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## 2,5-Diphenylpenta-2,4-dienenitrile

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Key indicators: single-crystal X-ray study; T = 110 K; mean  $\sigma$ (C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.121; data-to-parameter ratio = 14.8.

In the title compound, C<sub>17</sub>H<sub>13</sub>N, the dihedral angle between the two phenyl rings is 17.6 (1)°. An intermolecular  $C-H\cdots N$ hydrogen bond is found in the crystal structure, also a C- $H \cdots \pi$  interaction involving the phenyl ring at position 5.

### **Related literature**

For the prebiotic synthesis of biological molecules, see: Guillemin et al. (1998). For the preparation of flavonoid pigments, see: Fringuelli et al. (1994). For sexual pheromones, see: Liu et al. (1981). For the manufacture of light-emitting diodes (LEDs) with air-stable electrodes, see: Maruyama et al. (1998); Segura et al. (1999); Gómez et al. (1999).



## **Experimental**

Crystal data

C17H13N  $M_r = 231.28$ Monoclinic, C2/c a = 16.9390(5) Å b = 7.5869 (2) Å c = 19.3809 (6) Å  $\beta = 99.521 \ (3)^{\circ}$ 

 $V = 2456.42 (13) \text{ Å}^3$ Z = 8Cu Ka radiation  $\mu = 0.56 \text{ mm}^{-1}$ T = 110 K $0.53 \times 0.36 \times 0.29 \ \text{mm}$  4517 measured reflections

 $R_{\rm int} = 0.014$ 

2420 independent reflections 2322 reflections with  $I > 2\sigma(I)$ 

#### Data collection

Oxford Diffraction Xcalibur Ruby
Gemini diffractometer
Absorption correction: multi-scan
(CrysAlis Pro; Oxford
Diffraction, 2009)
$T_{\min} = 0.713, T_{\max} = 1.000$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$	163 parameters
$wR(F^2) = 0.121$	H-atom parameters constrained
S = 1.02	$\Delta \rho_{\rm max} = 0.34 \text{ e } \text{\AA}^{-3}$
2420 reflections	$\Delta \rho_{\rm min} = -0.22 \text{ e } \text{\AA}^{-3}$

### Table 1

Hydrogen-bond geometry (Å, °).

$D - H \cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdots A$
C54 $-$ H54 $\cdots$ N13 <sup>i</sup>	0.95	2.61	3.388 (2)	139
C56 $-$ H56 $\cdots$ Cg1 <sup>ii</sup>	0.95	2.83	3.657 (1)	146

Symmetry codes: (i)  $-x + \frac{1}{2}$ ,  $y - \frac{1}{2}$ ,  $-z + \frac{1}{2}$ ; (ii)  $-x + \frac{1}{2}$ ,  $y + \frac{1}{2}$ ,  $-z + \frac{1}{2}$ . Cg1 is the centroid of the C51-C56 phenyl ring

Data collection: CrysAlis Pro (Oxford Diffraction, 2009); cell refinement: CrysAlis Pro; data reduction: CrysAlis Pro; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: PLATON (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2360).

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## 2,5-Diphenylpenta-2,4-dienenitrile

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## S1. Comment

Unsaturated nitriles play a key role in many of the pathways proposed for the prebiotic synthesis of biological molecules (Guillemin *et al.*, 1998). Arylacrylonitriles are important synthons for the synthesis of several biologically active molecules in the preparation of flavonoid pigments (Fringuelli *et al.*, 1994) and sexual pheromones(Liu *et al.*, 1981). Recently arylacrylonitriles have been used to obtain high electron affinity polymers which can be used to manufacture light-emitting diodes (LEDs) with air-stable electrodes (Maruyama *et al.*, 1998; Segura *et al.*, 1999; Gómez *et al.*, 1999).

As part of our research, we have synthesized the title compound and report its crystal structure here. In the molecule, the dihedral angle between the two phenyl rings is 17.6 (1)°. The angle N13—C12—C2 is 178.90 (13)°, indicating that atom C12 is *sp* hybridized. Atoms C2,C3,C4 and C5 are essentially coplanar. An intermolecular C54—H54···N13(1/2 - *x*, -1/2 + y, 1/2 - z) hydrogen bond is found in the crystal structure. In addition, a C56—H56··· $\pi(1/2 - x, 1/2 + y, 1/2 - z)$  interaction involving the phenyl ring (C51—C56) at position 5 is also found.

## **S2. Experimental**

To a mixture of benzyl cyanide (1.12 ml, 0.01 mol) and potassium hydroxide (0.66 g, 0.01 mol) in 50 ml ethanol, *trans*cinnamaldehyde (1.3 ml, 0.01 mol) was added and the solution was stirred for five minutes at room temperature. The solid obtained was separated, dried and then recrystallized from absolute ethanol. The yield of isolated product was 1.81 g (82%).

## S3. Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95 Å;  $U_{iso}(H) = 1.2U_{eq}(C)$ .



Figure 1

The molecular structure of the title compound, showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius.



Figure 2

The packing of the title compound, viewed down the *b* axis. Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

## 2,5-Diphenylpenta-2,4-dienenitrile

## Crystal data

 $C_{17}H_{13}N$   $M_r = 231.28$ Monoclinic, C2/c Hall symbol: -C 2yc a = 16.9390 (5) Å b = 7.5869 (2) Å c = 19.3809 (6) Å  $\beta = 99.521$  (3)° V = 2456.42 (13) Å<sup>3</sup> Z = 8

## Data collection

Oxford Diffraction Xcalibur Ruby Gemini	4517 measured reflections
diffractometer	2420 independent reflections
Radiation source: Enhance (Cu) X-ray Source	2322 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{\rm int} = 0.014$
Detector resolution: 10.5081 pixels mm <sup>-1</sup>	$\theta_{\rm max} = 74.1^{\circ}, \ \theta_{\rm min} = 4.6^{\circ}$
$\omega$ scans	$h = -20 \rightarrow 15$
Absorption correction: multi-scan	$k = -8 \rightarrow 9$
(CrysAlis PRO; Oxford Diffraction, 2009)	<i>l</i> = −23→23
$T_{\min} = 0.713, \ T_{\max} = 1.000$	
Refinement	
<b>n</b> <i>a</i>	~

Refinement on $F^2$	Secondary atom site location: difference Fourier
Least-squares matrix: full	map
$R[F^2 > 2\sigma(F^2)] = 0.044$	Hydrogen site location: inferred from
$wR(F^2) = 0.121$	neighbouring sites
S = 1.02	H-atom parameters constrained
2420 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0729P)^2 + 1.834P]$
163 parameters	where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	$(\Delta/\sigma)_{\rm max} = 0.001$
Primary atom site location: structure-invariant	$\Delta \rho_{\rm max} = 0.34 \text{ e} \text{ Å}^{-3}$
direct methods	$\Delta \rho_{\rm min} = -0.22 \text{ e } \text{\AA}^{-3}$

F(000) = 976

 $\theta = 4.6 - 74.1^{\circ}$ 

 $\mu = 0.56 \text{ mm}^{-1}$ 

Prism, colourless

 $0.53 \times 0.36 \times 0.29 \text{ mm}$ 

T = 110 K

 $D_{\rm x} = 1.251 {\rm ~Mg} {\rm ~m}^{-3}$ Melting point: 440 K

Cu *K* $\alpha$  radiation,  $\lambda = 1.54178$  Å

Cell parameters from 4071 reflections

## Special details

**Geometry**. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**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  $F^2 > 2\sigma(F^2)$  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  $(Å^2)$ 

	x	У	Ζ	$U_{ m iso}$ */ $U_{ m eq}$	
N13	0.26391 (6)	0.47605 (14)	-0.01895 (5)	0.0260 (3)	
C2	0.40160 (7)	0.32134 (15)	0.01356 (6)	0.0195 (3)	
C3	0.42079 (7)	0.25057 (15)	0.07831 (6)	0.0211 (3)	
C4	0.37331 (7)	0.25955 (15)	0.13347 (6)	0.0209 (3)	

C5	0.39654 (7)	0.17874 (15)	0.19524 (6)	0.0214 (3)
C12	0.32517 (7)	0.40883 (15)	-0.00422 (6)	0.0204 (3)
C21	0.45270 (7)	0.31560 (14)	-0.04165 (6)	0.0189 (3)
C22	0.42867 (7)	0.40207 (16)	-0.10539 (6)	0.0224 (3)
C23	0.47643 (7)	0.39861 (16)	-0.15733 (6)	0.0250 (3)
C24	0.54848 (7)	0.30767 (16)	-0.14678 (6)	0.0245 (3)
C25	0.57313 (7)	0.22103 (16)	-0.08366 (6)	0.0242 (3)
C26	0.52583 (7)	0.22532 (16)	-0.03154 (6)	0.0224 (3)
C51	0.35609 (6)	0.18244 (15)	0.25646 (6)	0.0194 (3)
C52	0.37767 (7)	0.05962 (15)	0.31035 (6)	0.0212 (3)
C53	0.34045 (7)	0.05941 (15)	0.36908 (6)	0.0222 (3)
C54	0.28173 (7)	0.18303 (16)	0.37571 (6)	0.0230 (3)
C55	0.25983 (7)	0.30566 (16)	0.32272 (6)	0.0240 (3)
C56	0.29636 (7)	0.30601 (16)	0.26368 (6)	0.0219 (3)
Н3	0.47024	0.18917	0.08834	0.0254*
H4	0.32454	0.32395	0.12601	0.0250*
Н5	0.44452	0.11182	0.19968	0.0257*
H22	0.37921	0.46385	-0.11333	0.0269*
H23	0.45960	0.45882	-0.20022	0.0300*
H24	0.58077	0.30461	-0.18245	0.0294*
H25	0.62245	0.15873	-0.07614	0.0291*
H26	0.54331	0.16626	0.01150	0.0269*
H52	0.41827	-0.02457	0.30665	0.0254*
H53	0.35524	-0.02567	0.40485	0.0266*
H54	0.25673	0.18379	0.41613	0.0276*
Н55	0.21948	0.39005	0.32695	0.0288*
H56	0.28080	0.39060	0.22787	0.0263*

