

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

catena-Poly[[*(nitrate-κ²O,O')*silver(I)]-*μ*-*N,N'*-bis(3-pyridylmethylidene)benzene-1,4-diamine]

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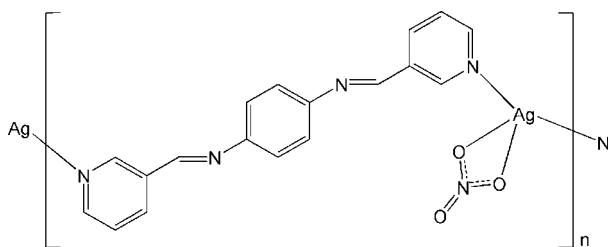
Received 13 June 2010; accepted 1 July 2010

 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.032; wR factor = 0.094; data-to-parameter ratio = 15.9.

In the title compound, $[\text{Ag}(\text{NO}_3)(\text{C}_{18}\text{H}_{14}\text{N}_4)]_n$, the Ag^{I} atom is coordinated by two N atoms from two *N,N'*-bis(3-pyridylmethylidene)benzene-1,4-diamine (bpbd) molecules and two O atoms from a bidentate nitrate anion. The bpbd molecules bridge the Ag atoms into a chain. Two adjacent chains are further connected by $\text{Ag} \cdots \text{Ag}$ interactions [3.1631 (8) Å], forming a double-chain structure. A π - π interaction [centroid-centroid distance = 3.758 (3) Å] occurs between the double chains. Interchain $\text{C}-\text{H} \cdots \text{O}$ hydrogen bonds are observed.

Related literature

For general background to metal-organic frameworks with bipyridine-type ligands, see: Biradha *et al.* (2006); Cunha-Silva *et al.* (2006); Lu *et al.* (2002); Ye *et al.* (2004).



Experimental

Crystal data

$[\text{Ag}(\text{NO}_3)(\text{C}_{18}\text{H}_{14}\text{N}_4)]$	$\gamma = 66.52$ (3)°
$M_r = 456.21$	$V = 857.6$ (4) Å ³
Triclinic, $P\bar{1}$	$Z = 2$
$a = 9.2148$ (18) Å	Mo $K\alpha$ radiation
$b = 9.771$ (2) Å	$\mu = 1.21$ mm ⁻¹
$c = 10.800$ (2) Å	$T = 293$ K
$\alpha = 81.51$ (3)°	$0.31 \times 0.30 \times 0.08$ mm
$\beta = 74.27$ (3)°	

Data collection

Rigaku R-Axis RAPID diffractometer	8493 measured reflections
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	3891 independent reflections
$T_{\text{min}} = 0.705$, $T_{\text{max}} = 0.908$	3163 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.019$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$	244 parameters
$wR(F^2) = 0.094$	H-atom parameters constrained
$S = 1.10$	$\Delta\rho_{\text{max}} = 0.72$ e Å ⁻³
3891 reflections	$\Delta\rho_{\text{min}} = -0.29$ e Å ⁻³

Table 1

Selected bond lengths (Å).

Ag1—N1	2.162 (2)	Ag1—O2	2.731 (3)
Ag1—N4 ⁱ	2.163 (2)	Ag1—O3	2.704 (3)

 Symmetry code: (i) $x + 2, y - 1, z - 1$.

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C1—H1A \cdots O3 ⁱⁱ	0.93	2.50	3.276 (4)	141
C16—H16A \cdots O2 ⁱⁱⁱ	0.93	2.44	3.280 (4)	151

 Symmetry codes: (ii) $-x + 3, -y, -z + 1$; (iii) $-x + 1, -y + 2, -z + 2$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

The authors thank the Natural Science Foundation of Heilongjiang Province (grant No. A200506), the Scientific Research Fund of Heilongjiang Provincial Education Department (grant No. 11553006) and the Doctoral Start-up Fund of Daqing Normal University (grant No. 08ZB02) for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2324).

