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catena-Poly[[dichloridonickel(II)]-μ-1,2-di-4-pyridylethane-κ^2N:N']

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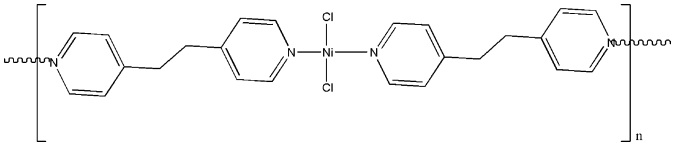
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.050; wR factor = 0.144; data-to-parameter ratio = 14.9.

The title compound, $[NiCl_2(C_{12}H_{12}N_2)]_n$, is a nickel complex polymer bridged by 1,2-bis(4-pyridyl)ethane ligands. The Ni^{II} center is coordinated in a distorted tetrahedral geometry by two Cl ligands and two N atoms from two 1,2-bis(4-pyridyl)-ethane ligands, forming a one-dimensional zigzag chain.

Related literature

For related literature, see: Brammer (2004); Carlucci *et al.* (2003); Ghosh *et al.* (2004); Hong *et al.* (2005); Luo *et al.* (2003); Moulton & Zaworotko (2001); Woodward *et al.* (2005).



Experimental

Crystal data

$[NiCl_2(C_{12}H_{12}N_2)]$
M_r = 313.85
Triclinic, $P\overline{1}$
a = 5.3979 (17) Å
b = 8.806 (3) Å
c = 14.018 (4) Å
α = 87.988 (5)°
β = 84.165 (5)°
γ = 84.475 (5)°
V = 659.6 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.85 mm^{-1}
T = 298 (2) K
0.38 × 0.30 × 0.30 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.511, T_{max} = 0.574
3306 measured reflections
2297 independent reflections
1942 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.144
S = 1.04
2297 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.98 e Å^{-3}
$\Delta\rho_{min}$ = −1.04 e Å^{-3}

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); 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: IS2165).

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supplementary materials

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catena-Poly[[dichloridonickel(II)]-μ-1,2-di-4-pyridylethane-κ^2N:N']

L. Zhang and J. Yu

Comment

Recently, there are of great interest in the design and synthesis of coordination complexes, such one-dimensional chains and ladders, two-dimensional grids, three-dimensional networks, interpenetrated modes and helical staircase networks, which are used as functional materials potentially applied in magnetism, molecular adsorption, optoelectronic devices, sensors, luminescent materials and catalysis (Moulton & Zaworotko, 2001; Carlucci *et al.*, 2003; Brammer, 2004). The flexible bridging ligand 1,2-bis(4-pyridyl)ethane (bpe) is useful in the formation of various frameworks (Luo *et al.*, 2003; Ghosh *et al.*, 2004; Hong *et al.*, 2005). We report here the crystal structure of the title Ni complex polymer, $[NiCl_2(bpe)]_n$, (I).

The Ni^{II} center has a distorted tetrahedral geometry, which is coordinated by two N atoms from two bpe ligands and two Cl ligands, forming a one-dimensional helical chain (Fig. 1 and 2). The dihedral angle between two pyridine rings, C1—C5/N1 and C7—C11/N2, is 61.93 (3)°. One bpe is almost planar as shown by the C8—C9—C12—$C12^{ii}$ torsion angle of −6.1 (9)°, while the other is not planar but parallel, the C2—C3—C6—$C6^{i}$ angle and the interplanar distance between the pyridine rings being 105.4 (6)° and 1.452 (2) Å, respectively [symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x, -y+2, -z+2$]. The angles of C3—C6—$C6^{i}$ and C9—C12—$C12^{ii}$ are also different, they are 111.6 (4) and 115.2 (5)°. The Ni···Ni^{i} and Ni···Ni^{ii} distances are 13.441 (3) and 13.279 (3) Å, respectively.

Experimental

The title complex was prepared by the addition of a stoichiometric amount of $NiSO_4$ (0.18 g, 20 mmol), NaOH (0.12 g, 30 mmol) and HCl (1 mol/*L*, 0.1 ml) to a hot aqueous solution of bpe (0.031 g, 12 mmol). The resulting solution was filtered, and green single crystals were obtained at room temperature over several days.

Refinement

H atoms were placed in calculated positions (C—H = 0.93–0.97 Å) refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$. The deepest hole in the difference Fourier map is located 0.95 Å from atom Ni1.

Figures

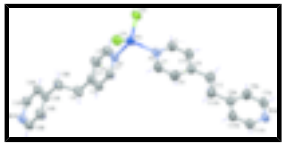

Fig. 1. Part of the polymeric structure of (I), showing the atomic numbering scheme. Non-H atoms are shown as 50% probability displacement ellipsoids. The suffixes A and B correspond to symmetry codes ($-x, -y+2, -z+2$) and ($-x+1, -y, -z+1$), respectively.

