

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Aqua[2-(2-pyridylmethyliminomethyl)-phenolato]nickel(II) nitrate monohydrate

Ning Sheng

Department of Chemistry & Chemical Engineering, Jining University, Qufu 273155, People's Republic of China

Correspondence e-mail: jn_sning@126.com

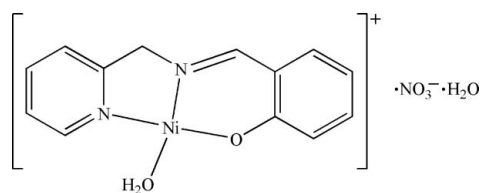
Received 8 August 2009; accepted 13 September 2009

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.033; wR factor = 0.086; data-to-parameter ratio = 12.5.

In the title compound, $[\text{Ni}(\text{C}_{13}\text{H}_{11}\text{N}_2\text{O})(\text{H}_2\text{O})]\text{NO}_3 \cdot \text{H}_2\text{O}$, the Ni(II) ion is coordinated by one O atom and two N atoms of the Schiff base ligand and the O atom from a water molecule, forming a slightly distorted square-planar geometry. A one-dimensional double-chain structure is formed along $[001]$ by $\text{O} \cdots \text{H}-\text{O}$ hydrogen bonds and the $\text{Ni} \cdots \text{O}$ $[2.617(3) \text{ \AA}]$ interactions.

Related literature

For background to Schiff bases in coordination chemistry, see: Boskovic *et al.* (2003); Koizumi *et al.* (2005); Oshio *et al.* (2005). For Ni—O and Ni—N bond distances in related structures, see: Wang *et al.* (2007).



Experimental

Crystal data

 $[\text{Ni}(\text{C}_{13}\text{H}_{11}\text{N}_2\text{O})(\text{H}_2\text{O})]\text{NO}_3 \cdot \text{H}_2\text{O}$ $M_r = 367.99$ Triclinic, $P\bar{1}$ $a = 7.7885(13) \text{ \AA}$ $b = 9.0155(15) \text{ \AA}$ $c = 11.3285(19) \text{ \AA}$ $\alpha = 71.244(2)^\circ$ $\beta = 85.846(3)^\circ$ $\gamma = 86.967(3)^\circ$ $V = 750.9(2) \text{ \AA}^3$ $Z = 2$ Mo $K\alpha$ radiation $\mu = 1.33 \text{ mm}^{-1}$ $T = 293 \text{ K}$ $0.27 \times 0.21 \times 0.15 \text{ mm}$

Data collection

Bruker APEXII CCD area-detector diffractometer

Absorption correction: multi-scan (SADABS; Sheldrick, 2003)

 $T_{\text{min}} = 0.716$, $T_{\text{max}} = 0.826$

3706 measured reflections

2610 independent reflections

2179 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.015$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.033$ $wR(F^2) = 0.086$ $S = 1.04$

2610 reflections

208 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.36 \text{ e \AA}^{-3}$ $\Delta\rho_{\text{min}} = -0.26 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{O6}-\text{H6A} \cdots \text{O1}^i$	0.83	2.12	2.930 (3)	165
$\text{O6}-\text{H6B} \cdots \text{O3}^{ii}$	0.82	2.00	2.819 (3)	172
$\text{O2}-\text{H2B} \cdots \text{O5}$	0.83	2.57	3.009 (3)	114
$\text{O2}-\text{H2B} \cdots \text{N3}$	0.83	2.53	3.234 (4)	143
$\text{O2}-\text{H2B} \cdots \text{O4}$	0.83	1.85	2.677 (3)	170
$\text{O2}-\text{H2A} \cdots \text{O6}$	0.83	1.86	2.681 (3)	168

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: XP (Sheldrick, 1998); software used to prepare material for publication: XP.

The author thanks Jining University for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2552).

References

- Boskovic, C., Bircher, R., Tregenna-Piggott, P. L. W., Gudel, H. U., Paulsen, C., Wernsdorfer, W., Barra, A. L., Khatsko, E., Neels, A. & Stoeckli-Evans, H. (2003). *J. Am. Chem. Soc.* **125**, 14046–14058.
- Bruker (2001). SAINT-Plus. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2004). APEX2. Bruker AXS Inc., Madison, Wisconsin, USA.
- Koizumi, S., Nihei, M., Nakano, M. & Oshio, H. (2005). *Inorg. Chem.* **44**, 1208–1210.
- Oshio, H., Nihei, M., Koizumi, S., Shiga, T., Nojiri, H., Nakano, M., Shirakawa, N. & Akatsu, M. (2005). *J. Am. Chem. Soc.* **127**, 4568–4569.
- Sheldrick, G. M. (1998). XP. Bruker AXS Inc., Madison, Wisconsin, USA.
- Sheldrick, G. M. (2003). SADABS. University of Göttingen, Germany.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Wang, Q., Li, X., Wang, X. & Zhang, Y. (2007). *Acta Cryst.* **E63**, m2537.

