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Tetra-μ-acetato-$\kappa^8O:O'$-bis{[2-methylsulfanyl-4-(pyridin-4-yl-κN)pyrimidine]copper(II)}(*Cu—Cu*)

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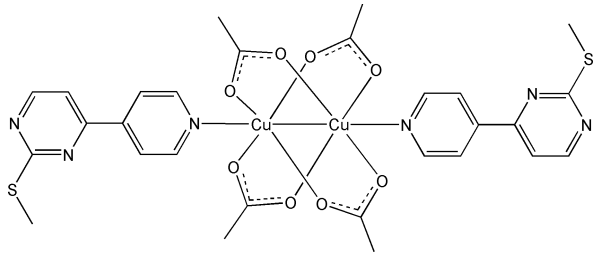
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.031; wR factor = 0.097; data-to-parameter ratio = 13.6.

The binuclear title compound, $[Cu_2(CH_3CO_2)_4(C_{10}H_9N_3S)_2]$, comprises a $Cu_2(CH_3CO_2)_4$ paddle-wheel core axially bound by two 2-methylsulfanyl-4-(pyridin-4-yl)pyrimidine ligands. The complex molecule has an inversion center lying at the mid-point of the Cu—Cu bond.

Related literature

For a related structure, see: Li *et al.* (2009).



Experimental

Crystal data

$[Cu_2(C_2H_3O_2)_4(C_{10}H_9N_3S)_2]$ M_r = 769.82
Monoclinic, $P2_1/c$
a = 15.192 (2) Å
b = 13.003 (2) Å
c = 8.6108 (13) Å
β = 103.781 (2)°
V = 1652.0 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.47 mm^{-1}
T = 298 K
0.41 × 0.25 × 0.18 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.650, T_{max} = 0.768
9568 measured reflections
2827 independent reflections
2354 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.097
S = 1.04
2827 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O1^{i}	1.970 (2)	Cu1—O4	1.967 (2)
Cu1—O2	1.967 (2)	Cu1—N1	2.183 (2)
Cu1—O3^{i}	1.974 (2)	Cu1—Cu1^{i}	2.6299 (7)

Symmetry code: (i) $-x+1, -y, -z+1$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT-Plus* (Bruker, 2007); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2450).

References

Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2007). *APEX2* and *SAINT-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.
Li, L., Xu, G. & Zhu, H.-B. (2009). *Acta Cryst.* E**65**, m476.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2011). E**67**, m1168 [doi:10.1107/S1600536811029837]

Tetra-μ-acetato-$\kappa^8O:O'$-bis{[2-methylsulfanyl-4-(pyridin-4-yl-κN)pyrimidine]-copper(II)}(*Cu—Cu*)

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S1. Comment

In our previous work, we have reported a mononuclear Cu(II) complex with 4-(pyridin-4-yl)pyrimidine-2-sulfonate ligand (Li *et al.*, 2009). Herein, we report a binuclear Cu(II) coordination compound with 2-(methylthio)-4-(pyridin-4-yl)pyrimidine (*L*) ligand. The title compound lies on an inversion center with a Cu—Cu separation of 2.6299 (7) Å (Fig. 1). The *L* ligand acts as a terminal ligand *via* its pyridine N atom, with a Cu—N distance of 2.183 (2) Å (Table 1).

S2. Experimental

A mixture of $Cu(CH_3CO_2)_2$ (0.1 mmol), *L* (0.1 mmol) in ethanol (15 ml) was stirred for 20 min at room temperature. After filtration, the mother liquid was allowed to stand for one week to give blue crystals suitable for X-ray diffraction analysis.

S3. Refinement

H atoms bound to C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (aromatic) and 0.96 (methyl) Å and U_{iso}(H) = 1.2(1.5 for methyl)U_{eq}(C).