Atomic displacement parameters  $(Å^2)$ 

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N13	0.0243 (5)	0.0299 (6)	0.0246 (5)	0.0032 (4)	0.0064 (4)	0.0016 (4)
C2	0.0198 (5)	0.0191 (6)	0.0198 (5)	-0.0021 (4)	0.0038 (4)	-0.0030 (4)
C3	0.0205 (6)	0.0216 (6)	0.0214 (6)	-0.0006 (4)	0.0037 (4)	-0.0013 (4)
C4	0.0199 (5)	0.0219 (6)	0.0209 (6)	-0.0005 (4)	0.0037 (4)	-0.0009 (4)
C5	0.0194 (5)	0.0229 (6)	0.0220 (6)	0.0003 (4)	0.0034 (4)	-0.0009 (4)
C12	0.0243 (6)	0.0216 (6)	0.0161 (5)	-0.0030 (4)	0.0060 (4)	-0.0010 (4)
C21	0.0206 (5)	0.0175 (5)	0.0188 (5)	-0.0036 (4)	0.0035 (4)	-0.0034 (4)
C22	0.0221 (5)	0.0240 (6)	0.0210 (6)	0.0010 (4)	0.0034 (4)	-0.0015 (4)
C23	0.0291 (6)	0.0274 (6)	0.0187 (5)	-0.0008(5)	0.0045 (4)	0.0001 (4)
C24	0.0267 (6)	0.0264 (6)	0.0228 (6)	-0.0032 (5)	0.0109 (5)	-0.0040 (4)
C25	0.0214 (6)	0.0243 (6)	0.0279 (6)	0.0004 (4)	0.0070 (5)	-0.0019 (5)
C26	0.0235 (6)	0.0230 (6)	0.0208 (6)	-0.0001 (4)	0.0036 (4)	0.0013 (4)
C51	0.0181 (5)	0.0215 (6)	0.0179 (5)	-0.0029 (4)	0.0010 (4)	-0.0009 (4)
C52	0.0188 (5)	0.0209 (5)	0.0228 (6)	0.0009 (4)	0.0002 (4)	0.0002 (4)
C53	0.0245 (6)	0.0219 (6)	0.0188 (5)	-0.0025 (4)	-0.0002 (4)	0.0037 (4)
C54	0.0250 (6)	0.0258 (6)	0.0190 (5)	-0.0039 (4)	0.0059 (4)	-0.0008 (4)
C55	0.0239 (6)	0.0248 (6)	0.0240 (6)	0.0036 (5)	0.0062 (4)	0.0005 (4)

