1252 independent reflections

714 reflections with  $I > 2\sigma(I)$ 

3 standard reflections

frequency: 120 min

intensity decay: 1%

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## 2-(1*H*-Benzimidazol-1-yl)-1-phenylethanone oxime

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Key indicators: single-crystal X-ray study; T = 294 K; mean  $\sigma$ (C–C) = 0.011 Å; *R* factor = 0.045; *wR* factor = 0.128; data-to-parameter ratio = 6.6.

In the molecule of the title compound,  $C_{15}H_{13}N_3O$ , intramolecular  $C-H \cdots O$  hydrogen bonding causes the formation of a planar five-membered ring. The oxime unit has an *E* configuration. In this configuration, the oxime groups are involved as donors in intermolecular  $O-H \cdots N$  hydrogen bonds, linking the molecules into chains elongated approximately parallel to the *c* axis and stacked along the *b* axis.

#### **Related literature**

For general background, see: Sevagapandian *et al.* (2000); Marsman *et al.* (1999); Karle *et al.* (1996); Etter *et al.* (1990); Chertanova *et al.* (1994). For related structures, see: Özel Güven *et al.* (2007); Hökelek, Batı *et al.* (2001); Hökelek, Zülfikaroğlu *et al.* (2001); Büyükgüngör *et al.* (2003); Hökelek *et al.* (2004); Hökelek *et al.* (2004*a,b*). For bond-length data, see: Allen *et al.* (1987).



#### **Experimental**

Crystal data

 $\begin{array}{l} C_{15}H_{13}N_{3}O\\ M_r = 251.29\\ Orthorhombic, Pna2_1\\ a = 9.3295 \ (1) \ \text{\AA}\\ b = 11.2863 \ (2) \ \text{\AA}\\ c = 12.5962 \ (2) \ \text{\AA} \end{array}$ 

 $V = 1326.32 (3) Å^{3}$ Z = 4 Mo K\alpha radiation \(\mu = 0.08 mm^{-1}\) T = 294 (2) K 0.35 \times 0.25 \times 0.20 mm

#### Data collection

```
Enraf–Nonius TurboCAD-4
diffractometer
Absorption correction: \psi scan
(North et al., 1968)
T_{\min} = 0.933, T_{\max} = 0.977
1252 measured reflections
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#### Refinement

$$\begin{split} R[F^2 > 2\sigma(F^2)] &= 0.045 & \text{H atoms treated by a mixture of} \\ wR(F^2) &= 0.128 & \text{independent and constrained} \\ S &= 1.00 & \text{refinement} \\ 1252 \text{ reflections} & \Delta\rho_{\text{max}} &= 0.16 \text{ e } \text{ Å}^{-3} \\ 189 \text{ parameters} & \Delta\rho_{\text{min}} &= -0.13 \text{ e } \text{ Å}^{-3} \end{split}$$

### Table 1

Hydrogen-bond geometry (Å,  $^{\circ}$ ).

$D - H \cdot \cdot \cdot A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdots A$
$\begin{array}{c} O - H \cdots N1^{i} \\ C8 - H82 \cdots O \end{array}$	0.87 (6)	1.84 (5)	2.654 (7)	155 (6)
	0.96 (6)	2.26 (6)	2.634 (9)	102 (4)

Symmetry code: (i)  $-x + \frac{1}{2}, y + \frac{1}{2}, z - \frac{1}{2}$ .

#### Table 2

Comparison of the bond lengths and angles (Å,  $^{\circ}$ ) in the oxime moieties of (I) with the corresponding values in the related structures (II)–(VII).

	(I)	(II)	(III)	(IV)	(V)	(VI)	(VII)
N3-O	1.383 (7)	1.403 (2)	1.423 (3)	1.4167 (10)	1.429 (4)	1.424 (2)	1.416 (3)
		1.396 (2)	1.396 (3)				1.397 (3)
N3-C9	1.300(7)	1.281 (2)	1.290 (3)	1.2897 (12)	1.241 (6)	1.289 (2)	1.282 (3)
		1.281 (2)	1.282 (3)				1.289 (3)
C9-C10	1.491 (8)	1.477 (3)	1.489 (3)	1.5098 (13)	1.551 (7)	1.513 (2)	1.501 (4)
		1.473 (3)					1.502 (4)
C10-C9-N3	115.3 (5)	115.2 (2)	116.6 (2)	114.32 (8)	118.3 (5)	113.2 (1)	114.4 (2)
		115.0 (2)	115.0 (2)				113.4 (2)
C9-N3-O	111.4 (5)	112.4 (1)	109.4 (2)	110.66 (8)	112.2 (4)	110.6 (1)	110.7 (2)
		112.2 (1)	111.5 (2)				111.1 (2)

Notes: (II) 2,3-dimethylquinoxaline–dimethylglyoxime (1/1) (Hökelek, Batı *et al.*, 2001); (III) 1-(2,6-dimethylphenyl-amino)propane-1,2-dione dioxime (Hökelek, Zülfikaroğlu & Batı, 2001); (IV) N-hydroxy-2-oxo-2,N'-diphenylacetamidine (Büyükgüngör *et al.*, 2003); (V) N-(3,4-dichlorophenyl)-N'-hydroxy-2-oxo-2-phenylacetamidine (Hökelek *et al.*, 2004*a*); (VI) N-hydroxy-N'-(1-naphthyl)-2-phenylacetamidin-2-one (Hökelek *et al.*, 2004*b*); (VII) N-(3-chloro-4-methylphenyl)-N'-hydroxy-2-oxo-2-phenylacetamidine-2,3dimethylquinoxaline–dimethylglyoxime (1/1) (Hökelek *et al.*, 2004c).

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2293).

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### 2-(1H-Benzimidazol-1-yl)-1-phenylethanone oxime

### Ö. Özel Güven, T. Erdogan, N. Çaylak and T. Hökelek

#### Comment

Oxime and dioxime derivatives are very important compounds in the chemical industry and medicine (Sevagapandian *et al.*, 2000\bbr018). The oxime (-C=N—OH) moiety is potentially ambidentate, with possibilities of coordination through nitrogen and/or oxygen atoms. It is a functional group that has not been extensively explored in crystal engineering. In the solid state, oximes are usually associated *via* O—H···N hydrogen bonds of length 2.8 Å.

Oxime groups possess stronger hydrogen-bonding capabilities than alcohols, phenols, and carboxylic acids (Marsman *et al.*, 1999\bbr015), in which intermolecular hydrogen bonding combines moderate strength and directionality (Karle *et al.*, 1996\bbr014) in linking molecules to form supramolecular structures; this has received considerable attention with respect to directional noncovalent intermolecular interactions (Etter *et al.*, 1990\bbr005).

The structures of oxime and dioxime derivatives have been the subject of much interest in our laboratory; examples are 2,3-dimethylquinoxaline-dimethyl- glyoxime (1/1), [(II) Hökelek, Batı *et al.*, 2001\bbr009], 1-(2,6-dimethylphenyl-amino)propane-1,2-dione dioxime, [(III) (Hökelek, Zülfikaroğlu *et al.*, 2001\bbr013), *N*-hydroxy-2-oxo-2,*N*-diphenylacet-amidine, [(IV) (Büyükgüngör *et al.*, 2003\bbr002], *N*-(3,4-dichlorophenyl)-*N*-hydroxy-2-oxo-2-phenylacetamidine, [(V) Hökelek *et al.*, 2004\bbr012], *N*-hydroxy-*N*-(1-naphthyl)-2-phenylacetamidin-2-one [(VI) Hökelek *et al.*, 2004\bbr010] and *N*-(3-chloro-4-methylphenyl)-*N*-hydroxy-2 -oxo-2-phenylacetamidine [(VII) Hökelek *et al.*, 2004\bbr011]. The structure determination of the title molecule, (I) was carried out in order to investigate the strength of the hydrogen bonding capability of the oxime groups and to compare the geometry of the oxime moieties with the previously reported ones.

In the molecule of the title compound (Fig. 1) the bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987\bbr001). The intramolecular C—H···O hydrogen bond (Table 1) causes to the formation of a five-membered planar ring A (O/N3/C8/C9/H82). The benzimidazol B (N1/N2/C7/C1—C6) and phenyl C (C10—C15) rings are, of course, planar and the dihedral angles between the rings are A/B = 89.6 (3)°, A/C = 31.4 (3) and B/C = 74.9 (2)°.

Some significant changes in the geometry of the oxime moieties are evident when the bond lengths and angles are compared with the corresponding values in compounds (II)-(VII) (Table 2). The oxime moiety has an E configuration [C10—C9—N3—O 174.9 (5)°; Chertanova *et al.*, 1994\bbr003]. In this configuration, the oxime groups are involved as donors in O—H…N intermolecular hydrogen bondings (Table 1).

In the crystal structure, the intermolecular O—H···N hydrogen bonds (Table 1) link the molecules into chains elongated approximately parallel to the c axis and stacked along the b axis (Fig. 2). The intra- and intermolecular hydrogen bonds seem to be effective in the stabilization of the crystal structure.

#### **Experimental**

The title compound was prepared from a mixture of 2-(1*H*-benzimidazol-1-yl)-1-phenylethanone (Özel Güven *et al.*, 2007\bbr017) (2.09 g, 8.84 mmol) in methanol (5 ml) and hydroxylaminehydrogensulfate (1.45 g, 8.84 mmol) in water

(3 ml), which was stirred for 24 h at room temperature. Then, methanol was evaporated and extracted with ether and the organic layer was dried and evaporated to dryness. The crude residue was purified by chromatography and recrystallized from methanol solution to obtain colorless crystals (yield; 1.44 g, 65%).

