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catena-Poly[[dichloridoiron(II)]-μ-4,4″-bis(benzimidazol-1-yl)-1,1′:4′,1″-terphenyl]

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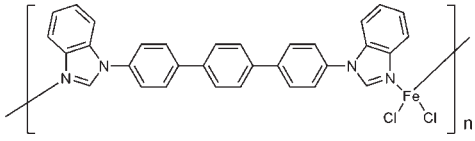
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.049; wR factor = 0.117; data-to-parameter ratio = 12.5.

In the title coordination polymer, $[FeCl_2(C_{32}H_{22}N_4)]_n$, the Fe^{II} atom lies on a crystallographic twofold axis and a distorted $FeCl_2N_2$ tetrahedral coordination geometry arises. The complete ligand is generated by crystallographic twofold symmetry, resulting in an infinite one-dimensional architecture along [101].

Related literature

For background to benzimidazoles as ligands, see: Vijayan *et al.* (2006).



Experimental

Crystal data

$[FeCl_2(C_{32}H_{22}N_4)]$ M_r = 589.29
Monoclinic, $C2/c$
a = 14.519 (3) Å
b = 14.303 (3) Å
c = 12.461 (3) Å
β = 101.94 (3)°
V = 2531.6 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.84 mm^{-1}
T = 293 K
0.20 × 0.18 × 0.15 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.846, T_{max} = 0.882
9515 measured reflections
2218 independent reflections
1960 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.117
S = 1.12
2218 reflections
177 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Table 1
Selected bond lengths (Å).

Fe1—N1	2.076 (2)	Fe1—Cl1	2.2489 (10)

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: HB5310).

References

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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
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supplementary materials

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catena-Poly[[dichloridoiron(II)]-μ-4,4''-bis(benzimidazol-1-yl)-1,1':4',1''-terphenyl]

H. Li, Z. Wei, Q. Gong and Q. Han

Comment

Benzimidazole has been well used in crystal engineering, and a large number of benzimidazole-containing flexible ligands have been extensively studied. However, to our knowledge, the research on benzoimidazole ligands bearing rigid spacers is still less developed.

Single-crystal X-ray diffraction analysis reveals that the title compound crystallizes in the monoclinic space group *C*2/*c*. The geometry of the Fe^{II} ion is surrounded by two benzimidazole 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 Fe^{II} center is bridged by the linear ligand **L** to form an infinite one-dimensional architecture along crystallographic [101] axis.

Experimental

A mixture of $(CH_3)_2CHOH$ and $CHCl_3$ (1:1, 8 ml), as a buffer layer, was carefully layered over a solution of 4,4'-Bis(benzimidazol-1-yl)terphenyl (**L**, 0.06 mmol) in $CHCl_3$ (6 ml). Then a solution of $FeCl_2$ (0.02 mmol) in $(CH_3)_2CHOH$ (6 ml) was layered over the buffer layer, and the resultant reaction was left to stand at room temperature. After *ca* three weeks, yellow blocks of (I) appeared at the boundary. Yield: ~10% (based on **L**).

Refinement

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

The N-bound H atoms were located in a difference map and their positions were freely refined with $U_{iso}(H) = 1.2U_{eq}(N)$.

Figures

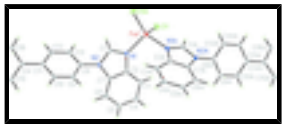


Fig. 1. A fragment of a polymeric chain in (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radius.

catena-Poly[[dichloridoiron(II)]-μ- 4,4''-bis(benzimidazol-1-yl)-1,1':4',1''-terphenyl]

Crystal data

$[FeCl_2(C_{32}H_{22}N_4)]$ $F(000) = 1208$

M_r = 589.29	D_x = 1.546 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 2574 reflections
a = 14.519 (3) Å	θ = 2.0–27.9°
b = 14.303 (3) Å	μ = 0.84 mm^{-1}
c = 12.461 (3) Å	*T* = 293 K
β = 101.94 (3)°	Block, yellow
V = 2531.6 (9) Å^3	0.20 × 0.18 × 0.15 mm
Z = 4	

