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Tetrakis(1*H*-imidazole-κN^3)(2-phenylpropanedioato-κ^2O^1,O^3)nickel(II)

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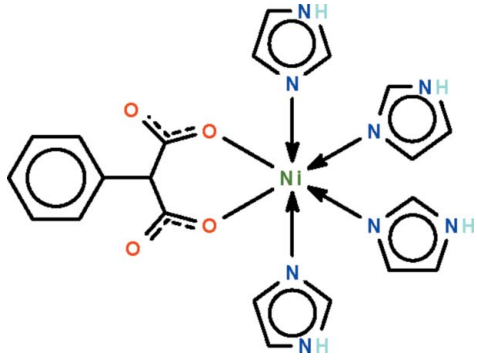
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.041; wR factor = 0.086; data-to-parameter ratio = 18.0.

In the title complex, $[Ni(C_9H_6O_4)(C_3H_4N_2)_4]$, the Ni^{II} ion is O,O'-chelated by the phenylmalonato ligand and coordinated by four imidazole ligands in a slightly distorted octahedral geometry. In the crystal structure, symmetry-related molecules are linked by N—H···O hydrogen bonds, generating a three-dimensional network.

Related literature

For the cobalt(II) analog, see: Zhang *et al.* (2007).



Experimental

Crystal data

$[Ni(C_9H_6O_4)(C_3H_4N_2)_4]$
M_r = 509.18
Orthorhombic, $P2_12_12_1$
a = 8.5358 (8) Å
b = 13.3148 (12) Å
c = 20.6996 (19) Å
V = 2352.6 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.87 mm^{-1}
T = 293 K
0.25 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.812, T_{max} = 0.881
15962 measured reflections
5516 independent reflections
4013 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.086
S = 0.98
5516 reflections
307 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Absolute structure: Flack (1983), 2344 Friedel pairs
Flack parameter: 0.082 (13)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O3^{i}	0.88	2.06	2.943 (3)	176
N4—H4···O1^{ii}	0.88	1.97	2.839 (3)	168
N6—H6···O2^{iii}	0.88	1.90	2.774 (3)	172
N8—H8···O4^{iv}	0.88	1.85	2.718 (3)	169

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5153).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2005). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Zhang, K.-L., Kuai, H.-W., Liu, W.-L. & Diao, G.-W. (2007). *J. Mol. Struct.* **831**, 114–118.

supplementary materials

Acta Cryst. (2010). E**66**, m1430 [**doi:10.1107/S1600536810041577**]

Tetrakis(1*H*-imidazole-κN^3)(2-phenylpropanedioato-$\kappa^2 O^1,O^3$)nickel(II)

K.-L. Zhang, G.-W. Diao and S. W. Ng

Comment

We have previously reported the crystal structure of the tetrakis(imidazole) adduct of cobalt(II) phenylmalonate. The structure features the carboxylate-chelated cobalt(II) atom bonded to four *N*-heterocycles; each of these has a nitrogen-donor site that enables the octahedrally coordinated mononuclear molecule to connect with each other to form a three-dimensional network (Zhang *et al.*, 2007). The nickel analog (Fig. 1) is isostructural, the two compounds crystallizing with similar unit cell dimensions.

Experimental

Imidazole (0.339 g. 0.56 mmol) was dissolved in methanol (10 ml) and to the solution was added nickel nitrate hexahydrate (0.480 g, 1.65 mmol) dissolved in water (6 ml). To the clear soluiton was added phenylmalonic acid (0.300 g, 1.65 mmol) and sodium hydroxide (0.120 g, 3.30 mmol) dissolved in water (10 ml). The filtered solution was set aside for the growth of green crystals over several days; yield 50%. CH&N elemental analysis. Calc. for $C_{21}H_{22}N_8NiO_4$: C 49.53, H 4.36, N 22.00%. Found: C 49.61, H 4.49, N 21.91%.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.93–0.98 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2U_{eq}(C).

The imidazolium H-atoms were similarly treated (N–H 0.88 Å; U_{iso}(H) 1.2U_{eq}(N)).

The crystal has several voids but these are too small (20Å^3) to accomodate a solvent molecule.

