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2-[(*E*)-(Naphthalen-2-ylimino)methyl]-4-(trifluoromethoxy)phenolMerve Pekdemir,^{a*} Zarife Sibel Şahin,^a Şamil Işık,^a Ayşen Alaman Açar,^b Sema Öztürk Yıldırım^{c,d} and Ray J. Butcher^d

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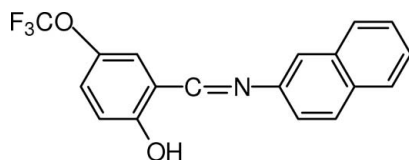
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Key indicators: single-crystal X-ray study; $T = 123$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.049; wR factor = 0.130; data-to-parameter ratio = 13.1.

In the title compound, $\text{C}_{18}\text{H}_{12}\text{F}_3\text{NO}_2$, the planes of the benzene ring and the naphthalene system form a dihedral angle of $47.21(3)^\circ$. The hydroxy group is involved in an intramolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bond. In the crystal, weak $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{F}$ interactions link the molecules related by translations along the c and a axes, respectively, into sheets.

Related literature

For background to photochromic and thermochromic characteristics and tautomerism of Schiff bases, see: Cohen *et al.* (1964); Hadjoudis *et al.* (1987). For related structures, see: Gül *et al.* (2007); Yüce *et al.* (2004). For classification of hydrogen-bonding patterns, see: Bernstein *et al.* (1995).



Experimental

Crystal data

 $\text{C}_{18}\text{H}_{12}\text{F}_3\text{NO}_2$ $M_r = 331.29$

Monoclinic, $P2_1/c$
 $a = 17.0813(10)$ Å
 $b = 14.1248(8)$ Å
 $c = 6.1900(5)$ Å
 $\beta = 99.669(6)^\circ$
 $V = 1472.25(17)$ Å³

$Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.12$ mm⁻¹
 $T = 123$ K
 $0.50 \times 0.40 \times 0.18$ mm

Data collection

Oxford Diffraction Gemini-R diffractometer
Absorption correction: analytical [CrysAlis RED (Oxford Diffraction, 2007) based on Clark

& Reid (1995)
 $T_{\min} = 0.941$, $T_{\max} = 0.978$
15270 measured reflections
2892 independent reflections
2497 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.050$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.049$
 $wR(F^2) = 0.130$
 $S = 1.09$
2892 reflections
221 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.31$ e Å⁻³
 $\Delta\rho_{\min} = -0.22$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---|----------|-------------|-------------|---------------|
| $\text{O1}-\text{H1}\cdots\text{N1}$ | 0.90 (3) | 1.77 (3) | 2.5904 (18) | 150 (2) |
| $\text{C10}-\text{H10}\cdots\text{O1}^i$ | 0.93 | 2.57 | 3.473 (2) | 165 |
| $\text{C5}-\text{H5}\cdots\text{F2}^{ii}$ | 0.93 | 2.57 | 3.487 (2) | 170 |

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2007); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2007); data reduction: *CrysAlis PRO* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5250).

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supporting information

Acta Cryst. (2012). E68, o1024 [https://doi.org/10.1107/S1600536812009361]

2-[(*E*)-(Naphthalen-2-ylimino)methyl]-4-(trifluoromethoxy)phenol

Merve Pekdemir, Zarife Sibel Şahin, Şamil Işık, Ayşen Alaman Ağar, Sema Öztürk Yıldırım and Ray J. Butcher

S1. Comment

There are two characteristic properties of Schiff bases, *viz.* photochromism and thermochromism (Cohen *et al.*, 1964). These properties result from proton transfer from the hydroxyl O atom to the imine N atom (Hadjoudis *et al.*, 1987). There are two types of intramolecular hydrogen bonds in Schiff bases, which may be stabilized in keto-amine (N—H \cdots O hydrogen bond) or phenol-imine (N \cdots H—O hydrogen bond) tautomeric forms (Hadjoudis *et al.*, 1987). Herewith we present the title compound (I), which exhibits the phenol-imine tautomeric form (Fig. 1).

