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# catena-Poly[ $\{\mu$ -cyanido-bis[(4,4'-dimethyl-2,2'-bipyridine- $\kappa^2N,N'$ )-copper(I)] $\}$ - $\mu$ -cyanido-copper(I)- $\mu$ -cyanido]

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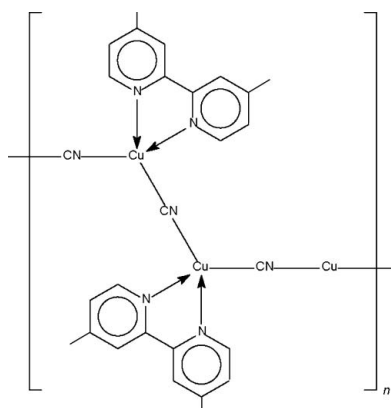
Received 10 July 2008; accepted 22 July 2008

Key indicators: single-crystal X-ray study;  $T = 295$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å; disorder in main residue;  $R$  factor = 0.038;  $wR$  factor = 0.110; data-to-parameter ratio = 18.4.

In the title compound,  $[\text{Cu}_3(\text{CN})_3(\text{C}_{12}\text{H}_{12}\text{N}_2)_2]$ , two 2,2'-bipyridine  $N,N'$ -chelated  $\text{Cu}^{\text{I}}$  atoms are linked by a cyanide bridge that lies about a center of inversion; the  $\text{Cu}^{\text{I}}$  atom exists in a tetrahedral coordination geometry. This dinuclear entity is linked to another  $\text{Cu}^{\text{I}}$  atom that lies on a twofold rotation axis by another cyanide bridge, these bridges giving rise to the formation of a linear chain motif.

## Related literature

Some copper(I) cyanide adducts with 2,2'-bipyridine-like ligands that adopt chain structures in which the cyanide group functions as a bridge are triscyano-bis(2,2'-biquinoline)tricopper (Chesnut *et al.*, 2001; Dessy *et al.*, 1985), tetrakis(cyano(2,2'-biquinoline)tetracopper (Chesnut & Zubieta, 1998) and biscyano-(4,4'-diphenyl-2,2'-bipyridine)dication (Chesnut *et al.*, 2001).



## Experimental

### Crystal data

$[\text{Cu}_3(\text{CN})_3(\text{C}_{12}\text{H}_{12}\text{N}_2)_2]$   
 $M_r = 637.15$

Monoclinic,  $C2/c$   
 $a = 10.7196$  (7) Å  
 $b = 12.3700$  (9) Å  
 $c = 20.9182$  (14) Å  
 $\beta = 100.146$  (1)°

$V = 2730.4$  (3) Å<sup>3</sup>  
 $Z = 4$

Mo  $K\alpha$  radiation  
 $\mu = 2.34$  mm<sup>-1</sup>  
 $T = 295$  (2) K  
 $0.30 \times 0.20 \times 0.16$  mm

### Data collection

Bruker SMART APEX  
 diffractometer  
 Absorption correction: multi-scan  
 (SADABS; Sheldrick, 1996)  
 $T_{\text{min}} = 0.540$ ,  $T_{\text{max}} = 0.705$

8685 measured reflections  
 3125 independent reflections  
 2491 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.024$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$   
 $wR(F^2) = 0.110$   
 $S = 1.03$   
 3125 reflections

170 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.53$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.21$  e Å<sup>-3</sup>

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: X-SEED (Barbour, 2001); software used to prepare material for publication: publCIF (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2103).

## References

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 Westrip, S. P. (2008). publCIF. In preparation.

## supporting information

*Acta Cryst.* (2008). E64, m1076 [doi:10.1107/S1600536808022964]

***catena*-Poly[ $\{\mu$ -cyanido-bis[(4,4'-dimethyl-2,2'-bipyridine- $\kappa^2$ N,N')]copper(I)] $\}$ - $\mu$ -cyanido-copper(I)- $\mu$ -cyanido]**

**Shi-Hong Lin, Ying-Yi Yang and Seik Weng Ng**

### S1. Comment

The cyanide group functions as a bridging group in a number of copper(I) adducts of 2,2'-bipyridine type of *N*-heterocycles. Those whose crystal structure have been described include the triscyano-bis(2,2'-biquinoline)tricopper (Chesnut *et al.*, 2001; Dessy *et al.*, 1985), tetrakis(cyano(2,2'-biquinoline)tetracopper (Chesnut & Zubieta, 1998) and bis(cyano-(4,4'-diphenyl-2,2'-bipyridine)dicopper (Chesnut *et al.*, 2001).

