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

# 1-(Biphenyl-4-ylcarbonyl)-3-(4-nitrophenyl)thiourea

**M. Sukeri M. Yusof,[a]* Sze Ting Wong[a] and Bohari M. Yamin[b]**

[a]Department of Chemical Sciences, Faculty of Science and Technology, Universiti Malaysia Terengganu, 21030 Kuala Terengganu, Terengganu, Malaysia, and [b]School of Chemical Sciences and Food Technology, Universiti Kebangsaan Malaysia, UKM 43500 Bangi Selangor, Malaysia
Correspondence e-mail: mohdsukeri@umt.edu.my

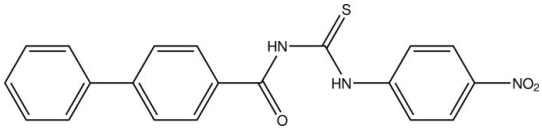
Received 8 August 2011; accepted 21 August 2011

Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.060; $wR$ factor = 0.143; data-to-parameter ratio = 12.8.

In the title compound, $C_{20}H_{15}N_3O_3S$, the two benzene rings of the biphenyl group form a dihedral angle of 40.11 (15)°. The conformation of the molecule is *trans–cis* and is stabilized by two intramolecular N—H···O and C—H···S hydrogen bonds. In the crystal structure, the molecules are linked by weak $\pi$–$\pi$ stacking interactions [centroid–centroid distance = 3.991 (2) Å].

## Related literature

For related structures, see: Arif &Yamin (2007); Yamin & Arif (2008). For standard bond lengths, see: Allen *et al.* (2003).




## Experimental

### Crystal data

$C_{20}H_{15}N_3O_3S$
$M_r$ = 377.41
Monoclinic, $P2_1/c$
$a$ = 12.154 (2) Å
$b$ = 9.4509 (18) Å
$c$ = 17.471 (3) Å
$\beta$ = 118.133 (9)°
$V$ = 1769.7 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.21 mm$^{-1}$
$T$ = 298 K
0.38 × 0.14 × 0.07 mm

### Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min}$ = 0.925, $T_{max}$ = 0.986
9891 measured reflections
3116 independent reflections
2268 reflections with $I > 2/s(I)$
$R_{int}$ = 0.043

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.143
$S$ = 0.88
3116 reflections
244 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2$A$···O1 | 0.86 | 1.90 | 2.633 (4) | 142 |
| C20—H20···S1 | 0.93 | 2.55 | 3.186 (4) | 126 |

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009), *SHELXTL* (Sheldrick, 2008), *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995).

The authors thank the Malaysian Government, Universiti Kebangsaan Malaysia, Faculty of Science and Technology, Universiti Malaysia Terengganu and the Ministry of Higher Education, Malaysia for research grant Nos. UKM-GUP-NBT-08-27-110 and FRGS 59178.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2367).

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# supporting information

*Acta Cryst.* (2011). E**67**, o2483 [doi:10.1107/S160053681103426X]

## 1-(Biphenyl-4-ylcarbonyl)-3-(4-nitrophenyl)thiourea

**M. Sukeri M. Yusof, Sze Ting Wong and Bohari M. Yamin**

### S1. Comment

The title compound, (I) is analogous to the previously reported *N*-(biphenyl-4-carbonyl)-*N*′-(4-chlorophenyl)thiourea (II) (Yamin & Arif, 2008) except the chlorine atom in (II) is replaced by a nitro group. The bond lengths and angles are in normal ranges (Allen *et al.*, 2003) and comparable to those previous reported (Arif & Yamin, 2007). The benzene rings (C1—C6, C7—C12, C15—C20) and thiourea moities (C14/N1/N2/S1) are all planar with maximum deviation of 0.043 (3) Å for atom N1 from the mean plane. The dihedral angle of two benzene rings of the biphenyl group are at an angle of 40.11 (15)° smaller compared in (II)(44.23 (12)°). The central thiourea fragment makes dihedral angles with the benzene-carbonyl (C7—C12) and nitrobenzene (C15—C20) rings of 16.14 (13) and 17.75 (14)°, respectively, smaller compared in (II) (55.96 (9) and 64.09 (9)°). The conformation of the molecule is *trans-cis* and is stabilized by two intramolecular hydrogen bonds N—H···O and C—H···S interactions. In the crystal structure, the molecules are linked by weak $\pi$-$\pi$ stacking interactions, Table1 & Table2, Fig2.

