# organic compounds

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# 2-[1-(3-Aminophenyl)ethylidene]propanedinitrile

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Key indicators: single-crystal X-ray study; T = 298 K; mean  $\sigma$ (C–C) = 0.003 Å; R factor = 0.051; wR factor = 0.124; data-to-parameter ratio = 13.3.

In the title compound,  $C_{11}H_9N_3$ , all bond lengths and angles are normal. The crystal packing is stabilized by intermolecular  $N-H\cdots N$  hydrogen-bond interactions involving the H atoms of the amino groups and N atoms of the cyano groups.

### **Related literature**

For related literature, see: Bigi et al. (2000); Freeman (1980); Wardell et al. (2006).



### **Experimental**

Crystal c	lata
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$C_{11}H_9N_3$
$M_r = 183.21$
Monoclinic, P21/n
a = 7.4654 (8) Å

b = 13.7051 (18) Å
c = 9.5361 (17)  Å
$\beta = 99.961 \ (2)^{\circ}$
$V = 961.0 (2) \text{ Å}^3$

Z = 4Mo  $K\alpha$  radiation  $\mu = 0.08 \text{ mm}^{-1}$ 

#### Data collection

Bruker SMART CCD area-detector	4744 measured reflections
diffractometer	1687 independent reflections
Absorption correction: multi-scan	944 reflections with $I > 2\sigma(I)$
(SADABS; Sheldrick, 1996)	$R_{\rm int} = 0.053$
$T_{\min} = 0.969, \ T_{\max} = 0.991$	

T = 298 (2) K

 $0.40 \times 0.35 \times 0.11 \text{ mm}$ 

#### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.051$ 127 parameters $wR(F^2) = 0.124$ H-atom parameters constrainedS = 1.00 $\Delta \rho_{max} = 0.16$  e Å $^{-3}$ 1687 reflections $\Delta \rho_{min} = -0.17$  e Å $^{-3}$ 

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

$D - H \cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdot \cdot \cdot A$
$N3-H3A\cdots N1^{i}$	0.86	2.35	3.209 (3)	173
$N3 - H3B \cdot \cdot \cdot N2^{ii}$	0.86	2.33	3.182 (3)	170

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000) and *DIAMOND* (Brandenburg, 2004); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZ2100).

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supplementary materials

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# 2-[1-(3-Aminophenyl)ethylidene]propanedinitrile

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#### Comment

Knoevenagel condensation of carbonyl compounds with compounds containing an active methylene group is one of the most important methods of preparing substituted alkenes. As a part of our study of benzylidenemalonontriles, which are effective anti-fouling agents, fungicides, cytotoxic agents and insecticides (Freeman, 1980; Bigi *et al.*, 2000), we report here the structure of the title compound, (I), synthesized by Knoevenagel condensation of *m*-aminoacetophenone with malononitrile.

In (I) (Fig. 1), all bond lengths and angles agree well with those reported for related compounds (Wardell *et al.*, 2006). The amino and cyano groups are involved in intermolecular N—H···N hydrogen bonds (Table 1), which link the molecules into 26-membered rings (Fig. 2). The amino N atom acts as a hydrogen-bond donor to the cyano N atom in a neighbouring molecule, thus forming layers along the *bc*-plane.

#### Experimental

A mixture of *m*-aminoacetophenone (15 mmol) and malononitrile (15 mmol) in distilled water (15 ml) was heated to 353 K for 2 h. Upon cooling to room temperature, a crude product crystallized. The precipitate was filtered off, washed with ethanol and recrystallized from ethanol to afford the desired product as a colourless solid. Colourless single crystals of (I) were obtained by slow evaporation of an aqueous ethanol (95%) solution at ambient temperatures after 10 d. Elemental analysis, calculated for C11 H9 N3: C 72.11, H 4.95, N 22.94%; found: C 72.04. H 4.91, N 22.98%.

#### Refinement

All hydrogen atoms were geometrically fixed at calculated positions and allowed to ride on their parent atoms with C—H = 0.93-0.96 Å, N—H = 0.86 Å, and with  $U_{iso}(H) = 1.2U_{eq}(C,N)$ .

#### **Figures**



Fig. 1. Molecular structure of the title complex showing the atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.



Fig. 2. Part of the crystal structure of (I), showing the 26-membered rings formed by N—H…N intermolecular hydrogen-bonds. Hydrogen bonds are shown as dashed lines.

# 2-[1-(3-Aminophenyl)ethylidene]propanedinitrile

## Crystal data

C<sub>11</sub>H<sub>9</sub>N<sub>3</sub>  $F_{000} = 384$  $M_r = 183.21$  $D_{\rm x} = 1.266 {\rm Mg m}^{-3}$ Mo Kα radiation Monoclinic,  $P2_1/n$  $\lambda = 0.71073 \text{ Å}$ Hall symbol: -P 2yn Cell parameters from 1277 reflections a = 7.4654 (8) Å  $\theta = 2.5 - 22.2^{\circ}$ *b* = 13.7051 (18) Å  $\mu = 0.08 \text{ mm}^{-1}$ *c* = 9.5361 (17) Å T = 298 (2) K $\beta = 99.961 \ (2)^{\circ}$ Needle, colourless  $0.40 \times 0.35 \times 0.11 \text{ mm}$  $V = 961.0(2) \text{ Å}^3$ Z = 4

#### Data collection

Bruker SMART CCD area-detector diffractometer	1687 independent reflections
Radiation source: fine-focus sealed tube	944 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\rm int} = 0.053$
T = 298(2)  K	$\theta_{\text{max}} = 25.0^{\circ}$
$\phi$ and $\omega$ scans	$\theta_{\min} = 2.6^{\circ}$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -8 \rightarrow 7$
$T_{\min} = 0.969, \ T_{\max} = 0.991$	$k = -12 \rightarrow 16$
4744 measured reflections	$l = -11 \rightarrow 11$

### Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier ma
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.051$	H-atom parameters constrained
$wR(F^2) = 0.124$	$w = 1/[\sigma^{2}(F_{o}^{2}) + (0.0469P)^{2}]$ where $P = (F_{o}^{2} + 2F_{c}^{2})/3$
S = 1.00	$(\Delta/\sigma)_{max} < 0.001$
1687 reflections	$\Delta \rho_{max} = 0.16 \text{ e } \text{\AA}^{-3}$
127 parameters	$\Delta \rho_{\rm min} = -0.17 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct	Extinction correction: none

methods

map

Extinction correction: none

## 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	$U_{\rm iso}$ */ $U_{\rm eq}$
N1	0.2598 (3)	0.98666 (15)	0.4529 (3)	0.0732 (7)
N2	0.1402 (3)	0.89557 (17)	0.0215 (3)	0.0784 (7)
N3	0.2430 (3)	0.53195 (15)	0.7174 (2)	0.0798 (7)
H3A	0.2525	0.5189	0.8066	0.096*
H3B	0.2815	0.4908	0.6613	0.096*
C1	0.2043 (3)	0.92393 (18)	0.3799 (3)	0.0536 (7)
C2	0.1377 (3)	0.84685 (16)	0.2806 (2)	0.0461 (6)
C3	0.1375 (3)	0.87283 (17)	0.1360 (3)	0.0553 (7)
C4	0.0880 (3)	0.75772 (16)	0.3203 (2)	0.0444 (6)
C5	0.0877 (3)	0.73249 (16)	0.4696 (2)	0.0435 (6)
C6	0.1566 (3)	0.64313 (16)	0.5219 (3)	0.0499 (6)
H6	0.1970	0.5988	0.4604	0.060*
C7	0.1666 (3)	0.61835 (18)	0.6645 (3)	0.0536 (7)
C8	0.1040 (3)	0.68524 (19)	0.7545 (3)	0.0577 (7)
H8	0.1115	0.6709	0.8507	0.069*
C9	0.0308 (3)	0.7728 (2)	0.7010 (3)	0.0592 (7)
Н9	-0.0139	0.8161	0.7616	0.071*
C10	0.0223 (3)	0.79763 (17)	0.5605 (3)	0.0509 (6)
H10	-0.0265	0.8573	0.5267	0.061*
C11	0.0328 (3)	0.68186 (16)	0.2086 (3)	0.0583 (7)
H11A	0.0460	0.7075	0.1172	0.088*
H11B	-0.0918	0.6640	0.2073	0.088*
H11C	0.1088	0.6254	0.2294	0.088*
Atomia displa	comont payameters ()	82)		
лотис иізрій	cement parameters (A	· /		

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N1	0.0955 (18)	0.0534 (14)	0.0705 (17)	-0.0135 (13)	0.0140 (14)	-0.0121 (13)
N2	0.1029 (19)	0.0718 (16)	0.0607 (16)	0.0024 (14)	0.0152 (14)	0.0081 (14)
N3	0.119 (2)	0.0599 (14)	0.0606 (15)	0.0067 (14)	0.0162 (14)	0.0154 (13)
C1	0.0626 (18)	0.0447 (15)	0.0532 (16)	0.0020 (13)	0.0090 (13)	0.0022 (14)
C2	0.0488 (15)	0.0424 (14)	0.0467 (15)	0.0022 (11)	0.0072 (12)	0.0003 (12)