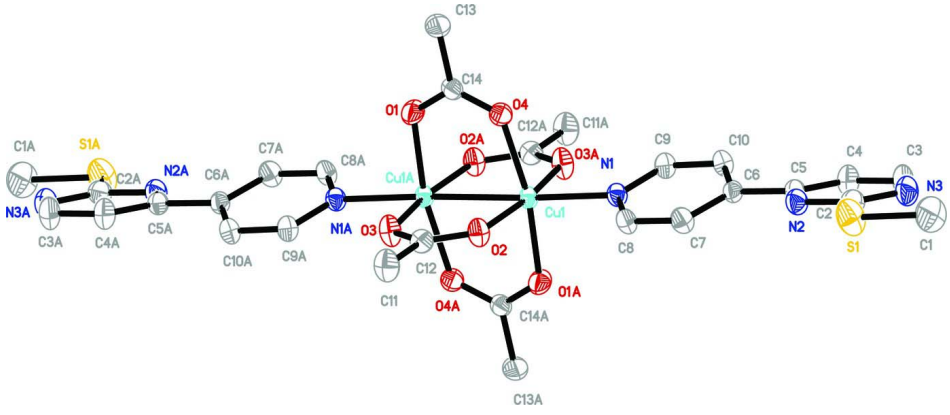

Figure 1

The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry code: (A) 1-*x*, -*y*, 1-*z*.]

Tetra-μ-acetato-κ^8O:O'-bis{[2-methylsulfanyl- 4-(pyridin-4-yl-κN)pyrimidine]copper(II)}(*Cu*—*Cu*)

Crystal data

$[Cu_2(C_2H_3O_2)_4(C_{10}H_9N_3S)_2]$
M_r = 769.82
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 15.192 (2) Å
b = 13.003 (2) Å
c = 8.6108 (13) Å
β = 103.781 (2)°
V = 1652.0 (4) Å^3
Z = 2
$F(000)$ = 788
D_x = 1.548 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2827 reflections
θ = 2.3–25.5°
μ = 1.47 mm^{-1}
T = 298 K
Block, blue
0.41 × 0.25 × 0.18 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.650, T_{max} = 0.768
9568 measured reflections
2827 independent reflections
2354 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 25.0°, θ_{min} = 2.1°
h = −15→18
k = −15→15
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.097
S = 1.04
2827 reflections
208 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0614P)^2 + 0.3763P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
Cu1	0.42790 (2)	0.03013 (2)	0.39231 (4)	0.03313 (14)
O2	0.39177 (14)	−0.11545 (15)	0.3826 (3)	0.0474 (5)
O4	0.50560 (15)	−0.00064 (17)	0.2452 (2)	0.0462 (5)
N1	0.31254 (16)	0.08776 (18)	0.2112 (3)	0.0380 (5)
O1	0.62838 (15)	−0.05037 (17)	0.4261 (3)	0.0522 (6)
O3	0.51441 (14)	−0.16651 (15)	0.5641 (3)	0.0518 (6)
C14	0.5845 (2)	−0.03341 (19)	0.2841 (4)	0.0396 (7)
C8	0.2390 (2)	0.0311 (2)	0.1478 (4)	0.0440 (7)
H8	0.2376	−0.0368	0.1810	0.053*
C6	0.16582 (19)	0.1693 (2)	−0.0149 (3)	0.0377 (6)
C10	0.2425 (2)	0.2277 (2)	0.0483 (3)	0.0427 (7)
H10	0.2459	0.2956	0.0164	0.051*
C9	0.3132 (2)	0.1843 (2)	0.1582 (3)	0.0410 (7)