### S2. Experimental

A solution of biphenylcarbomoylisothiocyanate (2.0 g, 8.4 mmol) in 20 ml acetone was added dropwise to a two-necked round-bottomed flask containing an equimolar amount of 4-nitroaniline (1.15 g, 8.4 mmol) in 20 ml of acetone. The mixture was refluxed for about 2.5 h. The light yellow solution was filtered and the filtrate allowed to evaporate at room temperature. Light yellow crystals were obtained after five days (yield 63%, m.p.: 164–166°C).

### S3. Refinement

H atoms on the parent carbon atoms were positioned geometrically with C—H= 0.93Å (benzene) and N—H = 0.86 Å, constrained to ride on their parent atoms with $U_{iso}$(H)= $xU_{eq}$(parent atom) where $x$=1.2 for CH and NH groups.

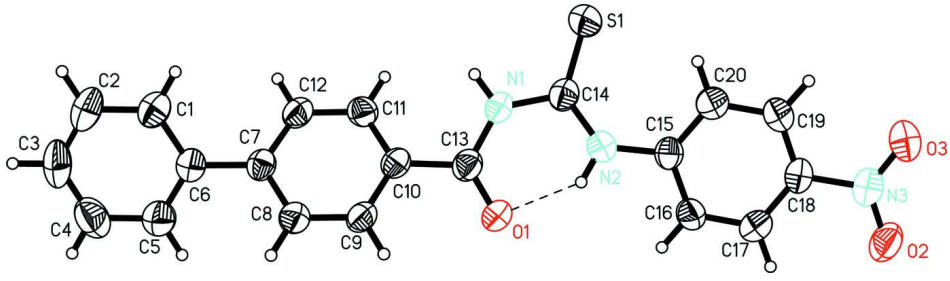


**Figure 1**

The molecular structure of (I), with displacement ellipsods drawn at the 50% probability level. The hydrogen bonds are shown by dashed lines.

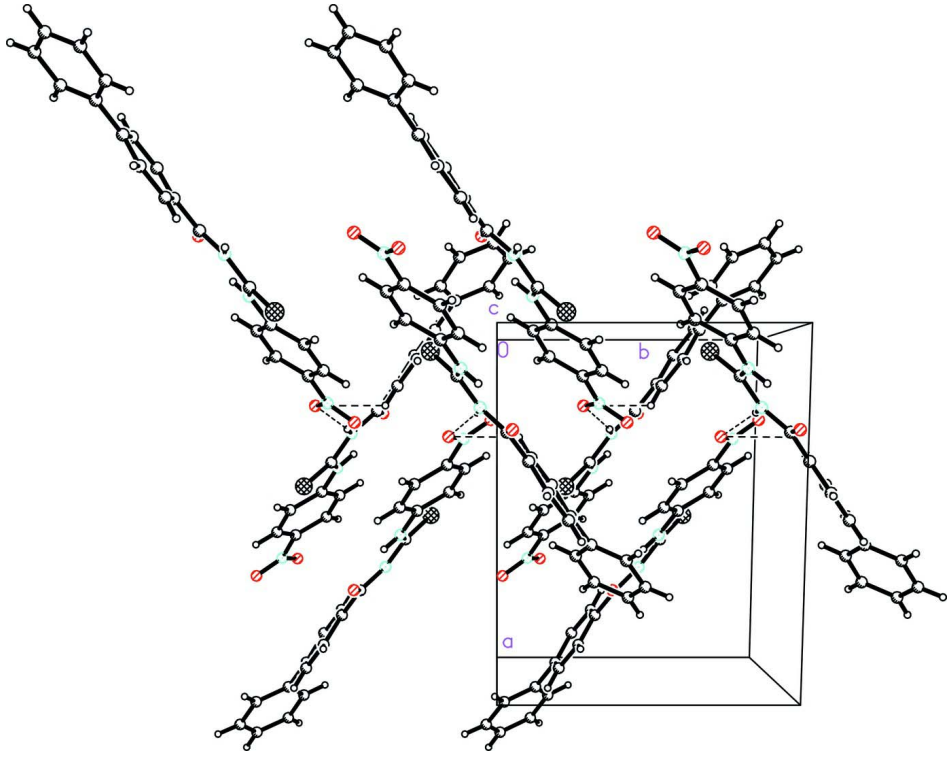


**Figure 2**

$\pi$-$\pi$ stacking interactions. The centroids are linked by dashed lines.