Data collection

Rigaku Saturn CCD area-detector diffractometer	2218 independent reflections
Radiation source: fine-focus sealed tube	1960 reflections with $I > 2\sigma(I)$
graphite	R_{int} = 0.052
Detector resolution: 9 pixels mm^{-1}	θ_{max} = 25.0°, θ_{min} = 2.0°
ω scans	*h* = −17→16
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)	*k* = −16→15
T_{min} = 0.846, T_{max} = 0.882	*l* = −14→14
9515 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.049	Hydrogen site location: inferred from neighbouring sites
$wR(F^2)$ = 0.117	H-atom parameters constrained
S = 1.12	$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2 + 2.1075P]$ where $P = (F_o^2 + 2F_c^2)/3$
2218 reflections	$(\Delta/\sigma)_{max}$ = 0.001
177 parameters	$\Delta\rho_{max}$ = 0.35 e Å^{-3}
0 restraints	$\Delta\rho_{min}$ = −0.41 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}
Fe1	0.0000	1.12084 (4)	0.7500	0.0240 (2)
Cl1	0.02255 (6)	1.20219 (6)	0.90773 (8)	0.0423 (3)
N2	0.20786 (16)	0.96985 (16)	0.63670 (19)	0.0186 (6)
N1	0.10013 (17)	1.02547 (17)	0.72169 (19)	0.0207 (6)
C15	0.4708 (2)	0.8783 (2)	0.2868 (2)	0.0176 (6)
H15	0.4516	0.8216	0.3115	0.021*
C11	0.3788 (2)	0.9625 (2)	0.4047 (2)	0.0181 (6)
C14	0.4398 (2)	0.9609 (2)	0.3250 (2)	0.0185 (6)
C8	0.2661 (2)	0.9662 (2)	0.5587 (2)	0.0187 (6)
C13	0.3223 (2)	1.0412 (2)	0.5485 (2)	0.0183 (6)
H13	0.3231	1.0931	0.5937	0.022*
C3	0.1067 (2)	0.8921 (2)	0.8545 (2)	0.0213 (7)
H3	0.0598	0.9141	0.8887	0.026*
C10	0.3213 (2)	0.8878 (2)	0.4174 (3)	0.0228 (7)
H10	0.3212	0.8351	0.3736	0.027*
C1	0.1466 (2)	1.0385 (2)	0.6442 (2)	0.0203 (7)
H1	0.1381	1.0905	0.5984	0.024*
C9	0.2649 (2)	0.8892 (2)	0.4924 (3)	0.0233 (7)
H9	0.2261	0.8387	0.4986	0.028*
C16	0.4710 (2)	1.0437 (2)	0.2859 (2)	0.0199 (6)
H16	0.4514	1.1005	0.3098	0.024*
C7	0.2006 (2)	0.9061 (2)	0.7177 (2)	0.0171 (6)
C12	0.3767 (2)	1.0395 (2)	0.4721 (2)	0.0184 (6)
H12	0.4137	1.0913	0.4647	0.022*
C2	0.1330 (2)	0.9411 (2)	0.7698 (2)	0.0177 (6)
C5	0.2242 (2)	0.7782 (2)	0.8350 (2)	0.0245 (7)
H5	0.2559	0.7235	0.8605	0.029*
C6	0.2490 (2)	0.8247 (2)	0.7494 (2)	0.0212 (7)
H6	0.2957	0.8027	0.7149	0.025*
C4	0.1526 (2)	0.8102 (2)	0.8854 (2)	0.0235 (7)
H4	0.1360	0.7750	0.9412	0.028*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0229 (4)	0.0202 (4)	0.0323 (4)	0.000	0.0134 (3)	0.000
Cl1	0.0413 (6)	0.0368 (5)	0.0522 (6)	−0.0083 (4)	0.0174 (5)	−0.0199 (4)
N2	0.0184 (13)	0.0194 (13)	0.0205 (13)	0.0010 (10)	0.0099 (10)	0.0014 (10)
N1	0.0213 (14)	0.0203 (14)	0.0226 (13)	0.0014 (11)	0.0097 (11)	0.0035 (11)
C15	0.0176 (16)	0.0168 (15)	0.0187 (14)	−0.0018 (12)	0.0041 (12)	0.0017 (12)
C11	0.0186 (16)	0.0178 (15)	0.0182 (14)	0.0007 (12)	0.0043 (12)	0.0020 (12)
C14	0.0170 (15)	0.0204 (16)	0.0185 (14)	−0.0008 (12)	0.0047 (12)	0.0003 (12)
C8	0.0172 (15)	0.0216 (16)	0.0192 (14)	0.0036 (12)	0.0082 (12)	0.0026 (12)
C13	0.0190 (16)	0.0155 (15)	0.0203 (15)	0.0014 (12)	0.0041 (12)	−0.0030 (12)

