dimensions are in Table 2. Fig. 1 shows the molecule and our numbering scheme.

**Related literature.** The $\eta^2$-derivatives $HB(Me_2pz)_3Mo(CO)_2(\eta^2\text{-}COR)$ ($R$ = $p$-$C_6H_4Me$ and $C_6H_{11}$) have been described previously (Desmond Lalor, O'Sullivan, Ferguson, Ruhl & Parvez, 1983). Curtis, Shiu & Butler (1986) have described $RBpz_3Mo(CO)_2(\eta^2\text{-}COR^1)$ ($R$ = H or pz, $R^1$ = alkyl, aryl).

We are indebted to the NSERC Canada for the award of an operating grant (to GF) and a Visiting Professorship (to BK). We are also pleased to acknowledge the award of a Postgraduate Maintenance Grant (to BO'S) from the Department of Education, Irish Republic, and financial support (to FJL) from Eolas (Irish Republic) *via* Grant No. SC-Chem-024-088.

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# Structure of *catena*-Poly{bis(1,1,1-trifluoro-2,4-pentanedionato-$\kappa^2O,O'$)copper-$\mu$-[(4,4′-bipyridine)-$\kappa N:\kappa N'$]}

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(*Received* 11 *March* 1991; *accepted* 2 *July* 1991)

**Abstract.** $[Cu(C_5H_4F_3O_2)_2(C_{10}H_8N_2)]$, $M_r$ = 525.55, tetragonal, $P4_2/m$, $a$ = 8.379 (1), $c$ = 15.832 (4) Å, $V$ = 1111.6 (4) Å$^3$, $Z$ = 2, $D_x$ = 1.57 g cm$^{-3}$, $\lambda$(Mo $K\alpha$) = 0.71073 Å, $\mu$ = 10.59 cm$^{-1}$, $F(000)$ = 530, $T$ = 295 K, $R$ = 0.043, $wR$ = 0.043 for 658 unique observed [$I > 1.5\sigma(I)$] reflections. Bis(1,1,1-trifluoropentane-2,4-dionato-$O,O'$)copper(II) and 4,4′-bipyridine form a one-dimensional infinite linear structure with molecular ratio 1:1. The coordination geometry around each copper(II) atom is that of an octahedron, where the basal plane is comprised of four O atoms at a distance of 1.968 (3) Å and the axial positions are occupied by two N atoms at 2.381 (5) Å. The distance between adjacent copper(II) atoms is 11.850 (4) Å.

**Experimental.** The title complex was prepared by addition of 4,4′-bipyridine (0.32 g) in absolute ethanol (10 ml) to a solution of bis(1,1,1-trifluoropentane-2,4-dionato-$O,O'$)copper(II) (1.48 g) in absolute ethanol (40 ml). After the resulting solution was stirred and refluxed for two hours, green crystals were obtained. Yield: 61%. The structure proposed is in agreement with microanalysis. $C_{20}H_{16}CuF_6N_2O_4$: Calc.: C 45.66, H 3.04, N 5.33; Found: C 45.50, H 3.15, N 5.16.

Light-green single crystals were developed from a $CH_3CN$–$C_2H_5OH$ solution of the complex at room temperature. A suitable crystal, dimensions 0.40 × 0.40 × 0.50 mm, *R3M/E* diffractometer, graphite-monochromatized Mo $K\alpha$ radiation; cell parameters from 19 reflections in $2\theta$ range 6.86–18.34°; data collected by $\omega$–$2\theta$ scans in $2\theta$ range 2–45°. *hkl* ranges: $h$ 0–9, $k$ 0–9, $l$ 0–17; 914 measured reflections, 658 unique with [$I > 1.5\sigma(I)$], $R_{int}$ = 0.0103. Corrections made for Lorentz–polarization factors, but not absorption effects. Three standard reflections monitored every 2 h, no significant variation during data collection.

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0108-2701/91/122653-02$03.00 

Cu atom located by direct methods and the remaining atoms found with successive Fourier syntheses. Refinement (on $F$) with 115 parameters performed by block-diagonal least-squares methods, using anisotropic thermal parameters for non-H atoms and isotropic thermal parameters for H atoms; final $R = 0.043$, $wR = 0.043$, $S = 1.881$, max. $\Delta/\sigma = 0.158$, $-0.23 < \Delta\rho < 0.30$ e Å$^{-3}$; $w = [1 - \exp(-5\sin^2\theta/\lambda^2)]/[\sigma^2(F) + gF^2]$, with $g = 0.0001$. Scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV). All calculations from *SHELXTL* (Sheldrick, 1983) on an Eclipse S/140 computer. Fig. 1 shows the asymmetric unit of the complex,* and Fig. 2 indicates the nature of the polymer. Final atomic coordinates are listed in Table 1,* and selected bond lengths and angles given in Table 2.†

**Related literature.** Recent research on one-dimensional molecular chains and polymers is due to their possible role as models for one-dimensional conductors (Shi & Xu, 1985; Xu & Shi, 1986; Gou, You, Xu, Zhou, Yu, Yu & Zhu, 1991). These complexes in which the 4,4′-bipyridine groups with the metal centres may enable transfer of electrons from one metal center to another; thus they may possess certain properties of conductivity similar to metals. In the title complex, each copper(II) atom is more closely located in the coordination plane composed of two 1,1,1-trifluoropentane-2,4-dionato-*O*,*O*′ groups than is found with other $\beta$-diketones.

