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Two-dimensional structure of poly[[[μ_2-1,4-bis(pyridin-4-yl)butane]bis(μ_4-pentanedioato)dicopper(II)] acetonitrile disolvate]

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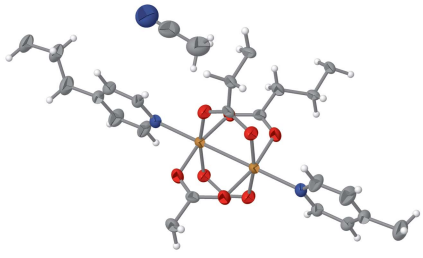
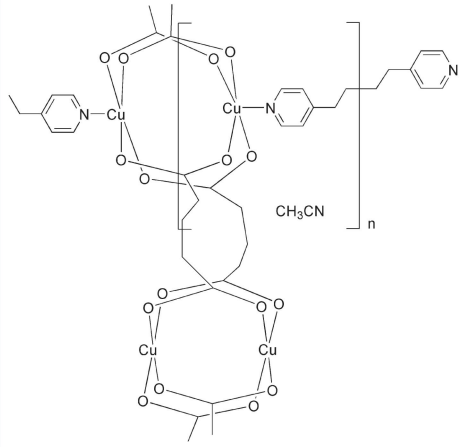
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, {[$Cu_2(\mu_4$-$C_5H_6O_4)_2(\mu_2$-$C_{14}H_{16}N_2)$]·2CH_3CN}$_n$, the Cu_2 dinuclear units are connected by glutartate ligands, forming one-dimensional double chains. These chains, are in turn bridged by 1,4-bis(pyridin-4-yl)butane ligands to form a two-dimensional layer structure parallel to (112). The carboxylate groups of the glutarate ligand bridge two copper(II) ions, forming a paddle-wheel-type $Cu_2(CO_2)_4$ dinuclear secondary building unit. A crystallographic inversion centre is located midway between two Cu^{II} ions, with a Cu···Cu distance of 2.639 (3) Å. The coordination geometry of the unique Cu^{II} ion is slightly disorted square pyramidal, formed by four equatorial carboxylate O atoms and an axial pyridyl N atom.

3D view



Chemical scheme



Structure description

Metal–organic frameworks (MOFs) have been constructed using metal ions and polytopic bridging ligands, and MOFs usually provide high surfaces and large pore volumes, and are thereby suitable for various advanced applications, such as selective gas sorption, heterogeneous catalysis, separation, sensors, drug delivery and biological imaging. Flexible dicarboxylates, as well as rigid aromatic dicarboxylates, have been used for the synthesis of MOFs, and flexible dicarboxylates, *e.g.* α,ω-alkanedicarboxylates, have been shown to be particularly suitable as ligands in MOFs of various topologies. Recently, various MOFs containing these α,ω-alkane(or alkene)dicarboxylate ligands have been reported (Hyun *et al.*, 2013; Hwang *et al.*, 2012, 2013; Lee *et al.*, 2014; Kim *et al.*, 2017), athough they are less frequently employed in MOFs than aromatic dicarboxylates. We report herein the crystal structure of poly[[[μ_2-1,4-bis(pyridin-4-yl)butane]bis(μ_4-pentanedioato)dicopper(II)] acetonitrile disolvate].