supporting information

Acta Cryst. (2009). E65, m1348 [https://doi.org/10.1107/S1600536809037027]

Aqua[2-(2-pyridylmethyliminomethyl)phenolato]nickel(II) nitrate monohydrate**Ning Sheng****S1. Comment**

Recently, Schiff base ligands, especially the relative flexible unsymmetrical tridentate Schiff base ligands and their hydrogenated derivatives have been employed to assembly alkoxo-or phenoxo-bridged clusters and polymers with beautiful molecular structures and interesting magnetic properties in the field of coordination chemistry. (Koizumi *et al.*, 2005; Boskovic *et al.*, 2003; Oshio *et al.*, 2005). Herein, we report the structure of a new nickel complex based on an unsymmetric tridentate Schiff base ligand. The title compound, which is comprised by $[\text{Ni}(L)(\text{H}_2\text{O})]^+$ ($L=2$ -(pyridin-2-ylmethyliminomethyl)phenol, nitrate anion and a free water molecule, crystallizes in triclinic cell setting and P-1 space group. The coordination sphere of the Ni ion can be described as slightly distorted square planar, in which three positions are occupied by two N atoms and one O atom from the asymmetric tridentate Schiff base ligand, and the other one coming from the O atom of the solvent water molecule. The bond distances of Ni—O and Ni—N are in the normal range compared to the reported complexes containing the N—Ni—O atoms (Wang *et al.*, 2007). The mean deviation of the plane formed by NiN_2O_2 unit is 0.0799 Å, and the Ni ion is only out of the plane 0.0514 Å. The distance between Ni and O5 is only 2.617 Å, indicative of significant interaction between these two atoms. Under the help of these interactions and the $\text{O}\cdots\text{H}-\text{O}$ hydrogen bonds between the O atoms of the water molecules (Table 1), the nitrate ion, and the Schiff base ligand, the asymmetric unit can be linked into one dimensional double chain supermolecular structure.

S2. Experimental

The Schiff base was synthesized by condensation 2-(aminomethyl)pyridine and 2-hydroxy-benzaldehyde with the ratio 1:1 in methanol. The synthesis of the title complex was carried out by treating $\text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (1 mmol, 290 mg) and the Schiff-base ligand (1 mmol, 212 mg) in methanol under the stirring condition at room temperature. The filtered solution was left to slowly evaporate in air to obtain single-crystal suitable for X-ray diffraction with a yield of about 202 mg, 55%.

S3. Refinement

All the H atoms bonded to the C atoms were placed using the HFIX commands in *SHELXL-97*, with C—H distances of 0.93 and 0.96 Å, and were allowed for as riding atoms with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. For the H atom of the water molecule, they were found from difference Fourier maps with the O—H bond length restrained to 0.82 Å and was allowed for as riding atoms with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$.