Figures

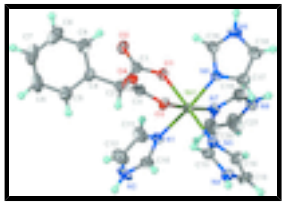


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $Ni(C_3H_4N_2)_4(C_9H_6O_4)$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

Tetrakis(1*H*-imidazole-κ*N*^{3})(2-phenylpropanedioato- κ^2*O*^{1},*O*^{3})nickel(II)

Crystal data

$[Ni(C_9H_6O_4)(C_3H_4N_2)_4]$	$F(000) = 1056$
$M_r = 509.18$	$D_x = 1.438$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 2481 reflections
$a = 8.5358$ (8) Å	$\theta = 2.6$–$21.7°$
$b = 13.3148$ (12) Å	$\mu = 0.87$ mm^{-1}
$c = 20.6996$ (19) Å	$T = 293$ K
$V = 2352.6$ (4) Å^3	Prism, green
$Z = 4$	0.25 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer	5516 independent reflections
Radiation source: fine-focus sealed tube	4013 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.051$
ω scans	$\theta_{max} = 27.8°$, $\theta_{min} = 1.8°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -11 \rightarrow 11$
$T_{min} = 0.812$, $T_{max} = 0.881$	$k = -17 \rightarrow 17$
15962 measured reflections	$l = -19 \rightarrow 27$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H-atom parameters constrained
$wR(F^2) = 0.086$	$w = 1/[\sigma^2(F_o^2) + (0.0326P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.98$	$(\Delta/\sigma)_{max} = 0.001$
5516 reflections	$\Delta\rho_{max} = 0.41$ e Å^{-3}
307 parameters	$\Delta\rho_{min} = -0.31$ e Å^{-3}
0 restraints	Absolute structure: Flack (1983), 2344 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.082 (13)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.66167 (4)	0.40568 (3)	0.336577 (18)	0.02636 (10)
O1	0.8851 (2)	0.40575 (17)	0.29819 (9)	0.0324 (4)

O2	1.0679 (2)	0.37546 (16)	0.22649 (12)	0.0433 (6)
O3	0.5823 (2)	0.41866 (15)	0.24132 (9)	0.0323 (5)
O4	0.6203 (3)	0.43579 (17)	0.13674 (11)	0.0515 (7)
N1	0.6652 (3)	0.24683 (16)	0.33088 (13)	0.0338 (6)
N2	0.5969 (3)	0.0939 (2)	0.30389 (16)	0.0597 (9)