#### Refinement

Atoms H, H7, H81 and H82 were located in difference syntheses and refined isotropically [O—H = 0.87 (5) Å,  $U_{iso}(H) = 0.11$  (3) Å<sup>2</sup>; C—H = 0.93 (6)–0.96 (6) Å,  $U_{iso}(H) = 0.053$  (17)–0.062 (19) Å<sup>2</sup>]. The remaining H atoms were positioned geometrically, with C—H = 0.93 Å, and constrained to ride on their parent atom, with  $U_{iso}(H) = 1.2U_{eq}(C)$ .

#### **Figures**



Fig. 1. The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.



Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity [symmetry codes: (') -x, -y, z + 1/2; ('') -x + 1/2, y + 1/2, z + 1/2; x + 1/2, -y + 1/2, z].

#### 2-(1*H*-Benzimidazol-1-yl)-1-phenylethanone oxime

Crystal data	
C <sub>15</sub> H <sub>13</sub> N <sub>3</sub> O	$D_{\rm x} = 1.258 {\rm ~Mg~m^{-3}}$
$M_r = 251.29$	Melting point: 465-468 K
Orthorhombic, <i>Pna</i> 2 <sub>1</sub>	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: P 2c -2n	Cell parameters from 25 reflections
a = 9.3295 (1)  Å	$\theta = 3.6 - 18.8^{\circ}$
<i>b</i> = 11.2863 (2) Å	$\mu = 0.08 \text{ mm}^{-1}$
c = 12.5962 (2) Å	T = 294 (2) K
V = 1326.32 (3) Å <sup>3</sup>	Block, colourless
Z = 4	$0.35\times0.25\times0.20\ mm$
$F_{000} = 528$	
Duta aultation	

Data collection

diffractometer

Radiation source: fine-focus sealed tube	$\theta_{\text{max}} = 25.3^{\circ}$
Monochromator: graphite	$\theta_{\min} = 2.4^{\circ}$
T = 294(2)  K	$h = -11 \rightarrow 0$
non–profiled $\omega$ scans	$k = 0 \rightarrow 13$
Absorption correction: $\psi$ scan (North <i>et al.</i> , 1968\bbr016)	$l = -15 \rightarrow 0$
$T_{\min} = 0.933, T_{\max} = 0.977$	3 standard reflections
1252 measured reflections	every 120 min
1252 independent reflections	intensity decay: 1%
714 reflections with $I > 2\sigma(I)$	

#### Refinement

Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.045$ 

H atoms treated by a mixture of independent and constrained refinement  $w = 1/[\sigma^2(F_o^2) + (0.0654P)^2]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{max} < 0.001$  $\Delta\rho_{max} = 0.16 \text{ e } \text{Å}^{-3}$  $\Delta\rho_{min} = -0.13 \text{ e } \text{Å}^{-3}$ Extinction correction: SHELXL97 (Sheldrick, 1997\bbr019), Fc\*=kFc[1+0.001xFc^2\lambda^3/sin(2\theta)]^{-1/4} Extinction coefficient: 0.017 (5)

1252 reflections

 $wR(F^2) = 0.128$ 

S = 1.00

189 parameters

4 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map Hydrogen site location: inferred from neighbouring sites

#### 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  $F^2 > 2 \operatorname{sigma}(F^2)$  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  $(A^2)$ 

	x	у	Ζ	$U_{\rm iso}*/U_{\rm eq}$
0	0.3005 (7)	1.2486 (4)	0.6439 (4)	0.0909 (16)
N1	0.2400 (7)	0.8842 (4)	0.9744 (4)	0.0668 (15)

N2	0.3004 (6)	1.0208 (4)	0.8558 (4)	0.0598 (14)
N3	0.3436 (6)	1.1408 (5)	0.6026 (5)	0.0700 (15)
C1	0.1192 (7)	0.9178 (5)	0.9184 (5)	0.0589 (16)
C2	-0.0212 (9)	0.8795 (6)	0.9275 (7)	0.080 (2)
C3	-0.1197 (9)	0.9278 (7)	0.8627 (7)	0.091 (2)
C4	-0.0845 (9)	1.0144 (8)	0.7884 (7)	0.095 (3)
C5	0.0541 (8)	1.0552 (6)	0.7774 (5)	0.074 (2)
C6	0.1554 (7)	1.0039 (5)	0.8440 (5)	0.0601 (17)
C7	0.3432 (10)	0.9469 (6)	0.9337 (5)	0.0697 (19)
C8	0.3909 (10)	1.1002 (7)	0.7907 (6)	0.070 (2)
C9	0.3845 (6)	1.0686 (5)	0.6770 (5)	0.0562 (16)
C10	0.4210 (7)	0.9465 (5)	0.6408 (5)	0.0613 (17)
C11	0.5217 (9)	0.8793 (7)	0.6923 (7)	0.091 (2)
C12	0.5529 (10)	0.7643 (9)	0.6562 (8)	0.119 (3)
C13	0.4857 (11)	0.7195 (8)	0.5701 (8)	0.111 (3)
C14	0.3855 (9)	0.7856 (7)	0.5190 (7)	0.091 (2)
C15	0.3517 (7)	0.8977 (6)	0.5544 (6)	0.074 (2)
Н	0.261 (7)	1.288 (5)	0.592 (4)	0.11 (3)*
H2	-0.0466	0.8220	0.9769	0.096*
H3	-0.2144	0.9026	0.8677	0.109*
H4	-0.1561	1.0455	0.7451	0.114*
H5	0.0783	1.1135	0.7285	0.089*
H7	0.437 (7)	0.951 (5)	0.959 (5)	0.062 (18)*
H11	0.5694	0.9098	0.7511	0.109*
H12	0.6204	0.7187	0.6920	0.142*
H13	0.5079	0.6439	0.5459	0.134*
H14	0.3393	0.7550	0.4596	0.109*
H15	0.2812	0.9411	0.5196	0.089*
H81	0.484 (6)	1.088 (5)	0.817 (5)	0.053 (17)*
H82	0.361 (6)	1.180 (5)	0.806 (5)	0.062 (19)*

## Atomic displacement parameters $(Å^2)$

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
0	0.151 (5)	0.060 (3)	0.062 (3)	-0.006 (3)	-0.015 (3)	0.017 (2)
N1	0.088 (4)	0.058 (3)	0.055 (3)	-0.005 (3)	0.001 (3)	0.018 (3)
N2	0.077 (4)	0.057 (3)	0.045 (3)	-0.010 (3)	-0.005 (3)	0.014 (3)
N3	0.086 (4)	0.055 (3)	0.069 (3)	-0.010 (3)	0.000 (3)	0.012 (3)
C1	0.073 (5)	0.053 (4)	0.050 (4)	0.001 (3)	0.010 (3)	0.007 (3)
C2	0.093 (6)	0.067 (4)	0.079 (5)	-0.004 (4)	0.016 (5)	0.016 (4)
C3	0.075 (5)	0.101 (5)	0.097 (6)	-0.001 (5)	0.015 (5)	0.012 (5)
C4	0.077 (6)	0.109 (6)	0.099 (6)	0.020 (5)	-0.008 (5)	0.017 (5)
C5	0.086 (6)	0.069 (4)	0.068 (5)	0.010 (4)	-0.007 (4)	0.015 (4)
C6	0.081 (5)	0.054 (3)	0.046 (4)	-0.002 (3)	-0.001 (4)	0.007 (3)
C7	0.091 (6)	0.069 (4)	0.049 (4)	-0.010 (4)	-0.021 (4)	0.020 (4)
C8	0.080 (5)	0.071 (5)	0.059 (4)	-0.025 (4)	-0.013 (4)	0.019 (4)
C9	0.066 (4)	0.057 (4)	0.046 (3)	-0.017 (3)	-0.008 (3)	0.019 (3)
C10	0.062 (4)	0.065 (4)	0.057 (4)	-0.009 (3)	0.010 (3)	0.019 (4)

$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C11	0.093 (5)	0.107 (6)	0.071 (5)	0.021 (5)	-0.005 (4)	0.015 (5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C12	0.132 (8)	0.123 (8)	0.102 (7)	0.064 (6)	0.009 (6)	0.014 (6)