H9	0.3644	0.2243	0.1980	0.049*
C12	0.4403 (2)	−0.1827 (2)	0.4653 (4)	0.0412 (7)
C7	0.1662 (2)	0.0681 (2)	0.0368 (4)	0.0477 (7)
H7	0.1169	0.0256	−0.0042	0.057*
N2	0.02885 (17)	0.1470 (2)	−0.2225 (3)	0.0491 (6)
C5	0.08668 (19)	0.2131 (2)	−0.1331 (3)	0.0417 (7)
C4	0.0726 (2)	0.3178 (3)	−0.1478 (4)	0.0573 (9)
H4	0.1123	0.3640	−0.0846	0.069*
S1	−0.11441 (7)	0.09520 (9)	−0.43675 (14)	0.0806 (3)
N3	−0.0610 (2)	0.2871 (3)	−0.3527 (4)	0.0620 (8)
C13	0.6315 (3)	−0.0562 (3)	0.1536 (4)	0.0579 (9)
H13A	0.5910	−0.0426	0.0517	0.087*
H13B	0.6494	−0.1271	0.1590	0.087*
H13C	0.6842	−0.0133	0.1664	0.087*
C2	−0.0421 (2)	0.1878 (3)	−0.3268 (4)	0.0514 (8)
C11	0.4090 (2)	−0.2928 (2)	0.4448 (5)	0.0609 (9)
H11A	0.4514	−0.3358	0.5166	0.091*
H11B	0.4050	−0.3141	0.3366	0.091*
H11C	0.3504	−0.2986	0.4681	0.091*
C3	−0.0023 (3)	0.3513 (3)	−0.2593 (5)	0.0657 (10)
H3	−0.0127	0.4216	−0.2707	0.079*
C1	−0.2020 (2)	0.1704 (4)	−0.5637 (5)	0.0900 (14)
H1A	−0.2452	0.1254	−0.6301	0.135*
H1B	−0.1757	0.2145	−0.6298	0.135*
H1C	−0.2319	0.2114	−0.4990	0.135*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0360 (2)	0.0322 (2)	0.0284 (2)	0.00451 (13)	0.00199 (15)	−0.00098 (13)
O2	0.0452 (12)	0.0375 (11)	0.0524 (13)	−0.0012 (9)	−0.0028 (10)	0.0009 (9)
O4	0.0511 (13)	0.0567 (12)	0.0316 (11)	0.0104 (10)	0.0111 (10)	0.0027 (9)
N1	0.0412 (14)	0.0382 (13)	0.0322 (13)	0.0043 (10)	0.0039 (11)	0.0004 (10)
O1	0.0528 (13)	0.0680 (15)	0.0362 (12)	0.0198 (11)	0.0116 (11)	0.0003 (10)
O3	0.0536 (14)	0.0350 (10)	0.0552 (13)	−0.0022 (10)	−0.0099 (11)	−0.0011 (9)
C14	0.0538 (19)	0.0307 (14)	0.0372 (17)	0.0042 (13)	0.0166 (15)	0.0001 (12)
C8	0.0453 (18)	0.0382 (15)	0.0444 (18)	0.0003 (13)	0.0024 (15)	0.0087 (13)
C6	0.0379 (16)	0.0397 (15)	0.0339 (15)	0.0062 (12)	0.0057 (13)	0.0037 (12)
C10	0.0484 (18)	0.0342 (14)	0.0410 (17)	0.0016 (13)	0.0019 (14)	0.0030 (12)
C9	0.0419 (16)	0.0369 (15)	0.0393 (16)	0.0005 (12)	0.0001 (13)	−0.0026 (12)
C12	0.0482 (18)	0.0357 (15)	0.0396 (17)	−0.0016 (13)	0.0103 (14)	−0.0075 (13)
C7	0.0403 (17)	0.0469 (17)	0.0503 (19)	−0.0071 (14)	−0.0002 (15)	0.0053 (14)
N2	0.0401 (15)	0.0544 (15)	0.0480 (16)	0.0030 (12)	0.0009 (13)	0.0101 (12)
C5	0.0365 (16)	0.0485 (16)	0.0384 (17)	0.0052 (13)	0.0056 (14)	0.0069 (13)
C4	0.053 (2)	0.0488 (18)	0.062 (2)	0.0087 (16)	−0.0018 (17)	0.0036 (16)
S1	0.0607 (6)	0.0805 (7)	0.0812 (8)	−0.0150 (5)	−0.0214 (5)	0.0158 (6)
N3	0.0477 (17)	0.0690 (19)	0.0622 (19)	0.0113 (14)	−0.0007 (15)	0.0157 (15)
C13	0.077 (3)	0.057 (2)	0.047 (2)	0.0175 (18)	0.0314 (19)	0.0038 (16)

C2	0.0376 (17)	0.067 (2)	0.0468 (19)	0.0017 (15)	0.0045 (15)	0.0123 (16)
C11	0.063 (2)	0.0362 (16)	0.076 (2)	−0.0064 (15)	0.0006 (19)	−0.0080 (16)
C3	0.062 (2)	0.052 (2)	0.076 (3)	0.0151 (18)	0.001 (2)	0.0134 (19)
C1	0.045 (2)	0.126 (4)	0.082 (3)	−0.004 (2)	−0.020 (2)	0.018 (3)

