7)	0.56640 (9)	0.0222 (2)
S3	-0.00410 (13)	0.47530 (7)	0.20539 (9)	0.0190 (2)
S4	0.08337 (14)	0.62113 (7)	-0.18194 (9)	0.0204 (2)
N1	0.4634 (4)	0.4796 (2)	0.6253 (3)	0.0162 (7)
N2	0.6965 (4)	0.5098 (2)	0.4548 (3)	0.0153 (7)
N3	-0.1094 (4)	0.5958 (2)	0.0928 (3)	0.0164 (7)
N4	0.2133 (4)	0.6157 (2)	0.0090 (3)	0.0162 (7)
C1	0.4158 (5)	0.4541 (3)	0.5306 (3)	0.0146 (7)
C2	0.5192 (5)	0.3993 (3)	0.4774 (3)	0.0144 (8)
C3	0.4778 (5)	0.3198 (3)	0.4598 (3)	0.0171 (8)
H3	0.386389	0.299324	0.485702	0.021*
C4	0.5714 (6)	0.2711 (3)	0.4041 (4)	0.0204 (9)
H4	0.543499	0.217087	0.392873	0.024*
C5	0.7043 (6)	0.2998 (3)	0.3646 (4)	0.0212 (9)
H5	0.766198	0.265992	0.325870	0.025*
C6	0.7464 (6)	0.3788 (3)	0.3824 (4)	0.0198 (9)
H6	0.837513	0.399221	0.355996	0.024*
C7	0.6547 (5)	0.4273 (3)	0.4388 (3)	0.0151 (8)
C8	0.6855 (6)	0.5620 (3)	0.3628 (4)	0.0217 (9)
H8A	0.634117	0.611580	0.379879	0.033*
H8B	0.626169	0.535327	0.305595	0.033*
H8C	0.789026	0.573784	0.341905	0.033*
C9	0.7461 (5)	0.5374 (3)	0.5481 (3)	0.0154 (8)
C10	0.7464 (5)	0.4825 (3)	0.6380 (3)	0.0145 (8)
C11	0.8864 (5)	0.4621 (3)	0.6920 (4)	0.0198 (9)
H11	0.980646	0.479671	0.667143	0.024*
C12	0.8874 (6)	0.4161 (3)	0.7817 (4)	0.0249 (10)
H12	0.982458	0.400997	0.816608	0.030*
C13	0.7496 (7)	0.3922 (3)	0.8204 (4)	0.0277 (11)
H13	0.750705	0.362301	0.882936	0.033*
C14	0.6102 (6)	0.4123 (3)	0.7675 (4)	0.0229 (10)
H14	0.516234	0.395693	0.793714	0.028*
C15	0.6084 (5)	0.4562 (3)	0.6768 (3)	0.0157 (8)
C16	0.3642 (6)	0.5304 (3)	0.6855 (4)	0.0233 (10)
H16A	0.322502	0.573708	0.641282	0.035*
H16B	0.424679	0.552509	0.745619	0.035*
H16C	0.279407	0.498618	0.709565	0.035*

C17	0.0011 (5)	0.5678 (3)	0.1588 (3)	0.0139 (8)
C18	0.1355 (5)	0.6197 (3)	0.1884 (3)	0.0145 (8)
C19	0.1655 (6)	0.6422 (3)	0.2922 (4)	0.0191 (9)
H19	0.096596	0.627427	0.342759	0.023*
C20	0.2965 (6)	0.6862 (3)	0.3212 (4)	0.0247 (10)
H20	0.316030	0.702008	0.391633	0.030*
C21	0.3989 (6)	0.7072 (3)	0.2483 (4)	0.0237 (10)
H21	0.488673	0.736819	0.269011	0.028*
C22	0.3702 (5)	0.6850 (3)	0.1447 (4)	0.0195 (9)
H22	0.439996	0.699159	0.094433	0.023*
C23	0.2381 (5)	0.6419 (3)	0.1157 (3)	0.0151 (8)
C24	0.3272 (6)	0.5599 (3)	-0.0291 (4)	0.0222 (10)
H24A	0.274897	0.521485	-0.076516	0.033*
H24B	0.378763	0.531628	0.030056	0.033*
H24C	0.403491	0.589373	-0.065973	0.033*
C25	0.1021 (5)	0.6461 (3)	-0.0558 (3)	0.0160 (8)
C26	-0.0062 (5)	0.7033 (3)	-0.0114 (3)	0.0148 (8)
C27	-0.0099 (5)	0.7823 (3)	-0.0445 (3)	0.0174 (8)
H27	0.060667	0.800521	-0.092065	0.021*
C28	-0.1179 (6)	0.8341 (3)	-0.0072 (4)	0.0205 (9)
H28	-0.121077	0.887881	-0.029652	0.025*
C29	-0.2209 (6)	0.8076 (3)	0.0628 (4)	0.0229 (9)
H29	-0.295034	0.843134	0.087105	0.027*
C30	-0.2162 (5)	0.7297 (3)	0.0971 (4)	0.0197 (9)
H30	-0.285263	0.711775	0.145920	0.024*
C31	-0.1093 (5)	0.6782 (3)	0.0594 (3)	0.0162 (8)
C32	-0.2420 (6)	0.5468 (3)	0.0555 (4)	0.0235 (10)
H32A	-0.205351	0.498557	0.022623	0.035*
H32B	-0.307424	0.576987	0.004693	0.035*
H32C	-0.301503	0.532172	0.114403	0.035*
N5	-0.2577 (6)	0.8188 (4)	0.3156 (4)	0.0391 (13)
C33	-0.1535 (6)	0.8101 (4)	0.3727 (4)	0.0268 (11)
C34	-0.0220 (7)	0.8001 (4)	0.4481 (5)	0.0307 (11)
H34A	0.070593	0.821076	0.418898	0.046*
H34B	-0.007665	0.743574	0.463914	0.046*
H34C	-0.040675	0.828993	0.511989	0.046*

Atomic displacement parameters (Å^2) for **[Cu_3Cl_4{(*R*)-(−)-(mdta)}$_2$(MeCN)]$_n$ (7)**

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0207 (3)	0.0206 (3)	0.0157 (2)	0.0016 (2)	-0.0024 (2)	0.0010 (2)

Cu2	0.0235 (3)	0.0191 (3)	0.0174 (3)	0.0006 (2)	-0.0048 (2)	-0.0019 (2)
Cu3	0.0193 (3)	0.0217 (3)	0.0160 (2)	0.0003 (2)	-0.00011 (19)	-0.0021 (2)
Cl1	0.0242 (5)	0.0211 (5)	0.0213 (5)	0.0048 (4)	-0.0010 (4)	-0.0039 (4)
Cl2	0.0261 (6)	0.0460 (8)	0.0310 (6)	-0.0035 (6)	0.0094 (5)	-0.0109 (6)
Cl3	0.0241 (5)	0.0156 (4)	0.0186 (5)	-0.0010 (4)	0.0002 (4)	-0.0006 (4)
Cl4	0.0213 (5)	0.0226 (6)	0.0205 (5)	-0.0020 (4)	0.0013 (4)	0.0019 (4)
S1	0.0189 (5)	0.0223 (5)	0.0161 (5)	0.0048 (4)	-0.0019 (4)	-0.0014 (4)
S2	0.0351 (6)	0.0144 (5)	0.0164 (5)	-0.0050 (5)	-0.0036 (4)	-0.0004 (4)
S3	0.0187 (5)	0.0176 (5)	0.0202 (5)	-0.0017 (4)	-0.0021 (4)	0.0037 (4)
S4	0.0220 (5)	0.0245 (6)	0.0144 (5)	0.0070 (4)	-0.0018 (4)	-0.0044 (4)
N1	0.0149 (16)	0.0196 (17)	0.0141 (16)	-0.0012 (14)	0.0004 (13)	-0.0047 (14)
N2	0.0177 (17)	0.0158 (17)	0.0121 (16)	-0.0022 (14)	-0.0016 (13)	0.0001 (13)
N3	0.0134 (16)	0.0193 (19)	0.0161 (16)	-0.0025 (14)	-0.0011 (13)	0.0015 (14)
N4	0.0135 (16)	0.0215 (18)	0.0134 (16)	0.0011 (14)	0.0005 (13)	0.0012 (14)
C1	0.0177 (19)	0.0131 (18)	0.0129 (17)	-0.0008 (16)	0.0010 (14)	0.0009 (15)
C2	0.018 (2)	0.0143 (18)	0.0106 (17)	0.0033 (16)	-0.0034 (15)	-0.0010 (15)
C3	0.0165 (19)	0.018 (2)	0.0167 (19)	0.0002 (16)	-0.0026 (15)	-0.0005 (16)
C4	0.024 (2)	0.016 (2)	0.019 (2)	0.0015 (18)	-0.0061 (17)	-0.0055 (17)
C5	0.026 (2)	0.020 (2)	0.018 (2)	0.0060 (18)	-0.0006 (16)	-0.0023 (17)
C6	0.019 (2)	0.026 (2)	0.0149 (19)	0.0020 (18)	0.0006 (16)	-0.0011 (17)
C7	0.018 (2)	0.0153 (19)	0.0110 (17)	-0.0011 (15)	-0.0031 (15)	-0.0010 (14)
C8	0.028 (2)	0.024 (2)	0.0128 (19)	-0.0042 (19)	-0.0010 (17)	0.0025 (16)
C9	0.0143 (19)	0.0156 (19)	0.0162 (19)	0.0005 (15)	0.0010 (15)	-0.0017 (16)
C10	0.0181 (19)	0.0115 (17)	0.0132 (18)	-0.0017 (16)	-0.0029 (15)	-0.0019 (15)
C11	0.020 (2)	0.019 (2)	0.019 (2)	-0.0017 (17)	-0.0057 (16)	-0.0006 (16)
C12	0.028 (2)	0.021 (2)	0.024 (2)	0.0009 (19)	-0.013 (2)	0.0016 (19)
C13	0.041 (3)	0.024 (2)	0.017 (2)	-0.005 (2)	-0.010 (2)	0.0046 (18)
C14	0.033 (3)	0.020 (2)	0.016 (2)	-0.0056 (19)	0.0000 (19)	0.0012 (17)
C15	0.0179 (19)	0.0154 (19)	0.0131 (17)	-0.0011 (16)	-0.0032 (14)	-0.0028 (15)
C16	0.022 (2)	0.029 (3)	0.019 (2)	0.0012 (19)	0.0026 (18)	-0.0081 (19)
C17	0.0132 (18)	0.0168 (19)	0.0120 (18)	-0.0011 (15)	0.0023 (15)	-0.0013 (14)
C18	0.0150 (19)	0.0142 (19)	0.0141 (18)	-0.0008 (15)	-0.0011 (15)	0.0026 (15)
C19	0.023 (2)	0.020 (2)	0.0138 (18)	-0.0014 (17)	-0.0016 (16)	0.0006 (15)
C20	0.031 (3)	0.021 (2)	0.020 (2)	-0.0012 (19)	-0.0102 (19)	-0.0018 (18)
C21	0.020 (2)	0.021 (2)	0.028 (2)	-0.0018 (18)	-0.0106 (19)	0.0038 (19)
C22	0.016 (2)	0.018 (2)	0.023 (2)	-0.0019 (16)	-0.0038 (17)	0.0053 (17)
C23	0.0118 (18)	0.018 (2)	0.0156 (18)	0.0019 (15)	-0.0021 (14)	0.0029 (15)
C24	0.017 (2)	0.031 (3)	0.019 (2)	0.0081 (18)	0.0040 (17)	0.0048 (18)
C25	0.0147 (18)	0.018 (2)	0.0149 (18)	0.0004 (16)	0.0008 (15)	0.0015 (16)

C26	0.0150 (18)	0.0176 (19)	0.0113 (17)	0.0015 (15)	-0.0029 (14)	-0.0018 (15)
C27	0.020 (2)	0.019 (2)	0.0128 (18)	0.0012 (17)	-0.0023 (15)	-0.0016 (15)
C28	0.024 (2)	0.020 (2)	0.017 (2)	0.0053 (18)	-0.0054 (17)	-0.0029 (17)
C29	0.021 (2)	0.027 (2)	0.020 (2)	0.0090 (19)	-0.0028 (16)	-0.0064 (19)
C30	0.015 (2)	0.027 (2)	0.0171 (19)	0.0019 (17)	0.0014 (15)	-0.0023 (18)
C31	0.0141 (18)	0.021 (2)	0.0130 (18)	0.0021 (16)	-0.0030 (15)	-0.0023 (15)
C32	0.017 (2)	0.028 (2)	0.025 (2)	-0.0063 (18)	-0.0062 (18)	0.0020 (19)
N5	0.031 (3)	0.058 (4)	0.029 (2)	-0.001 (2)	0.0016 (19)	-0.017 (2)
C33	0.022 (2)	0.033 (3)	0.027 (2)	-0.007 (2)	0.0097 (19)	-0.012 (2)
C34	0.028 (3)	0.029 (3)	0.035 (3)	-0.002 (2)	0.000 (2)	0.000 (2)

Geometric parameters (Å, °) for **[Cu_3Cl_4{(*R*)-(−)-(mdta)}$_2$(MeCN)]$_n$ (7)**

Cu1—Cl3	2.4867 (14)	C11—H11	0.9500
Cu1—Cl4	2.3378 (13)	C11—C12	1.390 (7)
Cu1—S1	2.2240 (13)	C12—H12	0.9500
Cu1—S3	2.2806 (13)	C12—C13	1.392 (8)
Cu2—Cl1^{i}	2.3601 (13)	C13—H13	0.9500
Cu2—Cl3^{i}	2.4871 (14)	C13—C14	1.393 (8)
Cu2—S2^{ii}	2.2880 (13)	C14—H14	0.9500
Cu2—S4	2.2362 (13)	C14—C15	1.382 (6)
Cu3—Cl1	2.2920 (14)	C16—H16A	0.9800
Cu3—Cl2	2.2266 (14)	C16—H16B	0.9800
Cu3—Cl3	2.3393 (13)	C16—H16C	0.9800
Cu3—Cl4	2.2901 (13)	C17—C18	1.490 (6)
S1—C1	1.689 (5)	C18—C19	1.397 (6)
S2—C9	1.676 (5)	C18—C23	1.391 (6)
S3—C17	1.671 (5)	C19—H19	0.9500
S4—C25	1.676 (5)	C19—C20	1.391 (7)
N1—C1	1.333 (5)	C20—H20	0.9500
N1—C15	1.441 (6)	C20—C21	1.387 (8)
N1—C16	1.475 (6)	C21—H21	0.9500
N2—C7	1.448 (6)	C21—C22	1.392 (7)
N2—C8	1.473 (6)	C22—H22	0.9500
N2—C9	1.333 (6)	C22—C23	1.390 (6)
N3—C17	1.326 (6)	C24—H24A	0.9800
N3—C31	1.453 (6)	C24—H24B	0.9800
N3—C32	1.474 (6)	C24—H24C	0.9800
N4—C23	1.446 (6)	C25—C26	1.491 (6)
N4—C24	1.476 (6)	C26—C27	1.396 (6)
N4—C25	1.337 (6)	C26—C31	1.390 (6)

C1—C2	1.490 (6)	C27—H27	0.9500
C2—C3	1.400 (6)	C27—C28	1.394 (6)
C2—C7	1.395 (6)	C28—H28	0.9500
C3—H3	0.9500	C28—C29	1.390 (7)
C3—C4	1.392 (7)	C29—H29	0.9500
C4—H4	0.9500	C29—C30	1.385 (7)
C4—C5	1.385 (7)	C30—H30	0.9500
C5—H5	0.9500	C30—C31	1.385 (6)
C5—C6	1.395 (7)	C32—H32A	0.9800
C6—H6	0.9500	C32—H32B	0.9800
C6—C7	1.384 (6)	C32—H32C	0.9800
C8—H8A	0.9800	N5—C33	1.138 (8)
C8—H8B	0.9800	C33—C34	1.459 (8)
C8—H8C	0.9800	C34—H34A	0.9800
C9—C10	1.482 (6)	C34—H34B	0.9800
C10—C11	1.405 (6)	C34—H34C	0.9800
C10—C15	1.407 (6)		
Cl4—Cu1—Cl3	84.72 (4)	C13—C12—H12	119.9
S1—Cu1—Cl3	112.14 (5)	C12—C13—H13	120.0
S1—Cu1—Cl4	123.56 (5)	C12—C13—C14	120.0 (5)
S1—Cu1—S3	122.64 (5)	C14—C13—H13	120.0
S3—Cu1—Cl3	92.26 (5)	C13—C14—H14	119.9
S3—Cu1—Cl4	109.16 (5)	C15—C14—C13	120.1 (5)
Cl1^{i}—Cu2—Cl3^{i}	82.64 (4)	C15—C14—H14	119.9
S2^{ii}—Cu2—Cl1^{i}	111.66 (5)	C10—C15—N1	119.6 (4)
S2^{ii}—Cu2—Cl3^{i}	94.00 (5)	C14—C15—N1	119.6 (4)
S4—Cu2—Cl1^{i}	122.44 (5)	C14—C15—C10	120.7 (4)
S4—Cu2—Cl3^{i}	115.88 (5)	N1—C16—H16A	109.5
S4—Cu2—S2^{ii}	119.86 (5)	N1—C16—H16B	109.5
Cl1—Cu3—Cl3	87.47 (5)	N1—C16—H16C	109.5
Cl2—Cu3—Cl1	92.20 (6)	H16A—C16—H16B	109.5
Cl2—Cu3—Cl3	178.17 (6)	H16A—C16—H16C	109.5
Cl2—Cu3—Cl4	91.14 (6)	H16B—C16—H16C	109.5
Cl4—Cu3—Cl1	176.02 (5)	N3—C17—S3	121.7 (3)
Cl4—Cu3—Cl3	89.26 (4)	N3—C17—C18	118.5 (4)
Cu3—Cl1—Cu2^{iii}	97.13 (5)	C18—C17—S3	119.7 (3)
Cu1—Cl3—Cu2^{iii}	177.05 (6)	C19—C18—C17	119.6 (4)
Cu3—Cl3—Cu1	90.44 (4)	C23—C18—C17	121.2 (4)
Cu3—Cl3—Cu2^{iii}	92.50 (4)	C23—C18—C19	119.0 (4)

Cu3—Cl4—Cu1	95.55 (5)	C18—C19—H19	120.1
C1—S1—Cu1	112.56 (15)	C20—C19—C18	119.8 (5)
C9—S2—Cu2^{iv}	110.99 (16)	C20—C19—H19	120.1
C17—S3—Cu1	110.30 (16)	C19—C20—H20	119.7
C25—S4—Cu2	113.15 (16)	C21—C20—C19	120.6 (5)
C1—N1—C15	122.7 (4)	C21—C20—H20	119.7
C1—N1—C16	120.8 (4)	C20—C21—H21	120.0
C15—N1—C16	116.4 (4)	C20—C21—C22	120.0 (5)
C7—N2—C8	117.2 (4)	C22—C21—H21	120.0
C9—N2—C7	121.7 (4)	C21—C22—H22	120.4
C9—N2—C8	121.1 (4)	C23—C22—C21	119.2 (5)
C17—N3—C31	121.0 (4)	C23—C22—H22	120.4
C17—N3—C32	121.8 (4)	C18—C23—N4	119.9 (4)
C31—N3—C32	117.1 (4)	C22—C23—N4	118.7 (4)
C23—N4—C24	116.8 (4)	C22—C23—C18	121.3 (4)
C25—N4—C23	122.1 (4)	N4—C24—H24A	109.5
C25—N4—C24	120.8 (4)	N4—C24—H24B	109.5
N1—C1—S1	121.1 (3)	N4—C24—H24C	109.5
N1—C1—C2	117.5 (4)	H24A—C24—H24B	109.5
C2—C1—S1	121.4 (3)	H24A—C24—H24C	109.5
C3—C2—C1	120.6 (4)	H24B—C24—H24C	109.5
C7—C2—C1	120.6 (4)	N4—C25—S4	121.8 (3)
C7—C2—C3	118.7 (4)	N4—C25—C26	117.3 (4)
C2—C3—H3	120.2	C26—C25—S4	120.9 (3)
C4—C3—C2	119.6 (4)	C27—C26—C25	120.0 (4)
C4—C3—H3	120.2	C31—C26—C25	120.8 (4)
C3—C4—H4	119.3	C31—C26—C27	119.2 (4)
C5—C4—C3	121.3 (5)	C26—C27—H27	120.2
C5—C4—H4	119.3	C28—C27—C26	119.6 (4)
C4—C5—H5	120.3	C28—C27—H27	120.2
C4—C5—C6	119.3 (4)	C27—C28—H28	119.9
C6—C5—H5	120.3	C29—C28—C27	120.3 (5)
C5—C6—H6	120.2	C29—C28—H28	119.9
C7—C6—C5	119.6 (4)	C28—C29—H29	119.8
C7—C6—H6	120.2	C30—C29—C28	120.4 (5)
C2—C7—N2	119.0 (4)	C30—C29—H29	119.8
C6—C7—N2	119.4 (4)	C29—C30—H30	120.4
C6—C7—C2	121.5 (4)	C29—C30—C31	119.1 (4)
N2—C8—H8A	109.5	C31—C30—H30	120.4
N2—C8—H8B	109.5	C26—C31—N3	119.9 (4)

