Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[dichloridocopper(II)]-μ-4,4′-bis(benzimidazol-1-yl)biphenyl]

Dan-Ni Xiao,[a] Hong-Yan Pan,[b] Min Yao[a] and Gang Xie[a]*

[a]Key Laboratory of Synthetic and Natural Functional Molecule Chemistry (Ministry of Education), College of Chemistry & Materials Science, Northwest University, Xi'an 710069, People's Republic of China, and [b]The College of Life Sciences, Northwest University, Xi'an 710069, People's Republic of China
Correspondence e-mail: nwuchem@126.com

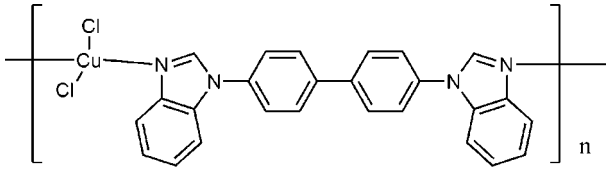
Received 14 March 2011; accepted 28 March 2011

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.026; wR factor = 0.066; data-to-parameter ratio = 12.6.

In the title compound, $[CuCl_2(C_{26}H_{18}N_4)]_n$, the Cu(II) ion is four-coordinated by two N atoms from two 4,4′-bis(benzoimidazol-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

$[CuCl_2(C_{26}H_{18}N_4)]$
M_r = 520.88
Monoclinic, $C2/c$
a = 12.599 (4) Å
b = 15.280 (4) Å
c = 11.233 (3) Å
β = 91.936 (4)°
V = 2161.3 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.28 mm^{-1}
T = 293 K
0.04 × 0.03 × 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_{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^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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*.

We gratefully acknowledge financial support from the Key Laboratory Foundation of the Education Committee of Shaanxi Province (grant No. 09JS089).

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.* A**64**, 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.

supporting information

Acta Cryst. (2011). E**67**, m521 [doi:10.1107/S1600536811011421]

catena-Poly[[dichloridocopper(II)]-μ-4,4′-bis(benzimidazol-1-yl)biphenyl]

Dan-Ni Xiao, Hong-Yan Pan, Min Yao and Gang Xie

S1. 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 benzoiimidazole 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.

S2. Experimental

A mixture of CH_3OH and $CHCl_3$ (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 $CHCl_3$ (6 ml). Then a solution of $CuCl_2$ (0.06 mmol) in CH_3OH (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**).

S3. Refinement

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

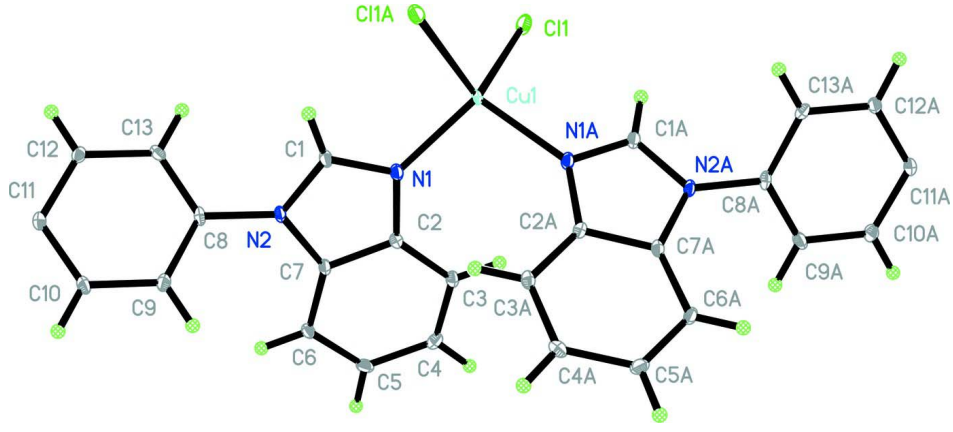


Figure 1

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.