# supplementary materials

$\begin{array}{cccccccccccccccccccccccccccccccccccc$							
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C3	0.0638 (17)	0.0450 (15)	0.0570 (17)	-0.0001 (12)	0.0107 (14)	0.0013 (14)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C4	0.0399 (13)	0.0436 (13)	0.0496 (15)	0.0053 (11)	0.0073 (11)	-0.0013 (12)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C5	0.0424 (14)	0.0403 (13)	0.0476 (15)	-0.0037 (11)	0.0074 (11)	-0.0027 (12)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C6	0.0580 (16)	0.0438 (14)	0.0487 (15)	-0.0029 (12)	0.0115 (12)	-0.0002 (13)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C7	0.0541 (16)	0.0506 (15)	0.0548 (17)	-0.0081 (13)	0.0062 (13)	0.0078 (15)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C8	0.0611 (17)	0.0674 (18)	0.0452 (15)	-0.0068 (15)	0.0113 (13)	0.0015 (15)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C9	0.0524 (16)	0.0719 (19)	0.0561 (18)	-0.0034 (14)	0.0175 (13)	-0.0129 (15)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C10	0.0471 (15)	0.0494 (14)	0.0572 (16)	-0.0003 (12)	0.0119 (12)	-0.0032 (13)
Geometric parameters (Å, $^{\circ}$ )N1—C11.138 (3)C6—C71.391 (3)N2—C31.139 (3)C6—H60.9300N3—C71.372 (3)C7—C81.390 (3)N3—H3A0.8600C8—C91.379 (3)N3—H3B0.8600C8—H80.9300C1—C21.448 (3)C9—C101.373 (3)C2—C41.350 (3)C9—H90.9300C2—C31.424 (3)C10—H100.9300C4—C51.466 (3)C11—H11A0.9600C4—C11.494 (3)C11—H11B0.9600C5—C61.387 (3)C11—H11C0.9600C5—C61.387 (3)C11—H11C0.9600C5—C101.391 (3)C11.444 (2)C7—N3—H3A120.0C8—C7—C6118.4 (2)N1—C1—C2176.8 (3)C9—C8—H8120.0C4—C2-C1123.8 (2)C10—C9—H8120.0C4—C2-C1123.8 (2)C10—C9—H9119.2C2—C4—C1119.0 (2)C3—C10—C5119.2 (2)C2—C4—C1113.2 (2)C10—C9—H9119.2C2—C4—C1119.0 (2)C3—C10—H10120.4C5—C4—C11119.4 (2)C4—C11—H11B109.5C5—C6—C7121.4 (2)C4—C11—H11B109.5C5—C6—C7121.4 (2)C4—C11—H11B109.5C5—C6—C7121.4 (2)C4—C11—H11B109.5C5—C6—C7121.4 (2)C4—C11—H11B109.5C5—C6—C7121.4 (2)C4—C11—H11B109.5C5—C6—C7121.4 (2) </td <td>C11</td> <td>0.0678 (17)</td> <td>0.0506 (15)</td> <td>0.0560 (17)</td> <td>-0.0070 (13)</td> <td>0.0089 (13)</td> <td>-0.0077 (13)</td>	C11	0.0678 (17)	0.0506 (15)	0.0560 (17)	-0.0070 (13)	0.0089 (13)	-0.0077 (13)
$\begin{split} \mathbf{N} &= \mathbf{C} & \mathbf{I} & \mathbf{I}$	Geometric paran	neters (Å, °)					
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N1 C1		1 138 (3)	C6 1	C7	1 30	(1)
N2-C31.137 (3)C0-103500N3-C71.372 (3)C7-C81.390 (3)N3-H3A0.8600C8-C91.379 (3)C1-C21.448 (3)C9-C101.373 (3)C2-C31.424 (3)C10-H100.9300C4-C51.466 (3)C11-H11A0.9600C4-C51.466 (3)C11-H11A0.9600C4-C51.466 (3)C11-H11B0.9600C5-C61.387 (3)C11-H11B0.9600C5-C61.387 (3)C11-H11C0.9600C5-C101.391 (3)C7-C6121 2 (2)C7-N3-H3A120.0C8-C7-C6118.4 (2)H3A-N3-H3B120.0C9-C8-C7119.9 (2)N1-C1-C2176.8 (3)C9-C8-H18120.0C4-C2-C3122.9 (2)C7-C8-H18120.0C4-C2-C1138.2 (2)C10-C9-C8121.7 (2)C3-C2-C1138.2 (2)C10-C9-H9119.2N2-C3-C2178.2 (3)C8-C9-H9119.2C2-C4-C11119.0 (2)C4-C11-H11A109.5C5-C4-C11119.0 (2)C4-C11-H11B109.5C5-C4-C11119.4 (2)C4-C11-H11B109.5C5-C6-C7121.4 (2)C4-C11-H11B109.5C5-C6-C7121.4 (2)C4-C11-H11B109.5C5-C6-C7121.4 (2)C4-C11-H11B109.5C5-C6-C7121.4 (2)C4-C11-H11C109.5C5-C6-C7121.4 (2)C4-C11-H11B109.5C5-C6-C7121.4 (2)C4-C11-H11C109.5 <td>N1 - C1</td> <td></td> <td>1.138(3) 1.139(3)</td> <td>C6</td> <td>U6</td> <td>0.03</td> <td>() ()</td>	N1 - C1		1.138(3) 1.139(3)	C6	U6	0.03	() ()