Geometric parameters (Å, º)

Cu1—O1^{i}	1.970 (2)	C12—C11	1.505 (4)
Cu1—O2	1.967 (2)	C7—H7	0.9300
Cu1—O3^{i}	1.974 (2)	N2—C2	1.338 (4)
Cu1—O4	1.967 (2)	N2—C5	1.335 (4)
Cu1—N1	2.183 (2)	C5—C4	1.379 (4)
Cu1—Cu1^{i}	2.6299 (7)	C4—C3	1.373 (5)
O2—C12	1.251 (4)	C4—H4	0.9300
O4—C14	1.241 (4)	S1—C2	1.748 (4)
N1—C9	1.337 (4)	S1—C1	1.796 (4)
N1—C8	1.341 (4)	N3—C2	1.330 (5)
O1—C14	1.265 (4)	N3—C3	1.341 (5)
O3—C12	1.257 (4)	C13—H13A	0.9600
C14—C13	1.498 (4)	C13—H13B	0.9600
C8—C7	1.366 (4)	C13—H13C	0.9600
C8—H8	0.9300	C11—H11A	0.9600
C6—C10	1.388 (4)	C11—H11B	0.9600
C6—C7	1.389 (4)	C11—H11C	0.9600
C6—C5	1.491 (4)	C3—H3	0.9300
C10—C9	1.372 (4)	C1—H1A	0.9600
C10—H10	0.9300	C1—H1B	0.9600
C9—H9	0.9300	C1—H1C	0.9600
O4—Cu1—O2	88.92 (9)	O2—C12—C11	118.1 (3)
O4—Cu1—O1^{i}	168.10 (9)	O3—C12—C11	116.5 (3)
O2—Cu1—O1^{i}	89.58 (9)	C8—C7—C6	119.9 (3)
O4—Cu1—O3^{i}	89.87 (9)	C8—C7—H7	120.0
O2—Cu1—O3^{i}	168.30 (8)	C6—C7—H7	120.0
O1^{i}—Cu1—O3^{i}	89.20 (10)	C2—N2—C5	116.5 (3)
O4—Cu1—N1	96.46 (9)	N2—C5—C4	121.1 (3)
O2—Cu1—N1	97.57 (9)	N2—C5—C6	117.4 (3)
O1^{i}—Cu1—N1	95.44 (9)	C4—C5—C6	121.5 (3)
O3^{i}—Cu1—N1	94.13 (9)	C3—C4—C5	117.5 (3)
O4—Cu1—Cu1^{i}	82.34 (7)	C3—C4—H4	121.3
O2—Cu1—Cu1^{i}	85.43 (6)	C5—C4—H4	121.3
O1^{i}—Cu1—Cu1^{i}	85.77 (7)	C2—S1—C1	103.5 (2)
O3^{i}—Cu1—Cu1^{i}	82.88 (6)	C2—N3—C3	114.7 (3)
N1—Cu1—Cu1^{i}	176.77 (7)	C14—C13—H13A	109.5
C12—O2—Cu1	121.89 (19)	C14—C13—H13B	109.5
C14—O4—Cu1	125.8 (2)	H13A—C13—H13B	109.5
C9—N1—C8	116.8 (2)	C14—C13—H13C	109.5
C9—N1—Cu1	119.7 (2)	H13A—C13—H13C	109.5

C8—N1—Cu1	123.46 (19)	H13B—C13—H13C	109.5
C14—O1—Cu1	65.15 (17)	N3—C2—N2	127.2 (3)
C12—O3—Cu1	66.66 (15)	N3—C2—S1	119.7 (3)
O4—C14—O1	125.0 (3)	N2—C2—S1	113.1 (3)
O4—C14—C13	117.9 (3)	C12—C11—H11A	109.5
O1—C14—C13	117.1 (3)	C12—C11—H11B	109.5
N1—C8—C7	123.3 (3)	H11A—C11—H11B	109.5
N1—C8—H8	118.4	C12—C11—H11C	109.5
C7—C8—H8	118.4	H11A—C11—H11C	109.5
C10—C6—C7	117.0 (3)	H11B—C11—H11C	109.5
C10—C6—C5	121.6 (3)	N3—C3—C4	123.0 (3)
C7—C6—C5	121.4 (3)	N3—C3—H3	118.5
C9—C10—C6	119.5 (3)	C4—C3—H3	118.5
C9—C10—H10	120.3	S1—C1—H1A	109.5
C6—C10—H10	120.3	S1—C1—H1B	109.5
N1—C9—C10	123.5 (3)	H1A—C1—H1B	109.5
N1—C9—H9	118.2	S1—C1—H1C	109.5
C10—C9—H9	118.2	H1A—C1—H1C	109.5
O2—C12—O3	125.4 (3)	H1B—C1—H1C	109.5