Geometric parameters (Å. ?)           N13C12         1.1491 (16)         C53C54         1.3885 (17)           C2-C3         1.3542 (16)         C54C55         1.3899 (17)           C2-C12         1.4450 (17)         C55C56         1.3899 (16)           C3C4         1.4411 (17)         C4-H4         0.9500           C4-C5         1.3447 (16)         C5-H5         0.9500           C2-C21         1.3985 (16)         C22-H22         0.9500           C2-C21         1.3985 (16)         C22-H22         0.9500           C21-C26         1.4006 (17)         C24-H24         0.9500           C22-C23         1.3921 (17)         C26-H26         0.9500           C24-C25         1.3097 (16)         C32-H52         0.9500           C25-C26         1.3897 (17)         C3-H53         0.9500           C51-C56         1.4032 (16)         C56-H56         0.9500	C56	0.0229 (6)	0.0233 (6)	0.0192 (5)	0.0020 (4)	0.0023 (4)	0.0039 (4)
N13-C12         1.1491 (16)         C33-C54         1.3885 (17)           C2-C3         1.3542 (16)         C34-C55         1.3899 (17)           C2-C12         1.4450 (17)         C3-H3         0.9500           C3-C4         1.4418 (17)         C3-H3         0.9500           C3-C4         1.4418 (17)         C4-H4         0.9500           C4-C5         1.3447 (16)         C2-H12         0.9500           C2-C21         1.3985 (16)         C23-H23         0.9500           C21-C26         1.4063 (16)         C24-H24         0.9500           C21-C26         1.3091 (17)         C24-H24         0.9500           C22-C23         1.3901 (16)         C52-H52         0.9500           C23-C24         1.3874 (17)         C3-H53         0.9500           C25-C26         1.3897 (17)         C3-H53         0.9500           C51-C56         1.4032 (16)         C56-H55         0.9500           C51-C54         1.4033 (16)         C56-H56         0.9500           C3-C44         3.3396 (16)         H3-C26         2.6600           N13-C54 <sup>41</sup> 3.3383 (15)         H3-H26         2.1000           N13-C54 <sup>41</sup> 3.3383 (15)         H3-H56	Geomet	ric parameters (Å	, °)				
$C2-C3$ $1.3542$ (16) $C34-C55$ $1.3899$ (17) $C2-C12$ $1.4450$ (17) $C3-C56$ $1.3880$ (16) $C2-C21$ $1.4451$ (17) $C3-H3$ $0.9500$ $C3-C4$ $1.4418$ (17) $C4-H4$ $0.9500$ $C4-C5$ $1.3447$ (16) $C2-H122$ $0.9500$ $C21-C22$ $1.3985$ (16) $C23-H23$ $0.9500$ $C22-C23$ $1.3921$ (17) $C24-H24$ $0.9500$ $C22-C23$ $1.3927$ (17) $C25-H25$ $0.9500$ $C22-C26$ $1.3897$ (17) $C25-H152$ $0.9500$ $C23-C26$ $1.3897$ (17) $C3-H153$ $0.9500$ $C25-C53$ $1.3907$ (16) $C54-H154$ $0.9500$ $C51-C56$ $1.4023$ (16) $C54-H154$ $0.9500$ $C52-C53$ $1.3894$ (16) $C56-H122^{*4}$ $3.1000$ $N13-C54^{*4}$ $3.3386$ (16) $H3-C26$ $2.6600$ $N13-C54^{*4}$ $3.3383$ (15) $H3-H26$ $2.1000$ $N13-H54^{*5}$ $2.8000$ $H4-H56$ $2.2800$ $N13-H54^{*4}$ $2.6100$	N13—C	212	1.1491	(16)	C53—C54		1.3885 (17)
$C2-C12$ 1.4450 (17) $C3-C56$ 1.3880 (16) $C2-C21$ 1.4841 (17) $C3-H3$ 0.9500 $C3-C4$ 1.4418 (17) $C4-H4$ 0.9500 $C4-C5$ 1.3447 (16) $C5-H5$ 0.9500 $C2-C22$ 1.3985 (16) $C22-H22$ 0.9500 $C21-C22$ 1.3985 (16) $C23-H25$ 0.9500 $C22-C23$ 1.3921 (17) $C24-H24$ 0.9500 $C23-C24$ 1.3874 (17) $C26-H26$ 0.9500 $C23-C24$ 1.3897 (16) $C52-H52$ 0.9500 $C25-C26$ 1.3897 (17) $C3-H53$ 0.9500 $C51-C52$ 1.4032 (16) $C56-H56$ 0.9500 $C51-C56$ 1.4032 (16) $C56-H56$ 0.9500 $C52-C53$ 1.3894 (16) $C56-H56$ 0.9500 $C3-C4^4$ 3.3450 (16)       H3-C26       2.1000 $N13-C4^4$ 3.4376 (15)       H3-H5       2.3500 $N13-C54^{su}$ 3.3883 (15)       H3-H26       2.1000 $N13-H54^{su}$ 2.6100       H4-C12       2.6100 $N13-H54^{su}$	C2—C3	;	1.3542	(16)	C54—C55		1.3899 (17)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C2-C1	2	1.4450	(17)	C55—C56		1.3880 (16)
C3-C4       1.4418 (17)       C4-H4       0.9500         C4-C5       1.3447 (16)       C3-H5       0.9500         C21-C2       1.3985 (16)       C22-H22       0.9500         C21-C22       1.3985 (16)       C23-H23       0.9500         C21-C23       1.3921 (17)       C25-H25       0.9500         C22-C23       1.3921 (17)       C25-H25       0.9500         C23-C24       1.3874 (17)       C26-H26       0.9500         C24-C25       1.3907 (16)       C52-H52       0.9500         C51-C52       1.4032 (16)       C54-H54       0.9500         C51-C56       1.4032 (16)       C56-H56       0.9500         C51-C56       1.4032 (16)       C56-H56       0.9500         C52-C53       1.3894 (16)       C56       1.300         N13-C12'       3.3510 (16)       C56-H56       0.9500         N13-C44'       3.4376 (15)       H3-H15       2.3500         N13-C54 <sup>ii</sup> 3.3883 (15)       H3-H26       2.1000         N13-H24'       2.8600       H4-C12       2.6100         N13-H54 <sup>ii</sup> 2.6100       H4-C156       2.7900         N13-H54 <sup>ii</sup> 2.6100       H4-H55       2.4200	C2—C2	21	1.4841	(17)	С3—Н3		0.9500
C4-C5         1.3447 (16)         C5-H5         0.9500           C5-C51         1.4653 (16)         C22-H22         0.9500           C21-C22         1.3985 (16)         C22-H23         0.9500           C21-C26         1.4006 (17)         C24-H24         0.9500           C22-C23         1.3921 (17)         C25-H25         0.9500           C24-C25         1.3907 (16)         C52-H52         0.9500           C24-C25         1.3897 (17)         C53-H53         0.9500           C51-C52         1.4023 (16)         C54-H54         0.9500           C51-C56         1.4032 (16)         C56-H56         0.9500           C52-C53         1.3894 (16)         C56-H56         0.9500           N13C12'         3.510 (16)         C56-H26         2.6600           N13C4'         3.4376 (15)         H3H5         2.3500           N13C54''         3.3883 (15)         H3H26         2.1000           N13H54''         2.8600         H4-·H56         2.2800           N13H54''         2.8900         H5-·H13         2.3500           N13H54''         2.8900         H5-·H13         2.3500           C3C25''         3.5805 (17)         H5-·H52	C3—C4	ŀ	1.4418	(17)	C4—H4		0.9500
C5-C51       1.4653 (16)       C22-H22       0.9500         C21-C22       1.3985 (16)       C23-H23       0.9500         C21-C26       1.4006 (17)       C24-H24       0.9500         C22-C23       1.3921 (17)       C25-H25       0.9500         C23-C24       1.3874 (17)       C26-H26       0.9500         C24-C25       1.3897 (17)       C3-H52       0.9500         C51-C52       1.4023 (16)       C54-H52       0.9500         C51-C56       1.4032 (16)       C56-H55       0.9500         C51-C56       1.4032 (16)       C56-H56       0.9500         C52-C53       3.3510 (16)       C56-H22"       3.1000         N13-··C54"       3.3396 (16)       H3-··C26       2.6600         N13-··C54"       3.3883 (15)       H3-··H5       2.3500         N13-··C54"       3.3883 (15)       H3-··H26       2.1000         N13-··C54"       3.3883 (15)       H3-··H26       2.1000         N13-··C54"       3.3883 (15)       H3-··H26       2.2800         N13-··H25"       2.8900       H5-··H3       2.3500         C3-··C25'       3.5805 (17)       H5-··H52       2.4200         C3-··C25'       3.5805 (17)       H5-··	C4—C5	5	1.3447	(16)	С5—Н5		0.9500
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C5—C5	51	1.4653	(16)	C22—H22		0.9500
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C21—C	22	1.3985	(16)	С23—Н23		0.9500
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C21—C	26	1.4006	(17)	C24—H24		0.9500
C23C24 $1.3874(17)$ C26H26 $0.9500$ C24C25 $1.3907(16)$ C52H52 $0.9500$ C25C26 $1.3897(17)$ C53H53 $0.9500$ C51C52 $1.4032(16)$ C54H54 $0.9500$ C51C56 $1.4032(16)$ C56H55 $0.9500$ C52C53 $1.3894(16)$ C56H56 $0.9500$ N13C12 <sup>i</sup> $3.3510(16)$ C56H56 $0.9500$ N13C24 <sup>ii</sup> $3.3396(16)$ H3C26 $2.6600$ N13C54 <sup>iii</sup> $3.383(15)$ H3H5 $2.500$ N13C54 <sup>iii</sup> $3.3883(15)$ H3H26 $2.1000$ N13C54 <sup>iii</sup> $2.8000$ H4C12 $2.6100$ N13H54 <sup>iii</sup> $2.8000$ H4H56 $2.2800$ N13H25 <sup>iii</sup> $2.8300$ H4H56 $2.2800$ N13H25 <sup>iii</sup> $2.8300$ H5H13 $2.3500$ C3C25 <sup>ii</sup> $3.5805(17)$ H5H52 $2.4200$ C3C25 <sup>ii</sup> $3.5805(17)$ H5H52 $2.4700$ C4C24 <sup>ii</sup> $3.5311(17)$ H5H52 <sup>ii</sup> $2.8900$ C4N13 <sup>ii</sup> $3.4376(15)$ H5H52 <sup>ii</sup> $2.8900$ C12N13 <sup>ii</sup> $3.510(16)$ H22N13 $2.8900$ C12C12 <sup>ii</sup> $3.5755(17)$ H22C12 <sup>ii</sup> $2.5500$ C23C3 <sup>ii</sup> $3.4028(17)$ H23H24 <sup>ii</sup> $2.5500$ C23C3 <sup>ii</sup> $3.5805(17)$ H22C12 <sup>ii</sup> $3.5755(17)$ C12N13 <sup>ii</sup> $2.8900$ C1C25 <sup>ii</sup> $3.1000$ C23C25 <sup>ii</sup> $3.5805(17)$ H22C12 <sup>ii</sup> $2.5500$ C23C25 <sup>ii</sup> <	С22—С	23	1.3921	(17)	C25—H25		0.9500