C14         0.095 (6)         0.007 (5)         0.000 (6)         -0.007 (4)         0.007 (5)         -0.017 (4)           C15         0.066 (5)         0.067 (4)         0.091 (5)         -0.007 (3)         -0.005 (4)         0.004 (4)           Geometric parameters (Å. ?)         0         0         -H         0.87 (5)         C7-H7         0.93 (6)           N1-C7         1.300 (9)         C8-H81         0.94 (6)         0.92 (6)         0.94 (6)           N2-C6         1.375 (8)         C8-H82         0.96 (6)         0.94 (6)           N2-C7         1.348 (8)         C9-C8         1.478 (10)           N3-C9         1.300 (7)         C10-C11         1.370 (10)           C1-C1         1.383 (8)         C10-C12         1.491 (8)           C2-C3         1.345 (11)         C12-C13         1.311 (9)           C1-C4         1.390 (0)         C11-H11         0.9300           C3-H3         0.9300         C12-C13         1.351 (13)           C3-H3         0.9300         C15-H14         1.358 (12)           C4-H4         0.9300         C15-H14         0.9300           C3-H3         0.9300         C15-H14         1.378 (9)           C5-H5         0.93	C13	0 130 (8)	0.092 (6)	0.112 (8)	0.019(6)	0.036(7)	0.002.(6)
C15         0.066 (5)         0.067 (4)         0.091 (5)         -0.007 (3)         -0.005 (4)         0.004 (4)           Geometric parameters (Å, ")           ON3         1.383 (7)         C5C6         1.389 (9)           OH         0.87 (5)         C7H7         0.93 (6)           N1-C7         1.300 (9)         C8H81         0.94 (6)           N2-C7         1.348 (8)         C9-C8         1.478 (10)           N2-C8         1.479 (8)         C10-C9         1.491 (8)           N3-C9         1.300 (7)         C10-C11         1.370 (10)           C1-N1         1.383 (8)         C10-C12         1.465 (11)           C2-C3         1.344 (10)         C11H11         0.9300           C1-C4         1.339 (11)         C14-C13         1.351 (13)           C3-C4         1.339 (11)         C14-C13         1.358 (12)           C4-H4         0.9300         C13H13         0.9300           C3-H2         0.9300         C15H14         0.9300           C3-H4         0.9300         C15H14         0.9300           C5-H5         0.9300         C15H15         0.9300           C5-H4         1.358 (12)         C4+-H44	C14	0.095 (6)	0.077 (5)	0.100(6)	-0.007(4)	0.000(7)	-0.017(4)
Geometric parameters (Å, ?)         Interest         Interest         Interest         Interest         Interest           Geometric parameters (Å, ?)         0–Ni         0.87 (5)         C7–H7         0.93 (6)           NI-C7         1.300 (9)         C8–H81         0.94 (6)           N2-C6         1.375 (8)         C8–H82         0.96 (6)           N2-C7         1.348 (8)         C9–C8         1.478 (10)           N2-C8         1.479 (8)         C10–C9         1.491 (8)           N3-C9         1.300 (7)         C10–C11         1.370 (10)           C1-C1         1.381 (9)         C1–C12         1.445 (11)           C2-C3         1.345 (11)         C12–H11         0.9300           C2-H2         0.9300         C12–C13         1.358 (12)           C4-H4         0.9300         C14–H14         0.9300           C3-C4         1.337 (9)         C15–C14         1.378 (9)           C5–C4         1.391 (9)         C15–C14         1.378 (9)           C5–H5         0.9300         C15–H15         0.9300           NI-C1-C2         1301 (6)         N2–C8–H81         104 (3)           NI-C1-C6         109.7 (6)         C9–C8–H22         111.5 (5)	C15	0.066 (5)	0.067 (4)	0.091 (5)	-0.007(3)	-0.005(4)	0.004 (4)
Geometric parameters (4. ?) $O-M3$ 1.383 (7) $C5-C6$ 1.389 (9) $O-H1$ 0.87 (5) $C7-H7$ 0.93 (6) $N1-C7$ 1.300 (9) $C8-H81$ 0.94 (6) $N2-C6$ 1.375 (8) $C8-H82$ 0.96 (6) $N2-C7$ 1.348 (8) $C9-C8$ 1.478 (10) $N2-C8$ 1.479 (8) $C10-C9$ 1.491 (8) $N3-C9$ 1.300 (7) $C10-C11$ 1.370 (10) $C1-N1$ 1.383 (8) $C10-C15$ 1.381 (9) $C1-C2$ 1.384 (10) $C11-H11$ 0.9300 $C1-C4$ 1.392 (8) $C11-C12$ 1.405 (11) $C2-C3$ 1.345 (11) $C12-H12$ 0.9300 $C2-H2$ 0.9300 $C13-H13$ 0.9300 $C3-H4$ 1.393 (11) $C14-C13$ 1.358 (12) $C4-H4$ 0.9300 $C15-H15$ 0.9300 $C3-C4$ 1.379 (9) $C15-C14$ 1.378 (9) $C5-H5$ 0.9300 $C15-H15$ 0.9300 $N3-O-H$ 107 (4) $N2-C8-H81$ 104 (3) $N1-C1-C2$ 130 (6) $N2-C8-H81$ 110 (4) $C-N2-C6$ 106 5 (6)H81-C8-H82107 (4) $N1-C1-C6$ 109 7 (6) $C9-C8-N2$ 111 5 (5) $C7-N2-C6$ 106 5 (6)H81-C8-H82106 (5) $C7-N2-C6$ 106 5 (6)H81-C8-H82110 (4) $C7-N2-C6$ 106 5 (6)H81-C8-H82106 (5) $C7-N2-C6$ 106 5 (6)H81-C8-H82106 (5) $C7-N2-C6$ 106 5 (6)H81-C8-H82106 (5) $C7-N2-C6$ <td></td> <td></td> <td></td> <td></td> <td></td> <td>()</td> <td></td>						()	
O = N3 $1.383$ (7) $CS = -C6$ $1.389$ (9) $O = H$ $0.87$ (5) $C7 = H7$ $0.93$ (6) $N1 = C7$ $1.300$ (9) $C8 = H81$ $0.94$ (6) $N2 = C6$ $1.375$ (8) $C8 = H82$ $0.96$ (6) $N2 = C7$ $1.348$ (8) $C9 = C8$ $1.478$ (10) $N2 = C8$ $1.479$ (8) $C10 = C11$ $1.370$ (10) $C1 = N1$ $1.383$ (8) $C10 = C11$ $1.370$ (10) $C1 = C6$ $1.392$ (8) $C11 = H11$ $0.9300$ $C1 = C6$ $1.392$ (8) $C12 = C13$ $1.351$ (13) $C2 = C3$ $1.345$ (11) $C12 = C13$ $1.358$ (12) $C4 = H12$ $0.9300$ $C13 = H13$ $0.9300$ $C3 = C4$ $1.379$ (9) $C15 = C14$ $1.378$ (9) $C5 = H5$ $0.9300$ $C15 = H15$ $0.9300$ $N = O = H$ $107$ (4) $N = C6 = H81$ $104$ (3) $N = C = C2$ $1301$ (6) $N = C8 = H81$ $104$ (4) $N = C = N2$ $111.5$ (5) $C7 = N2 = M18$ $106$ (4) $N = C = N2$ <td< td=""><td>Geometric param</td><td>neters (Å, °)</td><td></td><td></td><td></td><td></td><td></td></td<>	Geometric param	neters (Å, °)					
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0 N3		1 383 (7)	C5 C6			1 380 (0)