H2	0.5388	0.0432	0.2908	0.072*
N3	0.4310 (2)	0.4058 (2)	0.37002 (11)	0.0301 (5)
N4	0.1739 (3)	0.4091 (2)	0.36620 (12)	0.0388 (6)
H4	0.0782	0.4110	0.3504	0.047*
N5	0.6703 (3)	0.56328 (16)	0.33579 (12)	0.0312 (5)
N6	0.7570 (3)	0.7169 (2)	0.32201 (14)	0.0424 (8)
H6	0.8180	0.7667	0.3098	0.051*
N7	0.7489 (3)	0.4034 (2)	0.43160 (11)	0.0324 (6)
N8	0.8143 (4)	0.4576 (2)	0.52810 (14)	0.0500 (8)
H8	0.8359	0.4991	0.5599	0.060*
C1	0.9291 (3)	0.3761 (2)	0.24304 (17)	0.0300 (7)
C2	0.8045 (3)	0.3333 (2)	0.19607 (15)	0.0343 (8)
H2A	0.7662	0.2713	0.2161	0.041*
C3	0.6602 (3)	0.4033 (2)	0.19068 (14)	0.0315 (6)
C4	0.8732 (3)	0.3022 (2)	0.13164 (16)	0.0361 (8)
C5	0.8607 (4)	0.2032 (3)	0.11128 (17)	0.0468 (9)
H5	0.8055	0.1569	0.1360	0.056*
C6	0.9301 (5)	0.1738 (3)	0.0545 (2)	0.0635 (12)
H6A	0.9202	0.1075	0.0410	0.076*
C7	1.0126 (5)	0.2392 (4)	0.0179 (2)	0.0683 (13)
H7	1.0602	0.2173	−0.0199	0.082*
C8	1.0264 (5)	0.3368 (3)	0.0363 (2)	0.0643 (12)
H8A	1.0831	0.3817	0.0110	0.077*
C9	0.9556 (4)	0.3689 (3)	0.09264 (17)	0.0471 (9)
H9	0.9632	0.4360	0.1047	0.057*
C10	0.5503 (4)	0.1886 (2)	0.31110 (17)	0.0450 (9)
H10	0.4488	0.2108	0.3031	0.054*
C11	0.7919 (4)	0.1839 (2)	0.3360 (2)	0.0493 (9)
H11	0.8920	0.2036	0.3484	0.059*
C12	0.7502 (4)	0.0899 (3)	0.3204 (2)	0.0626 (12)
H12	0.8139	0.0333	0.3208	0.075*
C13	0.3064 (3)	0.4087 (2)	0.33245 (16)	0.0361 (7)
H13	0.3106	0.4102	0.2876	0.043*
C14	0.3722 (3)	0.4050 (3)	0.43166 (15)	0.0391 (7)
H14	0.4318	0.4040	0.4693	0.047*
C15	0.2137 (4)	0.4060 (3)	0.42918 (17)	0.0446 (8)
H15	0.1454	0.4048	0.4642	0.054*
C16	0.7835 (4)	0.6195 (2)	0.31334 (16)	0.0383 (8)
H16	0.8728	0.5941	0.2935	0.046*
C17	0.5650 (4)	0.6304 (2)	0.36077 (17)	0.0427 (9)
H17	0.4705	0.6132	0.3802	0.051*
C18	0.6178 (4)	0.7249 (2)	0.35329 (17)	0.0426 (9)
H18	0.5690	0.7837	0.3668	0.051*
C19	0.7768 (4)	0.4830 (3)	0.46802 (16)	0.0392 (8)

