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Key indicators

Single-crystal X-ray study
 T = 295 K
 Mean $\sigma(C-C)$ = 0.010 Å
 Disorder in main residue
 R factor = 0.054
 wR factor = 0.193
 Data-to-parameter ratio = 10.5

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

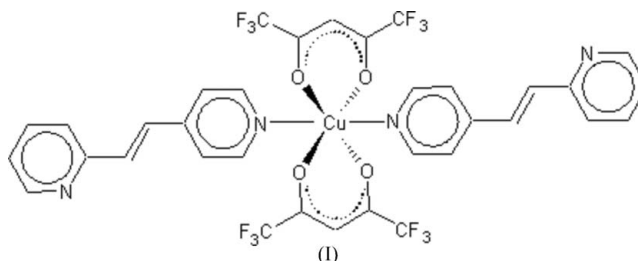
***trans*-Bis(hexafluoroacetylacetonato- κ^2O,O')-bis[*trans*-1-(2-pyridyl)-2-(4-pyridyl)ethylene- κN^4]-copper(II)**

The title compound, *trans*-[Cu(C₅HF₆O₂)₂(C₁₂H₁₀N₂)₂], consists of monomeric units built up by a copper metal ion (lying on a center of symmetry) octahedrally coordinated by one oxygen-chelating hexafluoroacetylacetonate (hfac) group, a nitrogen-bound 1-(2-pyridyl)-2-(4-pyridyl)ethylene (2,4-bpye) ligand, and their symmetry equivalents generated by the symmetry center at the metal site. The monomers interact with each other through π - π bonding between pyridine rings, and are organized as chains running along [11 $\bar{1}$]. The stabilization of this architecture of chains is associated with a number of weak C—H...F hydrogen bonds.

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Comment

There are few structural studies dealing with 1-(2-pyridyl)-2-(4-pyridyl)ethylene (2,4-bpye), and they show the ligand to adopt two binding modes to metal centers: monodentate, through the 4-pyridyl N atom, as in complexes with Mn^{II}, Fe^{II}, Co^{II}, Ni^{II}, Cu^{II} and Pb^{II} (Du *et al.*, 2006; Seidel *et al.*, 2001), and bridging bidentate, as in polymeric complexes with Ag^I (Rarig & Zubieta, 2001) and Cu^I (Zhong & Lu, 2005).



We present here a rather unusual copper complex, (I), containing both the 2,4-bpye ligand and the hfac anion (hfac is hexafluoroacetylacetonate); the only other known structure sharing both ligands is the Mn analog [Mn(hfac)₂(2,4-bpye)₂][Mn(hfac)₂(MeOH)₂], (II), reported by Seidel *et al.* (2001).

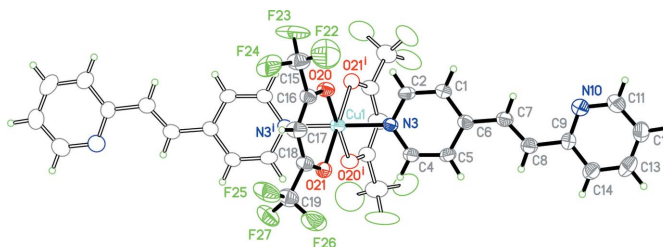


Figure 1
 The molecular structure of (I) with the atom numbering. Displacement ellipsoids are drawn at the 30% probability level. Only the major disorder components of F atoms are shown. [Symmetry code: (i) 1 - x, 1 - y, 1 - z.]

The copper(II) cation in (I), lying on a $\bar{1}$ site, is octahedrally coordinated by two *O,O'*-chelating hfac units, and two N-bonded 4-pyridyl groups from two 2,4-bpye ligands (Fig. 1). In spite of the chelation, the geometry around copper is rather regular due to the open character of the 2,4-bpye bite. The equatorial bonds differ by less than 2%, while the axial Cu1—O21 bond is only 12% longer (Table 1). The 2,4-bpye unit is basically planar (maximum deviation 0.057 Å for atom N3). The symmetry center forces the extended units to bind at *trans* positions and parallel to each other, expanding outwards and giving the molecule a highly prolate elliptical appearance with major/minor principal axes of ~ 22.6 and ~ 11.5 Å, respectively. The hfac CF₃ units exhibit some rotational disorder (see *Experimental*).

In spite of the striking monomeric similarities, the Mn and Cu analogs pack in very different ways; while (II) forms a hydrogen-bonded supramolecular structure involving hydroxyl protons and non-bonded 2-pyridyl units, in (I), the N atoms of the free 2-pyridyl groups do not participate in any kind of hydrogen bonding and it is the pyridyl rings instead that provide the main packing forces through their displaced π - π stacking interactions (shown in Fig. 2). This is characterized by a dihedral angle of 2.14 (1)° between the rings, a (nearly graphitic) interplanar separation of 3.46 (1) Å and a centroid-to-centroid distance [Cg1...Cg2ⁱⁱ; Cg1 and Cg2 are the centroids of the C1/C2/N3/C4/C5/C6 and C9/N10/C11/C12/C13/C14 rings, respectively; symmetry code: (ii) $-x, -y, 2-z$] of 3.917 (4) Å, with a (mean) slippage angle of 28.1 (7)° (Janiak, 2000). This interconnection between monomers leads to the formation of chains along [11 $\bar{1}$] (Fig. 2). The interlinkage between chains seems to be quite feeble as it involves only weak contacts in which the disordered F atoms and the pyridyl H atoms take part.