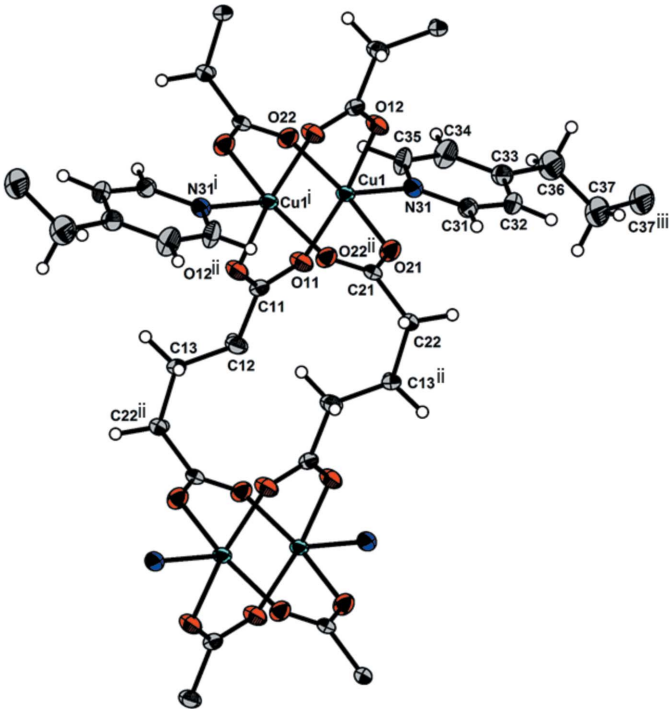


Figure 1
A fragment of the title compound, showing displacement ellipsoids at the 30% probability level. [Symmetry codes: (i) $1-x, 1-y, 2-z$; (ii) $1-x, -y, 2-z$; (iii) $3-x, 1-y, 1-z$.]

A fragment of the two-dimensional title compound is shown in Fig. 1. The Cu_2 dinuclear units are connected by glutartate ligands, forming one-dimensional double chains, and these chains are bridged by 1,4-bis(pyridin-4-yl)butane ligands to form a two-dimensional layer structure parallel to (112) (Fig. 2). The carboxylate groups of the glutarate ligands bridge two Cu^{II} ions, forming a paddle-wheel-type $Cu_2(CO_2)_4$ dinuclear secondary building unit. A crystallographic inversion centre is located midway between two Cu^{II} ions, with a Cu···Cu distance of 2.639 (3) Å. The coordination geometry of the unique Cu^{II} ion is slightly distorted square-pyramidal, constructed by four equatorial carboxylate O atoms and an axial pyridyl N atom.

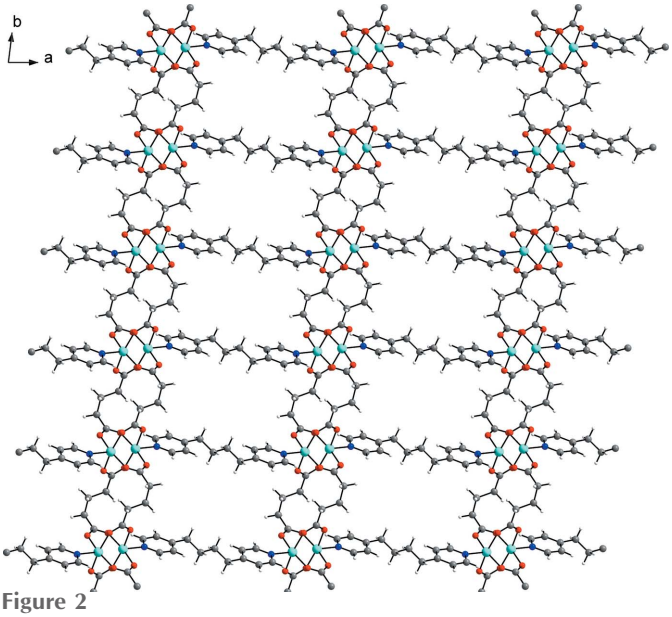


Figure 2
Two-dimensional structure of the title compound. The acetonitrile solvent molecules have been omitted for clarity.

Table 1
Experimental details.

Crystal data	
Chemical formula	$[Cu_2(C_5H_6O_4)_2(C_{14}H_{16}N_2)]\cdot 2C_2H_3N$
M_r	681.67
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	170
a, b, c (Å)	7.7525 (11), 7.9962 (11), 12.8132 (18)
α, β, γ (°)	87.867 (2), 81.875 (2), 82.674 (2)
V (Å^3)	779.76 (19)
Z	1
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.42
Crystal size (mm)	0.21 × 0.10 × 0.07
Data collection	
Diffractometer	Bruker APEX CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 1997)
T_{min}, T_{max}	0.804, 0.910
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4341, 2979, 1863
R_{int}	0.062
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.108, 0.89
No. of reflections	2979
No. of parameters	191
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.95, −0.38

Computer programs: *SMART* (Bruker, 1997), *SAINT* (Bruker, 1997), *SHELXS97* (Sheldrick, 2008), *SHELXL2013* (Sheldrick, 2015), *DIAMOND* (Brandenburg & Berndt, 1998) and *SHELXTL* (Sheldrick, 2008).