H19	0.7709	0.5489	0.4533	0.047*
C20	0.7710 (5)	0.3241 (3)	0.47194 (18)	0.0585 (12)
H20	0.7590	0.2571	0.4604	0.070*
C21	0.8133 (6)	0.3571 (3)	0.53140 (18)	0.0682 (13)
H21	0.8368	0.3179	0.5673	0.082*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.02413 (16)	0.02630 (16)	0.02864 (19)	−0.00065 (17)	−0.00168 (18)	−0.00153 (19)
O1	0.0262 (10)	0.0397 (11)	0.0312 (11)	−0.0002 (10)	0.0005 (9)	−0.0080 (11)
O2	0.0255 (11)	0.0565 (15)	0.0479 (15)	0.0019 (10)	0.0034 (11)	−0.0166 (12)
O3	0.0296 (10)	0.0422 (13)	0.0252 (11)	0.0041 (10)	0.0009 (9)	−0.0002 (10)
O4	0.0486 (14)	0.0700 (17)	0.0359 (14)	0.0183 (12)	0.0071 (12)	0.0217 (12)
N1	0.0380 (13)	0.0312 (13)	0.0322 (15)	−0.0052 (12)	−0.0028 (18)	0.0004 (11)
N2	0.0581 (18)	0.0281 (14)	0.093 (3)	−0.0143 (16)	−0.0013 (17)	−0.0146 (18)
N3	0.0258 (11)	0.0332 (12)	0.0313 (14)	−0.0023 (13)	−0.0017 (11)	−0.0005 (14)
N4	0.0232 (11)	0.0497 (15)	0.0436 (15)	0.0030 (15)	−0.0003 (13)	0.0011 (15)
N5	0.0278 (12)	0.0303 (12)	0.0356 (14)	−0.0031 (10)	0.0006 (17)	−0.0003 (11)
N6	0.0387 (15)	0.0343 (15)	0.054 (2)	−0.0088 (13)	−0.0008 (14)	0.0059 (15)
N7	0.0331 (12)	0.0349 (13)	0.0291 (14)	0.0015 (13)	−0.0029 (11)	−0.0033 (15)
N8	0.064 (2)	0.053 (2)	0.0330 (18)	0.0026 (18)	−0.0074 (17)	−0.0125 (15)
C1	0.0243 (15)	0.0255 (16)	0.040 (2)	0.0061 (12)	−0.0016 (14)	−0.0010 (13)
C2	0.0326 (18)	0.0358 (17)	0.0346 (18)	−0.0004 (14)	0.0001 (15)	0.0012 (15)
C3	0.0283 (13)	0.0343 (14)	0.0319 (15)	−0.0006 (18)	0.0009 (14)	−0.0023 (15)
C4	0.0273 (16)	0.049 (2)	0.0322 (17)	0.0077 (15)	−0.0009 (14)	−0.0051 (16)
C5	0.0362 (18)	0.051 (2)	0.053 (2)	0.0041 (18)	−0.0058 (18)	−0.0053 (18)
C6	0.064 (3)	0.069 (3)	0.057 (3)	0.018 (2)	−0.007 (2)	−0.031 (2)
C7	0.075 (3)	0.088 (3)	0.042 (3)	0.032 (3)	−0.001 (2)	−0.013 (2)
C8	0.060 (3)	0.088 (3)	0.045 (3)	0.018 (2)	0.015 (2)	0.015 (2)
C9	0.052 (2)	0.048 (2)	0.042 (2)	0.0090 (17)	0.0023 (19)	0.0043 (17)
C10	0.0379 (18)	0.0350 (18)	0.062 (3)	−0.0055 (15)	0.0071 (17)	−0.0004 (17)
C11	0.0431 (19)	0.0379 (18)	0.067 (3)	0.0085 (14)	−0.018 (2)	−0.004 (2)
C12	0.056 (2)	0.0342 (19)	0.098 (4)	0.006 (2)	−0.009 (2)	−0.003 (3)
C13	0.0293 (14)	0.0416 (16)	0.0374 (17)	−0.0031 (14)	−0.0022 (14)	−0.0015 (19)
C14	0.0350 (16)	0.0509 (18)	0.0313 (17)	0.0019 (18)	−0.0008 (14)	0.0026 (18)
C15	0.0366 (16)	0.056 (2)	0.041 (2)	0.0009 (19)	0.0089 (15)	0.006 (2)
C16	0.0365 (17)	0.0314 (19)	0.047 (2)	0.0011 (13)	0.0027 (15)	−0.0013 (15)
C17	0.0347 (17)	0.0400 (18)	0.053 (2)	0.0016 (14)	0.0081 (17)	0.0003 (16)
C18	0.0430 (19)	0.0261 (16)	0.059 (3)	0.0068 (14)	0.0016 (17)	0.0031 (15)
C19	0.0401 (19)	0.044 (2)	0.034 (2)	−0.0004 (16)	−0.0038 (16)	−0.0028 (17)
C20	0.102 (3)	0.038 (2)	0.036 (2)	0.003 (2)	−0.020 (2)	0.0050 (17)
C21	0.112 (4)	0.057 (3)	0.036 (2)	0.006 (3)	−0.025 (3)	0.0050 (19)

