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## (E)-2-{(2-Hydroxynaphthalen-1-yl)methylene}hydrazinecarboxamide

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Key indicators: single-crystal X-ray study; T = 200 K; mean  $\sigma$ (C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.124; data-to-parameter ratio = 13.8.

In the title molecule,  $C_{12}H_{11}N_3O_2$ , the dihedral angle between the mean planes of the naphthalene and carboxamide groups is 28.9 (8)°. The hydrazine N atoms are twisted slightly out of the plane of the carboxamide group [C-C-N-N] torsion angle =  $-175.06 (13)^{\circ}$ ]. The crystal packing is influenced by N-H···O hydrogen bonding which includes a bifurcated hydrogen bond between the amide N atom and nearby carboxyl and hydroxyl O atoms. A second bifurcated hydrogen bond occurs between the hydroxyl O atom and nearby amide (intermolecular) and hydrazine (intramolecular) N atoms. As a result, molecules are linked into a co-operative hydrogen-bonded network of infinite onedimensional  $O-H\cdots O-H\cdots O-H$  chains along the (101) plane of the unit cell in a zigzag pattern, the dihedral angle between the mean planes of the naphthalene groups of adjacent molecules in the chain being 86.9 (2)°. A MOPAC PM3 calculation provides support to these observations.

#### **Related literature**

For related semicarbazones, see: Noblia *et al.* (2005). For the bioactivity of semicarbazones, see: Beraldo & Gambino (2004). For their applications in polymers, see: Khuhawar *et al.* (2004) and in sensors, see: Oter *et al.* (2007).



### Experimental

#### Crystal data $C_{12}H_{11}N_3O_2$ $M_r = 229.24$ Monoclinic, $P2_1/c$ a = 16.0886 (4) Å b = 4.72900 (10) Å c = 15.6452 (4) Å $\beta = 114.647$ (3)°

#### Data collection

Oxford Diffraction Gemini R diffractometer Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)  $T_{\rm min} = 0.819, T_{\rm max} = 0.907$ 

#### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.047$  $wR(F^2) = 0.124$ S = 1.032135 reflections 7383 measured reflections 2135 independent reflections 1724 reflections with  $I > 2\sigma(I)$  $R_{int} = 0.031$ 

V = 1081.89 (5) Å<sup>3</sup>

Cu  $K\alpha$  radiation

 $0.57 \times 0.22 \times 0.12 \text{ mm}$ 

 $\mu = 0.82 \text{ mm}^{-1}$ 

T = 200 K

Z = 4

#### Table 1

Hydrogen-b	ond geometr	y (A,	°).

$D - H \cdot \cdot \cdot A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdot \cdot \cdot A$
01-H10···N1	0.84	1.82	2.5562 (17)	146
$N2-H2A\cdots O2^{i}$	0.88	1.98	2.8290 (17)	161
N3-H3A···O1 <sup>ii</sup>	0.88	2.10	2.9762 (18)	171
$N3-H3B\cdots O2^{iii}$	0.88	2.58	3.0618 (18)	116

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

Data collection: *CrysAlisPro* (Oxford Diffraction, 2007); cell refinement: *CrysAlisPro*; 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* and *WebMOPro* (Schmidt & Polik, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2136).

#### References

- Beraldo, H. & Gambino, D. (2004). *Mini Rev. Med. Chem.*, **4**, 31–39. Khuhawar, M. Y., Mughal, M. A. & Channar, A. H. (2004). *Eur. Polym. J.* **40**,
- Khuhawar, M. Y., Mughal, M. A. & Channar, A. H. (2004). Eur. Polym. J. 40 805–809.
- Noblia, P., Vieites, M., Parajon-Costa, B. S., Baran, E. J., Cerecetto, H., Draper, P., Gonzalez, M., Piro, O. E., Castellano, E. E., Azqueta, A., Lopez de Cerain, A., Monge-Vega, A. & Gambino, D. (2005). *J. Inorg. Biochem.* 99, 443–451.
- Oter, O., Ertekin, K., Kirilmis, C. & Koca, M. (2007). Anal. Chim. Acta, 584, 308–314.
- Oxford Diffraction (2007). CrysAlisPro and CrysAlis RED. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
- Schmidt, J. R. & Polik, W. F. (2007). WebMO Pro. WebMO, LLC, Holland, MI, USA. Available from http://www.webmo.net.
- Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.

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## (E)-2-{(2-Hydroxynaphthalen-1-yl)methylene}hydrazinecarboxamide

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#### Comment

The title compound,  $C_{12}H_{11}N_3O_2$ , is a tridentate semicarbazone ligand and forms complexes with a variety of metals. It coordinates with vanadium which forms complexes with potential antitumor activity (Noblia *et al.*, 2005). Semicarbazones show significant bioactivities including antiprotozoa and anticonvulsant types (Beraldo & Gambino, 2004), and additionally some derivatives have been used as selective fiber optic sensors for copper(II) (Oter *et al.*, 2007) or incorported into polymers (Khuhawar *et al.*, 2004).

The title molecule,  $C_{12}H_{11}N_3O_2$ , consists of a 2–hydroxynaphthalen–1–yl group and a hydrazinecarboxamide group bonded to a methylene carbon atom with the dihedral angle between the mean planes of the naphthalene and carboxamide groups measuring 28.9 (8)° (Fig. 1). The hydrazine nitrogen atoms are twisted slightly out of the plane of the carboxamide group [torsion angles C1–C11–N1–N2 = -175.06 (13)°]. The hydroxyl group is in the plane of the napthalene group [torsion angle = 179.62 (15)°]. Crystal packing is influenced by extensive strong intermolecular N—H···O hydrogen bonding which includes a bifurcated hydrogen bond between the amide nitrogen atom, N1, and a nearby carboxyl oxygen atom (O2) and hydroxyl oxygen atom (O1) (see Fig. 2, Table 1). A second bifurcated hydrogen bond occurs between the hydroxyl oxygen atom (O1) and nearby amide (N3) (intermolecular) and hydrazine (N1) (intramolecular) nitrogen atoms. As a result the molecules are linked into a cooperative hydrogen bond network of infinite one–dimensionsl O—H···O—H···O—H chains along the (1 0 1) plane of the unit cell in a zigzag pattern with the dihedral angle between the mean planes of the naphthalene groups of consecutive molecules in the chain measuring 86.9 (2)° (Fig. 3).

After a *MOPAC* PM3 calculation [Parameterized Model 3 approximation together with the Hartree–Fock closed–shell (restricted) wavefunction was used and minimizations were teminnated at an r.m.s. gradient of less than 0.01 kJ mol<sup>-1</sup> Å<sup>-1</sup>] of the molecule in the asymmetric unit with *WebMO Pro* (Schmidt & Polik, 2007), the mean planes between the naphthalene and carboxamide groups changes from 28.9 (8)° to 14.8 (1)°, producing a significantly less twisted, more planar, molecule than that observed in the crystalline environment. It is apparent that the extensive hydrogen bonding scheme described significantly influences the crystal packing in the unit cell highlighted by a network of infinite one–dimensionsl O–H···O–H chains.

#### **Experimental**

The title compound (I) was synthesized by adding a solution of 2–hydroxy–1–naphthaldehyde (1.72 g, 10 mmol) dissolved in 5 ml of ethanol to a solution of 1.15 g (10.4 mmol) of semicarbazide hydrochloride in 10 ml of water. The mixture was stirred at room temperature. A green precipitate formed. The mixture was stirred for 30 minutes then diluted with 50 ml of water, filtered and dried. Recrystallization from ethanol and slow evaporation of the solvent gave a light yellowish–green solid 1.55 g (68%). m.p. with decomposition > 503 K. <sup>1</sup>H NMR (*DMSO*–d6, 400 MHz)  $\delta$  (p.p.m.): 11.24 (br. s, 1H), 10.25 (br. s, 1H), 8.87 (s, 1H), 8.38 (d, J = 8.5 Hz, 1H), 7.85 (m, 2H), 7.55 (dt, J = 7.75, 1.4 Hz, 1 H), 7.37(t, J = 7.5 Hz, 1H),

7.17(d, J = 8.85, Hz, 1 H), 6.30 (br s, 2H); <sup>13</sup>C NMR (*DMSO*–d6, 100 MHz) δ (p.p.m.): 156.07, 155.83, 139.86, 131.40, 131.31, 128.67, 127.94, 127.47, 123.26, 121.99, 118.44, 109.79.

### Refinement

The atoms H3A, H3B and H10 were obtained from a difference fourier map. The remaining H atoms were placed in their calculated positions and then refined using the riding model with C—H = 0.95 Å, and with  $U_{iso}(H) = 1.18-1.21 U_{eq}(C,N,O)$ .

#### **Figures**



Fig. 1. The molecular structure of  $C_{12}H_{11}N_3O_2$ , showing the atom numbering scheme. Displacement ellipsoids are drawn at 50% probability level. H atoms are presented as a small cyrcles of arbitrary radius.