N2—C8—H8C	109.5	C30—C31—N3	118.6 (4)
H8A—C8—H8B	109.5	C30—C31—C26	121.4 (4)
H8A—C8—H8C	109.5	N3—C32—H32A	109.5
H8B—C8—H8C	109.5	N3—C32—H32B	109.5
N2—C9—S2	122.3 (4)	N3—C32—H32C	109.5
N2—C9—C10	118.0 (4)	H32A—C32—H32B	109.5
C10—C9—S2	119.7 (3)	H32A—C32—H32C	109.5
C11—C10—C9	119.6 (4)	H32B—C32—H32C	109.5
C11—C10—C15	118.8 (4)	N5—C33—C34	178.5 (6)
C15—C10—C9	121.3 (4)	C33—C34—H34A	109.5
C10—C11—H11	119.9	C33—C34—H34B	109.5
C12—C11—C10	120.2 (5)	C33—C34—H34C	109.5
C12—C11—H11	119.9	H34A—C34—H34B	109.5
C11—C12—H12	119.9	H34A—C34—H34C	109.5
C11—C12—C13	120.3 (5)	H34B—C34—H34C	109.5
Cu1—S1—C1—N1	169.0 (3)	C11—C10—C15—C14	1.2 (7)
Cu1—S1—C1—C2	-12.5 (4)	C11—C12—C13—C14	2.0 (8)
Cu1—S3—C17—N3	176.2 (3)	C12—C13—C14—C15	-0.4 (8)
Cu1—S3—C17—C18	-1.4 (4)	C13—C14—C15—N1	-177.2 (4)
$Cu2^{iv}$—S2—C9—N2	174.3 (3)	C13—C14—C15—C10	-1.2 (7)
$Cu2^{iv}$—S2—C9—C10	-4.9 (4)	C15—N1—C1—S1	178.4 (3)
Cu2—S4—C25—N4	166.0 (3)	C15—N1—C1—C2	-0.2 (6)
Cu2—S4—C25—C26	-13.6 (4)	C15—C10—C11—C12	0.4 (7)
S1—C1—C2—C3	-66.9 (5)	C16—N1—C1—S1	2.0 (6)
S1—C1—C2—C7	109.4 (4)	C16—N1—C1—C2	-176.6 (4)
S2—C9—C10—C11	-64.1 (5)	C16—N1—C15—C10	-115.3 (5)
S2—C9—C10—C15	109.9 (4)	C16—N1—C15—C14	60.7 (6)
S3—C17—C18—C19	-64.2 (5)	C17—N3—C31—C26	74.3 (5)
S3—C17—C18—C23	111.3 (4)	C17—N3—C31—C30	-107.6 (5)
S4—C25—C26—C27	-65.2 (5)	C17—C18—C19—C20	175.7 (4)
S4—C25—C26—C31	111.8 (4)	C17—C18—C23—N4	1.2 (6)
N1—C1—C2—C3	111.7 (5)	C17—C18—C23—C22	-174.8 (4)
N1—C1—C2—C7	-72.1 (5)	C18—C19—C20—C21	-0.8 (8)
N2—C9—C10—C11	116.6 (5)	C19—C18—C23—N4	176.8 (4)
N2—C9—C10—C15	-69.4 (6)	C19—C18—C23—C22	0.7 (7)
N3—C17—C18—C19	118.1 (5)	C19—C20—C21—C22	0.7 (8)
N3—C17—C18—C23	-66.4 (6)	C20—C21—C22—C23	0.1 (7)
N4—C25—C26—C27	115.2 (5)	C21—C22—C23—N4	-176.9 (4)
N4—C25—C26—C31	-67.9 (6)	C21—C22—C23—C18	-0.8 (7)

C1—N1—C15—C10	68.2 (6)	C23—N4—C25—S4	174.8 (3)
C1—N1—C15—C14	-115.8 (5)	C23—N4—C25—C26	-5.6 (6)
C1—C2—C3—C4	175.9 (4)	C23—C18—C19—C20	0.1 (7)
C1—C2—C7—N2	2.4 (6)	C24—N4—C23—C18	-113.4 (5)
C1—C2—C7—C6	-175.1 (4)	C24—N4—C23—C22	62.8 (6)
C2—C3—C4—C5	-0.6 (7)	C24—N4—C25—S4	1.5 (6)
C3—C2—C7—N2	178.7 (4)	C24—N4—C25—C26	-178.8 (4)
C3—C2—C7—C6	1.2 (6)	C25—N4—C23—C18	73.1 (6)
C3—C4—C5—C6	0.9 (7)	C25—N4—C23—C22	-110.7 (5)
C4—C5—C6—C7	-0.2 (7)	C25—C26—C27—C28	176.2 (4)
C5—C6—C7—N2	-178.4 (4)	C25—C26—C31—N3	1.6 (6)
C5—C6—C7—C2	-0.9 (7)	C25—C26—C31—C30	-176.5 (4)
C7—N2—C9—S2	176.2 (3)	C26—C27—C28—C29	0.2 (7)
C7—N2—C9—C10	-4.6 (6)	C27—C26—C31—N3	178.6 (4)
C7—C2—C3—C4	-0.4 (6)	C27—C26—C31—C30	0.5 (7)
C8—N2—C7—C2	-109.3 (5)	C27—C28—C29—C30	0.8 (7)
C8—N2—C7—C6	68.2 (6)	C28—C29—C30—C31	-1.2 (7)
C8—N2—C9—S2	-2.4 (6)	C29—C30—C31—N3	-177.6 (4)
C8—N2—C9—C10	176.9 (4)	C29—C30—C31—C26	0.5 (7)
C9—N2—C7—C2	72.0 (6)	C31—N3—C17—S3	175.2 (3)
C9—N2—C7—C6	-110.4 (5)	C31—N3—C17—C18	-7.2 (6)
C9—C10—C11—C12	174.5 (4)	C31—C26—C27—C28	-0.9 (6)
C9—C10—C15—N1	3.2 (6)	C32—N3—C17—S3	-0.9 (6)
C9—C10—C15—C14	-172.8 (4)	C32—N3—C17—C18	176.7 (4)
C10—C11—C12—C13	-2.1 (8)	C32—N3—C31—C26	-109.5 (5)
C11—C10—C15—N1	177.2 (4)	C32—N3—C31—C30	68.6 (5)

Symmetry codes: (i) -*x*, *y*+1/2, -*z*; (ii) *x*-1, *y*, *z*-1; (iii) -*x*, *y*-1/2, -*z*; (iv) *x*+1, *y*, *z*+1.

Crystal data for **[Cu_2I_2(bdta)(MeCN)]$_n$ (8)**

$C_{28}H_{22}Cu_2I_2N_2S_2$	$F(000)$ = 3200
M_r = 831.47	D_x = 1.787 Mg m^{-3}
Monoclinic, *I*2/*a*	Mo *K*α radiation, λ = 0.71073 Å
a = 19.2485 (11) Å	Cell parameters from 78720 reflections
b = 16.5225 (8) Å	θ = 2.1–29.7°
c = 21.3838 (11) Å	μ = 3.53 mm^{-1}
β = 114.655 (4)°	*T* = 120 K
V = 6180.8 (6) Å^3	Prism, yellow
Z = 8	0.45 × 0.23 × 0.19 mm

Data collection

STOE IPDS 2T diffractometer	8343 independent reflections
Radiation source: GeniX Mo, 0.05 x 0.05 mm2 microfocus	7370 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	$R_{int} = 0.060$
rotation method, ω scans	$\theta_{max} = 29.3°$, $\theta_{min} = 2.1°$
Absorption correction: integration STOE *X-RED32*, absorption correction by Gaussian integration, analogous to P. Coppens, "The Evaluation of Absorption and Extinction in Single-Crystal Structure Analysis", published in F. R. Ahmed (Editor), "Crystallographic Computing", Munksgaard, Copenhagen (1970), 255 - 270	$h = -26 \rightarrow 26$
$T_{min} = 0.175$, $T_{max} = 0.406$	$k = -22 \rightarrow 22$
42187 measured reflections	$l = -29 \rightarrow 29$

Refinement

Refinement on F^2	Primary atom site location: dual
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.056$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.159$	H-atom parameters constrained
$S = 1.09$	$w = 1/[\sigma^2(F_o^2) + (0.0937P)^2 + 44.3932P]$ where $P = (F_o^2 + 2F_c^2)/3$
8343 reflections	$(\Delta/\sigma)_{max} = 0.001$
326 parameters	$\Delta\rangle_{max} = 2.12$ e $Å^{-3}$
0 restraints	$\Delta\rangle_{min} = -3.30$ e $Å^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for **[Cu_2I_2(bdta)(MeCN)]$_n$ (8)**

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.23863 (2)	0.48315 (2)	0.09837 (2)	0.02929 (10)
I2	0.37161 (2)	0.29370 (2)	0.04851 (2)	0.02734 (10)
Cu1	0.31914 (3)	0.35616 (4)	0.13142 (3)	0.02824 (15)
Cu2	0.250000	0.30681 (6)	0.500000	0.02978 (19)
Cu3	0.250000	0.39612 (6)	0.000000	0.0309 (2)
S1	0.34478 (8)	0.28067 (8)	0.22490 (6)	0.0306 (3)
S2	0.20874 (7)	0.37554 (8)	0.39837 (6)	0.0284 (2)
N1	0.3860 (2)	0.3079 (2)	0.3573 (2)	0.0242 (7)
N2	0.2653 (2)	0.4467 (2)	0.3190 (2)	0.0245 (7)
C1	0.3693 (3)	0.3394 (3)	0.2954 (2)	0.0266 (9)
C2	0.3764 (3)	0.4281 (3)	0.2916 (2)	0.0253 (9)
C3	0.4322 (3)	0.4611 (3)	0.2728 (3)	0.0294 (9)
H3	0.466417	0.426408	0.263873	0.035*
C4	0.4373 (3)	0.5442 (4)	0.2673 (3)	0.0342 (11)
H4	0.475851	0.566503	0.255564	0.041*
C5	0.3866 (3)	0.5948 (3)	0.2787 (3)	0.0344 (11)
H5	0.390095	0.651683	0.274236	0.041*
C6	0.3302 (3)	0.5632 (3)	0.2967 (2)	0.0281 (9)
H6	0.295000	0.598037	0.303874	0.034*
C7	0.3264 (3)	0.4795 (3)	0.3041 (2)	0.0271 (9)
C8	0.1878 (3)	0.4518 (3)	0.2632 (2)	0.0277 (9)
H8A	0.156251	0.407741	0.269216	0.033*
H8B	0.190980	0.442940	0.218688	0.033*
C9	0.1480 (3)	0.5325 (3)	0.2604 (3)	0.0290 (10)
C10	0.1034 (3)	0.5649 (5)	0.1965 (3)	0.0462 (15)
H10	0.098791	0.537651	0.155901	0.055*
C11	0.0650 (4)	0.6378 (5)	0.1919 (4)	0.057 (2)
H11	0.034398	0.660175	0.148057	0.069*
C12	0.0714 (4)	0.6775 (4)	0.2504 (4)	0.0468 (15)
H12	0.044265	0.726533	0.247009	0.056*
C13	0.1172 (4)	0.6461 (4)	0.3144 (4)	0.0433 (14)
H13	0.122472	0.674128	0.354903	0.052*
C14	0.1555 (3)	0.5732 (4)	0.3192 (3)	0.0356 (11)
H14	0.186950	0.551563	0.363174	0.043*
C15	0.2787 (3)	0.4116 (3)	0.3792 (2)	0.0252 (9)
C16	0.3596 (3)	0.4057 (3)	0.4308 (2)	0.0256 (9)

C17	0.3829 (3)	0.4469 (3)	0.4935 (3)	0.0310 (10)
H17	0.347733	0.480339	0.502206	0.037*
C18	0.4577 (3)	0.4387 (4)	0.5431 (3)	0.0363 (11)
H18	0.473560	0.466721	0.585593	0.044*
C19	0.5082 (3)	0.3904 (4)	0.5307 (3)	0.0365 (11)
H19	0.559094	0.385345	0.564757	0.044*
C20	0.4863 (3)	0.3484 (3)	0.4689 (3)	0.0312 (10)
H20	0.521727	0.314696	0.460727	0.037*
C21	0.4114 (3)	0.3567 (3)	0.4191 (2)	0.0249 (9)
C22	0.3791 (3)	0.2195 (3)	0.3683 (2)	0.0242 (8)
H22A	0.340620	0.195644	0.325347	0.029*
H22B	0.360566	0.212413	0.404673	0.029*
C23	0.4542 (3)	0.1740 (3)	0.3888 (2)	0.0252 (9)
C24	0.5058 (3)	0.1935 (4)	0.3615 (3)	0.0370 (12)
H24	0.494805	0.236206	0.329020	0.044*
C25	0.5742 (3)	0.1500 (4)	0.3817 (3)	0.0351 (11)
H25	0.609363	0.162697	0.362551	0.042*
C26	0.5904 (4)	0.0889 (4)	0.4295 (4)	0.0472 (15)
H26	0.636531	0.058973	0.442905	0.057*
C27	0.5402 (4)	0.0710 (5)	0.4579 (5)	0.066 (3)
H27	0.551930	0.029386	0.491360	0.079*
C28	0.4716 (3)	0.1141 (4)	0.4376 (4)	0.0469 (16)
H28	0.437033	0.101768	0.457477	0.056*

Atomic displacement parameters (Å^2) for **[Cu_2I_2(bdta)(MeCN)]$_n$ (8)**

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.02693 (17)	0.0409 (2)	0.01975 (16)	0.00496 (12)	0.00948 (12)	-0.00064 (11)
I2	0.02395 (16)	0.0388 (2)	0.02004 (16)	0.00099 (11)	0.00995 (12)	-0.00146 (11)
Cu1	0.0284 (3)	0.0382 (3)	0.0177 (3)	0.0008 (2)	0.0092 (2)	0.0011 (2)
Cu2	0.0309 (4)	0.0400 (5)	0.0206 (4)	0.000	0.0129 (3)	0.000
Cu3	0.0292 (4)	0.0453 (5)	0.0179 (4)	0.000	0.0096 (3)	0.000
S1	0.0422 (7)	0.0330 (6)	0.0172 (5)	0.0033 (5)	0.0130 (5)	-0.0002 (4)
S2	0.0270 (5)	0.0399 (7)	0.0216 (5)	0.0008 (5)	0.0133 (4)	0.0037 (4)
N1	0.0227 (17)	0.030 (2)	0.0189 (17)	-0.0009 (14)	0.0081 (14)	-0.0004 (14)
N2	0.0294 (19)	0.0254 (19)	0.0215 (17)	0.0021 (15)	0.0134 (15)	0.0005 (14)
C1	0.025 (2)	0.035 (3)	0.023 (2)	0.0062 (18)	0.0136 (17)	0.0048 (18)
C2	0.024 (2)	0.033 (2)	0.0170 (18)	0.0009 (17)	0.0070 (16)	0.0023 (16)
C3	0.025 (2)	0.038 (3)	0.024 (2)	0.0010 (19)	0.0091 (17)	-0.0014 (19)
C4	0.030 (2)	0.045 (3)	0.029 (2)	-0.007 (2)	0.013 (2)	0.006 (2)
C5	0.037 (3)	0.034 (3)	0.032 (2)	-0.004 (2)	0.014 (2)	0.004 (2)

C6	0.032 (2)	0.030 (2)	0.023 (2)	0.0033 (18)	0.0117 (18)	0.0039 (17)
C7	0.029 (2)	0.033 (2)	0.019 (2)	-0.0024 (18)	0.0109 (17)	0.0001 (17)
C8	0.027 (2)	0.036 (3)	0.022 (2)	-0.0036 (18)	0.0109 (17)	-0.0030 (18)
C9	0.024 (2)	0.040 (3)	0.025 (2)	-0.0008 (18)	0.0116 (18)	0.0029 (19)
C10	0.033 (3)	0.070 (4)	0.034 (3)	0.018 (3)	0.013 (2)	0.007 (3)
C11	0.042 (3)	0.083 (5)	0.050 (4)	0.033 (3)	0.022 (3)	0.031 (4)
C12	0.037 (3)	0.042 (3)	0.070 (4)	0.012 (2)	0.030 (3)	0.019 (3)
C13	0.037 (3)	0.039 (3)	0.064 (4)	0.001 (2)	0.031 (3)	-0.005 (3)
C14	0.036 (3)	0.037 (3)	0.033 (3)	0.004 (2)	0.013 (2)	-0.001 (2)
C15	0.026 (2)	0.034 (2)	0.0177 (19)	0.0007 (17)	0.0121 (16)	-0.0027 (16)
C16	0.026 (2)	0.032 (2)	0.0192 (19)	-0.0015 (17)	0.0101 (17)	0.0011 (17)
C17	0.036 (3)	0.035 (3)	0.024 (2)	-0.004 (2)	0.014 (2)	-0.0014 (18)
C18	0.045 (3)	0.041 (3)	0.020 (2)	-0.005 (2)	0.010 (2)	-0.0028 (19)
C19	0.036 (3)	0.042 (3)	0.023 (2)	-0.005 (2)	0.004 (2)	0.000 (2)
C20	0.031 (2)	0.037 (3)	0.024 (2)	-0.002 (2)	0.0097 (19)	0.0004 (19)
C21	0.026 (2)	0.030 (2)	0.0149 (18)	-0.0005 (17)	0.0052 (16)	0.0003 (16)
C22	0.027 (2)	0.028 (2)	0.0197 (19)	0.0000 (17)	0.0118 (17)	0.0027 (16)
C23	0.025 (2)	0.032 (2)	0.0191 (19)	-0.0015 (17)	0.0104 (16)	-0.0048 (17)
C24	0.033 (3)	0.046 (3)	0.038 (3)	0.011 (2)	0.021 (2)	0.014 (2)
C25	0.030 (2)	0.048 (3)	0.034 (3)	0.011 (2)	0.021 (2)	0.009 (2)
C26	0.039 (3)	0.053 (4)	0.057 (4)	0.021 (3)	0.028 (3)	0.021 (3)
C27	0.047 (4)	0.076 (5)	0.091 (6)	0.029 (4)	0.044 (4)	0.056 (5)
C28	0.033 (3)	0.056 (4)	0.062 (4)	0.011 (3)	0.030 (3)	0.028 (3)

Geometric parameters (Å, °) for **$[Cu_2I_2(bdta)(MeCN)]_n$ (8)**

I1—Cu1	2.5278 (7)	C6—C7	1.397 (7)
I1—Cu3	2.6315 (6)	C8—C9	1.526 (7)
I2—Cu1	2.5926 (7)	C9—C10	1.383 (8)
I2—Cu2^{i}	2.6997 (7)	C9—C14	1.381 (7)
I2—Cu3	2.7190 (7)	C10—C11	1.394 (10)
Cu1—Cu3	2.6427 (6)	C11—C12	1.372 (11)
Cu1—S1	2.2298 (13)	C12—C13	1.382 (10)
Cu2—S2^{ii}	2.2811 (13)	C13—C14	1.393 (8)
Cu2—S2	2.2810 (13)	C15—C16	1.489 (6)
S1—C1	1.686 (5)	C16—C17	1.399 (7)
S2—C15	1.671 (5)	C16—C21	1.387 (7)
N1—C1	1.330 (6)	C17—C18	1.394 (8)
N1—C21	1.449 (6)	C18—C19	1.368 (9)
N1—C22	1.494 (6)	C19—C20	1.393 (7)
N2—C7	1.445 (6)	C20—C21	1.397 (7)

