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catena-Poly[nickel(II)-bis(μ-3,7-dichloroquinoline-8-carboxylato-$\kappa^3N,O:O'$)]

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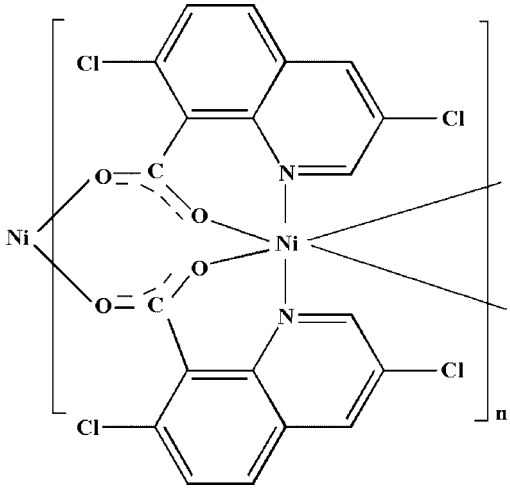
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.031; wR factor = 0.085; data-to-parameter ratio = 12.3.

In the crystal structure of the title compound, $[Ni(C_{10}H_4Cl_2NO_2)_2]_n$, the Ni^{II} atom, which lies on a symmetry plane, is *N*,*O*-chelated by the carboxylate anion, and adjacent formula units are linked by carboxylate bridges into a linear chain. The metal shows octahedral coordination.

Related literature

See Chen *et al.* (2001) and Yang *et al.* (2005) for related vanadium and cadmium complexes.

For related literature, see: Nuria *et al.* (1997); Pornprom *et al.* (2006); Sunohara & Matsumoto (2004); Tresch & Grossmann (2002).



Experimental

Crystal data

$[Ni(C_{10}H_4Cl_2NO_2)_2]$
M_r = 540.79
Orthorhombic, *Pccn*
a = 13.4603 (14) Å
b = 15.8837 (19) Å
c = 9.2040 (13) Å
V = 1967.8 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.56 mm^{-1}
T = 298 (2) K
0.62 × 0.21 × 0.18 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.68, T_{max} = 0.76
9136 measured reflections
1736 independent reflections
1407 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.085
S = 1.10
1736 reflections
141 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.71 e Å^{-3}
$\Delta\rho_{min}$ = −0.70 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O2^{i}	2.033 (2)	Ni1—N1	2.144 (2)
Ni1—O1	2.078 (2)		
O2^{i}—Ni1—O2^{iii}	103.47 (11)	O1^{iv}—Ni1—O1	84.91 (11)
O2^{i}—Ni1—O1^{iv}	85.86 (8)	O1—Ni1—N1	91.45 (9)
O2^{iii}—Ni1—O1^{iv}	170.43 (8)	N1^{iv}—Ni1—N1	176.44 (13)

Symmetry codes: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $-x+\frac{3}{2}, y, z-\frac{1}{2}$; (iv) $-x+\frac{3}{2}, -y+\frac{1}{2}, z$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: NG2259).

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supplementary materials

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catena-Poly[nickel(II)-bis(*μ*-3,7-dichloroquinoline-8-carboxylato-$\kappa^3N,O:O'$)]

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Comment

Quinolinecarboxylates generally chelate to metal atoms, and some metal quinolinecarboxylates have been reported such as, for example, bis(6-methyl-4-hydroxy-3-quinolinecarboxylate) mono(oxo)monohydroxyvanadium(V) and $Cd(H_2O)(4\text{-quinolinecarboxylato})_2$ (Chen *et al.*, 2001; Yang *et al.*, 2005). Quinclorac (3,7-dichloro-8-quinolinecarboxylic acid) is one of the most effective herbicides (Nuria *et al.*, 1997; Pornprom *et al.*, 2006; Sunohara & Matsumoto, 2004; Tresch & Grossmann, 2002). The title compound is a nickel derivative (I) (Fig. 1). The Ni^{II} center exhibits a distorted octahedral geometry defined by four carboxylato oxygen atoms from four quinclorac and two nitrogen atoms from two quinclorac units. The units chelate to the metal atom, and adjacent molecules are linked by carboxylate bridges into a linear chain. The chains are assembled into a three-dimensional supramolecular architecture by interchain π–π stacking interactions (perpendicular distance: 3.44 Å, centroid-centroid distance: 3.912 Å).