### 1-(Biphenyl-4-ylcarbonyl)-3-(4-nitrophenyl)thiourea

*Crystal data*

$C_{20}H_{15}N_3O_3S$
$M_r = 377.41$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 12.154$ (2) Å
$b = 9.4509$ (18) Å
$c = 17.471$ (3) Å
$\beta = 118.133$ (9)°
$V = 1769.7$ (5) Å$^3$
$Z = 4$
$F(000) = 784$
$D_x = 1.416$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 777 reflections
$\theta = 1.9$–25.0°
$\mu = 0.21$ mm$^{-1}$
$T = 298$ K
Slab, light yellow
0.38 × 0.14 × 0.07 mm

*Data collection*

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 83.66 pixels mm$^{-1}$
$\omega$ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.925$, $T_{max} = 0.986$
9891 measured reflections
3116 independent reflections
2268 reflections with $I > 2/s(I)$
$R_{int} = 0.043$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.9°$
$h = -13\rightarrow14$
$k = -10\rightarrow11$
$l = -20\rightarrow20$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.143$
$S = 0.88$
3116 reflections
244 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
$w = 1/[\sigma^2(F_o^2) + (0.0447P)^2 + 3.2573P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.26$ e Å$^{-3}$
$\Delta\rho_{min} = -0.22$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.34844 (10) | −0.26185 (12) | −0.10149 (6) | 0.0687 (4) |
| O1 | 0.3207 (2) | −0.5537 (3) | 0.09461 (16) | 0.0618 (7) |
| O2 | 1.0052 (2) | −0.1773 (3) | 0.30122 (17) | 0.0662 (7) |
| O3 | 0.9535 (3) | −0.0226 (3) | 0.19967 (19) | 0.0773 (9) |
| N1 | 0.2547 (2) | −0.4403 (3) | −0.03407 (17) | 0.0445 (7) |
| H1 | 0.1906 | −0.4296 | −0.0842 | 0.053* |
| N2 | 0.4557 (2) | −0.3739 (3) | 0.05899 (17) | 0.0473 (7) |
| H2A | 0.4451 | −0.4353 | 0.0913 | 0.057* |
| N3 | 0.9295 (3) | −0.1246 (3) | 0.2325 (2) | 0.0540 (8) |
| C1 | −0.3311 (3) | −0.7919 (4) | −0.1811 (2) | 0.0524 (9) |
| H1A | −0.3269 | −0.7079 | −0.2074 | 0.063* |
| C2 | −0.4442 (3) | −0.8619 (5) | −0.2122 (2) | 0.0612 (10) |
| H2B | −0.5157 | −0.8240 | −0.2578 | 0.073* |
| C3 | −0.4498 (4) | −0.9871 (5) | −0.1752 (3) | 0.0674 (12) |
| H3A | −0.5255 | −1.0347 | −0.1962 | 0.081* |
| C4 | −0.3461 (4) | −1.0434 (5) | −0.1080 (3) | 0.0717 (12) |
| H4 | −0.3508 | −1.1292 | −0.0837 | 0.086* |
| C5 | −0.2324 (4) | −0.9710 (4) | −0.0758 (2) | 0.0595 (10) |
| H5 | −0.1617 | −1.0090 | −0.0295 | 0.071* |
| C6 | −0.2238 (3) | −0.8443 (3) | −0.1117 (2) | 0.0423 (8) |
| C7 | −0.1055 (3) | −0.7659 (3) | −0.0786 (2) | 0.0402 (7) |
| C8 | −0.0235 (3) | −0.7554 (4) | 0.0100 (2) | 0.0468 (8) |
| H8 | −0.0436 | −0.7995 | 0.0493 | 0.056* |
| C9 | 0.0873 (3) | −0.6809 (4) | 0.0405 (2) | 0.0462 (8) |
| H9 | 0.1410 | −0.6763 | 0.0999 | 0.055* |