N2—C8	1.473 (6)	C22—C23	1.522 (7)
N2—C15	1.337 (6)	C23—C24	1.384 (7)
C1—C2	1.477 (7)	C23—C28	1.374 (7)
C2—C3	1.405 (7)	C24—C25	1.400 (7)
C2—C7	1.390 (7)	C25—C26	1.377 (8)
C3—C4	1.385 (8)	C26—C27	1.370 (9)
C4—C5	1.383 (8)	C27—C28	1.399 (8)
C5—C6	1.395 (7)		
Cu1—I1—Cu3	61.58 (2)	C3—C2—C1	120.0 (4)
Cu1—I2—Cu2^{i}	89.134 (19)	C7—C2—C1	120.5 (4)
Cu1—I2—Cu3	59.617 (15)	C7—C2—C3	119.5 (5)
Cu2^{i}—I2—Cu3	76.45 (3)	C4—C3—C2	119.9 (5)
I1—Cu1—I2	120.50 (2)	C5—C4—C3	120.2 (5)
I1—Cu1—Cu3	61.14 (2)	C4—C5—C6	120.7 (5)
I2—Cu1—Cu3	62.570 (19)	C5—C6—C7	119.1 (5)
S1—Cu1—I1	126.55 (4)	C2—C7—N2	120.3 (4)
S1—Cu1—I2	112.75 (4)	C2—C7—C6	120.6 (5)
S1—Cu1—Cu3	156.64 (5)	C6—C7—N2	118.9 (4)
I2^{i}—Cu2—I2^{iii}	104.07 (4)	N2—C8—C9	113.8 (4)
S2—Cu2—I2^{iii}	125.01 (3)	C10—C9—C8	118.2 (5)
S2^{ii}—Cu2—I2^{iii}	92.22 (3)	C14—C9—C8	122.0 (5)
S2^{ii}—Cu2—I2^{i}	125.01 (3)	C14—C9—C10	119.8 (5)
S2—Cu2—I2^{i}	92.22 (3)	C9—C10—C11	119.8 (6)
S2—Cu2—S2^{ii}	120.29 (8)	C12—C11—C10	120.3 (6)
I1—Cu3—I1^{iv}	113.76 (4)	C11—C12—C13	120.0 (6)
I1—Cu3—I2	112.368 (10)	C12—C13—C14	119.9 (6)
I1^{iv}—Cu3—I2^{iv}	112.367 (10)	C9—C14—C13	120.2 (6)
I1^{iv}—Cu3—I2	107.431 (11)	N2—C15—S2	122.7 (4)
I1—Cu3—I2^{iv}	107.430 (10)	N2—C15—C16	117.6 (4)
I1—Cu3—Cu1	57.276 (16)	C16—C15—S2	119.7 (3)
I1^{iv}—Cu3—Cu1	144.45 (3)	C17—C16—C15	119.7 (4)
I1—Cu3—Cu1^{iv}	144.45 (3)	C21—C16—C15	120.9 (4)
I1^{iv}—Cu3—Cu1^{iv}	57.272 (16)	C21—C16—C17	119.3 (4)
I2—Cu3—I2^{iv}	103.03 (4)	C18—C17—C16	119.9 (5)
Cu1—Cu3—I2	57.814 (19)	C19—C18—C17	120.1 (5)
Cu1^{iv}—Cu3—I2	102.81 (3)	C18—C19—C20	121.2 (5)
Cu1—Cu3—I2^{iv}	102.81 (3)	C19—C20—C21	118.7 (5)
Cu1^{iv}—Cu3—I2^{iv}	57.817 (19)	C16—C21—N1	119.7 (4)
Cu1—Cu3—Cu1^{iv}	151.06 (5)	C16—C21—C20	120.8 (4)

C1—S1—Cu1	110.76 (18)	C20—C21—N1	119.2 (4)
C15—S2—Cu2	114.49 (17)	N1—C22—C23	113.1 (4)
C1—N1—C21	122.6 (4)	C24—C23—C22	121.7 (4)
C1—N1—C22	122.6 (4)	C28—C23—C22	118.5 (4)
C21—N1—C22	114.8 (4)	C28—C23—C24	119.8 (5)
C7—N2—C8	116.2 (4)	C23—C24—C25	119.9 (5)
C15—N2—C7	121.9 (4)	C26—C25—C24	119.9 (5)
C15—N2—C8	121.8 (4)	C27—C26—C25	120.2 (5)
N1—C1—S1	121.7 (4)	C26—C27—C28	120.1 (6)
N1—C1—C2	117.0 (4)	C23—C28—C27	120.1 (5)
C2—C1—S1	121.3 (3)		
Cu1—S1—C1—N1	179.0 (3)	C8—C9—C10—C11	178.9 (6)
Cu1—S1—C1—C2	-3.7 (4)	C8—C9—C14—C13	-178.9 (5)
Cu2—S2—C15—N2	173.6 (3)	C9—C10—C11—C12	-0.1 (11)
Cu2—S2—C15—C16	-7.0 (4)	C10—C9—C14—C13	1.2 (9)
S1—C1—C2—C3	-63.6 (6)	C10—C11—C12—C13	1.4 (11)
S1—C1—C2—C7	114.1 (4)	C11—C12—C13—C14	-1.4 (10)
S2—C15—C16—C17	-63.4 (6)	C12—C13—C14—C9	0.1 (9)
S2—C15—C16—C21	113.4 (5)	C14—C9—C10—C11	-1.2 (9)
N1—C1—C2—C3	113.9 (5)	C15—N2—C7—C2	72.8 (6)
N1—C1—C2—C7	-68.4 (6)	C15—N2—C7—C6	-112.5 (5)
N1—C22—C23—C24	-36.9 (6)	C15—N2—C8—C9	97.0 (5)
N1—C22—C23—C28	140.9 (5)	C15—C16—C17—C18	177.2 (5)
N2—C8—C9—C10	141.7 (5)	C15—C16—C21—N1	-2.7 (7)
N2—C8—C9—C14	-38.2 (7)	C15—C16—C21—C20	-177.0 (5)
N2—C15—C16—C17	116.1 (5)	C16—C17—C18—C19	-0.2 (8)
N2—C15—C16—C21	-67.1 (6)	C17—C16—C21—N1	174.1 (4)
C1—N1—C21—C16	73.3 (6)	C17—C16—C21—C20	-0.2 (7)
C1—N1—C21—C20	-112.2 (5)	C17—C18—C19—C20	-0.2 (9)
C1—N1—C22—C23	95.6 (5)	C18—C19—C20—C21	0.3 (8)
C1—C2—C3—C4	178.1 (4)	C19—C20—C21—N1	-174.5 (5)
C1—C2—C7—N2	-1.8 (7)	C19—C20—C21—C16	-0.1 (8)
C1—C2—C7—C6	-176.4 (4)	C21—N1—C1—S1	176.4 (3)
C2—C3—C4—C5	-1.4 (8)	C21—N1—C1—C2	-1.0 (7)
C3—C2—C7—N2	175.9 (4)	C21—N1—C22—C23	-85.1 (5)
C3—C2—C7—C6	1.3 (7)	C21—C16—C17—C18	0.4 (8)
C3—C4—C5—C6	0.8 (8)	C22—N1—C1—S1	-4.4 (6)
C4—C5—C6—C7	0.9 (8)	C22—N1—C1—C2	178.1 (4)
C5—C6—C7—N2	-176.6 (4)	C22—N1—C21—C16	-105.9 (5)

C5—C6—C7—C2	-1.9 (7)	C22—N1—C21—C20	68.5 (6)
C7—N2—C8—C9	-84.8 (5)	C22—C23—C24—C25	-179.9 (5)
C7—N2—C15—S2	178.3 (4)	C22—C23—C28—C27	-179.9 (7)
C7—N2—C15—C16	-1.2 (7)	C23—C24—C25—C26	-0.9 (10)
C7—C2—C3—C4	0.4 (7)	C24—C23—C28—C27	-2.0 (11)
C8—N2—C7—C2	-105.4 (5)	C24—C25—C26—C27	-0.7 (12)
C8—N2—C7—C6	69.3 (6)	C25—C26—C27—C28	1.0 (14)
C8—N2—C15—S2	-3.7 (7)	C26—C27—C28—C23	0.4 (14)
C8—N2—C15—C16	176.9 (4)	C28—C23—C24—C25	2.3 (9)

Symmetry codes: (i) -*x*+1/2, -*y*+1/2, -*z*+1/2; (ii) -*x*+1/2, *y*, -*z*+1; (iii) *x*, -*y*+1/2, *z*+1/2; (iv) -*x*+1/2, *y*, -*z*.

Crystal data for **$[Cu_2Br_2(bdta)]_n$ (9)**

$C_{28}H_{22}Br_2Cu_2N_2S_2$	$Z = 2$
$M_r = 737.49$	$F(000) = 728$
Triclinic, $P\bar{1}$	$D_x = 1.857$ Mg m^{-3}
$a = 10.6426$ (12) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 11.6334$ (14) Å	Cell parameters from 2871 reflections
$c = 12.1551$ (15) Å	$\theta = 1.9–25.0°$
$\alpha = 108.021$ (9)°	$\mu = 4.82$ mm^{-1}
$\beta = 107.195$ (9)°	$T = 120$ K
$\gamma = 98.463$ (9)°	Block, yellow
$V = 1319.1$ (3) Å^3	0.16 × 0.09 × 0.08 mm

Data collection

STOE IPDS 2T diffractometer	5508 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	$R_{int} = 0.035$
rotation method, ω scans	$\theta_{max} = 29.2°$, $\theta_{min} = 2.1°$
Absorption correction: multi-scan STOE LANA, absorption correction by scaling of reflection intensities. J. Koziskova, F. Hahn, J. Richter, J. Kozisek, "Comparison of different absorption corrections on the model structure of tetrakis(μ_2-acetato)- diaqua-di-copper(II)", Acta Chimica Slovaca, vol. 9, no. 2, 2016, pp. 136 - 140. Afterwards a spherical absorption correction was performed within STOE LANA.	$h = -14\rightarrow12$
$T_{min} = 0.293$, $T_{max} = 0.701$	$k = -15\rightarrow15$
12200 measured reflections	$l = -16\rightarrow16$
6508 independent reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.031$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.082$	H-atom parameters constrained
$S = 1.03$	$w = 1/[\sigma^2(F_o^2) + (0.0535P)^2 + 0.0582P]$ where $P = (F_o^2 + 2F_c^2)/3$
6508 reflections	$(\Delta/\sigma)_{max} = 0.001$
325 parameters	$\Delta\rangle_{max} = 0.85$ e Å^{-3}
0 restraints	$\Delta\rangle_{min} = -0.83$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for **[Cu$_2$Br$_2$(bdta)]$_n$ (9)**

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.02722 (2)	0.80834 (2)	0.22317 (2)	0.01905 (7)
Br2	-0.01606 (2)	0.84772 (2)	0.53443 (2)	0.01487 (6)
Cu1	0.90430 (3)	0.91384 (3)	0.35321 (3)	0.02033 (8)
Cu2	0.15002 (3)	0.83259 (3)	0.43058 (3)	0.01833 (8)
S1	0.68786 (6)	0.90537 (6)	0.25357 (6)	0.01514 (12)
S2	0.36633 (6)	0.85125 (6)	0.53116 (6)	0.01900 (13)
N1	0.4416 (2)	0.77253 (18)	0.21006 (18)	0.0127 (4)
N2	0.55958 (19)	0.75762 (18)	0.47110 (18)	0.0119 (4)
C1	0.5761 (2)	0.7847 (2)	0.2481 (2)	0.0121 (4)
C2	0.6247 (2)	0.6856 (2)	0.2886 (2)	0.0124 (4)
C3	0.6883 (3)	0.6088 (2)	0.2221 (2)	0.0174 (5)
H3	0.696994	0.617804	0.149466	0.021*
C4	0.7386 (3)	0.5196 (2)	0.2623 (3)	0.0204 (5)
H4	0.780291	0.466712	0.216238	0.024*
C5	0.7285 (3)	0.5072 (2)	0.3688 (2)	0.0189 (5)
H5	0.763413	0.445992	0.395700	0.023*
C6	0.6673 (2)	0.5841 (2)	0.4373 (2)	0.0155 (4)

H6	0.662476	0.577187	0.511896	0.019*
C7	0.6136 (2)	0.6711 (2)	0.3948 (2)	0.0128 (4)
C8	0.6611 (2)	0.8533 (2)	0.5886 (2)	0.0142 (4)
H8A	0.631398	0.931659	0.605208	0.017*
H8B	0.749312	0.871109	0.577320	0.017*
C9	0.6835 (2)	0.8175 (2)	0.7015 (2)	0.0149 (5)
C10	0.7941 (3)	0.8915 (2)	0.8083 (3)	0.0232 (5)
H10	0.855226	0.959181	0.807397	0.028*
C11	0.8165 (3)	0.8677 (3)	0.9169 (2)	0.0271 (6)
H11	0.892146	0.919428	0.989954	0.033*
C12	0.7279 (3)	0.7682 (3)	0.9184 (3)	0.0255 (6)
H12	0.742071	0.752357	0.992655	0.031*
C13	0.6198 (3)	0.6928 (3)	0.8119 (3)	0.0223 (5)
H13	0.560767	0.623386	0.812320	0.027*
C14	0.5960 (3)	0.7173 (2)	0.7035 (2)	0.0180 (5)
H14	0.519966	0.665528	0.630844	0.022*
C15	0.4271 (2)	0.7549 (2)	0.4369 (2)	0.0132 (4)
C16	0.3340 (2)	0.6608 (2)	0.3136 (2)	0.0137 (4)
C17	0.2286 (2)	0.5672 (2)	0.3058 (3)	0.0184 (5)
H17	0.218134	0.562743	0.379411	0.022*
C18	0.1399 (3)	0.4813 (3)	0.1913 (3)	0.0235 (5)
H18	0.068247	0.418472	0.186622	0.028*
C19	0.1550 (3)	0.4863 (2)	0.0830 (3)	0.0225 (5)
H19	0.095184	0.425838	0.004670	0.027*
C20	0.2573 (3)	0.5797 (2)	0.0894 (2)	0.0174 (5)
H20	0.266716	0.584400	0.015416	0.021*
C21	0.3464 (2)	0.6667 (2)	0.2047 (2)	0.0132 (4)
C22	0.3781 (2)	0.8685 (2)	0.1752 (2)	0.0139 (4)
H22A	0.446543	0.950762	0.217642	0.017*
H22B	0.301845	0.875182	0.205609	0.017*
C23	0.3250 (2)	0.8402 (2)	0.0374 (2)	0.0138 (4)
C24	0.1844 (2)	0.8126 (2)	-0.0274 (2)	0.0179 (5)
H24	0.122607	0.805878	0.014343	0.021*
C25	0.1350 (3)	0.7952 (2)	-0.1528 (2)	0.0203 (5)
H25	0.039828	0.778065	-0.195995	0.024*
C26	0.2250 (3)	0.8028 (2)	-0.2146 (2)	0.0203 (5)
H26	0.191467	0.789774	-0.300376	0.024*
C27	0.3642 (3)	0.8297 (3)	-0.1505 (2)	0.0226 (5)
H27	0.425756	0.835445	-0.192655	0.027*
C28	0.4140 (3)	0.8481 (2)	-0.0262 (2)	0.0188 (5)

H28	0.509378	0.866190	0.016505	0.023*

Atomic displacement parameters (Å^2) for **[Cu_2Br_2(bdta)]$_n$ (9)**

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.01683 (12)	0.02696 (14)	0.01526 (12)	0.00888 (10)	0.00786 (10)	0.00700 (10)
Br2	0.01158 (11)	0.02015 (12)	0.01560 (11)	0.00562 (9)	0.00608 (9)	0.00850 (9)
Cu1	0.01399 (15)	0.02772 (17)	0.02147 (16)	0.00782 (13)	0.00633 (13)	0.01105 (14)
Cu2	0.01362 (15)	0.02322 (16)	0.01958 (16)	0.00784 (13)	0.00674 (13)	0.00782 (13)
S1	0.0121 (2)	0.0168 (3)	0.0192 (3)	0.0048 (2)	0.0060 (2)	0.0094 (2)
S2	0.0145 (3)	0.0287 (3)	0.0133 (3)	0.0107 (3)	0.0064 (2)	0.0036 (2)
N1	0.0129 (9)	0.0145 (9)	0.0133 (9)	0.0057 (8)	0.0061 (8)	0.0064 (8)
N2	0.0110 (8)	0.0151 (9)	0.0118 (9)	0.0053 (8)	0.0062 (8)	0.0051 (8)
C1	0.0134 (10)	0.0158 (10)	0.0086 (10)	0.0059 (9)	0.0053 (9)	0.0044 (8)
C2	0.0107 (9)	0.0115 (10)	0.0140 (10)	0.0027 (9)	0.0042 (9)	0.0038 (9)
C3	0.0204 (11)	0.0197 (12)	0.0173 (11)	0.0094 (10)	0.0110 (10)	0.0082 (10)
C4	0.0235 (12)	0.0197 (12)	0.0235 (13)	0.0128 (10)	0.0131 (11)	0.0077 (10)
C5	0.0207 (12)	0.0173 (11)	0.0221 (12)	0.0100 (10)	0.0087 (11)	0.0084 (10)
C6	0.0175 (11)	0.0160 (11)	0.0174 (11)	0.0061 (10)	0.0091 (10)	0.0086 (9)
C7	0.0103 (10)	0.0148 (10)	0.0153 (11)	0.0060 (9)	0.0067 (9)	0.0050 (9)
C8	0.0133 (10)	0.0166 (11)	0.0130 (10)	0.0036 (9)	0.0065 (9)	0.0046 (9)
C9	0.0156 (11)	0.0174 (11)	0.0145 (11)	0.0096 (10)	0.0068 (10)	0.0059 (9)
C10	0.0241 (13)	0.0173 (12)	0.0220 (13)	0.0045 (11)	0.0011 (11)	0.0065 (10)
C11	0.0327 (15)	0.0240 (13)	0.0140 (12)	0.0089 (13)	-0.0037 (12)	0.0039 (10)
C12	0.0341 (15)	0.0324 (14)	0.0158 (12)	0.0195 (13)	0.0093 (11)	0.0114 (11)
C13	0.0228 (12)	0.0275 (13)	0.0245 (13)	0.0102 (11)	0.0121 (11)	0.0150 (11)
C14	0.0162 (11)	0.0247 (12)	0.0164 (11)	0.0060 (10)	0.0088 (10)	0.0089 (10)
C15	0.0126 (10)	0.0173 (11)	0.0137 (10)	0.0061 (9)	0.0070 (9)	0.0079 (9)
C16	0.0113 (10)	0.0161 (11)	0.0152 (11)	0.0053 (9)	0.0054 (9)	0.0063 (9)
C17	0.0163 (11)	0.0193 (12)	0.0250 (13)	0.0055 (10)	0.0103 (11)	0.0124 (10)
C18	0.0151 (11)	0.0178 (12)	0.0344 (15)	0.0015 (10)	0.0062 (12)	0.0092 (11)
C19	0.0155 (11)	0.0168 (12)	0.0235 (13)	0.0036 (10)	-0.0032 (11)	0.0021 (10)
C20	0.0191 (12)	0.0158 (11)	0.0144 (11)	0.0075 (10)	0.0028 (10)	0.0034 (9)
C21	0.0108 (10)	0.0131 (10)	0.0166 (11)	0.0048 (9)	0.0054 (9)	0.0057 (9)
C22	0.0133 (10)	0.0164 (11)	0.0142 (11)	0.0079 (9)	0.0056 (9)	0.0063 (9)
C23	0.0163 (11)	0.0137 (10)	0.0126 (10)	0.0064 (9)	0.0052 (9)	0.0056 (9)
C24	0.0138 (11)	0.0218 (12)	0.0195 (12)	0.0050 (10)	0.0055 (10)	0.0098 (10)
C25	0.0174 (11)	0.0215 (12)	0.0177 (12)	0.0032 (11)	0.0007 (10)	0.0081 (10)
C26	0.0299 (13)	0.0188 (11)	0.0138 (11)	0.0106 (11)	0.0058 (11)	0.0084 (10)
C27	0.0283 (13)	0.0319 (14)	0.0190 (12)	0.0166 (12)	0.0149 (11)	0.0145 (11)
C28	0.0174 (11)	0.0270 (13)	0.0185 (12)	0.0109 (11)	0.0096 (10)	0.0118 (11)