Experimental

A mixture of quinclorac (0.5 mmol, 0.121 g), $NiCl_2{\cdot}6H_2O$ (1 mmol, 0.238 g) and H_2O (10 ml) was treated with aqueous HCl to a pH of 5. The mixture was placed in a Teflon-lined autoclave; this was heated at 403 K for three days. Green crystals were collected and washed with water. CH&N elemental analysis. Calculated for $C_{20}H_8Cl_4N_2O_4Ni$: C 44.36, H 1.48, N 5.18%; found: C 44.58, H 1.59, N 5.30%. Selected FT—IR (KBr, cm^{-1}): 3433(w), 1581(*s*), 1563(*s*), 1482(*m*), 1402(*s*), 1347(*s*), 1316(*m*), 1139 (*m*), 1101(*s*), 927(*s*), 908(*s*), 898(*s*), 814(*m*), 761(*m*), 671(*m*).

Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for all H atoms.

Figures

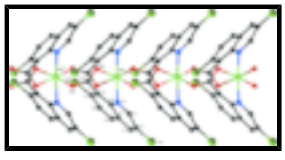

Fig. 1. The structure of (I), with the atomic numbering scheme and displacement ellipsoids at the 50% probability level. H atoms have been omitted for clarity [Symmetry codes: (i) *x*,-*y* + 1/2,*z* + 1/2.]

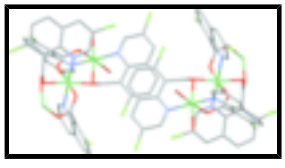

Fig. 2. Three dimensional supramolecular architecture constructed by interchain π–π stacking interactions.

catena-Poly[nickel(II)-bis(μ-3,7-dichloroquinoline-8-carboxylato- $\kappa^3N,O:O'$)]

Crystal data

$[Ni(C_{10}H_4Cl_2NO_2)_2]$	F_{000} = 1080
M_r = 540.79	D_x = 1.825 Mg m^{-3}
Orthorhombic, *Pccn*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ab 2ac	Cell parameters from 9136 reflections
a = 13.4603 (14) Å	θ = 2.0–25.0º
b = 15.8837 (19) Å	μ = 1.56 mm^{-1}
c = 9.2040 (13) Å	*T* = 298 (2) K
V = 1967.8 (4) Å^3	Block, green
Z = 4	0.62 × 0.21 × 0.18 mm

Data collection

Siemens SMART CCD area-detector diffractometer	1736 independent reflections
Radiation source: fine-focus sealed tube	1407 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.044
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −15→12
T_{min} = 0.68, T_{max} = 0.76	*k* = −18→17
9136 measured reflections	*l* = −10→10