| | | | | |
|---|---|---|---|---|
| C10 | 0.1184 (3) | −0.6134 (3) | −0.0165 (2) | 0.0398 (7) |
| C11 | 0.0382 (3) | −0.6242 (3) | −0.1049 (2) | 0.0435 (8) |
| H11 | 0.0586 | −0.5800 | −0.1440 | 0.052* |
| C12 | −0.0709 (3) | −0.6991 (4) | −0.1351 (2) | 0.0471 (8) |
| H12 | −0.1229 | −0.7055 | −0.1946 | 0.056* |
| C13 | 0.2392 (3) | −0.5352 (3) | 0.0202 (2) | 0.0450 (8) |
| C14 | 0.3579 (3) | −0.3590 (3) | −0.0200 (2) | 0.0433 (8) |
| C15 | 0.5734 (3) | −0.3067 (3) | 0.0989 (2) | 0.0407 (8) |
| C16 | 0.6628 (3) | −0.3681 (4) | 0.1744 (2) | 0.0458 (8) |
| H16 | 0.6438 | −0.4499 | 0.1954 | 0.055* |
| C17 | 0.7800 (3) | −0.3090 (4) | 0.2191 (2) | 0.0484 (8) |
| H17 | 0.8405 | −0.3504 | 0.2698 | 0.058* |
| C18 | 0.8055 (3) | −0.1871 (4) | 0.1869 (2) | 0.0452 (8) |
| C19 | 0.7179 (3) | −0.1240 (4) | 0.1130 (2) | 0.0557 (9) |
| H19 | 0.7372 | −0.0418 | 0.0926 | 0.067* |
| C20 | 0.5997 (3) | −0.1833 (4) | 0.0686 (2) | 0.0561 (9) |
| H20 | 0.5387 | −0.1401 | 0.0188 | 0.067* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0687 (7) | 0.0718 (7) | 0.0517 (6) | −0.0203 (6) | 0.0169 (5) | 0.0114 (5) |
| O1 | 0.0406 (14) | 0.0756 (18) | 0.0498 (15) | −0.0105 (12) | 0.0054 (12) | 0.0164 (13) |
| O2 | 0.0439 (15) | 0.0724 (18) | 0.0605 (17) | −0.0035 (13) | 0.0068 (13) | −0.0029 (14) |
| O3 | 0.0691 (19) | 0.075 (2) | 0.0768 (19) | −0.0285 (16) | 0.0255 (16) | 0.0006 (16) |
| N1 | 0.0330 (15) | 0.0523 (17) | 0.0412 (15) | −0.0026 (13) | 0.0118 (13) | 0.0020 (13) |
| N2 | 0.0439 (17) | 0.0477 (16) | 0.0481 (16) | −0.0050 (13) | 0.0198 (14) | 0.0046 (13) |
| N3 | 0.0472 (19) | 0.056 (2) | 0.0563 (19) | −0.0065 (15) | 0.0223 (17) | −0.0103 (16) |
| C1 | 0.045 (2) | 0.055 (2) | 0.050 (2) | −0.0013 (17) | 0.0155 (18) | −0.0062 (17) |
| C2 | 0.039 (2) | 0.075 (3) | 0.060 (2) | −0.0044 (19) | 0.0147 (18) | −0.022 (2) |
| C3 | 0.050 (2) | 0.082 (3) | 0.076 (3) | −0.028 (2) | 0.034 (2) | −0.032 (2) |
| C4 | 0.082 (3) | 0.066 (3) | 0.075 (3) | −0.026 (2) | 0.043 (3) | −0.006 (2) |
| C5 | 0.055 (2) | 0.058 (2) | 0.058 (2) | −0.0060 (19) | 0.0209 (19) | 0.0014 (19) |
| C6 | 0.0398 (19) | 0.0454 (19) | 0.0434 (18) | −0.0018 (15) | 0.0211 (16) | −0.0078 (15) |
| C7 | 0.0355 (18) | 0.0381 (18) | 0.0447 (18) | 0.0028 (14) | 0.0171 (15) | −0.0019 (14) |
| C8 | 0.0411 (19) | 0.055 (2) | 0.0437 (19) | −0.0005 (16) | 0.0192 (16) | 0.0033 (16) |
| C9 | 0.0369 (18) | 0.060 (2) | 0.0349 (17) | −0.0019 (16) | 0.0112 (15) | 0.0011 (16) |
| C10 | 0.0333 (17) | 0.0415 (18) | 0.0416 (18) | 0.0054 (14) | 0.0152 (15) | 0.0004 (14) |
| C11 | 0.0423 (19) | 0.049 (2) | 0.0438 (19) | 0.0019 (16) | 0.0239 (16) | 0.0039 (15) |
| C12 | 0.0409 (19) | 0.056 (2) | 0.0356 (17) | −0.0030 (16) | 0.0112 (15) | −0.0014 (15) |