Experimental

Ethanol was purchased from Merck and used without further purification. The compounds Cu(hfac)₂·H₂O and 2,4-bpye were obtained from the Aldrich Chemical Company. For the synthesis of (I), an ethanol solution (1.50 ml) of Cu(hfac)₂·H₂O (0.043 g, 0.087 mmol) was added to a solution of 2,4-bpye (0.032 g, 0.174 mmol) in ethanol (1.20 ml). The resulting dark-green solution was heated at 323 K for 10 min and then maintained at room temperature in a closed container. After a couple of days, crystals suitable for single-crystal X-ray diffraction were obtained (yield: 54.1%). The dark-green crystalline precipitate was washed with ethanol (3 × 2.5 ml) and dried *in vacuo* (m.p. 473 K). Analysis calculated for C₃₄H₂₂CuF₁₂N₄O₄: C 48.50, H 2.63, N 6.65%; found: C 48.65, H 2.68, N 6.56%.

Crystal data

[Cu(C ₅ HF ₆ O ₂) ₂ (C ₁₂ H ₁₀ N ₂) ₂]	$V = 913.9$ (3) Å ³
$M_r = 842.10$	$Z = 1$
Triclinic, $P\bar{1}$	$D_x = 1.530$ Mg m ⁻³
$a = 9.1513$ (18) Å	Mo $K\alpha$ radiation
$b = 10.009$ (2) Å	$\mu = 0.70$ mm ⁻¹
$c = 10.424$ (2) Å	$T = 295$ (2) K
$\alpha = 74.23$ (3)°	Plate, green
$\beta = 84.12$ (3)°	$0.35 \times 0.25 \times 0.12$ mm
$\gamma = 87.98$ (3)°	

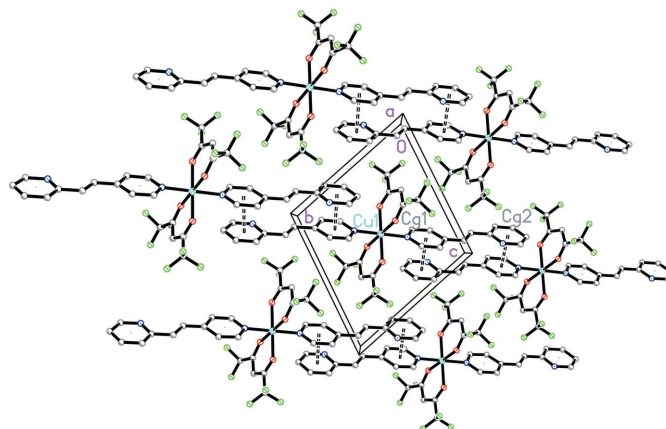


Figure 2
Packing view showing the formation of chains. π - π Contacts are shown as dashed lines. Cg1 and Cg2 are the centroids of the C1/C2/N3/C4/C5/C6 and C9/N10/C11/C12/C13/C14 rings, respectively.

Data collection

Rigaku AFC-6 diffractometer	1907 reflections with $I > 2\sigma(I)$
$\omega/2\theta$ scans	$R_{\text{int}} = 0.039$
Absorption correction: ψ scan	$\theta_{\text{max}} = 25.0^\circ$
(North <i>et al.</i> , 1968)	3 standard reflections
$T_{\text{min}} = 0.80, T_{\text{max}} = 0.91$	every 150 reflections
4174 measured reflections	intensity decay: 2%
3219 independent reflections	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0916P)^2 + 1.5666P]$
$R[F^2 > 2\sigma(F^2)] = 0.054$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.193$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 0.94$	$\Delta\rho_{\text{max}} = 0.41$ e Å ⁻³
3219 reflections	$\Delta\rho_{\text{min}} = -0.48$ e Å ⁻³
306 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (Å, °).

Cu1—N3	2.006 (5)	Cu1—O21	2.257 (4)
Cu1—O20	2.042 (4)		
N3—Cu1—O20	89.50 (18)	O20—Cu1—O21 ⁱ	94.11 (15)
N3—Cu1—O21 ⁱ	87.49 (16)		

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

H atoms were positioned geometrically (C—H = 0.96 Å) and allowed to ride with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. Both C—CF₃ units presented rotational disorder, and each one was refined with a split model, as two groups having common C atoms of full occupancy, and two sets of F atoms with partial occupancies of 0.60/0.40 (4) and 0.46/0.54 (2), respectively. These parameters were allowed to vary in the early stages of refinement but were kept fixed at their convergence values at the end of the process. In order to preserve a meaningful geometry, similarity restraints were applied to the C—F and F...F distances.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1988); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *MSC/AFC Diffractometer Control Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-NT*

(Sheldrick, 2000); software used to prepare material for publication: *SHELXTL-NT* and *PLATON* (Spek, 2003).

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