C3	0.0202 (16)	0.0266 (17)	0.0182 (15)	−0.0030 (13)	0.0066 (12)	−0.0023 (13)
C10	0.0272 (18)	0.0191 (17)	0.0253 (16)	−0.0050 (13)	0.0125 (14)	−0.0069 (13)
C1	0.0193 (16)	0.0190 (16)	0.0242 (15)	0.0009 (13)	0.0081 (13)	0.0044 (13)
C9	0.0243 (17)	0.0193 (16)	0.0281 (17)	−0.0046 (13)	0.0097 (14)	−0.0021 (13)
C16	0.0224 (16)	0.0167 (15)	0.0218 (15)	−0.0004 (12)	0.0074 (12)	−0.0023 (12)
C7	0.0199 (16)	0.0134 (14)	0.0189 (14)	−0.0024 (12)	0.0057 (12)	0.0013 (12)
C12	0.0183 (16)	0.0171 (15)	0.0200 (14)	−0.0018 (12)	0.0044 (12)	0.0004 (12)
C2	0.0159 (15)	0.0170 (15)	0.0211 (15)	0.0003 (12)	0.0058 (12)	−0.0011 (12)
C5	0.0288 (18)	0.0147 (16)	0.0284 (17)	0.0007 (13)	0.0018 (14)	0.0025 (13)
C6	0.0203 (16)	0.0185 (16)	0.0257 (16)	0.0001 (13)	0.0066 (13)	−0.0037 (13)
C4	0.0315 (18)	0.0207 (16)	0.0181 (15)	−0.0060 (13)	0.0048 (13)	0.0024 (13)

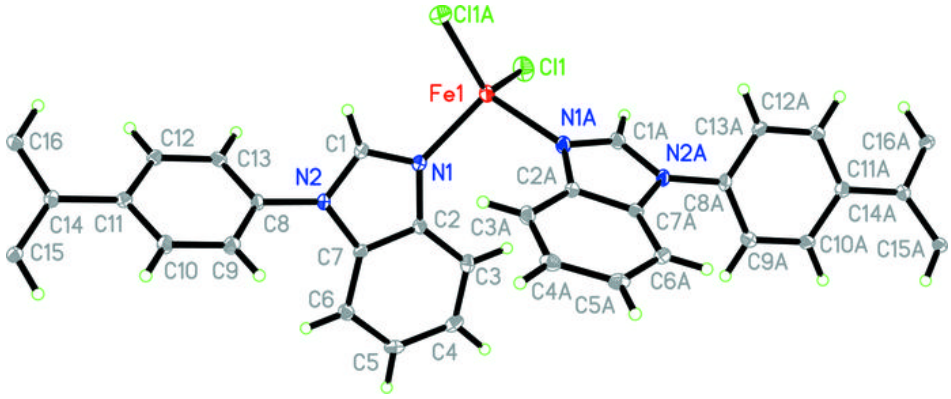
Geometric parameters (Å, °)

Fe1—N1^{i}	2.076 (2)	C13—H13	0.9300
Fe1—N1	2.076 (2)	C3—C4	1.362 (4)
Fe1—Cl1^{i}	2.2489 (10)	C3—C2	1.384 (4)
Fe1—Cl1	2.2489 (10)	C3—H3	0.9300
N2—C1	1.342 (4)	C10—C9	1.364 (4)
N2—C7	1.381 (4)	C10—H10	0.9300
N2—C8	1.415 (4)	C1—H1	0.9300
N1—C1	1.300 (4)	C9—H9	0.9300
N1—C2	1.388 (4)	C16—C16^{ii}	1.349 (6)
C15—C15^{ii}	1.373 (6)	C16—H16	0.9300
C15—C14	1.383 (4)	C7—C6	1.375 (4)
C15—H15	0.9300	C7—C2	1.379 (4)
C11—C10	1.386 (4)	C12—H12	0.9300
C11—C12	1.389 (4)	C5—C6	1.367 (4)
C11—C14	1.461 (4)	C5—C4	1.398 (4)
C14—C16	1.392 (4)	C5—H5	0.9300
C8—C13	1.368 (4)	C6—H6	0.9300
C8—C9	1.375 (4)	C4—H4	0.9300
C13—C12	1.358 (4)		
N1^{i}—Fe1—N1	97.86 (13)	C9—C10—C11	121.9 (3)
N1^{i}—Fe1—Cl1^{i}	120.53 (7)	C9—C10—H10	119.1
N1—Fe1—Cl1^{i}	99.90 (7)	C11—C10—H10	119.1
N1^{i}—Fe1—Cl1	99.90 (7)	N1—C1—N2	113.6 (3)
N1—Fe1—Cl1	120.53 (7)	N1—C1—H1	123.2
Cl1^{i}—Fe1—Cl1	117.69 (6)	N2—C1—H1	123.2
C1—N2—C7	106.3 (2)	C10—C9—C8	119.3 (3)
C1—N2—C8	125.0 (2)	C10—C9—H9	120.4
C7—N2—C8	128.6 (2)	C8—C9—H9	120.4
C1—N1—C2	105.1 (2)	C16^{ii}—C16—C14	121.72 (17)
C1—N1—Fe1	121.4 (2)	C16^{ii}—C16—H16	119.1
C2—N1—Fe1	133.50 (19)	C14—C16—H16	119.1
C15^{ii}—C15—C14	121.33 (17)	C6—C7—C2	122.9 (3)

