

## catena-Poly[[dichloridocopper(II)]- $\mu$ -4,4'-bis(benzimidazol-1-yl)biphenyl]

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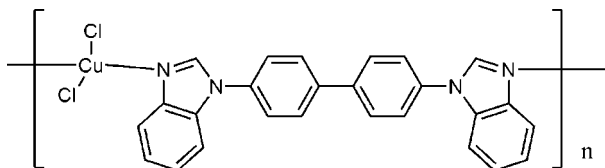
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.026;  $wR$  factor = 0.066; data-to-parameter ratio = 12.6.

In the title compound,  $[\text{CuCl}_2(\text{C}_{26}\text{H}_{18}\text{N}_4)]_n$ , the Cu(II) ion is four-coordinated by two N atoms from two 4,4'-bis(benzimidazol-1-yl)biphenyl ligands and two chloride anions, in a slightly distorted tetrahedral environment. The biphenyl ligand acts as a linear bidentate ligand, connecting the metal atoms into an infinite chain parallel to  $[101]$ . In the biphenyl ligand, the two benzene rings make a dihedral angle of  $33.19$  (7)°.

### Related literature

For background to benzimidazole-based ligands in crystal engineering, see: Jin *et al.* (2006); Li *et al.* (2009); Su *et al.* (2003).



### Experimental

#### Crystal data

$[\text{CuCl}_2(\text{C}_{26}\text{H}_{18}\text{N}_4)]$   
 $M_r = 520.88$   
Monoclinic,  $C2/c$   
 $a = 12.599$  (4) Å  
 $b = 15.280$  (4) Å  
 $c = 11.233$  (3) Å  
 $\beta = 91.936$  (4)°

$V = 2161.3$  (10) Å<sup>3</sup>  
 $Z = 4$   
Mo  $K\alpha$  radiation  
 $\mu = 1.28$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.04 \times 0.03 \times 0.02$  mm

#### Data collection

Rigaku Mercury CCD area-detector diffractometer  
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)  
 $T_{\min} = 0.955$ ,  $T_{\max} = 0.975$

6675 measured reflections  
1903 independent reflections  
1761 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.027$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.026$   
 $wR(F^2) = 0.066$   
 $S = 1.06$   
1903 reflections

151 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.50$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.27$  e Å<sup>-3</sup>

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: FJ2406).

### References

- Jin, C. M., Lu, H., Wu, L. Y. & Huang, J. (2006). *Chem. Commun.* pp. 5039–5041.  
Li, Z. X., Xu, Y., Zuo, Y., Li, L., Pan, Q., Hu, T. L. & Bu, X. H. (2009). *Cryst. Growth Des.* **9**, 3904–3909.  
Rigaku/MSC (2005). *CrystalClear*. Rigaku/MSC Inc., The Woodlands, Texas, USA.  
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
Su, C. Y., Cai, Y. P., Chen, C. L., Smith, M. D., Kaim, W. & zur Loye, H. C. (2003). *J. Am. Chem. Soc.* **125**, 8595–8613.

**supplementary materials**

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***catena*-Poly[[dichloridocopper(II)]- $\mu$ -4,4'-bis(benzimidazol-1-yl)biphenyl]**

**D.-N. Xiao, H.-Y. Pan, M. Yao and G. Xie**

**Comment**

Benzoimidazole has been well used in crystal engineering, and a large number of benzoimidazole-containing flexible ligands have been extensively studied (Su *et al.*,2003; Jin *et al.*,2006). However, to our knowledge, the research on benzoimidazole ligands bearing rigid spacers is still less developed (Li *et al.*,2009).

Single-crystal X-ray diffraction analysis reveals that the title compound (I) crystallizes in the monoclinic space group  $C2/c$ . The geometry of the Cu(II) ion is surrounded by two benzoimidazole rings of distinct L ligands and two chlorine anions, which illustrates a slightly distorted tetrahedral coordination environment (Fig. 1). Notably, as shown in Fig. 2, the four-coordinated Cu(II) center is bridged by the linear ligand L to form an infinite one-dimensional architecture.

