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Bis(pyrazine-2-carboxylato-κ^2N^1,O)-nickel(II)

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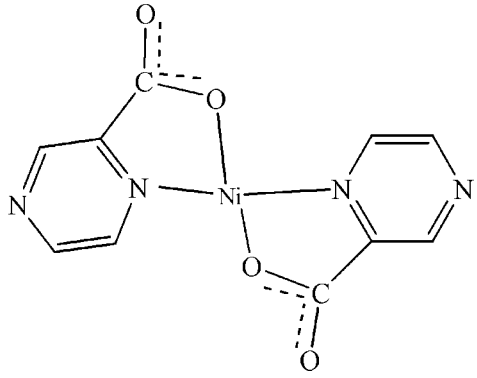
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.027; wR factor = 0.056; data-to-parameter ratio = 11.5.

In the title compound, $[Ni(C_5H_3N_2O_2)_2]$, the Ni^{II} cation is four-coordinated by two N and two O atoms belonging to two pyrazine-2-carboxylate ligands. The Ni^{II} cation lies on a centre of symmetry.

Related literature

For related literature, see: Ngo *et al.* (2004); Evans *et al.* (2001); Vioux *et al.* (2004); Sanchez *et al.* (2003); Evans & Lin (2001); Jannasch (2003); Javaid *et al.* (2001); Honma *et al.* (2001); Sudik *et al.* (2005); Rowsell *et al.* (2004); Kitaura *et al.* (2004).



Experimental

Crystal data

$[Ni(C_5H_3N_2O_2)_2]$
M_r = 304.90
Monoclinic, $P2_1/c$
a = 5.0501 (9) Å
b = 15.370 (3) Å
c = 7.0704 (13) Å
β = 106.60 (2)°
V = 525.9 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.86 mm^{-1}
T = 293 (2) K
0.10 × 0.10 × 0.10 mm

Data collection

Bruker $P4$ diffractometer
Absorption correction: none
4336 measured reflections
1014 independent reflections
776 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.056
S = 1.00
1014 reflections
88 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Data collection: *XSCANS* (Bruker, 2002); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Bruker, 1999); program(s) used to solve structure: *SHELXL97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; 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: BR2043).

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supplementary materials

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Bis(pyrazine-2-carboxylato-κ^2N^1,O)nickel(II)

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Comment

Hybrid organic–inorganic materials occupy a prominent position by virtue of their applications to catalysis, optical materials, membranes, and sorption (Ngo *et al.*, 2004; Evans *et al.*, 2001; Vioux *et al.*, 2004; Sanchez *et al.*, 2003; Evans & Lin, 2001; Jannasch, 2003; Javaid *et al.*, 2001; Honma *et al.*, 2001; Sudik *et al.*, 2005; Rowsell *et al.*, 2004; Kitaura *et al.*, 2002). The design of organic-inorganic hybrid materials is conceived of the metal, metal cluster, or metal oxide substructure as a node from which rigid or flexible multitopic organic ligands radiate to act as tethers to adjacent nodes in the bottom-up construction of complex extended architectures. While a variety of organic molecules have been investigated as potential tethers, materials incorporating multitopic carboxylates and pyridine ligands have witnessed the most significant development. However, ligands offering alternative tether lengths, different charge-balance requirements, and orientations of donor groups may afford advantages in the design of materials. One such ligand is 2-pyrazine caboxylate, a member of the polyazaheteroaromatic family of compounds, which exhibit an extensively documented ability to bridge metal ions to afford polynuclear compounds. 2-pyrazine caboxylate is an attractive ligand for the design of novel hybrid materials because of the unusual structural diversity associated with the di- and trinucleating properties of the neutral and anionic ligand forms, respectively. Herein, one new complex,[di(2-pyrazine caboxylato) nickel(II)], obtained from 2-pyrazine caboxylate and nickel acetate under hydrothermal reaction is reported.

The coordination of the nickel atom is shown in Fig. 1 which can be described as a co-planar. The nickel cation is four-coordinated by two nitrogen atoms and two oxygen atoms belonging to two 2-pyrazine caboxylate ligands. The Ni—N and Ni—O bond lengths are 1.9763 (18) and 1.9297 (15) Å, respectively. The angle of O(N)—Ni—O(N) are in the range of 83.71 (7)–96.29 (7) Å.

Experimental

All chemicals were used as purchased from Shanghai Chemical Co. Ltd. A mixture of Nickel(II) acetate (0.5 mmol), potassium hydroxide (0.5 mmol), 2-pyrazine caboxylic acid(0.5 mmol) and EtOH (8 ml) in a 25 ml Teflon-lined stainless steel autoclave was kept at 413 K for 2 d, and then cooled to room temperature. Green, block-shaped crystals of (I) were obtained in a yield of 12%. Anal. Calc. for $C_{10}H_6N_4NiO_4$: C 39.34, H 1.97, N 18.36, Ni 19.25%; Found: C 39.39, H 2.01, N 18.33, Ni 19.18%.

Refinement

All H atoms on C atoms were generated geometrically and refined as riding atoms with C—H = 0.93 Å and U_{iso}(H) = 1.2 times U_{eq}(C).

Figures

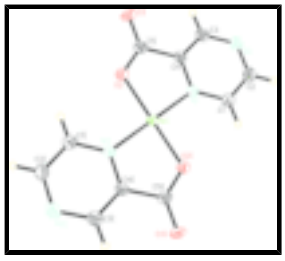

Fig. 1. A view of the structure for the title compound,showing 30% probability displacement ellipsoids. Atoms labeled with I at the symmetry positions (−*x* + 1,-*y* + 1,-*z* + 2).

