Bis(isonicotinamide-κN)silver(I) trifluoromethanesulfonate acetonitrile disolvate

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The central AgI atom of the title salt, [Ag(INAM)2](CF3SO3)·2CH3CN, where
INAM is isonicotinamide (C6H6N2O), is twofold coordinated by the pyridine N
atoms of two isonicotinamide ligands creating a slightly distorted linear
molecular geometry. The formation of polymeric chains [[Ag(INAM)2]+]n, held
together by discrete hydrogen bonds through the amide group of the INAM
ligand leaves voids for non-coordinating acetonitrile molecules that interact the
silver metal center via regium bonds.

Structure description
Silver(I) isonicotinamide complexes have been investigated for the ability to form
coordination complexes with a variety of molecular geometries due to amide hydrogen-
bond synthons in their structure (Aakerøy & Beatty, 1998; Aakerøy et al., 1998; Lian et al.
2007), luminescent properties (Yesīel et al., 2012), and antibacterial activity (Abu-
Youssef et al., 2007; Yu et al., 2020). Our research group interest currently lies in the
synthesis of novel metal complexes with biological activity; as part of our research in this
area, herein, we describe the synthesis and structure of the title silver(I) complex.

As depicted in Fig. 1, the asymmetric unit of the title compound shows the AgI ion in a
distorted linear coordination environment defined by two N-bonded isonicotamide
ligands. Two acetonitrile molecules and a trifluoromethanesulfonate ion complete the
asymmetric unit; the acetonitrile molecules sit at opposite sides of the plane defined by
N1—Ag1—N3 with the nitrile group facing the silver(I) metal center. All relevant bond
lengths and angles involving the Ag atom are presented in Table 1. The angle N1—Ag1—
N3 of 172.78 (7) is within the reported values (174.9, 180, and 171.1) in the comparable
silver(I) isonicotinamide structures currently available in the CSD (version 5.42 with
Two types of hydrogen-bonding motifs are present in the crystal lattice, with numerical values collated in Table 2. In the crystal packing, molecules self-assemble into layers aligned along the $a$-axis direction (Fig. 2) via $\mathrm{N—H—O}$ interactions. The trifluoromethanesulfonate anions fill the void between the layers and interact with the isonicotinamide ligands through additional $\mathrm{N—H—O}$ interactions. The pyridyl rings of the isonicotinamide ligand show $\pi—\pi$ stacking interactions with centroid-to-centroid ($\mathrm{Cg—Cg}$) distances ranging from 3.7005 (13) to 3.8503 (14) Å, and offset distances ranging from 1.940 to 2.056 Å, respectively.

| Table 1 | Selected geometric parameters (Å, °). |
|---------|---------------------------------------|
| Ag1—N3 | 2.162 (2) |
| Ag1—N1 | 2.162 (2) |
| N1—Ag1—N3 | 172.78 (7) |
| N4—Cl2—C9 | 118.3 (2) |

| Table 2 | Hydrogen-bond geometry (Å, °). |
|---------|---------------------------------|
| D—H—A—D' | D—H | H—A | D—A | D—H—A |
| N2—H2A—O2'' | 0.88 | 2.06 | 2.898 (3) | 160 |
| N2—H2B—O3 | 0.88 | 2.09 | 2.939 (3) | 162 |
| N4—H4A—O1'' | 0.88 | 2.05 | 2.927 (3) | 171 |
| N4—H4B—O5'' | 0.88 | 2.22 | 3.033 (3) | 154 |

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

| Table 3 | Experimental details. |
|---------|-----------------------|
| Crystal data | [Ag(\(\text{C}_6\text{H}_5\text{N}_2\text{O}_2\))_2(\text{CF}_3\text{O}_3\text{S})-2\text{C}_2\text{H}_3\text{N}] |
| Chemical formula | \(583.30\) |
| Crystal system, space group | Triclinic, $P\bar{1}$ |
| Temperature (K) | 100 |
| $a$, $b$, $c$ (Å) | 9.4566 (2), 11.0330 (3), 11.9848 (3) |
| $\alpha$, $\beta$, $\gamma$ (°) | 114.000 (2), 103.9287 (19), 95.129 (2) |
| $V$ (Å$^3$) | 1083.72 (5) |
| Data collection | XtaLAB Synergy, Dualflex, HyPix Gaussian (CrysAlis PRO; Rigaku OD, 2019) |
| No. of measured, independent and observed $|I| > 2\sigma(I)$ reflections | 24470, 4387, 4211 |
| Refinement | R($|F|^2 > 2\sigma(|F|^2)$), wR($|F|^2$), $S$ |
| No. of reflections | 4387 |
| No. of parameters | 300 |
| H-atom treatment | H-atom parameters constrained |
| Computer programs: CrysAlis PRO (Rigaku OD, 2019), SHELXT (Sheldrick, 2015a), SHELXL2018/5 (Sheldrick, 2015b), and OLEX2 (Dolomanov et al., 2009). |