**Experimental**

A mixture of CH<sub>3</sub>OH and CHCl<sub>3</sub> (1:1, 8 ml), as a buffer layer, was carefully layered over a solution of 4,4'-Bis(benzoimidazol-1-yl)terphenyl (L, 0.06 mmol) in CHCl<sub>3</sub> (6 ml). Then a solution of CuCl<sub>2</sub> (0.06 mmol) in CH<sub>3</sub>OH (6 ml) was layered over the buffer layer, and the resultant reaction was left to stand at room temperature. After *ca* three weeks, purple block single crystals appeared at the boundary. Yield: ~35% (based on L).

**Refinement**

C-bound H atoms were positioned geometrically and refined in the riding-model approximation, with C—H = 0.93 Å and  $U_{iso}(H) = 1.2U_{eq}$ .

**Figures**

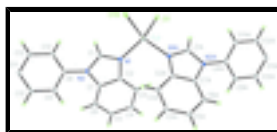


Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radius.

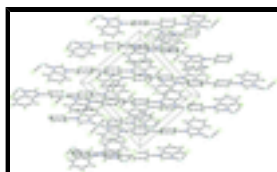


Fig. 2. The crystal packing for (I).

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### Crystal data

[CuCl <sub>2</sub> (C <sub>26</sub> H <sub>18</sub> N <sub>4</sub> )]	$F(000) = 1060$
$M_r = 520.88$	$D_x = 1.601 \text{ Mg m}^{-3}$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: -C 2yc	Cell parameters from 2903 reflections
$a = 12.599 (4) \text{ \AA}$	$\theta = 2.1\text{--}27.9^\circ$
$b = 15.280 (4) \text{ \AA}$	$\mu = 1.28 \text{ mm}^{-1}$
$c = 11.233 (3) \text{ \AA}$	$T = 293 \text{ K}$
$\beta = 91.936 (4)^\circ$	Block, brown
$V = 2161.3 (10) \text{ \AA}^3$	$0.04 \times 0.03 \times 0.02 \text{ mm}$
$Z = 4$	

### Data collection

Rigaku Mercury CCD area-detector diffractometer	1903 independent reflections
Radiation source: fine-focus sealed tube graphite	1761 reflections with $I > 2\sigma(I)$
Detector resolution: 9 pixels $\text{mm}^{-1}$	$R_{\text{int}} = 0.027$
$\omega$ scans	$\theta_{\text{max}} = 25.0^\circ$ , $\theta_{\text{min}} = 3.2^\circ$
Absorption correction: multi-scan ( <i>CrystalClear</i> ; Rigaku/MSC, 2005)	$h = -14 \rightarrow 14$
$T_{\text{min}} = 0.955$ , $T_{\text{max}} = 0.975$	$k = -18 \rightarrow 18$
6675 measured reflections	$l = -13 \rightarrow 13$

### Refinement

Refinement on $F^2$	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.026$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.066$	H-atom parameters constrained
$S = 1.06$	$w = 1/[\sigma^2(F_o^2) + (0.0296P)^2 + 3.937P]$
1903 reflections	where $P = (F_o^2 + 2F_c^2)/3$
151 parameters	$(\Delta/\sigma)_{\text{max}} = 0.002$
0 restraints	$\Delta\rho_{\text{max}} = 0.50 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.27 \text{ e \AA}^{-3}$