Fig. 2. The molecular packing for  $C_{12}H_{11}N_3O_2$  viewed down the *c* axis showing the cooperative hydrogen bond network of infinite one-dimensional O—H…O—H…O—H chains in a zigzag pattern. Dashed lines indicate intermolecular N—H…O and intramolecular O–H…N hydrogen bonds.



Fig. 3. The molecular packing for  $C_{12}H_{11}N_3O_2$  viewed down the *b* axis showing the cooperative hydrogen bond network of infinite one-dimensional O—H···O—H···O—H chains along the (1 0 1) plane of the unit cell in a zigzag pattern. Dashed lines indicate intermolecular N—H···O, and intramolecular O–H···N hydrogen bonds.

#### (E)-2-{(2-Hydroxynaphthalen-1-yl)methylene}hydrazinecarboxamide

Crystal data	
$C_{12}H_{11}N_3O_2$	$F_{000} = 480$
$M_r = 229.24$	$D_{\rm x} = 1.407 {\rm Mg m}^{-3}$
Monoclinic, $P2_1/c$	Cu K $\alpha$ radiation $\lambda = 1.54184$ Å
Hall symbol: -P 2ybc	Cell parameters from 4156 reflections
a = 16.0886 (4)  Å	$\theta = 5.2 - 73.5^{\circ}$
b = 4.72900 (10)  Å	$\mu = 0.82 \text{ mm}^{-1}$
c = 15.6452 (4) Å	T = 200  K
$\beta = 114.647 \ (3)^{\circ}$	Needle, pale yellow
V = 1081.89 (5) Å <sup>3</sup>	$0.57 \times 0.22 \times 0.12 \text{ mm}$

#### Z = 4

#### Data collection

Oxford Diffraction Gemini R diffractometer	2135 independent reflections
Radiation source: Fine-focus sealed tube	1724 reflections with $I > 2\sigma(I)$
Monochromator: Graphite	$R_{\rm int} = 0.031$
Detector resolution: 10.5081 pixels mm <sup>-1</sup>	$\theta_{\text{max}} = 73.5^{\circ}$
T = 200  K	$\theta_{\min} = 5.7^{\circ}$
$\varphi$ and $\omega$ scans	$h = -18 \rightarrow 20$
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	$k = -4 \rightarrow 5$
$T_{\min} = 0.819, \ T_{\max} = 0.907$	$l = -19 \rightarrow 19$
7383 measured reflections	

#### Refinement

Refinement on $F^2$	Secondary atom site location: Difmap
Least-squares matrix: Full	Hydrogen site location: Geom
$R[F^2 > 2\sigma(F^2)] = 0.047$	H-atom parameters constrained
$wR(F^2) = 0.124$	$w = 1/[\sigma^2(F_o^2) + (0.0706P)^2 + 0.3033P]$ where $P = (F_o^2 + 2F_c^2)/3$
<i>S</i> = 1.03	$(\Delta/\sigma)_{max} \le 0.001$
2135 reflections	$\Delta \rho_{max} = 0.30 \text{ e } \text{\AA}^{-3}$
155 parameters	$\Delta \rho_{min} = -0.26 \text{ e } \text{\AA}^{-3}$
Primary atom site location: Direct	Extinction correction: none

#### Special details

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 o	or	equivalent	isotropic	displ	lacement	parameters	(Å	²)
				1		1	1			1	1	

	x	У	Ζ	$U_{\rm iso}*/U_{\rm eq}$
01	0.31323 (8)	0.7964 (3)	0.22177 (8)	0.0437 (3)
H1O	0.3498	0.6774	0.2579	0.052*
02	0.56353 (8)	-0.0031 (2)	0.42849 (8)	0.0369 (3)
N1	0.38963 (8)	0.4986 (3)	0.37070 (9)	0.0317 (3)
N2	0.44479 (9)	0.2745 (3)	0.41411 (9)	0.0332 (3)

H2A	0.4322	0.1678	0.4533	0.040*
N3	0.54082 (10)	0.4022 (3)	0.34432 (10)	0.0391 (4)
H3A	0.5881	0.3706	0.3312	0.047*
H3B	0.5076	0.5557	0.3231	0.047*
C1	0.26235 (9)	0.7936 (3)	0.34640 (10)	0.0280 (3)
C2	0.25746 (10)	0.8928 (4)	0.26045 (10)	0.0325 (4)
C3	0.19255 (11)	1.0963 (4)	0.20808 (11)	0.0391 (4)
НЗС	0.1902	1.1586	0.1494	0.047*
C4	0.13328 (11)	1.2044 (4)	0.24071 (12)	0.0386 (4)
H4A	0.0896	1.3413	0.2044	0.046*
C5	0.13540 (10)	1.1162 (3)	0.32839 (11)	0.0325 (4)
C6	0.07427 (11)	1.2315 (4)	0.36314 (12)	0.0408 (4)
H6A	0.0312	1.3707	0.3274	0.049*
C7	0.07638 (12)	1.1455 (4)	0.44726 (13)	0.0438 (4)
H7A	0.0345	1.2225	0.4694	0.053*
C8	0.14048 (12)	0.9437 (4)	0.50068 (12)	0.0414 (4)
H8A	0.1419	0.8849	0.5593	0.050*
C9	0.20126 (10)	0.8293 (4)	0.46977 (11)	0.0348 (4)
H9A	0.2447	0.6942	0.5077	0.042*
C10	0.20044 (9)	0.9091 (3)	0.38214 (10)	0.0287 (3)
C11	0.32667 (10)	0.5704 (3)	0.39663 (10)	0.0291 (3)
H11A	0.3220	0.4782	0.4484	0.035*
C12	0.51931 (10)	0.2162 (3)	0.39678 (10)	0.0303 (3)

Atomic displacement parameters  $(\text{\AA}^2)$ 

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
01	0.0468 (7)	0.0513 (8)	0.0418 (6)	0.0135 (6)	0.0272 (5)	0.0132 (5)
O2	0.0394 (6)	0.0298 (6)	0.0446 (6)	0.0091 (5)	0.0208 (5)	0.0026 (5)
N1	0.0305 (6)	0.0290 (7)	0.0354 (6)	0.0038 (5)	0.0135 (5)	0.0024 (5)
N2	0.0337 (7)	0.0283 (7)	0.0408 (7)	0.0063 (5)	0.0187 (6)	0.0074 (5)
N3	0.0418 (7)	0.0330 (8)	0.0523 (8)	0.0081 (6)	0.0293 (6)	0.0057 (6)
C1	0.0251 (7)	0.0271 (8)	0.0302 (7)	-0.0010 (6)	0.0098 (6)	0.0006 (6)
C2	0.0321 (8)	0.0330 (9)	0.0334 (7)	0.0003 (6)	0.0145 (6)	0.0011 (6)
C3	0.0410 (9)	0.0404 (10)	0.0333 (8)	0.0023 (7)	0.0129 (7)	0.0090 (7)
C4	0.0319 (8)	0.0347 (9)	0.0408 (8)	0.0056 (7)	0.0068 (6)	0.0065 (7)
C5	0.0252 (7)	0.0282 (8)	0.0400 (8)	-0.0020 (6)	0.0095 (6)	-0.0039 (6)
C6	0.0293 (8)	0.0355 (9)	0.0531 (10)	0.0042 (7)	0.0127 (7)	-0.0048 (7)
C7	0.0355 (8)	0.0447 (10)	0.0569 (10)	-0.0011 (7)	0.0249 (8)	-0.0148 (8)
C8	0.0410 (9)	0.0459 (10)	0.0426 (9)	-0.0037 (8)	0.0226 (7)	-0.0081 (8)
C9	0.0332 (8)	0.0363 (9)	0.0352 (8)	0.0024 (6)	0.0146 (6)	-0.0016 (6)
C10	0.0247 (7)	0.0263 (8)	0.0333 (7)	-0.0036 (6)	0.0103 (6)	-0.0045 (6)
C11	0.0293 (7)	0.0279 (8)	0.0296 (7)	-0.0002 (6)	0.0119 (6)	0.0002 (6)
C12	0.0305 (7)	0.0289 (8)	0.0310 (7)	0.0008 (6)	0.0125 (6)	-0.0044 (6)

Geometric parameters (Å, °)

O1—C2	1.3534 (19)	С3—НЗС	0.9500
01—H10	0.8400	C4—C5	1.421 (2)