Two types of hydrogen-bonding motifs are present in the crystal lattice, with numerical values collated in Table 2. In the crystal packing, molecules self-assemble into layers aligned along the $a$-axis direction (Fig. 2) via $\mathrm{N—H—O}$ interactions. The trifluoromethanesulfonate anions fill the void between the layers and interact with the isonicotinamide ligands through additional $\mathrm{N—H—O}$ interactions. The pyridyl rings of the isonicotinamide ligand show $\pi—\pi$ stacking interactions with centroid-to-centroid ($\mathrm{Cg—Cg}$) distances ranging from 3.7005 (13) to 3.8503 (14) Å, and offset distances ranging from 1.940 to 2.056 Å, respectively.
Two different supramolecular interactions involving the silver atom are also responsible for the observed crystal packing: an Ag⋯Ag interaction with a distance between silver atoms of 3.4258 (3) Å, comparable to other silver complexes found in the CSD database (Titov et al., 2018; refcode FINWOR; Titov et al., 2019; refcode PIRCUR); and regio bonds, between the nitrogen of the acetonitrile solvent molecules and the silver atom (Alkorta et al., 2020; Zierkiewicz et al., 2018), with lengths of 2.916 Å for Ag1—N5 and 2.955 Å for Ag1—N6. (Fig. 3)

Synthesis and crystallization
Silver trifluoromethanesulfonate (0.200 g, 0.778 mmol) was added to an acetonitrile solution of isonicotinamide (0.190 g, 1.56 mmol) and stirred for 30 min. The resulting clear solution was used to grow crystals by vapor diffusion with diethyl ether at 278 K.

Refinement
Crystal data, data collection and structure refinement details are summarized in Table 3.

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full crystallographic data

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**Crystal data**

\[\text{[Ag(C}_6\text{H}_6\text{N}_2\text{O})_2](\text{CF}_3\text{O}_3\text{S})\cdot2\text{C}_2\text{H}_3\text{N}]\]

\[M_r = 583.30\]

Triclinic, \(P\overline{1}\)

\(a = 9.4566 \text{ (2) Å}\)

\(b = 11.0330 \text{ (3) Å}\)

\(c = 11.9848 \text{ (3) Å}\)

\(α = 114.000 \text{ (2)°}\)

\(β = 103.9287 \text{ (19)°}\)

\(γ = 95.129 \text{ (2)°}\)

\(V = 1083.72 \text{ (5) Å}^3\)

\(Z = 2\)

\(F(000) = 584\)

\(D_r = 1.788 \text{ Mg m}^{-3}\)

Cell parameters from 12499 reflections

\(θ = 4.2−76.2°\)

\(μ = 9.00 \text{ mm}^{-1}\)

\(T = 100 \text{ K}\)

Plate, clear colourless

\(0.27 \times 0.10 \times 0.07 \text{ mm}\)

**Data collection**

XtaLAB Synergy, Dualflex, HyPix diffractometer

Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source

Mirror monochromator

Detector resolution: 10.0000 pixels mm\(^{-1}\)

\(ω\) scans

Absorption correction: gaussian

(CrysAlisPro; Rigaku OD, 2019)

\(T_{\text{min}} = 0.544, T_{\text{max}} = 1.000\)

24470 measured reflections

4387 independent reflections

4211 reflections with \(I > 2σ(I)\)

\(R_{\text{int}} = 0.044\)

\(θ_{\text{max}} = 76.5°, θ_{\text{min}} = 4.2°\)

\(h = -10→11\)

\(k = -13→13\)

\(l = -15→14\)

**Refinement**

Refinement on \(F^2\)

Least-squares matrix: full

\(R[F^2 > 2σ(F^2)] = 0.027\)

\(wR(F^2) = 0.072\)

\(S = 1.08\)

