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2-[(*E*)-(1,10-Phenanthrolin-5-yl)iminomethyl]phenol methanol monosolvate

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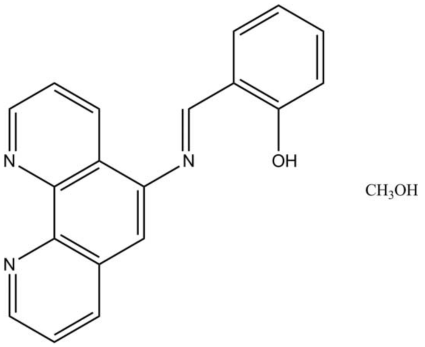
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.004 Å; R factor = 0.039; wR factor = 0.110; data-to-parameter ratio = 8.6.

In the title multi-donor Schiff base compound, $C_{19}H_{13}N_3O\cdot CH_3OH$, the dihedral angle between the mean planes of the phenanthroline and phenol rings is 59.3 (1)°. The Schiff base molecule is linked to the solvent molecule by an O—H⋯O hydrogen bond. In the crystal, the components are linked by O—H⋯N hydrogen bonds, weak O—H⋯N interactions and π–π stacking interactions [centroid–centroid distances = 3.701 (1) and 3.656 (1) Å].

Related literature

For the role played by 1,10-phenanthroline and its derivatives as molecular scaffolds for supramolecular assemblies, see: Balzani *et al.* (1996). For the metal-chelating properties of the 1,10-phenanthroline ligand, see: Sammes & Yahioglu (1994). For the photochemical and redox properties of phenanthroline rings, see: Camren *et al.* (1996); Bolger *et al.* (1996); Msood & Hodgson (1993). For Schiff bases as oxygen-carriers and as photochromic or thermochromic materials, see: Hobday & Smith (1973); Gul *et al.* (1986); Can & Bekaroglu (1988); Avciata *et al.* (1995, 1998); Demirhan *et al.* (2002). For the synthesis of 5-amino-1,10-phenanthroline, see: Gillard & Hill (1974). For related structures, see: Wu *et al.* (2011); Fun *et al.* (2010). For standard bond lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{19}H_{13}N_3O\cdot CH_4O$
M_r = 331.37
Monoclinic, Pc
a = 11.9398 (12) Å
b = 4.6680 (5) Å
c = 14.7818 (18) Å
β = 101.961 (11)°
V = 805.98 (16) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 0.73 mm^{-1}
T = 123 K
1.15 × 0.84 × 0.06 mm

Data collection

Oxford Diffraction Gemini-R diffractometer
Absorption correction: analytical [*CrysAlis RED* (Oxford Diffraction, 2007), using a multi-faceted crystal model (Clark & Reid, 1995)]
T_{min} = 0.505, T_{max} = 0.954
3176 measured reflections
1960 independent reflections
1885 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.110
S = 1.04
1960 reflections
229 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1—H1⋯O1S	0.84	1.81	2.640 (3)	172
O1S—H1S⋯N1^{i}	0.84	2.01	2.829 (3)	163
O1S—H1S⋯N2^{i}	0.84	2.68	3.242 (3)	126

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2007); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: JJ2127).

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o1174 Öztürk Yíldírím *et al.* • $C_{19}H_{13}N_3O{\cdot}CH_4O$ *Acta Cryst.* (2012). E**68**, o1173–o1174

supplementary materials

Acta Cryst. (2012). E**68**, o1173–o1174   [doi:10.1107/S1600536812011890]

2-[(*E*)-(1,10-Phenanthrolin-5-yl)iminomethyl]phenol methanol monosolvate

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Comment

1,10-Phenanthroline and its derivatives play important roles as molecular scaffolding for supramolecular assemblies (Balzani *et al.*, 1996). These have played a major role in the development of polypyridyl metal complexes. The metal chelating property of the 1,10-phenanthroline ligand and its derivatives have been utilized in a range of analytical reagents as well as for the development of bioinorganic probes (Sammes & Yahioglu, 1994). The photochemical and redox properties of complexes can be varied systematically through appropriate substitution on the phenanthroline rings (Camren *et al.*, 1996: Bolger *et al.*, 1996: Msood & Hodgson, 1993).