In (I), the C1—N1 bond length of 1.417 (2) Å agrees with the matching distance in 1-{4-[2-hydroxy-benzylidene)amino]phenyl}ethanone [1.4138 (17) Å; Yüce *et al.*, 2004]. The N1=C11 bond length of 1.284 (2) Å is typical of a double bond, like to the matching bond length in (*E*)-2-[(3-trifluoromethylphenylimino)methyl]-4-methylphenol [1.280 (2) Å; Gül *et al.*, 2007]. The O1—C17 distance of 1.349 (2) Å is similar to the worth of 1.352 (3) Å in (*E*)-2-[(3-trifluoromethylphenylimino)methyl]-4-methylphenol (Gül *et al.*, 2007). Fig.1 additionally shows a strong intramolecular hydrogen bond (O1—H1 \cdots N1) can be defined as an S(6) motif (Bernstein *et al.*, 1995). The O1—N1 distance of 2.590 (2) Å is comparable to those observed for same hydrogen bonds in 1-{4-[(2-hydroxy-benzylidene)amino]phenyl}ethanone [2.594 (2) Å; Yüce *et al.*, 2004].

The molecules are linked into sheets by a combination of C—H \cdots O and C—H \cdots F interactions (Table 1). The atom C10 in the reference molecule at (*x*, *y*, *z*) acts as a hydrogen-bond donor, *via* H10, to atom O1 in the molecule at (*x*, *y*, *z* + 1), so forming a C(8) chain running parallel to the [001] direction. Similarly, atom C5 in the molecule at (*x*, *y*, *z*) acts as a hydrogen-bond donor, *via* H5, to atom F2 in the molecule at (*x* + 1, *y*, *z*), so forming a C(14) chain running parallel to the [100] direction. The combination of the C(8) and C(14) chains generates a chain edge-fused $R_5^5(36)$ rings running parallel to the *ac* plane (Fig.2)

S2. Experimental

The title compound, (I), was prepared by reflux a mixture of a solution containing 2-hydroxy-5-(trifluoromethoxy)-benzaldehyde (0.045 g 0.23 mmol) in 20 ml ethanol and a solution containing 2-Naphthyamine (0.033 g 0.23 mmol) in 20 ml ethanol. The reaction mixture was stirred for 1 h under reflux. The crystals of (I) suitable for X-ray analysis were obtained from ethylalcohol by slow evaporation (yield % 68; m.p.369–371 K).

S3. Refinement

The H1 atom was located in a difference map, and isotropically refined with restraint of O—H=0.82 (2) Å. All other H atoms were placed in calculated positions and constrained to ride on their parents atoms, with C—H=0.93 Å and $U_{\text{iso}}(\text{H})=1.2U_{\text{eq}}(\text{C})$.

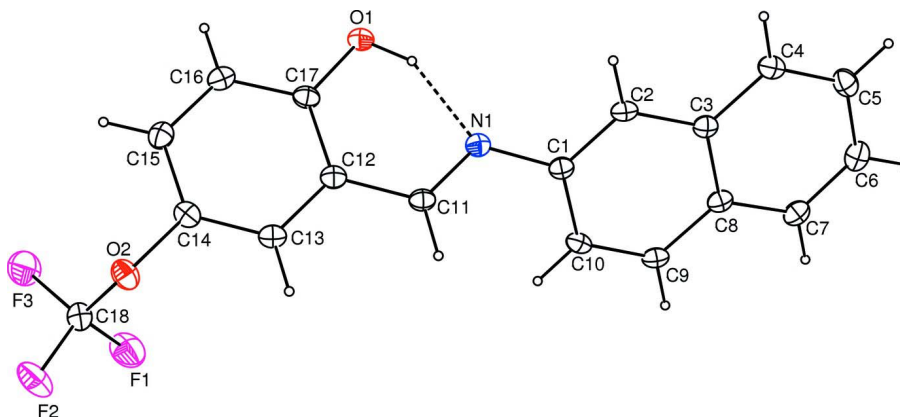


Figure 1

The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability. Dashed line denotes hydrogen bond.

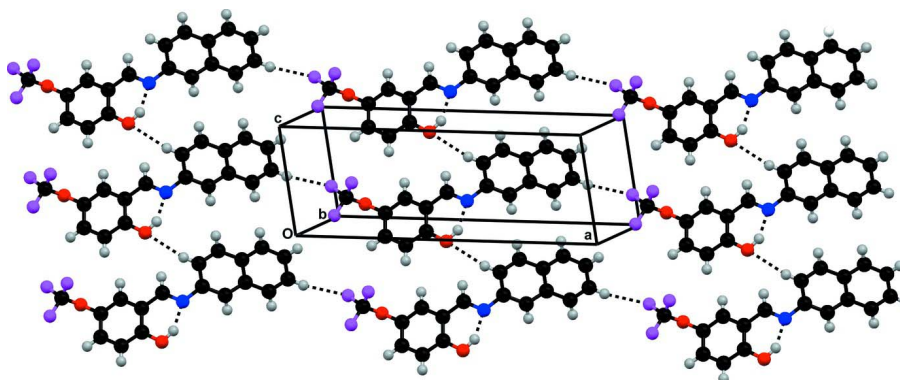


Figure 2

A portion of the crystal packing showing hydrogen bonds as dashed lines.