Geometric parameters (Å, °)

Ni1—O1	2.0662 (18)	C2—C4	1.515 (4)
Ni1—N3	2.087 (2)	C2—C3	1.549 (4)
Ni1—O3	2.092 (2)	C2—H2A	0.9800

Ni1—N5	2.100 (2)	C4—C5	1.388 (5)
Ni1—N7	2.103 (2)	C4—C9	1.391 (4)
Ni1—N1	2.118 (2)	C5—C6	1.372 (5)
O1—C1	1.265 (4)	C5—H5	0.9300
O2—C1	1.234 (3)	C6—C7	1.352 (6)
O3—C3	1.258 (3)	C6—H6A	0.9300
O4—C3	1.245 (3)	C7—C8	1.359 (5)
N1—C10	1.316 (4)	C7—H7	0.9300
N1—C11	1.373 (4)	C8—C9	1.382 (5)
N2—C10	1.330 (4)	C8—H8A	0.9300
N2—C12	1.353 (4)	C9—H9	0.9300
N2—H2	0.8800	C10—H10	0.9300
N3—C13	1.318 (3)	C11—C12	1.340 (5)
N3—C14	1.371 (4)	C11—H11	0.9300
N4—C13	1.329 (3)	C12—H12	0.9300
N4—C15	1.348 (4)	C13—H13	0.9300
N4—H4	0.8800	C14—C15	1.355 (4)
N5—C16	1.308 (4)	C14—H14	0.9300
N5—C17	1.369 (4)	C15—H15	0.9300
N6—C16	1.329 (4)	C16—H16	0.9300
N6—C18	1.357 (4)	C17—C18	1.345 (4)
N6—H6	0.8800	C17—H17	0.9300
N7—C19	1.323 (4)	C18—H18	0.9300
N7—C20	1.359 (4)	C19—H19	0.9300
N8—C19	1.328 (4)	C20—C21	1.356 (5)
N8—C21	1.339 (4)	C20—H20	0.9300
N8—H8	0.8800	C21—H21	0.9300
C1—C2	1.550 (4)		
O1—Ni1—N3	176.75 (9)	C5—C4—C2	119.8 (3)
O1—Ni1—O3	86.37 (7)	C9—C4—C2	122.2 (3)
N3—Ni1—O3	90.39 (8)	C6—C5—C4	119.9 (4)
O1—Ni1—N5	87.95 (9)	C6—C5—H5	120.1
N3—Ni1—N5	91.98 (10)	C4—C5—H5	120.1
O3—Ni1—N5	85.50 (9)	C7—C6—C5	121.4 (4)
O1—Ni1—N7	91.88 (8)	C7—C6—H6A	119.3
N3—Ni1—N7	91.36 (9)	C5—C6—H6A	119.3
O3—Ni1—N7	175.72 (9)	C6—C7—C8	120.3 (4)
N5—Ni1—N7	90.54 (10)	C6—C7—H7	119.9
O1—Ni1—N1	88.05 (10)	C8—C7—H7	119.9
N3—Ni1—N1	91.88 (10)	C7—C8—C9	119.6 (4)
O3—Ni1—N1	91.98 (9)	C7—C8—H8A	120.2
N5—Ni1—N1	175.40 (10)	C9—C8—H8A	120.2
N7—Ni1—N1	91.87 (10)	C8—C9—C4	120.9 (4)
C1—O1—Ni1	128.36 (18)	C8—C9—H9	119.5
C3—O3—Ni1	126.92 (18)	C4—C9—H9	119.5
C10—N1—C11	104.6 (2)	N1—C10—N2	111.8 (3)
C10—N1—Ni1	126.6 (2)	N1—C10—H10	124.1
C11—N1—Ni1	128.0 (2)	N2—C10—H10	124.1
C10—N2—C12	107.3 (3)	C12—C11—N1	110.0 (3)