Synthesis and crystallization

Glutaric acid (0.1 mmol, 13.3 mg) and $Cu(NO_3)_2\cdot H_2O$ (0.1 mmol, 23.7 mg) were dissolved in 4 ml H_2O and carefully layered by a 4 ml acetonitrile solution of 1,4-bis(pyridin-4-yl)-butane (0.2 mmol, 42.5 mg). Suitable crystals of the title compound were obtained within a few weeks.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Funding information

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References

Brandenburg, K. & Berndt, M. (1998). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.

Bruker (1997). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Hwang, I. H., Bae, J. M., Kim, W.-S., Jo, Y. D., Kim, C., Kim, Y., Kim, S.-J. & Huh, S. (2012). *Dalton Trans.* **41**, 12759–12763.

Hwang, I. H., Kim, H.-Y., Lee, M. M., Na, Y. J., Kim, J. H., Kim, H.-C., Kim, C., Huh, S., Kim, Y. & Kim, S.-J. (2013). *Cryst. Growth Des.* **13**, 4815–4823.

Hyun, M. Y., Hwang, I. H., Lee, M. M., Kim, H., Kim, K. B., Kim, C., Kim, H.-Y., Kim, Y. & Kim, S.-J. (2013). *Polyhedron*, **53**, 166–171.

Kim, H.-C., Huh, S., Kim, J. Y., Moon, H. R., Lee, D. N. & Kim, Y. (2017). *CrystEngComm*, **19**, 99–109.

Lee, M. M., Kim, H.-Y., Hwang, I. H., Bae, J. M., Kim, C., Yo, C.-H., Kim, Y. & Kim, S.-J. (2014). *Bull. Korean Chem. Soc.* **35**, 1777–1783.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

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

full crystallographic data

IUCrData (2017). **2**, x171448 [https://doi.org/10.1107/S2414314617014481]

Two-dimensional structure of poly[[[μ_2-1,4-bis(pyridin-4-yl)butane]bis(μ_4-pentanedioato)dicopper(II)] acetonitrile disolvate]

Do Nam Lee and Youngmee Kim

Poly[[[μ_2-1,4-bis(pyridin-4-yl)butane]bis(μ_4-pentanedioato)dicopper(II)] acetonitrile disolvate]

Crystal data

$[Cu_2(C_5H_6O_4)_2(C_{14}H_{16}N_2)]\cdot 2C_2H_3N$
M_r = 681.67
Triclinic, $P\overline{1}$
a = 7.7525 (11) Å
b = 7.9962 (11) Å
c = 12.8132 (18) Å
α = 87.867 (2)°
β = 81.875 (2)°
γ = 82.674 (2)°
V = 779.76 (19) Å^3
Z = 1
$F(000)$ = 352
D_x = 1.452 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2966 reflections
θ = 2.2–26.2°
μ = 1.42 mm^{-1}
T = 170 K
Block, blue
0.21 × 0.10 × 0.07 mm