4387 reflections

300 parameters

0 restraints

Primary atom site location: dual

H-atom site location: inferred from neighbouring sites

\(w = 1/\left[σ(F_c)^2 + (0.0394P)^2 + 0.7P\right]\)

where \(P = (F_c^2 + 2F_s^2)/3\)

\((Δ/σ)_{\text{max}} = 0.002\)

\(Δρ_{\text{max}} = 0.77 \text{ e Å}^{-3}\)

\(Δρ_{\text{min}} = -0.78 \text{ e Å}^{-3}\)

**Special details**

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.
Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

|   | x         | y         | z         | Uiso * / Ueq |
|---|-----------|-----------|-----------|-------------|
| Ag1 | 0.33026 (2) | 0.42666 (2) | 0.38452 (2) | 0.01913 (7) |
| S1  | 0.80813 (6) | 0.92406 (6) | 0.27008 (6) | 0.01835 (13) |
| F1  | 0.59457 (16) | 1.01941 (15) | 0.16879 (15) | 0.0272 (3) |
| F3  | 0.77762 (19) | 1.00737 (17) | 0.09034 (15) | 0.0314 (4) |
| F2  | 0.80186 (19) | 1.16528 (15) | 0.27750 (16) | 0.0353 (4) |
| O2  | −0.13731 (19) | 0.48669 (17) | 0.77676 (16) | 0.0195 (3) |
| O1  | 0.68870 (19) | 0.28645 (17) | −0.09989 (16) | 0.0209 (4) |
| O5  | 0.96843 (19) | 0.96695 (17) | 0.31236 (17) | 0.0238 (4) |
| O3  | 0.7525 (2) | 0.79175 (17) | 0.16192 (18) | 0.0263 (4) |
| N3  | 0.1996 (2) | 0.40757 (19) | 0.50408 (18) | 0.0151 (4) |
| N1  | 0.4587 (2) | 0.4184 (2) | 0.25573 (18) | 0.0156 (4) |
| O4  | 0.7400 (2) | 0.9518 (2) | 0.37019 (19) | 0.0350 (5) |
| N2  | 0.7732 (2) | 0.5144 (2) | −0.0006 (2) | 0.0191 (4) |
| H2A | 0.822879 | 0.511950 | −0.054633 | 0.023* |
| H2B | 0.774705 | 0.592520 | 0.062122 | 0.023* |
| N4  | −0.1246 (2) | 0.2695 (2) | 0.73398 (19) | 0.0184 (4) |
| H4A | −0.184009 | 0.264893 | 0.779082 | 0.022* |
| H4B | −0.088239 | 0.198602 | 0.695256 | 0.022* |
| N6  | 0.1601 (2) | 0.1602 (2) | 0.1866 (2) | 0.0262 (5) |
| N5  | 0.4275 (3) | 0.7251 (2) | 0.5268 (2) | 0.0325 (5) |
| C9  | 0.0129 (2) | 0.3874 (2) | 0.6467 (2) | 0.0150 (4) |
| C3  | 0.6141 (2) | 0.4105 (2) | 0.0827 (2) | 0.0149 (4) |
| C2  | 0.5905 (3) | 0.5331 (2) | 0.1669 (2) | 0.0164 (5) |
| H2  | 0.627509 | 0.615873 | 0.166627 | 0.020* |
| C10 | 0.0835 (2) | 0.5137 (2) | 0.6652 (2) | 0.0150 (4) |
| H10 | 0.068538 | 0.594775 | 0.726905 | 0.018* |
| C8  | 0.0393 (3) | 0.2713 (2) | 0.5556 (2) | 0.0167 (5) |
| H8  | −0.005429 | 0.183595 | 0.541580 | 0.020* |
| C11 | 0.1752 (3) | 0.5196 (2) | 0.5931 (2) | 0.0157 (4) |
| H11 | 0.223022 | 0.606106 | 0.606713 | 0.019* |
| C12 | −0.0895 (3) | 0.3837 (2) | 0.7243 (2) | 0.0158 (4) |
| C5  | 0.4811 (3) | 0.3005 (2) | 0.1740 (2) | 0.0174 (5) |
| H5  | 0.443286 | 0.219160 | 0.176380 | 0.021* |
| C6  | 0.6954 (3) | 0.3993 (2) | −0.0140 (2) | 0.0165 (5) |
| C1  | 0.5128 (3) | 0.5324 (2) | 0.2506 (2) | 0.0171 (5) |
| H1  | 0.496800 | 0.616240 | 0.307082 | 0.021* |
| C4  | 0.5567 (3) | 0.2924 (2) | 0.0869 (2) | 0.0165 (5) |
| H4  | 0.569408 | 0.206974 | 0.030278 | 0.020* |
| C7  | 0.1313 (3) | 0.2857 (2) | 0.4862 (2) | 0.0166 (5) |
| H7  | 0.147119 | 0.206188 | 0.423312 | 0.020* |
| C16 | 0.0818 (3) | 0.1753 (2) | 0.1065 (2) | 0.0220 (5) |
| C17 | −0.0166 (3) | 0.1959 (3) | 0.0045 (3) | 0.0261 (5) |
| H17A| −0.119652 | 0.152936 | −0.012235 | 0.039* |
| H17B| 0.012716 | 0.155320 | −0.073582 | 0.039* |
| H17C| −0.009032 | 0.293417 | 0.030980 | 0.039* |
|    |    |    |    |    |    |    |
|----|----|----|----|----|----|----|
| C14 | 0.5027 (3) | 0.8301 (3) | 0.5709 (3) | 0.0259 (6) |
| C13 | 0.7428 (3) | 1.0349 (2) | 0.1983 (2) | 0.0213 (5) |
| C15 | 0.6018 (3) | 0.9632 (3) | 0.6278 (3) | 0.0302 (6) |
| H15A | 0.642520 | 0.973096 | 0.563323 | 0.036* |
| H15B | 0.683648 | 0.971724 | 0.700319 | 0.036* |
| H15C | 0.545821 | 1.034243 | 0.657809 | 0.036* |