O-1         0.57 (5)         C + 11         0.53 (5)           N1-C7         1.300 (9)         C8-H81         0.94 (6)           N2-C6         1.375 (8)         C8-H82         0.96 (6)           N2-C7         1.348 (8)         C9-C8         1.478 (10)           N2-C8         1.479 (8)         C10-C9         1.491 (8)           N3-C9         1.300 (7)         C10-C11         1.370 (10)           C1-C2         1.384 (10)         C11-H11         0.9300           C1-C4         1.392 (8)         C11-C12         1.405 (11)           C2-H2         0.9300         C12-C13         1.351 (13)           C3-H3         0.9300         C13-H13         0.9300           C3-H4         0.9300         C14-H14         0.9300           C3-C4         1.393 (11)         C14-C13         1.358 (12)           C4-H4         0.9300         C15-H15         0.9300           C5-G4         1.379 (9)         C15-C14         1.378 (9)           C5-H5         0.9300         C15-H15         0.9300           N1-C1-C2         1.30.1 (6)         N2-C8-H81         104 (3)           N1-C1-C6         109.7 (6)         C9-C8-N2         111.5 (5)	0—N3		1.383(7)	С5—С0 С7 Н7	,		1.389(9)
$\begin{split} & \text{NI} = C^{-1} & \text{I} = 303 (5) & \text{CS} = 182 & 0.94 (6) \\ & \text{N2} = -C6 & 1.375 (8) & \text{CS} = -182 & 0.94 (6) \\ & \text{N2} = -C7 & 1.348 (8) & \text{C9} = -C8 & 1.478 (10) \\ & \text{N2} = -C8 & 1.479 (8) & \text{C10} = -C11 & 1.370 (10) \\ & \text{C1} = -N1 & 1.383 (8) & \text{C10} = -C11 & 1.370 (10) \\ & \text{C1} = -C2 & 1.384 (10) & \text{C1} = -H11 & 0.9300 \\ & \text{C1} = -C6 & 1.392 (8) & \text{C1} = -C12 & 1.495 (11) \\ & \text{C2} = -C3 & 1.345 (11) & \text{C1} = -H12 & 0.9300 \\ & \text{C2} = -H2 & 0.9300 & \text{C1} = -H12 & 0.9300 \\ & \text{C2} = -H2 & 0.9300 & \text{C1} = -H12 & 0.9300 \\ & \text{C2} = -H2 & 0.9300 & \text{C1} = -H12 & 0.9300 \\ & \text{C3} = -C4 & 1.393 (11) & \text{C1} = -H14 & 0.9300 \\ & \text{C3} = -C4 & 1.393 (11) & \text{C1} = -H14 & 0.9300 \\ & \text{C4} = -H4 & 0.9300 & \text{C1} = -H14 & 0.9300 \\ & \text{C5} = -C4 & 1.379 (9) & \text{C1} = -C14 & 1.378 (9) \\ & \text{C5} = -H5 & 0.9300 & \text{C1} = -H14 & 0.9300 \\ & \text{C5} = -C4 & 1.379 (9) & \text{C1} = -C14 & 1.378 (9) \\ & \text{C5} = -H5 & 0.9300 & \text{C1} = -H14 & 0.9300 \\ & \text{N1} = -C1 = -C2 & 130 (16) & \text{N2} = -C8 = -H81 & 104 (3) \\ & \text{N1} = -C1 = -C2 & 130 (16) & \text{N2} = -C8 = -H81 & 104 (3) \\ & \text{N1} = -C1 = -C2 & 130 (16) & \text{N2} = -C8 = -H82 & 107 (4) \\ & \text{N1} = -C1 = -C6 & 109.7 (6) & \text{C9} = -C8 = -H82 & 110 (5) \\ & \text{C7} = -N1 = C1 & 104.7 (5) & \text{C9} = -C8 = -H82 & 110 (5) \\ & \text{C7} = -N2 = -C8 & 125.9 (5) & \text{C9} = -C8 = -H82 & 110 (5) \\ & \text{C7} = -N2 = -C8 & 125.9 (5) & \text{C9} = -C8 = -H82 & 110 (5) \\ & \text{C7} = -N2 = -C8 & 127.5 (6) & \text{N3} = -O9 = -C10 & 120.7 (6) \\ & \text{C1} = -C2 = -H2 & 121.0 & \text{C1} = -C10 = -C13 & 118.2 (6) \\ & \text{C3} = -C2 = -H2 & 121.0 & \text{C1} = -C10 = -C13 & 118.2 (6) \\ & \text{C3} = -C2 = -H2 & 121.0 & \text{C1} = -C10 = -C13 & 118.2 (6) \\ & \text{C3} = -C2 = -H2 & 121.0 & \text{C1} = -C1 = -C11 & 120.0 (8) \\ & \text{C2} = -C3 = -H3 & 119.0 & \text{C1} = -C1 = -C11 & 120.0 (8) \\ & \text{C2} = -C3 = -H3 & 119.0 & \text{C1} = -C1 = -C11 & 120.0 (8) \\ & \text{C2} = -C3 = -H3 & 119.0 & \text{C1} = -C1 = -H11 & 120.0 \\ & \text{C4} = -C3 = -H3 & 119.0 & \text{C1} = -C1 = -H12 & 19.7 \\ & \text{C4} = -C5 = -H5 & 122.0 & \text{C1} = -C1 = -H13 & 120.2 \\ & \text{C4} = -$	0—11 N1—C7		1.300(9)	С?—Н?	1		0.93 (0)
N2-C3       1.373 (8)       C9-162       0.30 (9)         N2-C7       1.348 (8)       C9-C8       1.478 (10)         N2-C8       1.479 (8)       C10-C9       1.491 (8)         N3-C9       1.300 (7)       C10-C1       1.370 (10)         C1-C1       1.338 (8)       C10-C15       1.381 (9)         C1-C2       1.384 (10)       C11-H11       0.9300         C2-C3       1.345 (11)       C12-H12       0.9300         C2-H2       0.9300       C12-C13       1.351 (13)         C3-H3       0.9300       C13-H13       0.9300         C3-C4       1.393 (11)       C14-C13       1.358 (12)         C4-H4       0.9300       C15-C14       1.378 (9)         C5-C4       1.379 (9)       C15-C14       1.378 (9)         C5-C4       1.379 (9)       C15-C14       1.378 (9)         C5-C4       1.379 (9)       C15-H15       0.9300         N1-C1-C2       1301 (6)       N2-C8-H81       104 (3)         N1-C1-C4       109.7 (6)       C9-C8-H82       107 (4)         N1-C1-C5       109.7 (6)       C9-C8-H82       107 (4)         N1-C1       104.7 (5)       C9-C8-H81       110 (5)	N1 - C7		1.300(9)	C8 H8	2		0.94 (0)
N2-C3       1.349 (8)       CP-C3       1.449 (10)         N2-C3       1.490 (8)       CI0-C9       1.491 (8)         N3-C9       1.300 (7)       C10-C11       1.370 (10)         C1-N1       1.383 (8)       C10-C15       1.811 (9)         C1-C2       1.384 (10)       C11-H11       0.9300         C2-C3       1.345 (11)       C12-H12       0.9300         C2-H2       0.9300       C12-C13       1.51 (13)         C3-H3       0.9300       C14-H14       0.9300         C3-C4       1.393 (11)       C14-C13       1.358 (12)         C4-H4       0.9300       C15-C14       1.378 (9)         C5-C4       1.379 (9)       C15-C14       1.378 (9)         C5-H5       0.9300       C15-H15       0.9300         N1-C1-C2       130.1 (6)       N2-C8-H81       104 (3)         N1-C1-C2       130.1 (6)       N2-C8-H81       104 (3)         N1-C1-C2       130.1 (6)       N2-C8-H81       104 (4)         C7-N2-C8       125.9 (5)       C9-C8-H81       104 (4)         C7-N2-C8       125.9 (5)       C9-C8-H81       10 (4)         C6-N2-C1       106.5 (6)       H81-C8-H82       110 (5)	$N_2 = C_0$		1.373(8) 1.348(8)		52		1.478(10)
