Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 2-Methyl-3-nitro-*N*-{(*E*)-[5-(4-nitrophenyl)furan-2-yl]methylidene}aniline

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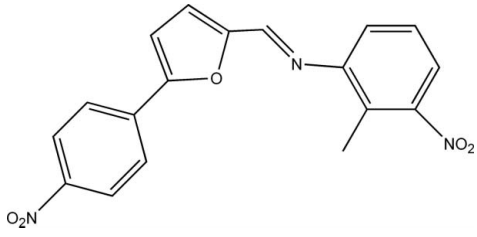
Received 17 May 2012; accepted 27 July 2012

Key indicators: single-crystal X-ray study; $T$ = 123 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.042; $wR$ factor = 0.118; data-to-parameter ratio = 13.4.

In the title Schiff-base type compound, $C_{18}H_{13}N_3O_5$, the central furan ring makes dihedral angles of 12.80 (7) and 51.43 (4)° with the terminal benzene rings. The dihedral angle between the benzene rings is 45.43 (3)°. In the crystal, C—H···O hydrogen bonds link the molecules into layers parallel to (010). In addition, there are $\pi$–$\pi$ stacking interactions within the layer [centroid–centroid distance = 3.584 (1) Å] and between the layers [centroid–centroid distance 3.751 (1) Å].

## Related literature

For similar Schiff bases, see: Yamada *et al.* (2002); Cukurovali *et al.* (2002); Isloor *et al.* (2009); Abu Thaher *et al.* (2012). For the biological activity of Schiff bases, see: Vijesh *et al.* (2010); Tarafder *et al.* (2002); Ghorab *et al.* (2010); Ali *et al.* (2002). For standard bond lengths, see: Allen *et al.* (1987).




## Experimental

### Crystal data

$C_{18}H_{13}N_3O_5$
$M_r$ = 351.31
Monoclinic, $P2_1/c$
$a$ = 10.9026 (3) Å
$b$ = 10.2798 (3) Å
$c$ = 14.2962 (3) Å
$\beta$ = 101.529 (2)°
$V$ = 1569.94 (7) Å$^3$
$Z$ = 4
Cu $K\alpha$ radiation
$\mu$ = 0.93 mm$^{-1}$
$T$ = 123 K
0.50 × 0.40 × 0.40 mm

### Data collection

Oxford Diffraction Gemini-R diffractometer
Absorption correction: multi-scan [*CrysAlis RED* (Oxford Diffraction, 2007), and Clark & Reid (1995)]
$T_{min}$ = 0.671, $T_{max}$ = 0.688
6460 measured reflections
3171 independent reflections
2764 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.118
$S$ = 1.05
3171 reflections
236 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.23 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C3—H3$A$···O5$^{i}$ | 0.93 | 2.58 | 3.4895 (19) | 165 |
| C13—H13$A$···O1$^{ii}$ | 0.93 | 2.53 | 3.432 (2) | 162 |
| C14—H14$A$···O2$^{iii}$ | 0.93 | 2.55 | 3.361 (2) | 147 |

Symmetry codes: (i) $x, y, z-1$; (ii) $x+1, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $x+1, y, z+1$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis CCD*; 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*.

RJB acknowledges the NSF–MRI program (grant No. CHE-0619278) for funds to purchase the diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2492).

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# supporting information

*Acta Cryst.* (2012). E**68**, o2630 [doi:10.1107/S1600536812033818]

## 2-Methyl-3-nitro-*N*-{(*E*)-[5-(4-nitrophenyl)furan-2-yl]methylidene}aniline

**Merve Pekdemir, Şamil Işık, Sümeyye Gümüş, Erbil Ağar, Sema Öztürk Yıldırım and Ray J. Butcher**

### S1. Comment

Schiff bases have been very important as ligands in the area of coordination chemistry. These ligands and their metal complexes have shown important activity in the field of biology in the past years. Several new examples have been tested for their antitumor, antimicrobial, anticancer and antibacterial activities (Ali *et al.*, 2002; Ghorab *et al.*, 2010; Tarafder *et al.*, 2002; Vijesh *et al.*, 2010). In view of these facts, the aim of this present study is to obtain a structure of the Schiff base, 2-methyl-3-nitro-*N*-{(*E*)-[5-(4-nitrophenyl)furan-2-yl]methylideneaniline.