* The $CF_3$ group was found to exhibit disorder.

† Lists of structure factors, anisotropic thermal parameters, full bond angles and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54417 (7 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

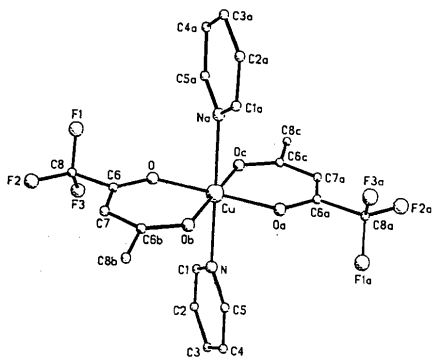


Fig. 1. View of complex showing the atomic labelling scheme.

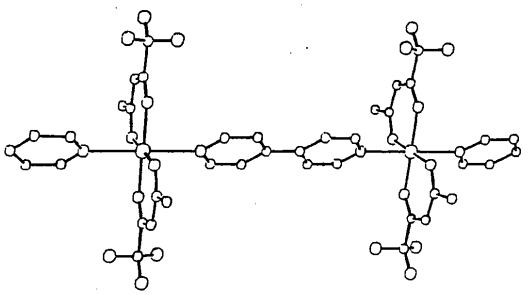

Fig. 2. View of one 4,4′-bipyridine group linking $Cu^{2+}$ atoms.

Table 1. *Atomic coordinates* ($\times 10^4$) *and isotropic thermal parameters* (Å$^2 \times 10^3$)

$U_{eq}$ is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor.

| | $x$ | $y$ | $z$ | $U_{eq}$ |
|---|---|---|---|---|
| Cu | 0 | 5000 | 0 | 55 (1) |
| N | 2009 (6) | 2991 (5) | 0 | 72 (2) |
| O | −1208 (3) | 3793 (3) | 854 (2) | 66 (1) |
| C1 | 1670 (7) | 1472 (8) | 0 | 105 (4) |
| C2 | 2773 (7) | 272 (8) | 0 | 102 (4) |
| C3 | 4367 (6) | 632 (6) | 0 | 54 (2) |
| C4 | 4731 (8) | 2214 (8) | 0 | 100 (4) |
| C5 | 3524 (7) | 3338 (7) | 0 | 105 (4) |
| C6 | −1032 (5) | 3973 (5) | 1640 (3) | 67 (2) |
| C7 | 0 | 5000 | 2040 (4) | 70 (2) |
| C8 | −2104 (7) | 2907 (8) | 2172 (5) | 100 (3) |
| F1 | −3539 (9) | 3188 (13) | 1958 (7) | 164 (5) |
| F2 | −1959 (12) | 3054 (12) | 2943 (5) | 148 (4) |
| F3 | −1874 (13) | 1482 (9) | 1940 (6) | 159 (5) |

Table 2. *Selected bond lengths* (Å) *and bond angles* (°)

| | | | |
|---|---|---|---|
| Cu—N | 2.381 (5) | Cu—O | 1.968 (3) |
| N—C1 | 1.304 (8) | N—C5 | 1.303 (8) |
| O—C6 | 1.262 (6) | C1—C2 | 1.365 (9) |
| C2—C3 | 1.369 (8) | C3—C4 | 1.360 (8) |
| C4—C5 | 1.382 (9) | C6—C7 | 1.375 (5) |
| C6—C8 | 1.521 (8) | C8—F1 | 1.271 (10) |
| C8—F2 | 1.233 (10) | C8—F3 | 1.264 (10) |

| | | | |
|---|---|---|---|
| N—Cu—O | 90.0 (1) | N—Cu—Na | 180.0 (1) |
| O—Cu—Na | 90.0 (1) | N—Cu—Oa | 90.0 (1) |
| O—Cu—Oa | 180.0 (1) | N—Cu—Ob | 90.0 (1) |
| O—Cu—Ob | 93.3 (2) | N—Cu—Oc | 90.0 (1) |
| O—Cu—Oc | 86.7 (2) | Cu—N—C1 | 122.4 (4) |
| Cu—N—C5 | 122.1 (4) | C1—N—C5 | 115.5 (5) |
| Cu—O—N6 | 123.7 (3) | N—C1—C2 | 124.9 (6) |
| C1—C2—C3 | 119.9 (6) | C2—C3—C4 | 115.7 (5) |
| C3—C4—C5 | 120.0 (6) | N—C5—C4 | 124.1 (6) |
| O—C6—C7 | 127.1 (4) | O—C6—C8 | 114.0 (4) |
| C7—C6—C8 | 118.9 (5) | C6—C7—C6a | 125.1 (6) |
| C6—C8—F1 | 107.6 (7) | C6—C8—F2 | 115.6 (7) |
| F1—C8—F2 | 109.8 (8) | C6—C8—F3 | 107.7 (7) |
| F1—C8—F3 | 104.0 (8) | F2—C8—F3 | 115.6 (7) |

We thank the National Science Foundation of China for support of the research.

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