2-[(E)-(Naphthalen-2-ylimino)methyl]-4-(trifluoromethoxy)phenol

Crystal data

$C_{18}H_{12}F_3NO_2$

$M_r = 331.29$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 17.0813$ (10) Å

$b = 14.1248$ (8) Å

$c = 6.1900$ (5) Å

$\beta = 99.669$ (6)°

$V = 1472.25$ (17) Å³

$Z = 4$

$F(000) = 680$

$D_x = 1.495$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 5076 reflections

$\theta = 3.1$ – 34.9 °

$\mu = 0.12$ mm⁻¹

$T = 123$ K

Plate, yellow

$0.50 \times 0.40 \times 0.18$ mm

Data collection

Oxford Diffraction Gemini-R
diffractometer

Radiation source: Enhance (Mo) X-ray Source

Graphite monochromator

Detector resolution: 10.5081 pixels mm⁻¹

ω scans

Absorption correction: analytical

[*CrysAlis RED* (Oxford Diffraction, 2007)

based on Clark & Reid (1995)

$T_{\min} = 0.941$, $T_{\max} = 0.978$

15270 measured reflections

2892 independent reflections

2497 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.050$ $\theta_{\text{max}} = 26.0^\circ$, $\theta_{\text{min}} = 3.1^\circ$ $h = -20 \rightarrow 21$ $k = -17 \rightarrow 17$ $l = -7 \rightarrow 6$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.049$ $wR(F^2) = 0.130$ $S = 1.09$

2892 reflections

221 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sitesH atoms treated by a mixture of independent
and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.062P)^2 + 0.5277P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} < 0.001$ $\Delta\rho_{\text{max}} = 0.31 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\text{min}} = -0.22 \text{ e } \text{\AA}^{-3}$ *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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|------------|----------------------------------|
| C1 | 0.52707 (9) | 0.88417 (11) | 0.3403 (3) | 0.0225 (4) |
| C2 | 0.59465 (10) | 0.90836 (11) | 0.2604 (3) | 0.0225 (3) |
| H2 | 0.5903 | 0.9338 | 0.1203 | 0.027* |
| C3 | 0.67071 (9) | 0.89512 (10) | 0.3876 (3) | 0.0222 (3) |
| C4 | 0.74184 (10) | 0.91509 (11) | 0.3061 (3) | 0.0268 (4) |
| H4 | 0.7390 | 0.9413 | 0.1672 | 0.032* |
| C5 | 0.81420 (10) | 0.89635 (12) | 0.4287 (3) | 0.0313 (4) |
| H5 | 0.8601 | 0.9103 | 0.3729 | 0.038* |
| C6 | 0.82014 (11) | 0.85608 (12) | 0.6391 (3) | 0.0320 (4) |
| H6 | 0.8698 | 0.8424 | 0.7201 | 0.038* |
| C7 | 0.75296 (10) | 0.83705 (11) | 0.7244 (3) | 0.0275 (4) |
| H7 | 0.7573 | 0.8114 | 0.8642 | 0.033* |
| C8 | 0.67680 (10) | 0.85604 (11) | 0.6021 (3) | 0.0232 (4) |
| C9 | 0.60574 (10) | 0.83457 (11) | 0.6822 (3) | 0.0246 (4) |
| H9 | 0.6089 | 0.8110 | 0.8237 | 0.029* |
| C10 | 0.53290 (10) | 0.84767 (11) | 0.5564 (3) | 0.0244 (4) |
| H10 | 0.4871 | 0.8327 | 0.6121 | 0.029* |
| C11 | 0.38798 (10) | 0.90319 (11) | 0.2662 (3) | 0.0241 (4) |
| H11 | 0.3894 | 0.9215 | 0.4112 | 0.029* |
| C12 | 0.31186 (10) | 0.89349 (11) | 0.1221 (3) | 0.0236 (4) |
| C13 | 0.24206 (10) | 0.92206 (11) | 0.1940 (3) | 0.0246 (4) |