In the title compound (Fig 1), the molecule presents an E configuration with the 2-(4-nitrophenyl)furan group opposite to 1-methyl-2-nitrobenzene group about the N2 ═C11 double bond. This N2 ═C11 double bond distance [1.2783 (19) Å] is longer than the N ═C typical bond distance (Allen *et al.*, 1987), probably due to $\pi$ conjugation along all the molecule. The torsion angle is 171.79 (14) ° formed by C10—C11—N2—C12. All other bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The central furan ring (C7—C10/O3) is planar, with an r.m.s. deviation for fitted atoms of 0.0019 Å. This plane makes dihedral angles of 12.80 (7) and 51.43 (4) ° with the terminal benzene rings C1—C6 and C12—C17, respectively. The dihedral angle between the two benzene ring is 45.43 (3)°.

In the crystal, C—H···O intermolecular interactions are observed (Table 1) as well as $\pi$–$\pi$ stacking interactions [*Cg*1···*Cg*3 (-*x*,1 - *y*,-*z*) = 3.584 (1) Å and *Cg*3···*Cg*3 (*x*, 1 + *y*, *z*) = 3.751 (1) Å, where *Cg*1(O3/C7—C10) and *Cg*3(C12—C17) are the centroids of the furan and benzene ring, respectively] (Fig. 2).

### S2. Experimental

The title compound was prepared by refluxing a mixture containing 5-(4-nitrophenyl)furan-2 carbaldehyde (0.011 g 0.051 mmol) and 2-methyl-3-nitroaniline (0.0077 g 0.051 mmol) in 40 ml of ethanol. The reaction mixture was stirred for 1 h under reflux. The crystals suitable for X-ray analysis were obtained from ethanol by slow evaporation (yield 62%; m.p: 471–474 K).

### S3. Refinement

All H atoms were positioned geometrically and refined using a riding model with C–H = 0.93–0.96 Å and $U_{iso}$(H) = 1.2 or 1.5 $U_{eq}$(C). A rotating-group model was applied for the methyl groups.

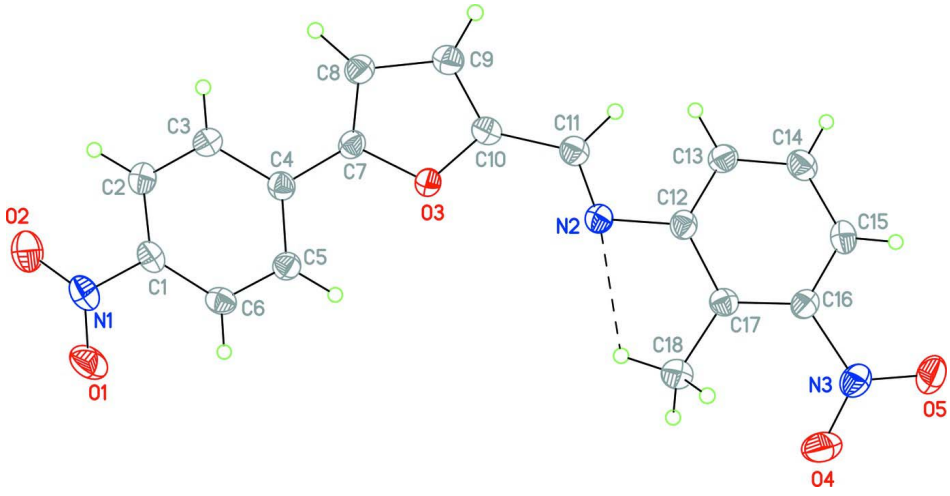


**Figure 1**

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. The intramolecular interaction is shown as a dashed line.