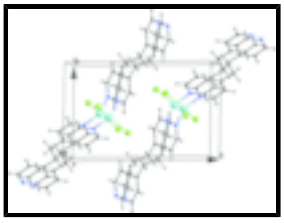

Fig. 2. A packing diagram of (I), viewed along the *a* axis.

catena-Poly[[dichloridonickel(II)]-μ-1,2-di-4-pyridylethane- $\kappa^2N:N'$]

Crystal data

$[NiCl_2(C_{12}H_{12}N_2)]$	$Z = 2$
$M_r = 313.85$	$F_{000} = 320$
Triclinic, $P\overline{1}$	$D_x = 1.580$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 5.3979$ (17) Å	Cell parameters from 1592 reflections
$b = 8.806$ (3) Å	$\theta = 2.7$–25.5º
$c = 14.018$ (4) Å	$\mu = 1.85$ mm^{-1}
$\alpha = 87.988$ (5)º	$T = 298$ (2) K
$\beta = 84.165$ (5)º	Block, green
$\gamma = 84.475$ (5)º	0.38 × 0.30 × 0.30 mm
$V = 659.6$ (4) Å^3	

Data collection

Bruker APEXII area-detector diffractometer	2297 independent reflections
Radiation source: fine-focus sealed tube	1942 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.022$
Detector resolution: none pixels mm^{-1}	$\theta_{max} = 25.1$º
$T = 298(2)$ K	$\theta_{min} = 1.5$º
φ and ω scan	$h = -4 \rightarrow 6$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$k = -9 \rightarrow 10$
$T_{min} = 0.511$, $T_{max} = 0.574$	$l = -16 \rightarrow 16$
3306 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.050$	H-atom parameters constrained
$wR(F^2) = 0.144$	$w = 1/[\sigma^2(F_o^2) + (0.1008P)^2 + 0.3P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$

2297 reflections	$\Delta\rho_{max} = 0.98$ e Å^{-3}
154 parameters	$\Delta\rho_{min} = -1.04$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
Ni1	0.88487 (9)	0.54655 (5)	0.74751 (3)	0.0401 (2)
Cl1	1.0080 (2)	0.70646 (11)	0.62712 (7)	0.0507 (3)
Cl2	1.1490 (2)	0.42178 (12)	0.84309 (7)	0.0505 (3)
N1	0.7275 (6)	0.3808 (3)	0.6836 (2)	0.0379 (7)
N2	0.6308 (6)	0.6763 (4)	0.8355 (2)	0.0397 (7)
C1	0.5435 (8)	0.4129 (4)	0.6284 (3)	0.0431 (9)
H1	0.4844	0.5148	0.6205	0.052*
C2	0.4336 (8)	0.3063 (5)	0.5819 (3)	0.0460 (10)
H2	0.3057	0.3359	0.5435	0.055*
C3	0.5183 (8)	0.1532 (5)	0.5935 (3)	0.0442 (9)
C4	0.7074 (9)	0.1187 (5)	0.6504 (3)	0.0541 (11)
H4	0.7696	0.0175	0.6592	0.065*
C5	0.8075 (9)	0.2329 (5)	0.6952 (3)	0.0491 (10)
H5	0.9343	0.2062	0.7346	0.059*
C6	0.4100 (9)	0.0308 (5)	0.5416 (3)	0.0517 (11)
H6A	0.2548	0.0729	0.5177	0.062*
H6B	0.3724	−0.0523	0.5864	0.062*
C7	0.4599 (9)	0.7752 (5)	0.7981 (3)	0.0536 (11)
H7	0.4614	0.7852	0.7317	0.064*
C8	0.2811 (9)	0.8629 (6)	0.8555 (3)	0.0604 (13)
H8	0.1651	0.9306	0.8274	0.072*
C9	0.2740 (8)	0.8505 (5)	0.9545 (3)	0.0481 (10)
C10	0.4500 (9)	0.7474 (5)	0.9904 (3)	0.0551 (11)
H10	0.4521	0.7342	1.0565	0.066*
C11	0.6215 (9)	0.6641 (5)	0.9308 (3)	0.0497 (10)
H11	0.7379	0.5953	0.9578	0.060*
C12	0.0849 (9)	0.9404 (5)	1.0231 (3)	0.0575 (12)
H12A	−0.0171	0.8695	1.0596	0.069*