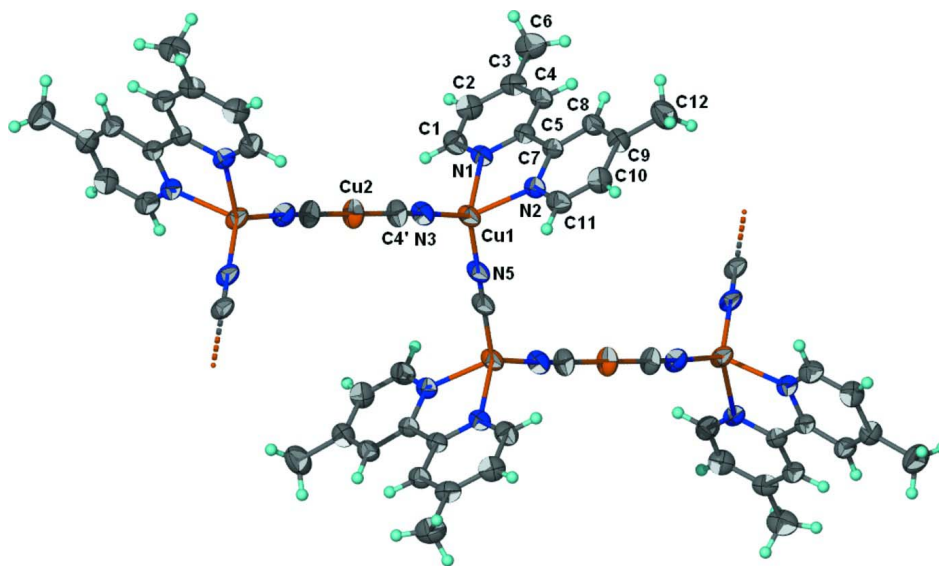
The copper(I) cyanide adduct with 4,4'-dimethyl-2,2'-bipyridine (Scheme 1, Fig. 1) adopts a similar chain motif. Two *N*-heterocycle-chelated copper(I) atoms are linked by a cyanide bridge that lies about a center-of-inversion; the copper(I) atom exists in a tetrahedral coordination geometry. This dinuclear entity is linked to copper(I) atom that lies on a twofold rotation axis by another cyanide bridge.

### S2. Experimental

4,4'-Dimethyl-2,2'-bipyridine (0.055 g, 0.3 mmol), cuprous cyanide (0.009 g, 0.1 mmol) and acetonitrile (8 ml) were placed in a 15-ml, teflon-lined autoclave. It was heated at 453 K for 72 hours, then was cooled to 333 K at a rate of 5 K per hour and then kept at this temperature for a further 10 hours before being cooled to room temperature. Red prisms were in 50% yield based on the *N*-heterocycle.

### S3. Refinement

The component atoms of the cyanide groups were each refined as a 50%:50% mixture of carbon and nitrogen. The pair of C/N atoms were restrained to the same site and also to have the same temperature factors. Hydrogen atoms were placed at calculated positions in the riding model approximation with C—H = 0.93–0.98 Å and  $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5U_{\text{eq}}(\text{C})$ .

**Figure 1**

Thermal ellipsoid plot (Barbour, 2001) of a portion of the linear chain motif; probability levels are set at 50%.

**catena-Poly**[ $\{\mu$ -cyano-bis[(4,4'-dimethyl-2,2'-bipyridine- $\kappa^2N,N'$ )copper(I)] $\}$ - $\mu$ -cyano-copper(I)- $\mu$ -cyano]

*Crystal data*

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Hall symbol:  $-C\ 2yc$

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$c = 20.9182\ (14)\ \text{\AA}$

$\beta = 100.146\ (1)^\circ$

$V = 2730.4\ (3)\ \text{\AA}^3$

$Z = 4$

$F(000) = 1288$

$D_x = 1.550\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 2750 reflections

$\theta = 2.5\text{--}27.0^\circ$

$\mu = 2.34\ \text{mm}^{-1}$

$T = 295\ \text{K}$

Block, red

$0.30 \times 0.20 \times 0.16\ \text{mm}$

*Data collection*

Bruker SMART APEX  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.540$ ,  $T_{\max} = 0.705$