Geometric parameters (Å, °) for **$[Cu_2Br_2(bdta)]_n$ (9)**

Br1—Cu1^{i}	2.4922 (5)	C6—C7	1.392 (3)
Br1—Cu2	2.3763 (5)	C8—C9	1.517 (3)
Br2—Cu1^{i}	2.5097 (5)	C9—C10	1.385 (4)
Br2—Cu1^{ii}	2.5881 (6)	C9—C14	1.393 (4)
Br2—Cu2	2.4540 (5)	C10—C11	1.392 (4)
Cu1—Cu2^{iii}	2.9053 (5)	C11—C12	1.389 (4)
Cu1—S1	2.2343 (7)	C12—C13	1.374 (4)
Cu2—S2	2.2059 (7)	C13—C14	1.392 (4)
S1—C1	1.672 (2)	C15—C16	1.488 (3)
S2—C15	1.686 (2)	C16—C17	1.403 (3)
N1—C1	1.338 (3)	C16—C21	1.390 (3)
N1—C21	1.446 (3)	C17—C18	1.383 (4)
N1—C22	1.492 (3)	C18—C19	1.390 (4)
N2—C7	1.453 (3)	C19—C20	1.387 (4)
N2—C8	1.482 (3)	C20—C21	1.393 (3)
N2—C15	1.340 (3)	C22—C23	1.509 (3)
C1—C2	1.488 (3)	C23—C24	1.403 (3)
C2—C3	1.402 (3)	C23—C28	1.398 (3)
C2—C7	1.388 (3)	C24—C25	1.395 (3)
C3—C4	1.388 (3)	C25—C26	1.390 (4)
C4—C5	1.378 (4)	C26—C27	1.390 (4)
C5—C6	1.396 (3)	C27—C28	1.379 (4)
Cu2—Br1—Cu1^{i}	73.231 (16)	C4—C5—C6	120.4 (2)
Cu1^{i}—Br2—Cu1^{ii}	81.050 (17)	C7—C6—C5	119.0 (2)
Cu2—Br2—Cu1^{ii}	89.212 (16)	C2—C7—N2	119.6 (2)
Cu2—Br2—Cu1^{i}	71.639 (14)	C2—C7—C6	121.1 (2)
Br1^{iii}—Cu1—Br2^{ii}	112.069 (17)	C6—C7—N2	118.9 (2)
Br1^{iii}—Cu1—Br2^{iii}	100.346 (16)	N2—C8—C9	115.1 (2)
Br1^{iii}—Cu1—Cu2^{iii}	51.550 (13)	C10—C9—C8	117.8 (2)
Br2^{iii}—Cu1—Br2^{ii}	98.951 (18)	C10—C9—C14	119.1 (2)
Br2^{iii}—Cu1—Cu2^{iii}	53.289 (12)	C14—C9—C8	123.1 (2)
Br2^{ii}—Cu1—Cu2^{iii}	97.053 (18)	C9—C10—C11	120.7 (3)
S1—Cu1—Br1^{iii}	116.58 (2)	C12—C11—C10	119.8 (3)
S1—Cu1—Br2^{iii}	124.93 (2)	C13—C12—C11	119.7 (3)
S1—Cu1—Br2^{ii}	102.72 (2)	C12—C13—C14	120.6 (3)
S1—Cu1—Cu2^{iii}	160.03 (2)	C13—C14—C9	120.1 (2)
Br1—Cu2—Br2	105.350 (16)	N2—C15—S2	121.60 (18)

Br1—Cu2—Cu1^{i}	55.219 (13)	N2—C15—C16	117.5 (2)
Br2—Cu2—Cu1^{i}	55.072 (13)	C16—C15—S2	120.90 (17)
S2—Cu2—Br1	132.64 (2)	C17—C16—C15	120.1 (2)
S2—Cu2—Br2	121.92 (2)	C21—C16—C15	121.0 (2)
S2—Cu2—Cu1^{i}	157.26 (2)	C21—C16—C17	118.9 (2)
C1—S1—Cu1	113.11 (8)	C18—C17—C16	120.3 (2)
C15—S2—Cu2	109.64 (8)	C17—C18—C19	120.3 (3)
C1—N1—C21	122.12 (19)	C20—C19—C18	120.0 (2)
C1—N1—C22	123.3 (2)	C19—C20—C21	119.7 (2)
C21—N1—C22	114.54 (18)	C16—C21—N1	119.7 (2)
C7—N2—C8	115.91 (18)	C16—C21—C20	120.8 (2)
C15—N2—C7	122.8 (2)	C20—C21—N1	119.2 (2)
C15—N2—C8	121.26 (19)	N1—C22—C23	113.95 (19)
N1—C1—S1	122.93 (18)	C24—C23—C22	119.8 (2)
N1—C1—C2	116.9 (2)	C28—C23—C22	121.1 (2)
C2—C1—S1	120.14 (16)	C28—C23—C24	118.9 (2)
C3—C2—C1	119.8 (2)	C25—C24—C23	120.2 (2)
C7—C2—C1	121.1 (2)	C26—C25—C24	120.0 (2)
C7—C2—C3	119.0 (2)	C27—C26—C25	119.7 (2)
C4—C3—C2	120.1 (2)	C28—C27—C26	120.6 (2)
C5—C4—C3	120.4 (2)	C27—C28—C23	120.5 (2)
Cu1—S1—C1—N1	169.52 (16)	C8—C9—C10—C11	176.7 (2)
Cu1—S1—C1—C2	-9.4 (2)	C8—C9—C14—C13	-177.4 (2)
Cu2—S2—C15—N2	172.97 (17)	C9—C10—C11—C12	0.5 (4)
Cu2—S2—C15—C16	-8.9 (2)	C10—C9—C14—C13	0.2 (4)
S1—C1—C2—C3	-65.1 (3)	C10—C11—C12—C13	0.9 (4)
S1—C1—C2—C7	112.0 (2)	C11—C12—C13—C14	-1.8 (4)
S2—C15—C16—C17	-60.5 (3)	C12—C13—C14—C9	1.2 (4)
S2—C15—C16—C21	117.0 (2)	C14—C9—C10—C11	-1.1 (4)
N1—C1—C2—C3	115.9 (2)	C15—N2—C7—C2	73.6 (3)
N1—C1—C2—C7	-67.0 (3)	C15—N2—C7—C6	-113.6 (3)
N1—C22—C23—C24	113.6 (2)	C15—N2—C8—C9	88.9 (3)
N1—C22—C23—C28	-70.2 (3)	C15—C16—C17—C18	178.5 (2)
N2—C8—C9—C10	168.1 (2)	C15—C16—C21—N1	-6.3 (3)
N2—C8—C9—C14	-14.2 (3)	C15—C16—C21—C20	-178.8 (2)
N2—C15—C16—C17	117.8 (2)	C16—C17—C18—C19	0.5 (4)
N2—C15—C16—C21	-64.7 (3)	C17—C16—C21—N1	171.3 (2)
C1—N1—C21—C16	76.0 (3)	C17—C16—C21—C20	-1.2 (3)
C1—N1—C21—C20	-111.4 (3)	C17—C18—C19—C20	-1.6 (4)

C1—N1—C22—C23	97.2 (3)	C18—C19—C20—C21	1.3 (4)
C1—C2—C3—C4	177.5 (2)	C19—C20—C21—N1	-172.4 (2)
C1—C2—C7—N2	-2.9 (3)	C19—C20—C21—C16	0.1 (3)
C1—C2—C7—C6	-175.6 (2)	C21—N1—C1—S1	179.31 (17)
C2—C3—C4—C5	-1.1 (4)	C21—N1—C1—C2	-1.7 (3)
C3—C2—C7—N2	174.2 (2)	C21—N1—C22—C23	-85.4 (2)
C3—C2—C7—C6	1.6 (3)	C21—C16—C17—C18	0.9 (3)
C3—C4—C5—C6	0.1 (4)	C22—N1—C1—S1	-3.4 (3)
C4—C5—C6—C7	1.7 (4)	C22—N1—C1—C2	175.5 (2)
C5—C6—C7—N2	-175.2 (2)	C22—N1—C21—C16	-101.5 (2)
C5—C6—C7—C2	-2.5 (4)	C22—N1—C21—C20	71.1 (3)
C7—N2—C8—C9	-93.1 (2)	C22—C23—C24—C25	175.4 (2)
C7—N2—C15—S2	176.47 (17)	C22—C23—C28—C27	-175.9 (2)
C7—N2—C15—C16	-1.7 (3)	C23—C24—C25—C26	1.1 (4)
C7—C2—C3—C4	0.2 (4)	C24—C23—C28—C27	0.3 (4)
C8—N2—C7—C2	-104.3 (2)	C24—C25—C26—C27	-0.9 (4)
C8—N2—C7—C6	68.5 (3)	C25—C26—C27—C28	0.4 (4)
C8—N2—C15—S2	-5.7 (3)	C26—C27—C28—C23	-0.1 (4)
C8—N2—C15—C16	176.1 (2)	C28—C23—C24—C25	-0.8 (4)

Symmetry codes: (i) *x*-1, *y*, *z*; (ii) -*x*+1, -*y*+2, -*z*+1; (iii) *x*+1, *y*, *z*.

Crystal data for **[Ag_2I_2(mdta)]$_n$ (10)**

$C_{16}H_{14}Ag_2I_2N_2S_2$	$F(000)$ = 1424
M_r = 767.95	D_x = 2.517 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, λ = 0.71073 Å
a = 13.3327 (8) Å	Cell parameters from 33275 reflections
b = 11.2308 (4) Å	θ = 2.1–29.7°
c = 13.8158 (8) Å	μ = 5.19 mm^{-1}
β = 101.542 (5)°	T = 120 K
V = 2026.90 (19) Å^3	Prism, yellow
Z = 4	0.22 × 0.17 × 0.05 mm

Data collection

STOE IPDS 2T diffractometer	5461 independent reflections
Radiation source: GeniX Mo, 0.05 x 0.05 mm2 microfocus	4861 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	R_{int} = 0.020

rotation method, ω scans	θ_{max} = 29.2°, θ_{min} = 1.9°
Absorption correction: integration STOE *X-RED32*, absorption correction by Gaussian integration, analogous to P. Coppens, "The Evaluation of Absorption and Extinction in Single-Crystal Structure Analysis", published in F. R. Ahmed (Editor), "Crystallographic Computing", Munksgaard, Copenhagen (1970), 255 - 270	h = -18→18
T_{min} = 0.288, T_{max} = 0.832	k = -15→15
24114 measured reflections	l = -18→18

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.019	Hydrogen site location: inferred from neighbouring sites
$wR(F^2)$ = 0.048	H-atom parameters constrained
S = 1.07	$w = 1/[\sigma^2(F_o^2) + (0.0267P)^2 + 1.616P]$ where $P = (F_o^2 + 2F_c^2)/3$
5461 reflections	$(\Delta/\sigma)_{max}$ = 0.002
219 parameters	$\Delta\rangle_{max}$ = 1.15 e Å^{-3}
0 restraints	$\Delta\rangle_{min}$ = -1.27 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for **[Ag_2I_2(mdta)]$_n$ (10)**

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.14221 (2)	0.01282 (2)	0.63152 (2)	0.01744 (4)
I2	0.15767 (2)	0.16980 (2)	0.33006 (2)	0.02748 (5)
Ag1	0.13918 (2)	0.22029 (2)	0.51858 (2)	0.02119 (5)
Ag2	0.08234 (2)	0.96916 (2)	0.42186 (2)	0.02321 (5)
S1	0.10400 (4)	0.40860 (5)	0.59887 (4)	0.01656 (11)
S2	0.09382 (4)	0.76872 (5)	0.33722 (4)	0.01585 (10)
N1	0.19058 (14)	0.61990 (15)	0.60269 (13)	0.0128 (3)
N2	0.20204 (14)	0.57081 (16)	0.37685 (13)	0.0122 (3)

C1	0.19272 (17)	0.50630 (18)	0.57675 (15)	0.0126 (4)
C2	0.27791 (17)	0.46594 (18)	0.52997 (16)	0.0129 (4)
C3	0.35346 (18)	0.3915 (2)	0.58235 (17)	0.0179 (4)
H3	0.352295	0.370932	0.648807	0.021*
C4	0.43026 (19)	0.3475 (2)	0.53787 (19)	0.0226 (5)
H4	0.482144	0.297825	0.574183	0.027*
C5	0.43140 (19)	0.3758 (2)	0.44063 (19)	0.0215 (5)
H5	0.483368	0.344198	0.410012	0.026*
C6	0.35697 (18)	0.4503 (2)	0.38746 (17)	0.0177 (4)
H6	0.357537	0.469337	0.320563	0.021*
C7	0.28162 (16)	0.49677 (18)	0.43330 (16)	0.0125 (4)
C8	0.13443 (18)	0.5162 (2)	0.29161 (16)	0.0171 (4)
H8A	0.158719	0.435652	0.281465	0.026*
H8B	0.134793	0.564327	0.232522	0.026*
H8C	0.064620	0.512031	0.303871	0.026*
C9	0.18885 (16)	0.68417 (18)	0.40030 (15)	0.0117 (4)
C10	0.26271 (16)	0.73756 (18)	0.48392 (15)	0.0119 (4)
C11	0.32801 (17)	0.8276 (2)	0.46444 (17)	0.0167 (4)
H11	0.327589	0.850944	0.398262	0.020*
C12	0.39357 (18)	0.8830 (2)	0.54209 (18)	0.0199 (5)
H12	0.438192	0.944091	0.528794	0.024*
C13	0.39446 (18)	0.8498 (2)	0.63880 (18)	0.0184 (4)
H13	0.439676	0.888113	0.691482	0.022*
C14	0.32947 (17)	0.76085 (19)	0.65886 (16)	0.0156 (4)
H14	0.329786	0.738136	0.725158	0.019*
C15	0.26396 (16)	0.70524 (18)	0.58134 (16)	0.0122 (4)
C16	0.11200 (19)	0.6633 (2)	0.65496 (19)	0.0194 (5)
H16A	0.043950	0.643723	0.616556	0.029*
H16B	0.118253	0.749831	0.663179	0.029*
H16C	0.121387	0.625301	0.720008	0.029*

Atomic displacement parameters (Å^2) for **$[Ag_2I_2(mdta)]_n$ (10)**

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.02103 (8)	0.01151 (7)	0.01905 (7)	0.00221 (5)	0.00225 (6)	-0.00038 (5)
I2	0.04606 (11)	0.01508 (8)	0.02712 (9)	-0.00476 (6)	0.02124 (7)	-0.00520 (6)
Ag1	0.02911 (10)	0.01310 (8)	0.02254 (9)	0.00050 (6)	0.00796 (7)	-0.00287 (6)
Ag2	0.02933 (10)	0.01439 (8)	0.02481 (10)	0.00096 (7)	0.00281 (7)	-0.00256 (6)
S1	0.0219 (3)	0.0110 (2)	0.0195 (3)	-0.00238 (19)	0.0108 (2)	-0.00091 (19)
S2	0.0171 (2)	0.0109 (2)	0.0171 (2)	0.00257 (19)	-0.0025 (2)	0.00015 (19)
N1	0.0149 (9)	0.0100 (8)	0.0146 (8)	0.0004 (6)	0.0058 (7)	-0.0001 (6)

N2	0.0133 (8)	0.0118 (8)	0.0109 (8)	0.0020 (6)	0.0011 (6)	-0.0011 (6)
C1	0.0170 (10)	0.0112 (9)	0.0097 (9)	0.0017 (7)	0.0029 (8)	0.0014 (7)
C2	0.0161 (10)	0.0100 (9)	0.0138 (10)	0.0021 (7)	0.0057 (8)	0.0000 (7)
C3	0.0216 (11)	0.0167 (10)	0.0153 (10)	0.0044 (8)	0.0038 (8)	0.0039 (8)
C4	0.0212 (12)	0.0209 (11)	0.0254 (12)	0.0101 (9)	0.0041 (10)	0.0047 (9)
C5	0.0195 (11)	0.0224 (11)	0.0252 (12)	0.0076 (9)	0.0107 (9)	0.0029 (9)
C6	0.0205 (11)	0.0187 (10)	0.0161 (10)	0.0035 (8)	0.0089 (8)	0.0009 (8)
C7	0.0141 (10)	0.0093 (9)	0.0138 (9)	0.0010 (7)	0.0024 (8)	0.0003 (7)
C8	0.0198 (11)	0.0152 (10)	0.0143 (10)	0.0015 (8)	-0.0012 (8)	-0.0026 (8)
C9	0.0129 (9)	0.0119 (9)	0.0116 (9)	0.0000 (7)	0.0052 (7)	0.0010 (7)
C10	0.0120 (9)	0.0091 (9)	0.0140 (9)	0.0015 (7)	0.0010 (7)	-0.0005 (7)
C11	0.0166 (10)	0.0169 (10)	0.0176 (10)	-0.0009 (8)	0.0054 (8)	0.0027 (8)
C12	0.0144 (10)	0.0198 (11)	0.0254 (12)	-0.0051 (8)	0.0034 (9)	-0.0010 (9)
C13	0.0148 (10)	0.0190 (10)	0.0205 (11)	-0.0024 (8)	0.0016 (8)	-0.0025 (9)
C14	0.0182 (10)	0.0139 (9)	0.0132 (9)	0.0011 (8)	-0.0006 (8)	0.0001 (8)
C15	0.0127 (9)	0.0077 (8)	0.0162 (10)	0.0010 (7)	0.0030 (8)	0.0016 (7)
C16	0.0231 (12)	0.0145 (10)	0.0251 (12)	0.0001 (8)	0.0158 (9)	-0.0022 (9)

Geometric parameters (Å, º) for **$[Ag_2I_2(mdta)]_n$ (10)**

I1—Ag1	2.8001 (2)	C4—C5	1.384 (4)
I1—Ag2^{i}	2.9435 (3)	C5—H5	0.9500
I1—Ag2^{ii}	2.8884 (3)	C5—C6	1.390 (3)
I2—Ag1	2.7245 (3)	C6—H6	0.9500
I2—Ag2^{ii}	2.8643 (3)	C6—C7	1.392 (3)
Ag1—Ag2^{ii}	3.1479 (3)	C8—H8A	0.9800
Ag1—S1	2.4761 (6)	C8—H8B	0.9800
Ag2—S2	2.5553 (6)	C8—H8C	0.9800
S1—C1	1.686 (2)	C9—C10	1.486 (3)
S2—C9	1.681 (2)	C10—C11	1.395 (3)
N1—C1	1.327 (3)	C10—C15	1.391 (3)
N1—C15	1.442 (3)	C11—H11	0.9500
N1—C16	1.470 (3)	C11—C12	1.388 (3)
N2—C7	1.447 (3)	C12—H12	0.9500
N2—C8	1.467 (3)	C12—C13	1.385 (3)
N2—C9	1.334 (3)	C13—H13	0.9500
C1—C2	1.486 (3)	C13—C14	1.386 (3)
C2—C3	1.394 (3)	C14—H14	0.9500
C2—C7	1.390 (3)	C14—C15	1.388 (3)
C3—H3	0.9500	C16—H16A	0.9800
C3—C4	1.387 (3)	C16—H16B	0.9800

C4—H4	0.9500	C16—H16C	0.9800
Ag1—I1—Ag2^{ii}	67.178 (7)	C4—C5—C6	120.4 (2)
Ag1—I1—Ag2^{i}	84.415 (8)	C6—C5—H5	119.8
Ag2^{ii}—I1—Ag2^{i}	72.381 (9)	C5—C6—H6	120.4
Ag1—I2—Ag2^{ii}	68.508 (7)	C5—C6—C7	119.3 (2)
I1—Ag1—Ag2^{ii}	57.751 (7)	C7—C6—H6	120.4
I2—Ag1—I1	111.442 (8)	C2—C7—N2	119.85 (19)
I2—Ag1—Ag2^{ii}	57.851 (6)	C2—C7—C6	120.8 (2)
S1—Ag1—I1	116.358 (15)	C6—C7—N2	119.23 (19)
S1—Ag1—I2	131.875 (15)	N2—C8—H8A	109.5
S1—Ag1—Ag2^{ii}	154.729 (16)	N2—C8—H8B	109.5
I1^{iii}—Ag2—I1^{i}	107.619 (9)	N2—C8—H8C	109.5
I1^{iii}—Ag2—Ag1^{iii}	55.073 (6)	H8A—C8—H8B	109.5
I1^{i}—Ag2—Ag1^{iii}	101.020 (7)	H8A—C8—H8C	109.5
I2^{iii}—Ag2—I1^{i}	105.316 (8)	H8B—C8—H8C	109.5
I2^{iii}—Ag2—I1^{iii}	105.039 (8)	N2—C9—S2	122.39 (16)
I2^{iii}—Ag2—Ag1^{iii}	53.639 (6)	N2—C9—C10	118.35 (18)
S2—Ag2—I1^{i}	95.564 (14)	C10—C9—S2	119.25 (15)
S2—Ag2—I1^{iii}	125.352 (14)	C11—C10—C9	118.97 (19)
S2—Ag2—I2^{iii}	115.597 (16)	C15—C10—C9	121.65 (19)
S2—Ag2—Ag1^{iii}	162.205 (16)	C15—C10—C11	119.25 (19)
C1—S1—Ag1	105.79 (8)	C10—C11—H11	120.1
C9—S2—Ag2	111.62 (7)	C12—C11—C10	119.8 (2)
C1—N1—C15	122.13 (19)	C12—C11—H11	120.1
C1—N1—C16	120.50 (19)	C11—C12—H12	119.7
C15—N1—C16	117.37 (17)	C13—C12—C11	120.5 (2)
C7—N2—C8	117.31 (17)	C13—C12—H12	119.7
C9—N2—C7	122.38 (17)	C12—C13—H13	119.9
C9—N2—C8	120.31 (18)	C12—C13—C14	120.1 (2)
N1—C1—S1	121.54 (17)	C14—C13—H13	119.9
N1—C1—C2	118.06 (19)	C13—C14—H14	120.3
C2—C1—S1	120.37 (15)	C13—C14—C15	119.5 (2)
C3—C2—C1	119.52 (19)	C15—C14—H14	120.3
C7—C2—C1	121.28 (19)	C10—C15—N1	119.62 (18)
C7—C2—C3	119.1 (2)	C14—C15—N1	119.30 (19)
C2—C3—H3	119.9	C14—C15—C10	120.9 (2)
C4—C3—C2	120.3 (2)	N1—C16—H16A	109.5
C4—C3—H3	119.9	N1—C16—H16B	109.5
C3—C4—H4	120.0	N1—C16—H16C	109.5