N3-H3AN3/2 (3)C/-C81.390 (3)N3-H3A0.8600C8-C91.379 (3)N3-H3B0.8600C8-H80.9300C1-C21.448 (3)C9-C101.373 (3)C2-C31.424 (3)C10-H100.9300C4-C51.466 (3)C11-H11A0.9600C4-C51.466 (3)C11-H11A0.9600C5-C61.387 (3)C11-H11B0.9600C5-C61.387 (3)C11-H11C0.9600C5-C61.387 (3)C11-H11C0.9600C5-C61.387 (3)C11-H11C0.9600C5-C61.387 (3)C11-H11C0.9600C5-C61.387 (3)C11-H11C0.9600C5-C101.391 (3)TTC7-N3-H3A120.0C8-C7-C6118.4 (2)H3A-N3-H3B120.0C9-C8-C7119.9 (2)N1-C1-C2176.8 (3)C9-C8-H8120.0C4-C2-C1123.8 (2)C10-C9-H9119.2C4-C2-C1123.8 (2)C10-C9-C8121.7 (2)C3-C2-C113.2 (2)C9-C10-C5119.2 (2)C2-C4-C5122.2 (2)C9-C10-C5119.2 (2)C2-C4-C11119.0 (2)C4-C11-H11A109.5C6-C5-C4119.7 (2)C4-C11-H11A109.5C5-C6-C7121.4 (2)C4-C11-H11B109.5C5-C6-C6120.3 (2)C5-C6-C7177.0 (2)C3-C2-C4-C53.5 (3)C5-C6-C7177.0 (2)C3-C2-C4-C53.5 (3)C5-C6-C7-C80.6 (3)C1-C2-C	N2-C7		1.139(3) 1.272(2)	C0—1	C 9	0.93	(0)
N3-H3A0.8000C8-C91.379 (3)N3-H3B0.8000C8-H80.9300C1-C21.448 (3)C9-C101.373 (3)C2-C41.350 (3)C9-H90.9300C2-C31.424 (3)C10-H100.9300C4-C51.466 (3)C11-H11A0.9600C4-C111.494 (3)C11-H11B0.9600C5-C61.387 (3)C11-H11C0.9600C5-C61.391 (3)C10.9600C5-C101.391 (3)C10.9600C5-C101.391 (3)C10.9600C5-C101.391 (3)C10.9600C4-C21.20.0C8-C7-C6118.4 (2)H3A-N3-H3B120.0C9-C8-C7119.9 (2)N1-C1-C2176.8 (3)C9-C8-H8120.0C4-C2-C3122.9 (2)C7-C8-H8120.0C4-C2-C4132.(2)C10-C9-C8121.7 (2)C3-C2-C1113.2 (2)C10-C9-H9119.2C2-C4-C5122.2 (2)C9-C10-H10120.4C5-C4-C11119.0 (2)C9-C10-H10120.4C5-C4-C11119.4 (2)C4-C11-H11A109.5C5-C6-C7121.4 (2)C4-C11-H11A109.5C5-C6-C7121.4 (2)C4-C11-H11B109.5C5-C6-C7121.4 (2)C4-C11-H11C109.5C5-C6-C7121.4 (2)C4-C11-H11C109.5C5-C6-C7121.4 (2)C4-C11-H11C109.5C5-C6-C7121.4 (2)C4-C11-H11C109.5C5-C6-C7120.3 (2)<	N3-C7		0.8600	C)—(		1.35	(0)(3)
N3-H3B $0.800^{-1}$ $C_{6}$ -H3 $0.9300^{-1}$ C1-C21.448 (3)C9-C101.373 (3)C2-C41.350 (3)C9-H90.9300C2-C31.424 (3)C10-H100.9300C4-C51.466 (3)C11-H11A0.9600C5-C61.387 (3)C11-H11B0.9600C5-C61.387 (3)C11-H11C0.9600C5-C101.391 (3) $C$ C7-N3-H3A120.0N3-C7-C6121.2 (2)C7-N3-H3B120.0C9-C8-C7119.9 (2)N1-C1-C2176.8 (3)C9-C8-H8120.0C4-C2-C3122.9 (2)C7-C8-H8120.0C4-C2-C1123.8 (2)C10-C9-C8121.7 (2)C3-C2-C1113.2 (2)C10-C9-H9119.2C2-C4-C5122.2 (2)C9-C10-C5119.2 (2)C2-C4-C5122.2 (2)C9-C10-C5119.2 (2)C2-C4-C11119.0 (2)C9-C10-H10120.4C5-C4-C11118.8 (2)C5-C10-H10120.4C5-C4-C11119.4 (2)C4-C11-H11A109.5C5-C5-C4119.7 (2)C4-C11-H11B109.5C5-C6-C7121.4 (2)C4-C11-H11B109.5C5-C6-C7121.4 (2)C4-C11-H11C109.5C5-C6-C7121.4 (2)C4-C11-H11C109.5C5-C6-C7120.3 (2)C1-C2-C4-C53.5 (3)C5-C6-C7C3-C2-C4-C53.5 (3)C5-C6-C7177.0 (2)C3-C2-C4-C53.5 (3)C5-C6-C70.6 (3)C1-C2-C4-C53.5 (3) <t< td=""><td>N3—H3A</td><td></td><td>0.8000</td><td>Co</td><td>C9</td><td>1.57</td><td>9(3)</td></t<>	N3—H3A		0.8000	Co	C9	1.57	9(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N3—ПЗВ		1.448(2)	C8—1	Пð С10	0.93	2 (2)
C2-C41.330 (5) $C9-H9$ 0.9300 $C2-C3$ 1.424 (3) $C10-H10$ 0.9300 $C4-C5$ 1.466 (3) $C11-H11A$ 0.9600 $C4-C11$ 1.494 (3) $C11-H11B$ 0.9600 $C5-C6$ 1.387 (3) $C11-H11C$ 0.9600 $C5-C6$ 1.387 (3) $C11-H11C$ 0.9600 $C5-C10$ 1.391 (3) $C7-N3-H3A$ 120.0 $N3-C7-C6$ 121.2 (2) $C7-N3-H3B$ 120.0 $C8-C7-C6$ 118.4 (2) $H3A-N3-H3B$ 120.0 $C9-C8-C7$ 119.9 (2) $N1-C1-C2$ 176.8 (3) $C9-C8-H8$ 120.0 $C4-C2-C3$ 122.9 (2) $C7-C8-H8$ 120.0 $C4-C2-C1$ 123.8 (2) $C10-C9-C8$ 121.7 (2) $C3-C2-C1$ 113.2 (2) $C10-C9-H9$ 119.2 $N2-C3-C2$ 178.2 (3) $C8-C9-H9$ 119.2 $C2-C4-C5$ 122.2 (2) $C9-C10-C5$ 119.2 (2) $C2-C4-C5$ 122.2 (2) $C9-C10-H10$ 120.4 $C5-C4-C11$ 119.0 (2) $C5-C10-H10$ 120.4 $C6-C5-C4$ 119.7 (2) $C4-C11-H11A$ 109.5 $C10-C5-C4$ 120.9 (2)H11A-C11-H11B109.5 $C5-C6-C7$ 121.4 (2) $C4-C11-H11B$ 109.5 $C5-C6-C7$ 121.4 (2) $C4-C1-H11C$ 109.5 $C5-C6-C7$ 120.3 (2) $C3-C2-C4-C5$ 3.5 (3) $C5-C6-C7-N3$ $C-C5-C6-C7-C8$ 3.5 (3) $C5-C6-C7-C8$ 0.6 (3) $C1-C2-C4-C5$ 3.5 (3) $C5-C6-C7-C8-C9$ 176.6 (2) $C3-C2-C4-C11$ 1.0 (3)	C1 - C2		1.448 (3)	C9—(		1.37	3 (3)