References

- Biradha, K., Sarkar, M. & Rajput, L. (2006). *Chem. Commun.* pp. 4169–4171.
- Brandenburg, K. (1999). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
- Cunha-Silva, L., Westcot, A., Whitford, N. & Hardie, M. J. (2006). *Cryst. Growth Des.* **6**, 726–733.
- Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
- Lu, C.-Z., Wu, C.-D., Zhuang, H.-H. & Huang, J.-S. (2002). *Chem. Mater.* **14**, 2649–2653.
- Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Ye, K.-Q., Kong, J.-F., Jiang, S.-M. & Wang, Y. (2004). *J. Mol. Sci.* **20**, 1–5.

supporting information

Acta Cryst. (2010). E66, m903 [https://doi.org/10.1107/S1600536810025997]

catena-Poly[[nitrate- κ^2 O,O']silver(I)]- μ -N,N'-bis(3-pyridylmethylidene)benzene-1,4-diamine]**Yong-Hao Liu, Quan Xu and Zhi-You Han****S1. Comment**

Bipyridine-type ligands have been extensively investigated in recent years, owing to their simple structures, readily availabilities and more predictable formation of network structures (Biradha *et al.*, 2006; Cunha-Silva *et al.*, 2006; Lu *et al.*, 2002). Moreover, when introducing double Schiff-base, a great deal of metal–organic frameworks with unusual network patterns and novel properties can be achieved due to the specific geometry including the different relative orientation of N-donors and the zigzag conformation of the space moiety between the two terminal coordination groups (Ye *et al.*, 2004).

Herein, we choose 3,3'-bipyridine-type Schiff-base as an organic linking ligand. In this simple compound, N=C—H group can act as a hydrogen bonding donor and the pyridyl N atom as an acceptor. In the title complex, the ligand takes a bidentate bridging coordination fashion and links two Ag^I centers with two pyridyl N atoms (Fig. 1), forming a zigzag chain, with Ag—N distances being 2.162 (2) and 2.163 (2) Å (Table 1). The two neighboring Ag atoms exhibit an Ag \cdots Ag interaction, with a distance of 3.1631 (8) Å. The Ag atoms are also coordinated by distant nitrate O atoms [Ag—O = 2.731 (3) and 2.704 (3) Å], leading to a deviation from linearity [N—Ag—N = 159.44 (9)°]. Two adjacent chains are connected by the Ag \cdots Ag interactions into a double-chain structure (Fig. 2). A π – π interaction [centroid–centroid distance = 3.758 (3) Å] occurs between the double-chains. Interchain C—H \cdots O hydrogen bonds are observed (Table 2).

S2. Experimental

The ligand *L* was prepared according to the previous method (Ye *et al.*, 2004). 1,4-Diaminobenzene (2.14 mg, 10 mmol) was dissolved in methanol (20 ml), followed by addition of 3-pyridinecarboxaldehyde (4.24 mg, 40 mmol). The mixture was stirred at room temperature for 2 h and filtered. The resulting yellow crystalline solid was washed with methanol several times and dried in air. A solution of AgNO₃ (33.9 mg, 0.2 mmol) in acetonitrile (10 ml) was slowly layered onto a solution of *L* (117 mg, 0.625 mmol) in methylene chloride (10 ml). Diffusion between the two phases over a week produced colorless crystals.

S3. Refinement

H atoms were placed at calculated positions and refined as riding atoms, with H—C = 0.93 Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

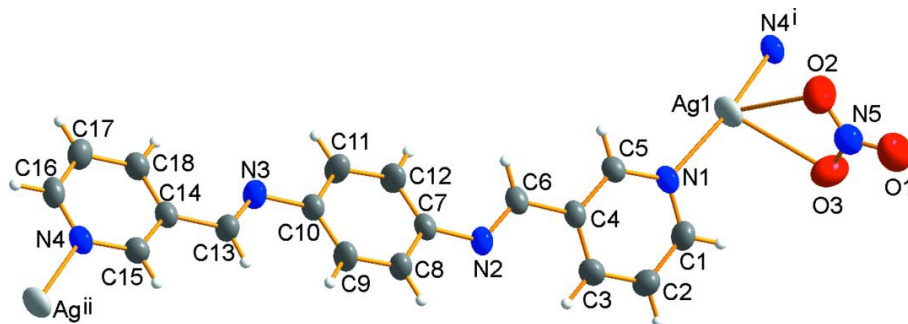


Figure 1

The asymmetric unit of the title compound with displacement ellipsoids shown at the 50% probability level. [Symmetry codes: (i) $2+x, -1+y, -1+z$; (ii) $-2+x, 1+y, 1+z$.]