C5—C4—C3	120.1 (2)	H16A—C16—H16B	109.5
C5—C4—H4	120.0	H16A—C16—H16C	109.5
C4—C5—H5	119.8	H16B—C16—H16C	109.5
Ag1—S1—C1—N1	174.27 (16)	C7—N2—C9—C10	3.7 (3)
Ag1—S1—C1—C2	-7.62 (18)	C7—C2—C3—C4	-1.0 (3)
Ag2—S2—C9—N2	171.99 (16)	C8—N2—C7—C2	-113.3 (2)
Ag2—S2—C9—C10	-9.43 (19)	C8—N2—C7—C6	62.1 (3)
S1—C1—C2—C3	-68.7 (3)	C8—N2—C9—S2	1.9 (3)
S1—C1—C2—C7	108.6 (2)	C8—N2—C9—C10	-176.7 (2)
S2—C9—C10—C11	-65.9 (3)	C9—N2—C7—C2	66.3 (3)
S2—C9—C10—C15	110.0 (2)	C9—N2—C7—C6	-118.2 (2)
N1—C1—C2—C3	109.5 (2)	C9—C10—C11—C12	176.5 (2)
N1—C1—C2—C7	-73.2 (3)	C9—C10—C15—N1	-1.4 (3)
N2—C9—C10—C11	112.7 (2)	C9—C10—C15—C14	-176.3 (2)
N2—C9—C10—C15	-71.3 (3)	C10—C11—C12—C13	-0.2 (4)
C1—N1—C15—C10	67.9 (3)	C11—C10—C15—N1	174.52 (19)
C1—N1—C15—C14	-117.1 (2)	C11—C10—C15—C14	-0.3 (3)
C1—C2—C3—C4	176.3 (2)	C11—C12—C13—C14	-0.1 (4)
C1—C2—C7—N2	0.8 (3)	C12—C13—C14—C15	0.2 (3)
C1—C2—C7—C6	-174.5 (2)	C13—C14—C15—N1	-174.9 (2)
C2—C3—C4—C5	-1.0 (4)	C13—C14—C15—C10	0.0 (3)
C3—C2—C7—N2	178.05 (19)	C15—N1—C1—S1	-177.92 (15)
C3—C2—C7—C6	2.7 (3)	C15—N1—C1—C2	3.9 (3)
C3—C4—C5—C6	1.3 (4)	C15—C10—C11—C12	0.4 (3)
C4—C5—C6—C7	0.4 (4)	C16—N1—C1—S1	2.1 (3)
C5—C6—C7—N2	-177.8 (2)	C16—N1—C1—C2	-176.07 (19)
C5—C6—C7—C2	-2.4 (3)	C16—N1—C15—C10	-112.1 (2)
C7—N2—C9—S2	-177.74 (16)	C16—N1—C15—C14	62.9 (3)

Symmetry codes: (i) -*x*, -*y*+1, -*z*+1; (ii) *x*, *y*-1, *z*; (iii) *x*, *y*+1, *z*.

Crystal data for **(bdta)**

$C_{28}H_{22}N_2S_2$	$F(000) = 944$
$M_r = 450.59$	$D_x = 1.335$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 9.3720$ (3) Å	Cell parameters from 10534 reflections
$b = 14.5073$ (9) Å	$\theta = 1.9$–$30.1°$
$c = 16.6745$ (7) Å	$\mu = 0.26$ mm^{-1}

β = 98.533 (3)°	T = 120 K
V = 2242.01 (18) Å^3	Prism, colourless
Z = 4	0.41 × 0.35 × 0.22 mm

Data collection

STOE IPDS 2T diffractometer	3451 reflections with $I > 2\sigma(I)$
Radiation source: GeniX Mo, 0.05 x 0.05 mm2 microfocus	R_{int} = 0.111
Detector resolution: 6.67 pixels mm^{-1}	θ_{max} = 26.0°, θ_{min} = 1.9°
rotation method, ω scans	h = -11→11
20437 measured reflections	k = -17→17
4270 independent reflections	l = -20→20

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.055	Hydrogen site location: inferred from neighbouring sites
$wR(F^2)$ = 0.154	H-atom parameters constrained
S = 1.15	$w = 1/[\sigma^2(F_o^2) + (0.0235P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
4270 reflections	$(\Delta/\sigma)_{max} < 0.001$
289 parameters	$\Delta\rangle_{max}$ = 0.53 e Å^{-3}
0 restraints	$\Delta\rangle_{min}$ = -0.36 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for **(bdta)**

	X	*y*	*z*	U_{iso}*/U_{eq}
S1	0.40411 (5)	0.30629 (5)	0.55959 (4)	0.0244 (2)
S2	0.82215 (6)	0.47184 (5)	0.42256 (4)	0.0248 (2)
N1	0.61625 (16)	0.25697 (14)	0.47813 (11)	0.0158 (4)
N2	0.78920 (17)	0.41777 (15)	0.57182 (11)	0.0181 (4)

C1	0.8272 (2)	0.39854 (18)	0.49921 (13)	0.0172 (5)
C2	0.8701 (2)	0.30090 (18)	0.48733 (13)	0.0169 (5)
C3	1.0143 (2)	0.2772 (2)	0.48581 (14)	0.0211 (5)
H3	1.087916	0.322497	0.496229	0.025*
C4	1.0488 (2)	0.1874 (2)	0.46904 (14)	0.0231 (6)
H4	1.147053	0.171156	0.469488	0.028*
C5	0.9436 (2)	0.12080 (19)	0.45162 (14)	0.0230 (5)
H5	0.968848	0.060040	0.437785	0.028*
C6	0.7996 (2)	0.14364 (19)	0.45457 (14)	0.0197 (5)
H6	0.726082	0.098389	0.443223	0.024*
C7	0.76512 (19)	0.23246 (18)	0.47408 (13)	0.0161 (5)
C8	0.5196 (2)	0.26583 (19)	0.40063 (13)	0.0182 (5)
H8A	0.578601	0.281797	0.358061	0.022*
H8B	0.453164	0.318042	0.405063	0.022*
C9	0.4303 (2)	0.18187 (18)	0.37305 (14)	0.0176 (5)
C10	0.3688 (2)	0.1787 (2)	0.29159 (14)	0.0233 (6)
H10	0.389097	0.226182	0.255662	0.028*
C11	0.2783 (2)	0.1068 (2)	0.26288 (16)	0.0297 (6)
H11	0.236106	0.105090	0.207466	0.036*
C12	0.2494 (2)	0.0371 (2)	0.31532 (18)	0.0292 (6)
H12	0.186372	-0.011958	0.295907	0.035*
C13	0.3121 (2)	0.0390 (2)	0.39548 (17)	0.0257 (6)
H13	0.292855	-0.009109	0.430997	0.031*
C14	0.4033 (2)	0.11092 (18)	0.42476 (14)	0.0203 (5)
H14	0.446976	0.111561	0.479937	0.024*
C15	0.5718 (2)	0.27873 (17)	0.54926 (13)	0.0165 (5)
C16	0.6850 (2)	0.27862 (19)	0.62223 (14)	0.0173 (5)
C17	0.6854 (2)	0.21155 (19)	0.68206 (14)	0.0208 (5)
H17	0.612699	0.165408	0.676585	0.025*
C18	0.7916 (2)	0.2118 (2)	0.74964 (15)	0.0245 (6)
H18	0.791853	0.165561	0.789998	0.029*
C19	0.8970 (2)	0.2793 (2)	0.75828 (14)	0.0240 (6)
H19	0.969944	0.278925	0.804372	0.029*
C20	0.8966 (2)	0.3474 (2)	0.69999 (15)	0.0224 (5)
H20	0.968486	0.394062	0.706222	0.027*
C21	0.7904 (2)	0.34704 (18)	0.63245 (14)	0.0169 (5)
C22	0.7277 (3)	0.5096 (2)	0.58549 (16)	0.0278 (6)
H22A	0.625961	0.511128	0.558892	0.033*
H22B	0.781144	0.556983	0.559280	0.033*
C23	0.7329 (2)	0.53408 (18)	0.67375 (15)	0.0210 (5)

C24	0.8472 (2)	0.58458 (19)	0.71462 (16)	0.0245 (6)
H24	0.923519	0.603205	0.686612	0.029*
C25	0.8517 (2)	0.6081 (2)	0.79507 (16)	0.0278 (6)
H25	0.931421	0.641811	0.822365	0.033*
C26	0.7392 (2)	0.5824 (2)	0.83605 (16)	0.0295 (6)
H26	0.740536	0.599052	0.891256	0.035*
C27	0.6251 (2)	0.5322 (2)	0.79551 (17)	0.0278 (6)
H27	0.548634	0.513848	0.823550	0.033*
C28	0.6206 (2)	0.5086 (2)	0.71543 (16)	0.0241 (6)
H28	0.540778	0.474821	0.688371	0.029*

Atomic displacement parameters (Å^2) for **(bdta)**

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0148 (3)	0.0322 (4)	0.0267 (4)	0.0038 (2)	0.0048 (2)	-0.0030 (3)
S2	0.0359 (4)	0.0211 (4)	0.0182 (4)	-0.0007 (3)	0.0061 (2)	0.0025 (2)
N1	0.0079 (8)	0.0205 (11)	0.0182 (10)	0.0003 (8)	-0.0004 (6)	-0.0010 (8)
N2	0.0194 (9)	0.0186 (12)	0.0161 (10)	0.0000 (8)	0.0020 (7)	0.0011 (9)
C1	0.0095 (9)	0.0240 (14)	0.0175 (12)	-0.0035 (9)	0.0002 (7)	-0.0002 (10)
C2	0.0148 (10)	0.0238 (14)	0.0124 (11)	-0.0011 (9)	0.0032 (7)	-0.0001 (9)
C3	0.0149 (10)	0.0292 (15)	0.0193 (12)	-0.0005 (10)	0.0030 (8)	0.0003 (11)
C4	0.0159 (10)	0.0345 (17)	0.0192 (12)	0.0077 (10)	0.0034 (8)	0.0027 (11)
C5	0.0259 (11)	0.0213 (14)	0.0230 (13)	0.0053 (10)	0.0082 (9)	0.0005 (11)
C6	0.0216 (11)	0.0189 (13)	0.0189 (12)	0.0003 (10)	0.0040 (8)	-0.0001 (10)
C7	0.0103 (9)	0.0209 (14)	0.0173 (11)	0.0028 (9)	0.0029 (7)	0.0021 (10)
C8	0.0145 (10)	0.0220 (14)	0.0170 (12)	-0.0020 (9)	-0.0013 (8)	0.0020 (10)
C9	0.0132 (10)	0.0212 (14)	0.0185 (12)	0.0021 (9)	0.0025 (8)	-0.0007 (10)
C10	0.0207 (11)	0.0293 (15)	0.0197 (13)	0.0034 (10)	0.0020 (8)	-0.0006 (11)
C11	0.0191 (11)	0.0391 (18)	0.0281 (14)	0.0025 (11)	-0.0059 (9)	-0.0087 (13)
C12	0.0196 (12)	0.0226 (16)	0.0445 (17)	-0.0015 (10)	0.0016 (10)	-0.0115 (13)
C13	0.0169 (11)	0.0237 (15)	0.0390 (16)	0.0015 (10)	0.0125 (9)	-0.0017 (12)
C14	0.0154 (10)	0.0258 (14)	0.0206 (12)	0.0006 (10)	0.0055 (8)	-0.0014 (11)
C15	0.0151 (10)	0.0147 (12)	0.0200 (12)	-0.0031 (9)	0.0033 (8)	-0.0001 (10)
C16	0.0117 (9)	0.0227 (13)	0.0181 (12)	0.0031 (9)	0.0040 (7)	-0.0013 (10)
C17	0.0224 (11)	0.0215 (13)	0.0202 (12)	0.0043 (10)	0.0092 (9)	0.0037 (10)
C18	0.0326 (12)	0.0255 (15)	0.0168 (12)	0.0101 (12)	0.0084 (9)	0.0057 (11)
C19	0.0302 (12)	0.0279 (15)	0.0124 (11)	0.0111 (11)	-0.0021 (8)	-0.0014 (11)
C20	0.0220 (11)	0.0224 (15)	0.0222 (13)	0.0025 (10)	0.0010 (8)	-0.0042 (11)
C21	0.0184 (10)	0.0176 (13)	0.0151 (11)	0.0020 (9)	0.0039 (8)	0.0014 (10)
C22	0.0421 (14)	0.0200 (15)	0.0222 (13)	0.0049 (12)	0.0074 (10)	-0.0007 (11)
C23	0.0241 (11)	0.0160 (14)	0.0233 (13)	0.0041 (9)	0.0050 (9)	0.0009 (10)

C24	0.0225 (11)	0.0229 (15)	0.0304 (14)	-0.0044 (10)	0.0108 (9)	-0.0009 (11)
C25	0.0258 (12)	0.0267 (15)	0.0307 (15)	-0.0059 (11)	0.0035 (9)	-0.0044 (12)
C26	0.0367 (13)	0.0308 (17)	0.0219 (13)	0.0062 (12)	0.0074 (10)	-0.0017 (12)
C27	0.0244 (12)	0.0284 (16)	0.0330 (15)	0.0035 (11)	0.0128 (10)	0.0072 (12)
C28	0.0186 (12)	0.0217 (14)	0.0315 (14)	-0.0031 (10)	0.0024 (9)	0.0011 (11)

Geometric parameters (Å, º) for **(bdta)**

S1—C15	1.655 (2)	C12—C13	1.378 (4)
S2—C1	1.658 (2)	C13—H13	0.9500
N1—C7	1.451 (2)	C13—C14	1.390 (3)
N1—C8	1.470 (2)	C14—H14	0.9500
N1—C15	1.351 (3)	C15—C16	1.491 (3)
N2—C1	1.341 (3)	C16—C17	1.393 (3)
N2—C21	1.439 (3)	C16—C21	1.393 (3)
N2—C22	1.483 (3)	C17—H17	0.9500
C1—C2	1.494 (4)	C17—C18	1.388 (3)
C2—C3	1.398 (3)	C18—H18	0.9500
C2—C7	1.392 (3)	C18—C19	1.383 (4)
C3—H3	0.9500	C19—H19	0.9500
C3—C4	1.380 (4)	C19—C20	1.386 (4)
C4—H4	0.9500	C20—H20	0.9500
C4—C5	1.380 (4)	C20—C21	1.388 (3)
C5—H5	0.9500	C22—H22A	0.9900
C5—C6	1.398 (3)	C22—H22B	0.9900
C6—H6	0.9500	C22—C23	1.507 (3)
C6—C7	1.379 (4)	C23—C24	1.390 (3)
C8—H8A	0.9900	C23—C28	1.395 (3)
C8—H8B	0.9900	C24—H24	0.9500
C8—C9	1.510 (3)	C24—C25	1.379 (3)
C9—C10	1.395 (3)	C25—H25	0.9500
C9—C14	1.390 (3)	C25—C26	1.391 (3)
C10—H10	0.9500	C26—H26	0.9500
C10—C11	1.385 (4)	C26—C27	1.384 (4)
C11—H11	0.9500	C27—H27	0.9500
C11—C12	1.390 (4)	C27—C28	1.373 (4)
C12—H12	0.9500	C28—H28	0.9500
C7—N1—C8	116.88 (17)	C9—C14—C13	119.8 (2)
C15—N1—C7	121.44 (18)	C9—C14—H14	120.1
C15—N1—C8	121.41 (17)	C13—C14—H14	120.1

C1—N2—C21	120.7 (2)	N1—C15—S1	124.66 (17)
C1—N2—C22	119.2 (2)	N1—C15—C16	116.21 (17)
C21—N2—C22	119.68 (18)	C16—C15—S1	119.12 (16)
N2—C1—S2	125.6 (2)	C17—C16—C15	120.8 (2)
N2—C1—C2	115.5 (2)	C21—C16—C15	120.3 (2)
C2—C1—S2	118.91 (16)	C21—C16—C17	118.9 (2)
C3—C2—C1	121.0 (2)	C16—C17—H17	119.8
C7—C2—C1	119.96 (17)	C18—C17—C16	120.3 (2)
C7—C2—C3	118.9 (2)	C18—C17—H17	119.8
C2—C3—H3	120.3	C17—C18—H18	120.0
C4—C3—C2	119.4 (2)	C19—C18—C17	120.1 (2)
C4—C3—H3	120.3	C19—C18—H18	120.0
C3—C4—H4	119.3	C18—C19—H19	119.9
C3—C4—C5	121.48 (19)	C18—C19—C20	120.3 (2)
C5—C4—H4	119.3	C20—C19—H19	119.9
C4—C5—H5	120.3	C19—C20—H20	120.2
C4—C5—C6	119.3 (2)	C19—C20—C21	119.6 (2)
C6—C5—H5	120.3	C21—C20—H20	120.2
C5—C6—H6	120.3	C16—C21—N2	119.38 (19)
C7—C6—C5	119.4 (2)	C20—C21—N2	119.8 (2)
C7—C6—H6	120.3	C20—C21—C16	120.8 (2)
C2—C7—N1	118.7 (2)	N2—C22—H22A	108.8
C6—C7—N1	120.0 (2)	N2—C22—H22B	108.8
C6—C7—C2	121.28 (18)	N2—C22—C23	113.9 (2)
N1—C8—H8A	108.3	H22A—C22—H22B	107.7
N1—C8—H8B	108.3	C23—C22—H22A	108.8
N1—C8—C9	116.0 (2)	C23—C22—H22B	108.8
H8A—C8—H8B	107.4	C24—C23—C22	120.9 (2)
C9—C8—H8A	108.3	C24—C23—C28	118.6 (2)
C9—C8—H8B	108.3	C28—C23—C22	120.4 (2)
C10—C9—C8	116.9 (2)	C23—C24—H24	119.4
C14—C9—C8	123.5 (2)	C25—C24—C23	121.2 (2)
C14—C9—C10	119.5 (2)	C25—C24—H24	119.4
C9—C10—H10	119.9	C24—C25—H25	120.2
C11—C10—C9	120.3 (2)	C24—C25—C26	119.7 (2)
C11—C10—H10	119.9	C26—C25—H25	120.2
C10—C11—H11	120.1	C25—C26—H26	120.4
C10—C11—C12	119.9 (2)	C27—C26—C25	119.3 (2)
C12—C11—H11	120.1	C27—C26—H26	120.4
C11—C12—H12	120.0	C26—C27—H27	119.5

C13—C12—C11	120.0 (3)	C28—C27—C26	121.1 (2)
C13—C12—H12	120.0	C28—C27—H27	119.5
C12—C13—H13	119.8	C23—C28—H28	119.9
C12—C13—C14	120.5 (3)	C27—C28—C23	120.1 (2)
C14—C13—H13	119.8	C27—C28—H28	119.9
S1—C15—C16—C17	70.3 (3)	C9—C10—C11—C12	-0.4 (3)
S1—C15—C16—C21	-108.3 (2)	C10—C9—C14—C13	-1.9 (3)
S2—C1—C2—C3	75.4 (3)	C10—C11—C12—C13	-0.8 (3)
S2—C1—C2—C7	-101.8 (2)	C11—C12—C13—C14	0.7 (3)
N1—C8—C9—C10	-162.98 (19)	C12—C13—C14—C9	0.7 (3)
N1—C8—C9—C14	19.3 (3)	C14—C9—C10—C11	1.8 (3)
N1—C15—C16—C17	-110.6 (2)	C15—N1—C7—C2	-70.2 (3)
N1—C15—C16—C21	70.8 (3)	C15—N1—C7—C6	112.1 (3)
N2—C1—C2—C3	-107.5 (2)	C15—N1—C8—C9	-89.9 (3)
N2—C1—C2—C7	75.3 (3)	C15—C16—C17—C18	179.7 (2)
N2—C22—C23—C24	93.8 (3)	C15—C16—C21—N2	-0.1 (3)
N2—C22—C23—C28	-88.1 (3)	C15—C16—C21—C20	-179.7 (2)
C1—N2—C21—C16	-72.1 (3)	C16—C17—C18—C19	0.6 (4)
C1—N2—C21—C20	107.6 (3)	C17—C16—C21—N2	-178.74 (19)
C1—N2—C22—C23	-161.8 (2)	C17—C16—C21—C20	1.6 (3)
C1—C2—C3—C4	-175.5 (2)	C17—C18—C19—C20	0.5 (4)
C1—C2—C7—N1	-4.5 (3)	C18—C19—C20—C21	-0.6 (4)
C1—C2—C7—C6	173.2 (2)	C19—C20—C21—N2	179.8 (2)
C2—C3—C4—C5	1.7 (4)	C19—C20—C21—C16	-0.5 (3)
C3—C2—C7—N1	178.2 (2)	C21—N2—C1—S2	176.52 (14)
C3—C2—C7—C6	-4.1 (3)	C21—N2—C1—C2	-0.3 (3)
C3—C4—C5—C6	-2.9 (4)	C21—N2—C22—C23	26.1 (3)
C4—C5—C6—C7	0.6 (3)	C21—C16—C17—C18	-1.6 (3)
C5—C6—C7—N1	-179.41 (19)	C22—N2—C1—S2	4.5 (3)
C5—C6—C7—C2	2.9 (3)	C22—N2—C1—C2	-172.41 (19)
C7—N1—C8—C9	95.9 (2)	C22—N2—C21—C16	100.0 (3)
C7—N1—C15—S1	-179.27 (19)	C22—N2—C21—C20	-80.4 (2)
C7—N1—C15—C16	1.7 (3)	C22—C23—C24—C25	179.2 (3)
C7—C2—C3—C4	1.8 (3)	C22—C23—C28—C27	-179.1 (2)
C8—N1—C7—C2	104.0 (2)	C23—C24—C25—C26	-1.1 (4)
C8—N1—C7—C6	-73.7 (3)	C24—C23—C28—C27	-0.9 (4)
C8—N1—C15—S1	6.8 (3)	C24—C25—C26—C27	0.9 (4)
C8—N1—C15—C16	-172.3 (2)	C25—C26—C27—C28	-0.8 (4)
C8—C9—C10—C11	-176.02 (18)	C26—C27—C28—C23	0.8 (4)

C8—C9—C14—C13	175.76 (19)	C28—C23—C24—C25	1.0 (4)

Tables generated using program *publCIF* [Westrip, S. P. “publCIF: software for editing, validating and formatting crystallographic information files” *J. Apply. Cryst.*, **2010**, *43*, 920-925], https://doi.org/10.1107/S0021889810022120.