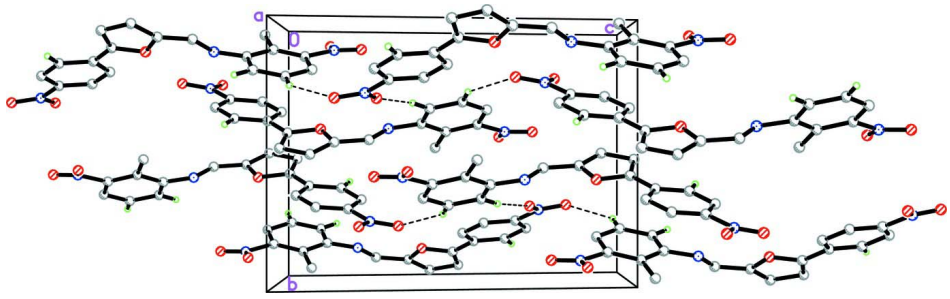


**Figure 2**

The crystal structure of the title compound, viewed along the *a* axis. H atoms not involved in hydrogen bonds (dashed lines) have been omitted for clarity.

### 2-Methyl-3-nitro-*N*-{(*E*)-[5-(4-nitrophenyl)furan- 2-yl]methylidene}aniline

*Crystal data*

$C_{18}H_{13}N_3O_5$
$M_r = 351.31$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.9026\ (3)$ Å
$b = 10.2798\ (3)$ Å
$c = 14.2962\ (3)$ Å
$\beta = 101.529\ (2)°$
$V = 1569.94\ (7)$ Å$^3$
$Z = 4$
$F(000) = 728$
$D_x = 1.486$ Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda = 1.5418$ Å
Cell parameters from 3039 reflections
$\theta = 3.2–75.5°$
$\mu = 0.93$ mm$^{-1}$
$T = 123$ K
Block, light yellow
0.50 × 0.40 × 0.40 mm

*Data collection*

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

Absorption correction: multi-scan
[*CrysAlis RED* (Oxford Diffraction, 2007), and Clark & Reid (1995)]
$T_{min}$ = 0.671, $T_{max}$ = 0.688
6460 measured reflections
3171 independent reflections

2764 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028
$\theta_{max}$ = 75.7°, $\theta_{min}$ = 4.1°
$h$ = −12→13
$k$ = −12→12
$l$ = −17→7

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.118
$S$ = 1.05
3171 reflections
236 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
$w = 1/[\sigma^2(F_o^2) + (0.0671P)^2 + 0.3233P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.31 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.23 e 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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | −0.22774 (12) | 0.22828 (14) | −0.24867 (10) | 0.0309 (3) |
| N2 | 0.28795 (11) | 0.40005 (12) | 0.30426 (9) | 0.0224 (3) |
| N3 | 0.26983 (13) | 0.41136 (13) | 0.64618 (9) | 0.0281 (3) |
| O1 | −0.32515 (11) | 0.21084 (14) | −0.21964 (10) | 0.0412 (3) |
| O2 | −0.21821 (12) | 0.20872 (15) | −0.33171 (9) | 0.0448 (3) |
| O3 | 0.20668 (9) | 0.40126 (10) | 0.10398 (7) | 0.0206 (2) |
| O4 | 0.15778 (13) | 0.43153 (18) | 0.63095 (9) | 0.0537 (4) |
| O5 | 0.33489 (12) | 0.41218 (14) | 0.72703 (8) | 0.0403 (3) |
| C1 | −0.11759 (13) | 0.27566 (15) | −0.18146 (10) | 0.0247 (3) |
| C2 | −0.01288 (15) | 0.31134 (16) | −0.21649 (11) | 0.0280 (3) |
| H2A | −0.0121 | 0.3041 | −0.2812 | 0.034* |
| C3 | 0.09029 (14) | 0.35784 (16) | −0.15327 (10) | 0.0258 (3) |
| H3A | 0.1611 | 0.3832 | −0.1756 | 0.031* |
| C4 | 0.08916 (13) | 0.36719 (14) | −0.05598 (10) | 0.0209 (3) |
| C5 | −0.01791 (13) | 0.32932 (14) | −0.02242 (10) | 0.0224 (3) |
| H5A | −0.0187 | 0.3345 | 0.0424 | 0.027* |
| C6 | −0.12221 (13) | 0.28430 (14) | −0.08556 (11) | 0.0242 (3) |
| H6A | −0.1940 | 0.2603 | −0.0641 | 0.029* |
| C7 | 0.20003 (13) | 0.41645 (14) | 0.00792 (10) | 0.0204 (3) |