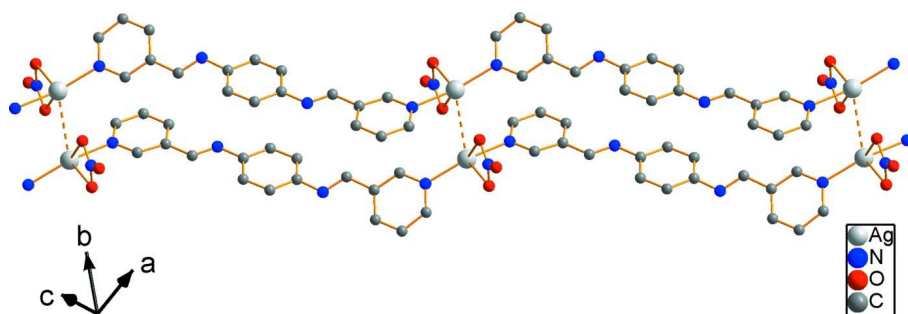


Figure 2

A view of the double-chain structure in the title compound.

catena-Poly[[*(nitrate-κ²O,O')*silver(I)]-*μ*-*N,N'*-bis(3-pyridylmethylidene)benzene-1,4-diamine]

Crystal data

[Ag(NO₃)(C₁₈H₁₄N₄)]

$M_r = 456.21$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 9.2148\ (18)\ \text{\AA}$

$b = 9.771\ (2)\ \text{\AA}$

$c = 10.800\ (2)\ \text{\AA}$

$\alpha = 81.51\ (3)^\circ$

$\beta = 74.27\ (3)^\circ$

$\gamma = 66.52\ (3)^\circ$

$V = 857.6\ (4)\ \text{\AA}^3$

$Z = 2$

$F(000) = 456$

$D_x = 1.767\ \text{Mg m}^{-3}$

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

Cell parameters from 3891 reflections

$\theta = 3.1\text{--}27.5^\circ$

$\mu = 1.21\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Block, colorless

$0.31 \times 0.30 \times 0.08\ \text{mm}$

Data collection

Rigaku R-AXIS RAPID

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: $10\ \text{pixels mm}^{-1}$

ω scans

Absorption correction: multi-scan

(*ABSCOR*; Higashi, 1995)

$T_{\min} = 0.705, T_{\max} = 0.908$

8493 measured reflections

3891 independent reflections

3163 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.019$

$\theta_{\max} = 27.5^\circ, \theta_{\min} = 3.1^\circ$

$h = -11 \rightarrow 11$

$k = -12 \rightarrow 12$

$l = -13 \rightarrow 14$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.032$ $wR(F^2) = 0.094$ $S = 1.10$