| C13 | 0.0371 (19) | 0.0444 (19) | 0.047 (2) | 0.0019 (15) | 0.0151 (17) | 0.0007 (16) |
| C14 | 0.0384 (19) | 0.0388 (18) | 0.0474 (19) | 0.0024 (15) | 0.0160 (16) | −0.0037 (15) |
| C15 | 0.0370 (18) | 0.0422 (18) | 0.0447 (18) | −0.0019 (15) | 0.0206 (16) | −0.0044 (15) |
| C16 | 0.042 (2) | 0.047 (2) | 0.050 (2) | −0.0038 (16) | 0.0229 (17) | 0.0040 (16) |
| C17 | 0.043 (2) | 0.055 (2) | 0.0412 (19) | 0.0029 (17) | 0.0151 (16) | 0.0006 (16) |
| C18 | 0.0373 (18) | 0.0473 (19) | 0.049 (2) | −0.0056 (16) | 0.0185 (16) | −0.0078 (16) |
| C19 | 0.054 (2) | 0.046 (2) | 0.061 (2) | −0.0100 (18) | 0.022 (2) | 0.0050 (18) |
| C20 | 0.046 (2) | 0.054 (2) | 0.057 (2) | −0.0009 (18) | 0.0153 (18) | 0.0103 (18) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—C14 | 1.652 (3) | C6—C7 | 1.472 (4) |
| O1—C13 | 1.219 (4) | C7—C12 | 1.393 (4) |
| O2—N3 | 1.222 (4) | C7—C8 | 1.394 (4) |
| O3—N3 | 1.226 (4) | C8—C9 | 1.384 (4) |
| N1—C13 | 1.382 (4) | C8—H8 | 0.9300 |
| N1—C14 | 1.391 (4) | C9—C10 | 1.378 (4) |
| N1—H1 | 0.8605 | C9—H9 | 0.9300 |
| N2—C14 | 1.338 (4) | C10—C11 | 1.387 (4) |
| N2—C15 | 1.413 (4) | C10—C13 | 1.492 (4) |
| N2—H2A | 0.8601 | C11—C12 | 1.370 (4) |
| N3—C18 | 1.457 (4) | C11—H11 | 0.9300 |
| C1—C2 | 1.385 (5) | C12—H12 | 0.9300 |
| C1—C6 | 1.388 (4) | C15—C20 | 1.379 (5) |
| C1—H1A | 0.9300 | C15—C16 | 1.381 (4) |
| C2—C3 | 1.365 (6) | C16—C17 | 1.379 (4) |
| C2—H2B | 0.9300 | C16—H16 | 0.9300 |
| C3—C4 | 1.361 (6) | C17—C18 | 1.380 (5) |
| C3—H3A | 0.9300 | C17—H17 | 0.9300 |
| C4—C5 | 1.400 (5) | C18—C19 | 1.363 (5) |
| C4—H4 | 0.9300 | C19—C20 | 1.389 (5) |
| C5—C6 | 1.378 (5) | C19—H19 | 0.9300 |
| C5—H5 | 0.9300 | C20—H20 | 0.9300 |
| | | | |
| C13—N1—C14 | 129.9 (3) | C8—C9—H9 | 119.8 |
| C13—N1—H1 | 115.1 | C9—C10—C11 | 118.8 (3) |
| C14—N1—H1 | 115.1 | C9—C10—C13 | 117.9 (3) |
| C14—N2—C15 | 131.5 (3) | C11—C10—C13 | 123.3 (3) |
| C14—N2—H2A | 114.3 | C12—C11—C10 | 120.7 (3) |
| C15—N2—H2A | 114.2 | C12—C11—H11 | 119.6 |
| O2—N3—O3 | 123.1 (3) | C10—C11—H11 | 119.6 |
| O2—N3—C18 | 118.5 (3) | C11—C12—C7 | 121.5 (3) |
| O3—N3—C18 | 118.4 (3) | C11—C12—H12 | 119.3 |
| C2—C1—C6 | 121.5 (4) | C7—C12—H12 | 119.3 |
| C2—C1—H1A | 119.3 | O1—C13—N1 | 121.3 (3) |
| C6—C1—H1A | 119.3 | O1—C13—C10 | 121.9 (3) |
| C3—C2—C1 | 119.4 (4) | N1—C13—C10 | 116.8 (3) |
| C3—C2—H2B | 120.3 | N2—C14—N1 | 114.4 (3) |
| C1—C2—H2B | 120.3 | N2—C14—S1 | 127.9 (3) |
| C4—C3—C2 | 120.9 (4) | N1—C14—S1 | 117.7 (2) |
| C4—C3—H3A | 119.5 | C20—C15—C16 | 120.2 (3) |
| C2—C3—H3A | 119.5 | C20—C15—N2 | 123.7 (3) |
| C3—C4—C5 | 119.5 (4) | C16—C15—N2 | 116.1 (3) |
| C3—C4—H4 | 120.2 | C17—C16—C15 | 120.5 (3) |
| C5—C4—H4 | 120.2 | C17—C16—H16 | 119.7 |
| C6—C5—C4 | 120.9 (4) | C15—C16—H16 | 119.7 |
| C6—C5—H5 | 119.5 | C16—C17—C18 | 118.5 (3) |