C2-C3 $1.424$ (3) $C10-H10$ $0.9500$ $C4-C5$ $1.466$ (3) $C11-H11A$ $0.9600$ $C5-C6$ $1.387$ (3) $C11-H11B$ $0.9600$ $C5-C6$ $1.387$ (3) $C11-H11C$ $0.9600$ $C5-C10$ $1.391$ (3) $C7-N3-H3A$ $120.0$ $N3-C7-C6$ $121.2$ (2) $C7-N3-H3B$ $120.0$ $C8-C7-C6$ $118.4$ (2) $H3A-N3-H3B$ $120.0$ $C9-C8-C7$ $119.9$ (2) $N1-C1-C2$ $76.8$ (3) $C9-C8-H8$ $120.0$ $C4-C2-C3$ $122.9$ (2) $C7-C8-H8$ $120.0$ $C4-C2-C1$ $123.8$ (2) $C10-C9-C8$ $121.7$ (2) $C3-C2-C1$ $113.2$ (2) $C10-C9-H9$ $119.2$ $V2-C3-C2$ $178.2$ (3) $C8-C9-H9$ $119.2$ $V2-C3-C2$ $178.2$ (3) $C8-C9-H9$ $119.2$ (2) $C2-C4-C5$ $122.2$ (2) $C9-C10-C5$ $119.2$ (2) $C2-C4-C5$ $122.2$ (2) $C9-C10-H10$ $120.4$ $C5-C4-C11$ $119.0$ (2) $C4-C11-H11A$ $109.5$ $C6-C5-C10$ $119.4$ (2) $C4-C11-H11A$ $109.5$ $C6-C5-C4$ $119.7$ (2) $C4-C11-H11B$ $109.5$ $C5-C6-C7$ $121.4$ (2) $C4-C11-H11B$ $109.5$ $C5-C6-C7$ $121.4$ (2) $C4-C11-H11C$ $109.5$ $C5-C6-H6$ $119.3$ $H11A-C11-H11C$ $109.5$ $C5-C6-H6$ $119.3$ $H11A-C11-H11C$ $109.5$ $C3-C2-C4-C5$ $35.(3)$ $C5-C6-C7-N3$ $-176.7$ (2) $C3-C2-C4-C5$ $35.(3)$ $C5-C6$	$C_2 - C_4$		1.350 (3)	C9—1	H9	0.93	00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_2 - C_3$		1.424 (3)	C10-	-HIU	0.93	500
C4-C11 $1.494 (3)$ $C11-H11B$ $0.9600$ $C5-C6$ $1.387 (3)$ $C11-H11C$ $0.9600$ $C5-C10$ $1.391 (3)$ $C7-N3-H3A$ $120.0$ $N3-C7-C6$ $121.2 (2)$ $C7-N3-H3B$ $120.0$ $C8-C7-C6$ $118.4 (2)$ $H3A-N3-H3B$ $120.0$ $C9-C8-C7$ $119.9 (2)$ $N1-C1-C2$ $176.8 (3)$ $C9-C8-H8$ $120.0$ $C4-C2-C3$ $122.9 (2)$ $C7-C8-H8$ $120.0$ $C4-C2-C1$ $133.8 (2)$ $C10-C9-C8$ $121.7 (2)$ $C3-C2-C1$ $113.2 (2)$ $C10-C9-H9$ $119.2$ $N2-C3-C2$ $178.2 (3)$ $C8-C9-H9$ $119.2$ $N2-C3-C2$ $178.2 (3)$ $C8-C9-H9$ $119.2 (2)$ $C2-C4-C11$ $119.0 (2)$ $C9-C10-C5$ $119.2 (2)$ $C2-C4-C11$ $119.0 (2)$ $C9-C10-H10$ $120.4$ $C5-C4-C11$ $119.4 (2)$ $C4-C11-H11A$ $109.5$ $C6-C5-C4$ $119.7 (2)$ $C4-C11-H11B$ $109.5$ $C5-C6-C7$ $121.4 (2)$ $C4-C11-H11B$ $109.5$ $C5-C6-C7$ $121.4 (2)$ $C4-C11-H11C$ $109.5$ $C5-C6-H6$ $119.3$ $H11A-C11-H11C$ $109.5$ $C7-C6-H6$ $19.3$ $H11B-C11-H11C$ $109.5$ $C5-C6-C7$ $121.6 (2)$ $C3-C6-C7$ $177.0 (2)$ $C3-C2-C4-C5$ $3.5 (3)$ $C5-C6-C7$ $177.0 (2)$ $C3-C2-C4-C5$ $3.5 (3)$ $C5-C6-C7$ $177.0 (2)$ $C3-C2-C4-C5$ $3.5 (3)$ $C5-C6-C7-C8$ $0.6 (3)$ $C1-C2-C4-C5$ <t< td=""><td>C4—C5</td><td></td><td>1.466 (3)</td><td>C11-</td><td>-HIIA</td><td>0.96</td><td>500</td></t<>	C4—C5		1.466 (3)	C11-	-HIIA	0.96	500
CS-C6 $1.387(3)$ $C11$ -H11C $0.9600$ C5-C10 $1.391(3)$ C7-M3-H3A120.0N3-C7-C6 $121.2(2)$ C7-M3-H3B120.0C9-C8-C7 $119.9(2)$ H3A-N3-H3B120.0C9-C8-H8120.0C4-C2-C3122.9(2)C7-C8-H8120.0C4-C2-C1133.8(2)C10-C9-C8121.7(2)C3-C2-C1113.2(2)C10-C9-H9119.2N2-C3-C2178.2(3)C8-C9-H9119.2C2-C4-C5122.2(2)C9-C10-C5119.2(2)C2-C4-C5122.2(2)C9-C10-H10120.4C5-C4-C11119.0(2)C9-C10-H10120.4C5-C4-C11119.4(2)C4-C11-H11A109.5C6-C5-C4119.7(2)C4-C11-H11B109.5C5-C6-C7121.4(2)C4-C11-H11B109.5C5-C6-C7121.4(2)C4-C11-H11C109.5C5-C6-C7121.4(2)C4-C11-H11C109.5C5-C6-C4119.3H11A-C11-H11C109.5C5-C6-C4119.3H11B-C11-H11C109.5C5-C6-C4120.3(2)C3-C2-C4-C5177.0(2)C3-C2-C4-C53.5(3)C5-C6-C7177.0(2)C3-C2-C4-C111.0(3)C5-C6-C7177.0(2)C3-C2-C4-C111.0(3)C5-C6-C7178.6(2)C2-C4-C5-C6-136.5(2)C6-C7-C8-C91.3(4)	C4—CII		1.494 (3)	CII-	-HIIB	0.96	500