3891 reflections

244 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.059P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.002$ $\Delta\rho_{\max} = 0.72 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.29 \text{ e } \text{\AA}^{-3}$ *Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	1.45799 (2)	0.37548 (2)	0.45603 (2)	0.05309 (11)
N1	1.2254 (3)	0.3738 (2)	0.5682 (2)	0.0379 (5)
N2	0.6797 (3)	0.6198 (2)	0.8049 (2)	0.0394 (5)
N3	0.1476 (3)	1.1322 (2)	1.0027 (2)	0.0451 (5)
N4	-0.3549 (3)	1.3921 (2)	1.2898 (2)	0.0409 (5)
N5	1.7214 (3)	0.1260 (3)	0.5841 (3)	0.0519 (6)
O1	1.8206 (4)	0.0262 (4)	0.6349 (3)	0.0910 (9)
O2	1.6959 (3)	0.2598 (3)	0.5904 (3)	0.0794 (8)
O3	1.6440 (4)	0.0949 (3)	0.5224 (3)	0.0686 (7)
C1	1.2039 (3)	0.2446 (3)	0.5801 (3)	0.0447 (6)
H1A	1.2915	0.1601	0.5462	0.054*
C2	1.0576 (4)	0.2313 (3)	0.6405 (3)	0.0530 (7)
H2A	1.0457	0.1405	0.6437	0.064*
C3	0.9290 (3)	0.3543 (3)	0.6960 (3)	0.0468 (6)
H3A	0.8302	0.3470	0.7394	0.056*
C4	0.9491 (3)	0.4889 (3)	0.6862 (2)	0.0338 (5)
C5	1.0982 (3)	0.4942 (3)	0.6205 (2)	0.0358 (5)
H5A	1.1113	0.5850	0.6119	0.043*
C6	0.8148 (3)	0.6244 (3)	0.7420 (2)	0.0373 (5)
H6A	0.8299	0.7145	0.7306	0.045*
C7	0.5498 (3)	0.7521 (3)	0.8539 (2)	0.0356 (5)
C8	0.4388 (3)	0.7368 (3)	0.9655 (3)	0.0426 (6)
H8A	0.4528	0.6424	1.0046	0.051*
C9	0.3077 (3)	0.8597 (3)	1.0195 (3)	0.0464 (7)
H9A	0.2364	0.8481	1.0960	0.056*
C10	0.2824 (3)	1.0000 (3)	0.9596 (2)	0.0379 (5)
C11	0.3917 (4)	1.0142 (3)	0.8472 (3)	0.0492 (7)
H11A	0.3757	1.1081	0.8065	0.059*
C12	0.5248 (3)	0.8915 (3)	0.7937 (3)	0.0475 (7)
H12A	0.5968	0.9031	0.7176	0.057*
C13	0.0370 (3)	1.1306 (3)	1.0983 (3)	0.0421 (6)
H13A	0.0434	1.0412	1.1449	0.051*
C14	-0.1040 (3)	1.2686 (3)	1.1388 (2)	0.0372 (5)
C15	-0.2228 (3)	1.2683 (3)	1.2502 (3)	0.0405 (6)