Atomic displacement parameters (Å²)

|    |    |    |    |    |    |    |
|----|----|----|----|----|----|----|
| Ag1 | 0.02101 (11) | 0.02377 (11) | 0.01987 (11) | 0.00738 (7) | 0.01347 (7) | 0.01206 (8) |
| S1 | 0.0220 (3) | 0.0175 (3) | 0.0209 (3) | 0.0087 (2) | 0.0108 (2) | 0.0103 (2) |
| F1 | 0.0224 (7) | 0.0293 (8) | 0.0322 (8) | 0.0106 (6) | 0.0075 (6) | 0.0153 (7) |
| F3 | 0.0405 (9) | 0.0372 (9) | 0.0328 (9) | 0.0161 (7) | 0.0204 (7) | 0.0243 (7) |
| F2 | 0.0379 (9) | 0.0142 (7) | 0.0423 (10) | 0.0057 (6) | 0.0000 (8) | 0.0083 (7) |
| O2 | 0.0237 (9) | 0.0203 (8) | 0.0220 (8) | 0.0116 (7) | 0.0139 (7) | 0.0113 (7) |
| O1 | 0.0266 (9) | 0.0191 (8) | 0.0220 (9) | 0.0069 (7) | 0.0151 (7) | 0.0093 (7) |
| O5 | 0.0220 (9) | 0.0198 (8) | 0.0302 (10) | 0.0066 (7) | 0.0069 (7) | 0.0117 (7) |
| O3 | 0.0290 (10) | 0.0154 (8) | 0.0335 (10) | 0.0036 (7) | 0.0094 (8) | 0.0100 (8) |
| N3 | 0.0163 (9) | 0.0182 (9) | 0.0141 (9) | 0.0071 (7) | 0.0076 (7) | 0.0080 (8) |
| N1 | 0.0157 (9) | 0.0194 (9) | 0.0153 (9) | 0.0062 (7) | 0.0073 (8) | 0.0092 (8) |
| O4 | 0.0402 (12) | 0.0530 (13) | 0.0336 (11) | 0.0270 (10) | 0.0243 (9) | 0.0294 (10) |
| N2 | 0.0229 (10) | 0.0198 (10) | 0.0190 (10) | 0.0041 (8) | 0.0137 (8) | 0.0089 (8) |
| N4 | 0.0220 (10) | 0.0187 (10) | 0.0229 (10) | 0.0086 (8) | 0.0154 (8) | 0.0116 (8) |
| N6 | 0.0259 (11) | 0.0295 (11) | 0.0251 (11) | 0.0045 (9) | 0.0108 (9) | 0.0125 (10) |
| N5 | 0.0456 (15) | 0.0285 (13) | 0.0290 (12) | 0.0141 (11) | 0.0177 (11) | 0.0133 (10) |
| C9 | 0.0143 (11) | 0.0192 (11) | 0.0139 (11) | 0.0049 (9) | 0.0044 (9) | 0.0093 (9) |
| C3 | 0.0132 (10) | 0.0173 (11) | 0.0165 (11) | 0.0050 (8) | 0.0047 (9) | 0.0092 (9) |
| C2 | 0.0174 (11) | 0.0175 (11) | 0.0178 (11) | 0.0058 (9) | 0.0069 (9) | 0.0098 (9) |
| C10 | 0.0163 (11) | 0.0156 (10) | 0.0135 (10) | 0.0061 (8) | 0.0054 (9) | 0.0058 (9) |
| C8 | 0.0178 (11) | 0.0167 (11) | 0.0184 (11) | 0.0047 (9) | 0.0075 (9) | 0.0091 (9) |
| C11 | 0.0161 (11) | 0.0164 (11) | 0.0164 (11) | 0.0052 (8) | 0.0053 (9) | 0.0085 (9) |
| C12 | 0.0151 (11) | 0.0198 (11) | 0.0147 (11) | 0.0057 (9) | 0.0055 (9) | 0.0088 (9) |
| C5 | 0.0175 (11) | 0.0171 (11) | 0.0200 (12) | 0.0040 (9) | 0.0074 (9) | 0.0094 (9) |
| C6 | 0.0143 (10) | 0.0207 (11) | 0.0180 (11) | 0.0068 (9) | 0.0057 (9) | 0.0107 (9) |
| C1 | 0.0184 (11) | 0.0183 (11) | 0.0174 (11) | 0.0060 (9) | 0.0072 (9) | 0.0091 (9) |
| C4 | 0.0177 (11) | 0.0169 (11) | 0.0162 (11) | 0.0054 (9) | 0.0074 (9) | 0.0070 (9) |
| C7 | 0.0201 (11) | 0.0161 (11) | 0.0158 (11) | 0.0059 (9) | 0.0082 (9) | 0.0072 (9) |
| C16 | 0.0253 (13) | 0.0204 (11) | 0.0227 (13) | 0.0038 (10) | 0.0143 (11) | 0.0081 (10) |
| C17 | 0.0293 (14) | 0.0265 (13) | 0.0261 (13) | 0.0082 (11) | 0.0116 (11) | 0.0131 (11) |
| C14 | 0.0328 (14) | 0.0335 (15) | 0.0226 (13) | 0.0188 (12) | 0.0154 (11) | 0.0170 (12) |
| C13 | 0.0243 (12) | 0.0169 (11) | 0.0247 (13) | 0.0077 (9) | 0.0091 (10) | 0.0095 (10) |
| C15 | 0.0310 (15) | 0.0315 (14) | 0.0327 (15) | 0.0113 (12) | 0.0126 (12) | 0.0162 (12) |