$C24-C25$ $1.3907(16)$ $C52-H52$ $0.9500$ $C25-C26$ $1.3897(17)$ $C53-H53$ $0.9500$ $C51-C52$ $1.4023(16)$ $C54-H54$ $0.9500$ $C52-C53$ $1.4023(16)$ $C55-H55$ $0.9500$ $C52-C53$ $1.3894(16)$ $C56-H56$ $0.9500$ $N13-C54^{ii}$ $3.3510(16)$ $C56-H22^{vii}$ $3.1000$ $N13-C54^{ii}$ $3.3396(16)$ $H3-C26$ $2.6000$ $N13-C54^{iii}$ $3.383(15)$ $H3-H26$ $2.1000$ $N13-K54^{iii}$ $2.8000$ $H4-C12$ $2.6100$ $N13-H54^{iii}$ $2.6100$ $H4-C56$ $2.7900$ $N13-H54^{iii}$ $2.8000$ $H4-H56$ $2.2800$ $N13-H54^{iii}$ $2.6100$ $H4-K56$ $2.2800$ $N13-H54^{iii}$ $2.6100$ $H4-H56$ $2.2800$ $N13-H22$ $2.8900$ $H5-H33$ $2.3500$ $C3-C25^{vi}$ $3.5805(17)$ $H5-H52$ $2.4200$ $C3-C23^{vi}$ $3.4028(17)$ $H5-H52^{vi}$ $2.4700$ $C4-N13^{13}$ $3.4376(15)$ $H5-H52^{vi}$ $2.8900$ $C12-C23^{vi}$ $3.5296(17)$ $H22-C51^{ii}$ $2.8900$ $C12-C25^{vi}$ $3.5296(17)$ $H22-C56^{ii}$ $3.1000$ $C23-C3^{vi}$ $3.4028(17)$ $H22-C56^{ii}$ $3.1000$ $C23-C3^{vi}$ $3.5296(17)$ $H22-C56^{ii}$ $3.1000$ $C23-C3^{vi}$ $3.5805(17)$ $H22-C56^{ii}$ $2.8000$ $C12-C12^{i}$ $3.5296(17)$ $H22-C56^{ii}$ $2.8000$ $C2-C25^{vi}$ $3.5$	С23—С	24	1.3874	(17)	C26—H26		0.9500
C25-C261.3897 (17)C33-H530.9500C51-C521.4023 (16)C54-H540.9500C51-C561.4032 (16)C55-H550.9500C52-C531.3894 (16)C56-H560.9500N13-C12 <sup>1</sup> 3.3510 (16)C56-H22 <sup>vii</sup> 3.1000N13-C54 <sup>iii</sup> 3.3396 (16)H3-··C262.6600N13-C54 <sup>iii</sup> 3.3883 (15)H3-··H52.3500N13-C54 <sup>iii</sup> 3.3883 (15)H3-··H262.1000N13-··C54 <sup>iii</sup> 3.3883 (15)H3-··H262.2800N13-··H54 <sup>ii</sup> 2.6100H4-··C562.7900N13-··H54 <sup>iii</sup> 2.8300H4-··H562.2800N13-··H222.8900H5-··H32.3500C3-··C25 <sup>v</sup> 3.5805 (17)H5-··H5 <sup>x</sup> 2.4700C4-··N13 <sup>1</sup> 3.4376 (15)H5-··H5 <sup>x</sup> 2.4700C4-··C24 <sup>vii</sup> 3.5341 (17)H5-··H5 <sup>x</sup> 2.5700C12-··N13 <sup>1</sup> 3.5755 (17)H22-··C55 <sup>ii</sup> 2.8000C12-··C12 <sup>1</sup> 3.5296 (17)H22-··C56 <sup>ii</sup> 3.1000C23-··C23 <sup>vii</sup> 3.5755 (17)H22-··C56 <sup>ii</sup> 3.1000C23-··C2 <sup>3vii</sup> 3.5341 (17)H23-··H23 <sup>xii</sup> 2.5500C24-··C24 <sup>vii</sup> 3.5341 (17)H23-··H24 <sup>xiii</sup> 2.5500C25-··C12 <sup>ii</sup> 3.5755 (17)H22-··C56 <sup>iii</sup> 3.1000C25-··C12 <sup>ii</sup> 3.5805 (17)H23-··H24 <sup>xiii</sup> 2.5500C25-··C2 <sup>svii</sup> 3.5755 (17)H23-··H24 <sup>xiii</sup> 2.5500C25-··C12 <sup>iii</sup> 3.5805 (17)H25-··H3 <sup>xiii</sup> 2.8300C54-·N13 <sup>xiii</sup> 3.38	C24—C	25	1.3907	(16)	С52—Н52		0.9500
C51-C521.4023 (16)C54-H540.9500C51-C561.4032 (16)C55-H550.9500C52-C531.3894 (16)C56-H560.9500N13···C12i3.3510 (16)C56···H22 <sup>vii</sup> 3.1000N13···C54ii3.3396 (16)H3···C262.6600N13···C54iii3.3883 (15)H3···H52.3500N13···C54iii3.3883 (15)H3···H262.1000N13···C54iii3.883 (15)H3···H262.1000N13···C54iii2.6100H4···C122.6100N13···H54ii2.6000H4···C122.6100N13···H54ii2.8000H4···H562.2800N13···H222.8900H5···H32.3500C3···C25v3.5805 (17)H5···H522.4200C3···C25v3.5805 (17)H5···H5*2.4700C4-··N13i3.4376 (15)H5···H5*2.4700C12···N13i3.510 (16)H22···N132.8900C12···C12i3.5755 (17)H22···C12i2.4700C12···C12i3.5296 (17)H22···C55 <sup>ii</sup> 2.8000C24···C4vi3.5341 (17)H23···H23 <sup>vi</sup> 2.5500C23···C23vi3.5805 (17)H22···C25 <sup>ii</sup> 3.5500C24···C12i3.5755 (17)H24···H23 <sup>vi</sup> 2.5500C24···C2vi3.5755 (17)H24···H23 <sup>vi</sup> 2.5500C24···C12i3.5805 (17)H26···C332.7000C24···C2vi3.5805 (17)H26···C332.5000C24···C12vi3.5805 (17)H26···C332.9000C44···N13 <sup>viii</sup> <td>C25—C</td> <td>26</td> <td>1.3897</td> <td>(17)</td> <td>С53—Н53</td> <td></td> <td>0.9500</td>	C25—C	26	1.3897	(17)	С53—Н53		0.9500
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C51—C	252	1.4023	(16)	С54—Н54		0.9500
C52—C531.3894 (16)C56—H560.9500N13—C12 <sup>i</sup> 3.3510 (16)C56—H22 <sup>+ii</sup> 3.1000N13—C54 <sup>ii</sup> 3.3396 (16)H3—C262.6600N13—C54 <sup>ii</sup> 3.3383 (15)H3—H52.3500N13—C54 <sup>iii</sup> 3.3883 (15)H3—H262.1000N13—H54 <sup>ii</sup> 2.8600H4—C122.6100N13—H54 <sup>iii</sup> 2.8600H4—C562.2800N13—H54 <sup>iii</sup> 2.8300H4—H562.2800N13—H25 <sup>iv</sup> 2.8300H4—H562.2800N13—H222.8900H5—H52.3500C3—C25 <sup>iv</sup> 3.5805 (17)H5—H522.4200C3—C25 <sup>iv</sup> 3.5805 (17)H5—H522.4700C4—C24 <sup>ii</sup> 3.5341 (17)H5—H52 <sup>is</sup> 2.5700C12—N13 <sup>i</sup> 3.3510 (16)H22—N132.8900C12—C12 <sup>i</sup> 3.5296 (17)H22—C55 <sup>is</sup> 2.8000C21—C12 <sup>ii</sup> 3.5296 (17)H22—C56 <sup>ii</sup> 3.1000C23—C3 <sup>ii</sup> 3.4028 (17)H23—H23 <sup>ii</sup> 2.5400C23-C3 <sup>ii</sup> 3.4028 (17)H23—H23 <sup>ii</sup> 2.5500C23-C3 <sup>ii</sup> 3.5805 (17)H24—H23 <sup>ii</sup> 2.5500C23-C3 <sup>ii</sup> 3.5805 (17)H26—N13 <sup>iii</sup> 2.8300C54-N13 <sup>iii</sup> 3.3396 (16)H25—N13 <sup>iii</sup> 2.8300C54-N13 <sup>iii</sup> 3.3396 (16)H25—H54 <sup>iiii</sup> 2.6000C54-N13 <sup>iii</sup> 3.3883 (15)H26-C32.7000C25-C12 <sup>ii</sup> 3.5805 (17)H26-C32.7000C25-C13 <sup>iii</sup> 3.0900H26-H32.1000C3-H262.7800H26-H3	C51—C	256	1.4032	(16)	С55—Н55		0.9500
N13C12 <sup>i</sup> 3.3510 (16)C56H22 <sup>vii</sup> 3.1000N13C54 <sup>ii</sup> 3.3396 (16)H3C262.6600N13C54 <sup>iii</sup> 3.3896 (15)H3H52.3500N13C54 <sup>iii</sup> 3.3833 (15)H3H262.1000N13H54 <sup>ii</sup> 2.8600H4C122.6100N13H54 <sup>iii</sup> 2.6100H4C562.7900N13H25 <sup>iv</sup> 2.8300H4H562.2800N13H222.8900H5H32.3500C3C25 <sup>v</sup> 3.5805 (17)H5H522.4200C3C25 <sup>v</sup> 3.5805 (17)H5H5 <sup>x</sup> 2.4700C4N13 <sup>i</sup> 3.4376 (15)H5H5 <sup>x</sup> 2.4700C4C24 <sup>vi</sup> 3.5341 (17)H5H52 <sup>x</sup> 2.5700C12N13 <sup>i</sup> 3.3510 (16)H22N132.8900C12C12 <sup>i</sup> 3.5296 (17)H22C55 <sup>ii</sup> 3.1000C23C25 <sup>vi</sup> 3.5755 (17)H22C55 <sup>ii</sup> 3.1000C23C2 <sup>ivi</sup> 3.5755 (17)H22C55 <sup>ii</sup> 3.1000C23C2 <sup>ivi</sup> 3.5755 (17)H22C56 <sup>ii</sup> 3.1000C23C2 <sup>ivi</sup> 3.5341 (17)H23H23 <sup>xii</sup> 2.5400C24C4 <sup>vi</sup> 3.5341 (17)H23H24 <sup>xii</sup> 2.5500C25C12 <sup>vi</sup> 3.5805 (17)H24H23 <sup>xii</sup> 2.6500C25C12 <sup>xii</sup> 3.5805 (17)H24H23 <sup>xii</sup> 2.6500C25C12 <sup>xii</sup> 3.5805 (17)H25H154 <sup>xiii</sup> 2.6000C54N13 <sup>xiii</sup> 3.3883 (15)H26C32.7000C54N13 <sup>xiii</sup> 3.3883 (15)H26C32.7000C2H53 <sup>xk</sup> 3.0900H26H3	C52—C	253	1.3894	(16)	С56—Н56		0.9500
N13···C12 <sup>i</sup> 3.3510 (16)C56···H22 <sup>*ii</sup> 3.1000N13···C54 <sup>ii</sup> 3.3396 (16)H3···C262.6600N13···C54 <sup>iii</sup> 3.4376 (15)H3···H52.3500N13···C54 <sup>iii</sup> 3.3883 (15)H3···H262.1000N13···H54 <sup>iii</sup> 2.8600H4···C122.6100N13···H54 <sup>iii</sup> 2.6100H4···C562.7900N13···H25 <sup>iv</sup> 2.8300H4···H562.2800N13···H222.8900H5···H32.3500C3···C25 <sup>iv</sup> 3.5805 (17)H5···H522.4200C3···C23 <sup>ii</sup> 3.4028 (17)H5···H5 <sup>x</sup> 2.4700C4···N13 <sup>i</sup> 3.4376 (15)H5···H5 <sup>x</sup> 2.4700C4···N13 <sup>i</sup> 3.3510 (16)H22···N132.8900C12···C25 <sup>ii</sup> 3.5555 (17)H22···C122.4700C12···C12 <sup>i</sup> 3.5296 (17)H22···C56 <sup>ii</sup> 3.1000C23···C21 <sup>ii</sup> 3.4028 (17)H22···C56 <sup>ii</sup> 3.1000C23···C21 <sup>ii</sup> 3.590 (17)H22···C56 <sup>ii</sup> 3.1000C23···C12 <sup>ii</sup> 3.595 (17)H24··H23 <sup>ii</sup> 2.5500C24···C4 <sup>ii</sup> 3.5341 (17)H23···H23 <sup>ii</sup> 2.5400C24···C4 <sup>ii</sup> 3.5351 (16)H22···C56 <sup>ii</sup> 3.1000C23···C3 <sup>ii</sup> 3.4028 (17)H23···H23 <sup>ii</sup> 2.5500C25···C12 <sup>ii</sup> 3.585 (17)H24···H23 <sup>ii</sup> 2.5500C25···C13 <sup>ii</sup> 3.396 (16)H25···H54 <sup>iii</sup> 2.6000C54··N13 <sup>iii</sup> 3.386 (15)H26···C332.7000C54··N13 <sup>iii</sup> 3.386 (15)H26···C3i2.7000C2-··H53 <sup>ik</sup>							
N13···C54 <sup>ii</sup> 3.3396 (16)H3···C262.6600N13···C4i3.4376 (15)H3···H52.3500N13···C54 <sup>ii</sup> 3.3883 (15)H3···H262.1000N13···H54 <sup>ii</sup> 2.8600H4···C122.6100N13···H54 <sup>iii</sup> 2.6100H4···C662.7900N13···H54 <sup>iii</sup> 2.8300H4···H562.2800N13···H25 <sup>iv</sup> 2.8300H5···H32.3500C3···C25 <sup>v</sup> 3.5805 (17)H5···H522.4200C3···C23 <sup>vi</sup> 3.4028 (17)H5···H522.4700C4···C24 <sup>vi</sup> 3.5341 (17)H5···H552.4700C12···N13 <sup>i</sup> 3.3510 (16)H22···N132.8900C12···C25 <sup>vi</sup> 3.5755 (17)H22···C122.4700C12···C25 <sup>vi</sup> 3.5756 (17)H22···C122.4700C12···C25 <sup>vi</sup> 3.5296 (17)H22···C56 <sup>ii</sup> 3.1000C23···C25 <sup>vi</sup> 3.54028 (17)H22···C122.4700C12···C12 <sup>ii</sup> 3.54028 (17)H22···C122.4700C24···C24 <sup>vii</sup> 3.5341 (17)H22···C122.4700C21···C21 <sup>vii</sup> 3.4853 (16)H22···L12 <sup>vii</sup> 2.5500C25···C12 <sup>vii</sup> 3.5755 (17)H24···H23 <sup>vii</sup> 2.5500C25···C12 <sup>vii</sup> 3.5805 (17)H25···N13 <sup>viii</sup> 2.8300C54···N13 <sup>viii</sup> 3.3833 (15)H26···C32.7000C25···C3 <sup>vi</sup> 3.5805 (17)H25···N13 <sup>viii</sup> 2.8300C54···N13 <sup>viii</sup> 3.3833 (15)H26···C3 <sup>×</sup> 2.9000C54···N13 <sup>viii</sup> 3.3833 (15)H26···C3 <sup>×</sup> 2.9000C54···N13 <sup>vi</sup>	N13…C	12 <sup>i</sup>	3.3510	(16)	C56···H22 <sup>vii</sup>		3.1000