| | | | |
|---|---|---|---|
| C4—C5—H5 | 119.5 | C16—C17—H17 | 120.7 |
| C5—C6—C1 | 117.8 (3) | C18—C17—H17 | 120.7 |
| C5—C6—C7 | 121.9 (3) | C19—C18—C17 | 121.7 (3) |
| C1—C6—C7 | 120.3 (3) | C19—C18—N3 | 119.0 (3) |
| C12—C7—C8 | 117.2 (3) | C17—C18—N3 | 119.2 (3) |
| C12—C7—C6 | 121.0 (3) | C18—C19—C20 | 119.6 (3) |
| C8—C7—C6 | 121.7 (3) | C18—C19—H19 | 120.2 |
| C9—C8—C7 | 121.3 (3) | C20—C19—H19 | 120.2 |
| C9—C8—H8 | 119.3 | C15—C20—C19 | 119.5 (3) |
| C7—C8—H8 | 119.3 | C15—C20—H20 | 120.3 |
| C10—C9—C8 | 120.4 (3) | C19—C20—H20 | 120.3 |
| C10—C9—H9 | 119.8 | | |

| | | | |
|---|---|---|---|
| C6—C1—C2—C3 | −1.8 (5) | C9—C10—C13—O1 | 15.8 (5) |
| C1—C2—C3—C4 | 0.5 (6) | C11—C10—C13—O1 | −162.5 (3) |
| C2—C3—C4—C5 | 0.7 (6) | C9—C10—C13—N1 | −164.2 (3) |
| C3—C4—C5—C6 | −0.6 (6) | C11—C10—C13—N1 | 17.4 (5) |
| C4—C5—C6—C1 | −0.6 (5) | C15—N2—C14—N1 | −177.0 (3) |
| C4—C5—C6—C7 | 179.7 (3) | C15—N2—C14—S1 | 5.4 (5) |
| C2—C1—C6—C5 | 1.8 (5) | C13—N1—C14—N2 | −1.4 (5) |
| C2—C1—C6—C7 | −178.5 (3) | C13—N1—C14—S1 | 176.4 (3) |
| C5—C6—C7—C12 | 139.9 (3) | C14—N2—C15—C20 | 16.4 (5) |
| C1—C6—C7—C12 | −39.8 (5) | C14—N2—C15—C16 | −166.6 (3) |
| C5—C6—C7—C8 | −40.0 (5) | C20—C15—C16—C17 | −1.7 (5) |
| C1—C6—C7—C8 | 140.3 (3) | N2—C15—C16—C17 | −178.8 (3) |
| C12—C7—C8—C9 | 0.5 (5) | C15—C16—C17—C18 | 0.4 (5) |
| C6—C7—C8—C9 | −179.7 (3) | C16—C17—C18—C19 | 0.5 (5) |
| C7—C8—C9—C10 | 0.7 (5) | C16—C17—C18—N3 | −179.0 (3) |
| C8—C9—C10—C11 | −1.3 (5) | O2—N3—C18—C19 | 176.0 (3) |
| C8—C9—C10—C13 | −179.8 (3) | O3—N3—C18—C19 | −4.9 (5) |
| C9—C10—C11—C12 | 0.7 (5) | O2—N3—C18—C17 | −4.5 (5) |
| C13—C10—C11—C12 | 179.1 (3) | O3—N3—C18—C17 | 174.6 (3) |
| C10—C11—C12—C7 | 0.5 (5) | C17—C18—C19—C20 | −0.1 (5) |
| C8—C7—C12—C11 | −1.1 (5) | N3—C18—C19—C20 | 179.5 (3) |
| C6—C7—C12—C11 | 179.0 (3) | C16—C15—C20—C19 | 2.2 (5) |
| C14—N1—C13—O1 | 3.9 (5) | N2—C15—C20—C19 | 179.0 (3) |
| C14—N1—C13—C10 | −176.1 (3) | C18—C19—C20—C15 | −1.3 (6) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2*A*···O1 | 0.86 | 1.90 | 2.633 (4) | 142 |
| C20—H20···S1 | 0.93 | 2.55 | 3.186 (4) | 126 |