H15A	-0.2108	1.1795	1.2992	0.049*
C16	-0.3680 (3)	1.5191 (3)	1.2194 (3)	0.0432 (6)
H16A	-0.4579	1.6051	1.2464	0.052*
C17	-0.2541 (3)	1.5289 (3)	1.1081 (3)	0.0456 (6)
H17A	-0.2665	1.6197	1.0622	0.055*
C18	-0.1215 (3)	1.4008 (3)	1.0666 (3)	0.0408 (6)
H18A	-0.0447	1.4036	0.9909	0.049*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.03204 (13)	0.06102 (16)	0.05624 (16)	-0.01785 (10)	0.01587 (10)	-0.02131 (11)
N1	0.0264 (10)	0.0419 (10)	0.0382 (11)	-0.0094 (9)	0.0035 (8)	-0.0110 (9)
N2	0.0282 (10)	0.0374 (10)	0.0411 (11)	-0.0048 (8)	0.0019 (9)	-0.0082 (9)
N3	0.0340 (11)	0.0366 (10)	0.0471 (12)	-0.0048 (9)	0.0079 (10)	-0.0068 (10)
N4	0.0270 (10)	0.0442 (11)	0.0430 (12)	-0.0088 (9)	0.0045 (9)	-0.0137 (10)
N5	0.0433 (13)	0.0540 (14)	0.0494 (14)	-0.0170 (12)	0.0032 (11)	-0.0059 (12)
O1	0.0671 (18)	0.092 (2)	0.106 (2)	-0.0279 (16)	-0.0287 (17)	0.0307 (18)
O2	0.0651 (16)	0.0626 (14)	0.111 (2)	-0.0149 (12)	-0.0198 (16)	-0.0331 (14)
O3	0.0859 (19)	0.0556 (12)	0.0735 (16)	-0.0326 (13)	-0.0263 (14)	0.0020 (12)
C1	0.0350 (13)	0.0367 (12)	0.0483 (15)	-0.0050 (11)	0.0031 (11)	-0.0087 (11)
C2	0.0443 (16)	0.0356 (12)	0.067 (2)	-0.0132 (12)	0.0051 (14)	-0.0053 (13)
C3	0.0344 (13)	0.0434 (13)	0.0524 (16)	-0.0143 (11)	0.0057 (12)	-0.0025 (12)
C4	0.0253 (11)	0.0378 (11)	0.0317 (11)	-0.0066 (9)	-0.0010 (9)	-0.0074 (10)
C5	0.0282 (11)	0.0388 (12)	0.0369 (12)	-0.0109 (10)	-0.0007 (10)	-0.0091 (10)
C6	0.0268 (11)	0.0417 (12)	0.0390 (13)	-0.0084 (10)	-0.0023 (10)	-0.0123 (11)
C7	0.0240 (11)	0.0386 (12)	0.0380 (12)	-0.0080 (9)	-0.0003 (10)	-0.0071 (10)
C8	0.0297 (12)	0.0362 (12)	0.0475 (15)	-0.0064 (10)	0.0032 (11)	-0.0002 (11)
C9	0.0316 (13)	0.0423 (13)	0.0453 (15)	-0.0056 (11)	0.0096 (11)	-0.0022 (12)
C10	0.0283 (12)	0.0352 (11)	0.0406 (13)	-0.0074 (10)	0.0033 (10)	-0.0073 (10)
C11	0.0411 (14)	0.0357 (12)	0.0488 (16)	-0.0065 (11)	0.0100 (12)	0.0018 (12)
C12	0.0365 (14)	0.0432 (13)	0.0432 (14)	-0.0090 (11)	0.0132 (11)	-0.0034 (12)
C13	0.0336 (13)	0.0327 (11)	0.0468 (14)	-0.0070 (10)	0.0049 (11)	-0.0053 (11)
C14	0.0269 (11)	0.0363 (11)	0.0413 (13)	-0.0084 (10)	0.0016 (10)	-0.0091 (10)
C15	0.0324 (12)	0.0390 (12)	0.0420 (13)	-0.0117 (10)	0.0026 (11)	-0.0044 (11)
C16	0.0290 (12)	0.0416 (13)	0.0487 (15)	-0.0033 (10)	-0.0023 (11)	-0.0127 (12)
C17	0.0398 (14)	0.0408 (13)	0.0461 (15)	-0.0073 (11)	-0.0069 (12)	-0.0004 (12)
C18	0.0319 (12)	0.0431 (13)	0.0391 (13)	-0.0113 (11)	0.0022 (10)	-0.0052 (11)

Geometric parameters (Å, °)

Ag1—N1	2.162 (2)	C4—C6	1.474 (3)
Ag1—N4 ⁱ	2.163 (2)	C5—H5A	0.9300
Ag1—O2	2.731 (3)	C6—H6A	0.9300
Ag1—O3	2.704 (3)	C7—C12	1.378 (4)
Ag1—Ag1 ⁱⁱ	3.1631 (8)	C7—C8	1.386 (3)
N1—C1	1.337 (4)	C8—C9	1.382 (3)
N1—C5	1.347 (3)	C8—H8A	0.9300