N13···C4i $3.4376$ (15)H3···H5 $2.3500$ N13···C54 <sup>iii</sup> $3.3883$ (15)H3···H26 $2.1000$ N13···H54 <sup>ii</sup> $2.8600$ H4···C12 $2.6100$ N13···H54 <sup>iii</sup> $2.6100$ H4···C66 $2.7900$ N13···H27 <sup>iii</sup> $2.8300$ H4···H56 $2.2800$ N13···H22 $2.8900$ H5···H3 $2.3500$ C3···C25 <sup>v</sup> $3.5805$ (17)H5···H52 $2.4200$ C3···C25 <sup>v</sup> $3.5805$ (17)H5···H52 $2.4200$ C3···C25 <sup>vi</sup> $3.4028$ (17)H5···C52 <sup>x</sup> $3.0800$ C4···N13 <sup>i</sup> $3.4376$ (15)H5···H5 <sup>s</sup> $2.4700$ C12···C24 <sup>vi</sup> $3.5341$ (17)H5···H5 <sup>x</sup> $2.4700$ C12···C25 <sup>vi</sup> $3.5755$ (17)H22···C12 $2.4700$ C12···C12 <sup>i</sup> $3.5296$ (17)H22···C12 $2.4700$ C12···C21 <sup>vi</sup> $3.5755$ (17)H22···C12 $2.4700$ C21···C21 <sup>vi</sup> $3.5341$ (17)H22···C12 $2.4700$ C21···C21 <sup>vi</sup> $3.5341$ (17)H22···C12 $2.4700$ C21···C21 <sup>vi</sup> $3.5341$ (17)H22···C12 $2.4700$ C23···C3 <sup>vi</sup> $3.4028$ (17)H23···H24 <sup>ii</sup> $2.5500$ C25···C12 <sup>vi</sup> $3.5755$ (17)H24···H23 <sup>vi</sup> $2.5500$ C25···C12 <sup>vi</sup> $3.3805$ (17)H25···N13 <sup>viii</sup> $2.8300$ C54···N13 <sup>viii</sup> $3.3805$ (16)H25····H54 <sup>viiii</sup> $2.6000$ C54···N13 <sup>viii</sup> $3.3805$ (17)H25···N13 <sup>viii</sup> $2.8300$ C54···N13 <sup>viii</sup> $3.3805$ (17)H25····T54 <sup>viii</sup> $2.9000$ C54·	N13…C	54 <sup>ii</sup>	3.3396	(16)	H3…C26		2.6600
N13···C54 <sup>iii</sup> 3.3883 (15)H3···H262.1000N13···H54 <sup>iii</sup> 2.8600H4···C122.6100N13···H54 <sup>iii</sup> 2.6100H4···C562.7900N13···H25 <sup>iv</sup> 2.8300H4···H562.2800N13···H222.8900H5···H32.3500C3···C25 <sup>v</sup> 3.5805 (17)H5···H522.4200C3···C23 <sup>vi</sup> 3.4028 (17)H5···C52 <sup>x</sup> 3.0800C4···N13 <sup>i</sup> 3.4376 (15)H5···H5 <sup>x</sup> 2.4700C4···C24 <sup>vi</sup> 3.5341 (17)H5···H52 <sup>x</sup> 2.5700C12···C25 <sup>vi</sup> 3.5755 (17)H22···C122.4700C12···C25 <sup>vi</sup> 3.5755 (17)H22···C122.4700C12···C21 <sup>vi</sup> 3.5296 (17)H22···C56 <sup>ii</sup> 2.8000C21···C21 <sup>vi</sup> 3.5341 (17)H23 <sup>vi</sup> H24 <sup>xi</sup> 2.5500C23···C21 <sup>vi</sup> 3.5755 (17)H22···C122.4700C24···C4 <sup>vi</sup> 3.5341 (17)H23 <sup>xi</sup> H24 <sup>xi</sup> 2.5500C25···C12 <sup>vi</sup> 3.5755 (17)H24··H23 <sup>xi</sup> 2.5500C25···C12 <sup>vi</sup> 3.5805 (17)H24··H23 <sup>xi</sup> 2.5500C25···C12 <sup>vii</sup> 3.5805 (17)H25···H34 <sup>xiii</sup> 2.8300C54···N13 <sup>viii</sup> 3.3883 (15)H26···C32.7000C2···C3 <sup>x</sup> 3.0900H26···H32.1000C3···H262.7000H26···C3 <sup>x</sup> 2.9000C4···H562.7800H52···H52.4200C5···H55 <sup>viii</sup> 2.9300H52···H5 <sup>x</sup> 2.5700	N13…C	4 <sup>i</sup>	3.4376	(15)	Н3…Н5		2.3500
N13···H54 <sup>ii</sup> 2.8600H4···C122.6100N13···H54 <sup>iii</sup> 2.6100H4···C562.7900N13···H25 <sup>iv</sup> 2.8300H4···H562.2800N13···H222.8900H5···H32.3500C3···C25 <sup>v</sup> 3.5805 (17)H5···H522.4200C3···C23 <sup>vi</sup> 3.4028 (17)H5···F5 <sup>x</sup> 2.4700C4···C24 <sup>vi</sup> 3.5341 (17)H5···H5 <sup>x</sup> 2.4700C12···C12 <sup>vi</sup> 3.5341 (17)H5···H5 <sup>x</sup> 2.4700C12···C25 <sup>vi</sup> 3.5755 (17)H22···C122.4700C12···C25 <sup>vi</sup> 3.5755 (17)H22···C55 <sup>ii</sup> 2.8000C21···C21 <sup>vi</sup> 3.4928 (17)H22···C56 <sup>ii</sup> 3.1000C23···C3 <sup>vi</sup> 3.4028 (17)H22···C56 <sup>ii</sup> 3.1000C23···C12 <sup>vi</sup> 3.5341 (17)H23···H23 <sup>xi</sup> 2.5500C25···C12 <sup>vi</sup> 3.5755 (17)H22···C56 <sup>ii</sup> 3.1000C23···C3 <sup>vi</sup> 3.4028 (17)H23···H23 <sup>xii</sup> 2.5500C25···C12 <sup>vi</sup> 3.5755 (17)H24···H23 <sup>xii</sup> 2.5500C25···C12 <sup>vi</sup> 3.5805 (17)H25···N13 <sup>xii</sup> 2.8300C54···N13 <sup>viii</sup> 3.388 (15)H26···C32.7000C54···N13 <sup>viii</sup> 3.3883 (15)H26···C32.7000C54···N13 <sup>viii</sup> 3.0900H26···H32.1000C3···H262.7000H26···H32.1000C3···H262.7800H52···H5 <sup>x</sup> 2.4200C5···H55 <sup>viii</sup> 2.9300H52···H5 <sup>x</sup> 3.0500	N13…C	54 <sup>iii</sup>	3.3883	(15)	H3…H26		2.1000
N13···H54 <sup>iii</sup> 2.6100H4···C562.7900N13···H25 <sup>iv</sup> 2.8300H4···H562.2800N13···H222.8900H5···H32.3500C3···C25 <sup>v</sup> 3.5805 (17)H5···H522.4200C3···C23 <sup>vi</sup> 3.4028 (17)H5···C52 <sup>x</sup> 3.0800C4···N13 <sup>i</sup> 3.4376 (15)H5···H5 <sup>x</sup> 2.4700C4···C24 <sup>vi</sup> 3.5341 (17)H5···H52 <sup>x</sup> 2.5700C12···N13 <sup>i</sup> 3.3510 (16)H22···N132.8900C12···C25 <sup>vi</sup> 3.5755 (17)H22···C122.4700C12···C25 <sup>vi</sup> 3.5755 (17)H22···C55 <sup>ii</sup> 2.8000C21···C21 <sup>vi</sup> 3.5296 (17)H22···C55 <sup>ii</sup> 2.8000C23···C3 <sup>vi</sup> 3.4028 (17)H23···H23 <sup>xi</sup> 2.5400C24···C4 <sup>vii</sup> 3.5341 (17)H23···H23 <sup>xii</sup> 2.5500C25···C12 <sup>vi</sup> 3.5755 (17)H24···H23 <sup>xii</sup> 2.5500C25···C12 <sup>vi</sup> 3.5805 (17)H25···N13 <sup>xii</sup> 2.8300C54···N13 <sup>viii</sup> 3.3396 (16)H25···H34 <sup>xiii</sup> 2.6000C54···N13 <sup>viii</sup> 3.3883 (15)H26···C32.7000C5···L55 <sup>xiii</sup> 3.0900H26···H32.1000C3···H262.7000H26···H32.1000C3···H262.7800H52···H5 <sup>x</sup> 2.4200C5···H55 <sup>viii</sup> 2.9300H52···H5 <sup>x</sup> 3.0500	N13…H	54 <sup>ii</sup>	2.8600		H4…C12		2.6100
N13···H25 <sup>iv</sup> 2.8300H4···H562.2800N13···H222.8900H5···H32.3500C3···C25 <sup>v</sup> 3.5805 (17)H5···H522.4200C3···C23 <sup>vii</sup> 3.4028 (17)H5···C52 <sup>s</sup> 3.0800C4···N13 <sup>i</sup> 3.4376 (15)H5···H5 <sup>x</sup> 2.4700C4···C24 <sup>vii</sup> 3.5341 (17)H5···H52 <sup>s</sup> 2.5700C12···N13 <sup>i</sup> 3.3510 (16)H22···N132.8900C12···C25 <sup>vii</sup> 3.5755 (17)H22···C122.4700C12···C12 <sup>i</sup> 3.5296 (17)H22···C56 <sup>ii</sup> 3.1000C23···C3 <sup>vii</sup> 3.4028 (17)H23···H23 <sup>xii</sup> 2.5400C24···C4 <sup>vii</sup> 3.5341 (17)H23···H24 <sup>xii</sup> 2.5500C25···C12 <sup>vii</sup> 3.5755 (17)H24···H23 <sup>xii</sup> 2.5500C25···C12 <sup>vii</sup> 3.5805 (17)H25···N13 <sup>xiii</sup> 2.8300C54···N13 <sup>viii</sup> 3.3883 (15)H26···C32.7000C54···N13 <sup>viii</sup> 3.0900H26···H32.1000C3···H262.7000H26···C3 <sup>x</sup> 2.9000C4···H562.7800H52···H52.4200C5···H55 <sup>viii</sup> 2.9300H52···H52.4200	N13…H	54 <sup>iii</sup>	2.6100		H4…C56		2.7900
N13···H222.8900H5···H32.3500C3···C25 <sup>v</sup> 3.5805 (17)H5···H522.4200C3···C23 <sup>vi</sup> 3.4028 (17)H5···F523.0800C4···N13 <sup>i</sup> 3.4376 (15)H5···H5x2.4700C4···C24 <sup>vi</sup> 3.5341 (17)H5···H52x2.5700C12···N13 <sup>i</sup> 3.3510 (16)H22···N132.8900C12···C25 <sup>vi</sup> 3.5755 (17)H22···C122.4700C12···C12 <sup>i</sup> 3.5296 (17)H22···C55 <sup>ii</sup> 2.8000C21···C21 <sup>vi</sup> 3.4853 (16)H22···C56 <sup>ii</sup> 3.1000C23···C3 <sup>vi</sup> 3.4028 (17)H23···H23 <sup>vi</sup> 2.5400C24···C4 <sup>vi</sup> 3.5341 (17)H23···H23 <sup>vi</sup> 2.5500C25···C12 <sup>vi</sup> 3.5755 (17)H24···H23 <sup>vi</sup> 2.5500C25···C12 <sup>vi</sup> 3.5755 (17)H25···N13 <sup>xii</sup> 2.8300C54···N13 <sup>viii</sup> 3.3806 (16)H25···H54 <sup>xiii</sup> 2.6000C54···N13 <sup>viii</sup> 3.3883 (15)H26···C32.7000C3···H262.7000H26···C3 <sup>x</sup> 2.9000C4···H562.7800H52···H52.4200C5···H55 <sup>viii</sup> 2.9300H52···H5 <sup>x</sup> 3.0500	N13…H	25 <sup>iv</sup>	2.8300		H4…H56		2.2800
C3···C25 <sup>v</sup> 3.5805 (17)H5···H522.4200C3···C23 <sup>vi</sup> 3.4028 (17)H5···H523.0800C4···N13 <sup>i</sup> 3.4376 (15)H5···H5 <sup>x</sup> 2.4700C4···C24 <sup>vi</sup> 3.5341 (17)H5···H52 <sup>x</sup> 2.5700C12···N13 <sup>i</sup> 3.3510 (16)H22···N132.8900C12···C25 <sup>vi</sup> 3.5755 (17)H22···C122.4700C12···C12 <sup>i</sup> 3.5296 (17)H22···C55 <sup>ii</sup> 2.8000C21···C21 <sup>vi</sup> 3.4853 (16)H22···C56 <sup>ii</sup> 3.1000C23···C3 <sup>vi</sup> 3.4028 (17)H23···H23 <sup>vi</sup> 2.5400C24···C4 <sup>vi</sup> 3.5341 (17)H23···H23 <sup>vi</sup> 2.5500C25···C12 <sup>vi</sup> 3.5755 (17)H24···H23 <sup>vi</sup> 2.5500C25···C12 <sup>vi</sup> 3.5805 (17)H25···N13 <sup>viii</sup> 2.8300C54···N13 <sup>viii</sup> 3.386 (16)H25···H54 <sup>viiii</sup> 2.6000C54···N13 <sup>viii</sup> 3.3883 (15)H26···C32.7000C2···H53 <sup>ix</sup> 3.0900H26···H32.1000C3···H262.7800H26···F152.4200C5···H55 <sup>viii</sup> 2.9300H52···H5 <sup>x</sup> 2.5700C12···H222.4700H52···F5 <sup>x</sup> 3.0500	N13…H	22	2.8900		Н5…Н3		2.3500
C3C23vi $3.4028(17)$ $H5C52x$ $3.0800$ C4N13i $3.4376(15)$ $H5H5x$ $2.4700$ C4C24vi $3.5341(17)$ $H5H5x$ $2.5700$ C12N13i $3.3510(16)$ $H22N13$ $2.8900$ C12C25vi $3.5755(17)$ $H22C12$ $2.4700$ C12C25vi $3.5755(17)$ $H22C55ii$ $2.8000$ C21C21vi $3.4853(16)$ $H22C56ii$ $3.1000$ C23C2vi $3.5755(17)$ $H23H23xii$ $2.5400$ C24C4vi $3.5341(17)$ $H23H23xii$ $2.5500$ C25C12vi $3.5755(17)$ $H24H23xii$ $2.5500$ C25C12vi $3.5755(17)$ $H24H23xii$ $2.6000$ C54N13vii $3.396(16)$ $H25H54xiii$ $2.6000$ C54N13viii $3.3883(15)$ $H26C3$ $2.7000$ C2H53ix $3.0900$ $H26H3$ $2.1000$ C3H26 $2.7000$ $H26C53x$ $2.9000$ C4H26 $2.7800$ $H52H5x$ $2.5700$ C12H22 $2.4700$ $H52C23^{xiv}$ $3.0500$	C3…C2	5 <sup>v</sup>	3.5805	(17)	Н5…Н52		2.4200
