5691 measured reflections 2721 independent reflections

 $R_{\rm int} = 0.028$

203 parameters

 $\Delta \rho_{\text{max}} = 0.16 \text{ e } \text{\AA}^{-3}$ $\Delta \rho_{\text{min}} = -0.20 \text{ e } \text{\AA}^{-3}$

1467 reflections with $I > 2\sigma(I)$

H-atom parameters constrained

Acta Crystallographica Section E Structure Reports Online

ISSN 1600-5368

4,4'-(Anthracene-9,10-diyl)dibenzoic acid dimethylformamide disolvate

Hong Li,^a* Zhi-Qiang Wang,^b Liu-Zhi Yang,^a Yan-Qi Liu^a and Duo-Bin Mao^a

^aSchool of Food and Biological Engineering, Zhengzhou University of Light Industry, Zhengzhou 450002, People's Republic of China, and ^bCollege of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang 471022, People's Republic of China

Correspondence e-mail: lihong@zzuli.edu.cn

Received 26 March 2009; accepted 22 April 2009

Key indicators: single-crystal X-ray study; T = 295 K; mean σ (C–C) = 0.004 Å; disorder in solvent or counterion; R factor = 0.053; wR factor = 0.162; data-to-parameter ratio = 13.4.

In the title compound, $C_{28}H_{18}O_4 \cdot 2C_3H_7NO$, the dihedral angle between the benzene rings and the anthracene system is 74.05 (12)°. A crystallographic inversion centre is located in the middle of the anthracene unit. The dimethylformamide solvent molecules are partially disordered over two positions of approximately equal occupancy [0.529 (6):0.471 (6)]. Intermolecular O-H···O hydrogen bonds with the major occupancy formamide O atom as acceptor result in the formation of 2:1 solvate-complex aggregates, which are alternately linked to shorter solvate units via weak intermolecular C-H···O contacts generated from the rotational disorder of the formamide O atom (minor occupancy component). Weak $C-H\cdots\pi$ interactions between the solvent molecules as the donor and the outer anthracene rings support these contacts in the crystal structure for both disorder components.

Related literature

For the structure of 4-(2,5-dihexyloxyphenyl)benzoic acid and the syntheses of related compounds, see: Li *et al.* (2008). For palladium-catalysed Suzuki coupling reactions, see: Xu *et al.* (2006, 2008); Li *et al.* (2006) and literature cited therein.



Experimental

Crystal data

$C_{28}H_{18}O_4 \cdot 2C_3H_7NO$	$\gamma = 79.754 \ (3)^{\circ}$
$M_r = 564.62$	V = 738.0 (3) Å ³
Triclinic, P1	Z = 1
a = 7.3692 (15) Å	Mo $K\alpha$ radiation
b = 8.9981 (18) Å	$\mu = 0.09 \text{ mm}^{-1}$
c = 12.124 (2) Å	$T = 295 { m K}$
$\alpha = 71.157 \ (3)^{\circ}$	$0.23 \times 0.16 \times 0.06 \text{ mm}$
$\beta = 77.640 \ (3)^{\circ}$	

Data collection

Bruker SMART APEX CCD areadetector diffractometer Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) *T*_{min} = 0.980, *T*_{max} = 0.994

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.162$
S = 1.02
2721 reflections

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdots A$
D2−H2D···O3 ⁱ	0.82	1.79	2.603 (4)	170
C5−H5···O3′	0.93	2.63	3.478 (5)	152
C16−H16A···Cg1	0.96	2.91	3.485 (3)	120

Symmetry code: (i) -x, -y, -z + 1. Cg1 is the centroid of the anthracene ring C8,C9,C10,C12A-C14A.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; 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 *PLATON* (Spek, 2009).

This work was supported by the Doctoral Foundation of Zhengzhou University of Light Industry (000420).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2166).

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supplementary materials

Acta Cryst. (2009). E65, o1223 [doi:10.1107/S1600536809014858]

4,4'-(Anthracene-9,10-diyl)dibenzoic acid dimethylformamide disolvate

H. Li, Z.-Q. Wang, L.-Z. Yang, Y.-Q. Liu and D.-B. Mao

Comment

Cyclopalladated ferrocenylimine complexs with monophosphino ligands were successfully used as catalysts for Suzuki reactions (Xu *et al.* 2006; Li *et al.*, 2006; Xu *et al.* 2008). We have recently reported that the structure of 4-(2,5-dihexyloxyphenyl)benzoic acid was obtained from the Suzuki coupling reaction (Li *et al.*, 2008). The title compound was derived from the Suzuki reaction of 9,10-dibromoanthracene and 4-carboxyphenylboronic acid.