C10—N2—H2	126.3	C12—C11—H11	125.0
C12—N2—H2	126.3	N1—C11—H11	125.0
C13—N3—C14	104.7 (2)	C11—C12—N2	106.3 (4)
C13—N3—Ni1	124.44 (19)	C11—C12—H12	126.8
C14—N3—Ni1	130.84 (18)	N2—C12—H12	126.8
C13—N4—C15	107.1 (2)	N3—C13—N4	112.1 (3)
C13—N4—H4	126.5	N3—C13—H13	123.9
C15—N4—H4	126.5	N4—C13—H13	123.9
C16—N5—C17	104.2 (3)	C15—C14—N3	109.3 (3)
C16—N5—Ni1	126.9 (2)	C15—C14—H14	125.4
C17—N5—Ni1	128.8 (2)	N3—C14—H14	125.4
C16—N6—C18	106.8 (3)	N4—C15—C14	106.8 (3)
C16—N6—H6	126.6	N4—C15—H15	126.6
C18—N6—H6	126.6	C14—C15—H15	126.6
C19—N7—C20	104.3 (3)	N5—C16—N6	112.7 (3)
C19—N7—Ni1	125.8 (2)	N5—C16—H16	123.7
C20—N7—Ni1	129.4 (2)	N6—C16—H16	123.7
C19—N8—C21	107.5 (3)	C18—C17—N5	110.3 (3)
C19—N8—H8	126.2	C18—C17—H17	124.8
C21—N8—H8	126.2	N5—C17—H17	124.8
O2—C1—O1	122.5 (3)	C17—C18—N6	106.0 (3)
O2—C1—C2	118.9 (3)	C17—C18—H18	127.0
O1—C1—C2	118.5 (3)	N6—C18—H18	127.0
C4—C2—C3	114.1 (2)	N7—C19—N8	111.9 (3)
C4—C2—C1	112.8 (2)	N7—C19—H19	124.1
C3—C2—C1	111.7 (2)	N8—C19—H19	124.1
C4—C2—H2A	105.8	C21—C20—N7	110.1 (3)
C3—C2—H2A	105.8	C21—C20—H20	125.0
C1—C2—H2A	105.8	N7—C20—H20	125.0
O4—C3—O3	123.1 (3)	N8—C21—C20	106.2 (4)
O4—C3—C2	119.4 (3)	N8—C21—H21	126.9
O3—C3—C2	117.2 (3)	C20—C21—H21	126.9
C5—C4—C9	118.0 (3)		
O3—Ni1—O1—C1	−28.3 (3)	Ni1—O3—C3—O4	−161.4 (2)
N5—Ni1—O1—C1	−113.9 (3)	Ni1—O3—C3—C2	23.8 (4)
N7—Ni1—O1—C1	155.7 (3)	C4—C2—C3—O4	−6.3 (4)
N1—Ni1—O1—C1	63.9 (3)	C1—C2—C3—O4	123.0 (3)
O1—Ni1—O3—C3	15.1 (2)	C4—C2—C3—O3	168.7 (3)
N3—Ni1—O3—C3	−164.7 (2)	C1—C2—C3—O3	−61.9 (4)
N5—Ni1—O3—C3	103.4 (2)	C3—C2—C4—C5	−111.2 (3)
N1—Ni1—O3—C3	−72.8 (2)	C1—C2—C4—C5	120.0 (3)
O1—Ni1—N1—C10	−137.2 (3)	C3—C2—C4—C9	71.8 (4)
N3—Ni1—N1—C10	39.6 (3)	C1—C2—C4—C9	−57.1 (4)
O3—Ni1—N1—C10	−50.9 (3)	C9—C4—C5—C6	0.6 (5)
N7—Ni1—N1—C10	131.0 (3)	C2—C4—C5—C6	−176.6 (3)
O1—Ni1—N1—C11	30.7 (3)	C4—C5—C6—C7	0.8 (6)
N3—Ni1—N1—C11	−152.6 (3)	C5—C6—C7—C8	−1.1 (7)
O3—Ni1—N1—C11	117.0 (3)	C6—C7—C8—C9	0.1 (7)
N7—Ni1—N1—C11	−61.1 (3)	C7—C8—C9—C4	1.4 (6)