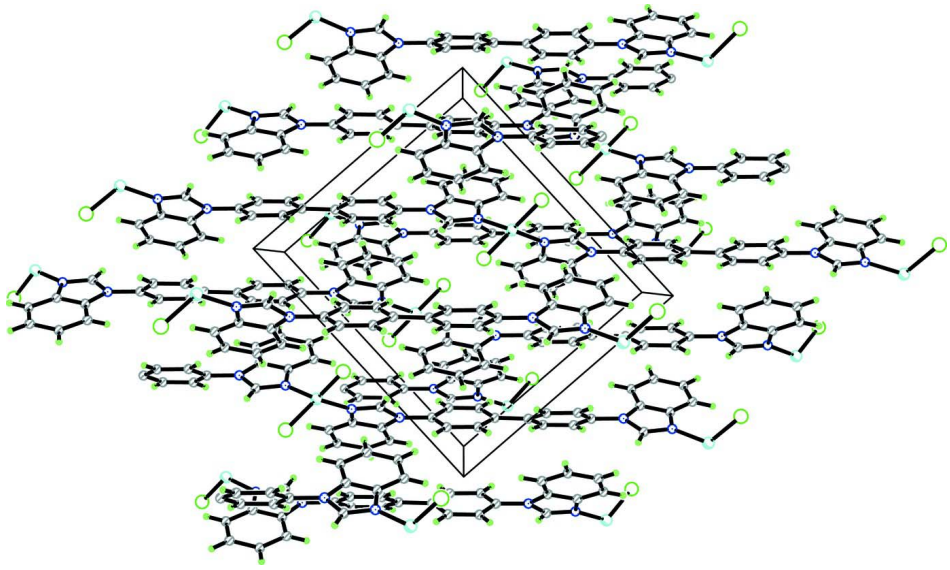


Figure 2

The crystal packing for (I).

catena-Poly[[dichloridocopper(II)]-μ-4,4′- bis(benzimidazol-1-yl)biphenyl]

Crystal data

$[CuCl_2(C_{26}H_{18}N_4)]$
$M_r = 520.88$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 12.599$ (4) Å
$b = 15.280$ (4) Å
$c = 11.233$ (3) Å
$\beta = 91.936$ (4)°
$V = 2161.3$ (10) Å^3
$Z = 4$
$F(000) = 1060$
$D_x = 1.601$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2903 reflections
$\theta = 2.1$–$27.9°$
$\mu = 1.28$ mm^{-1}
$T = 293$ K
Block, brown
0.04 × 0.03 × 0.02 mm

Data collection

Rigaku Mercury CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 9 pixels mm^{-1}
ω scans
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 $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 25.0°$, $\theta_{min} = 3.2°$
$h = -14 \rightarrow 14$
$k = -18 \rightarrow 18$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.066$
$S = 1.06$
1903 reflections
151 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
$w = 1/[\sigma^2(F_o^2) + (0.0296P)^2 + 3.937P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.50$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{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 (Å^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)
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 (Å, º)

Cu1—N1^{i}	1.9851 (17)	C5—C6	1.383 (3)
Cu1—N1	1.9851 (17)	C5—H5	0.9300
Cu1—Cl1^{i}	2.2378 (7)	C6—C7	1.392 (3)
Cu1—Cl1	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^{ii}	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^{i}—Cu1—N1	102.49 (10)	C4—C5—H5	119.0
N1^{i}—Cu1—Cl1^{i}	130.22 (5)	C5—C6—C7	116.19 (19)
N1—Cu1—Cl1^{i}	97.44 (5)	C5—C6—H6	121.9
N1^{i}—Cu1—Cl1	97.44 (5)	C7—C6—H6	121.9
N1—Cu1—Cl1	130.22 (5)	C6—C7—N2	131.90 (19)
Cl1^{i}—Cu1—Cl1	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^{ii}	119.99 (13)
C4—C3—C2	117.44 (19)	C12—C11—C11^{ii}	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^{i}—Cu1—N1—C1	151.17 (19)	C8—N2—C7—C6	3.6 (3)
Cl1^{i}—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^{i}—Cu1—N1—C2	−37.46 (15)	C3—C2—C7—C6	−1.3 (3)
Cl1^{i}—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^{ii}	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^{ii}—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.