NI-C11 $12844(2)$ CS-C6 $1446(2)$ NI-N2 $13674(18)$ CS-C10 $1444(2)$ N2-C12 $13367(19)$ C6-C7 $1354(3)$ N2-H2A $0.8800$ C6-H6A $0.9500$ N3-H3B $0.8800$ C7-H7A $0.9500$ N3-H3B $0.8800$ C8-C9 $1.370(2)$ C1-C10 $1.438(2)$ C9-C10 $1.417(2)$ C1-C11 $1.457(2)$ C9-H9A $0.9500$ C2-C3 $1.405(2)$ C1-H11A $0.9500$ C2-C3 $1.405(2)$ C1-H11A $0.9500$ C12-N2-N1 $120.02(13)$ C7-C6-H6A $119.6$ C12-N2-H2A $120.0$ C6-C7-L8 $119.71(6)$ C12-N3-H3A $120.0$ C6-C7-C8 $119.71(6)$ C12-N3-H3A $120.0$ C6-C7-L8A $120.1$ C12-N3-H3A $120.0$ C6-C7-H7A $120.1$ C12-N3-H3B $120.0$ C6-C7-L8A $119.5$ C12-N3-H3B $120.0$ C6-C7-L8A $119.5$ C12-N3-H3A $120.0$ C6-C7-L7A	O2—C12	1.2386 (18)	C4—H4A	0.9500
$\begin{split} & \text{N1} - \text{N2} & 1.3674 (18) & \text{C5} - \text{C10} & 1.424 (2) \\ & \text{N2} - \text{C12} & 1.360 (19) & \text{C6} - \text{C7} & 1.364 (3) \\ & \text{N2} - \text{H2A} & 0.8800 & \text{C6} - \text{H6A} & 0.9500 \\ & \text{N3} - \text{C12} & 1.343 (2) & \text{C7} - \text{C8} & 1.398 (3) \\ & \text{N3} - \text{H3A} & 0.8800 & \text{C8} - \text{C9} & 1.370 (2) \\ & \text{C1} - \text{C2} & 1.395 (2) & \text{C8} - \text{H8A} & 0.9500 \\ & \text{C1} - \text{C10} & 1.438 (2) & \text{C9} - \text{C10} & 1.417 (2) \\ & \text{C1} - \text{C1} & 1.457 (2) & \text{C9} - \text{H9A} & 0.9500 \\ & \text{C2} - \text{C3} & 1.405 (2) & \text{C1} - \text{H1A} & 0.9500 \\ & \text{C2} - \text{C3} & 1.405 (2) & \text{C1} - \text{H1A} & 0.9500 \\ & \text{C2} - \text{C3} & 1.405 (2) & \text{C1} - \text{H1A} & 0.9500 \\ & \text{C2} - \text{C4} & 1.255 (2) & \text{C2} - \text{C10} & 119 23 (14) \\ & \text{C1} - \text{N1} - \text{N2} & 118 82 (13) & \text{C7} - \text{C6} - \text{C5} & 120.90 (16) \\ & \text{C1} - \text{N1} - \text{N2} & 118 82 (13) & \text{C7} - \text{C6} - \text{C6} & 119 20 (16) \\ & \text{C1} - \text{N1} - \text{N2} & 118 82 (13) & \text{C7} - \text{C6} - \text{H6A} & 119 6 \\ & \text{C1} - \text{N1} - \text{N2} & 120.0 & \text{C6} - \text{C7} - \text{C8} & 119.71 (16) \\ & \text{C1} - \text{N1} - \text{N2} & 120.0 & \text{C6} - \text{C7} - \text{C8} & 119.71 (16) \\ & \text{C1} - \text{N3} - \text{H3A} & 120.0 & \text{C6} - \text{C7} - \text{N1} & 120.1 \\ & \text{H3} - \text{N3} - \text{H3B} & 120.0 & \text{C8} - \text{C7} - \text{N1} & 120.1 \\ & \text{H3} - \text{N3} - \text{H3B} & 120.0 & \text{C8} - \text{C7} & 121.05 (16) \\ & \text{C2} - \text{C1} - \text{C10} & 118.52 (13) & \text{C9} - \text{C8} - \text{H8A} & 119.5 \\ & \text{C1} - \text{C1} - \text{C11} & 121.01 (13) & \text{C8} - \text{C9} - \text{C10} & 121.09 (15) \\ & \text{O1} - \text{C2} - \text{C1} & 122.44 (14) & \text{C8} - \text{C9} - \text{H9A} & 119.5 \\ & \text{C1} - \text{C1} - \text{C1} & 123.44 (14) \\ & \text{C4} - \text{C3} - \text{H3C} & 119.5 & \text{C1} - \text{C1} & 119.82 (13) \\ & \text{C1} - \text{C2} - \text{C3} & 121.45 (14) & \text{C9} - \text{C10} - \text{C1} & 119.82 (13) \\ & \text{C3} - \text{C4} - \text{C4} & 119.5 & \text{C1} - \text{C1} & 119.82 (13) \\ & \text{C3} - \text{C4} - \text{C4} & 119.5 & \text{C1} - \text{C1} & 119.82 (13) \\ & \text{C3} - \text{C4} - \text{C5} & 12.03 (15) & \text{N1} - \text{C1} - \text{C1} & 119.82 (13) \\ & \text{C3} - \text{C4} - \text{C4} & 119.6 & \text{C3} - \text{C1} - \text{C1} & 119.82 (13) \\ & \text{C3} - \text{C4} - \text{C4} & 119.5 & \text{C1} - \text{C1} - \text{C1} & 119.82 (13) \\ & \text{C3} - \text{C4} - \text$	N1—C11	1.284 (2)	C5—C6	1.416 (2)
N2-Cl2       1.3630 (19)       C6-C7       1.364 (3)         N2-H2A       0.8800       C6-H6A       0.9500         N3-Cl2       1.343 (2)       C7-C8       1.398 (3)         N3-H3A       0.8800       C8-C9       1.370 (2)         Cl-C2       1.395 (2)       C8-H8A       0.9500         Cl-C10       1.438 (2)       C9-C10       1.417 (2)         Cl-C11       1.457 (2)       C9-H9A       0.9500         C3-C3       1.405 (2)       C1-H11A       0.9500         C3-C4       1.355 (2)       1.000 (13)       C7-C6-H6A       1196         C12-N2-N1       120.0 (213)       C7-C6-H6A       119.6         C12-N2-H12A       120.0 (26-C7-H7A       120.1       120.1         I3A-N3-H3B       120.1	N1—N2	1.3674 (18)	C5—C10	1.424 (2)
$\begin{split} & \text{N2}-\text{H2A} & 0.8800 & \text{C6}-\text{H6A} & 0.9500 \\ & \text{N3}-\text{C12} & 1.343 (2) & \text{C7}-\text{C8} & 1.398 (3) \\ & \text{N3}-\text{H3A} & 0.8800 & \text{C8}-\text{C9} & 1.370 (2) \\ & \text{C1}-\text{C2} & 1.395 (2) & \text{C8}-\text{H8A} & 0.9500 \\ & \text{C1}-\text{C10} & 1.438 (2) & \text{C9}-\text{C10} & 1.417 (2) \\ & \text{C1}-\text{C1} & 1.457 (2) & \text{C9}-\text{H9A} & 0.9500 \\ & \text{C2}-\text{C3} & 1.405 (2) & \text{C1}-\text{H1A} & 0.9500 \\ & \text{C3}-\text{C4} & 1.355 (2) & \text{C2}-\text{C3} & 1.405 (2) & \text{C1}-\text{H1A} & 0.9500 \\ & \text{C3}-\text{C4} & 1.355 (2) & \text{C2}-\text{C3} & 1.405 (2) & \text{C1}-\text{H1A} & 0.9500 \\ & \text{C2}-\text{C3} & 1.405 (2) & \text{C1}-\text{H1A} & 0.9500 \\ & \text{C3}-\text{C4} & 1.355 (2) & \text{C2}-\text{C3} & 1.200 & \text{C5}-\text{C6}-\text{H6A} & 119.6 \\ & \text{C1}-\text{N1}-\text{N2} & 118.82 (13) & \text{C7}-\text{C6}-\text{C5} & 120.90 (16) \\ & \text{C1}2-\text{N2}-\text{M1} & 120.02 (13) & \text{C7}-\text{C6}-\text{H6A} & 119.6 \\ & \text{N1}-\text{N2}-\text{H2A} & 120.0 & \text{C5}-\text{C6}-\text{H6A} & 119.6 \\ & \text{N1}-\text{N2}-\text{H2A} & 120.0 & \text{C6}-\text{C7}-\text{H7A} & 120.1 \\ & \text{H3A}-\text{N3}-\text{H3B} & 120.0 & \text{C6}-\text{C7}-\text{H7A} & 120.1 \\ & \text{H3A}-\text{N3}-\text{H3B} & 120.0 & \text{C8}-\text{C7}-\text{H7A} & 120.1 \\ & \text{H3A}-\text{N3}-\text{H3B} & 120.0 & \text{C9}-\text{C8}-\text{C7} & 121.05 (16) \\ & \text{C2}-\text{C1}-\text{C1} & 118.52 (13) & \text{C9}-\text{C8}-\text{H8A} & 119.5 \\ & \text{C1}-\text{C1}-\text{C1} & 122.44 (14) & \text{C8}-\text{C9}-\text{H9A} & 119.5 \\ & \text{C1}-\text{C1}-\text{C1} & 122.44 (14) & \text{C8}-\text{C9}-\text{H9A} & 119.5 \\ & \text{C1}-\text{C2}-\text{C3} & 116.10 (14) & \text{C1}-\text{C5} & 117.57 (14) \\ & \text{C4}-\text{C3}-\text{H3C} & 119.8 & \text{N1}-\text{C1}-\text{C1} & 119.82 (13) \\ & \text{C3}-\text{C4}-\text{C5} & 121.03 (15) & \text{N1}-\text{C1}-\text{C1} & 119.82 (13) \\ & \text{C3}-\text{C4}-\text{C5} & 121.03 (15) & \text{N1}-\text{C1}-\text{C1} & 119.82 (13) \\ & \text{C3}-\text{C4}-\text{C5} & 121.03 (15) & \text{N1}-\text{C1}-\text{C1} & 119.82 (13) \\ & \text{C3}-\text{C4}-\text{C5} & 122.01 \\ & \text{C2}-\text{C3} & 121.03 (15) & \text{N1}-\text{C1}-\text{C1} & 119.82 (13) \\ & \text{C3}-\text{C4}-\text{C5} & 122.02 & 119.57 (14) \\ & \text{C4}-\text{C3}-\text{H3C} & 119.8 & \text{N1}-\text{C1}-\text{C1} & 119.82 (13) \\ & \text{C3}-\text{C4}-\text{C5} & 120.0 & 119.58 & 122.81 (14) \\ & \text{C4}-\text{C3}-\text{H3C} & 119.57 & 122.81 (14) \\ & \text{C4}-\text{C3}-\text{C1} & 119.82 (13) & \text{C3}-\text{C1}-\text{C1} & 119.82 (13) \\ & \text{C3}-\text{C4}-\text{C5} & 12.2 (2) & \text$	N2—C12	1.3630 (19)	C6—C7	1.364 (3)
$\begin{split} & \text{N3}-\text{Cl}2 & 1.343 (2) & \text{C7}-\text{C8} & 1.398 (3) \\ & \text{N3}-\text{H3A} & 0.8800 & \text{C7}-\text{H7A} & 0.9500 \\ & \text{N3}-\text{H3B} & 0.8800 & \text{C8}-\text{C9} & 1.370 (2) \\ & \text{Cl}-\text{C2} & 1.395 (2) & \text{C8}-\text{H8A} & 0.9500 \\ & \text{Cl}-\text{C10} & 1.438 (2) & \text{C9}-\text{Cl0} & 1.417 (2) \\ & \text{Cl}-\text{C11} & 1.457 (2) & \text{C9}-\text{H9A} & 0.9500 \\ & \text{C3}-\text{C4} & 1.355 (2) & \\ & \text{C2}-\text{C3} & 1.405 (2) & \text{C1}-\text{H1IA} & 0.9500 \\ & \text{C3}-\text{C4} & 1.355 (2) & \\ & \text{C2}-\text{C1} & 1.182 (13) & \text{C7}-\text{C6}-\text{C5} & 120.90 (16) \\ & \text{C1}-\text{N2}-\text{N1} & 120.02 (13) & \text{C7}-\text{C6}-\text{H6A} & 119.6 \\ & \text{C1}-\text{N2}-\text{N1} & 120.0 & \text{C5}-\text{C6}-\text{H6A} & 119.6 \\ & \text{C1}-\text{N2}-\text{N1} & 120.0 & \text{C5}-\text{C6}-\text{H6A} & 119.6 \\ & \text{N1}-\text{N2}-\text{H2A} & 120.0 & \text{C6}-\text{C7}-\text{H7A} & 120.1 \\ & \text{C1}-\text{C2}-\text{N3}-\text{H3B} & 120.0 & \text{C6}-\text{C7}-\text{H7A} & 120.1 \\ & \text{C1}-\text{C2}-\text{N3}-\text{H3B} & 120.0 & \text{C6}-\text{C7}-\text{H7A} & 120.1 \\ & \text{C1}-\text{N3}-\text{H3B} & 120.0 & \text{C9}-\text{C8}-\text{C7} & 121.05 (16) \\ & \text{C2}-\text{C1}-\text{C1} & 118.52 (13) & \text{C9}-\text{C8}-\text{H8A} & 119.5 \\ & \text{C1}-\text{C1}-\text{C1} & 123.44 (14) & \text{C7}-\text{C8}-\text{H8A} & 119.5 \\ & \text{C1}-\text{C1}-\text{C1} & 122.44 (14) & \text{C9}-\text{C1}-\text{H7A} & 120.5 (16) \\ & \text{C2}-\text{C1}-\text{C1} & 122.44 (14) & \text{C9}-\text{C1}-\text{C1} & 123.14 (14) \\ & \text{C1}-\text{C2}-\text{C3} & 116.10 (14) & \text{C1}-\text{C9}-\text{H9A} & 119.5 \\ & \text{C1}-\text{C2}-\text{C3} & 116.10 (14) & \text{C1}-\text{C9}-\text{H9A} & 119.5 \\ & \text{C1}-\text{C2}-\text{C3} & 121.45 (14) & \text{C9}-\text{C1}-\text{C1} & 123.14 (14) \\ & \text{C3}-\text{C3}-\text{H3C} & 119.8 & \text{N}-\text{C1}-\text{C1} & 119.29 (14) \\ & \text{C3}-\text{C4}-\text{C5} & 121.03 (15) & \text{N1}-\text{C1}-\text{C1} & 119.22 (13) \\ & \text{C3}-\text{C4}-\text{C5} & 121.03 (15) & \text{N1}-\text{C1}-\text{C1} & 119.52 (13) \\ & \text{C3}-\text{C4}-\text{C5} & 120.31 & \text{C5}-\text{C1}-\text{C1} & 119.52 (13) \\ & \text{C3}-\text{C4}-\text{C5} & 12.03 (15) & \text{N1}-\text{C1}-\text{C1} & 119.52 (13) \\ & \text{C3}-\text{C4}-\text{C5} & 12.03 (15) & \text{N1}-\text{C1}-\text{C1} & 119.52 (13) \\ & \text{C3}-\text{C4}-\text{C5} & 12.03 (15) & \text{C3}-\text{C1}-\text{C1} & -179.55 (15) \\ & \text{C1}-\text{C1}-\text{C2}-\text{C3} & 117.45 (14) & \text{C9}-\text{C1}-\text{C1} & -179.55 (15) \\ & \text{C1}-\text{C1}-\text{C2}-\text{C3} & 119.47 (14) \\ & \text{C4}-\text{C3}-\text{C4} & 19.5 & \text{C3}-\text{C1}-\text$	N2—H2A	0.8800	С6—Н6А	0.9500
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	N3—C12	1.343 (2)	С7—С8	1.398 (3)