8685 measured reflections

3125 independent reflections

2491 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.024$

$\theta_{\max} = 27.5^\circ$ ,  $\theta_{\min} = 2.5^\circ$

$h = -13 \rightarrow 13$

$k = -16 \rightarrow 15$

$l = -16 \rightarrow 27$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.110$

$S = 1.03$

3125 reflections

170 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

$$w = 1/[\sigma^2(F_o^2) + (0.065P)^2 + 0.8323P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 0.53 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.22 \text{ e } \text{\AA}^{-3}$$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Cu1	0.74268 (3)	0.41078 (2)	0.072850 (16)	0.04716 (14)	
Cu2	0.5000	0.41827 (4)	0.2500	0.05469 (16)	
N1	0.75592 (19)	0.54384 (16)	0.01065 (10)	0.0420 (5)	
N2	0.92273 (18)	0.47469 (15)	0.11124 (9)	0.0406 (4)	
N3	0.6442 (3)	0.41773 (18)	0.14085 (14)	0.0519 (6)	0.50
N4	0.5915 (2)	0.4184 (2)	0.18400 (12)	0.0502 (6)	0.50
N5	0.7489 (2)	0.28632 (17)	0.01721 (11)	0.0487 (6)	0.50
C3'	0.6442 (3)	0.41773 (18)	0.14085 (14)	0.0519 (6)	0.50
C4'	0.5915 (2)	0.4184 (2)	0.18400 (12)	0.0502 (6)	0.50
C5'	0.7489 (2)	0.28632 (17)	0.01721 (11)	0.0487 (6)	0.50
C1	0.6717 (3)	0.5725 (2)	-0.04135 (14)	0.0531 (6)	
H1	0.5932	0.5384	-0.0485	0.064*	
C2	0.6951 (3)	0.6501 (2)	-0.08494 (13)	0.0562 (7)	
H2	0.6325	0.6680	-0.1200	0.067*	
C3	0.8105 (3)	0.7011 (2)	-0.07670 (12)	0.0493 (6)	
C4	0.8992 (2)	0.67121 (18)	-0.02273 (12)	0.0450 (6)	
H4	0.9791	0.7030	-0.0154	0.054*	
C5	0.8687 (2)	0.59363 (16)	0.02044 (12)	0.0385 (5)	
C6	0.8409 (4)	0.7858 (2)	-0.12307 (15)	0.0699 (9)	
H6A	0.8117	0.7623	-0.1669	0.105*	
H6B	0.9309	0.7970	-0.1164	0.105*	
H6C	0.7997	0.8523	-0.1156	0.105*	
C7	0.9594 (2)	0.56084 (18)	0.07973 (11)	0.0391 (5)	
C8	1.0699 (2)	0.61388 (19)	0.10154 (13)	0.0461 (6)	
H8	1.0910	0.6739	0.0789	0.055*	
C9	1.1516 (3)	0.5801 (2)	0.15691 (14)	0.0523 (6)	
C10	1.1131 (3)	0.4918 (2)	0.18924 (14)	0.0559 (7)	
H10	1.1634	0.4661	0.2270	0.067*	
C11	1.0006 (3)	0.4430 (2)	0.16498 (13)	0.0516 (6)	
H11	0.9766	0.3837	0.1873	0.062*	
C12	1.2752 (3)	0.6366 (3)	0.18039 (18)	0.0781 (10)	
H12A	1.3038	0.6203	0.2255	0.117*	
H12B	1.2635	0.7133	0.1751	0.117*	
H12C	1.3372	0.6125	0.1556	0.117*	

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cu1	0.0535 (2)	0.0446 (2)	0.0483 (2)	-0.01261 (12)	0.02281 (16)	-0.00397 (12)
Cu2	0.0494 (3)	0.0793 (4)	0.0406 (3)	0.000	0.0223 (2)	0.000
N1	0.0483 (11)	0.0401 (10)	0.0402 (12)	-0.0070 (8)	0.0149 (9)	-0.0055 (8)