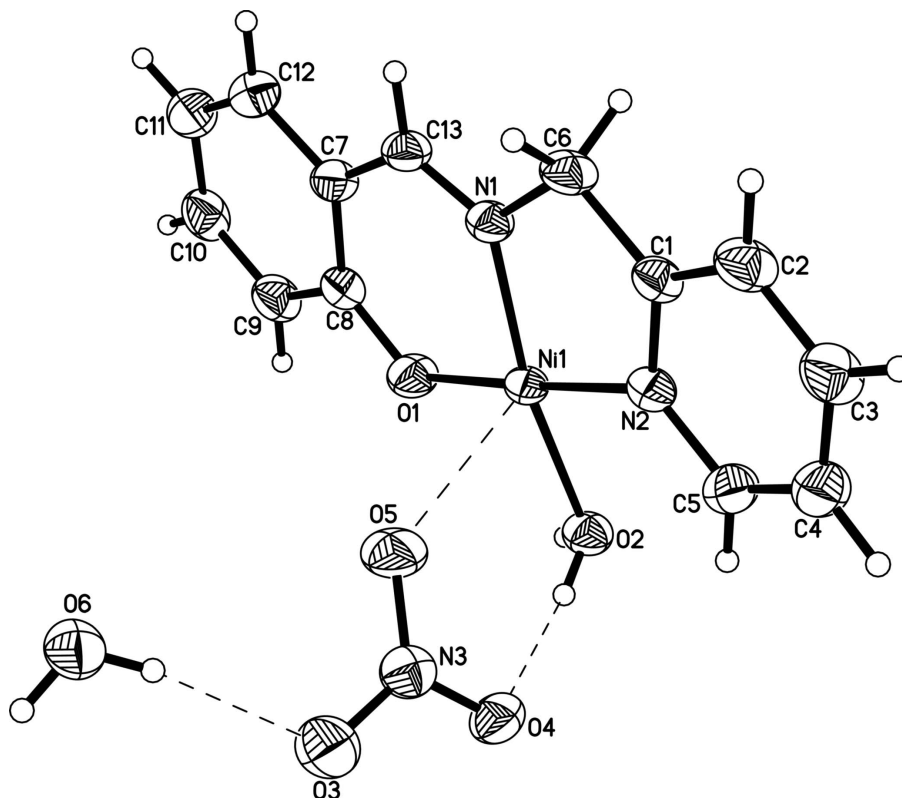


Figure 1

View of the title compound containing the hydrogen bonds with the atom-labelling scheme displacement ellipsoids are drawn at the 30% probability level.

Aqua[2-(2-pyridylmethyliminomethyl)phenolato]nickel(II) nitrate monohydrate

Crystal data

$[\text{Ni}(\text{C}_{13}\text{H}_{11}\text{N}_2\text{O})(\text{H}_2\text{O})]\text{NO}_3 \cdot \text{H}_2\text{O}$

$M_r = 367.99$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 7.7885(13) \text{ \AA}$

$b = 9.0155(15) \text{ \AA}$

$c = 11.3285(19) \text{ \AA}$

$\alpha = 71.244(2)^\circ$

$\beta = 85.846(3)^\circ$

$\gamma = 86.967(3)^\circ$

$V = 750.9(2) \text{ \AA}^3$

$Z = 2$

$F(000) = 380$

$D_x = 1.628 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 1525 reflections

$\theta = 2.5\text{--}25.8^\circ$

$\mu = 1.33 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Block, red-brown

$0.27 \times 0.21 \times 0.15 \text{ mm}$

Data collection

Bruker APEXII CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(SADABS; Sheldrick, 2003)

$T_{\text{min}} = 0.716$, $T_{\text{max}} = 0.826$

3706 measured reflections

2610 independent reflections

2179 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.015$

$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.4^\circ$

$h = -9 \rightarrow 9$

$k = -7 \rightarrow 10$

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.086$
 $S = 1.04$
 2610 reflections
 208 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0417P)^2 + 0.2147P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.36 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.26 \text{ e } \text{Å}^{-3}$

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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ni1	0.65546 (5)	0.59075 (4)	0.61677 (3)	0.03862 (14)
O1	0.6180 (3)	0.7356 (2)	0.45717 (19)	0.0534 (5)
O2	0.5125 (3)	0.7279 (2)	0.69276 (19)	0.0502 (5)
H2A	0.4512	0.7909	0.6414	0.060*
H2B	0.5764	0.7774	0.7215	0.060*
O3	1.0146 (3)	0.9237 (3)	0.7257 (3)	0.0827 (8)
O4	0.7495 (3)	0.8666 (3)	0.7775 (2)	0.0646 (6)
O5	0.8974 (3)	0.7562 (3)	0.6573 (3)	0.0743 (7)
O6	0.2993 (3)	0.9471 (2)	0.5530 (2)	0.0651 (6)
H6B	0.2135	0.9322	0.6016	0.078*
H6A	0.3320	1.0375	0.5370	0.078*
N1	0.7643 (3)	0.4328 (3)	0.5523 (2)	0.0427 (6)
N2	0.7069 (3)	0.4333 (3)	0.7799 (2)	0.0455 (6)
N3	0.8871 (4)	0.8476 (3)	0.7206 (2)	0.0550 (7)
C1	0.7858 (4)	0.2991 (3)	0.7729 (3)	0.0437 (7)
C2	0.8364 (4)	0.1813 (4)	0.8778 (3)	0.0586 (9)
H2	0.8902	0.0897	0.8707	0.070*
C3	0.8059 (5)	0.2014 (4)	0.9927 (3)	0.0642 (9)
H3	0.8397	0.1239	1.0646	0.077*
C4	0.7247 (5)	0.3378 (4)	1.0002 (3)	0.0626 (9)
H4	0.7027	0.3534	1.0771	0.075*
C5	0.6771 (4)	0.4494 (4)	0.8938 (3)	0.0583 (8)
H5	0.6215	0.5407	0.8999	0.070*
C6	0.8153 (4)	0.2851 (3)	0.6448 (3)	0.0511 (8)
H6C	0.9361	0.2608	0.6296	0.061*