N3-H3B       0.8800       C8-C9       1.370 (2)         C1-C2       1.395 (2)       C8-H8A       0.9500         C1-C10       1.438 (2)       C9-C10       1.417 (2)         C1-C11       1.457 (2)       C9-H9A       0.9500         C2-C3       1.405 (2)       C11-H11A       0.9500         C3-C4       1.355 (2)       C11-H11A       0.9500         C1-NI-N2       118.82 (13)       C7-C6-C5       120.90 (16)         C12-N2-N1       120.02 (13)       C7-C6-H6A       119.6         N1-N2-H2A       120.0       C6-C7-C8       119.71 (16)         C12-N3-H3A       120.0       C8-C7       120.1         C12-N3-H3B       120.0       C9-C8-C7       121.05 (16)         C2-C1-C10       118.52 (13)       C9-C8-M8A       119.5         C3-C1-C11       120.34 (14)       C7-C8-H8A       119.5         C1-C1-C11       121.10 (13)       C8-C9-C10       121.09 (15)         C1-C2-C3       116.10 (14)       C10-C5       117.57 (14)         C4-C3-C2       120.48 (15)       C9-C10-C1       123.14 (14)         C4-C3-C3       121.45 (14)       C9-C10-C1       123.14 (14)         C4-C3-C3       121.45 (13)       C	N3—H3A	0.8800	С7—Н7А	0.9500
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N3—H3B	0.8800	С8—С9	1.370 (2)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C1—C2	1.395 (2)	C8—H8A	0.9500
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C1—C10	1.438 (2)	C9—C10	1.417 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C1—C11	1.457 (2)	С9—Н9А	0.9500
C3-C4       1355 (2)       111 1011       119 101         C2-O1-HIO       109.5       C4-C5-C10       119.23 (14)         C11-N1-N2       118.82 (13)       C7-C6-C5       120.90 (16)         C12-N2-N1       120.02 (13)       C7-C6-H6A       119.6         C12-N2-H2A       120.0       C6-C7-H7A       120.1         C12-N3-H3B       120.0       C6-C7-H7A       120.1         C12-N3-H3B       120.0       C9-C8-H8A       119.5         C2-C1-C10       118.52 (13)       C9-C8-H8A       119.5         C2-C1-C11       120.34 (14)       C7-C8-H8A       119.5         C1-C1-C11       121.10 (13)       C8-C9-H0A       119.5         C1-C2-C1       122.44 (14)       C8-C9-H9A       119.5         C1-C2-C3       116.10 (14)       C10-C9-H9A       119.5         C1-C2-C3       124.5 (14)       C9-C10-C1       123.14 (14)         C4-C3-H3C       119.8       C5-C10-C1       123.14 (14)         C4-C3-H3C       119.8       C1-C1-C1       119.29 (14)         C3-C4-C5       121.03 (15)       N1-C1-H11A       120.1         C3-C4-H4A       119.5       C1-C1-H11A       120.1         C3-C4-H4A       119.5 <t< td=""><td>C2—C3</td><td>1.405 (2)</td><td>C11—H11A</td><td>0.9500</td></t<>	C2—C3	1.405 (2)	C11—H11A	0.9500
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C3—C4	1.355 (2)		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C2	109 5	C4—C5—C10	119 23 (14)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C11N1N2	118 82 (13)	C7 - C6 - C5	120.90 (16)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C12N2N1	120.02(13)	C7-C6-H6A	119.6
$\begin{split} & \text{C12} - \text{C12} - \text{C12} & \text{C12} - \text{C13} & \text{C12} - \text{C14} & \text{C14} \\ & \text{C12} - \text{N3} - \text{H3A} & \text{120.0} & \text{C6} - \text{C7} - \text{C8} & \text{119.71} (16) \\ & \text{C12} - \text{N3} - \text{H3B} & \text{120.0} & \text{C6} - \text{C7} - \text{C7} & \text{121.05} (16) \\ & \text{C12} - \text{N3} - \text{H3B} & \text{120.0} & \text{C9} - \text{C8} - \text{C7} & \text{121.05} (16) \\ & \text{C2} - \text{C1} - \text{C10} & \text{118.52} (13) & \text{C9} - \text{C8} - \text{C7} & \text{121.05} (16) \\ & \text{C2} - \text{C1} - \text{C11} & \text{120.34} (14) & \text{C7} - \text{C8} - \text{H8A} & \text{119.5} \\ & \text{C10} - \text{C1} - \text{C11} & \text{121.10} (13) & \text{C8} - \text{C9} - \text{C10} & \text{121.09} (15) \\ & \text{O1} - \text{C2} - \text{C3} & \text{116.10} (14) & \text{C10} - \text{C9} - \text{H9A} & \text{119.5} \\ & \text{C1} - \text{C2} - \text{C3} & \text{116.10} (14) & \text{C10} - \text{C9} - \text{H9A} & \text{119.5} \\ & \text{C1} - \text{C2} - \text{C3} & \text{121.45} (14) & \text{C9} - \text{C10} - \text{C1} & \text{123.14} (14) \\ & \text{C4} - \text{C3} - \text{C2} & \text{120.48} (15) & \text{C9} - \text{C10} - \text{C1} & \text{123.14} (14) \\ & \text{C4} - \text{C3} - \text{C2} & \text{120.48} (15) & \text{C9} - \text{C10} - \text{C1} & \text{123.14} (14) \\ & \text{C4} - \text{C3} - \text{H3C} & \text{119.8} & \text{N1} - \text{C11} - \text{C1} & \text{119.82} (13) \\ & \text{C3} - \text{C4} - \text{C5} & \text{121.03} (15) & \text{N1} - \text{C11} - \text{H11A} & \text{120.1} \\ & \text{C3} - \text{C4} - \text{H4A} & \text{119.5} & \text{C1} - \text{C11} - \text{H11A} & \text{120.1} \\ & \text{C5} - \text{C4} - \text{H4A} & \text{119.5} & \text{C2} - \text{C12} - \text{N3} & \text{122.81} (14) \\ & \text{C6} - \text{C5} - \text{C10} & \text{119.81} (14) & \text{C8} - \text{C9} - \text{C10} - \text{C5} & \text{1.2} (2) \\ & \text{C1} - \text{C1} - \text{C2} - \text{C1} & \text{119.57} (13) & \text{C8} - \text{C9} - \text{C10} - \text{C5} & \text{1.2} (2) \\ & \text{C1} - \text{C1} - \text{C2} - \text{C1} & \text{119.57} (15) & \text{N3} - \text{C1} - \text{C1} & - \text{179.55} (15) \\ & \text{C1} - \text{C1} - \text{C2} - \text{C1} & - \text{C1} & \text{C1} - \text{C1} & - \text{C1} \\ & \text{C1} - \text{C1} - \text{C2} - \text{C1} & - \text{C1} & - 179.55 (15) \\ & \text{C1} - \text{C1} - \text{C2} - \text{C1} & - 179.55 (15) \\ & \text{C1} - \text{C1} - \text{C2} - \text{C2} & - 171.55 (13) & \text{C8} - \text{C9} - \text{C10} - \text{C5} & 1.2 (2) \\ & \text{C1} - \text{C1} - \text{C2} - \text{C1} & - 179.81 (14) \\ & \text{C1} - \text{C1} - \text{C1} - \text{C1} & - 179.86 (14) \\ & \text{C1} - \text{C1} - \text{C2} - \text{C3} & 176.35 (15) & \text{C6} - \text{C5} - \text{C10} - \text{C9} & - 179.18 $	C12 - N2 - H2A	120.02 (13)	C5-C6-H6A	119.6