| | | | | |
|-----|--------------|--------------|-------------|------------|
| H13 | 0.2443 | 0.9475 | 0.3334 | 0.030* |
| C14 | 0.17025 (10) | 0.91238 (11) | 0.0580 (3) | 0.0265 (4) |
| C15 | 0.16428 (10) | 0.87238 (12) | -0.1487 (3) | 0.0285 (4) |
| H15 | 0.1150 | 0.8661 | -0.2381 | 0.034* |
| C16 | 0.23260 (10) | 0.84183 (12) | -0.2206 (3) | 0.0279 (4) |
| H16 | 0.2290 | 0.8130 | -0.3570 | 0.034* |
| C17 | 0.30663 (10) | 0.85398 (11) | -0.0901 (3) | 0.0248 (4) |
| C18 | 0.05121 (10) | 0.89134 (14) | 0.1960 (3) | 0.0335 (4) |
| F1 | 0.08590 (7) | 0.83013 (9) | 0.3436 (2) | 0.0551 (4) |
| F2 | -0.00045 (7) | 0.94076 (10) | 0.2849 (2) | 0.0537 (4) |
| F3 | 0.01029 (7) | 0.84060 (11) | 0.0357 (2) | 0.0614 (4) |
| N1 | 0.45326 (8) | 0.88684 (9) | 0.1961 (2) | 0.0241 (3) |
| O1 | 0.37203 (7) | 0.82747 (9) | -0.1701 (2) | 0.0301 (3) |
| O2 | 0.10202 (7) | 0.95092 (8) | 0.1277 (2) | 0.0328 (3) |
| H1 | 0.4140 (16) | 0.8422 (18) | -0.067 (5) | 0.066 (8)* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|------------|-------------|-------------|-------------|-------------|-------------|
| C1 | 0.0276 (8) | 0.0185 (8) | 0.0218 (8) | 0.0017 (6) | 0.0051 (7) | -0.0016 (6) |
| C2 | 0.0325 (9) | 0.0176 (7) | 0.0184 (8) | 0.0003 (6) | 0.0072 (7) | 0.0002 (6) |
| C3 | 0.0282 (8) | 0.0162 (7) | 0.0228 (8) | 0.0003 (6) | 0.0060 (7) | -0.0030 (6) |
| C4 | 0.0327 (9) | 0.0225 (8) | 0.0268 (9) | -0.0017 (7) | 0.0095 (7) | -0.0011 (7) |
| C5 | 0.0279 (9) | 0.0273 (9) | 0.0402 (10) | -0.0031 (7) | 0.0102 (8) | -0.0038 (8) |
| C6 | 0.0299 (9) | 0.0266 (9) | 0.0370 (10) | 0.0026 (7) | -0.0018 (8) | -0.0041 (8) |
| C7 | 0.0349 (9) | 0.0205 (8) | 0.0256 (9) | 0.0014 (6) | 0.0013 (7) | -0.0025 (6) |
| C8 | 0.0317 (9) | 0.0158 (7) | 0.0220 (8) | 0.0005 (6) | 0.0043 (7) | -0.0026 (6) |
| C9 | 0.0345 (9) | 0.0215 (8) | 0.0185 (8) | 0.0009 (6) | 0.0070 (7) | 0.0011 (6) |
| C10 | 0.0282 (8) | 0.0223 (8) | 0.0253 (9) | -0.0004 (6) | 0.0118 (7) | -0.0016 (6) |
| C11 | 0.0304 (9) | 0.0207 (8) | 0.0222 (8) | 0.0005 (6) | 0.0069 (7) | -0.0012 (6) |
| C12 | 0.0292 (8) | 0.0191 (8) | 0.0231 (8) | -0.0001 (6) | 0.0063 (7) | 0.0026 (6) |
| C13 | 0.0323 (9) | 0.0191 (8) | 0.0235 (8) | 0.0006 (6) | 0.0076 (7) | -0.0003 (6) |
| C14 | 0.0277 (8) | 0.0224 (8) | 0.0303 (9) | 0.0020 (6) | 0.0080 (7) | 0.0031 (7) |
| C15 | 0.0291 (9) | 0.0270 (8) | 0.0282 (9) | -0.0026 (7) | 0.0014 (7) | 0.0036 (7) |
| C16 | 0.0350 (9) | 0.0264 (8) | 0.0221 (8) | -0.0016 (7) | 0.0041 (7) | 0.0003 (7) |
| C17 | 0.0303 (9) | 0.0213 (8) | 0.0245 (9) | -0.0010 (6) | 0.0092 (7) | 0.0010 (6) |
| C18 | 0.0257 (9) | 0.0413 (11) | 0.0330 (10) | 0.0012 (7) | 0.0035 (8) | -0.0022 (8) |
| F1 | 0.0503 (7) | 0.0630 (8) | 0.0554 (8) | 0.0110 (6) | 0.0188 (6) | 0.0264 (6) |
| F2 | 0.0386 (7) | 0.0587 (8) | 0.0701 (9) | 0.0065 (5) | 0.0274 (6) | -0.0067 (6) |
| F3 | 0.0440 (7) | 0.0829 (10) | 0.0581 (8) | -0.0267 (7) | 0.0108 (6) | -0.0259 (7) |
| N1 | 0.0275 (7) | 0.0215 (7) | 0.0236 (7) | -0.0009 (5) | 0.0052 (6) | 0.0006 (5) |
| O1 | 0.0299 (7) | 0.0375 (7) | 0.0244 (6) | 0.0001 (5) | 0.0085 (5) | -0.0058 (5) |
| O2 | 0.0283 (6) | 0.0289 (7) | 0.0428 (8) | 0.0036 (5) | 0.0103 (5) | -0.0008 (5) |