H12B	0.1743	0.9897	1.0681	0.069*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0508 (4)	0.0359 (3)	0.0341 (3)	−0.0033 (2)	−0.0084 (2)	−0.0001 (2)
Cl1	0.0616 (7)	0.0437 (6)	0.0459 (6)	−0.0056 (5)	−0.0051 (5)	0.0136 (4)
Cl2	0.0571 (7)	0.0537 (6)	0.0419 (6)	−0.0005 (5)	−0.0174 (4)	0.0064 (4)
N1	0.0468 (18)	0.0331 (17)	0.0346 (16)	−0.0041 (13)	−0.0069 (13)	−0.0018 (13)
N2	0.0473 (18)	0.0357 (17)	0.0371 (17)	−0.0009 (14)	−0.0109 (14)	−0.0021 (13)
C1	0.053 (2)	0.033 (2)	0.043 (2)	−0.0005 (17)	−0.0095 (18)	0.0001 (17)
C2	0.052 (2)	0.046 (2)	0.042 (2)	−0.0053 (18)	−0.0135 (18)	−0.0006 (18)
C3	0.054 (2)	0.043 (2)	0.037 (2)	−0.0115 (18)	−0.0039 (17)	−0.0038 (17)
C4	0.073 (3)	0.032 (2)	0.060 (3)	−0.004 (2)	−0.018 (2)	−0.001 (2)
C5	0.061 (3)	0.037 (2)	0.053 (2)	−0.0020 (18)	−0.022 (2)	−0.0007 (18)
C6	0.064 (3)	0.048 (2)	0.046 (2)	−0.018 (2)	−0.007 (2)	−0.0066 (19)
C7	0.067 (3)	0.057 (3)	0.034 (2)	0.012 (2)	−0.0090 (19)	0.0016 (19)
C8	0.064 (3)	0.064 (3)	0.048 (3)	0.022 (2)	−0.008 (2)	0.005 (2)
C9	0.056 (3)	0.045 (2)	0.041 (2)	0.0023 (19)	−0.0028 (18)	−0.0019 (18)
C10	0.068 (3)	0.060 (3)	0.035 (2)	0.011 (2)	−0.0083 (19)	−0.0005 (19)
C11	0.059 (3)	0.048 (2)	0.041 (2)	0.0075 (19)	−0.0082 (19)	−0.0005 (18)
C12	0.066 (3)	0.058 (3)	0.044 (2)	0.012 (2)	−0.001 (2)	0.001 (2)

Geometric parameters (Å, °)

Ni1—N1	2.034 (3)	C5—H5	0.9300
Ni1—N2	2.040 (3)	C6—C6^{i}	1.520 (9)
Ni1—Cl2	2.2402 (12)	C6—H6A	0.9700
Ni1—Cl1	2.2490 (12)	C6—H6B	0.9700
N1—C1	1.324 (5)	C7—C8	1.385 (6)
N1—C5	1.342 (5)	C7—H7	0.9300
N2—C11	1.333 (5)	C8—C9	1.386 (6)
N2—C7	1.340 (5)	C8—H8	0.9300
C1—C2	1.373 (6)	C9—C10	1.371 (6)
C1—H1	0.9300	C9—C12	1.514 (6)
C2—C3	1.391 (6)	C10—C11	1.359 (6)
C2—H2	0.9300	C10—H10	0.9300
C3—C4	1.363 (6)	C11—H11	0.9300
C3—C6	1.515 (5)	C12—C12^{ii}	1.500 (9)
C4—C5	1.384 (6)	C12—H12A	0.9700
C4—H4	0.9300	C12—H12B	0.9700
N1—Ni1—N2	112.52 (13)	C3—C6—C6^{i}	111.6 (4)
N1—Ni1—Cl2	105.23 (9)	C3—C6—H6A	109.3
N2—Ni1—Cl2	105.99 (10)	C6^{i}—C6—H6A	109.3
N1—Ni1—Cl1	105.07 (10)	C3—C6—H6B	109.3
N2—Ni1—Cl1	104.95 (10)	C6^{i}—C6—H6B	109.3
Cl2—Ni1—Cl1	123.23 (5)	H6A—C6—H6B	108.0
C1—N1—C5	116.7 (3)	N2—C7—C8	121.8 (4)