In the title compound (Fig.1), the dihedral angle between benzene rings and anthracene rings is 74.05 (12)°. A crystallographic inversion centre is in the middle of the anthracene unit, and an approximate two-fold pseudo rotation axis is running along the plane of the anthracene unit. The dimethylformamide solvent molecules are partially disordered over two positions, O3 and O3', of approximately equal occupancy, (0.529 (6) and 0.471 (6), respectively. The different intermolecular hydrogen bonding contacts are shown in Fig. 1 (O3' is the acceptor) and Fig. 2 (with O3 as acceptor). The intermolecular O—H…O hydrogen bonds result in the formation of long 2:1 solvate:complex aggregates, (Table 1) which are alternately linked *via* weak intermolecular C—H…O contacts generated from the rotational disorder of the formamide oxygen atom (0.471 (6) site occupancy). C—H… π interactions support these contacts in the crystal structure foming a one-dimensional supramolecular architecture (Fig. 1 and Fig. 2).

Experimental

The title compound was obtained from the Suzuki coupling reaction of 9,10-dibromoanthracene and 4-carboxyphenylboronic acid as described in the literature (Li *et al.*, 2008) and recrystallized from dimethylformamide at room temperature to give the desired crystals suitable for single-crystal X-ray diffraction.

Refinement

H atoms attached to C atoms of the title compound were placed in geometrically idealized positions and treated as riding with C—H distances constrained to 0.93 (aromatic CH), or 0.96 Å (methyl CH₃), and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$ (1.5 U_{eq} for methyl H). The atom-site occupancies for the rotational disordered formamide oxygen atoms O3 and O3' refined to a ratio of 0.53/0.47.

Alert levels A and B for short intermolecular O1···O3' and H2D···H15' contacts with distances of2.50 Å and 2.01 Å may be explained by the difficulties to split the whole solvent molecule due to the pseudo two-fold rotation of the methyl groups around the N1—C15 axis. BUMP instruction or splitting of the whole solvent molecule resulted in unstable refinements. Introduction of shift-limiting restraints (DAMP instruction) resulted in larger R-values without improving the geometries. Therefore the partial disorder refinement (O3, O3', H15, H15') was preferred as a compromise.

Figures



Fig. 1. The molecular structure of the title compound with displacement ellipsoids at the 30% probability level (suffix A denotes the symmetry code: -x + 1, -y + 1, -z). Weak C—H··· π and C—H···O hydrogen bonding contacts are indicated with dashed lines. Cg1 is the centroid of the anthracene ring C8, C9, C10, C12A, C13A, C14A.

Fig. 2. Partial view of the crystal packing showing the intermolecular O—H···O hydrogen bonds and weak C—H··· π interactions. Cg1 is the centroid of the anthracene ring (C8, C9, C10, C12A, C13A, C14A).

4,4'-(Anthracene-9,10-diyl)dibenzoic acid dimethylformamide disolvate

Crystal data

$C_{28}H_{18}O_4 \cdot 2C_3H_7NO$	Z = 1
$M_r = 564.62$	$F_{000} = 298$
Triclinic, PT	$D_{\rm x} = 1.270 {\rm ~Mg~m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
a = 7.3692 (15) Å	Cell parameters from 879 reflections
<i>b</i> = 8.9981 (18) Å	$\theta = 2.9 - 22.0^{\circ}$
c = 12.124 (2) Å	$\mu = 0.09 \text{ mm}^{-1}$
$\alpha = 71.157 \ (3)^{\circ}$	T = 295 K
$\beta = 77.640 \ (3)^{\circ}$	Block, colourless
$\gamma = 79.754 \ (3)^{\circ}$	$0.23\times0.16\times0.06~mm$
$V = 738.0 (3) \text{ Å}^3$	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	2721 independent reflections
Radiation source: fine-focus sealed tube	1467 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\rm int} = 0.028$
T = 295 K	$\theta_{\text{max}} = 25.5^{\circ}$
φ and ω scans	$\theta_{\min} = 2.4^{\circ}$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -8 \rightarrow 8$
$T_{\min} = 0.980, \ T_{\max} = 0.994$	$k = -10 \rightarrow 9$
5691 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

 $R[F^{2} > 2\sigma(F^{2})] = 0.053$ H-atom parameters constrained $wR(F^{2}) = 0.162$ S = 1.02 $\Delta \rho_{max} = 0.16 \text{ e}^{A^{-3}}$ Primary atom site location: structure-invariant direct

Primary atom site location: structure-invariant direct methods Extinction correction: none