O4—Cu1—O2—C12	81.3 (2)	Cu1—O4—C14—C13	177.6 (2)
O1^{i}—Cu1—O2—C12	−86.9 (2)	C9—N1—C8—C7	−1.4 (4)
O3^{i}—Cu1—O2—C12	−2.9 (6)	Cu1—N1—C8—C7	178.6 (2)
N1—Cu1—O2—C12	177.7 (2)	C7—C6—C10—C9	−0.9 (4)
Cu1^{i}—Cu1—O2—C12	−1.1 (2)	C5—C6—C10—C9	179.2 (3)
O2—Cu1—O4—C14	−85.3 (2)	C8—N1—C9—C10	2.1 (4)
O1^{i}—Cu1—O4—C14	−2.5 (6)	Cu1—N1—C9—C10	−178.0 (2)
O3^{i}—Cu1—O4—C14	83.0 (2)	C6—C10—C9—N1	−0.9 (4)
N1—Cu1—O4—C14	177.2 (2)	Cu1—O2—C12—C11	−177.5 (2)
Cu1^{i}—Cu1—O4—C14	0.2 (2)	N1—C8—C7—C6	−0.4 (5)
O4—Cu1—N1—C9	−80.7 (2)	C10—C6—C7—C8	1.5 (4)
O2—Cu1—N1—C9	−170.5 (2)	C5—C6—C7—C8	−178.6 (3)
O1^{i}—Cu1—N1—C9	99.2 (2)	C2—N2—C5—C4	0.6 (4)
O3^{i}—Cu1—N1—C9	9.6 (2)	C2—N2—C5—C6	179.4 (3)
O4—Cu1—N1—C8	99.3 (2)	C10—C6—C5—N2	160.4 (3)
O2—Cu1—N1—C8	9.5 (2)	C7—C6—C5—N2	−19.5 (4)
O1^{i}—Cu1—N1—C8	−80.8 (2)	C10—C6—C5—C4	−20.7 (4)
O3^{i}—Cu1—N1—C8	−170.4 (2)	C7—C6—C5—C4	159.4 (3)
O4—Cu1—O1^{i}—C14^{i}	4.2 (6)	N2—C5—C4—C3	−0.9 (5)
O2—Cu1—O1^{i}—C14^{i}	86.9 (2)	C6—C5—C4—C3	−179.7 (3)
O3^{i}—Cu1—O1^{i}—C14^{i}	−81.4 (2)	C3—N3—C2—N2	−1.7 (5)
N1—Cu1—O1^{i}—C14^{i}	−175.5 (2)	C3—N3—C2—S1	178.5 (3)
Cu1^{i}—Cu1—O1^{i}—C14^{i}	1.5 (2)	C5—N2—C2—N3	0.8 (5)
O4—Cu1—O3^{i}—C12^{i}	−82.5 (2)	C5—N2—C2—S1	−179.4 (2)
O2—Cu1—O3^{i}—C12^{i}	1.5 (6)	C1—S1—C2—N3	−0.4 (3)
O1^{i}—Cu1—O3^{i}—C12^{i}	85.6 (2)	C1—S1—C2—N2	179.7 (2)

N1—Cu1—O3^{i}—C12^{i}	−179.0 (2)	C2—N3—C3—C4	1.2 (5)
Cu1^{i}—Cu1—O3^{i}—C12^{i}	−0.2 (2)	C5—C4—C3—N3	0.0 (6)

Symmetry code: (i) −*x*+1, −*y*, −*z*+1.