| | | | | |
|---|---|---|---|---|
| C8 | 0.30432 (14) | 0.47801 (15) | −0.00873 (10) | 0.0236 (3) |
| H8A | 0.3217 | 0.4999 | −0.0679 | 0.028* |
| C9 | 0.38082 (14) | 0.50202 (15) | 0.08172 (10) | 0.0236 (3) |
| H9A | 0.4585 | 0.5428 | 0.0936 | 0.028* |
| C10 | 0.31886 (13) | 0.45401 (14) | 0.14813 (10) | 0.0215 (3) |
| C11 | 0.35804 (13) | 0.44480 (14) | 0.25000 (10) | 0.0222 (3) |
| H11A | 0.4382 | 0.4727 | 0.2778 | 0.027* |
| C12 | 0.34377 (13) | 0.38033 (14) | 0.40136 (10) | 0.0216 (3) |
| C13 | 0.46195 (14) | 0.32360 (15) | 0.42596 (11) | 0.0248 (3) |
| H13A | 0.5056 | 0.3028 | 0.3783 | 0.030* |
| C14 | 0.51519 (14) | 0.29778 (15) | 0.52044 (11) | 0.0270 (3) |
| H14A | 0.5945 | 0.2608 | 0.5361 | 0.032* |
| C15 | 0.45026 (14) | 0.32705 (15) | 0.59109 (10) | 0.0248 (3) |
| H15A | 0.4849 | 0.3099 | 0.6548 | 0.030* |
| C16 | 0.33171 (13) | 0.38282 (14) | 0.56546 (10) | 0.0221 (3) |
| C17 | 0.27330 (13) | 0.41176 (14) | 0.47145 (10) | 0.0208 (3) |
| C18 | 0.14791 (14) | 0.47584 (16) | 0.43966 (11) | 0.0267 (3) |
| H18A | 0.1486 | 0.5596 | 0.4694 | 0.040* |
| H18B | 0.0841 | 0.4227 | 0.4577 | 0.040* |
| H18C | 0.1310 | 0.4861 | 0.3715 | 0.040* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0263 (7) | 0.0291 (7) | 0.0333 (7) | 0.0015 (5) | −0.0037 (5) | −0.0025 (6) |
| N2 | 0.0224 (6) | 0.0234 (6) | 0.0213 (6) | 0.0002 (5) | 0.0040 (5) | −0.0015 (5) |
| N3 | 0.0339 (7) | 0.0280 (7) | 0.0237 (6) | −0.0029 (6) | 0.0091 (5) | 0.0007 (5) |
| O1 | 0.0234 (6) | 0.0482 (8) | 0.0492 (7) | −0.0046 (5) | 0.0003 (5) | −0.0067 (6) |
| O2 | 0.0407 (7) | 0.0580 (9) | 0.0306 (6) | −0.0050 (6) | −0.0051 (5) | −0.0087 (6) |
| O3 | 0.0211 (5) | 0.0228 (5) | 0.0177 (5) | −0.0007 (4) | 0.0034 (4) | −0.0005 (4) |
| O4 | 0.0355 (7) | 0.0957 (13) | 0.0336 (7) | 0.0182 (8) | 0.0155 (5) | 0.0061 (7) |