The coordination chemistry of Schiff bases derived from salicylaldehyde has been the subject of many studies because of their interesting properties; *e.g.* as oxygen-carriers to mimic some complicated biological systems, as photochromic or thermochromic materials (Hobday & Smith, 1973: Gul *et al.*, 1986: Can & Bekaroglu, 1988: Avciata *et al.* 1995; Avciata *et al.* 1998; Demirhan *et al.* 2002).

We report here the synthesis and characterization a new multidonor Schiff base derivative, (I), carrying N_3O donor atoms and prepared from the condensation reaction of 5-amino-1,10-phenanthroline with salicylaldehyde.

The title molecule $C_{19}H_{13}N_3O.CH_3OH$, crystallized as a methanol monosolvate (Fig. 1). All bond lengths are as expected (Allen *et al.*, 1987) and are comparable to those observed in related structures (Wu *et al.*, 2011; Fun *et al.*, 2010). The molecule is not planar, forming a dihedral angle of 59.3 (1)° between the mean planes of the phenanthroline (N1/N2/C1—C12) and phenol (C14—C19) rings.

In the crystal, O—H···N hydrogen bonds and weak O—H···N intermolecular interactions are observed (Table 1) as well as weak *π*-*π* stacking interactions [*Cg*1···*Cg*2 (*x*, 1+*y*, *z*) = 3.701 (1) Å and *Cg*1···*Cg*3 (*x*, 1+*y*,*z*) = 3.656 (1) Å, where *Cg*1(N1/C1—C4/C12), *Cg*2(N2/C7—C11) and *Cg*3(C4—C7/C11—C12) are the centroids of the phenonthroline ring], (Fig. 2).

Experimental

5-Amino-1,10-phenanthroline (Gillard & Hill, 1974) (1.5 g, 7.69 mmol) in 50 ml absolute methanol was added to salicylaldehyde (0.93 g, 7.69 mmol) dissolved in 20 ml diethylether and 100 ml absolute ethanol. After refluxing this mixture for 4.5 h, the precipitate was filtered off and then washed with water and ether. The product was obtained as a yellow precipitate (70° yield). It was soluble in methanol, ethanol and chloroform. Yield 1.79 g (78%). m.p. 451–453 K; Anal. Calcd. for $C_{19}H_{13}N_3O.CH_3OH$ (299.32 g/mol) C, 74.24; H, 4.38; N, 14.04. Found: C, 74.86; H, 4.12; N, 14.66.

Refinement

H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with O—H = 0.84 Å, C—H = 0.95–0.98 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ or $U_{iso}(H) = 1.5\ U_{eq}(CH_3$ and O).

Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2007); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

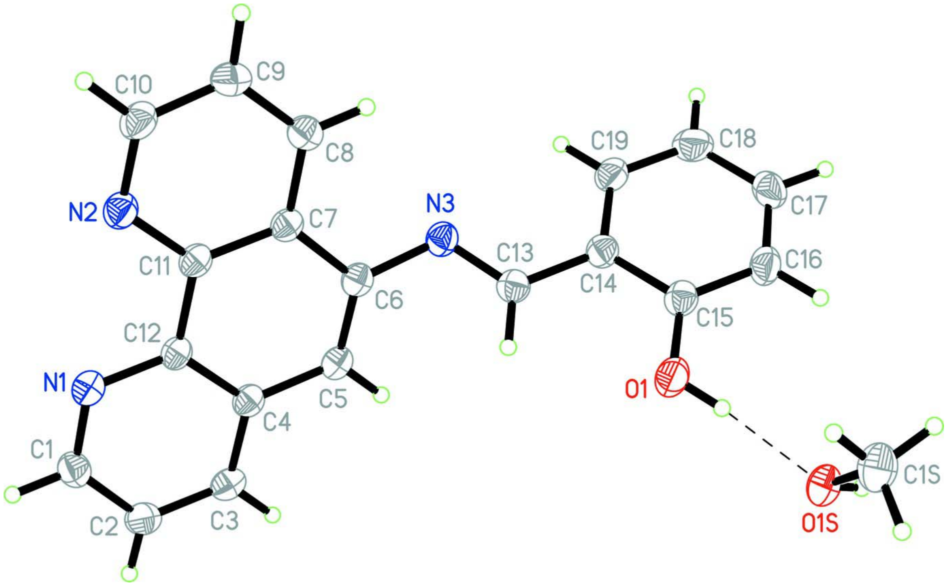

Figure 1

View of the molecular structure of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level for non-hydrogen atoms. Hydrogen bonds are drawn as dashed lines.