C1—N1—Ni1	122.1 (3)	N2—C7—H7	119.1
C5—N1—Ni1	121.2 (3)	C8—C7—H7	119.1
C11—N2—C7	117.4 (3)	C7—C8—C9	120.4 (4)
C11—N2—Ni1	122.4 (3)	C7—C8—H8	119.8
C7—N2—Ni1	120.1 (3)	C9—C8—H8	119.8
N1—C1—C2	124.7 (4)	C10—C9—C8	116.3 (4)
N1—C1—H1	117.7	C10—C9—C12	119.4 (4)
C2—C1—H1	117.7	C8—C9—C12	124.3 (4)
C1—C2—C3	118.4 (4)	C11—C10—C9	120.9 (4)
C1—C2—H2	120.8	C11—C10—H10	119.6
C3—C2—H2	120.8	C9—C10—H10	119.6
C4—C3—C2	117.4 (4)	N2—C11—C10	123.2 (4)
C4—C3—C6	121.6 (4)	N2—C11—H11	118.4
C2—C3—C6	120.9 (4)	C10—C11—H11	118.4
C3—C4—C5	120.6 (4)	C12^{ii}—C12—C9	115.2 (5)
C3—C4—H4	119.7	C12^{ii}—C12—H12A	108.5
C5—C4—H4	119.7	C9—C12—H12A	108.5
N1—C5—C4	122.1 (4)	C12^{ii}—C12—H12B	108.5
N1—C5—H5	119.0	C9—C12—H12B	108.5
C4—C5—H5	119.0	H12A—C12—H12B	107.5
N2—Ni1—N1—C1	58.7 (3)	C6—C3—C4—C5	178.4 (4)
Cl2—Ni1—N1—C1	173.7 (3)	C1—N1—C5—C4	1.3 (7)
Cl1—Ni1—N1—C1	−54.9 (3)	Ni1—N1—C5—C4	−178.3 (4)
N2—Ni1—N1—C5	−121.7 (3)	C3—C4—C5—N1	−1.2 (8)
Cl2—Ni1—N1—C5	−6.7 (4)	C4—C3—C6—C6^{i}	−72.3 (7)
Cl1—Ni1—N1—C5	124.7 (3)	C2—C3—C6—C6^{i}	105.4 (6)
N1—Ni1—N2—C11	106.5 (3)	C11—N2—C7—C8	0.6 (7)
Cl2—Ni1—N2—C11	−8.0 (4)	Ni1—N2—C7—C8	178.6 (4)
Cl1—Ni1—N2—C11	−139.8 (3)	N2—C7—C8—C9	−0.1 (8)
N1—Ni1—N2—C7	−71.4 (4)	C7—C8—C9—C10	−0.5 (8)
Cl2—Ni1—N2—C7	174.1 (3)	C7—C8—C9—C12	−179.5 (5)
Cl1—Ni1—N2—C7	42.3 (3)	C8—C9—C10—C11	0.5 (7)
C5—N1—C1—C2	−1.0 (7)	C12—C9—C10—C11	179.6 (5)
Ni1—N1—C1—C2	178.6 (3)	C7—N2—C11—C10	−0.6 (7)
N1—C1—C2—C3	0.6 (7)	Ni1—N2—C11—C10	−178.5 (4)
C1—C2—C3—C4	−0.4 (6)	C9—C10—C11—N2	0.0 (8)
C1—C2—C3—C6	−178.1 (4)	C10—C9—C12—C12^{ii}	174.9 (6)
C2—C3—C4—C5	0.7 (7)	C8—C9—C12—C12^{ii}	−6.1 (9)

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

Fig. 1

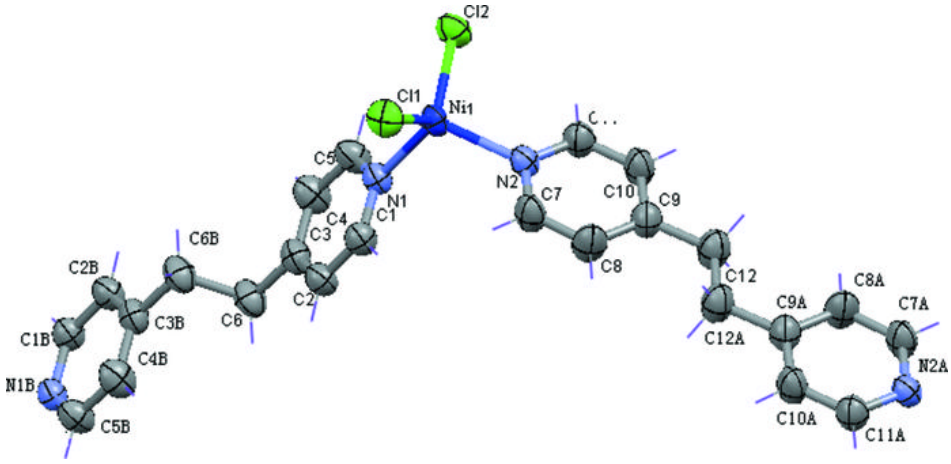
Cl2
Cl1
Ni1
C..
C5
N2
C7
C10
C9
N1
C1
C4
C3
C6B
C2B
C8
C12
C8A
C9A
C7A
C2
C3B
C6
C1B
C12A
N2A
C4B
N1B
C10A
C11A
C5B

Fig. 2