N3-C3       1.437 (6)       C10-C3       1.437 (6)         N3-C9       1.300 (7)       C10-C11       1.370 (10)         C1-N1       1.383 (8)       C10-C15       1.381 (9)         C1-C2       1.384 (10)       C11-H11       0.9300         C1-C6       1.392 (8)       C11-C12       1.405 (11)         C2-C3       1.345 (11)       C12-H12       0.9300         C3-C4       1.393 (11)       C14-C13       1.358 (12)         C4-H4       0.9300       C14-H14       0.9300         C5-C4       1.379 (9)       C15-C14       1.378 (9)         C5-H5       0.9300       C15-H15       0.9300         N3-O-H       107 (4)       N2-C8-H81       104 (3)         N1-C1-C2       130.1 (6)       N2-C8-H81       104 (3)         N1-C1-C4       1097 (6)       C9-C8-H81       110 (4)         C6-N2-C8       125 (5)       C9-C8-H81       110 (4)         C6-N2-C8       125 (5)       C9-C8-H81       110 (5)         C7-N2-C6       106 (5) (6)       H81-C8-H82       110 (5)         C7-N2-C6       106 (5) (6)       H81-C9-C10       125 (5)         C3-C2-C1       111 (5)       N3-C9-C10       120 (6)	N2_C8		1.348 (8)	C10 C	0		1.478 (10)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$N_2 = C_0$		1.479(0) 1 300(7)	C10—C	<i>5</i> 11		1.491(0) 1 370(10)
CI-MI1.505 (8)CI-CL31.536 (9)CI-C21.384 (10)CI1-H110.9300CI-C61.392 (8)CI1-C121.405 (11)C2-C31.345 (11)CI2-H120.9300C3-H30.9300CI3-H130.9300C3-C41.393 (11)CI4-C131.358 (12)C4-H40.9300CI3-H140.9300C5-C41.379 (9)CI5-C141.378 (9)C5-H50.9300CI5-H150.9300C5-C41.379 (9)CI5-H150.9300C5-C41.301 (6)N2-C8-H81104 (3)NI-C1-C2130.1 (6)N2-C8-H81104 (3)NI-C1-C4130.1 (6)N2-C8-H81110 (4)C7-N2-C5109.7 (6)C9-C8-N2111.5 (5)C7-N1-C1104.7 (5)C9-C8-H82114 (4)C6-N2-C8125.9 (5)C9-C8-H82110 (5)C7-N2-C6106.5 (6)H81-C8-H82110 (5)C7-N2-C6106.5 (6)N3-C9-C10153.3 (5)C2-C1-C6120.2 (6)C8-C9-C10120.7 (6)C3-C2-C1118.1 (7)C11-C10-C9121.6 (7)C3-C2-C1118.1 (7)C11-C10-C9120.2 (6)C2-C3-C4121.0C10-C11-H11120.0C3-C2-C1121.6 (8)C10-C11-C12120.0 (6)C2-C3-H3119.0C10-C1-C1-H11120.0C3-C4-C3121.5 (8)C13-C12-C11120.6 (9)C3-C4-C4122.0C12-C13-H13120.2C4-C5-H5122.0C12-C13-H13	NJC3		1.300(7) 1.383(8)	C10—C	11		1.370 (10)
C1-C21.364 (10)C11-H110.9500C1-C61.392 (8)C11-C121.405 (11)C2-C31.345 (11)C12-H120.9300C2-H20.9300C12-C131.351 (13)C3-H30.9300C13-H130.9300C3-C41.393 (11)C14-C131.358 (12)C4-H40.9300C14-H140.9300C5-C41.379 (9)C15-C141.378 (9)C5-H50.9300C15-H150.9300N3-O-H107 (4)N2-C8-H81104 (3)N1-C1-C2103.1 (6)N2-C8-H81104 (3)N1-C1-C6109.7 (6)C9-C8-N2111.5 (5)C7-N1-C1104.7 (5)C9-C8-H81110 (4)C6-N2-C8125.9 (5)C9-C8-H82114 (4)C7-N2-C6106.5 (6)H81-C8-H82110 (5)C7-N2-C6106.5 (6)H81-C8-H82110 (5)C7-N2-C6106.5 (6)H81-C8-H82110 (6)C9-N3-O111.4 (5)N3-C9-C10115.3 (5)C2-C1-C6120.2 (6)C8-C9-C1020.7 (6)C3-C2-H2121.0C11-C10-C15118.2 (6)C3-C2-H2121.0C11-C10-C15118.2 (6)C3-C2-H2121.0C10-C11-H11120.0C4-C3-H3119.0C10-C11-H11120.0C3-C4-H4119.3C11-C12-H12119.7C5-C4-C5121.5 (8)C13-C12-C11120.6 (9)C5-C4-C5122.0C14-C13-H13120.2C4-C5-H5122.0C14-C13-H13120.2 <td>C1 - C1</td> <td></td> <td>1.383(8)</td> <td>C10—C</td> <td>15</td> <td></td> <td>0.0200</td>	C1 - C1		1.383(8)	C10—C	15		0.0200
C1-C01.392 (8)C11-C121.405 (11)C2-C31.345 (11)C12-H120.9300C2-H20.9300C12-C131.351 (13)C3-H30.9300C13-H130.9300C3-C41.379 (9)C15-C141.378 (9)C5-C41.379 (9)C15-C141.378 (9)C5-H50.9300C15-H150.9300N3-O-H107 (4)N2-C8-H81104 (3)N1-C1-C2130.1 (6)N2-C8-H81104 (3)N1-C1-C6109.7 (6)C9-C8-H82114 (4)C7-N1-C1104.7 (5)C9-C8-H81110 (4)C6-N2-C8125.9 (5)C9-C8-H81110 (4)C6-N2-C8125.9 (5)C9-C8-H82114 (4)C7-N2-C6106.5 (6)H81-C8-H82110 (5)C2-C1-C6120.2 (6)C8-C9-C10123.7 (6)C2-C1-C6120.2 (6)C8-C9-C10120.7 (6)C1-C2-H2121.0C11-C10-C15118.2 (6)C3-C2-C1118.1 (7)C11-C10-C9121.6 (7)C3-C2-H2121.0C15-C10-C9120.2 (6)C2-C3-C4122.1 (8)C10-C11-H11120.0C4-C3-H3119.0C12-C11-H11120.0C4-C3-H3119.0C12-C11-H11120.0C4-C3-H4119.3C13-C12-C14119.7C5-C4-C3121.5 (8)C13-C12-C11119.7C5-C4-C4122.0C14-C13-H13120.2C4-C5-H5122.0C14-C13-H13120.2C4-C5-H5122.0C13-C14-H14119	C1 = C2		1.364(10) 1.302(8)	C11—fi	12		1 405 (11)
C2-C3 $1.340$ (11) $C12-C13$ $0.9300$ $C3-H2$ $0.9300$ $C13-H13$ $0.9300$ $C3-C4$ $1.393$ (11) $C14-C13$ $1.358$ (12) $C4-H4$ $0.9300$ $C14-H14$ $0.9300$ $C5-C4$ $1.379$ (9) $C15-C14$ $1.378$ (9) $C5-H5$ $0.9300$ $C15-H15$ $0.9300$ $N-C-I-C2$ $130.1$ (6) $N2-C8-H81$ $104$ (3) $NI-C1-C2$ $130.1$ (6) $N2-C8-H81$ $104$ (3) $NI-C1-C6$ $109.7$ (6) $C9-C8-N2$ $111.5$ (5) $C7-N1-C1$ $104.7$ (5) $C9-C8-H81$ $110$ (4) $C6-N2-C8$ $125.9$ (5) $C9-C8-H82$ $114$ (4) $C7-N2-C6$ $106.5$ (6) $H81-C8-H82$ $110$ (5) $C7-N2-C6$ $106.5$ (6) $H81-C8-H82$ $110$ (5) $C7-N2-C6$ $120.2$ (6) $C8-C9-C10$ $15.3$ (5) $C2-C1-C6$ $120.2$ (6) $C8-C9-C10$ $120.7$ (6) $C1-C2-H2$ $121.0$ $C11-C10-C15$ $118.2$ (6) $C3-C2-C1$ $118.1$ (7) $C11-C10-C9$ $121.6$ (7) $C3-C2-C1$ $118.1$ (7) $C11-C10-C9$ $120.6$ (8) $C2-C3-C4$ $122.1$ (8) $C10-C11-H11$ $120.0$ $C4-C3-H3$ $119.0$ $C12-C1-H12$ $119.7$ $C5-C4-C3$ $121.5$ (8) $C13-C12-H12$ $119.7$ $C4-C5-C6$ $116.0$ (7) $C12-C13-C14$ $119.6$ (9) $C5-C4-C1$ $122.0$ $C14-C13-H13$ $120.2$ $C6-C5-H5$ $122.0$ $C12-C13-H14$ $119.7$ <t< td=""><td>C1 = C0</td><td></td><td>1.392(0) 1.345(11)</td><td>C12 U</td><td>12</td><td></td><td>0.0200</td></t<>	C1 = C0		1.392(0) 1.345(11)	C12 U	12		0.0200
C2-H20.9300C12-C131.51 (15)C3-H30.9300C13-H130.9300C3-C41.393 (11)C14-C131.358 (12)C4-H40.9300C14-H140.9300C5-C41.379 (9)C15-C141.378 (9)C5-H50.9300C15-H150.9300N3-O-H107 (4)N2-C8-H81104 (3)N1-C1-C2130.1 (6)N2-C8-H82107 (4)N1-C1-C6109.7 (6)C9-C8-N2111.5 (5)C7-N1-C1104.7 (5)C9-C8-H81110 (4)C6-N2-C8125.9 (5)C9-C8-H82114 (4)C7-N2-C6106.5 (6)H81-C8-H82110 (5)C7-N2-C6106.5 (6)N3-C9-C10115.3 (5)C2-C1-C6120.2 (6)C8-C9-C10120.7 (6)C1-C2-H2121.0C11-C10-C15118.2 (6)C3-C2-C1118.1 (7)C11-C10-C19120.6 (6)C2-C3-C4122.1 (8)C10-C11-H11120.0C4-C3-H3119.0C12-C11-H11120.0C4-C3-H3119.0C12-C11-H11120.0C3-C4-H4119.3C13-C12-H12119.7C5-C4-C3121.5 (8)C13-C12-H12119.7C4-C5-C6116.0 (7)C12-C13-H13120.2C6-C5132.6 (6)C13-C14-C15120.5 (8)C3-C4-C4122.0C14-C13-H13120.2C4-C5-C6132.6 (6)C13-C14-H14119.7C5-C6-C1132.6 (6)C13-C14-H14119.7	C2—C3		0.0300	C12—II	12		1 351 (13)