Data collection

Bruker APEX CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 1997)
T_{min} = 0.804, T_{max} = 0.910
4341 measured reflections
2979 independent reflections
1863 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
θ_{max} = 26.0°, θ_{min} = 2.6°
h = −9→9
k = −9→9
l = −15→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.108
S = 0.89
2979 reflections
191 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0347P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.95 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.62490 (7)	0.51464 (6)	0.92000 (4)	0.0290 (2)
O11	0.5339 (4)	0.3241 (4)	0.8619 (2)	0.0412 (8)
O12	0.6750 (4)	0.7057 (4)	1.0021 (2)	0.0404 (8)
O21	0.7596 (4)	0.3508 (4)	1.0043 (2)	0.0404 (8)
O22	0.4478 (4)	0.6742 (4)	0.8592 (2)	0.0381 (8)
N31	0.8414 (5)	0.5371 (4)	0.7959 (3)	0.0331 (9)
C11	0.4123 (6)	0.2480 (5)	0.9120 (4)	0.0306 (10)
C12	0.3767 (6)	0.0878 (5)	0.8647 (4)	0.0380 (11)
H12A	0.4735	−0.0019	0.8752	0.046*
H12B	0.3788	0.1067	0.7877	0.046*
C13	0.2032 (5)	0.0246 (5)	0.9092 (4)	0.0347 (11)
H13A	0.1965	0.0125	0.9868	0.042*
H13B	0.1051	0.1095	0.8937	0.042*
C21	0.7012 (6)	0.2860 (5)	1.0915 (4)	0.0307 (10)
C22	0.8184 (6)	0.1436 (5)	1.1359 (3)	0.0343 (11)
H22A	0.7890	0.1389	1.2136	0.041*
H22B	0.9424	0.1650	1.1189	0.041*
C31	1.0050 (6)	0.4805 (5)	0.8086 (3)	0.0336 (11)
H31	1.0250	0.4252	0.8735	0.040*
C32	1.1470 (6)	0.4962 (6)	0.7344 (4)	0.0377 (11)
H32	1.2613	0.4501	0.7475	0.045*
C33	1.1231 (6)	0.5799 (6)	0.6399 (4)	0.0396 (12)
C34	0.9544 (6)	0.6400 (7)	0.6260 (4)	0.0554 (15)
H34	0.9313	0.6981	0.5625	0.067*
C35	0.8182 (6)	0.6158 (6)	0.7042 (4)	0.0468 (13)
H35	0.7020	0.6571	0.6923	0.056*
C36	1.2771 (7)	0.6114 (7)	0.5565 (4)	0.0684 (17)
H36A	1.2327	0.6280	0.4876	0.082*
H36B	1.3180	0.7186	0.5729	0.082*
C37	1.4299 (7)	0.4809 (7)	0.5443 (4)	0.0622 (16)
H37A	1.3902	0.3717	0.5311	0.075*
H37B	1.4812	0.4690	0.6111	0.075*
N1S	1.1372 (9)	0.0804 (8)	0.6005 (5)	0.105 (2)
C1S	1.0053 (11)	0.0854 (8)	0.6449 (6)	0.077 (2)
C2S	0.8316 (9)	0.0914 (9)	0.7021 (6)	0.106 (2)
H2S1	0.7528	0.0535	0.6569	0.160*
H2S2	0.7891	0.2073	0.7238	0.160*
H2S3	0.8342	0.0174	0.7647	0.160*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0282 (3)	0.0198 (3)	0.0365 (3)	−0.0045 (2)	0.0048 (2)	0.0014 (2)
O11	0.045 (2)	0.0324 (18)	0.044 (2)	−0.0143 (16)	0.0101 (16)	−0.0085 (15)
O12	0.043 (2)	0.0332 (19)	0.045 (2)	−0.0158 (16)	0.0044 (16)	−0.0070 (15)