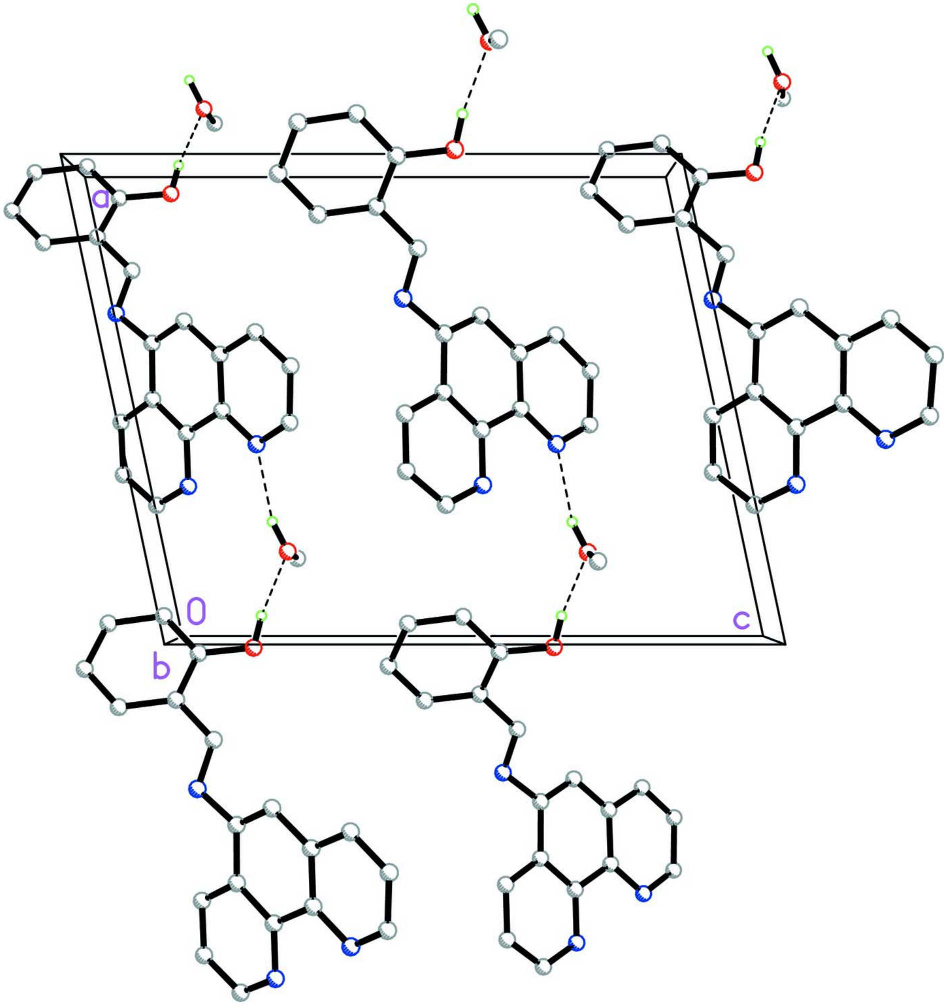

Figure 2

The molecular packing of the title compound. Hydrogen bonds are drawn as dashed lines.