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.031	H-atom parameters constrained
$wR(F^2)$ = 0.085	$w = 1/[\sigma^2(F_o^2) + (0.0301P)^2 + 3.058P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.10	$(\Delta/\sigma)_{max}$ = 0.001
1736 reflections	$\Delta\rho_{max}$ = 0.71 e Å^{-3}
141 parameters	$\Delta\rho_{min}$ = −0.70 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	0.7500	0.2500	0.23917 (6)	0.02149 (17)
Cl1	1.11039 (8)	0.21431 (6)	−0.04748 (13)	0.0600 (3)
Cl2	0.77760 (7)	−0.04046 (5)	0.58593 (10)	0.0409 (2)
N1	0.89128 (18)	0.18780 (15)	0.2319 (3)	0.0249 (6)
O1	0.70164 (15)	0.17179 (12)	0.4057 (2)	0.0272 (5)
O2	0.79907 (15)	0.15853 (12)	0.6024 (2)	0.0261 (5)
C1	0.9549 (2)	0.2156 (2)	0.1354 (4)	0.0302 (7)
H1	0.9477	0.2705	0.1020	0.036*
C2	1.0329 (2)	0.1673 (2)	0.0798 (4)	0.0346 (8)
C3	1.0437 (3)	0.0855 (2)	0.1215 (4)	0.0374 (8)
H3	1.0937	0.0521	0.0821	0.045*
C4	0.9774 (2)	0.05242 (19)	0.2259 (3)	0.0302 (7)
C5	0.9032 (2)	0.10672 (18)	0.2842 (3)	0.0248 (7)
C6	0.8412 (2)	0.07861 (18)	0.3988 (3)	0.0242 (7)
C7	0.8512 (2)	−0.00314 (19)	0.4443 (3)	0.0292 (7)
C8	0.9196 (3)	−0.05881 (19)	0.3816 (4)	0.0382 (8)
H8	0.9215	−0.1147	0.4116	0.046*
C9	0.9832 (3)	−0.0313 (2)	0.2771 (4)	0.0375 (8)
H9	1.0307	−0.0677	0.2392	0.045*
C10	0.7738 (2)	0.14138 (17)	0.4749 (3)	0.0233 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0241 (3)	0.0229 (3)	0.0175 (3)	0.0024 (2)	0.000	0.000
Cl1	0.0521 (6)	0.0519 (6)	0.0761 (8)	0.0056 (5)	0.0362 (6)	0.0096 (5)
Cl2	0.0442 (5)	0.0345 (4)	0.0441 (5)	−0.0039 (4)	0.0032 (4)	0.0102 (4)
N1	0.0245 (13)	0.0264 (13)	0.0238 (14)	0.0024 (10)	0.0015 (11)	−0.0010 (10)
O1	0.0294 (12)	0.0308 (11)	0.0215 (11)	0.0044 (9)	0.0012 (9)	0.0039 (9)
O2	0.0299 (11)	0.0279 (11)	0.0205 (12)	0.0016 (9)	−0.0001 (9)	−0.0026 (9)
C1	0.0282 (17)	0.0291 (16)	0.0334 (19)	0.0003 (14)	0.0015 (15)	−0.0011 (14)
C2	0.0289 (17)	0.0380 (18)	0.037 (2)	0.0013 (14)	0.0080 (15)	0.0012 (15)
C3	0.0310 (18)	0.043 (2)	0.038 (2)	0.0080 (15)	0.0058 (16)	−0.0067 (16)
C4	0.0309 (17)	0.0318 (16)	0.0280 (18)	0.0044 (14)	−0.0009 (14)	−0.0043 (13)
C5	0.0245 (15)	0.0272 (16)	0.0227 (16)	0.0037 (12)	−0.0049 (13)	−0.0048 (12)
C6	0.0240 (16)	0.0259 (15)	0.0227 (16)	0.0027 (12)	−0.0047 (13)	−0.0040 (12)
C7	0.0314 (17)	0.0302 (17)	0.0262 (17)	−0.0029 (14)	−0.0032 (14)	−0.0004 (13)

C8	0.048 (2)	0.0227 (16)	0.044 (2)	0.0058 (15)	−0.0031 (18)	−0.0004 (15)
C9	0.040 (2)	0.0315 (17)	0.042 (2)	0.0109 (15)	0.0027 (17)	−0.0067 (15)
C10	0.0297 (17)	0.0195 (14)	0.0207 (16)	−0.0029 (12)	0.0040 (13)	0.0010 (12)

Geometric parameters (Å, °)