C3-C41.393 (11)C14-C131.358 (12)C4-H40.9300C14-H140.9300C5-C41.379 (9)C15-C141.378 (9)C5-H50.9300C15-H150.9300N3-O-H107 (4)N2-C8-H81104 (3)N1-C1-C2130.1 (6)N2-C8-H81104 (3)N1-C1-C6109.7 (6)C9-C8-N2111.5 (5)C7-N1-C1104.7 (5)C9-C8-H81110 (4)C6-N2-C8125.9 (5)C9-C8-H82114 (4)C7-N2-C6106.5 (6)H81-C8-H82110 (5)C7-N2-C6106.5 (6)H81-C8-H82110 (5)C2-C1-C6120.2 (6)C8-C9-C1015.3 (5)C2-C1-C6120.2 (6)C8-C9-C10120.7 (6)C1-C2-H2121.0C11-C10-C15118.2 (6)C3-C2-C1118.1 (7)C11-C10-C9121.6 (7)C3-C2-H2121.0C15-C10-C9120.2 (6)C2-C3-C4122.1 (8)C10-C11-H11120.0C4-C3-H3119.0C12-C11-H11120.0C4-C3-H3119.0C12-C12-H12119.7C5-C4-C4121.5 (8)C13-C12-H12119.7C4-C5-C6116.0 (7)C12-C13-C14119.6 (9)C4-C5-H5122.0C12-C13-H13120.2C6-C5132.6 (6)C13-C14-H14119.7C5-C6-C1122.2 (7)C13-C14-H14119.7	C2—H2		0.9300	C12—C	13		0.0300
C3-C41.55 (11)C14-C131.53 (12)C4-H40.9300C14-H140.9300C5-C41.379 (9)C15-C141.378 (9)C5-H50.9300C15-H150.9300N3-O-H107 (4)N2-C8-H81104 (3)N1-C1-C2130.1 (6)N2-C8-H82107 (4)N1-C1-C6109.7 (6)C9-C8-N2111.5 (5)C7-N1-C1104.7 (5)C9-C8-H82110 (4)C6-N2-C8125.9 (5)C9-C8-H82110 (4)C6-N2-C6106.5 (6)H81-C8-H82110 (5)C7-N2-C6106.5 (6)N3-C9-C10115.3 (5)C2-C1-C6120.2 (6)C8-C9-C10120.7 (6)C3-C2-C1118.1 (7)C11-C10-C15118.2 (6)C3-C2-C1118.1 (7)C11-C10-C9121.6 (7)C3-C2-H2121.0C15-C10-C9120.2 (6)C2-C3-C4122.1 (8)C10-C11-C12120.0 (8)C2-C3-H3119.0C12-C11-H11120.0C4-C3-H3119.0C12-C11-H11120.0C4-C3-H319.3C13-C12-C11119.7C5-C4-C3121.5 (8)C13-C12-C11119.7C4-C5-C6116.0 (7)C12-C13-C14119.6 (9)C4-C5-H5122.0C14-C13-H13120.2C6-C5132.6 (6)C13-C14-H14119.7C5-C6-C1105.2 (5)C13-C14-H14119.7	$C_3 = C_4$		1.302(11)	C13—11	12		1 258 (12)
C4-140.5300C14-1140.5300C5-C41.379 (9)C15-C141.378 (9)C5-H50.9300C15-C141.378 (9)N3-O-H107 (4)N2-C8-H81104 (3)N1-C1-C2130.1 (6)N2-C8-H82107 (4)N1-C1-C6109.7 (6)C9-C8-N2111.5 (5)C7-N1-C1104.7 (5)C9-C8-H81110 (4)C6-N2-C8125.9 (5)C9-C8-H81110 (4)C7-N2-C6106.5 (6)H81-C8-H82110 (5)C7-N2-C6106.5 (6)H81-C9-C10115.3 (5)C2-C1-C6120.2 (6)C8-C9-C10120.7 (6)C1-C2-H2121.0C11-C10-C15118.2 (6)C3-C2-C1118.1 (7)C11-C10-C9121.6 (7)C3-C2-H2121.0C15-C10-C9120.2 (6)C2-C3-C4122.1 (8)C10-C11-H11120.0C4-C3-H3119.0C12-C11-H11120.0C3-C4-H4119.3C13-C12-C11119.7C5-C4-C3121.5 (8)C13-C12-C11120.6 (9)C5-C4-C4122.0C14-C13-H13120.2C4-C5-H5122.0C14-C13-H13120.2C6-C5-H5122.0C14-C13-H13120.2C6-C5-H5122.0C14-C13-H13120.2C6-C5-H5122.0C14-C13-H13120.2C6-C5-H5122.0C14-C13-H13120.2C6-C5-H5122.0C14-C13-H14119.7C5-C6-C1105.2 (5)C13-C14-H14119.7	$C_3 = C_4$		0.0300	C14—C	13		0.0300
C3-C41.375 (5)C13-C141.378 (5)C5-H50.9300C15-H150.9300N3-O-H107 (4)N2-C8-H81104 (3)N1-C1-C2130.1 (6)N2-C8-H82107 (4)N1-C1-C6109.7 (6)C9-C8-N2111.5 (5)C7-N1-C1104.7 (5)C9-C8-H81110 (4)C6-N2-C8125.9 (5)C9-C8-H82114 (4)C7-N2-C6106.5 (6)H81-C8-H82110 (5)C7-N2-C8127.5 (6)N3-C9-C8124.0 (6)C9-N3-O111.4 (5)N3-C9-C1015.3 (5)C2-C1-C6120.2 (6)C8-C9-C10120.7 (6)C1-C2-H2121.0C11-C10-C15118.2 (6)C3-C2-C1118.1 (7)C11-C10-C9121.6 (7)C3-C2-H2121.0C15-C10-C9120.2 (6)C2-C3-C4122.1 (8)C10-C11-C12120.0 (8)C2-C3-H3119.0C10-C11-H11120.0C4-C3-H3119.0C12-C11-H11120.0C3-C4-H4119.3C13-C12-C11119.7C5-C4-C3121.5 (8)C13-C12-C11119.7C5-C4-C4122.0C14-C13-H13120.2C4-C5-H5122.0C14-C13-H13120.2C4-C5-H5122.0C14-C13-H13120.2C4-C5-H5122.0C14-C13-H13120.2C4-C5-H5122.0C14-C13-H13120.2C5-C4-C1132.2 (7)C13-C14-H14119.7C5-C6-C1122.2 (7)C13-C14-H14119.7	$C_{4}$		1 379 (9)	C14—II	14		1 378 (0)
N3-O-H107 (4)N2-C8-H81104 (3)N1-C1-C2130.1 (6)N2-C8-H82107 (4)N1-C1-C2130.1 (6)N2-C8-H82107 (4)N1-C1-C6109.7 (6)C9-C8-N211.5 (5)C7-N1-C1104.7 (5)C9-C8-H81110 (4)C6-N2-C8125.9 (5)C9-C8-H82114 (4)C7-N2-C6106.5 (6)H81-C8-H82110 (5)C7-N2-C8127.5 (6)N3-C9-C8124.0 (6)C9-N3-O111.4 (5)N3-C9-C10115.3 (5)C2-C1-C6120.2 (6)C8-C9-C10120.7 (6)C1-C2-H2121.0C11-C10-C15118.2 (6)C3-C2-C1118.1 (7)C11-C10-C9121.6 (7)C3-C2-H212.0C15-C10-C9120.2 (6)C2-C3-C4122.1 (8)C10-C11-C12120.0 (8)C2-C3-H3119.0C12-C11-H11120.0C4-C3-H3119.0C12-C11-H11120.0C3-C4-H4119.3C13-C12-C11119.7C5-C4-C3121.5 (8)C13-C12-C11119.7C4-C5-C6116.0 (7)C12-C13-C14119.6 (9)C4-C5-H5122.0C14-C13-H13120.2C4-C5-H5122.0C14-C13-H13120.2C4-C5-H5122.0C14-C13-H13120.2C4-C5-H5122.0C14-C13-H13120.2C5-C4-C1132.2 (7)C13-C14-H14119.7C5-C6-C1122.2 (7)C13-C14-H14119.7	С5—Н5		0.9300	С15—Н	15		0.9300
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N3—0—H		107 (4)	N2—C8	—H81		104 (3)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	N1-C1-C2		130.1 (6)	N2—C8	-H82		107 (4)
C7 - N1 - C1 $104.7 (5)$ $C9 - C8 - H81$ $110 (4)$ $C6 - N2 - C8$ $125.9 (5)$ $C9 - C8 - H82$ $114 (4)$ $C7 - N2 - C6$ $106.5 (6)$ $H81 - C8 - H82$ $110 (5)$ $C7 - N2 - C8$ $127.5 (6)$ $N3 - C9 - C8$ $124.0 (6)$ $C9 - N3 - O$ $111.4 (5)$ $N3 - C9 - C10$ $115.3 (5)$ $C2 - C1 - C6$ $120.2 (6)$ $C8 - C9 - C10$ $120.7 (6)$ $C1 - C2 - H2$ $121.0$ $C11 - C10 - C15$ $118.2 (6)$ $C3 - C2 - C1$ $118.1 (7)$ $C11 - C10 - C9$ $121.6 (7)$ $C3 - C2 - H2$ $121.0$ $C15 - C10 - C9$ $120.2 (6)$ $C2 - C3 - C4$ $122.1 (8)$ $C10 - C11 - C12$ $120.0 (8)$ $C2 - C3 - H3$ $119.0$ $C10 - C11 - H11$ $120.0$ $C4 - C3 - H3$ $119.0$ $C12 - C11 - H11$ $120.0$ $C3 - C4 - H4$ $119.3$ $C13 - C12 - C11$ $119.7$ $C5 - C4 - C3$ $121.5 (8)$ $C13 - C12 - C11$ $119.7$ $C4 - C5 - C6$ $116.0 (7)$ $C12 - C13 - H13$ $120.2$ $C4 - C5 - H5$ $122.0$ $C14 - C13 - H13$ $120.2$ $C4 - C5 - H5$ $122.0$ $C14 - C13 - H13$ $120.2$ $C4 - C5 - H5$ $122.0$ $C14 - C13 - H13$ $120.2$ $C4 - C5 - H5$ $122.0$ $C14 - C13 - H13$ $120.2$ $C4 - C5 - H5$ $122.0$ $C14 - C13 - H13$ $120.2$ $C5 - C6 - C1$ $105.2 (5)$ $C13 - C14 - H14$ $119.7$	N1-C1-C6		109.7 (6)	C9—C8	—N2		111.5 (5)