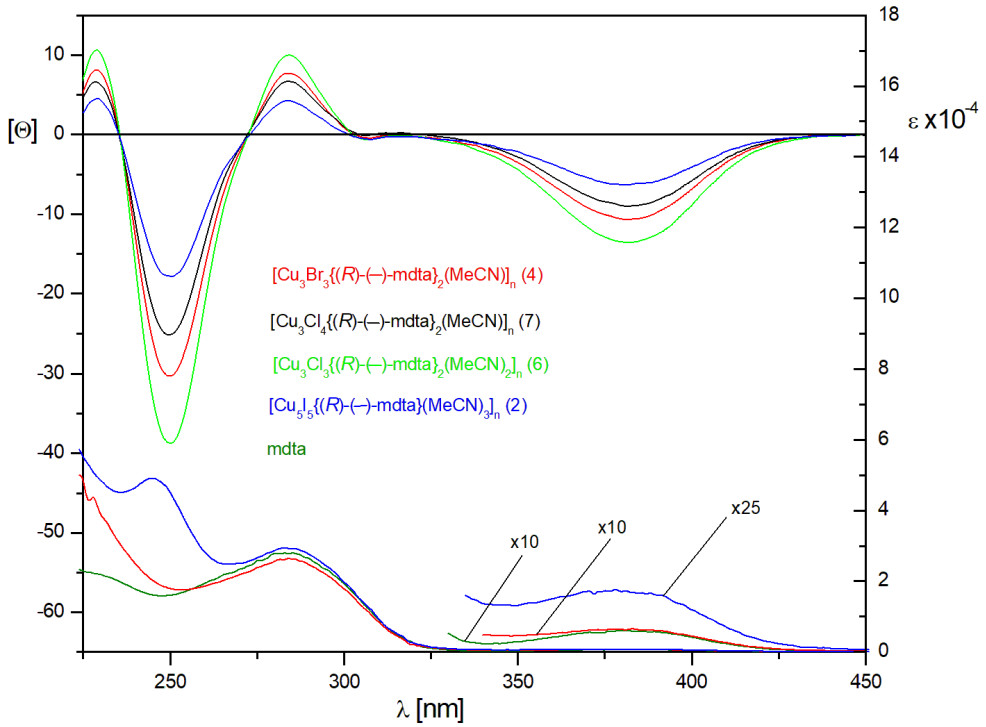

Figure S11. CD spectra of **2**, **4**, **6**, **7** and UV-vis (lower curves) spectra of **2**, **4** and free ligand **mdta** taken in acetonitrile.

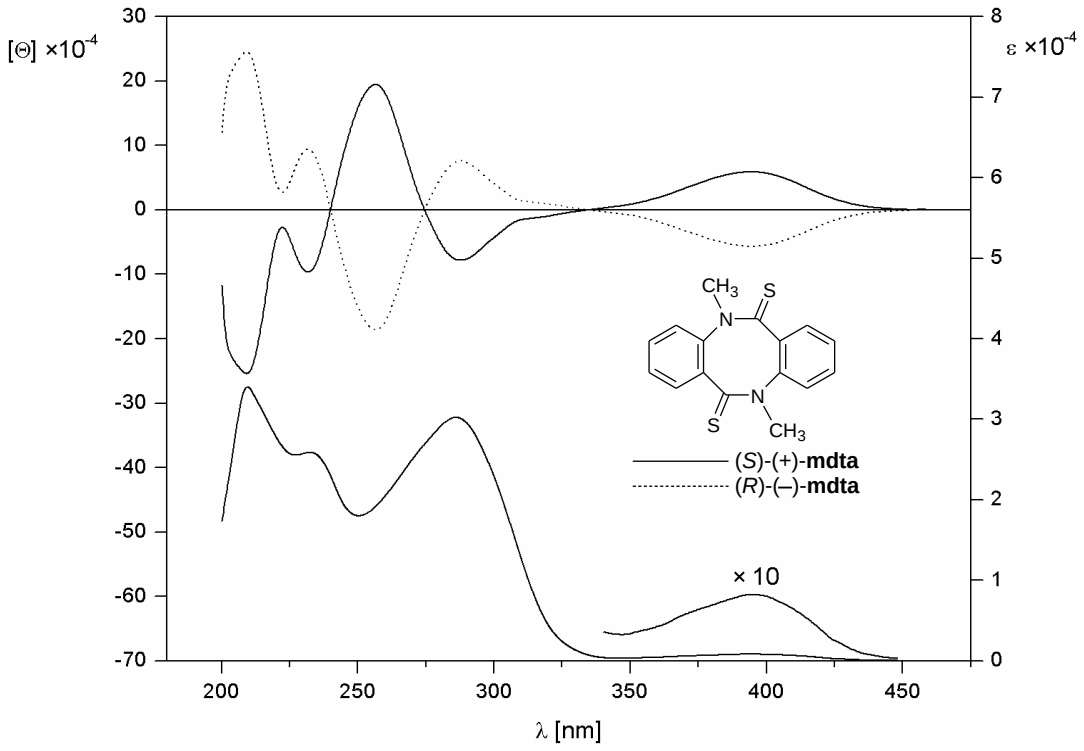

Figure S12. CD and UV-vis (lower curve) spectra of enantiomers of **mdta** taken in cyclohexane–dioxane (5:1 v/v).

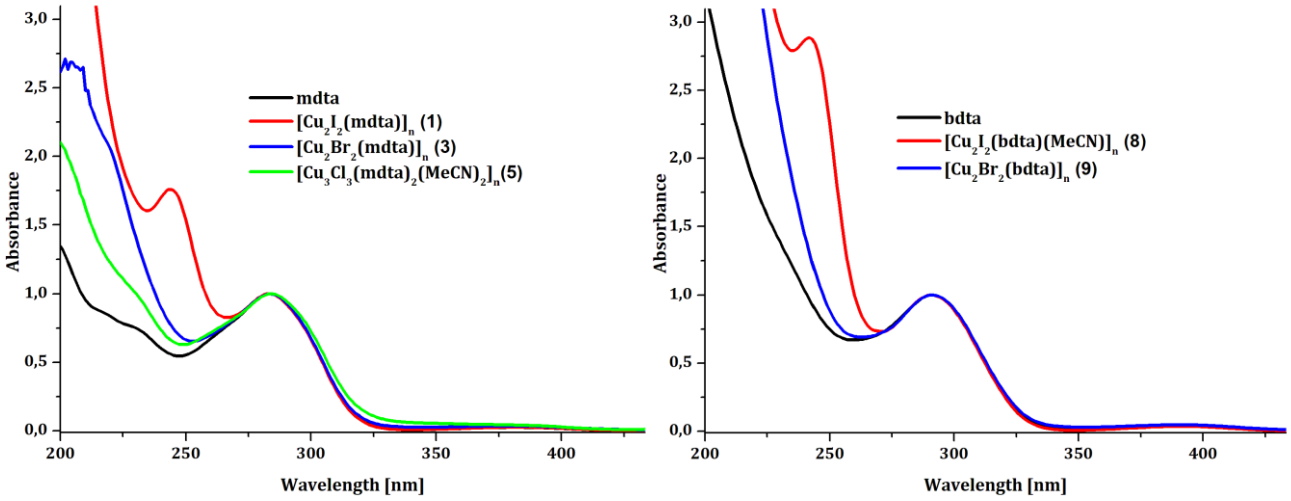

Figure S13. Absorption spectra of ligands and some complexes dissolved in MeCN.

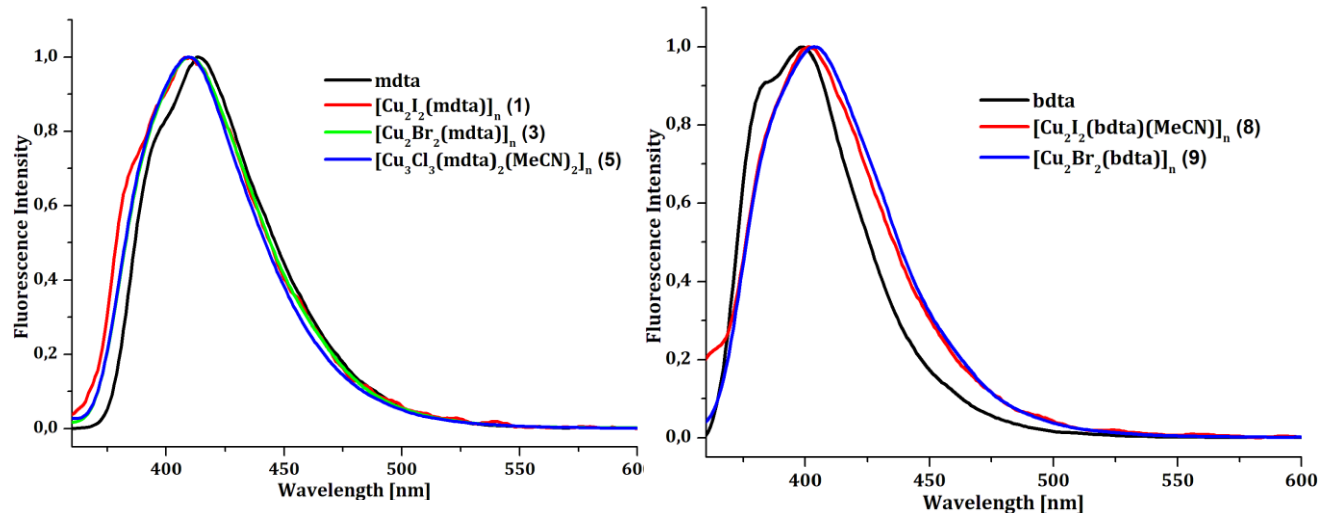

Figure S14. Fluorescence spectra of ligands and some complexes dissolved in MeCN.

Table S2. Average lifetimes and fitting parameters of luminescence decays of complexes in crystal state at various temperatures*

Compound	T [K]	A_1	τ_1 [μs]	f_1	A_2	τ_2 [μs]	f_2	A_3	τ_3 [μs]	f_3	A_4	τ_4 [μs]	f_4	τ_{av} [μs]
$[Cu_5I_5\{(R)$-(−)-mdta)$\}(MeCN)_3]_n$ (2)	298	0.43	1.1	0.14	0.49	5.6	0.78	0.02	13.1	0.09				5.6
	10	0.54	0.6	0.01	0.30	15.0	0.10	0.45	91.6	0.89				83.4
$[Cu_3Br_3\{(R)$-(−)-mdta$\}_2(MeCN)]_n$ (4)	10	0.47	13.0	0.15	0.24	67.0	0.39	0.27	68.0	0.45				59.3
$[Cu_2I_2(mdta)]_n$ (1)	10	0.40	0.1	0.00	0.31	3.2	0.08	0.24	45.0	0.91				41.3
$[Cu_2I_2$ (bdta)(MeCN)$]_n$ (8)	298	0.30	0.1	0.05	0.32	0.3	0.22	0.36	0.9	0.74				0.7
	10	0.12	0.1	0.00	0.62	23.9	0.97	0.23	1.9	0.03				23.3
$[Cu_2Br_2(bdta)]_n$ (9)	298	0.39	0.1	0.06	0.49	0.5	0.56	0.12	1.5	0.38				0.9
	10	0.25	0.1	0.00	0.38	0.5	0.04	0.30	4.1	0.29	0.12	24	0.66	17.1
$[Ag_2I_2(mdta)]_n$ (10)	10	0.12	15.8	0.03	0.68	50.1	0.54	0.215	128.0	0.43				82.8

*τ_i –lifetime of emission component; A_i – pre-exponential factor, f_i – fractional contribution, calculated as $f_i = A_i \cdot \tau_i / \sum A_i \cdot \tau_i$,

τ_{av} – intensity-weighted emission lifetime calculated as $\tau_{av} = \sum f_i \cdot \tau_i$.

