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catena-Poly[[(2,2′-bipyridine-κ^2N,N')-neodymium(III)]-μ-dichloroacetato-1$\kappa^2O:O'$:2κO-di-μ-dichloroacetato-$\kappa^4O:O'$]

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The title compound, $[Nd(C_2HCl_2O_2)_3(C_{10}H_8N_2)]_n$, was synthesized by reaction of neodymium(III) dichloroacetate with 2,2′-bipyridine in a water–ethanol (1:1) solution. The structure consists of chains running along the *a* axis. The Nd^{3+} ions are coordinated by seven O and two N atoms, giving a distorted monocapped square antiprism.

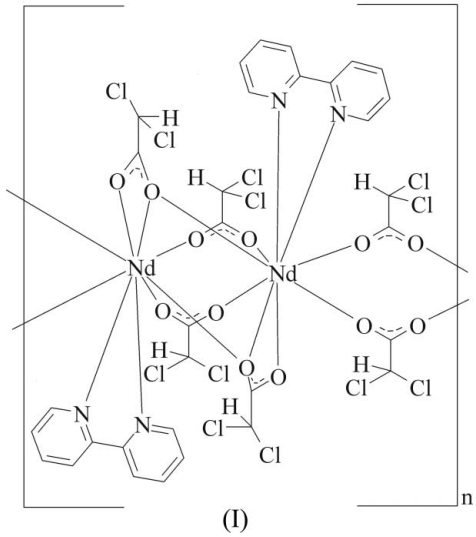
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.009 Å
R factor = 0.031
wR factor = 0.073
Data-to-parameter ratio = 15.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

In connection with our investigation of the structural chemistry of lanthanide (Ln) carboxylates with 2,2′-bipyridine (bipy) (Rohde *et al.*, 2005; John & Urland, 2005), we have paid attention to complexes with dichloroacetic acid, of which, until now, only the erbium compound is known (Lu *et al.*, 1995). In contrast to this compound, which consists of monomeric units, the title compound, (I), consists of chains.



(I)

The structure of (I) is shown in Fig. 1. The Nd^{3+} ion is coordinated by seven O atoms from six carboxylate groups, and by two N atoms from the bipy molecule (Table 1), giving a distorted monocapped square antiprism.

The characteristic structural units are polymeric $[Nd(C_2HCl_2O_2)_3(bipy)]_n$ chains, running along [100]. The chains are made up by dimers, which are connected by two carboxylate groups in a bidentate bridging mode (Fig. 2). In the dimers, the Nd^{3+} ions are bridged by four carboxylate groups, two in bidentate and two in tridentate bridging modes. As a consequence of this structural behaviour, there are two different Nd···Nd distances within the chain [4.310 (1) and 6.089 (1) Å].

The extended structure is formed by π–π stacking of the bipy molecule (Janiak, 2000). The shortest distance between two aromatic fragments of neighbouring chains is 3.333 (6) Å.

Experimental

The title compound was prepared by the reaction of neodymium(III) dichloroacetate (1 mmol, 0.56 g) with 2,2′-bipyridine (1 mmol, 0.16 g) in a water–ethanol (1:1) solution (5 ml) at room temperature. After a few weeks, violet crystals formed.

Crystal data

$[Nd(C_2HCl_2O_2)_3(C_{10}H_8N_2)]$
M_r = 684.21
Triclinic, $P\overline{1}$
a = 8.8492 (8) Å
b = 12.2399 (12) Å
c = 12.3403 (12) Å
α = 109.336 (11)°
β = 104.427 (11)°
γ = 102.457 (11)°
V = 1154.6 (3) Å^3
Z = 2
D_x = 1.968 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.98 mm^{-1}
T = 293 (2) K
Needle, violet
0.22 × 0.09 × 0.07 mm

Data collection

Stoe IPDS area-detector diffractometer
φ scans
Absorption correction: none
16610 measured reflections
4248 independent reflections
3542 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 26.2°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.073
S = 0.98
4248 reflections
280 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0442P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −1.14 e Å^{-3}

Table 1
Selected bond lengths (Å).

Nd1—O11^{i}	2.385 (3)	Nd1—O12	2.559 (4)
Nd1—O31	2.421 (3)	Nd1—N2	2.607 (4)
Nd1—O21	2.436 (3)	Nd1—N1	2.622 (4)
Nd1—O22	2.438 (4)	Nd1—O11	2.860 (4)
Nd1—O32	2.476 (3)		

Symmetry code: (i) $-x+1, -y, -z$.

All H atoms on C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.98 (Csp^3) or 0.93 Å (Csp^2) and U_{iso}(H) = 1.2U_{eq}(C). The deepest hole is located 0.89 Å from atom Nd1.

Data collection: *IPDS Software* (Stoe & Cie, 1998); cell refinement: *IPDS Software*; data reduction: *IPDS Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *SHELXL97*.

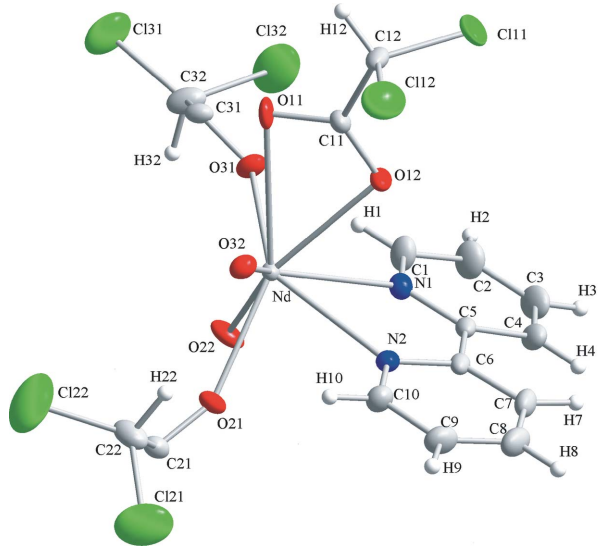


Figure 1
View of the asymmetric unit of (I) with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

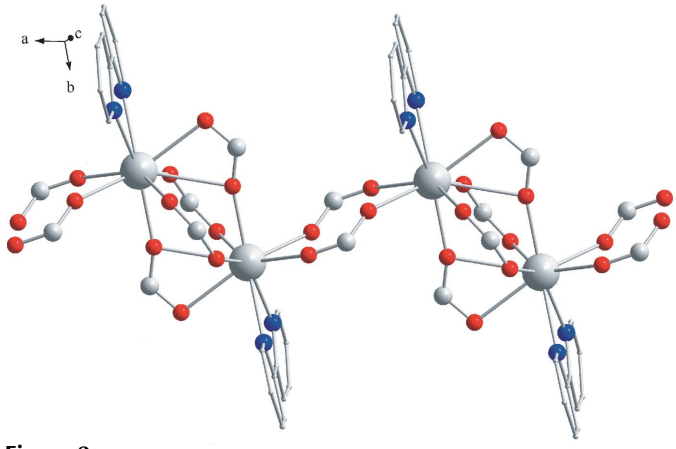


Figure 2
Polymeric chain of the type $[Nd(C_2HCl_2O_2)_3(bipy)]_n$, where only Nd atoms, carboxylate groups and 2,2′-bipyridine molecules are displayed. H atoms have been omitted.

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