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N1_N2_H2A	120.0	C6-C7-C8	119.0
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	120.0	$C_{0} = C_{1} = C_{0}$	120.1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_{12}$ N3 $H_{2R}$	120.0	$C^{\circ}$ $C^{-}$ $U^{-}$	120.1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C12— $N3$ — $H3B$	120.0	$C_{8}$ $C_{1}$ $H/A$	120.1
$C_2 \rightarrow C_1 \rightarrow C_10$ 118.52 (13) $C_3 \rightarrow C_4 \rightarrow HAA$ 119.5 $C_2 - C_1 - C_11$ 120.34 (14) $C_7 - C_8 \rightarrow HAA$ 119.5 $O_1 - C_2 - C_1$ 121.10 (13) $C_8 - C_9 \rightarrow C_10$ 121.09 (15) $O_1 - C_2 - C_1$ 122.44 (14) $C_8 - C_9 \rightarrow H9A$ 119.5 $O_1 - C_2 - C_3$ 116.10 (14) $C_1 - C_9 \rightarrow H9A$ 119.5 $C_1 - C_2 - C_3$ 121.45 (14) $C_9 - C_1 0 - C_5$ 117.57 (14) $C_4 - C_3 - C_2$ 120.48 (15) $C_9 - C_1 0 - C_1$ 123.14 (14) $C_4 - C_3 - H3C$ 119.8 $C_5 - C_1 0 - C_1$ 119.29 (14) $C_2 - C_3 - H3C$ 119.8 $N_1 - C_1 1 - C_1$ 119.22 (13) $C_3 - C_4 - C_5$ 121.03 (15) $N_1 - C_1 1 - H11A$ 120.1 $C_3 - C_4 - C_5$ 121.03 (15) $N_1 - C_1 1 - H11A$ 120.1 $C_3 - C_4 - H4A$ 119.5 $O_2 - C_1 2 - N3$ 122.81 (14) $C_6 - C_5 - C_4$ 121.10 (15) $O_2 - C_1 2 - N2$ 119.71 (14) $C_6 - C_5 - C_10$ 119.67 (15) $N_3 - C_1 2 - N2$ 117.48 (14) $C_1 - N_1 - N_2 - C_12$ $-171.55$ (13) $C_8 - C_9 - C_1 0 - C_5$ 1.2 (2) $C_1 - C_2 - O_1$ 179.81 (14) $C_8 - C_9 - C_1 0 - C_5$ 1.2 (2) $C_1 - C_1 - C_2 - C_3$ $-1.4$ (2) $C_4 - C_5 - C_1 0 - C_1$ $-179.56$ (15) $C_1 - C_2 - C_3$ $-1.4$ (2) $C_4 - C_5 - C_1 0 - C_1$ $-179.86$ (14) $O_1 - C_2 - C_3 - C_4$ 0.8 (3) $C_2 - C_1 - C_1 0 - C_5$ $-1.1$ (2) $C_1 - C_2 - C_3 - C_4$ 0.8 (3) $C_2 - C_1 - C_1 0 - C_5$ $-1.79.8$	$\Pi SA = NS = \Pi SB$	120.0	$C_{2} = C_{2} = C_{2}$	121.03 (10)
$C_2 = C_1 = C_1 1$ 120.34 (14) $C_1 = C_8 = H8A$ 119.5 $C10 = C_1 = C_1 1$ 121.10 (13) $C8 = C_9 = C_1 0$ 121.09 (15) $O1 = C_2 = C_1 1$ 122.44 (14) $C8 = C_9 = H9A$ 119.5 $O1 = C_2 = C_3 1$ 121.45 (14) $C9 = C_1 0 = C_5 1$ 117.57 (14) $C4 = C_3 = C_2 2$ 120.48 (15) $C9 = C_1 0 = C_5 1$ 123.14 (14) $C4 = C_3 = H3C 1$ 119.8 $C5 = C_1 0 = C_1 1$ 129.29 (14) $C2 = C_3 = H3C 1$ 119.8 $N1 = C_1 1 = C_1 1$ 119.82 (13) $C3 = C4 = C_5 1$ 121.03 (15) $N1 = C_1 1 = H11A 120.1$ 120.1 $C3 = C4 = H4A 119.5 1$ $C1 = C_1 1 = H11A 120.1$ 122.81 (14) $C6 = C_5 = C_1 0$ 119.67 (15) $O2 = C_1 2 = N3 122.81 (14)$ $C6 = C_5 = C_1 0$ 119.67 (15) $N3 = C_1 2 = N2 117.48 (14)$ $C6 = C_5 = C_1 0$ 119.67 (15) $N3 = C_1 2 = N2 117.48 (14)$ $C1 = -N1 = N2 = C_1 2 = -171.55 (13) C8 = C_9 = C_1 0 = C_5 1.2 (2)$ 117.48 (14) $C1 = -C_2 = -O_1 1$ 79.81 (14) C8 = C_9 = C_1 0 = C_5 1.2 (2) $C1 = -C_2 = -C_3 1 = -C_3 176.35 (15) C6 = C_5 = C_1 0 = C_1 1 = -179.86 (14)$ $C1 = -C_2 = -C_3 = -1.4 (2) C4 = C_5 = C_1 0 = C_1 1 = -179.86 (14)$ $C1 = -C_2 = -C_3 = -1.4 (2) C4 = C_5 = C_1 0 = C_1 1 = -179.86 (14)$ $C1 = -C_2 = -C_3 = -1.4 (2) C4 = -C_5 = -C_1 0 = -C_1 1 = -179.86 (14)$ $O1 = -C_2 = -C_3 = -C_4 = 0.8 (3) C2 = -C_1 = -C_1 0 = -C_9 = -178.19 (14)$ $C2 = -C_3 = -C_4 = -C_5 = 0.2 (3) C11 = -C_1 = -C_1 0 = -C_5 = -176.66 (13)$ $C4 = -C_5 = -C_1 0 = -C_7 = -C_7 = 0.5 (2) C1 = -C_1 = -C_1 0 = -C_5 = -176.66 (13)$ <	$C_2 = C_1 = C_{10}$	118.52 (13)	$C_{2} = C_{3} = H_{3}$	119.5
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		120.34 (14)	C/-C8-H8A	119.5
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		121.10(13)	C8—C9—C10	121.09 (15)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	01	122.44 (14)	С8—С9—Н9А	119.5
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	01	116.10 (14)	С10—С9—Н9А	119.5
C4-C3-C2 $120.48 (15)$ $C9-C10-C1$ $123.14 (14)$ $C4-C3-H3C$ $119.8$ $C5-C10-C1$ $119.29 (14)$ $C2-C3-H3C$ $119.8$ $N1-C11-C1$ $119.82 (13)$ $C3-C4-C5$ $121.03 (15)$ $N1-C11-H11A$ $120.1$ $C3-C4-H4A$ $119.5$ $C1-C11-H11A$ $120.1$ $C5-C4-H4A$ $119.5$ $O2-C12-N3$ $122.81 (14)$ $C6-C5-C4$ $121.10 (15)$ $O2-C12-N2$ $119.71 (14)$ $C6-C5-C10$ $119.67 (15)$ $N3-C12-N2$ $117.48 (14)$ $C11-N1-N2-C12$ $-171.55 (13)$ $C8-C9-C10-C5$ $1.2 (2)$ $C10-C1-C2-O1$ $179.81 (14)$ $C8-C9-C10-C5$ $1.2 (2)$ $C10-C1-C2-O1$ $-2.4 (2)$ $C6-C5-C10-C9$ $-0.6 (2)$ $C10-C1-C2-C3$ $-1.4 (2)$ $C4-C5-C10-C9$ $-179.86 (14)$ $O1-C2-C3-C4$ $0.8 (3)$ $C2-C1-C10-C9$ $-178.19 (14)$ $C2-C3-C4-C5$ $0.2 (3)$ $C11-C1-C10-C9$ $-178.19 (14)$ $C2-C3-C4-C5-C6$ $179.19 (15)$ $C2-C1-C10-C5$ $1.1 (2)$ $C3-C4-C5-C6$ $179.19 (15)$ $C2-C1-C10-C5$ $1.1 (2)$ $C3-C4-C5-C6$ $179.19 (15)$ $C2-C1-C10-C5$ $-176.66 (13)$ $C4-C5-C6-C7$ $-0.5 (2)$ $C1-C1-C10-C5$ $-175.06 (13)$ $C4-C5-C6-C7$ $-0.5 (2)$ $C2-C1-C11-N1$ $-175.06 (13)$ $C10-C5-C6-C7$ $-0.5 (2)$ $C2-C1-C11-N1$ $-175.06 (13)$	C1—C2—C3	121.45 (14)	C9—C10—C5	117.57 (14)