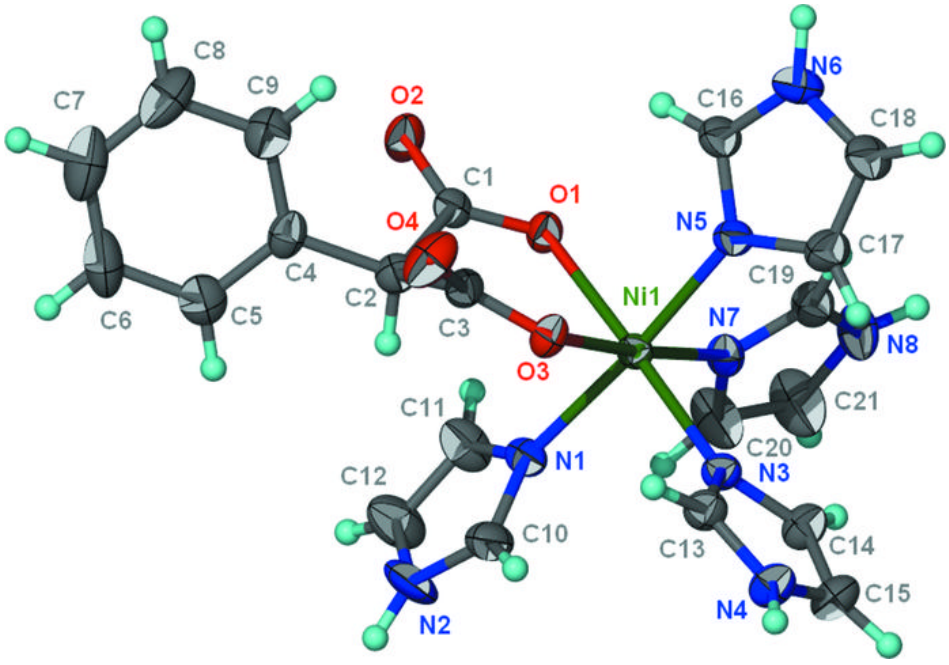
O3—Ni1—N3—C13	2.8 (3)	C5—C4—C9—C8	−1.7 (5)
N5—Ni1—N3—C13	88.3 (3)	C2—C4—C9—C8	175.4 (3)
N7—Ni1—N3—C13	178.9 (3)	C11—N1—C10—N2	0.3 (4)
N1—Ni1—N3—C13	−89.2 (3)	Ni1—N1—C10—N2	170.4 (2)
O3—Ni1—N3—C14	−175.9 (3)	C12—N2—C10—N1	0.5 (4)
N5—Ni1—N3—C14	−90.4 (3)	C10—N1—C11—C12	−1.0 (4)
N7—Ni1—N3—C14	0.2 (3)	Ni1—N1—C11—C12	−171.0 (3)
N1—Ni1—N3—C14	92.1 (3)	N1—C11—C12—N2	1.3 (5)
O1—Ni1—N5—C16	3.4 (3)	C10—N2—C12—C11	−1.1 (5)
N3—Ni1—N5—C16	−173.4 (3)	C14—N3—C13—N4	−0.4 (4)
O3—Ni1—N5—C16	−83.1 (3)	Ni1—N3—C13—N4	−179.4 (2)
N7—Ni1—N5—C16	95.3 (3)	C15—N4—C13—N3	−0.2 (4)
O1—Ni1—N5—C17	−173.2 (3)	C13—N3—C14—C15	0.8 (4)
N3—Ni1—N5—C17	10.1 (3)	Ni1—N3—C14—C15	179.7 (2)
O3—Ni1—N5—C17	100.3 (3)	C13—N4—C15—C14	0.7 (4)
N7—Ni1—N5—C17	−81.3 (3)	N3—C14—C15—N4	−1.0 (4)
O1—Ni1—N7—C19	92.3 (2)	C17—N5—C16—N6	−0.3 (4)
N3—Ni1—N7—C19	−87.6 (3)	Ni1—N5—C16—N6	−177.6 (2)
N5—Ni1—N7—C19	4.4 (3)	C18—N6—C16—N5	1.1 (4)
N1—Ni1—N7—C19	−179.5 (3)	C16—N5—C17—C18	−0.5 (4)
O1—Ni1—N7—C20	−96.5 (3)	Ni1—N5—C17—C18	176.7 (2)
N3—Ni1—N7—C20	83.5 (3)	N5—C17—C18—N6	1.2 (4)
N5—Ni1—N7—C20	175.5 (3)	C16—N6—C18—C17	−1.3 (4)
N1—Ni1—N7—C20	−8.4 (3)	C20—N7—C19—N8	−0.1 (4)
Ni1—O1—C1—O2	−176.5 (2)	Ni1—N7—C19—N8	172.8 (2)
Ni1—O1—C1—C2	−0.1 (4)	C21—N8—C19—N7	0.9 (5)
O2—C1—C2—C4	−4.3 (4)	C19—N7—C20—C21	−0.6 (5)
O1—C1—C2—C4	179.1 (3)	Ni1—N7—C20—C21	−173.2 (3)
O2—C1—C2—C3	−134.4 (3)	C19—N8—C21—C20	−1.2 (6)
O1—C1—C2—C3	49.0 (4)	N7—C20—C21—N8	1.2 (6)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O3^{i}	0.88	2.06	2.943 (3)	176
N4—H4···O1^{ii}	0.88	1.97	2.839 (3)	168
N6—H6···O2^{iii}	0.88	1.90	2.774 (3)	172
N8—H8···O4^{iv}	0.88	1.85	2.718 (3)	169

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

Fig. 1


C8
C9
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C5
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Ni1
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C18
N5
C17
C19
N7
N8
C21
C20
N3
C11
N1
C12
C10
C13
C14
C15
N4
N2