2-[(*E*)-(1,10-Phenanthrolin-5-yl)iminomethyl]phenol methanol monosolvate

Crystal data

$C_{19}H_{13}N_3O{\cdot}CH_4O$	$F(000) = 348$
$M_r = 331.37$	$D_x = 1.365$ Mg m^{-3}
Monoclinic, *Pc*	Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Hall symbol: P -2yc	Cell parameters from 1347 reflections
$a = 11.9398$ (12) Å	$\theta = 3.1$–$75.2°$
$b = 4.6680$ (5) Å	$\mu = 0.73$ mm^{-1}
$c = 14.7818$ (18) Å	$T = 123$ K
$\beta = 101.961$ (11)°	Triangular plate, yellow
$V = 805.98$ (16) Å^3	$1.15 \times 0.84 \times 0.06$ mm
$Z = 2$	

Data collection

Oxford Diffraction Gemini-R diffractometer	Graphite monochromator
Radiation source: Enhance (Cu) X-ray Source	Detector resolution: 10.5081 pixels mm^{-1}
	ω scans

Absorption correction: analytical [*CrysAlis RED* (Oxford Diffraction, 2007), using a multi-faceted crystal model (Clark & Reid, 1995)]
T_{min} = 0.505, T_{max} = 0.954
3176 measured reflections
1960 independent reflections
1885 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 75.2°, θ_{min} = 3.1°
$h = -13 \rightarrow 14$
$k = -5 \rightarrow 5$
$l = -18 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.110$
$S = 1.04$
1960 reflections
229 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0747P)^2 + 0.0897P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Absolute structure: Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881, 303 Friedel pairs
Flack parameter: −1.5 (18)

Special details

Experimental. The crystal was very fragile. On cutting the crystal shattered so an incident collimator of 1.0 mm was used.
IR (KBr): 3435(Ar—OH), 3020(Ar), 1616 (C=N—C). ^{13} C NMR, 167 (C—OH), 165 (C=C—N), 150,152 and 148 (C=N) p.p.m.. LC—MS, m/*z* (%): 298 (*M*-1). In the electronic spectrum two band appears at 281 and 340 nm which can be assigned to the π -π * and n-π * transition of C=C and C=N group.
The FTIR spectra were obtained on a Perkin Elmer Spectrum One Bv 5.0 spectrophotometer. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Varian UNITY INOVA 500 MHz s pectrometer. Mass spectra were measured on a FinniganTM LCQTM Advantage MAX spectrometer. Electronic spectra were obtained on a Agilent 8453 UV-Vis. Spectroscopy System. Elemental analyses were obtained on a Thermo Finnigan Flash EA 112. All other chemicals employed were of the highest grade available.
Absorption correction: CrysAlis RED, (Oxford Diffraction, 2007) Analytical numeric absorption correction using a multifaceted crystal model (Clark & Reid, 1995).

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}
O1	0.98484 (16)	1.4695 (5)	0.63127 (14)	0.0337 (4)
H1	1.0514	1.5260	0.6545	0.051*
O1S	1.18635 (15)	1.6610 (4)	0.71862 (14)	0.0307 (4)
H1S	1.2497	1.6321	0.7038	0.046*
N1	0.41348 (18)	0.5215 (5)	0.70687 (15)	0.0254 (4)
N2	0.32594 (18)	0.8980 (5)	0.56783 (15)	0.0268 (4)
N3	0.70428 (17)	1.0456 (5)	0.50248 (15)	0.0256 (4)