### Special details

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations

between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

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

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	1.0000	1.09184 (2)	0.7500	0.01275 (12)
Cl1	0.98903 (4)	1.18252 (3)	0.59365 (5)	0.02221 (15)
N1	0.89293 (14)	1.01051 (11)	0.81368 (14)	0.0136 (4)
N2	0.75910 (13)	0.96997 (11)	0.92601 (15)	0.0128 (4)
C1	0.83320 (16)	1.03097 (13)	0.90401 (18)	0.0138 (4)
H1	0.8414	1.0822	0.9480	0.017*
C2	0.85403 (16)	0.92994 (13)	0.77153 (18)	0.0121 (4)
C3	0.88572 (16)	0.87841 (13)	0.67670 (17)	0.0133 (4)
H3	0.9422	0.8949	0.6304	0.016*
C4	0.83018 (17)	0.80212 (13)	0.65424 (19)	0.0158 (4)
H4	0.8493	0.7666	0.5913	0.019*
C5	0.74523 (17)	0.77700 (13)	0.72469 (19)	0.0168 (5)
H5	0.7089	0.7255	0.7064	0.020*
C6	0.71401 (17)	0.82661 (13)	0.82038 (19)	0.0142 (4)
H6	0.6584	0.8095	0.8676	0.017*
C7	0.77056 (16)	0.90357 (13)	0.84203 (17)	0.0125 (4)
C8	0.68519 (16)	0.97360 (13)	1.02045 (18)	0.0132 (4)
C9	0.66932 (17)	0.89992 (14)	1.08940 (19)	0.0177 (5)
H9	0.7071	0.8488	1.0756	0.021*
C10	0.59681 (17)	0.90309 (14)	1.17892 (19)	0.0177 (5)
H10	0.5857	0.8533	1.2245	0.021*
C11	0.53980 (16)	0.97924 (13)	1.20262 (17)	0.0129 (4)
C12	0.55967 (16)	1.05353 (13)	1.13412 (18)	0.0129 (4)
H12	0.5247	1.1056	1.1502	0.015*
C13	0.63069 (16)	1.05066 (13)	1.04257 (18)	0.0137 (4)
H13	0.6418	1.1000	0.9962	0.016*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cu1	0.0123 (2)	0.01272 (19)	0.01364 (19)	0.000	0.00700 (14)	0.000
Cl1	0.0252 (3)	0.0219 (3)	0.0202 (3)	0.0108 (2)	0.0105 (2)	0.0070 (2)
N1	0.0132 (9)	0.0158 (9)	0.0121 (9)	-0.0018 (7)	0.0043 (7)	-0.0008 (7)
N2	0.0121 (9)	0.0151 (8)	0.0114 (8)	-0.0016 (7)	0.0052 (7)	0.0000 (7)
C1	0.0118 (11)	0.0166 (10)	0.0131 (10)	-0.0021 (8)	0.0037 (8)	-0.0004 (8)
C2	0.0110 (10)	0.0138 (10)	0.0114 (10)	-0.0011 (8)	0.0011 (8)	0.0014 (8)
C3	0.0119 (11)	0.0172 (10)	0.0108 (10)	0.0016 (8)	0.0022 (8)	0.0018 (8)

## supplementary materials

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C4	0.0178 (11)	0.0155 (10)	0.0141 (10)	0.0043 (8)	0.0010 (9)	-0.0024 (8)
C5	0.0164 (11)	0.0115 (10)	0.0226 (11)	-0.0030 (8)	0.0003 (9)	0.0013 (9)
C6	0.0112 (10)	0.0140 (10)	0.0177 (11)	-0.0012 (8)	0.0035 (8)	0.0036 (8)
C7	0.0106 (10)	0.0155 (10)	0.0114 (10)	0.0011 (8)	0.0031 (8)	0.0018 (8)
C8	0.0100 (10)	0.0198 (11)	0.0099 (10)	-0.0020 (8)	0.0033 (8)	-0.0003 (8)
C9	0.0183 (12)	0.0173 (11)	0.0181 (11)	0.0054 (9)	0.0082 (9)	0.0019 (9)
C10	0.0197 (12)	0.0180 (11)	0.0160 (11)	0.0011 (9)	0.0082 (9)	0.0055 (9)
C11	0.0101 (11)	0.0175 (11)	0.0112 (10)	-0.0003 (8)	0.0018 (8)	-0.0009 (8)
C12	0.0103 (10)	0.0141 (10)	0.0142 (10)	-0.0003 (8)	0.0015 (8)	-0.0028 (8)
C13	0.0146 (11)	0.0135 (10)	0.0130 (10)	-0.0045 (8)	0.0018 (8)	0.0016 (8)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