N2	0.0469 (10)	0.0416 (10)	0.0376 (11)	-0.0031 (8)	0.0193 (9)	0.0007 (8)
N3	0.0530 (13)	0.0527 (14)	0.0522 (15)	-0.0098 (10)	0.0152 (12)	-0.0068 (10)
N4	0.0469 (13)	0.0700 (16)	0.0387 (13)	-0.0049 (10)	0.0214 (11)	-0.0049 (10)
N5	0.0560 (13)	0.0453 (12)	0.0514 (15)	-0.0154 (10)	0.0281 (11)	-0.0066 (9)
C3'	0.0530 (13)	0.0527 (14)	0.0522 (15)	-0.0098 (10)	0.0152 (12)	-0.0068 (10)
C4'	0.0469 (13)	0.0700 (16)	0.0387 (13)	-0.0049 (10)	0.0214 (11)	-0.0049 (10)
C5'	0.0560 (13)	0.0453 (12)	0.0514 (15)	-0.0154 (10)	0.0281 (11)	-0.0066 (9)
C1	0.0539 (15)	0.0559 (15)	0.0491 (16)	-0.0090 (12)	0.0082 (13)	-0.0071 (12)
C2	0.0655 (16)	0.0599 (16)	0.0415 (15)	0.0020 (13)	0.0047 (13)	0.0003 (12)
C3	0.0678 (16)	0.0432 (12)	0.0409 (14)	0.0022 (12)	0.0206 (13)	0.0002 (10)
C4	0.0525 (14)	0.0423 (13)	0.0451 (14)	-0.0055 (10)	0.0221 (11)	-0.0005 (10)
C5	0.0457 (12)	0.0370 (11)	0.0365 (13)	-0.0020 (9)	0.0175 (10)	-0.0035 (9)
C6	0.098 (2)	0.0630 (18)	0.0550 (19)	0.0058 (16)	0.0312 (17)	0.0142 (14)
C7	0.0456 (13)	0.0367 (11)	0.0400 (13)	-0.0031 (9)	0.0216 (11)	-0.0021 (9)
C8	0.0501 (14)	0.0424 (12)	0.0482 (15)	-0.0047 (10)	0.0153 (12)	0.0046 (10)
C9	0.0506 (14)	0.0537 (15)	0.0530 (17)	-0.0049 (11)	0.0103 (12)	-0.0013 (11)
C10	0.0554 (15)	0.0640 (17)	0.0473 (16)	0.0013 (13)	0.0066 (12)	0.0101 (13)
C11	0.0628 (16)	0.0484 (13)	0.0474 (15)	-0.0050 (12)	0.0201 (13)	0.0069 (12)
C12	0.0605 (18)	0.080 (2)	0.086 (2)	-0.0172 (16)	-0.0074 (17)	0.0093 (19)

*Geometric parameters (Å, °)*

Cu1—N1	2.118 (2)	C4—C5	1.395 (3)
Cu1—N2	2.109 (2)	C4—H4	0.9300
Cu1—N3	1.917 (3)	C5—C7	1.491 (3)
Cu1—N5	1.938 (2)	C6—H6A	0.9600
Cu2—N4	1.829 (2)	C6—H6B	0.9600
Cu2—N4 <sup>i</sup>	1.829 (2)	C6—H6C	0.9600
N1—C1	1.333 (3)	C7—C8	1.361 (4)
N1—C5	1.340 (3)	C8—C9	1.388 (4)
N2—C11	1.336 (3)	C8—H8	0.9300
N2—C7	1.347 (3)	C9—C10	1.385 (4)
N3—N4	1.146 (4)	C9—C12	1.502 (4)
N5—C5 <sup>ii</sup>	1.154 (4)	C10—C11	1.364 (4)
C1—C2	1.377 (4)	C10—H10	0.9300
C1—H1	0.9300	C11—H11	0.9300
C2—C3	1.372 (4)	C12—H12A	0.9600
C2—H2	0.9300	C12—H12B	0.9600
C3—C4	1.392 (4)	C12—H12C	0.9600
C3—C6	1.503 (4)		
N3—Cu1—N5	124.25 (9)	N1—C5—C4	121.7 (2)
N3—Cu1—N2	106.70 (9)	N1—C5—C7	116.1 (2)
N5—Cu1—N2	113.61 (9)	C4—C5—C7	122.2 (2)
N3—Cu1—N1	121.75 (9)	C3—C6—H6A	109.5
N5—Cu1—N1	103.61 (9)	C3—C6—H6B	109.5
N2—Cu1—N1	77.69 (7)	H6A—C6—H6B	109.5
N4—Cu2—C4 <sup>i</sup>	179.88 (15)	C3—C6—H6C	109.5