Ni1—O2^{i}	2.033 (2)	C1—H1	0.9300
Ni1—O2^{ii}	2.033 (2)	C2—C3	1.362 (5)
Ni1—O1^{iii}	2.078 (2)	C3—C4	1.412 (5)
Ni1—O1	2.078 (2)	C3—H3	0.9300
Ni1—N1^{iii}	2.144 (2)	C4—C9	1.413 (5)
Ni1—N1	2.144 (2)	C4—C5	1.425 (4)
Cl1—C2	1.738 (3)	C5—C6	1.417 (4)
Cl2—C7	1.741 (3)	C6—C7	1.371 (4)
N1—C1	1.310 (4)	C6—C10	1.519 (4)
N1—C5	1.384 (4)	C7—C8	1.402 (4)
O1—C10	1.258 (3)	C8—C9	1.360 (5)
O2—C10	1.251 (3)	C8—H8	0.9300
O2—Ni1^{iv}	2.033 (2)	C9—H9	0.9300
C1—C2	1.398 (4)		
O2^{i}—Ni1—O2^{ii}	103.47 (11)	C1—C2—Cl1	117.5 (2)
O2^{i}—Ni1—O1^{iii}	85.86 (8)	C2—C3—C4	118.6 (3)
O2^{ii}—Ni1—O1^{iii}	170.43 (8)	C2—C3—H3	120.7
O2^{i}—Ni1—O1	170.43 (8)	C4—C3—H3	120.7
O2^{ii}—Ni1—O1	85.86 (8)	C3—C4—C9	122.8 (3)
O1^{iii}—Ni1—O1	84.91 (11)	C3—C4—C5	118.3 (3)
O2^{i}—Ni1—N1^{iii}	86.54 (9)	C9—C4—C5	118.9 (3)
O2^{ii}—Ni1—N1^{iii}	91.26 (9)	N1—C5—C6	118.9 (3)
O1^{iii}—Ni1—N1^{iii}	91.45 (9)	N1—C5—C4	120.9 (3)
O1—Ni1—N1^{iii}	91.18 (9)	C6—C5—C4	120.2 (3)
O2^{i}—Ni1—N1	91.26 (9)	C7—C6—C5	117.9 (3)
O2^{ii}—Ni1—N1	86.54 (9)	C7—C6—C10	122.6 (3)
O1^{iii}—Ni1—N1	91.18 (9)	C5—C6—C10	119.2 (2)
O1—Ni1—N1	91.45 (9)	C6—C7—C8	122.4 (3)
N1^{iii}—Ni1—N1	176.44 (13)	C6—C7—Cl2	119.7 (2)
C1—N1—C5	118.3 (3)	C8—C7—Cl2	117.9 (2)
C1—N1—Ni1	116.4 (2)	C9—C8—C7	120.2 (3)
C5—N1—Ni1	121.36 (19)	C9—C8—H8	119.9
C10—O1—Ni1	111.16 (18)	C7—C8—H8	119.9
C10—O2—Ni1^{iv}	130.39 (19)	C8—C9—C4	120.2 (3)
N1—C1—C2	123.6 (3)	C8—C9—H9	119.9
N1—C1—H1	118.2	C4—C9—H9	119.9
C2—C1—H1	118.2	O2—C10—O1	126.9 (3)
C3—C2—C1	120.1 (3)	O2—C10—C6	114.4 (3)
C3—C2—Cl1	122.4 (3)	O1—C10—C6	118.6 (3)