Geometric parameters (Å, °)

| | | | |
|-------|-----------|---------|-----------|
| C1—C2 | 1.373 (2) | C11—N1 | 1.284 (2) |
| C1—N1 | 1.417 (2) | C11—C12 | 1.454 (2) |

| | | | |
|------------|-------------|-------------|-------------|
| C1—C10 | 1.421 (2) | C11—H11 | 0.9300 |
| C2—C3 | 1.414 (2) | C12—C13 | 1.400 (2) |
| C2—H2 | 0.9300 | C12—C17 | 1.416 (2) |
| C3—C4 | 1.420 (2) | C13—C14 | 1.373 (2) |
| C3—C8 | 1.425 (2) | C13—H13 | 0.9300 |
| C4—C5 | 1.363 (2) | C14—C15 | 1.387 (2) |
| C4—H4 | 0.9300 | C14—O2 | 1.4176 (19) |
| C5—C6 | 1.409 (3) | C15—C16 | 1.386 (2) |
| C5—H5 | 0.9300 | C15—H15 | 0.9300 |
| C6—C7 | 1.368 (3) | C16—C17 | 1.392 (2) |
| C6—H6 | 0.9300 | C16—H16 | 0.9300 |
| C7—C8 | 1.416 (2) | C17—O1 | 1.349 (2) |
| C7—H7 | 0.9300 | C18—F2 | 1.316 (2) |
| C8—C9 | 1.419 (2) | C18—F1 | 1.324 (2) |
| C9—C10 | 1.365 (2) | C18—F3 | 1.324 (2) |
| C9—H9 | 0.9300 | C18—O2 | 1.328 (2) |
| C10—H10 | 0.9300 | O1—H1 | 0.90 (3) |
| | | | |
| C2—C1—N1 | 118.63 (14) | N1—C11—C12 | 120.90 (15) |
| C2—C1—C10 | 119.94 (15) | N1—C11—H11 | 119.5 |
| N1—C1—C10 | 121.10 (14) | C12—C11—H11 | 119.5 |
| C1—C2—C3 | 121.05 (15) | C13—C12—C17 | 118.92 (15) |
| C1—C2—H2 | 119.5 | C13—C12—C11 | 119.96 (15) |
| C3—C2—H2 | 119.5 | C17—C12—C11 | 121.11 (15) |
| C2—C3—C4 | 122.47 (15) | C14—C13—C12 | 119.83 (15) |
| C2—C3—C8 | 119.10 (14) | C14—C13—H13 | 120.1 |
| C4—C3—C8 | 118.35 (15) | C12—C13—H13 | 120.1 |
| C5—C4—C3 | 120.90 (16) | C13—C14—C15 | 121.73 (15) |
| C5—C4—H4 | 119.6 | C13—C14—O2 | 118.08 (15) |
| C3—C4—H4 | 119.6 | C15—C14—O2 | 120.04 (15) |
| C4—C5—C6 | 120.71 (16) | C16—C15—C14 | 119.18 (16) |
| C4—C5—H5 | 119.6 | C16—C15—H15 | 120.4 |
| C6—C5—H5 | 119.6 | C14—C15—H15 | 120.4 |
| C7—C6—C5 | 120.07 (16) | C15—C16—C17 | 120.49 (16) |
| C7—C6—H6 | 120.0 | C15—C16—H16 | 119.8 |
| C5—C6—H6 | 120.0 | C17—C16—H16 | 119.8 |
| C6—C7—C8 | 120.76 (16) | O1—C17—C16 | 118.72 (15) |
| C6—C7—H7 | 119.6 | O1—C17—C12 | 121.51 (15) |
| C8—C7—H7 | 119.6 | C16—C17—C12 | 119.77 (15) |
| C7—C8—C9 | 122.39 (15) | F2—C18—F1 | 108.15 (15) |
| C7—C8—C3 | 119.20 (15) | F2—C18—F3 | 107.09 (14) |
| C9—C8—C3 | 118.38 (15) | F1—C18—F3 | 106.41 (17) |
| C10—C9—C8 | 121.55 (15) | F2—C18—O2 | 108.49 (16) |
| C10—C9—H9 | 119.2 | F1—C18—O2 | 113.14 (14) |
| C8—C9—H9 | 119.2 | F3—C18—O2 | 113.28 (15) |
| C9—C10—C1 | 119.93 (15) | C11—N1—C1 | 121.55 (14) |
| C9—C10—H10 | 120.0 | C17—O1—H1 | 106.7 (17) |
| C1—C10—H10 | 120.0 | C18—O2—C14 | 117.93 (13) |