CS-C101.391 (3) $C7-N3-H3A$ 120.0 $N3-C7-C6$ 121.2 (2) $C7-N3-H3B$ 120.0 $C8-C7-C6$ 118.4 (2) $H3A-N3-H3B$ 120.0 $C9-C8-C7$ 119.9 (2) $N1-C1-C2$ 176.8 (3) $C9-C8-H8$ 120.0 $C4-C2-C3$ 122.9 (2) $C7-C8-H8$ 120.0 $C4-C2-C1$ 133.8 (2) $C10-C9-C8$ 121.7 (2) $C3-C2-C1$ 113.2 (2) $C10-C9-H9$ 119.2 $V2-C3-C2$ 178.2 (3) $C8-C9-H9$ 119.2 (2) $C2-C4-C5$ 122.2 (2) $C9-C10-C5$ 119.2 (2) $C2-C4-C5$ 122.2 (2) $C9-C10-H10$ 120.4 $C5-C4-C11$ 119.0 (2) $C9-C10-H10$ 120.4 $C5-C4-C11$ 119.4 (2) $C4-C11-H11A$ 109.5 $C6-C5-C4$ 119.7 (2) $C4-C11-H11B$ 109.5 $C5-C6-C7$ 121.4 (2) $C4-C11-H11B$ 109.5 $C5-C6-C7$ 121.4 (2) $C4-C11-H11C$ 109.5 $C5-C6-H6$ 119.3H11A-C11-H11C109.5 $C7-C6-H6$ 119.3H11A-C11-H11C109.5 $N3-C7-C8$ 120.3 (2) $C3-C6-C7$ 177.0 (2) $C3-C2-C4-C5$ $3.5$ (3) $C5-C6-C7-R8$ 0.6 (3) $C1-C2-C4-C5$ $3.5$ (3) $C5-C6-C7-R8$ 0.6 (3) $C1-C2-C4-C5-C6$ $-136.5$ (2) $C6-C7-C8-C9$ 1.3 (4)	C5—C6		1.387 (3)	CII-	-нпс	0.96	600
C7-M3-H3A $120.0$ $N3-C7-C6$ $121.2 (2)$ $C7-M3-H3B$ $120.0$ $C8-C7-C6$ $118.4 (2)$ $H3A-N3-H3B$ $120.0$ $C9-C8-C7$ $119.9 (2)$ $N1-C1-C2$ $176.8 (3)$ $C9-C8-H8$ $120.0$ $C4-C2-C3$ $122.9 (2)$ $C7-C8-H8$ $120.0$ $C4-C2-C1$ $123.8 (2)$ $C10-C9-C8$ $121.7 (2)$ $C3-C2-C1$ $113.2 (2)$ $C10-C9-H9$ $119.2$ $N2-C3-C2$ $178.2 (3)$ $C8-C9-H9$ $119.2$ $C2-C4-C5$ $122.2 (2)$ $C9-C10-C5$ $119.2 (2)$ $C2-C4-C11$ $119.0 (2)$ $C9-C10-H10$ $120.4$ $C5-C4-C11$ $119.4 (2)$ $C4-C11-H11A$ $109.5$ $C6-C5-C4$ $119.7 (2)$ $C4-C11-H11B$ $109.5$ $C5-C6-C7$ $121.4 (2)$ $C4-C11-H11B$ $109.5$ $C5-C6-C7$ $121.4 (2)$ $C4-C11-H11B$ $109.5$ $C5-C6-C7$ $121.4 (2)$ $C4-C11-H11C$ $109.5$ $C5-C6-C7$ $121.4 (2)$ $C4-C11-H11C$ $109.5$ $C7-C6-H6$ $119.3$ $H11A-C11-H11C$ $109.5$ $C7-C6-H6$ $119.3$ $H11B-C11-H11C$ $109.5$ $N3-C7-C8$ $120.3 (2)$ $C3-C2-C4-C5$ $-179.5 (2)$ $C4-C5-C6-C7$ $177.0 (2)$ $C1-C2-C4-C5$ $3.5 (3)$ $C5-C6-C7-C8$ $0.6 (3)$ $C1-C2-C4-C11$ $1.0 (3)$ $C5-C6-C7-C8-C9$ $13.(4)$	C5-C10		1.391 (3)				
C7-N3-H3B $120.0$ $C8-C7-C6$ $118.4 (2)$ $H3A-N3-H3B$ $120.0$ $C9-C8-C7$ $119.9 (2)$ $N1-C1-C2$ $176.8 (3)$ $C9-C8-H8$ $120.0$ $C4-C2-C3$ $122.9 (2)$ $C7-C8-H8$ $120.0$ $C4-C2-C1$ $123.8 (2)$ $C10-C9-C8$ $121.7 (2)$ $C3-C2-C1$ $113.2 (2)$ $C10-C9-H9$ $119.2$ $N2-C3-C2$ $178.2 (3)$ $C8-C9-H9$ $119.2 (2)$ $C2-C4-C5$ $122.2 (2)$ $C9-C10-C5$ $119.2 (2)$ $C2-C4-C5$ $122.2 (2)$ $C9-C10-H10$ $120.4$ $C5-C4-C11$ $119.0 (2)$ $C9-C10-H10$ $120.4$ $C5-C4-C11$ $119.4 (2)$ $C4-C11-H11A$ $109.5$ $C6-C5-C4$ $119.7 (2)$ $C4-C11-H11B$ $109.5$ $C5-C6-C7$ $121.4 (2)$ $C4-C11-H11B$ $109.5$ $C5-C6-C7$ $121.4 (2)$ $C4-C11-H11C$ $109.5$ $C5-C6-H6$ $119.3$ $H11A-C11-H11C$ $109.5$ $C7-C6-H6$ $119.3$ $H11B-C11-H11C$ $109.5$ $C3-C2-C4-C5$ $-179.5 (2)$ $C4-C5-C6-C7$ $177.0 (2)$ $C3-C2-C4-C5$ $3.5 (3)$ $C5-C6-C7-R3$ $-176.7 (2)$ $C3-C2-C4-C11$ $10.0 (3)$ $C5-C6-C7-C8$ $0.6 (3)$ $C1-C2-C4-C5-C6$ $-136.5 (2)$ $C6-C7-C8-C9$ $13.(4)$	C7—N3—H3A		120.0	N3—	С7—С6	121	.2 (2)
H3A—N3—H3B120.0C9—C8—C7119.9 (2)N1—C1—C2176.8 (3)C9—C8—H8120.0C4—C2—C3122.9 (2)C7—C8—H8120.0C4—C2—C1123.8 (2)C10—C9—C8121.7 (2)C3—C2—C1113.2 (2)C10—C9—H9119.2N2—C3—C2178.2 (3)C8—C9—H9119.2C2—C4—C5122.2 (2)C9—C10—C5119.2 (2)C2—C4—C11119.0 (2)C9—C10—H10120.4C5—C4—C11119.4 (2)C4—C11—H11A109.5C6—C5—C4119.7 (2)C4—C11—H11B109.5C5—C6—C7121.4 (2)C4—C11—H11B109.5C5—C6—H6119.3H11A—C11—H11C109.5C7—C6—H6119.3H11B—C11—H11C109.5C3—C2—C4—C5-179.5 (2)C4—C5—C6—C7177.0 (2)C1—C2—C4—C53.5 (3)C5—C6—C7—R3-176.7 (2)C3—C2—C4—C51.0 (3)C5—C6—C7—R3-176.7 (2)C3—C2—C4—C111.0 (3)C5—C6—C7—C80.6 (3)C1—C2—C4—C53.5 (2)C6—C7—C8—C91.3 (4)	C7—N3—H3B		120.0	C8—0	С7—С6	118.	.4 (2)