| O5 | 0.0425 (7) | 0.0572 (8) | 0.0218 (6) | −0.0081 (6) | 0.0076 (5) | −0.0048 (5) |
| C1 | 0.0221 (7) | 0.0231 (7) | 0.0263 (7) | 0.0025 (6) | −0.0015 (6) | −0.0012 (6) |
| C2 | 0.0282 (7) | 0.0338 (8) | 0.0212 (7) | 0.0010 (6) | 0.0031 (6) | −0.0012 (6) |
| C3 | 0.0238 (7) | 0.0314 (8) | 0.0230 (7) | 0.0001 (6) | 0.0067 (5) | 0.0022 (6) |
| C4 | 0.0213 (7) | 0.0194 (7) | 0.0215 (7) | 0.0028 (5) | 0.0031 (5) | 0.0013 (5) |
| C5 | 0.0234 (7) | 0.0221 (7) | 0.0220 (7) | 0.0029 (6) | 0.0056 (5) | 0.0008 (6) |
| C6 | 0.0209 (7) | 0.0226 (7) | 0.0295 (8) | 0.0024 (6) | 0.0061 (6) | 0.0025 (6) |
| C7 | 0.0229 (7) | 0.0206 (7) | 0.0182 (7) | 0.0043 (5) | 0.0051 (5) | 0.0020 (5) |
| C8 | 0.0234 (7) | 0.0265 (7) | 0.0218 (7) | 0.0022 (6) | 0.0064 (5) | 0.0030 (6) |
| C9 | 0.0212 (7) | 0.0245 (7) | 0.0254 (7) | −0.0009 (6) | 0.0052 (5) | 0.0004 (6) |
| C10 | 0.0190 (6) | 0.0206 (7) | 0.0247 (7) | −0.0002 (5) | 0.0043 (5) | −0.0011 (6) |
| C11 | 0.0217 (7) | 0.0208 (7) | 0.0239 (7) | −0.0005 (6) | 0.0038 (5) | −0.0022 (6) |
| C12 | 0.0229 (7) | 0.0211 (7) | 0.0205 (7) | −0.0037 (6) | 0.0037 (5) | −0.0014 (5) |
| C13 | 0.0246 (7) | 0.0262 (7) | 0.0246 (7) | 0.0001 (6) | 0.0073 (6) | −0.0020 (6) |
| C14 | 0.0226 (7) | 0.0270 (8) | 0.0299 (8) | 0.0025 (6) | 0.0016 (6) | −0.0013 (6) |
| C15 | 0.0271 (7) | 0.0234 (7) | 0.0219 (7) | −0.0036 (6) | −0.0001 (5) | 0.0000 (6) |
| C16 | 0.0254 (7) | 0.0205 (7) | 0.0215 (7) | −0.0050 (6) | 0.0069 (5) | −0.0023 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C17 | 0.0204 (7) | 0.0189 (7) | 0.0236 (7) | −0.0033 (5) | 0.0053 (5) | −0.0012 (5) |
| C18 | 0.0237 (7) | 0.0295 (8) | 0.0270 (7) | 0.0022 (6) | 0.0056 (6) | 0.0001 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—O1 | 1.2282 (18) | C7—C8 | 1.363 (2) |
| N1—O2 | 1.2288 (19) | C8—C9 | 1.413 (2) |
| N1—C1 | 1.4633 (19) | C8—H8A | 0.9300 |