| | | | |
|----------------|--------------|-----------------|--------------|
| N1—C1—C2—C3 | -171.57 (13) | C17—C12—C13—C14 | -0.7 (2) |
| C10—C1—C2—C3 | 1.8 (2) | C11—C12—C13—C14 | -179.68 (14) |
| C1—C2—C3—C4 | 176.90 (14) | C12—C13—C14—C15 | 1.8 (2) |
| C1—C2—C3—C8 | 0.0 (2) | C12—C13—C14—O2 | -173.65 (14) |
| C2—C3—C4—C5 | -176.17 (15) | C13—C14—C15—C16 | -0.4 (2) |
| C8—C3—C4—C5 | 0.8 (2) | O2—C14—C15—C16 | 174.97 (14) |
| C3—C4—C5—C6 | 0.4 (3) | C14—C15—C16—C17 | -2.1 (2) |
| C4—C5—C6—C7 | -1.3 (3) | C15—C16—C17—O1 | -176.85 (14) |
| C5—C6—C7—C8 | 1.0 (3) | C15—C16—C17—C12 | 3.2 (2) |
| C6—C7—C8—C9 | 178.00 (15) | C13—C12—C17—O1 | 178.27 (14) |
| C6—C7—C8—C3 | 0.2 (2) | C11—C12—C17—O1 | -2.7 (2) |
| C2—C3—C8—C7 | 175.98 (14) | C13—C12—C17—C16 | -1.8 (2) |
| C4—C3—C8—C7 | -1.1 (2) | C11—C12—C17—C16 | 177.22 (14) |
| C2—C3—C8—C9 | -1.9 (2) | C12—C11—N1—C1 | -171.85 (13) |
| C4—C3—C8—C9 | -178.95 (14) | C2—C1—N1—C11 | -151.42 (15) |
| C7—C8—C9—C10 | -175.68 (15) | C10—C1—N1—C11 | 35.3 (2) |
| C3—C8—C9—C10 | 2.1 (2) | F2—C18—O2—C14 | 170.19 (14) |
| C8—C9—C10—C1 | -0.4 (2) | F1—C18—O2—C14 | 50.2 (2) |
| C2—C1—C10—C9 | -1.6 (2) | F3—C18—O2—C14 | -71.0 (2) |
| N1—C1—C10—C9 | 171.60 (14) | C13—C14—O2—C18 | -105.77 (18) |
| N1—C11—C12—C13 | -172.63 (14) | C15—C14—O2—C18 | 78.7 (2) |
| N1—C11—C12—C17 | 8.4 (2) | | |

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

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|----------------------------------|----------|-------------|-------------|---------------|
| O1—H1 \cdots N1 | 0.90 (3) | 1.77 (3) | 2.5904 (18) | 150 (2) |
| C10—H10 \cdots O1 ⁱ | 0.93 | 2.57 | 3.473 (2) | 165 |
| C5—H5 \cdots F2 ⁱⁱ | 0.93 | 2.57 | 3.487 (2) | 170 |

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