C4 <sup>i</sup> —Cu2—N4 <sup>i</sup>	0.00 (12)	H6A—C6—H6C	109.5
C1—N1—C5	117.7 (2)	H6B—C6—H6C	109.5
C1—N1—Cu1	126.79 (17)	N2—C7—C8	121.9 (2)
C5—N1—Cu1	114.80 (16)	N2—C7—C5	114.8 (2)
C11—N2—C7	116.8 (2)	C8—C7—C5	123.3 (2)
C11—N2—Cu1	127.21 (16)	C7—C8—C9	121.3 (2)
C7—N2—Cu1	115.86 (16)	C7—C8—H8	119.4
N4—N3—Cu1	175.6 (3)	C9—C8—H8	119.4
N3—N4—Cu2	177.1 (3)	C10—C9—C8	116.5 (2)
C5 <sup>ii</sup> —N5—Cu1	178.3 (3)	C10—C9—C12	121.9 (3)
N5 <sup>ii</sup> —N5—Cu1	178.3 (3)	C8—C9—C12	121.6 (3)
N1—C1—C2	123.4 (2)	C11—C10—C9	119.2 (3)
N1—C1—H1	118.3	C11—C10—H10	120.4
C2—C1—H1	118.3	C9—C10—H10	120.4
C3—C2—C1	120.2 (3)	N2—C11—C10	124.3 (2)
C3—C2—H2	119.9	N2—C11—H11	117.8
C1—C2—H2	119.9	C10—C11—H11	117.8
C2—C3—C4	116.8 (2)	C9—C12—H12A	109.5
C2—C3—C6	122.2 (3)	C9—C12—H12B	109.5
C4—C3—C6	120.9 (2)	H12A—C12—H12B	109.5
C3—C4—C5	120.2 (2)	C9—C12—H12C	109.5
C3—C4—H4	119.9	H12A—C12—H12C	109.5
C5—C4—H4	119.9	H12B—C12—H12C	109.5
N3—Cu1—N1—C1	-81.2 (2)	C1—N1—C5—C7	178.9 (2)
N5—Cu1—N1—C1	64.9 (2)	Cu1—N1—C5—C7	-9.9 (2)
N2—Cu1—N1—C1	176.6 (2)	C3—C4—C5—N1	1.8 (3)
N3—Cu1—N1—C5	108.54 (18)	C3—C4—C5—C7	-178.5 (2)
N5—Cu1—N1—C5	-105.30 (17)	C11—N2—C7—C8	-0.4 (3)
N2—Cu1—N1—C5	6.36 (15)	Cu1—N2—C7—C8	176.04 (18)
N3—Cu1—N2—C11	54.7 (2)	C11—N2—C7—C5	-179.5 (2)
N5—Cu1—N2—C11	-85.9 (2)	Cu1—N2—C7—C5	-3.0 (2)
N1—Cu1—N2—C11	174.5 (2)	N1—C5—C7—N2	8.7 (3)
N3—Cu1—N2—C7	-121.34 (17)	C4—C5—C7—N2	-171.0 (2)
N5—Cu1—N2—C7	98.09 (17)	N1—C5—C7—C8	-170.4 (2)
N1—Cu1—N2—C7	-1.55 (15)	C4—C5—C7—C8	10.0 (4)
C5—N1—C1—C2	0.0 (4)	N2—C7—C8—C9	1.3 (4)
Cu1—N1—C1—C2	-170.0 (2)	C5—C7—C8—C9	-179.7 (2)
N1—C1—C2—C3	1.1 (4)	C7—C8—C9—C10	-1.5 (4)
C1—C2—C3—C4	-0.7 (4)	C7—C8—C9—C12	178.5 (3)
C1—C2—C3—C6	179.7 (3)	C8—C9—C10—C11	1.0 (4)
C2—C3—C4—C5	-0.7 (4)	C12—C9—C10—C11	-179.1 (3)
C6—C3—C4—C5	179.0 (2)	C7—N2—C11—C10	-0.2 (4)
C1—N1—C5—C4	-1.4 (3)	Cu1—N2—C11—C10	-176.2 (2)
Cu1—N1—C5—C4	169.76 (17)	C9—C10—C11—N2	-0.1 (5)

Symmetry codes: (i)  $-x+1, y, -z+1/2$ ; (ii)  $-x+3/2, -y+1/2, -z$ .