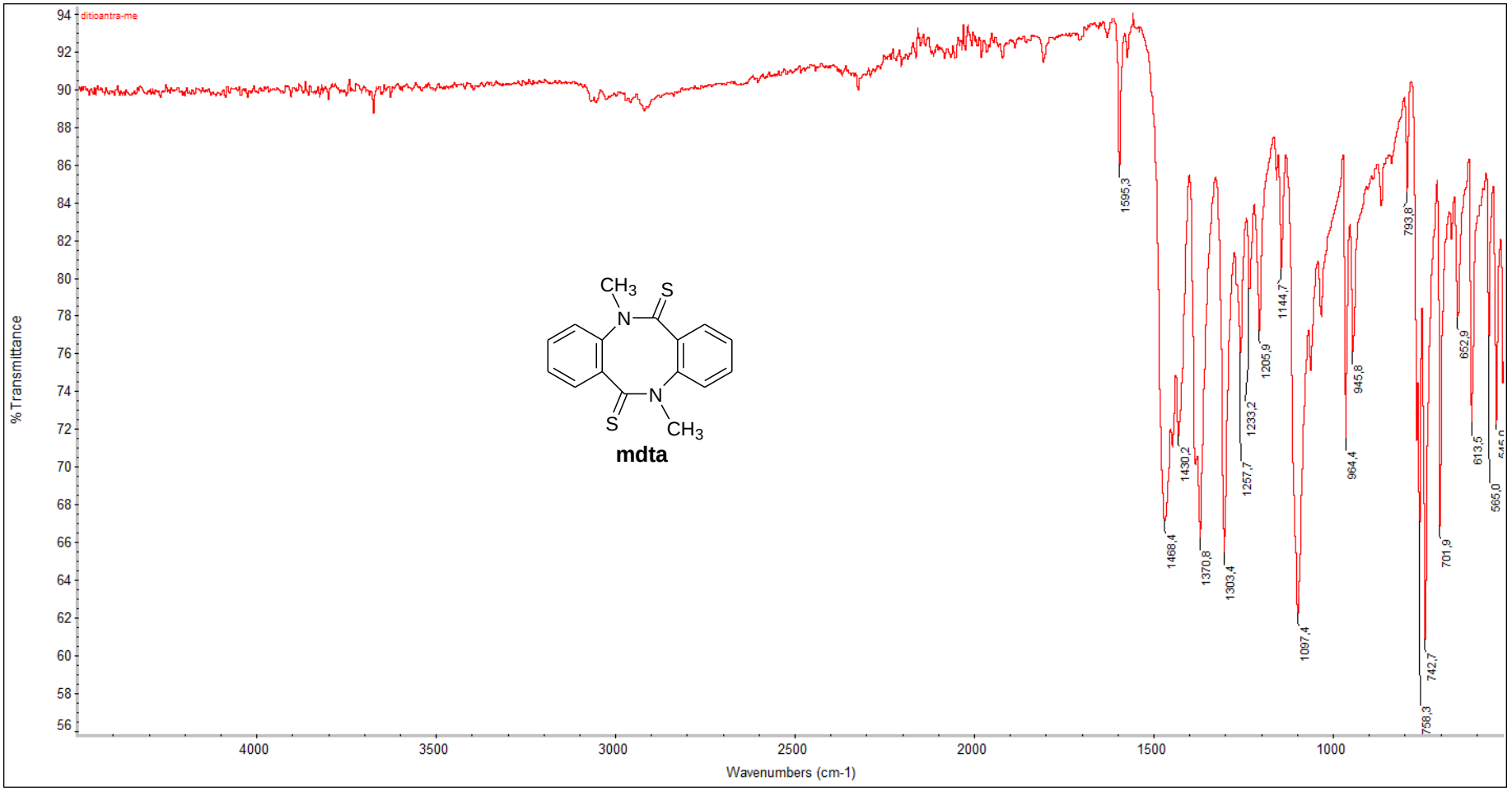

Figure S15. IR spectrum of **mdta**

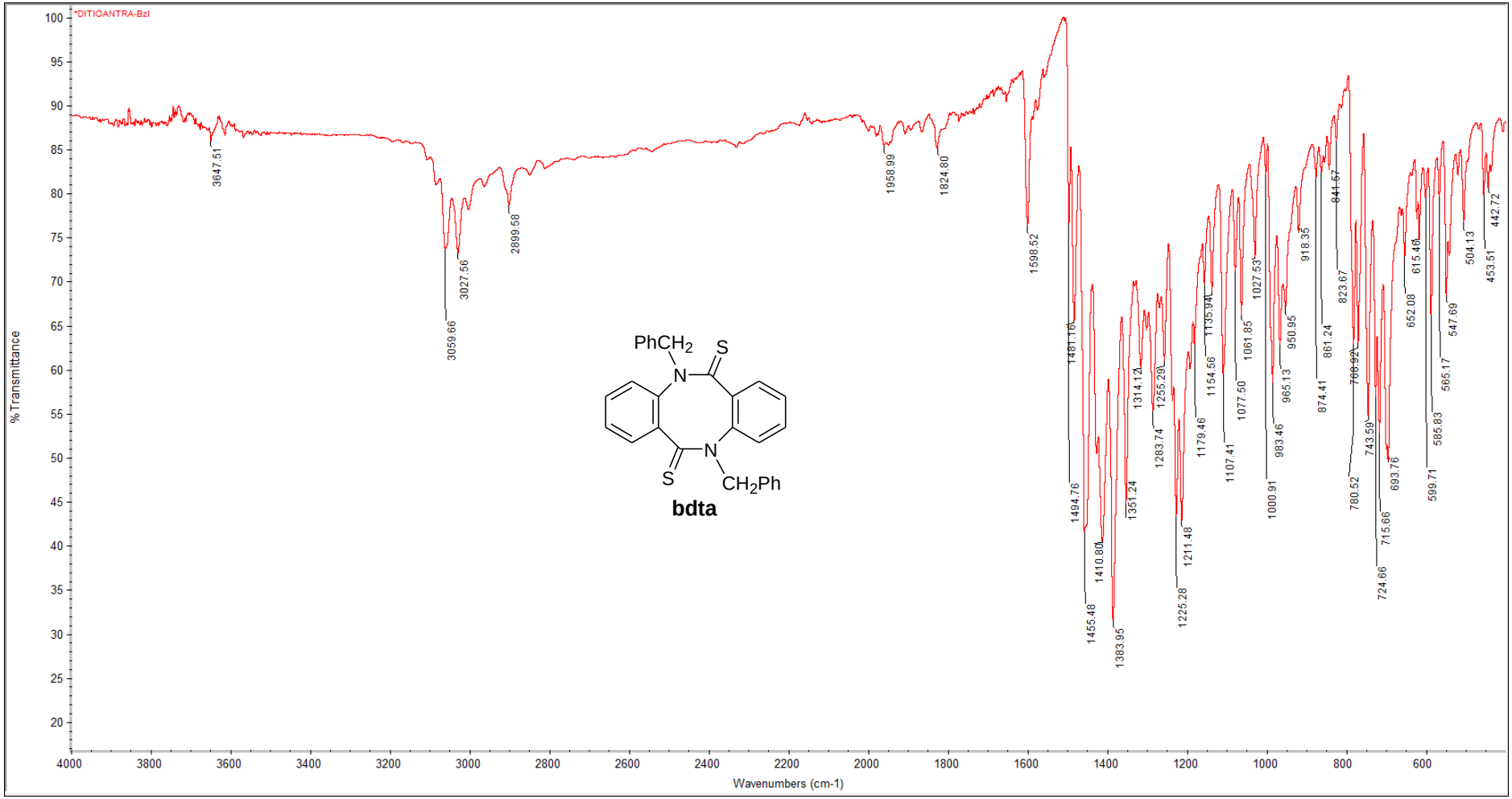

Figure S16. IR spectrum of **bdta**

Figure S17. IR spectrum of **$[Cu_2I_2(mdta)]_n$ (1)**

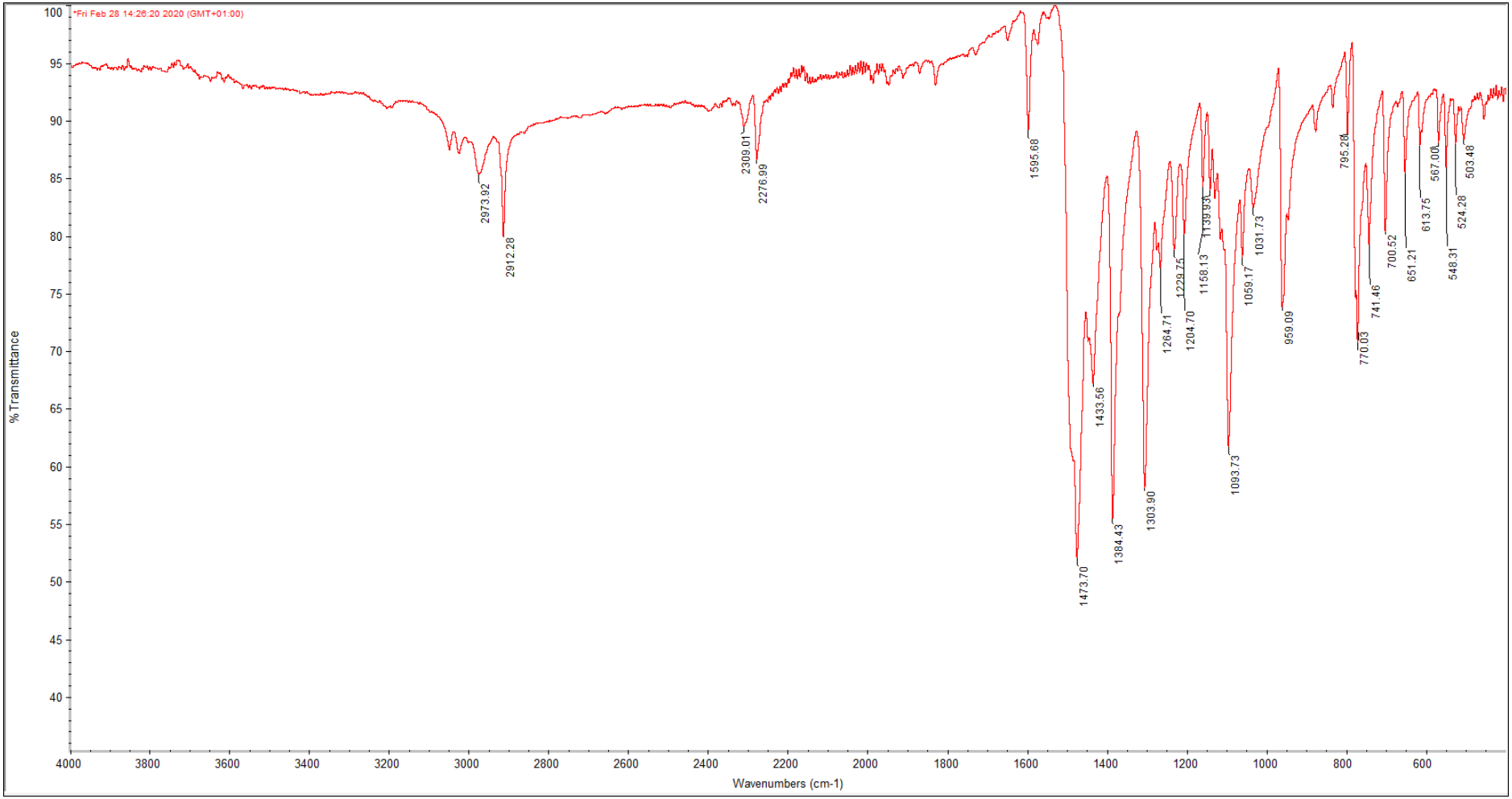

Figure S18. IR spectrum of **$[Cu_5I_5\{(R)\text{-}(-)\text{-}(mdta)\}(MeCN)_3]_n$ (2)**

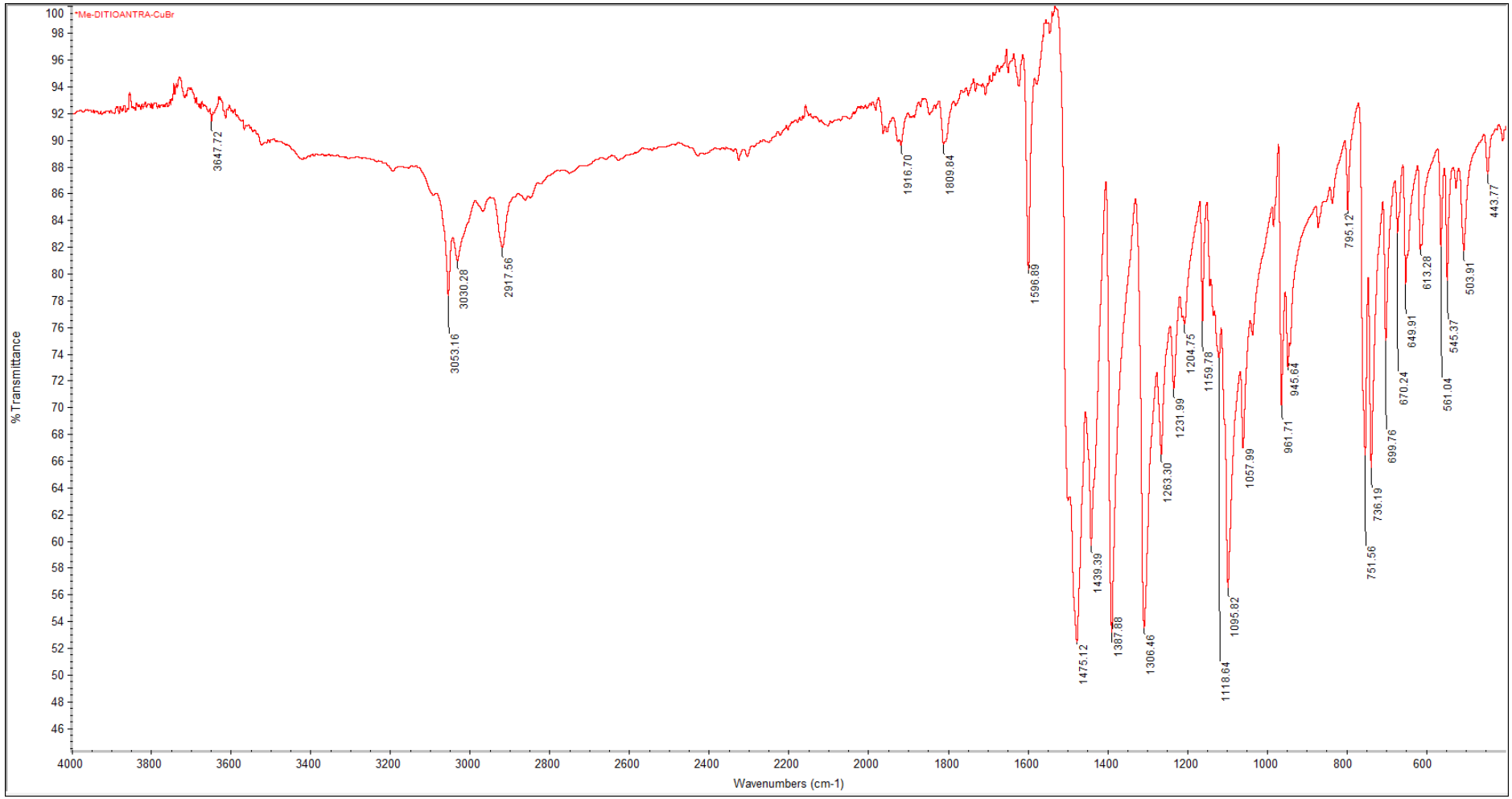

Figure S19. IR spectrum of **$[Cu_2Br_2(mdta)]_n$ (3)**

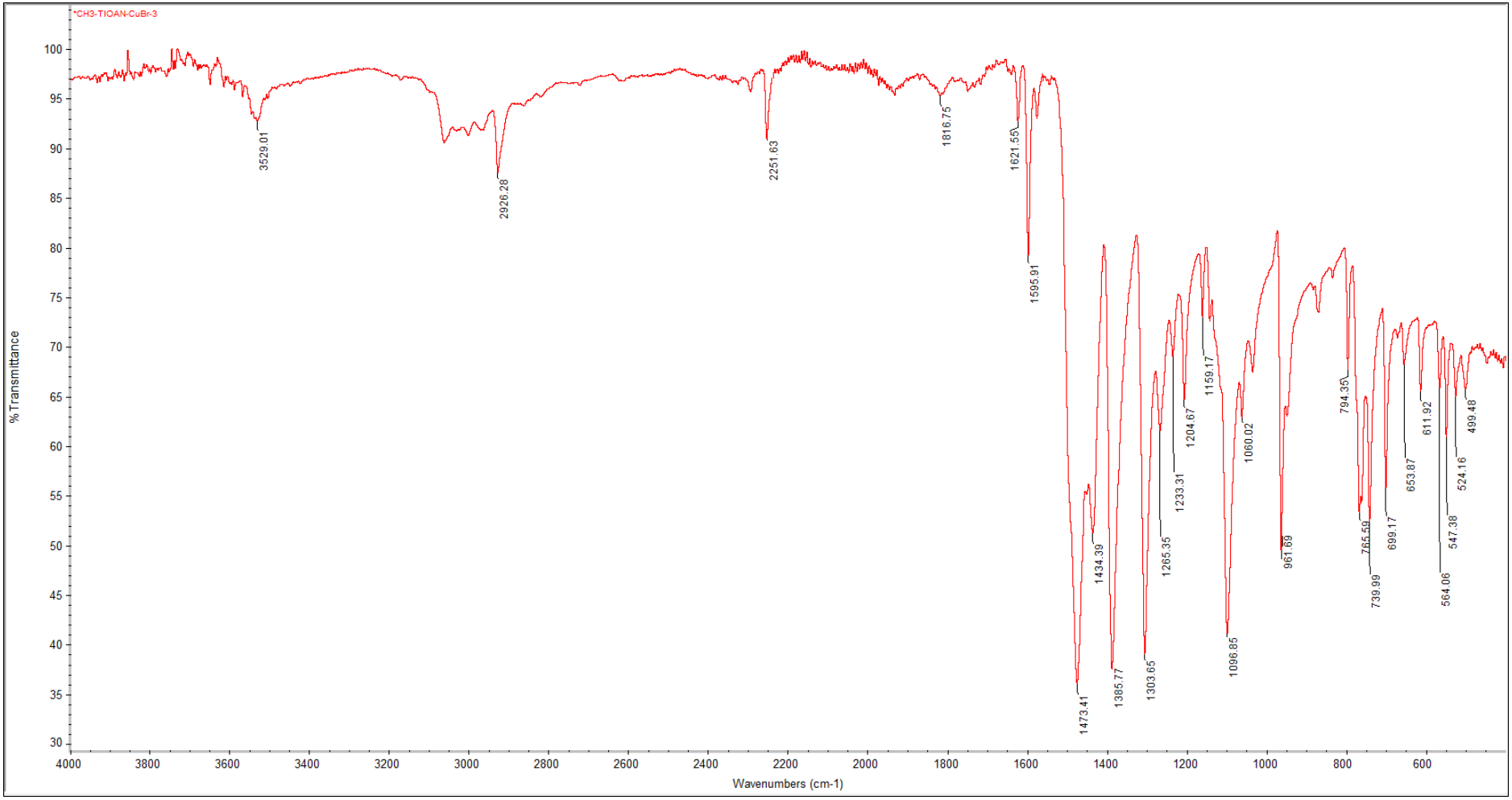

Figure S20. IR spectrum of **[Cu_3Br_3{(*R*)-(−)-(mdta)}$_2$(MeCN)]$_n$ (4)**

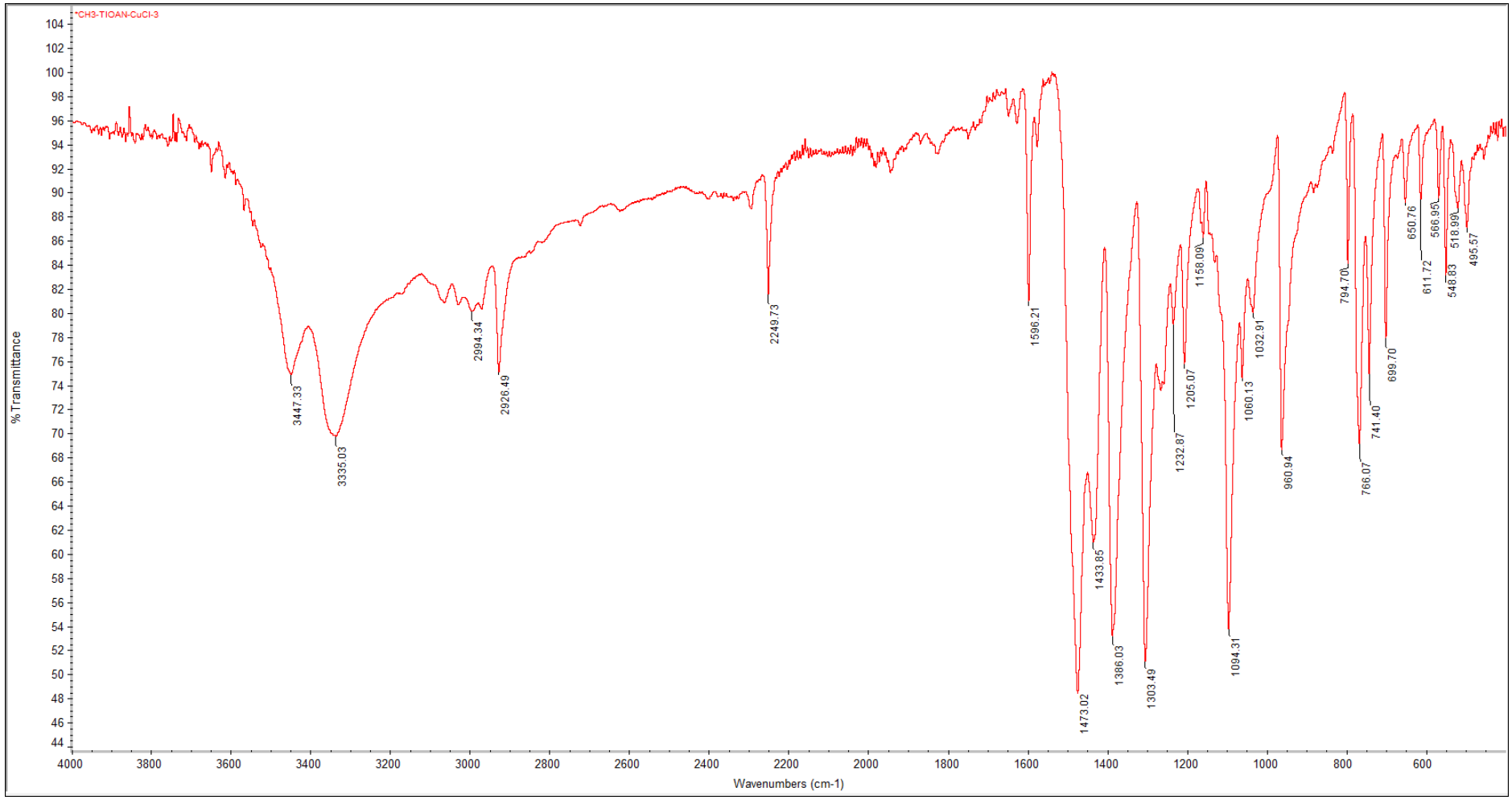

Figure S21. IR spectrum of **$[Cu_3Cl_3\{(R)\text{-}(-)\text{-}(mdta)\}_2(MeCN)_2]_n$ (6)**

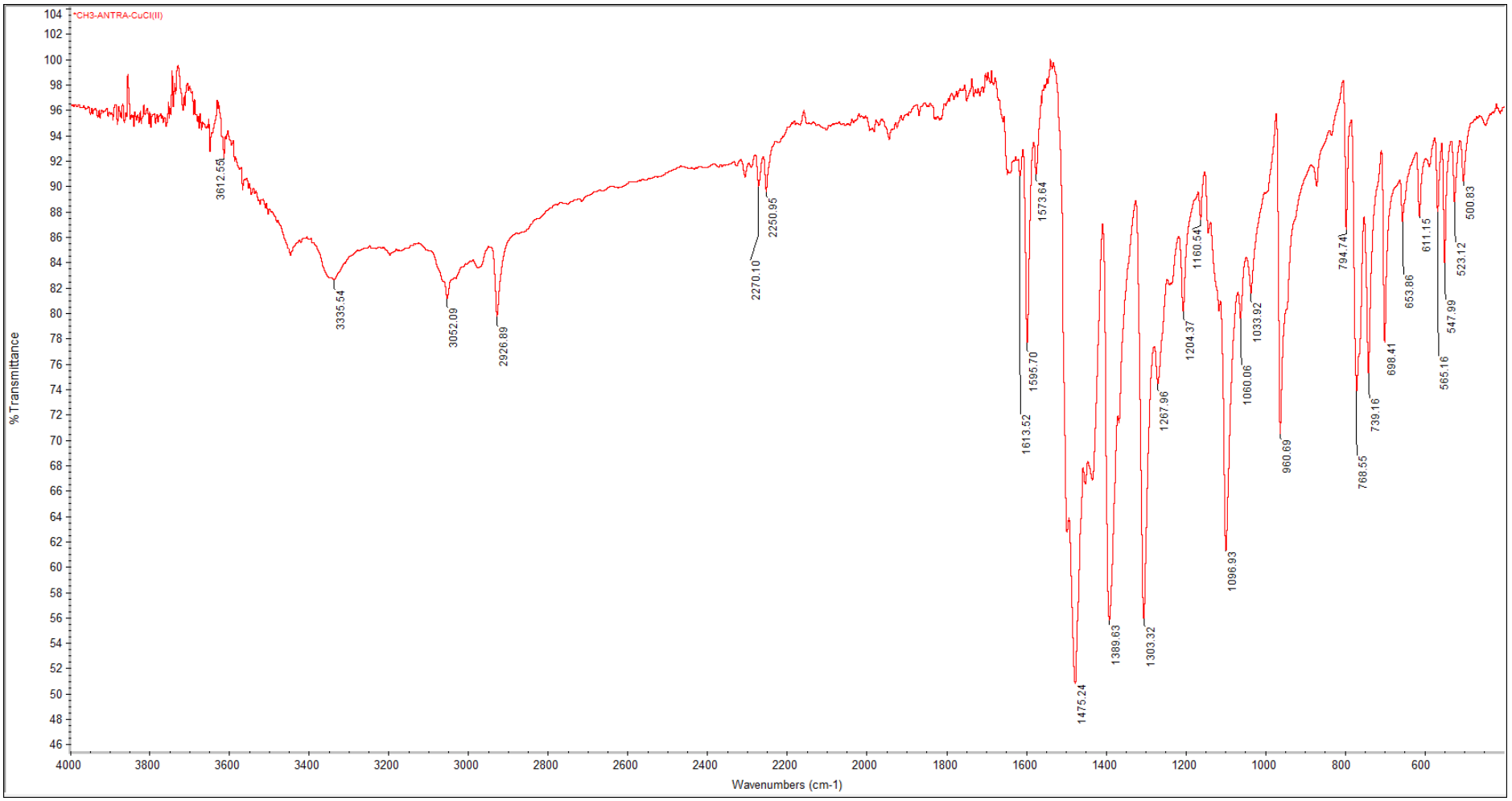

Figure S22. IR spectrum of **$[Cu_3Cl_4\{(R)\text{-}(-)\text{-}(mdta)\}_2(MeCN)]_n$ (7)**