C 6 - N2 - C 8125.9 (5)C 9 - C 8 - H 82114 (4)C 7 - N2 - C 6106.5 (6)H 81 - C 8 - H 82110 (5)C 7 - N2 - C 8127.5 (6)N 3 - C 9 - C 8124.0 (6)C 9 - N 3 - O111.4 (5)N 3 - C 9 - C 10115.3 (5)C 2 - C 1 - C 6120.2 (6)C 8 - C 9 - C 10120.7 (6)C 1 - C 2 - H 2121.0C 11 - C 10 - C 15118.2 (6)C 3 - C 2 - C 1118.1 (7)C 11 - C 10 - C 9120.2 (6)C 2 - C 3 - C 4122.1 (8)C 10 - C 11 - C 12120.0 (8)C 2 - C 3 - C 4122.1 (8)C 10 - C 11 - C 12120.0 (8)C 2 - C 3 - H 3119.0C 12 - C 11 - H 11120.0C 4 - C 3 - H 3119.0C 12 - C 11 - H 11120.0C 3 - C 4 - H 4119.3C 11 - C 12 - H 12119.7C 5 - C 4 - C 3121.5 (8)C 13 - C 12 - C 11120.6 (9)C 5 - C 4 - C 3121.5 (8)C 13 - C 12 - H 12119.7C 4 - C 5 - H 5122.0C 12 - C 1 - C 1 - H 13120.2C 6 - C 5 - H 5122.0C 12 - C 1 - H 13120.2N - C 6 - C 5132.6 (6)C 13 - C 1 - C 15120.5 (8)N - C 6 - C 1105.2 (5)C 13 - C 1 - H 14119.7	C7—N1—C1		104.7 (5)	С9—С8	—H81		110 (4)
C7 - N2 - C6 $106.5(6)$ $H81 - C8 - H82$ $110(5)$ $C7 - N2 - C8$ $127.5(6)$ $N3 - C9 - C8$ $124.0(6)$ $C9 - N3 - O$ $111.4(5)$ $N3 - C9 - C10$ $115.3(5)$ $C2 - C1 - C6$ $120.2(6)$ $C8 - C9 - C10$ $120.7(6)$ $C1 - C2 - H2$ $121.0$ $C11 - C10 - C15$ $118.2(6)$ $C3 - C2 - C1$ $118.1(7)$ $C11 - C10 - C9$ $121.6(7)$ $C3 - C2 - H2$ $121.0$ $C15 - C10 - C9$ $120.2(6)$ $C2 - C3 - C4$ $122.1(8)$ $C10 - C11 - C12$ $120.0(8)$ $C2 - C3 - C4$ $122.1(8)$ $C10 - C11 - H11$ $120.0$ $C4 - C3 - H3$ $119.0$ $C12 - C11 - H11$ $120.0$ $C3 - C4 - H4$ $119.3$ $C13 - C12 - C11$ $119.7$ $C5 - C4 - C3$ $121.5(8)$ $C13 - C12 - C11$ $119.7$ $C4 - C5 - C6$ $116.0(7)$ $C12 - C13 - C14$ $119.6(9)$ $C4 - C5 - H5$ $122.0$ $C12 - C13 - H13$ $120.2$ $C6 - C5 - H5$ $122.0$ $C14 - C13 - H13$ $120.2$ $N2 - C6 - C5$ $132.6(6)$ $C13 - C14 - C15$ $120.5(8)$ $N2 - C6 - C1$ $105.2(5)$ $C13 - C14 - H14$ $119.7$	C6—N2—C8		125.9 (5)	C9—C8	-H82		114 (4)
C7-N2-C8127.5 (6)N3-C9-C8124.0 (6)C9-N3-O111.4 (5)N3-C9-C10115.3 (5)C2-C1-C6120.2 (6)C8-C9-C10120.7 (6)C1-C2-H2121.0C11-C10-C15118.2 (6)C3-C2-C1118.1 (7)C11-C10-C9121.6 (7)C3-C2-H2121.0C15-C10-C9120.2 (6)C2-C3-C4122.1 (8)C10-C11-H11120.0 (8)C2-C3-H3119.0C10-C11-H11120.0C4-C3-H3119.0C12-C11-H11120.0C3-C4-H4119.3C11-C12-H12119.7C5-C4-C3121.5 (8)C13-C12-C11120.6 (9)C5-C4-H4119.3C13-C12-H12119.7C4-C5-C6116.0 (7)C12-C13-C14119.6 (9)C4-C5-H5122.0C14-C13-H13120.2C6-C5-H5122.0C14-C13-H13120.2N2-C6-C5132.6 (6)C13-C14-C15120.5 (8)N2-C6-C1105.2 (5)C13-C14-H14119.7C5-C6-C1122.2 (7)C15-C14-H14119.7	C7—N2—C6		106.5 (6)	H81—C	8—H82		110 (5)
C9-N3-O111.4 (5)N3-C9-C10115.3 (5)C2-C1-C6120.2 (6)C8-C9-C10120.7 (6)C1-C2-H2121.0C11-C10-C15118.2 (6)C3-C2-C1118.1 (7)C11-C10-C9121.6 (7)C3-C2-H2121.0C15-C10-C9120.2 (6)C2-C3-C4122.1 (8)C10-C11-C12120.0 (8)C2-C3-H3119.0C10-C11-H11120.0C4-C3-H3119.0C12-C11-H11120.0C3-C4-H4119.3C11-C12-H12119.7C5-C4-C3121.5 (8)C13-C12-C11120.6 (9)C5-C4-H4119.3C13-C12-H12119.7C4-C5-C6116.0 (7)C12-C13-C14119.6 (9)C4-C5-H5122.0C12-C13-H13120.2C6-C5-H5122.0C14-C13-H13120.2N2-C6-C5132.6 (6)C13-C14-C15120.5 (8)N2-C6-C1105.2 (5)C13-C14-H14119.7C5-C6-C1122.2 (7)C15-C14-H14119.7	C7—N2—C8		127.5 (6)	N3—C9			124.0 (6)
C2-C1-C6120.2 (6)C8-C9-C10120.7 (6)C1-C2-H2121.0C11-C10-C15118.2 (6)C3-C2-C1118.1 (7)C11-C10-C9121.6 (7)C3-C2-H2121.0C15-C10-C9120.2 (6)C2-C3-C4122.1 (8)C10-C11-C12120.0 (8)C2-C3-H3119.0C10-C11-H11120.0C4-C3-H3119.0C12-C11-H11120.0C3-C4-H4119.3C11-C12-H12119.7C5-C4-C3121.5 (8)C13-C12-C11120.6 (9)C5-C4-H4119.3C13-C12-H12119.7C4-C5-C6116.0 (7)C12-C13-C14119.6 (9)C4-C5-H5122.0C12-C13-H13120.2C6-C5-H5122.0C14-C13-H13120.2N2-C6-C5132.6 (6)C13-C14-C15120.5 (8)N2-C6-C1105.2 (5)C13-C14-H14119.7C5-C6-C1122.2 (7)C15-C14-H14119.7	C9—N3—O		111.4 (5)	N3—C9	—C10		115.3 (5)
C1-C2-H2121.0C11-C10-C15118.2 (6)C3-C2-C1118.1 (7)C11-C10-C9121.6 (7)C3-C2-H2121.0C15-C10-C9120.2 (6)C2-C3-C4122.1 (8)C10-C11-C12120.0 (8)C2-C3-H3119.0C10-C11-H11120.0C4-C3-H3119.0C12-C11-H11120.0C3-C4-H4119.3C11-C12-H12119.7C5-C4-C3121.5 (8)C13-C12-C11120.6 (9)C5-C4-H4119.3C13-C12-H12119.7C4-C5-C6116.0 (7)C12-C13-C14119.6 (9)C4-C5-H5122.0C14-C13-H13120.2C6-C5-H5122.0C14-C13-H13120.2N2-C6-C5132.6 (6)C13-C14-C15120.5 (8)N2-C6-C1105.2 (5)C13-C14-H14119.7C5-C6-C1122.2 (7)C15-C14-H14119.7	C2—C1—C6		120.2 (6)	C8—C9			120.7 (6)
C3-C2-C1 $118.1 (7)$ $C11-C10-C9$ $121.6 (7)$ C3-C2-H2 $121.0$ $C15-C10-C9$ $120.2 (6)$ C2-C3-C4 $122.1 (8)$ $C10-C11-C12$ $120.0 (8)$ C2-C3-H3 $119.0$ $C10-C11-H11$ $120.0$ C4-C3-H3 $119.0$ $C12-C11-H11$ $120.0$ C3-C4-H4 $119.3$ $C11-C12-H12$ $119.7$ C5-C4-C3 $121.5 (8)$ $C13-C12-C11$ $120.6 (9)$ C5-C4-H4 $119.3$ $C13-C12-H12$ $119.7$ C4-C5-C6 $116.0 (7)$ $C12-C13-C14$ $119.6 (9)$ C4-C5-H5 $122.0$ $C12-C13-H13$ $120.2$ C6-C5-H5 $122.0$ $C14-C13-H13$ $120.2$ N2-C6-C5 $132.6 (6)$ $C13-C14-C15$ $120.5 (8)$ N2-C6-C1 $105.2 (5)$ $C13-C14-H14$ $119.7$	C1—C2—H2		121.0	C11—C	10—C15		118.2 (6)
C3-C2-H2121.0C15-C10-C9120.2 (6)C2-C3-C4122.1 (8)C10-C11-C12120.0 (8)C2-C3-H3119.0C10-C11-H11120.0C4-C3-H3119.0C12-C11-H11120.0C3-C4-H4119.3C11-C12-H12119.7C5-C4-C3121.5 (8)C13-C12-C11120.6 (9)C5-C4-H4119.3C13-C12-H12119.7C4-C5-C6116.0 (7)C12-C13-C14119.6 (9)C4-C5-H5122.0C12-C13-H13120.2C6-C5-H5122.0C14-C13-H13120.2N2-C6-C5132.6 (6)C13-C14-C15120.5 (8)N2-C6-C1105.2 (5)C13-C14-H14119.7C5-C6-C1122.2 (7)C15-C14-H14119.7	C3—C2—C1		118.1 (7)	C11—C	10—C9		121.6 (7)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С3—С2—Н2		121.0	C15—C	10—С9		120.2 (6)
C2-C3-H3119.0C10-C11-H11120.0C4-C3-H3119.0C12-C11-H11120.0C3-C4-H4119.3C11-C12-H12119.7C5-C4-C3121.5 (8)C13-C12-C11120.6 (9)C5-C4-H4119.3C13-C12-H12119.7C4-C5-C6116.0 (7)C12-C13-C14119.6 (9)C4-C5-H5122.0C12-C13-H13120.2C6-C5-H5122.0C14-C13-H13120.2N2-C6-C5132.6 (6)C13-C14-C15120.5 (8)N2-C6-C1105.2 (5)C13-C14-H14119.7C5-C6-C1122.2 (7)C15-C14-H14119.7	C2—C3—C4		122.1 (8)	C10—C	11—C12		120.0 (8)