O21	0.0339 (19)	0.0395 (19)	0.043 (2)	0.0011 (15)	0.0032 (15)	0.0080 (15)
O22	0.0339 (19)	0.0339 (18)	0.0423 (19)	0.0012 (15)	0.0019 (15)	0.0093 (15)
N31	0.031 (2)	0.031 (2)	0.036 (2)	−0.0069 (18)	−0.0005 (18)	0.0012 (17)
C11	0.032 (3)	0.023 (2)	0.037 (3)	0.001 (2)	−0.007 (2)	0.000 (2)
C12	0.044 (3)	0.027 (3)	0.044 (3)	−0.010 (2)	−0.004 (2)	−0.004 (2)
C13	0.031 (3)	0.020 (2)	0.053 (3)	−0.001 (2)	−0.008 (2)	−0.005 (2)
C21	0.031 (3)	0.019 (2)	0.044 (3)	−0.008 (2)	−0.006 (2)	−0.003 (2)
C22	0.028 (3)	0.023 (2)	0.053 (3)	−0.006 (2)	−0.009 (2)	0.003 (2)
C31	0.031 (3)	0.031 (3)	0.037 (3)	−0.004 (2)	0.001 (2)	0.004 (2)
C32	0.027 (3)	0.039 (3)	0.046 (3)	−0.001 (2)	−0.002 (2)	−0.001 (2)
C33	0.036 (3)	0.036 (3)	0.043 (3)	−0.006 (2)	0.011 (2)	−0.001 (2)
C34	0.043 (3)	0.071 (4)	0.046 (3)	0.001 (3)	0.002 (3)	0.020 (3)
C35	0.025 (3)	0.062 (4)	0.050 (3)	0.002 (2)	−0.002 (2)	0.014 (3)
C36	0.051 (4)	0.074 (4)	0.071 (4)	−0.010 (3)	0.019 (3)	0.015 (3)
C37	0.044 (3)	0.076 (4)	0.058 (4)	−0.008 (3)	0.020 (3)	0.001 (3)
N1S	0.108 (5)	0.103 (5)	0.098 (5)	−0.003 (5)	−0.001 (4)	0.017 (4)
C1S	0.090 (6)	0.062 (4)	0.072 (5)	0.008 (4)	−0.004 (4)	0.004 (4)
C2S	0.102 (6)	0.084 (5)	0.125 (6)	0.007 (5)	−0.002 (5)	−0.003 (4)

Geometric parameters (Å, º)

Cu1—O21	1.959 (3)	C22—H22A	0.9900
Cu1—O11	1.970 (3)	C22—H22B	0.9900
Cu1—O22	1.976 (3)	C31—C32	1.364 (6)
Cu1—O12	1.994 (3)	C31—H31	0.9500
Cu1—N31	2.163 (3)	C32—C33	1.386 (6)
Cu1—Cu1^{i}	2.6392 (11)	C32—H32	0.9500
O11—C11	1.271 (5)	C33—C34	1.368 (6)
O12—C11^{i}	1.251 (5)	C33—C36	1.526 (6)
O21—C21	1.263 (5)	C34—C35	1.376 (6)
O22—C21^{i}	1.245 (5)	C34—H34	0.9500
N31—C31	1.321 (5)	C35—H35	0.9500
N31—C35	1.337 (5)	C36—C37	1.470 (7)
C11—O12^{i}	1.251 (5)	C36—H36A	0.9900
C11—C12	1.510 (5)	C36—H36B	0.9900
C12—C13	1.525 (6)	C37—C37^{iii}	1.508 (9)
C12—H12A	0.9900	C37—H37A	0.9900
C12—H12B	0.9900	C37—H37B	0.9900
C13—C22^{ii}	1.521 (5)	N1S—C1S	1.094 (8)
C13—H13A	0.9900	C1S—C2S	1.435 (9)
C13—H13B	0.9900	C2S—H2S1	0.9800
C21—O22^{i}	1.245 (5)	C2S—H2S2	0.9800
C21—C22	1.510 (5)	C2S—H2S3	0.9800
C22—C13^{ii}	1.521 (5)		
O21—Cu1—O11	88.10 (13)	C21—C22—C13^{ii}	111.1 (3)
O21—Cu1—O22	167.84 (12)	C21—C22—H22A	109.4
O11—Cu1—O22	90.17 (12)	C13^{ii}—C22—H22A	109.4

