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The ribbon structure of nickel(II) acetate–4,4′-bipyridine

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.009 Å
R factor = 0.074
wR factor = 0.148
Data-to-parameter ratio = 12.0

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

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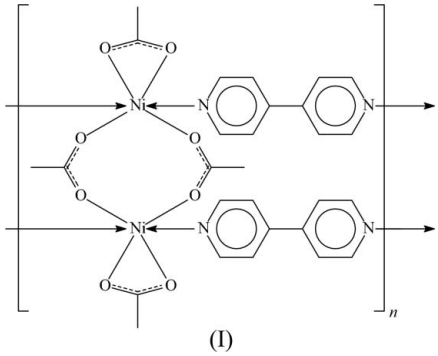
One acetate chelates to an Ni atom and the other bridges two Ni atoms in the title compound, *catena*-poly[[di-μ-acetato-1κ*O*:2κ*O*′-bis[(acetato-κ^2*O*,*O*′)nickel(II)]]-di-μ-4,4′-bipyridine-1κ*N*:1′κ*N*′;2κ*N*:2′κ*N*′], $[Ni_2(C_2H_3O_2)_4(C_{10}H_8N_2)_2]_n$. The Ni atoms in the centrosymmetric $[Ni_2(C_2H_3O_2)_4]$ arrangement are bridged by the $C_{10}H_8N_2$ ligands to afford a ribbon structure. The Ni atom, both acetates and the heterocyclic ligand all lie on special positions of *m* site symmetry.

Comment

The 4,4′-bipyridine heterocycle has been used in the formation of a large number of metal complexes; in these, the ligand typically functions as a rigid spacer in the resulting linear, layer and network motifs. With nickel(II) carboxylates in particular, the crystallographically authenticated adducts include the 2-methylbut-2-enedioate (Liao *et al.*, 2001), benzoate (Biradha *et al.*, 1999), phthalate (Yang *et al.*, 2003), benzene-1,2,4,5-tetracarboxylate (Wu *et al.*, 2002), pyridine-2,6-dicarboxylate (Wang *et al.*, 2004) and pyridine-1,3,5-tricarboxylate (Prior *et al.*, 2003). The list now includes the title acetate homologue, (I).



(I)

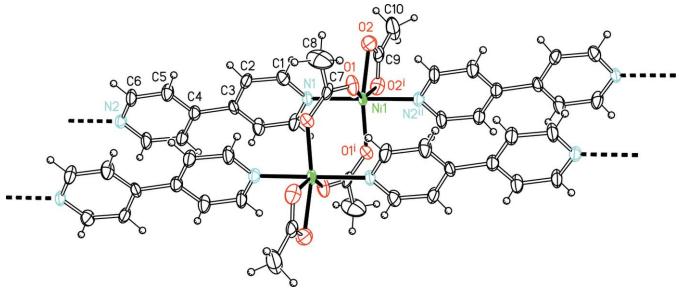


Figure 1
A plot showing the numbering scheme of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. Symmetry codes are as given in Table 1.

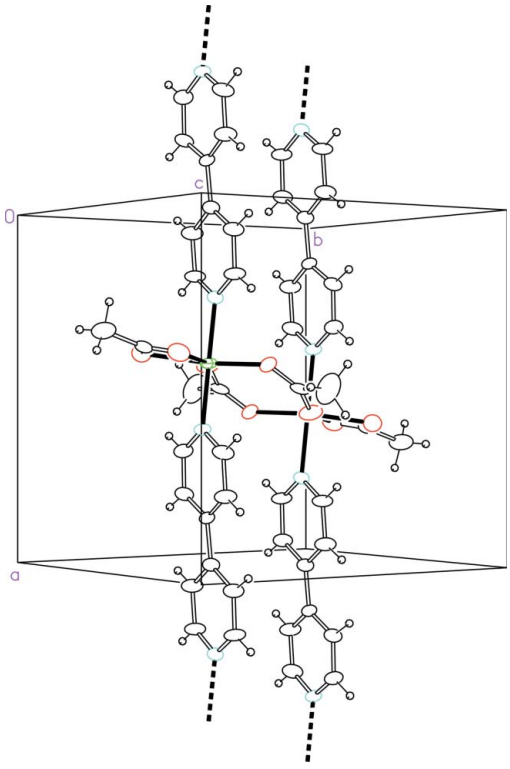


Figure 2
A plot showing the formation of the ribbon in the unit cell.

The title adduct of nickel(II) acetate with 4,4′-bipyridine is a centrosymmetric compound in which two acetates coordinate in the bridging mode to two acetate-chelated Ni atoms across a centre of inversion. The planar four-membered Ni—O···C···O ring lies on a mirror plane so that the two C—O distances are equivalent. The buckled eight-membered Ni—O···C···O—Ni—O···C···O— ring lies on another special position of *m* site symmetry. The O atoms surrounding the Ni atom comprise a rhombus, and the presence of the N atoms above and below it leads to a distorted octahedral environment for the metal atom (Fig. 1). The mode of coordination of the pair of *N*-heterocycles gives rise to the formation of a ribbon structure that propagates along the *a* axis (Fig. 2).

Only a few metal acetates of this spacer heterocycle have been reported to date, these being the cobalt(II) derivative, a diaqua compound that crystallizes with both methanol and water (Zhang *et al.*, 1999), and a copper(II) monohydrate that crystallizes in two forms (Castiñeiras *et al.*, 2002; Conerney *et al.*, 2003).

Experimental

Nickel acetate tetrahydrate (0.5 mmol) and 4,4′-bipyridine (0.5 mmol) were dissolved in *N*,*N*-dimethylformamide (8 ml). The mixture was placed in a 15 ml Teflon-lined Parr bomb which was then heated at 383 K for 48 h. Blue crystals of (I) were obtained from the cooled solution in about 50% yield.

Crystal data

$[Ni_2(C_2H_3O_2)_4(C_{10}H_8N_2)_2]$
M_r = 332.96
Orthorhombic, *Pnnm*
a = 11.278 (2) Å
b = 11.532 (2) Å
c = 10.802 (2) Å
V = 1404.9 (4) Å^3
Z = 4
D_x = 1.574 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 416 reflections
θ = 2.5–19.2°
μ = 1.40 mm^{-1}
T = 295 (2) K
Block, blue
0.11 × 0.08 × 0.06 mm

Data collection

Bruker APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.440, T_{max} = 0.921
5686 measured reflections
1307 independent reflections
975 reflections with $I > 2\sigma(I)$
R_{int} = 0.094
θ_{max} = 25.0°
$h = -8 \rightarrow 13$
$k = -13 \rightarrow 9$
$l = -11 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.148
S = 1.18
1307 reflections
109 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.059P)^2 + 0.0628P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.69 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	2.017 (4)	Ni1—N1	2.101 (6)
Ni1—O2	2.139 (4)		
O1—Ni1—O1^{i}	113.9 (2)	O2—Ni1—O2^{i}	60.7 (2)
O1—Ni1—O2	92.5 (2)	O2—Ni1—N1	92.9 (2)
O1—Ni1—O2^{i}	152.9 (2)	O2—Ni1—N2^{ii}	87.4 (2)
O1—Ni1—N1	92.1 (2)	N1—Ni1—N2^{ii}	179.7 (3)
O1—Ni1—N2^{ii}	87.8 (2)		

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

The C-bound H atoms were positioned geometrically, with C—$H_{pyridyl}$ = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C), and C—H_{methyl} = 0.98 Å and U_{iso}(H) = 1.5U_{eq}(C)], and were included in the refinement in the riding-model approximation. The methyl groups were rotated to fit the electron density.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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