C4···N13i3.4376 (15)H5···H5x2.4700C4···C24vi3.5341 (17)H5···H52x2.5700C12···N13i3.3510 (16)H22···N132.8900C12···C25vi3.5755 (17)H22···C122.4700C12···C12i3.5296 (17)H22···C55ii2.8000C21···C21vi3.5296 (17)H22···C56ii3.1000C23···C3vi3.4028 (17)H23···H23xii2.5400C24···C4vi3.5341 (17)H23···H24xii2.5500C25···C12vi3.5755 (17)H24···H23xii2.5500C25···C3v3.5805 (17)H25···N13xii2.8300C54···N13vii3.3396 (16)H25···N13xii2.8000C54···N13viii3.3883 (15)H26···C32.7000C2···H53ix3.0900H26···H32.1000C3···H262.7000H26···C53x2.9000C4···H562.7800H52···H5x2.4200C5···H55viii2.9300H52···H5x2.5700C12···H222.4700H52···C23xiv3.0500	C3…C2	3 <sup>vi</sup>	3.4028	(17)	H5…C52 <sup>x</sup>		3.0800
C4···C24vi $3.5341(17)$ H5···H52x $2.5700$ C12···N13i $3.3510(16)$ H22···N13 $2.8900$ C12···C25vi $3.5755(17)$ H22···C12 $2.4700$ C12···C12i $3.5296(17)$ H22···C55ii $2.8000$ C21···C21vi $3.4853(16)$ H22···C56ii $3.1000$ C23···C3vi $3.4028(17)$ H23···H23xi $2.5400$ C24···C4vii $3.5341(17)$ H23···H24xii $2.5500$ C25···C12vi $3.5755(17)$ H24···H23xii $2.5500$ C25···C12vi $3.5755(17)$ H24···H23xii $2.5500$ C25···C3v $3.5805(17)$ H25···N13xii $2.8300$ C54···N13vii $3.3396(16)$ H25···H54xiii $2.6000$ C54···N13viii $3.3883(15)$ H26···C3 $2.7000$ C2···H53ix $3.0900$ H26···H3 $2.1000$ C3···H26 $2.7000$ H26···C53x $2.9000$ C4···H56 $2.7800$ H52···H55 $2.4200$ C5···H55viii $2.9300$ H52···H5x $2.5700$ C12···H22 $2.4700$ H52···C23xiv $3.0500$	C4…N1	3 <sup>i</sup>	3.4376	(15)	H5…H5 <sup>x</sup>		2.4700
C12···N13i3.3510 (16)H22···N132.8900C12···C25vi3.5755 (17)H22···C122.4700C12···C12i3.5296 (17)H22···C55ii2.8000C21···C21vi3.4853 (16)H22···C56ii3.1000C23···C3vi3.4028 (17)H23···H23xii2.5400C24···C4vi3.5341 (17)H23···H24xii2.5500C25···C12vi3.5755 (17)H24···H23xii2.5500C25···C12vi3.5755 (17)H24···H23xii2.8300C4···N13vii3.396 (16)H25···N13xii2.8300C54···N13viii3.3883 (15)H26···C32.7000C2···H53ix3.0900H26···H32.1000C3···H262.7000H26···C3x2.9000C4···H562.7800H52···H52.4200C5···H55viii2.9300H52···H5x2.5700C12···H222.4700H52···C23xiv3.0500	C4…C2	4 <sup>vi</sup>	3.5341	(17)	H5…H52 <sup>x</sup>		2.5700
C12···C25 <sup>vi</sup> $3.5755 (17)$ H22···C12 $2.4700$ C12···C12 <sup>i</sup> $3.5296 (17)$ H22···C55 <sup>ii</sup> $2.8000$ C21···C21 <sup>vi</sup> $3.4853 (16)$ H22···C56 <sup>ii</sup> $3.1000$ C23···C3 <sup>vi</sup> $3.4028 (17)$ H23···H23 <sup>xi</sup> $2.5400$ C24···C4 <sup>vi</sup> $3.5341 (17)$ H23···H24 <sup>xi</sup> $2.5500$ C25···C12 <sup>vi</sup> $3.5755 (17)$ H24···H23 <sup>xi</sup> $2.5500$ C25···C12 <sup>vi</sup> $3.5805 (17)$ H25···N13 <sup>xii</sup> $2.8300$ C54···N13 <sup>vii</sup> $3.3396 (16)$ H25···H54 <sup>xiii</sup> $2.6000$ C54···N13 <sup>viii</sup> $3.3883 (15)$ H26···C3 $2.7000$ C2···H53 <sup>ix</sup> $3.0900$ H26···H3 $2.1000$ C3···H26 $2.7000$ H26···C53 <sup>x</sup> $2.9000$ C4···H56 $2.7800$ H52···H5 $2.4200$ C5···H55 <sup>viii</sup> $2.9300$ H52···H5 $2.5700$ C12···H22 $2.4700$ H52···C23 <sup>xiv</sup> $3.0500$	C12…N	13 <sup>i</sup>	3.3510	(16)	H22…N13		2.8900
C12···C12i $3.5296 (17)$ $H22···C55^{ii}$ $2.8000$ C21···C21vi $3.4853 (16)$ $H22···C56^{ii}$ $3.1000$ C23···C3vi $3.4028 (17)$ $H23···H23^{xi}$ $2.5400$ C24···C4vi $3.5341 (17)$ $H23···H24^{xi}$ $2.5500$ C25···C12vi $3.5755 (17)$ $H24···H23^{xi}$ $2.5500$ C25···C3v $3.5805 (17)$ $H25···N13^{xii}$ $2.8300$ C54···N13 <sup>viii</sup> $3.396 (16)$ $H25···H54^{xiii}$ $2.6000$ C54···N13 <sup>viii</sup> $3.383 (15)$ $H26···C3$ $2.7000$ C2···H53 <sup>ix</sup> $3.0900$ $H26···C3^{x}$ $2.9000$ C3···H26 $2.7000$ $H26···C53^{x}$ $2.9000$ C4···H56 $2.7800$ $H52···H5^{xii}$ $2.4200$ C5···H55 <sup>viii</sup> $2.9300$ $H52···H5^{x}$ $2.5700$ C12···H22 $2.4700$ $H52···C23^{xiv}$ $3.0500$	C12…C	25 <sup>vi</sup>	3.5755	(17)	H22…C12		2.4700
C21…C21 <sup>vi</sup> $3.4853(16)$ $H22…C56^{ii}$ $3.1000$ C23…C3 <sup>vi</sup> $3.4028(17)$ $H23…H23^{xi}$ $2.5400$ C24…C4 <sup>vi</sup> $3.5341(17)$ $H23…H24^{xi}$ $2.5500$ C25…C12 <sup>vi</sup> $3.5755(17)$ $H24…H23^{xi}$ $2.5500$ C25…C3 <sup>v</sup> $3.5805(17)$ $H25…N13^{xii}$ $2.8300$ C54…N13 <sup>viii</sup> $3.3396(16)$ $H25…H54^{xiii}$ $2.6000$ C54…N13 <sup>viii</sup> $3.3883(15)$ $H26…C3$ $2.7000$ C2…H53 <sup>ix</sup> $3.0900$ $H26…C3^x$ $2.9000$ C3…H26 $2.7000$ $H26…C53^x$ $2.9000$ C4…H56 $2.7800$ $H52…H5^x$ $2.5700$ C12…H22 $2.4700$ $H52…C23^{xiv}$ $3.0500$	C12…C	12 <sup>i</sup>	3.5296	(17)	H22…C55 <sup>ii</sup>		2.8000
C23···C3 <sup>vi</sup> $3.4028(17)$ $H23···H23^{xi}$ $2.5400$ C24···C4 <sup>vi</sup> $3.5341(17)$ $H23···H24^{xi}$ $2.5500$ C25···C12 <sup>vi</sup> $3.5755(17)$ $H24···H23^{xi}$ $2.5500$ C25···C3 <sup>v</sup> $3.5805(17)$ $H25···N13^{xii}$ $2.8300$ C54···N13 <sup>vii</sup> $3.3396(16)$ $H25···H54^{xiii}$ $2.6000$ C54···N13 <sup>viii</sup> $3.3883(15)$ $H26···C3$ $2.7000$ C2···H53 <sup>ix</sup> $3.0900$ $H26···H3$ $2.1000$ C3···H26 $2.7000$ $H26···C53^{x}$ $2.9000$ C4···H56 $2.7800$ $H52···H5^{xiii}$ $2.4200$ C5···H55 <sup>viii</sup> $2.9300$ $H52···H5^{x}$ $2.5700$ C12···H22 $2.4700$ $H52···C23^{xiv}$ $3.0500$	C21…C	21 <sup>vi</sup>	3.4853	(16)	H22…C56 <sup>ii</sup>		3.1000
C24···C4vi $3.5341 (17)$ H23···H24xi $2.5500$ C25···C12vi $3.5755 (17)$ H24···H23xi $2.5500$ C25···C3v $3.5805 (17)$ H25···N13xii $2.8300$ C54···N13vii $3.3396 (16)$ H25···H54xiii $2.6000$ C54···N13viii $3.3883 (15)$ H26···C3 $2.7000$ C2···H53 <sup>ix</sup> $3.0900$ H26···H3 $2.1000$ C3···H26 $2.7000$ H26···C53 <sup>x</sup> $2.9000$ C4···H56 $2.7800$ H52···H5 $2.4200$ C5···H55 <sup>viii</sup> $2.9300$ H52···H5 <sup>x</sup> $2.5700$ C12···H22 $2.4700$ H52···C23 <sup>xiv</sup> $3.0500$	C23…C	3 <sup>vi</sup>	3.4028	(17)	H23····H23 <sup>xi</sup>		2.5400
C25···C12vi $3.5755 (17)$ H24···H23xi $2.5500$ C25···C3v $3.5805 (17)$ H25···N13xii $2.8300$ C54···N13vii $3.3396 (16)$ H25···H54xiii $2.6000$ C54···N13viii $3.3883 (15)$ H26···C3 $2.7000$ C2···H53 <sup>ix</sup> $3.0900$ H26···C3 $2.1000$ C3···H26 $2.7000$ H26···C53 <sup>x</sup> $2.9000$ C4···H56 $2.7800$ H52···H5 $2.4200$ C5···H55viii $2.9300$ H52···H5 $2.5700$ C12···H22 $2.4700$ H52···C23xiv $3.0500$	C24…C	4 <sup>vi</sup>	3.5341	(17)	H23…H24 <sup>xi</sup>		2.5500
C25···C3 <sup>v</sup> 3.5805 (17)       H25···N13 <sup>xii</sup> 2.8300         C54···N13 <sup>vii</sup> 3.3396 (16)       H25···H54 <sup>xiii</sup> 2.6000         C54···N13 <sup>viii</sup> 3.3883 (15)       H26···C3       2.7000         C2···H53 <sup>ix</sup> 3.0900       H26···H3       2.1000         C3···H26       2.7000       H26···C53 <sup>x</sup> 2.9000         C4···H56       2.7800       H52···H5       2.4200         C5···H55 <sup>viii</sup> 2.9300       H52···H5 <sup>x</sup> 2.5700         C12···H22       2.4700       H52···C23 <sup>xiv</sup> 3.0500	C25…C	12 <sup>vi</sup>	3.5755	(17)	H24…H23 <sup>xi</sup>		2.5500
C54···N13vii       3.3396 (16)       H25···H54xiii       2.6000         C54···N13viii       3.3883 (15)       H26···C3       2.7000         C2···H53 <sup>ix</sup> 3.0900       H26···H3       2.1000         C3···H26       2.7000       H26···C53 <sup>x</sup> 2.9000         C4···H56       2.7800       H52···H5       2.4200         C5···H55 <sup>viii</sup> 2.9300       H52···H5 <sup>x</sup> 2.5700         C12···H22       2.4700       H52···C23 <sup>xiv</sup> 3.0500	C25…C	3 <sup>v</sup>	3.5805	(17)	H25…N13 <sup>xii</sup>		2.8300
C54···N13viii       3.3883 (15)       H26···C3       2.7000         C2···H53 <sup>ix</sup> 3.0900       H26···H3       2.1000         C3···H26       2.7000       H26···C53 <sup>x</sup> 2.9000         C4···H56       2.7800       H52···H5       2.4200         C5···H55 <sup>viii</sup> 2.9300       H52···H5 <sup>x</sup> 2.5700         C12···H22       2.4700       H52···C23 <sup>xiv</sup> 3.0500	C54…N	13 <sup>vii</sup>	3.3396	(16)	H25…H54 <sup>xiii</sup>		2.6000
C2···H53 <sup>ix</sup> 3.0900       H26···H3       2.1000         C3···H26       2.7000       H26···C53 <sup>x</sup> 2.9000         C4···H56       2.7800       H52···H5       2.4200         C5···H55 <sup>viii</sup> 2.9300       H52···H5 <sup>x</sup> 2.5700         C12···H22       2.4700       H52···C23 <sup>xiv</sup> 3.0500	C54…N	13 <sup>viii</sup>	3.3883	(15)	H26…C3		2.7000
C3…H26       2.7000       H26…C53x       2.9000         C4…H56       2.7800       H52…H5       2.4200         C5…H55 <sup>viii</sup> 2.9300       H52…H5x       2.5700         C12…H22       2.4700       H52…C23 <sup>xiv</sup> 3.0500	С2…Н5	3 <sup>ix</sup>	3.0900	× - /	H26…H3		2.1000
C4···H56       2.7800       H52···H5       2.4200         C5···H55 <sup>viii</sup> 2.9300       H52···H5 <sup>x</sup> 2.5700         C12···H22       2.4700       H52···C23 <sup>xiv</sup> 3.0500	C3…H2	6	2.7000		H26C53x		2.9000
C5···H55 <sup>viii</sup> 2.9300       H52···H5 <sup>x</sup> 2.5700         C12···H22       2.4700       H52···C23 <sup>xiv</sup> 3.0500	C4…H5	6	2.7800		Н52…Н5		2.4200
C12···H22 2.4700 H52···C23 <sup>xiv</sup> 3.0500	С5…Н5	5 <sup>viii</sup>	2.9300		H52H5x		2.5700
	С12…Н	22	2.4700		H52C23 <sup>xiv</sup>		3.0500