| N2—C11 | 1.2783 (19) | C9—C10 | 1.363 (2) |
| N2—C12 | 1.4145 (18) | C9—H9A | 0.9300 |
| N3—O4 | 1.2151 (19) | C10—C11 | 1.437 (2) |
| N3—O5 | 1.2294 (18) | C11—H11A | 0.9300 |
| N3—C16 | 1.4779 (18) | C12—C13 | 1.394 (2) |
| O3—C7 | 1.3696 (16) | C12—C17 | 1.417 (2) |
| O3—C10 | 1.3711 (17) | C13—C14 | 1.385 (2) |
| C1—C2 | 1.385 (2) | C13—H13A | 0.9300 |
| C1—C6 | 1.385 (2) | C14—C15 | 1.378 (2) |
| C2—C3 | 1.380 (2) | C14—H14A | 0.9300 |
| C2—H2A | 0.9300 | C15—C16 | 1.394 (2) |
| C3—C4 | 1.397 (2) | C15—H15A | 0.9300 |
| C3—H3A | 0.9300 | C16—C17 | 1.399 (2) |
| C4—C5 | 1.403 (2) | C17—C18 | 1.504 (2) |
| C4—C7 | 1.453 (2) | C18—H18A | 0.9600 |
| C5—C6 | 1.383 (2) | C18—H18B | 0.9600 |
| C5—H5A | 0.9300 | C18—H18C | 0.9600 |
| C6—H6A | 0.9300 | | |
| | | | |
| O1—N1—O2 | 123.25 (14) | C10—C9—H9A | 126.6 |
| O1—N1—C1 | 118.58 (14) | C8—C9—H9A | 126.6 |
| O2—N1—C1 | 118.17 (14) | C9—C10—O3 | 110.08 (12) |
| C11—N2—C12 | 117.06 (12) | C9—C10—C11 | 129.92 (13) |
| O4—N3—O5 | 122.54 (14) | O3—C10—C11 | 119.85 (12) |
| O4—N3—C16 | 119.57 (13) | N2—C11—C10 | 123.11 (13) |
| O5—N3—C16 | 117.89 (13) | N2—C11—H11A | 118.4 |
| C7—O3—C10 | 106.26 (11) | C10—C11—H11A | 118.4 |
| C2—C1—C6 | 122.47 (14) | C13—C12—N2 | 120.15 (13) |
| C2—C1—N1 | 118.59 (14) | C13—C12—C17 | 121.44 (13) |
| C6—C1—N1 | 118.94 (14) | N2—C12—C17 | 118.28 (13) |
| C3—C2—C1 | 118.55 (14) | C14—C13—C12 | 120.82 (14) |
| C3—C2—H2A | 120.7 | C14—C13—H13A | 119.6 |
| C1—C2—H2A | 120.7 | C12—C13—H13A | 119.6 |
| C2—C3—C4 | 120.52 (14) | C15—C14—C13 | 119.77 (14) |
| C2—C3—H3A | 119.7 | C15—C14—H14A | 120.1 |
| C4—C3—H3A | 119.7 | C13—C14—H14A | 120.1 |
| C3—C4—C5 | 119.67 (13) | C14—C15—C16 | 118.84 (14) |
| C3—C4—C7 | 118.58 (13) | C14—C15—H15A | 120.6 |
| C5—C4—C7 | 121.76 (13) | C16—C15—H15A | 120.6 |
| C6—C5—C4 | 120.11 (13) | C15—C16—C17 | 124.04 (14) |