Cu1—N1 <sup>i</sup>	1.9851 (17)	C5—C6	1.383 (3)
Cu1—N1	1.9851 (17)	C5—H5	0.9300
Cu1—C11 <sup>i</sup>	2.2378 (7)	C6—C7	1.392 (3)
Cu1—C11	2.2378 (7)	C6—H6	0.9300
N1—C1	1.321 (3)	C8—C9	1.385 (3)
N1—C2	1.402 (3)	C8—C13	1.390 (3)
N2—C1	1.348 (3)	C9—C10	1.382 (3)
N2—C7	1.396 (3)	C9—H9	0.9300
N2—C8	1.436 (3)	C10—C11	1.398 (3)
C1—H1	0.9300	C10—H10	0.9300
C2—C3	1.394 (3)	C11—C12	1.399 (3)
C2—C7	1.397 (3)	C11—C11 <sup>ii</sup>	1.487 (4)
C3—C4	1.379 (3)	C12—C13	1.387 (3)
C3—H3	0.9300	C12—H12	0.9300
C4—C5	1.406 (3)	C13—H13	0.9300
C4—H4	0.9300		
N1 <sup>i</sup> —Cu1—N1	102.49 (10)	C4—C5—H5	119.0
N1 <sup>i</sup> —Cu1—C11 <sup>i</sup>	130.22 (5)	C5—C6—C7	116.19 (19)
N1—Cu1—C11 <sup>i</sup>	97.44 (5)	C5—C6—H6	121.9
N1 <sup>i</sup> —Cu1—C11	97.44 (5)	C7—C6—H6	121.9
N1—Cu1—C11	130.22 (5)	C6—C7—N2	131.90 (19)
C11 <sup>i</sup> —Cu1—C11	103.48 (4)	C6—C7—C2	122.36 (19)
C1—N1—C2	105.40 (17)	N2—C7—C2	105.69 (17)
C1—N1—Cu1	122.71 (14)	C9—C8—C13	120.48 (19)
C2—N1—Cu1	131.47 (14)	C9—C8—N2	119.42 (18)
C1—N2—C7	106.89 (17)	C13—C8—N2	120.10 (18)
C1—N2—C8	125.39 (17)	C10—C9—C8	119.3 (2)
C7—N2—C8	127.71 (17)	C10—C9—H9	120.3
N1—C1—N2	113.16 (18)	C8—C9—H9	120.3
N1—C1—H1	123.4	C9—C10—C11	121.6 (2)
N2—C1—H1	123.4	C9—C10—H10	119.2
C3—C2—C7	120.72 (18)	C11—C10—H10	119.2
C3—C2—N1	130.42 (19)	C10—C11—C12	117.91 (19)
C7—C2—N1	108.85 (18)	C10—C11—C11 <sup>ii</sup>	119.99 (13)