H6D	0.7483	0.2008	0.6381	0.061*
C7	0.7468 (4)	0.5799 (3)	0.3335 (3)	0.0461 (7)
C8	0.6592 (4)	0.7162 (3)	0.3475 (3)	0.0452 (7)
C9	0.6142 (4)	0.8354 (4)	0.2387 (3)	0.0588 (9)
H9	0.5550	0.9250	0.2453	0.071*
C10	0.6560 (5)	0.8222 (4)	0.1225 (3)	0.0629 (9)
H10	0.6235	0.9025	0.0519	0.075*
C11	0.7465 (5)	0.6902 (4)	0.1084 (3)	0.0643 (9)
H11	0.7764	0.6833	0.0293	0.077*
C12	0.7902 (4)	0.5718 (4)	0.2126 (3)	0.0575 (8)
H12	0.8500	0.4836	0.2037	0.069*
C13	0.7934 (4)	0.4472 (3)	0.4359 (3)	0.0457 (7)
H13	0.8501	0.3636	0.4169	0.055*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0453 (2)	0.0280 (2)	0.0426 (2)	0.00371 (14)	0.00055 (15)	-0.01290 (15)
O1	0.0696 (14)	0.0374 (11)	0.0513 (13)	0.0101 (10)	-0.0023 (11)	-0.0135 (10)
O2	0.0555 (12)	0.0402 (11)	0.0564 (13)	0.0045 (9)	-0.0031 (10)	-0.0186 (10)
O3	0.0580 (16)	0.108 (2)	0.097 (2)	-0.0215 (15)	-0.0002 (14)	-0.0517 (18)
O4	0.0579 (14)	0.0783 (17)	0.0680 (15)	-0.0067 (12)	0.0113 (12)	-0.0402 (14)
O5	0.0684 (16)	0.0642 (15)	0.104 (2)	0.0061 (12)	0.0087 (14)	-0.0506 (16)
O6	0.0666 (15)	0.0451 (13)	0.0814 (17)	0.0045 (11)	0.0029 (13)	-0.0196 (12)
N1	0.0493 (14)	0.0332 (12)	0.0459 (14)	0.0027 (10)	-0.0025 (11)	-0.0138 (11)
N2	0.0533 (15)	0.0344 (13)	0.0489 (15)	-0.0009 (11)	-0.0015 (11)	-0.0140 (11)
N3	0.0629 (18)	0.0470 (16)	0.0534 (17)	0.0057 (13)	-0.0081 (14)	-0.0137 (13)
C1	0.0502 (17)	0.0327 (15)	0.0477 (17)	-0.0004 (12)	-0.0062 (14)	-0.0115 (13)
C2	0.077 (2)	0.0391 (17)	0.059 (2)	0.0045 (16)	-0.0157 (17)	-0.0128 (16)
C3	0.089 (3)	0.0478 (19)	0.052 (2)	-0.0025 (18)	-0.0216 (18)	-0.0066 (16)
C4	0.086 (3)	0.056 (2)	0.0450 (19)	-0.0036 (18)	-0.0088 (17)	-0.0147 (17)
C5	0.075 (2)	0.0503 (19)	0.051 (2)	0.0010 (16)	0.0011 (17)	-0.0200 (16)
C6	0.065 (2)	0.0321 (15)	0.0563 (19)	0.0097 (14)	-0.0091 (16)	-0.0153 (14)
C7	0.0525 (18)	0.0422 (17)	0.0462 (17)	-0.0014 (14)	-0.0051 (14)	-0.0174 (14)
C8	0.0491 (17)	0.0373 (16)	0.0490 (18)	-0.0039 (13)	-0.0041 (14)	-0.0126 (14)
C9	0.071 (2)	0.0417 (18)	0.060 (2)	-0.0040 (16)	-0.0066 (17)	-0.0100 (16)
C10	0.082 (2)	0.054 (2)	0.046 (2)	-0.0157 (18)	-0.0108 (17)	-0.0043 (16)
C11	0.082 (3)	0.067 (2)	0.047 (2)	-0.0143 (19)	-0.0020 (17)	-0.0204 (18)
C12	0.064 (2)	0.060 (2)	0.054 (2)	-0.0020 (16)	-0.0017 (16)	-0.0248 (17)
C13	0.0476 (17)	0.0392 (16)	0.0542 (19)	0.0031 (13)	-0.0008 (14)	-0.0215 (14)