Geometric parameters (Å, °)

|        |        |        |        |        |        |
|--------|--------|--------|--------|--------|--------|
| Ag1—N3 | 2.162 (2) | C9—C12 | 1.505 (3) |
| Ag1—N1 | 2.162 (2) | C3—C2  | 1.396 (3) |
| Bond      | Length  | Bond      | Length  |
|-----------|---------|-----------|---------|
| S1—O5     | 1.4442 (18) | C3—C6     | 1.510 (3) |
| S1—O3     | 1.4433 (18) | C3—C4     | 1.390 (3) |
| S1—O4     | 1.434 (2)  | C2—H2     | 0.9500   |
| S1—C13    | 1.831 (2)  | C2—C1     | 1.380 (3) |
| F1—C13    | 1.337 (3)  | C10—H10   | 0.9500   |
| F3—C13    | 1.333 (3)  | C10—C11   | 1.378 (3) |
| F2—C13    | 1.331 (3)  | C8—H8     | 0.9500   |
| O2—C12    | 1.240 (3)  | C8—C7     | 1.380 (3) |
| O1—C6     | 1.235 (3)  | C11—H11   | 0.9500   |
| N3—C11    | 1.348 (3)  | C5—H5     | 0.9500   |
| N3—C7     | 1.347 (3)  | C5—C4     | 1.380 (3) |
| N1—C5     | 1.346 (3)  | C1—H1     | 0.9500   |
| N1—C1     | 1.345 (3)  | C4—H4     | 0.9500   |
| N2—H2A    | 0.8800    | C7—H7     | 0.9500   |
| N2—H2B    | 0.8800    | C16—C17   | 1.459 (4) |
| N2—C6     | 1.338 (3)  | C17—H17A  | 0.9800   |
| N4—H4A    | 0.8800    | C17—H17B  | 0.9800   |
| N4—H4B    | 0.8800    | C17—H17C  | 0.9800   |
| N4—C12    | 1.331 (3)  | C14—C15   | 1.460 (4) |
| N6—C16    | 1.144 (3)  | C15—H15A  | 0.9800   |
| N5—C14    | 1.141 (4)  | C15—H15B  | 0.9800   |
| C9—C10    | 1.395 (3)  | C15—H15C  | 0.9800   |
| C9—C8     | 1.395 (3)  |            |          |