C4—C3—H3119.0C12—C11—H11120.0C3—C4—H4119.3C11—C12—H12119.7C5—C4—C3121.5 (8)C13—C12—C11120.6 (9)C5—C4—H4119.3C13—C12—H12119.7C4—C5—C6116.0 (7)C12—C13—C14119.6 (9)C4—C5—H5122.0C12—C13—H13120.2C6—C5—H5122.0C14—C13—H13120.2N2—C6—C5132.6 (6)C13—C14—C15120.5 (8)N2—C6—C1105.2 (5)C13—C14—H14119.7C5—C6—C1122.2 (7)C15—C14—H14119.7	С2—С3—Н3		119.0	C10—C	11—H11		120.0
C3—C4—H4       119.3       C11—C12—H12       119.7         C5—C4—C3       121.5 (8)       C13—C12—C11       120.6 (9)         C5—C4—H4       119.3       C13—C12—H12       119.7         C4—C5—C6       116.0 (7)       C12—C13—C14       119.6 (9)         C4—C5—H5       122.0       C14—C13—H13       120.2         C6—C5—H5       122.0       C14—C13—H13       120.2         N2—C6—C5       132.6 (6)       C13—C14—C15       120.5 (8)         N2—C6—C1       105.2 (5)       C13—C14—H14       119.7         C5—C6—C1       122.2 (7)       C15—C14—H14       119.7	С4—С3—Н3		119.0	C12—C	11—H11		120.0
C5-C4-C3121.5 (8)C13-C12-C11120.6 (9)C5-C4-H4119.3C13-C12-H12119.7C4-C5-C6116.0 (7)C12-C13-C14119.6 (9)C4-C5-H5122.0C12-C13-H13120.2C6-C5-H5122.0C14-C13-H13120.2N2-C6-C5132.6 (6)C13-C14-C15120.5 (8)N2-C6-C1105.2 (5)C13-C14-H14119.7C5-C6-C1122.2 (7)C15-C14-H14119.7	С3—С4—Н4		119.3	C11—C	12—H12		119.7
C5—C4—H4       119.3       C13—C12—H12       119.7         C4—C5—C6       116.0 (7)       C12—C13—C14       119.6 (9)         C4—C5—H5       122.0       C12—C13—H13       120.2         C6—C5—H5       122.0       C14—C13—H13       120.2         N2—C6—C5       132.6 (6)       C13—C14—C15       120.5 (8)         N2—C6—C1       105.2 (5)       C13—C14—H14       119.7         C5—C6—C1       122.2 (7)       C15—C14—H14       119.7	C5—C4—C3		121.5 (8)	C13—C	12—C11		120.6 (9)
C4—C5—C6116.0 (7)C12—C13—C14119.6 (9)C4—C5—H5122.0C12—C13—H13120.2C6—C5—H5122.0C14—C13—H13120.2N2—C6—C5132.6 (6)C13—C14—C15120.5 (8)N2—C6—C1105.2 (5)C13—C14—H14119.7C5—C6—C1122.2 (7)C15—C14—H14119.7	С5—С4—Н4		119.3	C13—C	12—H12		119.7
C4—C5—H5       122.0       C12—C13—H13       120.2         C6—C5—H5       122.0       C14—C13—H13       120.2         N2—C6—C5       132.6 (6)       C13—C14—C15       120.5 (8)         N2—C6—C1       105.2 (5)       C13—C14—H14       119.7         C5—C6—C1       122.2 (7)       C15—C14—H14       119.7	C4—C5—C6		116.0 (7)	C12—C	13—C14		119.6 (9)
C6—C5—H5122.0C14—C13—H13120.2N2—C6—C5132.6 (6)C13—C14—C15120.5 (8)N2—C6—C1105.2 (5)C13—C14—H14119.7C5—C6—C1122.2 (7)C15—C14—H14119.7	С4—С5—Н5		122.0	C12—C	13—H13		120.2
N2—C6—C5132.6 (6)C13—C14—C15120.5 (8)N2—C6—C1105.2 (5)C13—C14—H14119.7C5—C6—C1122.2 (7)C15—C14—H14119.7	С6—С5—Н5		122.0	C14—C	13—H13		120.2
N2—C6—C1         105.2 (5)         C13—C14—H14         119.7           C5—C6—C1         122.2 (7)         C15—C14—H14         119.7	N2—C6—C5		132.6 (6)	C13—C	14—C15		120.5 (8)
C5—C6—C1 122.2 (7) C15—C14—H14 119.7	N2—C6—C1		105.2 (5)	C13—C	14—H14		119.7
	C5—C6—C1		122.2 (7)	C15—C	14—H14		119.7

N1—C7—N2	113.9 (7)	C10-C15-H15	119.5
N1—C7—H7	126 (4)	C14—C15—C10	121.0 (7)
N2—C7—H7	120 (4)	C14—C15—H15	119.5
C1—N1—C7—N2	0.8 (7)	C1—C2—C3—C4	-0.3 (12)
C7—N2—C6—C5	179.4 (7)	C2—C3—C4—C5	0.0 (13)
C8—N2—C6—C5	-3.6 (11)	C6—C5—C4—C3	0.6 (12)
C7—N2—C6—C1	0.0 (6)	C4—C5—C6—N2	179.8 (7)
C8—N2—C6—C1	177.0 (6)	C4—C5—C6—C1	-0.9 (10)
C6—N2—C7—N1	-0.5 (7)	N3—C9—C8—N2	121.9 (7)
C8—N2—C7—N1	-177.5 (6)	C10-C9-C8-N2	-55.9 (10)
C7—N2—C8—C9	117.9 (8)	C11-C10-C9-N3	149.8 (6)
C6—N2—C8—C9	-58.5 (10)	С11—С10—С9—С8	-32.2 (9)
O—N3—C9—C8	-3.0 (9)	C15—C10—C9—N3	-31.0 (8)
O—N3—C9—C10	174.9 (5)	C15—C10—C9—C8	147.0 (7)
C2—C1—N1—C7	179.6 (7)	C15-C10-C11-C12	0.5 (11)
C6—C1—N1—C7	-0.8 (6)	C9-C10-C11-C12	179.7 (7)
N1-C1-C2-C3	179.6 (7)	C9-C10-C15-C14	179.1 (6)
C6—C1—C2—C3	0.0 (10)	C11-C10-C15-C14	-1.7 (10)
N1—C1—C6—N2	0.5 (6)	C10-C11-C12-C13	0.9 (13)
C2C1C6N2	-179.9 (6)	C11-C12-C13-C14	-1.0 (14)
N1—C1—C6—C5	-179.0 (6)	C15-C14-C13-C12	-0.1 (13)
C2—C1—C6—C5	0.6 (9)	C10-C15-C14-C13	1.6 (11)

Hydrogen-bond geometry (Å, °)

D—H···A	<i>D</i> —Н	$H \cdots A$	$D \cdots A$	D—H··· $A$
O—H…N1 <sup>i</sup>	0.87 (6)	1.84 (5)	2.654 (7)	155 (6)
С8—Н82…О	0.96 (6)	2.26 (6)	2.634 (9)	102 (4)
(1)				

Symmetry codes: (i) -*x*+1/2, *y*+1/2, *z*-1/2.

Comparison of the bond lengths and angles  $(\mathring{A}, \circ)$  in the oxime moieties of (I) with the corresponding values in the related structures (II)–(VII)

	(I)	(II)	(III)	(IV)	(V)	(VI)	(VII)
N3—O	1.383 (7)	1.403 (2)	1.423 (3)	1.4167 (10)	1.429 (4)	1.424 (2)	1.416 (3)
		1.396 (2)	1.396 (3)				1.397 (3)
N3—C9	1.300(7)	1.281 (2)	1.290 (3)	1.2897 (12)	1.241 (6)	1.289 (2)	1.282 (3)
		1.281 (2)	1.282 (3)				1.289 (3)
C9—C10	1.491 (8)	1.477 (3)	1.489 (3)	1.5098 (13)	1.551 (7)	1.513 (2)	1.501 (4)
		1.473 (3)					1.502 (4)
C10-C9-N3	115.3 (5)	115.2 (2)	116.6 (2)	114.32 (8)	118.3 (5)	113.2 (1)	114.4 (2)
		115.0 (2)	115.0 (2)				113.4 (2)
C9—N3—O	111.4 (5)	112.4 (1)	109.4 (2)	110.66 (8)	112.2 (4)	110.6 (1)	110.7 (2)
		112.2 (1)	111.5 (2)				111.1 (2)

Notes: (II) 2,3-dimethylquinoxaline–dimethylglyoxime (1/1) (Hökelek, Batı *et al.*, 2001\bbr009); (III) 1-(2,6-dimethylphenylamino)propane-1,2-dione dioxime (Hökelek, Zülfikar-oğlu *et al.*, 2001); (IV) *N*-hydroxy-2-oxo-2,*N*-diphenylacetamidine (Büyükgüngör *et al.*, 2003\bbr002); (V) *N*-(3,4-dichlorophenyl)-*N*-hydroxy-2-oxo-2-phenylacetamidine (Hökelek *et al.*, 2004a\bbr010); (VI) *N*-hydroxy-*N*-(1-naphthyl)-2-phenylacetamidin-2-one (Hökelek *et al.*, 2004b\bbr011); (VII) *N*-(3-chloro-4-methylphenyl)-*N*<sup>-</sup>hydroxy-2-oxo-2-phenylacetamidine-2,3- dimethylquinoxaline–dimethyl–glyoxime (1/1) (Hökelek *et al.*, 2004\bbr012*c*).