C12…H4	2.6100	H53····C2 <sup>xiv</sup>	3.0900
C21···H53 <sup>ix</sup>	2.8400	H53····C21 <sup>xiv</sup>	2.8400
C23····H52 <sup>ix</sup>	3.0500	H54…N13 <sup>vii</sup>	2.8600
С26…Н3	2.6600	H54…N13 <sup>viii</sup>	2.6100
C51····H55 <sup>viii</sup>	2.9100	H54…H25 <sup>xv</sup>	2.6000
C52…H5 <sup>x</sup>	3.0800	H55…C5 <sup>iii</sup>	2.9300
C52····H56 <sup>viii</sup>	2.9600	H55…C51 <sup>iii</sup>	2.9100
C53····H56 <sup>viii</sup>	2.8500	H56…C4	2.7800
C53…H26 <sup>x</sup>	2.9000	Н56…Н4	2.2800
C54…H56 <sup>viii</sup>	3.0600	H56…C52 <sup>iii</sup>	2.9600
C55····H22 <sup>vii</sup>	2.8000	H56…C53 <sup>iii</sup>	2.8500
С56…Н4	2.7900	H56…C54 <sup>iii</sup>	3.0600
C3—C2—C12	118.13 (11)	C3—C4—H4	119.00
$C_{3}$ — $C_{2}$ — $C_{21}$	125.26 (11)	C5—C4—H4	119.00
$C_{12} - C_{2} - C_{21}$	116.61 (10)	C4—C5—H5	116.00
$C^2 - C^3 - C^4$	126 20 (11)	C51—C5—H5	116.00
$C_{3}$ $C_{4}$ $C_{5}$	120.20 (11)	$C_{21} = C_{22} = H_{22}$	120.00
C4-C5-C51	127.77(11)	$C_{23}$ $C_{22}$ $H_{22}$	120.00
N13_C12_C2	178 90 (13)	$C_{23} = C_{23} = H_{23}$	120.00
$C_2 = C_2 = C_2$	170.90(19) 120.26(10)	$C_{22} = C_{23} = H_{23}$	120.00
$C_2 = C_2 $	120.20(10) 121.42(10)	$C_{24} = C_{23} = H_{23}$	120.00
$C_2 = C_2 I = C_2 C_2 C_2 I$	121.42(10) 118.32(11)	$C_{25} = C_{24} = H_{24}$	120.00
$C_{22} = C_{21} = C_{20}$	118.32(11) 120.72(11)	$C_{23} = C_{24} = 1124$	120.00
$C_{21} = C_{22} = C_{23}$	120.72(11) 120.24(11)	$C_{24} = C_{25} = H_{25}$	120.00
$C_{22} = C_{23} = C_{24}$	120.34(11)	$C_{20} = C_{23} = H_{23}$	120.00
$C_{23} = C_{24} = C_{23}$	119.57 (11)	$C_{21} = C_{20} = H_{20}$	120.00
$C_{24} = C_{25} = C_{26}$	120.20 (11)	C25—C26—H26	120.00
$C_{21} = C_{26} = C_{25}$	120.84 (11)	С51—С52—Н52	120.00
C5C51C52	119.42 (10)	С53—С52—Н52	120.00
C5-C51-C56	122.34 (10)	С52—С53—Н53	120.00
C52—C51—C56	118.24 (10)	С54—С53—Н53	120.00
C51—C52—C53	120.88 (11)	С53—С54—Н54	120.00
C52—C53—C54	120.27 (11)	С55—С54—Н54	120.00
C53—C54—C55	119.44 (11)	С54—С55—Н55	120.00
C54—C55—C56	120.63 (11)	С56—С55—Н55	120.00
C51—C56—C55	120.54 (11)	C51—C56—H56	120.00
С2—С3—Н3	117.00	С55—С56—Н56	120.00
С4—С3—Н3	117.00		
C12—C2—C3—C4	-2.66 (18)	C22—C21—C26—C25	-0.32 (17)
C21—C2—C3—C4	177.83 (11)	C21—C22—C23—C24	0.57 (18)
$C_{3}$ $C_{2}$ $C_{2}$ $C_{2}$ $C_{2}$ $C_{2}$	-176.35(12)	$C_{22}$ $C_{23}$ $C_{24}$ $C_{25}$	-0.55(18)
$C_{3}$ $C_{2}$ $C_{21}$ $C_{26}$	3.30 (18)	$C_{23}$ $C_{24}$ $C_{25}$ $C_{26}$	0.10 (19)
$C_{12} = C_{21} = C_{21} = C_{22}$	4 13 (16)	$C_{24}$ $C_{25}$ $C_{26}$ $C_{21}$	0.34(18)
$C_{12} = C_{2} = C_{21} = C_{26}$	-176 22 (11)	$C_{5}$ $C_{51}$ $C_{52}$ $C_{53}$	-179 94 (11)
$C_2 = C_3 = C_4 = C_5$	177 44 (12)	$C_{56} - C_{51} - C_{52} - C_{53}$	0 50 (17)
$C_{3}$ $C_{4}$ $C_{5}$ $C_{51}$	177 45 (11)	$C_{5}$ $C_{5$	-17963(11)
C4 - C5 - C51 - C52	165 27 (12)	$C_{52} = C_{51} = C_{56} = C_{55}$	-0.08(17)
$\cup \neg - \cup J = \cup J I = \cup J L$	103.27 (12)	0.52 - 0.51 - 0.50 - 0.55	0.00 (17)