C1	0.4567 (2)	0.3337 (6)	0.77219 (17)	0.0275 (5)
H1A	0.4061	0.2468	0.8058	0.033*
C2	0.5729 (2)	0.2556 (6)	0.79469 (18)	0.0291 (5)
H2A	0.5997	0.1206	0.8424	0.035*
C3	0.6463 (2)	0.3780 (5)	0.74647 (18)	0.0265 (5)
H3A	0.7252	0.3282	0.7600	0.032*
C4	0.60430 (19)	0.5796 (5)	0.67619 (16)	0.0233 (5)
C5	0.6784 (2)	0.7166 (5)	0.62454 (17)	0.0237 (5)
H5A	0.7577	0.6711	0.6372	0.028*
C6	0.63612 (19)	0.9123 (5)	0.55719 (16)	0.0234 (5)
C7	0.5151 (2)	0.9788 (5)	0.53588 (16)	0.0227 (5)
C8	0.4682 (2)	1.1790 (6)	0.46665 (17)	0.0258 (5)
H8A	0.5159	1.2761	0.4326	0.031*
C9	0.3527 (2)	1.2309 (6)	0.44944 (19)	0.0299 (5)
H9A	0.3191	1.3639	0.4030	0.036*
C10	0.2852 (2)	1.0854 (6)	0.50113 (19)	0.0297 (5)
H10A	0.2052	1.1223	0.4879	0.036*
C11	0.4404 (2)	0.8465 (5)	0.58528 (16)	0.0233 (5)
C12	0.48604 (19)	0.6424 (5)	0.65842 (16)	0.0221 (5)
C13	0.8014 (2)	1.1466 (6)	0.54239 (17)	0.0252 (5)
H13A	0.8229	1.1375	0.6079	0.030*
C14	0.8805 (2)	1.2756 (5)	0.49080 (18)	0.0258 (5)
C15	0.9738 (2)	1.4372 (5)	0.53890 (18)	0.0268 (5)
C16	1.0503 (2)	1.5581 (6)	0.4904 (2)	0.0311 (5)
H16A	1.1138	1.6655	0.5226	0.037*
C17	1.0351 (2)	1.5235 (6)	0.3963 (2)	0.0358 (6)
H17A	1.0878	1.6080	0.3641	0.043*
C18	0.9425 (2)	1.3650 (8)	0.3476 (2)	0.0382 (6)
H18A	0.9323	1.3405	0.2826	0.046*
C19	0.8661 (2)	1.2446 (6)	0.39525 (18)	0.0305 (5)
H19A	0.8027	1.1387	0.3623	0.037*
C1S	1.1695 (2)	1.9603 (6)	0.7274 (2)	0.0368 (6)
H1S1	1.2045	2.0217	0.7903	0.055*
H1S2	1.0873	2.0020	0.7150	0.055*
H1S3	1.2051	2.0636	0.6829	0.055*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0270 (8)	0.0449 (11)	0.0295 (9)	−0.0100 (8)	0.0067 (7)	−0.0060 (8)
O1S	0.0226 (8)	0.0333 (9)	0.0364 (10)	−0.0025 (7)	0.0064 (7)	−0.0027 (8)
N1	0.0220 (9)	0.0255 (10)	0.0282 (10)	−0.0003 (8)	0.0040 (8)	−0.0010 (9)
N2	0.0228 (9)	0.0262 (10)	0.0310 (11)	0.0006 (8)	0.0047 (8)	0.0015 (8)
N3	0.0223 (10)	0.0280 (10)	0.0269 (10)	−0.0002 (8)	0.0061 (8)	−0.0011 (8)
C1	0.0298 (12)	0.0264 (12)	0.0271 (12)	−0.0032 (10)	0.0081 (10)	0.0005 (10)
C2	0.0306 (12)	0.0284 (12)	0.0262 (12)	−0.0009 (10)	0.0011 (9)	0.0011 (9)
C3	0.0243 (11)	0.0253 (11)	0.0277 (12)	0.0021 (9)	0.0002 (9)	−0.0014 (10)
C4	0.0227 (12)	0.0209 (10)	0.0255 (12)	−0.0011 (9)	0.0029 (9)	−0.0024 (9)
C5	0.0203 (10)	0.0243 (11)	0.0260 (11)	0.0004 (9)	0.0035 (8)	−0.0032 (9)
C6	0.0236 (11)	0.0220 (10)	0.0244 (11)	−0.0013 (9)	0.0044 (9)	−0.0041 (9)