| Bond      | Angle   | Bond      | Angle   |
|-----------|---------|-----------|---------|
| N1—Ag1—N3 | 172.78 (7) | O2—C12—C9 | 118.8 (2) |
| O5—S1—C13 | 103.79 (11) | N4—C12—C9 | 118.3 (2) |
| O3—S1—O5  | 113.68 (11) | N1—C5—H5  | 118.5   |
| O3—S1—C13 | 101.70 (11) | N1—C5—C4  | 122.9 (2) |
| O4—S1—O5  | 115.49 (12) | C4—C5—H5  | 118.5   |
| O4—S1—O3  | 116.01 (13) | O1—C6—N2  | 123.2 (2) |
| O4—S1—C13 | 103.62 (11) | O1—C6—C3  | 119.5 (2) |
| C11—N3—Ag1 | 119.93 (16) | N2—C6—C3  | 117.3 (2) |
| C7—N3—Ag1 | 121.89 (15) | N1—C1—C2  | 123.0 (2) |
| C7—N3—C11 | 118.0 (2)  | N1—C1—H1  | 118.5   |
| C5—N1—Ag1 | 122.04 (16) | C2—C1—H1  | 118.5   |
| C1—N1—Ag1 | 120.28 (16) | C3—C4—H4  | 120.3   |
| C1—N1—C5  | 117.6 (2)  | C5—C4—C3  | 119.4 (2) |
| H2A—N2—H2B | 120.0     | C5—C4—H4  | 120.3   |
| C6—N2—H2A | 120.0     | N3—C7—C8  | 122.9 (2) |
| C6—N2—H2B | 120.0     | N3—C7—H7  | 118.5   |
| H4A—N4—H4B | 120.0     | C8—C7—H7  | 118.5   |
| C12—N4—H4A | 120.0     | N6—C16—C17 | 179.3 (3) |
| C12—N4—H4B | 120.0     | C16—C17—H17A | 109.5 |
| C10—C9—C12 | 118.3 (2) | C16—C17—H17B | 109.5 |
| C8—C9—C10 | 118.2 (2) | C16—C17—H17C | 109.5 |
| C8—C9—C12 | 123.5 (2) | H17A—C17—H17B | 109.5 |
| C2—C3—C6  | 123.5 (2) | H17A—C17—H17C | 109.5 |
| C4—C3—C2  | 117.9 (2) | H17B—C17—H17C | 109.5 |
C4—C3—C6 118.5 (2) N5—C14—C15 178.8 (3)
C3—C2—H2 120.5 F1—C13—S1 110.99 (17)
C1—C2—C3 119.1 (2) F3—C13—S1 111.58 (16)
C1—C2—H2 120.5 F3—C13—F1 107.2 (2)
C9—C10—H10 120.3 F2—C13—F3 107.6 (2)
C9—C8—H8 120.5 C14—C15—H15A 109.5
C7—C8—C9 118.9 (2) C14—C15—H15B 109.5
C7—C8—H8 120.5 C14—C15—H15C 109.5
N3—C11—C10 122.6 (2) H15A—C15—H15B 109.5
N3—C11—H11 118.7 H15A—C15—H15C 109.5
C10—C11—H11 118.7 H15B—C15—H15C 109.5
O2—C12—N4 122.8 (2)

Hydrogen-bond geometry (Å, °)

| D—H···A | D—H | H···A | D···A | D—H···A |
|----------|------|-------|-------|---------|
| N2—H2,A···O2|i | 0.88 | 2.06 | 2.898 (3) | 160 |
| N2—H2,B···O3 | 0.88 | 2.09 | 2.939 (3) | 162 |
| N4—H4,A···O1 | 0.88 | 2.05 | 2.927 (3) | 171 |
| N4—H4,B···O5 | 0.88 | 2.22 | 3.033 (3) | 154 |

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