N1C1C2176.8 (3)C9C8H8120.0C4C2C3122.9 (2)C7C8H8120.0C4C2C1123.8 (2)C10C9C8121.7 (2)C3C2C1113.2 (2)C10C9H9119.2N2C3C2178.2 (3)C8C9H9119.2C2C4C5122.2 (2)C9C10C5119.2 (2)C2C4C11119.0 (2)C9C10H10120.4C5C4C11119.4 (2)C4C11H11A109.5C6C5C4119.7 (2)C4C11H11B109.5C5C6C7121.4 (2)C4C11H11B109.5C5C6H6119.3H11AC11H11C109.5C7C6H6119.3H11BC11H11C109.5N3C7C8120.3 (2)C4C5C6C7177.0 (2)C3C2-C4C53.5 (3)C5C6C7N3-176.7 (2)C3C2-C4C53.5 (3)C5C6C7C80.6 (3)C1C2C4C111.0 (3)C5C6C7C8C9178.6 (2)C2C4C5C6-136.5 (2)C6C7C8C91.3 (4)	H3A—N3—H3B		120.0	С9—(	С8—С7	119.	.9 (2)
C4-C2-C3 $122.9 (2)$ $C7-C8-H8$ $120.0$ $C4-C2-C1$ $123.8 (2)$ $C10-C9-C8$ $121.7 (2)$ $C3-C2-C1$ $113.2 (2)$ $C10-C9-H9$ $119.2$ $N2-C3-C2$ $178.2 (3)$ $C8-C9-H9$ $119.2$ $C2-C4-C5$ $122.2 (2)$ $C9-C10-C5$ $119.2 (2)$ $C2-C4-C11$ $119.0 (2)$ $C9-C10-H10$ $120.4$ $C5-C4-C11$ $119.4 (2)$ $C4-C11-H11A$ $109.5$ $C6-C5-C10$ $119.4 (2)$ $C4-C11-H11B$ $109.5$ $C6-C5-C4$ $119.7 (2)$ $C4-C11-H11B$ $109.5$ $C5-C6-C7$ $121.4 (2)$ $C4-C11-H11B$ $109.5$ $C5-C6-H6$ $119.3$ $H11A-C11-H11C$ $109.5$ $C7-C6-H6$ $119.3$ $H11B-C11-H11C$ $109.5$ $C3-C2-C4-C5$ $-179.5 (2)$ $C4-C5-C6-C7$ $177.0 (2)$ $C3-C2-C4-C5$ $3.5 (3)$ $C5-C6-C7-N3$ $-176.7 (2)$ $C3-C2-C4-C5$ $3.5 (3)$ $C5-C6-C7-C8$ $0.6 (3)$ $C1-C2-C4-C11$ $1.0 (3)$ $C5-C6-C7-C8$ $0.6 (3)$ $C1-C2-C4-C11$ $-176.0 (2)$ $N3-C7-C8-C9$ $1.3 (4)$	N1—C1—C2		176.8 (3)	С9—(	С8—Н8	120	.0
C4—C2—C1123.8 (2)C10—C9—C8121.7 (2)C3—C2—C1113.2 (2)C10—C9—H9119.2N2—C3—C2178.2 (3)C8—C9—H9119.2C2—C4—C5122.2 (2)C9—C10—C5119.2 (2)C2—C4—C11119.0 (2)C9—C10—H10120.4C5—C4—C11118.8 (2)C5—C10—H10120.4C6—C5—C10119.4 (2)C4—C11—H11A109.5C6—C5—C4119.7 (2)C4—C11—H11B109.5C5—C6—C7121.4 (2)C4—C11—H11B109.5C5—C6—H6119.3H11A—C11—H11C109.5C7—C6—H6119.3H11B—C11—H11C109.5N3—C7—C8120.3 (2)C4—C5—C6—C7177.0 (2)C3—C2—C4—C5-179.5 (2)C4—C5—C6—C7177.0 (2)C3—C2—C4—C53.5 (3)C5—C6—C7176.7 (2)C3—C2—C4—C111.0 (3)C5—C6—C7—C80.6 (3)C1—C2—C4—C111.0 (2)N3—C7—C80.6 (3)C1—C2—C4—C11-176.0 (2)N3—C7—C8—C9178.6 (2)C2—C4—C5—C6-136.5 (2)C6—C7—C8—C91.3 (4)	C4—C2—C3		122.9 (2)	С7—(	С8—Н8	120	.0
C3-C2-C1113.2 (2)C10-C9-H9119.2N2-C3-C2178.2 (3)C8-C9-H9119.2C2-C4-C5122.2 (2)C9-C10-C5119.2 (2)C2-C4-C11119.0 (2)C9-C10-H10120.4C5-C4-C11118.8 (2)C5-C10-H10120.4C6-C5-C10119.4 (2)C4-C11-H11A109.5C6-C5-C4119.7 (2)C4-C11-H11B109.5C5-C6-C7121.4 (2)C4-C11-H11B109.5C5-C6-H6119.3H11A-C11-H11C109.5C7-C6-H6119.3H11B-C11-H11C109.5N3-C7-C8120.3 (2)C5-C6-C7177.0 (2)C3-C2-C4-C53.5 (3)C5-C6-C7-N3-176.7 (2)C3-C2-C4-C111.0 (3)C5-C6-C7-C80.6 (3)C1-C2-C4-C111.0 (2)N3-C7-C80.6 (3)C1-C2-C4-C111.0 (2)N3-C7-C8-C9178.6 (2)C2-C4-C5-C6-136.5 (2)C6-C7-C8-C91.3 (4)	C4—C2—C1		123.8 (2)	C10-	-C9C8	121	.7 (2)
N2-C3-C2178.2 (3) $C8-C9-H9$ 119.2C2-C4-C5122.2 (2) $C9-C10-C5$ 119.2 (2)C2-C4-C11119.0 (2) $C9-C10-H10$ 120.4C5-C4-C11118.8 (2) $C5-C10-H10$ 120.4C6-C5-C10119.4 (2) $C4-C11-H11A$ 109.5C6-C5-C4119.7 (2) $C4-C11-H11B$ 109.5C10-C5-C4120.9 (2)H11A-C11-H11B109.5C5-C6-C7121.4 (2) $C4-C11-H11C$ 109.5C7-C6-H6119.3H11A-C11-H11C109.5N3-C7-C8120.3 (2) $C5-C6-C7$ 177.0 (2)C1-C2-C4-C5-179.5 (2) $C4-C5-C6-C7$ 177.0 (2)C1-C2-C4-C53.5 (3) $C5-C6-C7-C8$ 0.6 (3)C1-C2-C4-C111.0 (3) $C5-C6-C7-C8-C9$ 178.6 (2)C2-C4-C5-C6-136.5 (2) $C6-C7-C8-C9$ 1.3 (4)	C3—C2—C1		113.2 (2)	C10-	-С9—Н9	119	.2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N2-C3-C2		178.2 (3)	C8—4	С9—Н9	119.	.2
C2—C4—C11119.0 (2)C9—C10—H10120.4C5—C4—C11118.8 (2)C5—C10—H10120.4C6—C5—C10119.4 (2)C4—C11—H11A109.5C6—C5—C4119.7 (2)C4—C11—H11B109.5C10—C5—C4120.9 (2)H11A—C11—H11B109.5C5—C6—C7121.4 (2)C4—C11—H11C109.5C5—C6—H6119.3H11A—C11—H11C109.5C7—C6—H6119.3H11B—C11—H11C109.5N3—C7—C8120.3 (2)C4—C5—C6—C7177.0 (2)C1—C2—C4—C53.5 (3)C5—C6—C7—N3-176.7 (2)C3—C2—C4—C111.0 (3)C5—C6—C7—C80.6 (3)C1—C2—C4—C11-176.0 (2)N3—C7—C8—C9178.6 (2)C2—C4—C5—C6-136.5 (2)C6—C7—C8—C91.3 (4)	C2—C4—C5		122.2 (2)	С9—(	С10—С5	119.	.2 (2)