Bis(pyrazine-2-caboxylato-κ^2*N*^{1},*O*)nickel(II)

Crystal data

$[Ni(C_5H_3N_2O_2)_2]$	F_{000} = 308
M_r = 304.90	D_x = 1.925 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 4678 reflections
a = 5.0501 (9) Å	θ = 2.0–26.0º
b = 15.370 (3) Å	μ = 1.86 mm^{-1}
c = 7.0704 (13) Å	*T* = 293 (2) K
β = 106.60 (2)º	Block, green
V = 525.9 (3) Å^3	0.10 × 0.10 × 0.10 mm
Z = 2	

Data collection

Bruker P4 diffractometer	776 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.039
Monochromator: graphite	θ_{max} = 26.0º
T = 293(2) K	θ_{min} = 2.7º
ω scans	*h* = −6→6
Absorption correction: none	*k* = −18→19
4336 measured reflections	*l* = −8→8
1014 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.028	$w = 1/[\sigma^2(F_o^2) + (0.0234P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.056	$(\Delta/\sigma)_{max}$ = 0.011

S = 1.00	$\Delta\rho_{max}$ = 0.43 e Å^{-3}
1014 reflections	$\Delta\rho_{min}$ = −0.24 e Å^{-3}
88 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.036 (3)
Secondary atom site location: difference Fourier map	

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	0.5000	0.5000	1.0000	0.03121 (15)
O2	0.1700 (3)	0.43181 (10)	0.8941 (2)	0.0391 (4)
N1	0.2849 (4)	0.59243 (12)	0.8293 (3)	0.0319 (5)
C5	−0.0329 (5)	0.47318 (15)	0.7773 (4)	0.0352 (6)
O3	−0.2701 (3)	0.44533 (12)	0.7132 (3)	0.0500 (5)
C4	0.0334 (5)	0.56447 (14)	0.7293 (3)	0.0312 (5)
N2	−0.0889 (4)	0.70172 (14)	0.5766 (3)	0.0466 (6)
C3	−0.1486 (5)	0.61873 (16)	0.6001 (3)	0.0393 (6)
H3	−0.3187	0.5968	0.5270	0.047*
C2	0.1568 (5)	0.72928 (16)	0.6837 (4)	0.0435 (6)
H2	0.2012	0.7876	0.6755	0.052*
C1	0.3507 (5)	0.67537 (15)	0.8072 (4)	0.0374 (6)
H1	0.5247	0.6966	0.8741	0.045*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0198 (2)	0.0274 (2)	0.0392 (3)	−0.00080 (18)	−0.00327 (17)	0.0042 (2)
O2	0.0307 (9)	0.0315 (9)	0.0469 (11)	−0.0020 (7)	−0.0024 (8)	0.0036 (8)
N1	0.0272 (11)	0.0318 (11)	0.0342 (11)	−0.0005 (8)	0.0045 (8)	−0.0011 (9)
C5	0.0309 (14)	0.0379 (14)	0.0338 (14)	−0.0008 (11)	0.0042 (11)	−0.0033 (11)
O3	0.0283 (10)	0.0493 (11)	0.0597 (12)	−0.0116 (8)	−0.0077 (8)	0.0042 (9)
C4	0.0267 (12)	0.0324 (13)	0.0319 (13)	0.0024 (10)	0.0041 (10)	−0.0028 (11)
N2	0.0473 (14)	0.0392 (13)	0.0464 (13)	0.0084 (10)	0.0026 (11)	0.0058 (10)
C3	0.0341 (15)	0.0429 (15)	0.0375 (15)	0.0028 (11)	0.0046 (12)	0.0007 (12)

C2	0.0494 (17)	0.0321 (14)	0.0487 (16)	−0.0001 (12)	0.0137 (14)	0.0023 (13)
C1	0.0338 (14)	0.0355 (15)	0.0413 (15)	−0.0033 (10)	0.0081 (12)	−0.0024 (12)

Geometric parameters (Å, °)

Ni1—O2^{i}	1.9297 (15)	C5—O3	1.230 (3)
Ni1—O2	1.9297 (15)	C5—C4	1.504 (3)
Ni1—N1^{i}	1.9763 (18)	C4—C3	1.377 (3)
Ni1—N1	1.9763 (18)	N2—C2	1.325 (3)
O2—C5	1.286 (3)	N2—C3	1.332 (3)
N1—C4	1.336 (3)	C2—C1	1.386 (3)
N1—C1	1.338 (3)		
O2^{i}—Ni1—N1^{i}	83.71 (7)	O3—C5—C4	119.9 (2)
O2—Ni1—N1^{i}	96.29 (7)	O2—C5—C4	114.74 (19)
O2^{i}—Ni1—N1	96.29 (7)	N1—C4—C3	120.7 (2)
O2—Ni1—N1	83.71 (7)	N1—C4—C5	114.85 (19)
C5—O2—Ni1	114.96 (14)	C3—C4—C5	124.4 (2)
C4—N1—C1	118.4 (2)	C2—N2—C3	116.3 (2)
C4—N1—Ni1	111.44 (15)	N2—C3—C4	122.1 (2)
C1—N1—Ni1	130.15 (16)	N2—C2—C1	123.2 (2)
O3—C5—O2	125.3 (2)	N1—C1—C2	119.3 (2)

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

Fig. 1