O2^{i}—Ni1—N1—C1	−9.6 (2)	C9—C4—C5—N1	−176.6 (3)
O2^{ii}—Ni1—N1—C1	93.8 (2)	C3—C4—C5—C6	−174.1 (3)
O1^{iii}—Ni1—N1—C1	−95.5 (2)	C9—C4—C5—C6	4.5 (4)
O1—Ni1—N1—C1	179.6 (2)	N1—C5—C6—C7	177.1 (3)
O2^{i}—Ni1—N1—C5	−166.9 (2)	C4—C5—C6—C7	−3.9 (4)
O2^{ii}—Ni1—N1—C5	−63.5 (2)	N1—C5—C6—C10	−8.4 (4)
O1^{iii}—Ni1—N1—C5	107.2 (2)	C4—C5—C6—C10	170.5 (3)
O1—Ni1—N1—C5	22.3 (2)	C5—C6—C7—C8	−0.1 (5)
O2^{ii}—Ni1—O1—C10	109.87 (19)	C10—C6—C7—C8	−174.4 (3)
O1^{iii}—Ni1—O1—C10	−67.61 (18)	C5—C6—C7—Cl2	179.4 (2)
N1^{iii}—Ni1—O1—C10	−158.96 (19)	C10—C6—C7—Cl2	5.1 (4)
N1—Ni1—O1—C10	23.44 (19)	C6—C7—C8—C9	3.8 (5)
C5—N1—C1—C2	1.4 (5)	Cl2—C7—C8—C9	−175.8 (3)
Ni1—N1—C1—C2	−156.6 (3)	C7—C8—C9—C4	−3.2 (5)
N1—C1—C2—C3	2.6 (5)	C3—C4—C9—C8	177.6 (3)
N1—C1—C2—Cl1	−179.9 (3)	C5—C4—C9—C8	−0.9 (5)
C1—C2—C3—C4	−2.7 (5)	Ni1^{iv}—O2—C10—O1	−9.3 (4)
Cl1—C2—C3—C4	179.9 (3)	Ni1^{iv}—O2—C10—C6	169.08 (18)
C2—C3—C4—C9	−179.4 (3)	Ni1—O1—C10—O2	110.4 (3)
C2—C3—C4—C5	−0.9 (5)	Ni1—O1—C10—C6	−67.9 (3)
C1—N1—C5—C6	173.8 (3)	C7—C6—C10—O2	64.5 (4)
Ni1—N1—C5—C6	−29.3 (4)	C5—C6—C10—O2	−109.7 (3)
C1—N1—C5—C4	−5.1 (4)	C7—C6—C10—O1	−117.0 (3)
Ni1—N1—C5—C4	151.8 (2)	C5—C6—C10—O1	68.8 (4)
C3—C4—C5—N1	4.9 (4)		

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

Fig. 1

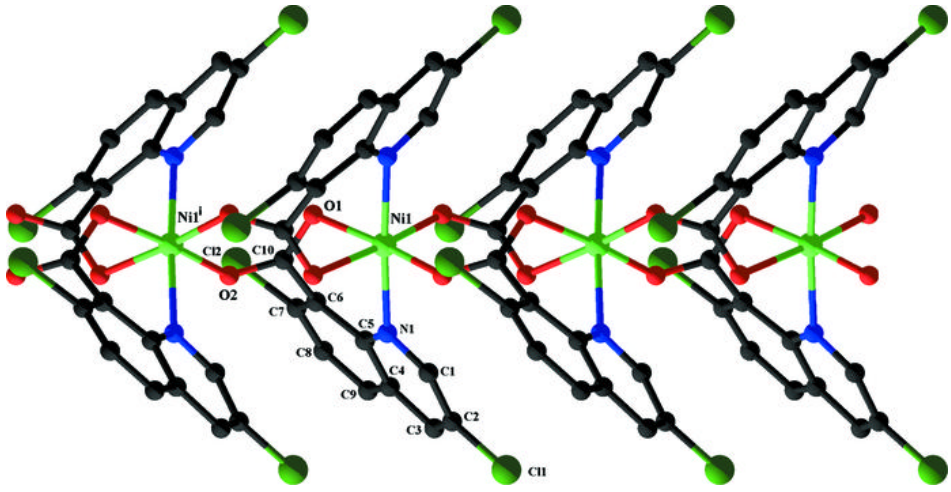

Fig. 2