C5—C4—C11118.8 (2)C5—C10—H10120.4C6—C5—C10119.4 (2)C4—C11—H11A109.5C6—C5—C4119.7 (2)C4—C11—H11B109.5C10—C5—C4120.9 (2)H11A—C11—H11B109.5C5—C6—C7121.4 (2)C4—C11—H11C109.5C5—C6—H6119.3H11A—C11—H11C109.5C7—C6—H6119.3H11B—C11—H11C109.5N3—C7—C8120.3 (2)C4—C5—C6—C7177.0 (2)C1—C2—C4—C53.5 (3)C5—C6—C7—N3-176.7 (2)C3—C2—C4—C111.0 (3)C5—C6—C7—C80.6 (3)C1—C2—C4—C11-176.0 (2)N3—C7—C8—C9178.6 (2)C2—C4—C5—C6-136.5 (2)C6—C7—C8—C91.3 (4)	C2—C4—C11		119.0 (2)	С9—(	С10—Н10	120	.4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C5-C4-C11		118.8 (2)	C5—(	С10—Н10	120	.4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C6—C5—C10		119.4 (2)	C4—0	C11—H11A	109	.5
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C6—C5—C4		119.7 (2)	C4—0	C11—H11B	109	.5
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C10—C5—C4		120.9 (2)	H11A	—С11—Н11В	109	.5
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С5—С6—С7		121.4 (2)	C4—0	С11—Н11С	109	.5
C7—C6—H6       119.3       H11B—C11—H11C       109.5         N3—C7—C8       120.3 (2)       C3—C2—C4—C5       -179.5 (2)       C4—C5—C6—C7       177.0 (2)         C1—C2—C4—C5       3.5 (3)       C5—C6—C7—N3       -176.7 (2)         C3—C2—C4—C11       1.0 (3)       C5—C6—C7—C8       0.6 (3)         C1—C2—C4—C11       -176.0 (2)       N3—C7—C8—C9       178.6 (2)         C2—C4—C5—C6       -136.5 (2)       C6—C7—C8—C9       1.3 (4)	С5—С6—Н6		119.3	H11A	—С11—Н11С	109	.5
N3—C7—C8 $120.3 (2)$ C3—C2—C4—C5 $-179.5 (2)$ C4—C5—C6—C7 $177.0 (2)$ C1—C2—C4—C5 $3.5 (3)$ C5—C6—C7—N3 $-176.7 (2)$ C3—C2—C4—C11 $1.0 (3)$ C5—C6—C7—C8 $0.6 (3)$ C1—C2—C4—C11 $-176.0 (2)$ N3—C7—C8—C9 $178.6 (2)$ C2—C4—C5—C6 $-136.5 (2)$ C6—C7—C8—C9 $1.3 (4)$	С7—С6—Н6		119.3	H11B	—С11—Н11С	109	.5
C3-C2-C4-C5 $-179.5$ (2)C4-C5-C6-C7 $177.0$ (2)C1-C2-C4-C5 $3.5$ (3)C5-C6-C7-N3 $-176.7$ (2)C3-C2-C4-C11 $1.0$ (3)C5-C6-C7-C8 $0.6$ (3)C1-C2-C4-C11 $-176.0$ (2) $N3-C7-C8-C9$ $178.6$ (2)C2-C4-C5-C6 $-136.5$ (2)C6-C7-C8-C9 $1.3$ (4)	N3—C7—C8		120.3 (2)				
C1-C2-C4-C5 $3.5 (3)$ $C5-C6-C7-N3$ $-176.7 (2)$ $C3-C2-C4-C11$ $1.0 (3)$ $C5-C6-C7-C8$ $0.6 (3)$ $C1-C2-C4-C11$ $-176.0 (2)$ $N3-C7-C8-C9$ $178.6 (2)$ $C2-C4-C5-C6$ $-136.5 (2)$ $C6-C7-C8-C9$ $1.3 (4)$	C3—C2—C4—C5	5	-179.5 (2)	C4—4	С5—С6—С7	177	.0 (2)
C3-C2-C4-C11       1.0 (3)       C5-C6-C7-C8       0.6 (3)         C1-C2-C4-C11       -176.0 (2)       N3-C7-C8-C9       178.6 (2)         C2-C4-C5-C6       -136.5 (2)       C6-C7-C8-C9       1.3 (4)	C1—C2—C4—C5	5	3.5 (3)	C5—4	C6—C7—N3	-17	6.7 (2)
C1C2C4C11-176.0 (2)N3C7C8C9178.6 (2)C2C4C5C6-136.5 (2)C6C7C8C91.3 (4)	C3—C2—C4—C1	1	1.0 (3)	C5—0	С6—С7—С8	0.6	(3)
C2-C4-C5-C6 -136.5 (2) C6-C7-C8-C9 1.3 (4)	C1—C2—C4—C1	1	-176.0 (2)	N3—	С7—С8—С9	178	.6 (2)
	C2-C4-C5-C6						
C11—C4—C5—C6 43.0 (3) C7—C8—C9—C10 $-1.9$ (4)	e2 e1 e5 et	5	-136.5 (2)	C6—4	С7—С8—С9	1.3	(4)
	C11—C4—C5—C	6 26	-136.5 (2) 43.0 (3)	C6—( C7—(	C7—C8—C9 C8—C9—C10	1.3 -1.9	(4) 9 (4)

# supplementary materials

C11—C4—C5—C10	-138.2 (2)	C6—C5—C10—C9		1.3 (3)			
C10—C5—C6—C7	-1.9 (3)	C4—C5—C10—C9		-177.5 (2)			
Hydrogen-bond geometry (Å, °)							
D—H···A	<i>D</i> —Н	H···A	$D \cdots A$	D—H··· $A$			
N3—H3A…N1 <sup>i</sup>	0.86	2.35	3.209 (3)	173			
N3—H3B···N2 <sup>ii</sup>	0.86	2.33	3.182 (3)	170			
Symmetry codes: (i) $-x+1/2$ , $y-1/2$ , $-z+3/2$ ; (ii) $-x+1/2$ , $y-1/2$ , $-z+1/2$ .							