O21—Cu1—O12	91.43 (12)	C21—C22—H22B	109.4
O11—Cu1—O12	168.18 (12)	C13^{ii}—C22—H22B	109.4
O22—Cu1—O12	87.80 (12)	H22A—C22—H22B	108.0
O21—Cu1—N31	94.73 (13)	N31—C31—C32	124.2 (4)
O11—Cu1—N31	97.41 (12)	N31—C31—H31	117.9
O22—Cu1—N31	97.42 (13)	C32—C31—H31	117.9
O12—Cu1—N31	94.39 (13)	C31—C32—C33	119.4 (4)
O21—Cu1—Cu1^{i}	82.35 (9)	C31—C32—H32	120.3
O11—Cu1—Cu1^{i}	84.67 (9)	C33—C32—H32	120.3
O22—Cu1—Cu1^{i}	85.51 (9)	C34—C33—C32	117.0 (4)
O12—Cu1—Cu1^{i}	83.57 (9)	C34—C33—C36	120.9 (4)
N31—Cu1—Cu1^{i}	176.38 (10)	C32—C33—C36	122.1 (5)
C11—O11—Cu1	123.1 (3)	C33—C34—C35	119.8 (4)
C11^{i}—O12—Cu1	123.7 (3)	C33—C34—H34	120.1
C21—O21—Cu1	125.6 (3)	C35—C34—H34	120.1
C21^{i}—O22—Cu1	121.4 (3)	N31—C35—C34	123.2 (4)
C31—N31—C35	116.3 (4)	N31—C35—H35	118.4
C31—N31—Cu1	121.7 (3)	C34—C35—H35	118.4
C35—N31—Cu1	121.9 (3)	C37—C36—C33	117.4 (4)
O12^{i}—C11—O11	124.6 (4)	C37—C36—H36A	108.0
O12^{i}—C11—C12	118.6 (4)	C33—C36—H36A	108.0
O11—C11—C12	116.8 (4)	C37—C36—H36B	108.0
C11—C12—C13	115.4 (4)	C33—C36—H36B	108.0
C11—C12—H12A	108.4	H36A—C36—H36B	107.2
C13—C12—H12A	108.4	C36—C37—C37^{iii}	113.3 (6)
C11—C12—H12B	108.4	C36—C37—H37A	108.9
C13—C12—H12B	108.4	C37^{iii}—C37—H37A	108.9
H12A—C12—H12B	107.5	C36—C37—H37B	108.9
C22^{ii}—C13—C12	112.7 (4)	C37^{iii}—C37—H37B	108.9
C22^{ii}—C13—H13A	109.0	H37A—C37—H37B	107.7
C12—C13—H13A	109.0	N1S—C1S—C2S	179.4 (10)
C22^{ii}—C13—H13B	109.0	C1S—C2S—H2S1	109.5
C12—C13—H13B	109.0	C1S—C2S—H2S2	109.5
H13A—C13—H13B	107.8	H2S1—C2S—H2S2	109.5
O22^{i}—C21—O21	124.9 (4)	C1S—C2S—H2S3	109.5
O22^{i}—C21—C22	117.9 (4)	H2S1—C2S—H2S3	109.5
O21—C21—C22	117.1 (4)	H2S2—C2S—H2S3	109.5

Cu1—O11—C11—O12^{i}	7.5 (6)	N31—C31—C32—C33	1.7 (7)
Cu1—O11—C11—C12	−170.5 (3)	C31—C32—C33—C34	−1.2 (7)
O12^{i}—C11—C12—C13	17.0 (6)	C31—C32—C33—C36	176.2 (4)
O11—C11—C12—C13	−164.8 (4)	C32—C33—C34—C35	0.0 (7)
C11—C12—C13—C22^{ii}	−175.8 (3)	C36—C33—C34—C35	−177.4 (5)
Cu1—O21—C21—O22^{i}	−5.5 (6)	C31—N31—C35—C34	−0.6 (7)
Cu1—O21—C21—C22	171.3 (2)	Cu1—N31—C35—C34	176.5 (4)
O22^{i}—C21—C22—C13^{ii}	91.8 (5)	C33—C34—C35—N31	0.9 (8)
O21—C21—C22—C13^{ii}	−85.2 (5)	C34—C33—C36—C37	−147.8 (5)

C35—N31—C31—C32	−0.7 (6)	C32—C33—C36—C37	34.8 (8)
Cu1—N31—C31—C32	−177.8 (3)	C33—C36—C37—C37^{iii}	176.6 (5)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+2; (ii) −*x*+1, −*y*, −*z*+2; (iii) −*x*+3, −*y*+1, −*z*+1.