C4—C5—C51—C56	-15.19 (19)	C51—C52—C53—C54	-0.85 (18)
C2-C21-C22-C23	179.52 (11)	C52—C53—C54—C55	0.76 (18)
C26—C21—C22—C23	-0.14 (17)	C53—C54—C55—C56	-0.34 (18)
C2-C21-C26-C25	-179.97 (10)	C54—C55—C56—C51	0.00 (18)

Symmetry codes: (i) -*x*+1/2, -*y*+1/2, -*z*; (ii) *x*, -*y*+1, *z*-1/2; (iii) -*x*+1/2, *y*+1/2, -*z*+1/2; (iv) *x*-1/2, *y*+1/2, *z*; (v) -*x*+1, -*y*, -*z*; (vi) -*x*+1, -*y*+1, -*z*; (vii) *x*, -*y*+1, *z*+1/2; (viii) -*x*+1/2, *y*-1/2, *z*; (vi) -*x*+1, -*y*+1, -*z*; (vii) *x*, -*y*+1/2, *z*+1/2; (viii) -*x*+1/2, *y*-1/2, *z*; (xiii) *x*+1/2, -*y*+1/2, *z*-1/2; (xi) *x*, -*y*, *z*+1/2; (xi) -*x*+1, *y*, -*z*+1/2; (xi) -*x*+1, *y*, -*z*+1/2; (xii) *x*+1/2, *y*-1/2, *z*; (xiii) *x*+1/2, -*y*+1/2, *z*-1/2; (xiv) *x*, -*y*, *z*+1/2; (xv) *x*-1/2, -*y*+1/2, *z*+1/2.

## Hydrogen-bond geometry (Å, °)

D—H···A	<i>D</i> —Н	H···A	D····A	<i>D</i> —H··· <i>A</i>
C54—H54…N13 <sup>viii</sup>	0.95	2.61	3.388 (2)	139
С56—Н56…Сд1 <sup>ііі</sup>	0.95	2.83	3.657 (1)	146

Symmetry codes: (iii) -x+1/2, y+1/2, -z+1/2; (viii) -x+1/2, y-1/2, -z+1/2.