C7	0.0227 (10)	0.0212 (10)	0.0233 (11)	−0.0013 (8)	0.0025 (9)	−0.0029 (9)
C8	0.0286 (12)	0.0246 (11)	0.0242 (11)	−0.0008 (9)	0.0053 (9)	−0.0010 (9)
C9	0.0309 (13)	0.0298 (11)	0.0272 (11)	0.0032 (10)	0.0022 (10)	0.0041 (10)
C10	0.0225 (12)	0.0290 (12)	0.0363 (13)	0.0035 (9)	0.0032 (10)	0.0019 (11)
C11	0.0221 (11)	0.0217 (10)	0.0250 (11)	−0.0013 (8)	0.0024 (9)	−0.0033 (9)
C12	0.0206 (10)	0.0206 (11)	0.0246 (11)	−0.0011 (8)	0.0034 (9)	−0.0023 (9)
C13	0.0241 (11)	0.0259 (11)	0.0257 (11)	0.0017 (9)	0.0057 (8)	0.0000 (9)
C14	0.0214 (10)	0.0268 (11)	0.0294 (12)	0.0020 (9)	0.0056 (9)	0.0022 (10)
C15	0.0222 (10)	0.0275 (11)	0.0308 (12)	0.0021 (9)	0.0056 (9)	0.0002 (10)
C16	0.0215 (11)	0.0326 (13)	0.0397 (14)	−0.0031 (10)	0.0072 (10)	0.0021 (11)
C17	0.0248 (11)	0.0432 (14)	0.0417 (15)	0.0030 (11)	0.0123 (10)	0.0150 (12)
C18	0.0313 (13)	0.0560 (18)	0.0273 (12)	0.0040 (12)	0.0061 (10)	0.0063 (12)
C19	0.0228 (11)	0.0403 (14)	0.0279 (12)	−0.0011 (10)	0.0039 (9)	0.0007 (11)
C1S	0.0318 (13)	0.0350 (14)	0.0451 (16)	−0.0016 (11)	0.0115 (11)	−0.0054 (12)

Geometric parameters (Å, º)

O1—C15	1.353 (3)	C7—C8	1.413 (3)
O1—H1	0.8400	C8—C9	1.371 (4)
O1S—C1S	1.421 (3)	C8—H8A	0.9500
O1S—H1S	0.8400	C9—C10	1.396 (4)
N1—C1	1.327 (3)	C9—H9A	0.9500
N1—C12	1.356 (3)	C10—H10A	0.9500
N2—C10	1.333 (3)	C11—C12	1.459 (3)
N2—C11	1.359 (3)	C13—C14	1.462 (3)
N3—C13	1.277 (3)	C13—H13A	0.9500
N3—C6	1.406 (3)	C14—C19	1.395 (4)
C1—C2	1.406 (4)	C14—C15	1.410 (3)
C1—H1A	0.9500	C15—C16	1.393 (3)
C2—C3	1.365 (4)	C16—C17	1.374 (4)
C2—H2A	0.9500	C16—H16A	0.9500
C3—C4	1.414 (4)	C17—C18	1.399 (4)
C3—H3A	0.9500	C17—H17A	0.9500
C4—C12	1.412 (3)	C18—C19	1.382 (4)
C4—C5	1.434 (3)	C18—H18A	0.9500
C5—C6	1.368 (3)	C19—H19A	0.9500
C5—H5A	0.9500	C1S—H1S1	0.9800
C6—C7	1.447 (3)	C1S—H1S2	0.9800
C7—C11	1.407 (3)	C1S—H1S3	0.9800
C15—O1—H1	109.5	C9—C10—H10A	118.0
C1S—O1S—H1S	109.5	N2—C11—C7	123.0 (2)
C1—N1—C12	117.7 (2)	N2—C11—C12	117.5 (2)
C10—N2—C11	117.1 (2)	C7—C11—C12	119.5 (2)
C13—N3—C6	118.4 (2)	N1—C12—C4	122.6 (2)
N1—C1—C2	124.0 (2)	N1—C12—C11	118.80 (19)
N1—C1—H1A	118.0	C4—C12—C11	118.6 (2)
C2—C1—H1A	118.0	N3—C13—C14	122.3 (2)
C3—C2—C1	118.5 (2)	N3—C13—H13A	118.9
C3—C2—H2A	120.8	C14—C13—H13A	118.9