Geometric parameters (Å, °)

Ni1—O1	1.891 (2)	C3—C4	1.377 (5)
Ni1—N1	1.931 (2)	C3—H3	0.9300
Ni1—O2	1.9777 (19)	C4—C5	1.359 (4)
Ni1—N2	1.987 (2)	C4—H4	0.9300
O1—C8	1.324 (3)	C5—H5	0.9300

O2—H2A	0.8290	C6—H6C	0.9700
O2—H2B	0.8324	C6—H6D	0.9700
O3—N3	1.251 (3)	C7—C12	1.411 (4)
O4—N3	1.243 (3)	C7—C8	1.422 (4)
O5—N3	1.251 (3)	C7—C13	1.425 (4)
O6—H6B	0.8225	C8—C9	1.402 (4)
O6—H6A	0.8261	C9—C10	1.374 (5)
N1—C13	1.287 (4)	C9—H9	0.9300
N1—C6	1.462 (4)	C10—C11	1.399 (5)
N2—C5	1.347 (4)	C10—H10	0.9300
N2—C1	1.350 (4)	C11—C12	1.363 (5)
C1—C2	1.381 (4)	C11—H11	0.9300
C1—C6	1.497 (4)	C12—H12	0.9300
C2—C3	1.374 (5)	C13—H13	0.9300
C2—H2	0.9300		
O1—Ni1—N1	94.39 (9)	C3—C4—H4	120.3
O1—Ni1—O2	89.12 (8)	N2—C5—C4	122.8 (3)
N1—Ni1—O2	170.48 (9)	N2—C5—H5	118.6
O1—Ni1—N2	176.56 (9)	C4—C5—H5	118.6
N1—Ni1—N2	82.56 (10)	N1—C6—C1	109.4 (2)
O2—Ni1—N2	94.14 (9)	N1—C6—H6C	109.8
C8—O1—Ni1	127.20 (18)	C1—C6—H6C	109.8
Ni1—O2—H2A	111.9	N1—C6—H6D	109.8
Ni1—O2—H2B	109.2	C1—C6—H6D	109.8
H2A—O2—H2B	109.2	H6C—C6—H6D	108.2
H6B—O6—H6A	110.5	C12—C7—C8	119.4 (3)
C13—N1—C6	118.2 (2)	C12—C7—C13	116.9 (3)
C13—N1—Ni1	125.4 (2)	C8—C7—C13	123.6 (3)
C6—N1—Ni1	116.37 (18)	O1—C8—C9	118.8 (3)
C5—N2—C1	117.8 (3)	O1—C8—C7	123.5 (3)
C5—N2—Ni1	127.0 (2)	C9—C8—C7	117.7 (3)
C1—N2—Ni1	115.2 (2)	C10—C9—C8	121.2 (3)
O4—N3—O5	120.7 (3)	C10—C9—H9	119.4
O4—N3—O3	118.9 (3)	C8—C9—H9	119.4
O5—N3—O3	120.4 (3)	C9—C10—C11	121.2 (3)
N2—C1—C2	122.1 (3)	C9—C10—H10	119.4
N2—C1—C6	116.1 (2)	C11—C10—H10	119.4
C2—C1—C6	121.8 (3)	C12—C11—C10	118.8 (3)
C3—C2—C1	119.0 (3)	C12—C11—H11	120.6
C3—C2—H2	120.5	C10—C11—H11	120.6
C1—C2—H2	120.5	C11—C12—C7	121.6 (3)
C2—C3—C4	119.1 (3)	C11—C12—H12	119.2
C2—C3—H3	120.5	C7—C12—H12	119.2
C4—C3—H3	120.5	N1—C13—C7	125.9 (3)
C5—C4—C3	119.3 (3)	N1—C13—H13	117.1
C5—C4—H4	120.3	C7—C13—H13	117.1

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O6—H6A \cdots O1 ⁱ	0.83	2.12	2.930 (3)	165
O6—H6B \cdots O3 ⁱⁱ	0.82	2.00	2.819 (3)	172
O2—H2B \cdots O5	0.83	2.57	3.009 (3)	114
O2—H2B \cdots N3	0.83	2.53	3.234 (4)	143
O2—H2B \cdots O4	0.83	1.85	2.677 (3)	170
O2—H2A \cdots O6	0.83	1.86	2.681 (3)	168

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