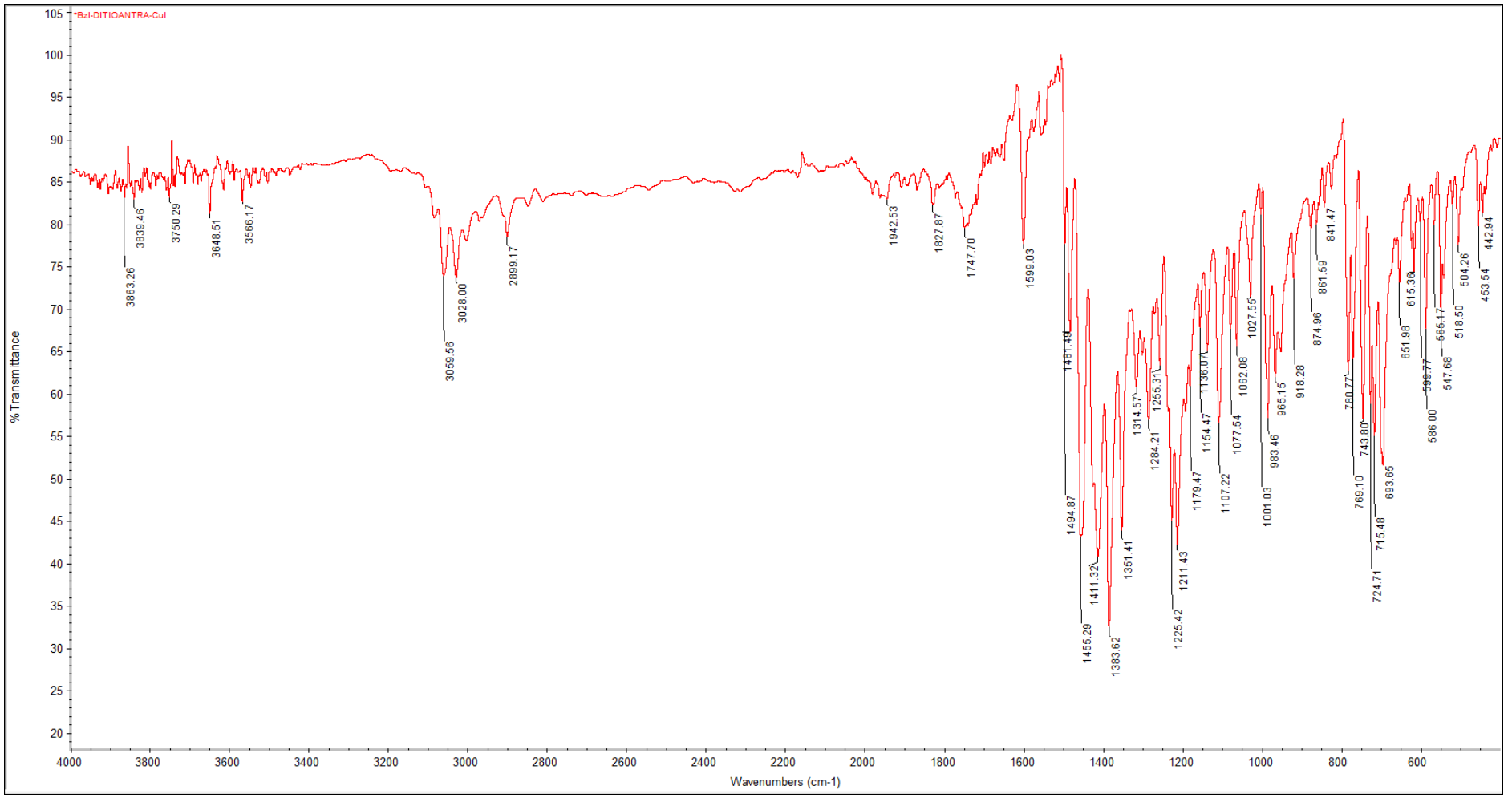

Figure S23. IR spectrum of **$[Cu_2I_2(bdta)(MeCN)]_n$ (8)**

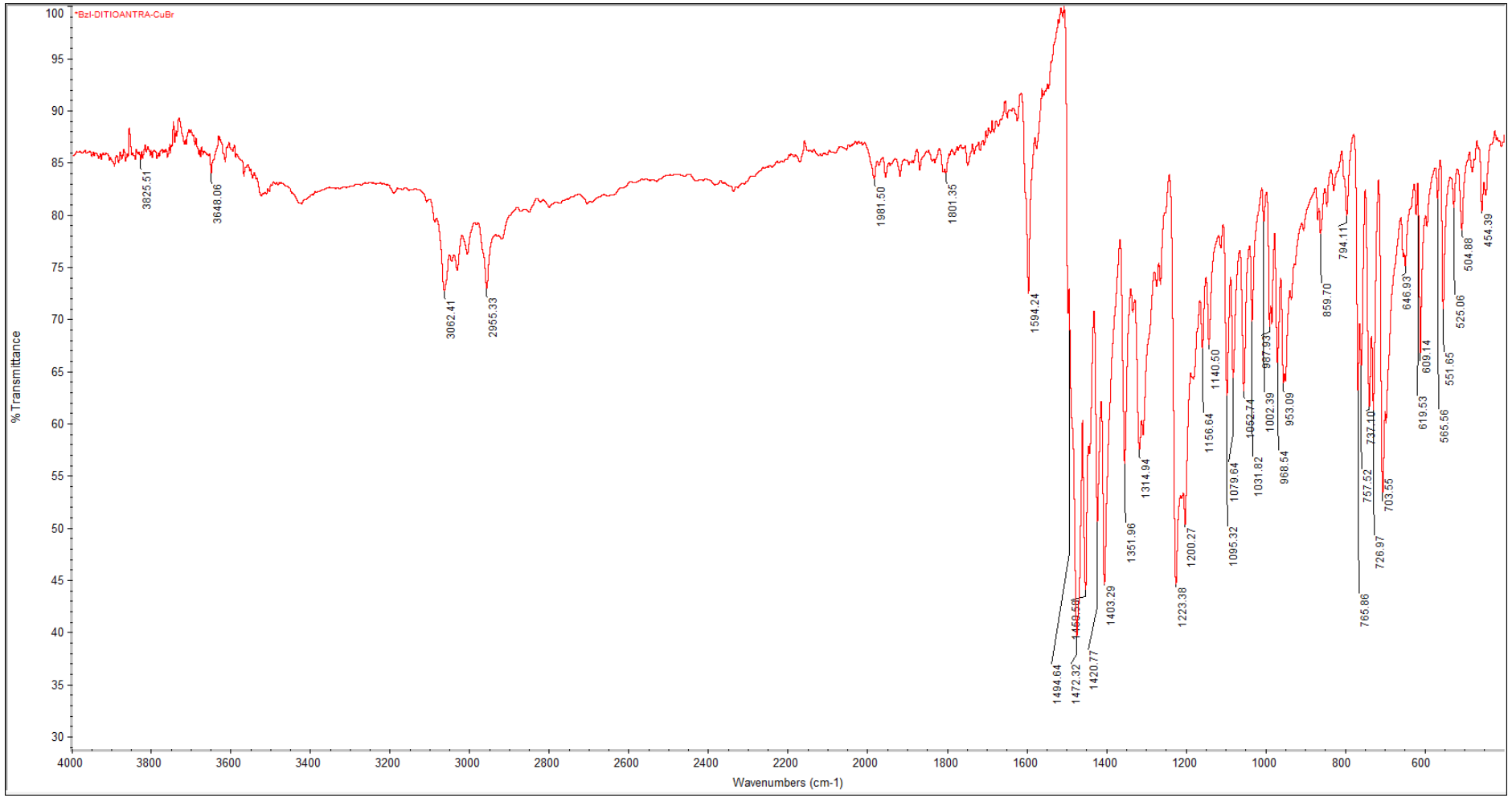

Figure S24. IR spectrum of **$[Cu_2Br_2(bdta)]_n$ (9)**

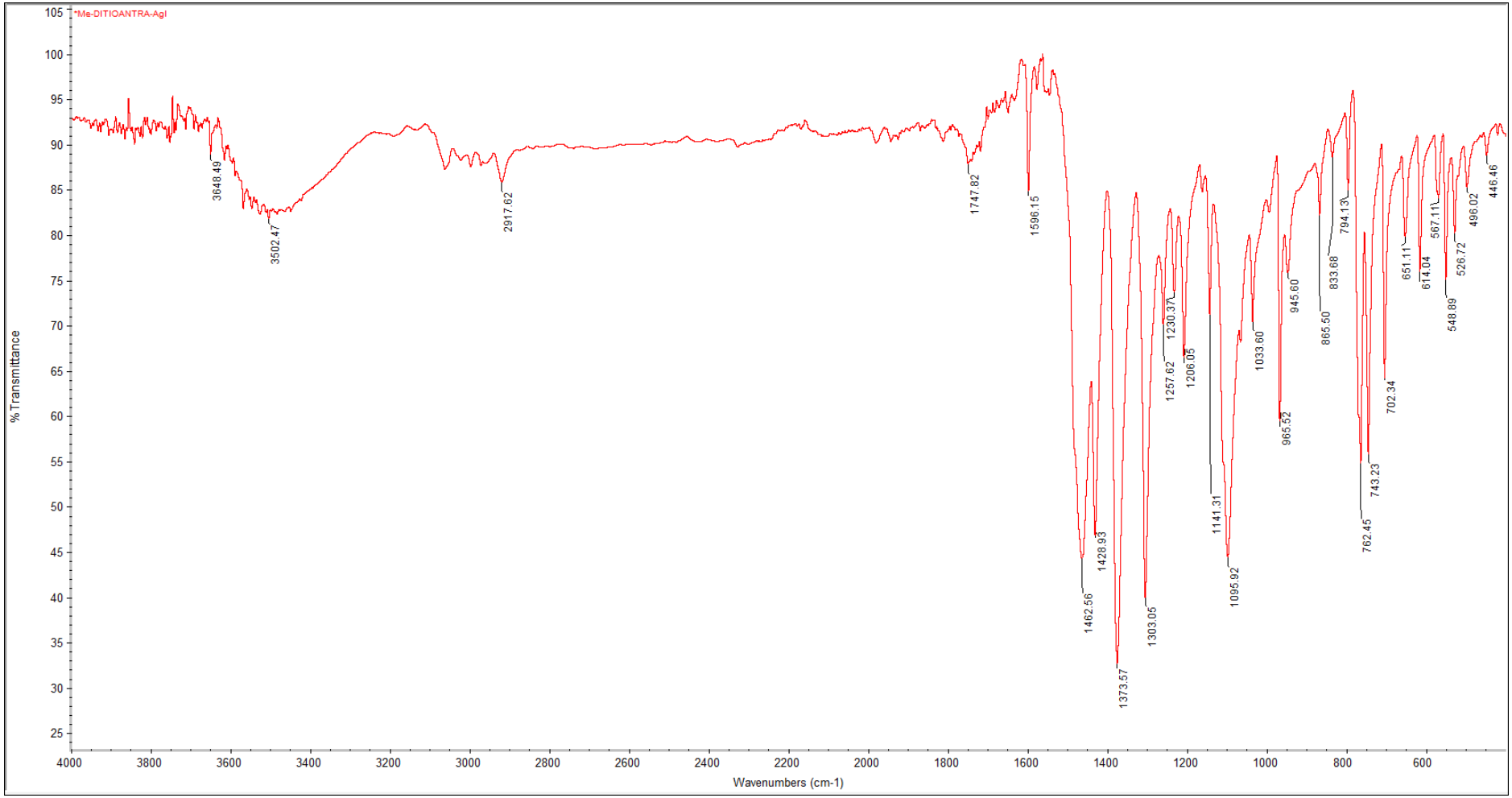

Figure S25. IR spectrum of **$[Ag_2I_2(mdta)]_n$ (10)**

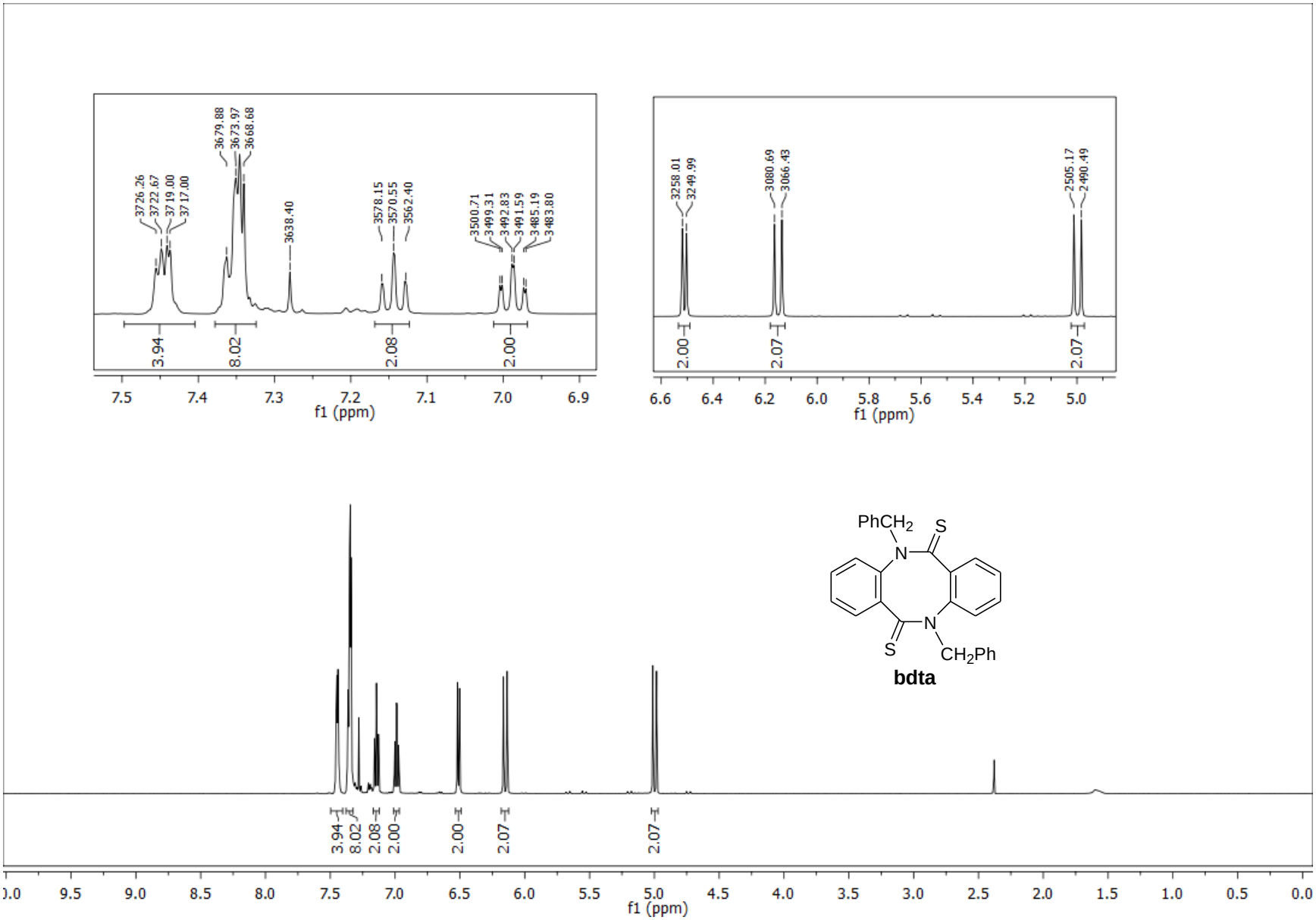

Figure S26. ^{1}H NMR spectrum of **bdta** taken in $CDCl_3$

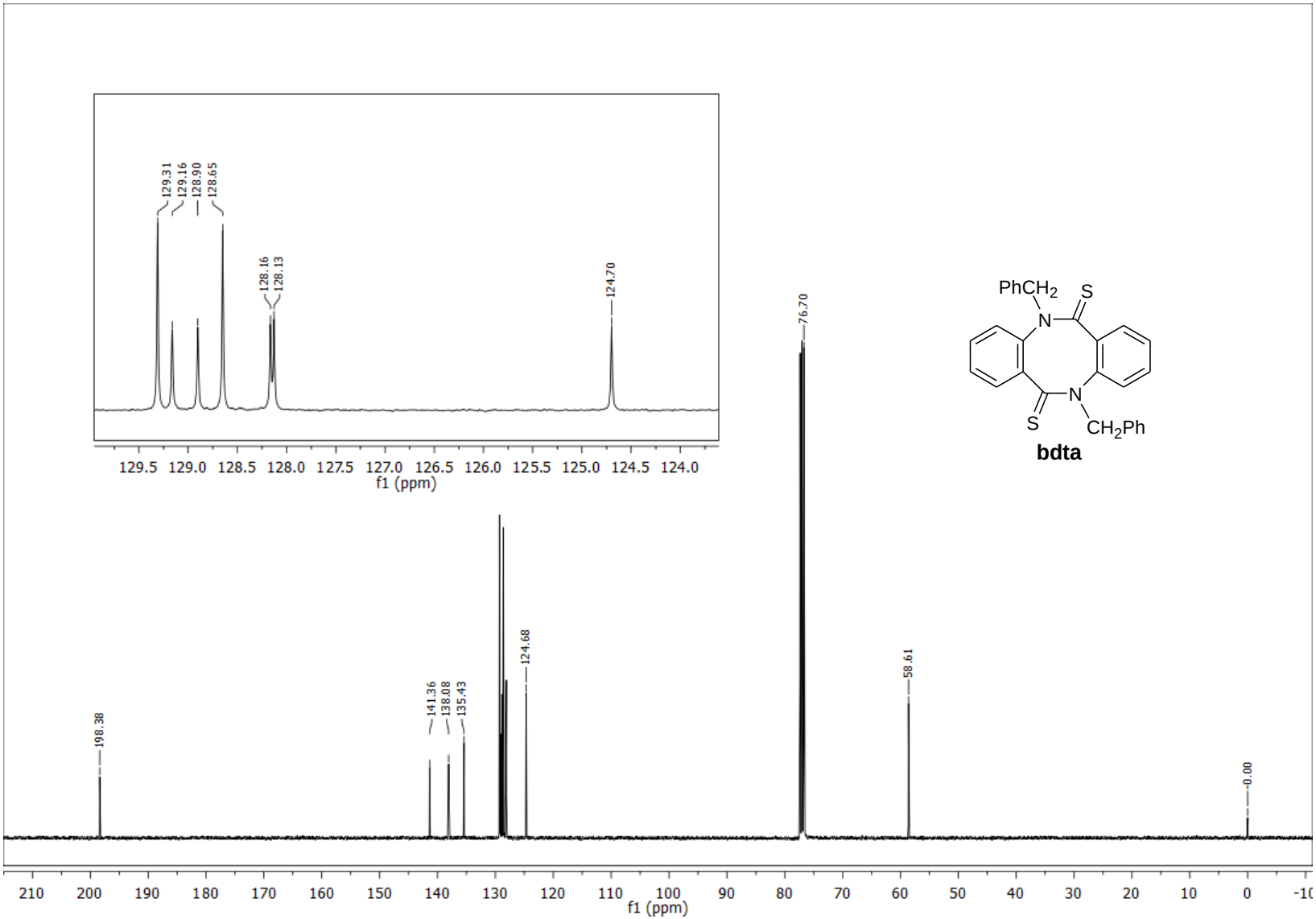

Figure S27. ^{13}C NMR spectrum of **bdta** taken in $CDCl_3$

References

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G. M. Sheldrick, *Acta Cryst.* 2015, C**71**, 3–8