C15^{ii}—C15—H15	119.3	C6—C7—N2	131.2 (3)
C14—C15—H15	119.3	C2—C7—N2	105.9 (2)
C10—C11—C12	117.0 (3)	C13—C12—C11	121.8 (3)
C10—C11—C14	122.0 (3)	C13—C12—H12	119.1
C12—C11—C14	121.0 (3)	C11—C12—H12	119.1
C15—C14—C16	117.0 (3)	C7—C2—C3	120.7 (3)
C15—C14—C11	122.2 (3)	C7—C2—N1	109.1 (2)
C16—C14—C11	120.8 (3)	C3—C2—N1	130.2 (3)
C13—C8—C9	120.3 (3)	C6—C5—C4	122.1 (3)
C13—C8—N2	119.2 (3)	C6—C5—H5	118.9
C9—C8—N2	120.5 (3)	C4—C5—H5	118.9
C12—C13—C8	119.7 (3)	C5—C6—C7	115.8 (3)
C12—C13—H13	120.1	C5—C6—H6	122.1
C8—C13—H13	120.1	C7—C6—H6	122.1
C4—C3—C2	117.1 (3)	C3—C4—C5	121.3 (3)
C4—C3—H3	121.5	C3—C4—H4	119.3
C2—C3—H3	121.5	C5—C4—H4	119.3
N1^{i}—Fe1—N1—C1	139.0 (3)	N2—C8—C9—C10	179.6 (3)
Cl1^{i}—Fe1—N1—C1	16.0 (2)	C15—C14—C16—C16^{ii}	−0.1 (5)
Cl1—Fe1—N1—C1	−114.6 (2)	C11—C14—C16—C16^{ii}	178.6 (3)
N1^{i}—Fe1—N1—C2	−40.2 (2)	C1—N2—C7—C6	−177.4 (3)
Cl1^{i}—Fe1—N1—C2	−163.2 (3)	C8—N2—C7—C6	3.3 (5)
Cl1—Fe1—N1—C2	66.2 (3)	C1—N2—C7—C2	0.4 (3)
C15^{ii}—C15—C14—C16	−0.3 (5)	C8—N2—C7—C2	−178.9 (3)
C15^{ii}—C15—C14—C11	−179.0 (3)	C8—C13—C12—C11	−1.3 (4)
C10—C11—C14—C15	−23.9 (4)	C10—C11—C12—C13	1.1 (4)
C12—C11—C14—C15	155.5 (3)	C14—C11—C12—C13	−178.3 (3)
C10—C11—C14—C16	157.5 (3)	C6—C7—C2—C3	−3.6 (5)
C12—C11—C14—C16	−23.2 (4)	N2—C7—C2—C3	178.3 (3)
C1—N2—C8—C13	53.0 (4)	C6—C7—C2—N1	177.6 (3)
C7—N2—C8—C13	−127.8 (3)	N2—C7—C2—N1	−0.5 (3)
C1—N2—C8—C9	−125.7 (3)	C4—C3—C2—C7	2.0 (4)
C7—N2—C8—C9	53.5 (4)	C4—C3—C2—N1	−179.4 (3)
C9—C8—C13—C12	0.3 (4)	C1—N1—C2—C7	0.4 (3)
N2—C8—C13—C12	−178.4 (3)	Fe1—N1—C2—C7	179.6 (2)
C12—C11—C10—C9	0.1 (5)	C1—N1—C2—C3	−178.3 (3)
C14—C11—C10—C9	179.5 (3)	Fe1—N1—C2—C3	1.0 (5)
C2—N1—C1—N2	−0.1 (3)	C4—C5—C6—C7	1.4 (4)
Fe1—N1—C1—N2	−179.48 (19)	C2—C7—C6—C5	1.8 (4)
C7—N2—C1—N1	−0.2 (3)	N2—C7—C6—C5	179.3 (3)
C8—N2—C1—N1	179.1 (3)	C2—C3—C4—C5	1.1 (4)
C11—C10—C9—C8	−1.2 (5)	C6—C5—C4—C3	−2.9 (5)
C13—C8—C9—C10	0.9 (5)		

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

Fig. 1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Fe1
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C13A
C16A
C11A
C14A
C15A
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C13
C1
N2
N1
C14
C11
C8
C2
C15
C10
C9
C7
C3
C6
C4
C5