N2—C6	1.261 (3)	C9—C10	1.385 (4)
N2—C7	1.417 (3)	C9—H9A	0.9300
N3—C13	1.242 (3)	C10—C11	1.381 (4)
N3—C10	1.419 (3)	C11—C12	1.388 (4)
N4—C16	1.336 (4)	C11—H11A	0.9300
N4—C15	1.351 (3)	C12—H12A	0.9300
N5—O1	1.221 (4)	C13—C14	1.472 (3)
N5—O3	1.240 (4)	C13—H13A	0.9300
N5—O2	1.242 (4)	C14—C18	1.382 (4)
C1—C2	1.378 (4)	C14—C15	1.390 (3)
C1—H1A	0.9300	C15—H15A	0.9300
C2—C3	1.379 (4)	C16—C17	1.385 (4)
C2—H2A	0.9300	C16—H16A	0.9300
C3—C4	1.385 (4)	C17—C18	1.382 (4)
C3—H3A	0.9300	C17—H17A	0.9300
C4—C5	1.382 (3)	C18—H18A	0.9300
N1—Ag1—N4 ⁱ	159.44 (9)	C12—C7—C8	119.2 (2)
N1—Ag1—Ag1 ⁱⁱ	111.41 (6)	C12—C7—N2	123.7 (2)
N4 ⁱ —Ag1—Ag1 ⁱⁱ	79.97 (7)	C8—C7—N2	117.0 (2)
N1—Ag1—O2	112.93 (10)	C9—C8—C7	121.0 (2)
N1—Ag1—O3	97.63 (10)	C9—C8—H8A	119.5
N4 ⁱ —Ag1—O2	87.07 (9)	C7—C8—H8A	119.5
N4 ⁱ —Ag1—O3	92.98 (9)	C8—C9—C10	120.0 (2)
C1—N1—C5	117.7 (2)	C8—C9—H9A	120.0
C1—N1—Ag1	117.05 (16)	C10—C9—H9A	120.0
C5—N1—Ag1	125.13 (18)	C11—C10—C9	118.7 (2)
C6—N2—C7	120.2 (2)	C11—C10—N3	116.5 (2)
C13—N3—C10	121.8 (2)	C9—C10—N3	124.8 (2)
C16—N4—C15	117.8 (2)	C10—C11—C12	121.4 (3)
C16—N4—Ag1 ⁱⁱⁱ	122.67 (17)	C10—C11—H11A	119.3
C15—N4—Ag1 ⁱⁱⁱ	119.45 (18)	C12—C11—H11A	119.3
O1—N5—O3	119.9 (3)	C7—C12—C11	119.6 (2)
O1—N5—O2	122.2 (3)	C7—C12—H12A	120.2
O3—N5—O2	117.9 (3)	C11—C12—H12A	120.2
N1—C1—C2	122.8 (2)	N3—C13—C14	120.8 (2)
N1—C1—H1A	118.6	N3—C13—H13A	119.6
C2—C1—H1A	118.6	C14—C13—H13A	119.6
C1—C2—C3	119.1 (3)	C18—C14—C15	118.7 (2)
C1—C2—H2A	120.5	C18—C14—C13	120.7 (2)
C3—C2—H2A	120.5	C15—C14—C13	120.7 (2)
C2—C3—C4	119.1 (3)	N4—C15—C14	122.5 (2)
C2—C3—H3A	120.5	N4—C15—H15A	118.8
C4—C3—H3A	120.5	C14—C15—H15A	118.8
C5—C4—C3	118.3 (2)	N4—C16—C17	123.2 (2)
C5—C4—C6	120.4 (2)	N4—C16—H16A	118.4
C3—C4—C6	121.3 (2)	C17—C16—H16A	118.4
N1—C5—C4	123.0 (2)	C18—C17—C16	118.5 (3)

N1—C5—H5A	118.5	C18—C17—H17A	120.7
C4—C5—H5A	118.5	C16—C17—H17A	120.7
N2—C6—C4	120.9 (2)	C14—C18—C17	119.3 (2)
N2—C6—H6A	119.6	C14—C18—H18A	120.3
C4—C6—H6A	119.6	C17—C18—H18A	120.3

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

Hydrogen-bond geometry (Å, °)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C1—H1A \cdots O3 ^{iv}	0.93	2.50	3.276 (4)	141
C16—H16A \cdots O2 ^v	0.93	2.44	3.280 (4)	151

Symmetry codes: (iv) $-x+3, -y, -z+1$; (v) $-x+1, -y+2, -z+2$.