C4-C3-H3C $119.8$ $C5-C10-C1$ $119.29 (14)$ $C2-C3-H3C$ $119.8$ $N1-C11-C1$ $119.82 (13)$ $C3-C4-C5$ $121.03 (15)$ $N1-C11-H11A$ $120.1$ $C3-C4-H4A$ $119.5$ $C1-C11-H11A$ $120.1$ $C5-C4-H4A$ $119.5$ $O2-C12-N3$ $122.81 (14)$ $C6-C5-C4$ $121.10 (15)$ $O2-C12-N2$ $119.71 (14)$ $C6-C5-C10$ $119.67 (15)$ $N3-C12-N2$ $117.48 (14)$ $C11-N1-N2-C12$ $-171.55 (13)$ $C8-C9-C10-C5$ $1.2 (2)$ $C10-C1-C2-O1$ $179.81 (14)$ $C8-C9-C10-C5$ $1.2 (2)$ $C10-C1-C2-C3$ $-1.4 (2)$ $C4-C5-C10-C9$ $-0.6 (2)$ $C10-C1-C2-C3$ $-1.4 (2)$ $C4-C5-C10-C9$ $-179.86 (14)$ $O1-C2-C3-C4$ $0.8 (3)$ $C2-C1-C10-C9$ $-178.19 (14)$ $C2-C3-C4-C5$ $0.2 (3)$ $C11-C1-C10-C9$ $-178.19 (14)$ $C2-C3-C4-C5$ $0.2 (3)$ $C11-C1-C10-C9$ $-178.19 (14)$ $C2-C3-C4-C5-C6$ $179.19 (15)$ $C2-C1-C10-C5$ $-176.66 (13)$ $C3-C4-C5-C6$ $-0.5 (2)$ $C11-C1-C10-C5$ $-176.66 (13)$ $C4-C5-C6-C7$ $179.81 (15)$ $N2-N1-C11-C1$ $-175.06 (13)$ $C4-C5-C6-C7$ $-0.5 (2)$ $C2-C1-C10-N1$ $12.1 (2)$ $C5-C6-C7$ $-0.5 (2)$ $C2-C1-C10-N1$ $-170.23 (13)$	C4—C3—C2	120.48 (15)	C9—C10—C1	123.14 (14)
C2=C3=H3C $119.8$ $N1=C11=C1$ $119.82 (13)$ $C3=C4=C5$ $121.03 (15)$ $N1=C11=H11A$ $120.1$ $C3=C4=H4A$ $119.5$ $C1=C11=H11A$ $120.1$ $C5=C4=H4A$ $119.5$ $O2=C12=N3$ $122.81 (14)$ $C6=C5=C4$ $121.10 (15)$ $O2=C12=N2$ $119.71 (14)$ $C6=C5=C10$ $119.67 (15)$ $N3=C12=N2$ $117.48 (14)$ $C11=N1=N2=C12$ $-171.55 (13)$ $C8=C9=C10=C5$ $1.2 (2)$ $C10=C1=C2=O1$ $-79.81 (14)$ $C8=C9=C10=C1$ $-179.55 (15)$ $C11=C1=C2=O1$ $-2.4 (2)$ $C6=C5=C10=C9$ $-0.6 (2)$ $C10=C1=C2=C3$ $-1.4 (2)$ $C4=C5=C10=C9$ $-179.86 (14)$ $O1=C2=C3=C4$ $179.62 (15)$ $C4=C5=C10=C1$ $-0.1 (2)$ $C1=C2=C3=C4$ $0.8 (3)$ $C2=C1=C10=C9$ $-178.19 (14)$ $C2=C3=C4=C5$ $0.2 (3)$ $C11=C1=C10=C5$ $-176.66 (13)$ $C4=C5=C6=C7$ $179.81 (15)$ $N2=N1=C11=C1$ $-175.06 (13)$ $C4=C5=C6=C7$ $-0.5 (2)$ $C1=C1=N1$ $-170.23 (13)$	С4—С3—Н3С	119.8	C5—C10—C1	119.29 (14)
C3-C4-C5121.03 (15)N1-C11-H11A120.1C3-C4-H4A119.5C1-C11-H11A120.1C5-C4-H4A119.5O2-C12-N3122.81 (14)C6-C5-C4121.10 (15)O2-C12-N2119.71 (14)C6-C5-C10119.67 (15)N3-C12-N2117.48 (14)C11-N1-N2-C12-171.55 (13)C8-C9-C10-C51.2 (2)C10-C1-C2-O1179.81 (14)C8-C9-C10-C1-179.55 (15)C11-C1-C2-O1-2.4 (2)C6-C5-C10-C9-0.6 (2)C10-C1-C2-C3-1.4 (2)C4-C5-C10-C9179.18 (14)C11-C1-C2-C3176.35 (15)C6-C5-C10-C1-179.86 (14)C11-C1-C2-C3-C4179.62 (15)C4-C5-C10-C1-0.1 (2)C1-C2-C3-C40.8 (3)C2-C1-C10-C9-178.19 (14)C2-C3-C4-C50.2 (3)C11-C1-C10-C94.1 (2)C3-C4-C5-C6179.19 (15)C2-C1-C10-C51.1 (2)C3-C4-C5-C6179.19 (15)N2-N1-C11-C1-176.66 (13)C4-C5-C6-C7179.81 (15)N2-N1-C11-C1-176.06 (13)C4-C5-C6-C70.5 (2)C11-C1-C10-C5-176.66 (13)C4-C5-C6-C70.9 (3)C10-C1-C1-170.33 (13)	С2—С3—Н3С	119.8	N1—C11—C1	119.82 (13)
C3-C4-H4A119.5C1-C11-H11A120.1C5-C4-H4A119.5 $02-C12-N3$ 122.81 (14)C6-C5-C4121.10 (15) $02-C12-N2$ 119.71 (14)C6-C5-C10119.67 (15) $N3-C12-N2$ 117.48 (14)C11-N1-N2-C12-171.55 (13)C8-C9-C10-C51.2 (2)C10-C1-C2-O1179.81 (14)C8-C9-C10-C9-0.6 (2)C10-C1-C2-C3-1.4 (2)C4-C5-C10-C9179.18 (14)C11-C1-C2-C3176.35 (15)C6-C5-C10-C1-179.86 (14)C1-C2-C3-C40.8 (3)C2-C1-C10-C9-178.19 (14)C2-C3-C4-C50.2 (3)C11-C1-C10-C9-178.19 (14)C3-C4-C5-C6179.19 (15)C2-C1-C10-C51.1 (2)C3-C4-C5-C10-0.5 (2)C11-C1-C10-C5-176.66 (13)C4-C5-C6-C7179.81 (15)N2-N1-C11-C1-175.06 (13)C10-C5-C6-C7-0.5 (2)C2-C1-C10-N112.1 (2)C5-C6-C70.9 (3)C10-C1-C1-N112.1 (2)	C3—C4—C5	121.03 (15)	N1—C11—H11A	120.1
C5-C4-H4A119.5 $02-C12-N3$ $122.81 (14)$ C6-C5-C4121.10 (15) $02-C12-N2$ $119.71 (14)$ C6-C5-C10119.67 (15) $N3-C12-N2$ $117.48 (14)$ C11-N1-N2-C12 $-171.55 (13)$ $C8-C9-C10-C5$ $1.2 (2)$ C10-C1-C2-01179.81 (14) $C8-C9-C10-C1$ $-179.55 (15)$ C11-C1-C2-01 $-2.4 (2)$ $C6-C5-C10-C9$ $-0.6 (2)$ C10-C1-C2-C3 $-1.4 (2)$ $C4-C5-C10-C9$ $179.18 (14)$ C11-C1-C2-C3 $176.35 (15)$ $C6-C5-C10-C1$ $-179.86 (14)$ C1-C2-C3-C4 $179.62 (15)$ $C4-C5-C10-C1$ $-0.1 (2)$ C1-C2-C3-C4 $0.8 (3)$ $C2-C1-C10-C9$ $-178.19 (14)$ C2-C3-C4-C5 $0.2 (3)$ $C11-C1-C10-C9$ $4.1 (2)$ C3-C4-C5-C6 $179.19 (15)$ $C2-C1-C10-C5$ $1.1 (2)$ C3-C4-C5-C10 $-0.5 (2)$ $C11-C1-C10-C5$ $-176.66 (13)$ C4-C5-C6-C7 $179.81 (15)$ $N2-N1-C11-C1$ $-175.06 (13)$ C10-C5-C6-C7 $-0.5 (2)$ $C1-C1-N1$ $12.1 (2)$	С3—С4—Н4А	119.5	C1—C11—H11A	120.1
C6—C5—C4121.10 (15)O2—C12—N2119.71 (14)C6—C5—C10119.67 (15)N3—C12—N2117.48 (14)C11—N1—N2—C12 $-171.55 (13)$ C8—C9—C10—C51.2 (2)C10—C1—C2—O1179.81 (14)C8—C9—C10—C1 $-179.55 (15)$ C11—C1—C2—O1 $-2.4 (2)$ C6—C5—C10—C9 $-0.6 (2)$ C10—C1—C2—C3 $-1.4 (2)$ C4—C5—C10—C9 $179.18 (14)$ C11—C1—C2—C3 $176.35 (15)$ C6—C5—C10—C1 $-179.86 (14)$ O1—C2—C3—C4179.62 (15)C4—C5—C10—C9 $-178.19 (14)$ C2—C3—C40.8 (3)C2—C1—C10—C9 $-178.19 (14)$ C3—C4—C5—C6179.19 (15)C2—C1—C10—C5 $1.1 (2)$ C3—C4—C5—C10 $-0.5 (2)$ C11—C1—C10—C5 $-176.66 (13)$ C4—C5—C6—C7179.81 (15)N2—N1—C11—C1 $-175.06 (13)$ C10—C5—C6—C7 $-0.5 (2)$ C10—C1—C11—N1 $12.1 (2)$ C5—C6—C7 $0.9 (3)$ C10—C1—C11—N1 $12.1 (2)$	С5—С4—Н4А	119.5	O2—C12—N3	122.81 (14)
C6—C5—C10119.67 (15)N3—C12—N2117.48 (14)C11—N1—N2—C12 $-171.55 (13)$ C8—C9—C10—C51.2 (2)C10—C1—C2—O1179.81 (14)C8—C9—C10—C1 $-179.55 (15)$ C11—C1—C2—O1 $-2.4 (2)$ C6—C5—C10—C9 $-0.6 (2)$ C10—C1—C2—C3 $-1.4 (2)$ C4—C5—C10—C9 $179.18 (14)$ C11—C1—C2—C3176.35 (15)C6—C5—C10—C1 $-179.86 (14)$ O1—C2—C3—C4179.62 (15)C4—C5—C10—C1 $-0.1 (2)$ C1—C2—C3—C40.8 (3)C2—C1—C10—C9 $-178.19 (14)$ C2—C3—C4—C50.2 (3)C11—C1—C10—C9 $4.1 (2)$ C3—C4—C5—C6179.19 (15)C2—C1—C10—C5 $1.1 (2)$ C3—C4—C5—C679.19 (15)N2—N1—C11—C1 $-175.06 (13)$ C4—C5—C6—C7179.81 (15)N2—N1—C11—C1 $-175.06 (13)$ C10—C5—C6—C7 $-0.5 (2)$ C11—C1—C10—N1 $12.1 (2)$	C6—C5—C4	121.10 (15)	O2—C12—N2	119.71 (14)
