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{4,4′-Dichloro-2,2′-[2,2-dimethylpropane-1,3-diylbis(nitrilomethanylylidene)]diphenolato-κ^4O,N,N',O'}nickel(II)

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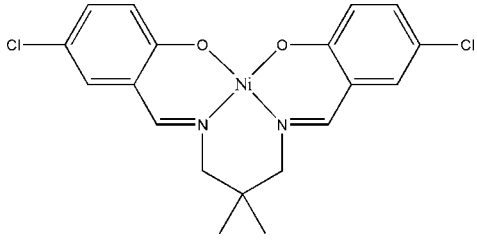
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.039; wR factor = 0.081; data-to-parameter ratio = 14.2.

In the title compound, $[Ni(C_{19}H_{18}Cl_2N_2O_2)]$, the Ni^{II} atom shows a slightly distorted square-planar geometry. The dihedral angle between the mean planes of the coordination rings is 9.15 (12)° while the dihedral angle between the mean planes of the two aromatic rings is 3.48 (16)°. In the crystal, pairs of intermolecular C—H···O hydrogen bonds link neighboring molecules into a chain along the a axis. The crystal structure is further stabilized by π–π interactions [centroid–centroid distance = 3.883 (2) Å].

Related literature

For standard bond lengths, see: Allen *et al.* (1987). For background to Schiff base metal complexes, see: Granovski *et al.* (1993); Blower (1998); Elmali *et al.* (2000). For related structures, see: Fun *et al.* (2008); Kargar *et al.* (2008); Rayati *et al.* (2011).



Experimental

Crystal data

$[Ni(C_{19}H_{18}Cl_2N_2O_2)]$
M_r = 435.96
Monoclinic, $P2_1/n$
a = 6.9781 (3) Å
b = 23.2517 (11) Å
c = 11.8395 (5) Å
β = 105.828 (3)°
V = 1848.16 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.36 mm^{-1}
T = 296 K
0.22 × 0.15 × 0.09 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.755, T_{max} = 0.888
14131 measured reflections
3354 independent reflections
2373 reflections with $I > 2\sigma(I)$
R_{int} = 0.062

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.081
S = 1.02
3354 reflections
237 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8A···O1^{i}	0.97	2.44	3.266 (4)	143
C12—H12A···O2^{ii}	0.97	2.49	3.346 (4)	148

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KJ2181).

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