C1—C2—H2A	120.8	C19—C14—C15	119.0 (2)
C2—C3—C4	119.6 (2)	C19—C14—C13	121.9 (2)
C2—C3—H3A	120.2	C15—C14—C13	119.1 (2)
C4—C3—H3A	120.2	O1—C15—C16	122.5 (2)
C12—C4—C3	117.6 (2)	O1—C15—C14	118.0 (2)
C12—C4—C5	120.8 (2)	C16—C15—C14	119.4 (2)
C3—C4—C5	121.6 (2)	C17—C16—C15	120.7 (2)
C6—C5—C4	120.6 (2)	C17—C16—H16A	119.7
C6—C5—H5A	119.7	C15—C16—H16A	119.7
C4—C5—H5A	119.7	C16—C17—C18	120.5 (3)
C5—C6—N3	122.9 (2)	C16—C17—H17A	119.7
C5—C6—C7	120.2 (2)	C18—C17—H17A	119.7
N3—C6—C7	116.8 (2)	C19—C18—C17	119.2 (3)
C11—C7—C8	117.9 (2)	C19—C18—H18A	120.4
C11—C7—C6	120.3 (2)	C17—C18—H18A	120.4
C8—C7—C6	121.8 (2)	C18—C19—C14	121.2 (2)
C9—C8—C7	118.9 (2)	C18—C19—H19A	119.4
C9—C8—H8A	120.5	C14—C19—H19A	119.4
C7—C8—H8A	120.5	O1S—C1S—H1S1	109.5
C8—C9—C10	119.0 (2)	O1S—C1S—H1S2	109.5
C8—C9—H9A	120.5	H1S1—C1S—H1S2	109.5
C10—C9—H9A	120.5	O1S—C1S—H1S3	109.5
N2—C10—C9	124.1 (2)	H1S1—C1S—H1S3	109.5
N2—C10—H10A	118.0	H1S2—C1S—H1S3	109.5

C12—N1—C1—C2	0.7 (4)	C6—C7—C11—C12	0.2 (3)
N1—C1—C2—C3	−0.4 (4)	C1—N1—C12—C4	−1.2 (3)
C1—C2—C3—C4	0.4 (4)	C1—N1—C12—C11	179.1 (2)
C2—C3—C4—C12	−0.8 (3)	C3—C4—C12—N1	1.2 (3)
C2—C3—C4—C5	179.2 (2)	C5—C4—C12—N1	−178.7 (2)
C12—C4—C5—C6	0.3 (3)	C3—C4—C12—C11	−179.1 (2)
C3—C4—C5—C6	−179.6 (2)	C5—C4—C12—C11	1.0 (3)
C4—C5—C6—N3	−177.8 (2)	N2—C11—C12—N1	−2.0 (3)
C4—C5—C6—C7	−1.3 (3)	C7—C11—C12—N1	178.5 (2)
C13—N3—C6—C5	−46.2 (3)	N2—C11—C12—C4	178.3 (2)
C13—N3—C6—C7	137.3 (2)	C7—C11—C12—C4	−1.2 (3)
C5—C6—C7—C11	1.1 (3)	C6—N3—C13—C14	176.8 (2)
N3—C6—C7—C11	177.8 (2)	N3—C13—C14—C19	−13.4 (4)
C5—C6—C7—C8	−179.8 (2)	N3—C13—C14—C15	166.3 (2)
N3—C6—C7—C8	−3.1 (3)	C19—C14—C15—O1	178.7 (2)
C11—C7—C8—C9	−1.3 (3)	C13—C14—C15—O1	−1.0 (3)
C6—C7—C8—C9	179.6 (2)	C19—C14—C15—C16	−1.0 (3)
C7—C8—C9—C10	0.3 (4)	C13—C14—C15—C16	179.3 (2)
C11—N2—C10—C9	−0.4 (4)	O1—C15—C16—C17	−179.1 (2)
C8—C9—C10—N2	0.6 (4)	C14—C15—C16—C17	0.7 (4)
C10—N2—C11—C7	−0.7 (3)	C15—C16—C17—C18	−0.3 (4)
C10—N2—C11—C12	179.8 (2)	C16—C17—C18—C19	0.3 (4)
C8—C7—C11—N2	1.6 (3)	C17—C18—C19—C14	−0.7 (4)
C6—C7—C11—N2	−179.3 (2)	C15—C14—C19—C18	1.1 (4)

C8—C7—C11—C12	−178.9 (2)	C13—C14—C19—C18	−179.2 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O1*S*	0.84	1.81	2.640 (3)	172
O1*S*—H1*S*···N1^{i}	0.84	2.01	2.829 (3)	163
O1*S*—H1*S*···N2^{i}	0.84	2.68	3.242 (3)	126

Symmetry code: (i) *x*+1, *y*+1, *z*.