C11—N1—N2—C12 $-171.55(13)$ C8—C9—C10—C5 $1.2(2)$ C10—C1—C2—O1179.81(14)C8—C9—C10—C1 $-179.55(15)$ C11—C1—C2—O1 $-2.4(2)$ C6—C5—C10—C9 $-0.6(2)$ C10—C1—C2—C3 $-1.4(2)$ C4—C5—C10—C9179.18(14)C11—C1—C2—C3176.35(15)C6—C5—C10—C1 $-179.86(14)$ O1—C2—C3—C4179.62(15)C4—C5—C10—C1 $-0.1(2)$ C1—C2—C3—C40.8(3)C2—C1—C10—C9 $-178.19(14)$ C2—C3—C4—C50.2(3)C11—C1—C10—C9 $4.1(2)$ C3—C4—C5—C6179.19(15)C2—C1—C10—C5 $1.1(2)$ C3—C4—C5—C60.5(2)C11—C1—C10—C5 $-176.66(13)$ C4—C5—C6—C7179.81(15)N2—N1—C11—C1 $-175.06(13)$ C10—C5—C6—C7 $-0.5(2)$ C2—C1—C11—N1 $12.1(2)$ C5C6C7C8 $0.9(3)$ C10	C6—C5—C10	119.67 (15)	N3—C12—N2	117.48 (14)
C10—C1—C2—O1179.81 (14)C8—C9—C10—C1 $-179.55 (15)$ C11—C1—C2—O1 $-2.4 (2)$ C6—C5—C10—C9 $-0.6 (2)$ C10—C1—C2—C3 $-1.4 (2)$ C4—C5—C10—C9179.18 (14)C11—C1—C2—C3176.35 (15)C6—C5—C10—C1 $-179.86 (14)$ O1—C2—C3—C4179.62 (15)C4—C5—C10—C1 $-0.1 (2)$ C1—C2—C3—C40.8 (3)C2—C1—C10—C9 $-178.19 (14)$ C2—C3—C4—C50.2 (3)C11—C1—C10—C9 $4.1 (2)$ C3—C4—C5—C6179.19 (15)C2—C1—C10—C5 $1.1 (2)$ C3—C4—C5—C10 $-0.5 (2)$ C11—C1—C10—C5 $-176.66 (13)$ C4—C5—C6—C7179.81 (15)N2—N1—C11—C1 $-175.06 (13)$ C10—C5—C6—C7 $-0.5 (2)$ C2—C1—C11—N1 $12.1 (2)$ C5C6C7C8 $0.9 (3)$ C10	C11—N1—N2—C12	-171.55 (13)	C8—C9—C10—C5	1.2 (2)
C11C1C2O1-2.4 (2)C6C5C10C9-0.6 (2)C10C1C2C3-1.4 (2)C4C5C10C9179.18 (14)C11C1C2C3176.35 (15)C6C5C10C1-179.86 (14)O1C2C3C4179.62 (15)C4C5C10C1-0.1 (2)C1C2C3C40.8 (3)C2C1C10C9-178.19 (14)C2C3C4C50.2 (3)C11C1C10C94.1 (2)C3C4C5C6179.19 (15)C2C1C10C51.1 (2)C3C4C5C6179.19 (15)C2C1C10C5-176.66 (13)C4C5C6C7179.81 (15)N2N1C11C1-175.06 (13)C10C5C6C7-0.5 (2)C2C1C11N112.1 (2)C5C6C70.9 (3)C10C1C11N112.1 (2)	C10-C1-C2-O1	179.81 (14)	C8—C9—C10—C1	-179.55 (15)
C10C1C2C3 $-1.4$ (2)C4C5C10C9179.18 (14)C11C1C2C3176.35 (15)C6C5C10C1 $-179.86$ (14)O1C2C3C4179.62 (15)C4C5C10C1 $-0.1$ (2)C1C2C3C40.8 (3)C2C1C10C9 $-178.19$ (14)C2C3C4C50.2 (3)C11C1C10C9 $4.1$ (2)C3C4C5C6179.19 (15)C2C1C10C5 $1.1$ (2)C3C4C5C10 $-0.5$ (2)C11C1C10C5 $-176.66$ (13)C4C5C6C7179.81 (15)N2N1C11C1 $-175.06$ (13)C10C5C6C7 $-0.5$ (2)C2C1C11N1 $12.1$ (2)C5C6C70.9 (3)C10C1C11N1 $12.1$ (2)	C11—C1—C2—O1	-2.4 (2)	C6—C5—C10—C9	-0.6 (2)
C11C1C2C3176.35 (15)C6C5C10C1 $-179.86 (14)$ O1C2C3C4179.62 (15)C4C5C10C1 $-0.1 (2)$ C1C2C3C40.8 (3)C2C1C10C9 $-178.19 (14)$ C2C3C4C50.2 (3)C11C1C10C9 $4.1 (2)$ C3C4C5C6179.19 (15)C2C1C10C5 $1.1 (2)$ C3C4C5C6C70.5 (2)C11C1C10C5 $-176.66 (13)$ C4C5C6C7179.81 (15)N2N1C11C1 $-175.06 (13)$ C10C5C6C7-0.5 (2)C2C1C11N1 $12.1 (2)$ C5C6C70.9 (3)C10C1C11N1 $12.7 (23 (13))$	C10-C1-C2-C3	-1.4 (2)	C4—C5—C10—C9	179.18 (14)
01-C2-C3-C4 $179.62 (15)$ $C4-C5-C10-C1$ $-0.1 (2)$ $C1-C2-C3-C4$ $0.8 (3)$ $C2-C1-C10-C9$ $-178.19 (14)$ $C2-C3-C4-C5$ $0.2 (3)$ $C11-C1-C10-C9$ $4.1 (2)$ $C3-C4-C5-C6$ $179.19 (15)$ $C2-C1-C10-C5$ $1.1 (2)$ $C3-C4-C5-C10$ $-0.5 (2)$ $C11-C1-C10-C5$ $-176.66 (13)$ $C4-C5-C6-C7$ $179.81 (15)$ $N2-N1-C11-C1$ $-175.06 (13)$ $C10-C5-C6-C7$ $-0.5 (2)$ $C2-C1-C11-N1$ $12.1 (2)$ $C5-C6-C7-C8$ $0.9 (3)$ $C10-C1-C11-N1$ $12.7 (2)$	C11—C1—C2—C3	176.35 (15)	C6—C5—C10—C1	-179.86 (14)
C1-C2-C3-C4 $0.8 (3)$ $C2-C1-C10-C9$ $-178.19 (14)$ $C2-C3-C4-C5$ $0.2 (3)$ $C11-C1-C10-C9$ $4.1 (2)$ $C3-C4-C5-C6$ $179.19 (15)$ $C2-C1-C10-C5$ $1.1 (2)$ $C3-C4-C5-C10$ $-0.5 (2)$ $C11-C1-C10-C5$ $-176.66 (13)$ $C4-C5-C6-C7$ $179.81 (15)$ $N2-N1-C11-C1$ $-175.06 (13)$ $C10-C5-C6-C7$ $-0.5 (2)$ $C2-C1-C11-N1$ $12.1 (2)$ $C5-C6-C7-C8$ $0.9 (3)$ $C10-C1-C11-N1$ $12.70 (23 (13))$	O1—C2—C3—C4	179.62 (15)	C4—C5—C10—C1	-0.1 (2)
C2-C3-C4-C5 $0.2 (3)$ $C11-C1-C10-C9$ $4.1 (2)$ $C3-C4-C5-C6$ $179.19 (15)$ $C2-C1-C10-C5$ $1.1 (2)$ $C3-C4-C5-C10$ $-0.5 (2)$ $C11-C1-C10-C5$ $-176.66 (13)$ $C4-C5-C6-C7$ $179.81 (15)$ $N2-N1-C11-C1$ $-175.06 (13)$ $C10-C5-C6-C7$ $-0.5 (2)$ $C2-C1-C11-N1$ $12.1 (2)$ $C5-C6-C7$ $0.9 (3)$ $C10-C1-C11-N1$ $12.7 (2)$	C1—C2—C3—C4	0.8 (3)	C2-C1-C10-C9	-178.19 (14)
C3-C4-C5-C6179.19 (15)C2-C1-C10-C51.1 (2)C3-C4-C5-C10 $-0.5$ (2)C11-C1-C10-C5 $-176.66$ (13)C4-C5-C6-C7179.81 (15)N2-N1-C11-C1 $-175.06$ (13)C10-C5-C6-C7 $-0.5$ (2)C2-C1-C11-N112.1 (2)C5-C6-C7 $0.9$ (3)C10-C1-C11-N1 $-170.23$ (13)	C2—C3—C4—C5	0.2 (3)	C11—C1—C10—C9	4.1 (2)
C3-C4-C5-C10 $-0.5$ (2)C11-C1-C10-C5 $-176.66$ (13)C4-C5-C6-C7179.81 (15)N2-N1-C11-C1 $-175.06$ (13)C10-C5-C6-C7 $-0.5$ (2)C2-C1-C11-N112.1 (2)C5-C6-C7C80.9 (3)C10-C1-C11-N1 $-170.23$ (13)	C3—C4—C5—C6	179.19 (15)	C2-C1-C10-C5	1.1 (2)
$C4\_C5\_C6\_C7$ $179.81 (15)$ $N2\_N1\_C11\_C1$ $-175.06 (13)$ $C10\_C5\_C6\_C7$ $-0.5 (2)$ $C2\_C1\_C11\_N1$ $12.1 (2)$ $C5\_C6\_C7$ $C8$ $0.9 (3)$ $C10\_C1\_C11\_N1$ $-170.23 (13)$	C3—C4—C5—C10	-0.5 (2)	C11—C1—C10—C5	-176.66 (13)
C10—C5—C6—C7 $-0.5$ (2) C2—C1—C11—N1 12.1 (2) C5 C6 C7 C8 $0.9$ (3) $C10$ C1 C11 N1 $-170$ 23 (13)	C4—C5—C6—C7	179.81 (15)	N2—N1—C11—C1	-175.06 (13)
$C_{5} = C_{6} = C_{7} = C_{8} = 0.0(3)$ $C_{10} = C_{11} = 0.11 = -170(23)(13)$	C10—C5—C6—C7	-0.5 (2)	C2—C1—C11—N1	12.1 (2)
$C_{3} = C_{6} = C_{7} = C_{6} = C_{7} = C_{7$	C5—C6—C7—C8	0.9 (3)	C10-C1-C11-N1	-170.23 (13)

C6—C7—C8—C9 C7—C8—C9—C10	-0.3 (3) -0.8 (3)	N1—N2—C12—O2 N1—N2—C12—N3		-172.55 (13) 6.8 (2)
Hydrogen-bond geometry (Å, °)				
D—H···A	<i>D</i> —Н	H···A	$D \cdots A$	D—H··· $A$
01—H1O…N1	0.84	1.82	2.5562 (17)	146
N2—H2A···O2 <sup>i</sup>	0.88	1.98	2.8290 (17)	161
N3—H3A···O1 <sup>ii</sup>	0.88	2.10	2.9762 (18)	171
N3—H3B···O2 <sup>iii</sup>	0.88	2.58	3.0618 (18)	116
Symmetry codes: (i) $-x+1$ , $-y$ , $-z+1$ ; (ii)	i) $-x+1$ , $y-1/2$ , $-z+1/2$ ; (iii	x, y+1, z.		



Fig. 1

Fig. 2



Fig. 3

