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***catena*-Poly[[bis(α -thenoyltrifluoroacetato- κ^2 O,O')copper(II)]- μ -1,4-di-3-pyridyl-2,3-diaza-1,3-butadiene- κ^2 N:N']**

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Key indicators

Single-crystal X-ray study

$T = 294$ K

Mean $\sigma(C-C) = 0.004$ Å

Disorder in main residue

R factor = 0.045

wR factor = 0.131

Data-to-parameter ratio = 14.0

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

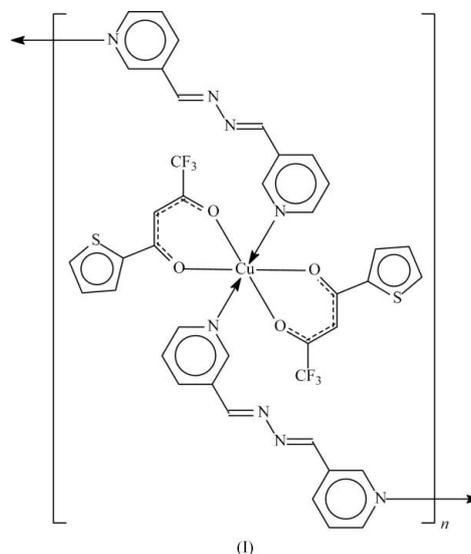
The title compound, $[Cu(C_8H_4F_3O_2S)_2(C_{12}H_{10}N_4)]_n$ or $[Cu(tta)_2(L2)]_n$ ($L2 = 1,4$ -di-3-pyridyl-2,3-diaza-1,3-butadiene and $tta = \alpha$ -thenoyltrifluoroacetate), consists of undulating chains containing two crystallographically distinct Cu^{II} centers that are each located on inversion centers. Each Cu^{II} center exhibits distorted octahedral coordination provided by two pyridyl N atoms from two equivalent $L2$ ligands and four O atoms from two equivalent tta ligands. The chains interact through weak $C-F \cdots H-C$ contacts.

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Comment

The synthesis of coordination polymers is of current interest due to their potential applications in a variety of areas, including catalysis, gas storage and nonlinear optics (Chin *et al.*, 1993; Kitagawa *et al.*, 2004; Janiak, 2003). Our group has been interested in utilizing N,N' -bipyridine-type ligands for the construction of new inorganic-organic coordination polymers, and we have synthesized several Schiff base ligands such as 1,4-bis(4-pyridyl)-2,3-diaza-1,3-butadiene ($L1$) and 1,4-bis(3-pyridyl)-2,3-diaza-1,3-butadiene ($L2$) for this purpose (Ciurtin *et al.*, 2001; Dong *et al.*, 2000). These efforts have resulted in the generation of many new coordination polymers (Perkins *et al.*, 2005; Davis *et al.*, 2004; Khalil *et al.*, 2005; Dong *et al.*, 2000*a,b*) including the title compound, (I), which is an example of a one-dimensional coordination polymer that utilizes $L2$ and tta ($tta = \alpha$ -thenoyltrifluoroacetate) in its construction.



The structure of (I) contains two distinct Cu^{II} centers that are both located on inversion centers and both are octa-

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.131$
 $S = 1.04$
 6101 reflections
 435 parameters
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0817P)^2 + 0.2214P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.45 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.34 \text{ e } \text{\AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

Cu1—O1	2.0225 (19)	Cu2—O4	2.0108 (18)
Cu1—N1	2.111 (2)	Cu2—N4	2.086 (2)
Cu1—O2	2.1426 (18)	Cu2—O3	2.164 (2)
O1 ⁱ —Cu1—N1	88.71 (8)	O4—Cu2—N4	89.81 (8)
O1 ⁱ —Cu1—O2 ⁱ	88.10 (7)	O4 ⁱⁱ —Cu2—N4	90.19 (8)
O1—Cu1—O2 ⁱ	91.90 (7)	O4—Cu2—O3	88.84 (7)
N1—Cu1—O2 ⁱ	91.14 (7)	O4 ⁱⁱ —Cu2—O3	91.16 (7)

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

H atoms were placed in geometrically idealized positions and included as riding atoms with C—H distances fixed at 0.93 \AA . Both independent thiophene rings were found to be rotationally disordered about the *ipso* carbon bonds (C16—C17 and C24—C25). The disorder components of each ring lie essentially in the same plane. For each ring, the geometry of the minor component (C17B—C20B/S1B and C25B—C28B/S2B) was restrained to be similar to that of the major (C17A—C20A/S1A and C25A—C28A/S2A). The pivot atom C10(A/B) is common to both components, and atoms less than 0.5 \AA from their disorder counterparts were assigned equal displacement parameters. The total occupancy was restrained to sum to unity. The final refined occupancies are C17—C20/S1 (A/B) = 0.776 (4)/0.224 (4) and C25—C28/S2 (A/B) = 0.818 (4)/0.182 (4).

Data collection: SMART-NT (Bruker, 2001); cell refinement: SAINT-Plus-NT (Bruker, 2001); data reduction: SAINT-Plus-NT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997);

molecular graphics: SHELXTL (Sheldrick, 2000) and DIAMOND (Brandenburg, 2005); software used to prepare material for publication: SHELXTL.

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