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| C6—C5—H5A | 119.9 | C15—C16—N3 | 114.85 (13) |
| C4—C5—H5A | 119.9 | C17—C16—N3 | 121.10 (13) |
| C5—C6—C1 | 118.68 (14) | C16—C17—C12 | 115.08 (13) |
| C5—C6—H6A | 120.7 | C16—C17—C18 | 126.53 (13) |
| C1—C6—H6A | 120.7 | C12—C17—C18 | 118.35 (13) |
| C8—C7—O3 | 110.44 (13) | C17—C18—H18A | 109.5 |
| C8—C7—C4 | 132.08 (13) | C17—C18—H18B | 109.5 |
| O3—C7—C4 | 117.48 (12) | H18A—C18—H18B | 109.5 |
| C7—C8—C9 | 106.36 (13) | C17—C18—H18C | 109.5 |
| C7—C8—H8A | 126.8 | H18A—C18—H18C | 109.5 |
| C9—C8—H8A | 126.8 | H18B—C18—H18C | 109.5 |
| C10—C9—C8 | 106.86 (13) | | |

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| O1—N1—C1—C2 | −171.75 (15) | C7—O3—C10—C9 | 0.44 (15) |
| O2—N1—C1—C2 | 7.8 (2) | C7—O3—C10—C11 | −175.51 (13) |
| O1—N1—C1—C6 | 7.7 (2) | C12—N2—C11—C10 | 171.79 (14) |
| O2—N1—C1—C6 | −172.80 (15) | C9—C10—C11—N2 | 178.09 (15) |
| C6—C1—C2—C3 | −0.3 (2) | O3—C10—C11—N2 | −6.9 (2) |
| N1—C1—C2—C3 | 179.05 (14) | C11—N2—C12—C13 | −43.4 (2) |
| C1—C2—C3—C4 | 0.7 (2) | C11—N2—C12—C17 | 140.62 (14) |
| C2—C3—C4—C5 | −0.2 (2) | N2—C12—C13—C14 | −176.78 (14) |
| C2—C3—C4—C7 | 179.87 (14) | C17—C12—C13—C14 | −0.9 (2) |
| C3—C4—C5—C6 | −0.7 (2) | C12—C13—C14—C15 | 0.7 (2) |
| C7—C4—C5—C6 | 179.25 (13) | C13—C14—C15—C16 | −0.2 (2) |
| C4—C5—C6—C1 | 1.0 (2) | C14—C15—C16—C17 | −0.1 (2) |
| C2—C1—C6—C5 | −0.5 (2) | C14—C15—C16—N3 | −179.66 (13) |
| N1—C1—C6—C5 | −179.91 (13) | O4—N3—C16—C15 | −163.26 (16) |
| C10—O3—C7—C8 | −0.50 (15) | O5—N3—C16—C15 | 15.9 (2) |
| C10—O3—C7—C4 | 179.55 (12) | O4—N3—C16—C17 | 17.2 (2) |
| C3—C4—C7—C8 | 12.5 (2) | O5—N3—C16—C17 | −163.65 (14) |
| C5—C4—C7—C8 | −167.42 (15) | C15—C16—C17—C12 | −0.1 (2) |
| C3—C4—C7—O3 | −167.53 (13) | N3—C16—C17—C12 | 179.45 (12) |
| C5—C4—C7—O3 | 12.5 (2) | C15—C16—C17—C18 | −177.78 (14) |
| O3—C7—C8—C9 | 0.36 (17) | N3—C16—C17—C18 | 1.8 (2) |
| C4—C7—C8—C9 | −179.70 (15) | C13—C12—C17—C16 | 0.6 (2) |
| C7—C8—C9—C10 | −0.08 (17) | N2—C12—C17—C16 | 176.52 (12) |
| C8—C9—C10—O3 | −0.23 (17) | C13—C12—C17—C18 | 178.50 (14) |
| C8—C9—C10—C11 | 175.19 (15) | N2—C12—C17—C18 | −5.6 (2) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C18—H18*C*···N2 | 0.96 | 2.30 | 2.8047 (19) | 112 |
| C3—H3*A*···O5$^{i}$ | 0.93 | 2.58 | 3.4895 (19) | 165 |
| C13—H13*A*···O1$^{ii}$ | 0.93 | 2.53 | 3.432 (2) | 162 |
| C14—H14*A*···O2$^{iii}$ | 0.93 | 2.55 | 3.361 (2) | 147 |

Symmetry codes: (i) *x*, *y*, *z*−1; (ii) *x*+1, −*y*+1/2, *z*+1/2; (iii) *x*+1, *y*, *z*+1.