C4—C3—C2	117.44 (19)	C12—C11—C11 <sup>ii</sup>	122.10 (13)
C4—C3—H3	121.3	C13—C12—C11	120.95 (19)
C2—C3—H3	121.3	C13—C12—H12	119.5
C3—C4—C5	121.28 (19)	C11—C12—H12	119.5
C3—C4—H4	119.4	C12—C13—C8	119.64 (19)
C5—C4—H4	119.4	C12—C13—H13	120.2
C6—C5—C4	121.99 (19)	C8—C13—H13	120.2
C6—C5—H5	119.0		
N1 <sup>i</sup> —Cu1—N1—C1	151.17 (19)	C8—N2—C7—C6	3.6 (3)
Cl1 <sup>i</sup> —Cu1—N1—C1	17.06 (16)	C1—N2—C7—C2	-0.2 (2)
Cl1—Cu1—N1—C1	-97.67 (16)	C8—N2—C7—C2	-178.85 (18)
N1 <sup>i</sup> —Cu1—N1—C2	-37.46 (15)	C3—C2—C7—C6	-1.3 (3)
Cl1 <sup>i</sup> —Cu1—N1—C2	-171.56 (17)	N1—C2—C7—C6	178.54 (18)
Cl1—Cu1—N1—C2	73.71 (19)	C3—C2—C7—N2	-179.11 (18)
C2—N1—C1—N2	0.9 (2)	N1—C2—C7—N2	0.7 (2)
Cu1—N1—C1—N2	174.20 (13)	C1—N2—C8—C9	-134.1 (2)
C7—N2—C1—N1	-0.4 (2)	C7—N2—C8—C9	44.3 (3)
C8—N2—C1—N1	178.25 (18)	C1—N2—C8—C13	45.5 (3)
C1—N1—C2—C3	178.8 (2)	C7—N2—C8—C13	-136.1 (2)
Cu1—N1—C2—C3	6.4 (3)	C13—C8—C9—C10	1.5 (3)
C1—N1—C2—C7	-1.0 (2)	N2—C8—C9—C10	-178.90 (19)
Cu1—N1—C2—C7	-173.47 (14)	C8—C9—C10—C11	-0.7 (3)
C7—C2—C3—C4	1.4 (3)	C9—C10—C11—C12	-1.2 (3)
N1—C2—C3—C4	-178.4 (2)	C9—C10—C11—C11 <sup>ii</sup>	178.2 (2)
C2—C3—C4—C5	-0.4 (3)	C10—C11—C12—C13	2.4 (3)
C3—C4—C5—C6	-0.8 (3)	C11 <sup>ii</sup> —C11—C12—C13	-176.9 (2)
C4—C5—C6—C7	0.9 (3)	C11—C12—C13—C8	-1.8 (3)
C5—C6—C7—N2	177.3 (2)	C9—C8—C13—C12	-0.2 (3)
C5—C6—C7—C2	0.2 (3)	N2—C8—C13—C12	-179.86 (18)
C1—N2—C7—C6	-177.7 (2)		

Symmetry codes: (i)  $-x+2, y, -z+3/2$ ; (ii)  $-x+1, y, -z+5/2$ .

Fig. 1

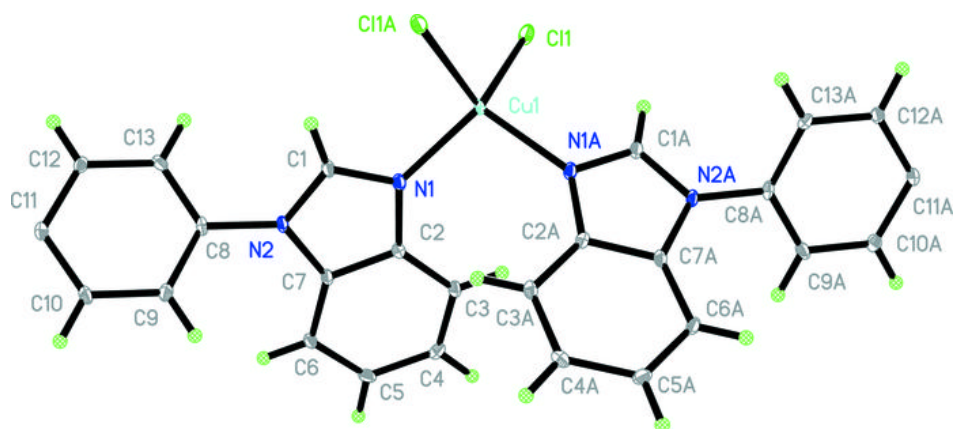




Fig. 2