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2 , conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic aisplacement parameters (A	lent isotropic displacement parameters (A^2)	equivalent isotropic a	l isotropic or	coordinates and	l atomic	Fractional
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	x	У	Ζ	Uiso*/Ueq	Occ. (<1)
C15	0.5707 (5)	0.2790 (4)	0.4860 (3)	0.0742 (9)	0.529 (6)
H15	0.4771	0.2595	0.4536	0.089*	0.529 (6)
O3	0.5840 (5)	0.2039 (5)	0.5938 (4)	0.0918 (18)	0.529 (6)
C15'	0.5707 (5)	0.2790 (4)	0.4860 (3)	0.0742 (9)	0.471 (6)
H15'	0.5944	0.2141	0.5598	0.089*	0.471 (6)
O3'	0.4309 (7)	0.2700 (6)	0.4479 (4)	0.096 (2)	0.471 (6)
N1	0.6843 (3)	0.3826 (3)	0.41928 (19)	0.0637 (6)	
C16	0.6620 (5)	0.4705 (4)	0.2994 (3)	0.0999 (12)	
H16A	0.5498	0.4476	0.2831	0.150*	
H16B	0.7677	0.4407	0.2459	0.150*	
H16C	0.6535	0.5816	0.2895	0.150*	
C17	0.8377 (4)	0.4104 (5)	0.4627 (3)	0.0945 (11)	
H17A	0.8375	0.3450	0.5429	0.142*	
H17B	0.8249	0.5196	0.4598	0.142*	
H17C	0.9532	0.3852	0.4146	0.142*	
01	-0.1924 (3)	-0.0937 (3)	0.42504 (19)	0.1024 (9)	
O2	-0.3377 (3)	-0.0181 (3)	0.2730 (2)	0.1090 (9)	
H2D	-0.4140	-0.0728	0.3213	0.163*	
C1	-0.0616 (3)	0.0915 (3)	0.2520(2)	0.0496 (6)	
C2	-0.0651 (4)	0.1757 (3)	0.1348 (2)	0.0638 (8)	
H2	-0.1589	0.1662	0.0978	0.077*	
C3	0.0713 (4)	0.2746 (3)	0.0719 (2)	0.0594 (7)	
H3	0.0669	0.3313	-0.0068	0.071*	
C4	0.2133 (3)	0.2901 (3)	0.1243 (2)	0.0445 (6)	

supplementary materials

C5	0.2169 (3)	0.2037 (3)	0.2414 (2)	0.0525 (7)
Н5	0.3117	0.2117	0.2783	0.063*
C6	0.0805 (3)	0.1053 (3)	0.3045 (2)	0.0537 (7)
H6	0.0852	0.0480	0.3831	0.064*
C7	-0.2053 (4)	-0.0146 (3)	0.3219 (3)	0.0643 (8)
C8	0.6573 (4)	0.1754 (3)	-0.1369 (2)	0.0640 (8)
H8	0.6611	0.0821	-0.1552	0.077*
C9	0.5159 (4)	0.2148 (3)	-0.0568 (2)	0.0549 (7)
Н9	0.4239	0.1477	-0.0204	0.066*
C10	0.5040 (3)	0.3575 (3)	-0.02629 (19)	0.0432 (6)
C11	0.3592 (3)	0.3985 (3)	0.05850 (19)	0.0419 (6)
C12	0.3533 (3)	0.5398 (3)	0.08512 (19)	0.0419 (6)
C13	0.2061 (3)	0.5896 (3)	0.1681 (2)	0.0514 (7)
H13	0.1110	0.5259	0.2059	0.062*
C14	0.2008 (4)	0.7263 (3)	0.1932 (2)	0.0620 (8)
H14	0.1031	0.7554	0.2478	0.074*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C15	0.066 (2)	0.089 (2)	0.066 (2)	-0.0197 (18)	-0.0072 (17)	-0.0164 (19)
O3	0.082 (3)	0.114 (4)	0.071 (3)	-0.054 (3)	-0.012 (2)	0.006 (3)
C15'	0.066 (2)	0.089 (2)	0.066 (2)	-0.0197 (18)	-0.0072 (17)	-0.0164 (19)
O3'	0.087 (4)	0.120 (4)	0.079 (3)	-0.060 (3)	-0.015 (3)	0.000 (3)
N1	0.0574 (14)	0.0753 (17)	0.0547 (14)	-0.0202 (12)	-0.0040 (11)	-0.0113 (12)
C16	0.088 (2)	0.119 (3)	0.071 (2)	-0.022 (2)	-0.0099 (18)	0.004 (2)
C17	0.079 (2)	0.125 (3)	0.086 (2)	-0.045 (2)	-0.0063 (19)	-0.028 (2)
01	0.0933 (16)	0.128 (2)	0.0722 (15)	-0.0639 (15)	-0.0176 (13)	0.0188 (14)
O2	0.0826 (16)	0.137 (2)	0.0938 (17)	-0.0672 (15)	-0.0245 (14)	0.0188 (15)
C1	0.0454 (14)	0.0470 (15)	0.0548 (16)	-0.0134 (12)	-0.0041 (12)	-0.0114 (12)
C2	0.0535 (16)	0.0701 (19)	0.0652 (18)	-0.0227 (14)	-0.0159 (14)	-0.0045 (15)
C3	0.0605 (16)	0.0624 (18)	0.0512 (15)	-0.0233 (14)	-0.0133 (13)	-0.0001 (13)
C4	0.0460 (14)	0.0408 (14)	0.0468 (14)	-0.0098 (11)	-0.0061 (11)	-0.0115 (12)
C5	0.0541 (15)	0.0553 (16)	0.0474 (15)	-0.0189 (13)	-0.0085 (12)	-0.0077 (13)
C6	0.0593 (16)	0.0519 (16)	0.0453 (14)	-0.0170 (13)	-0.0041 (12)	-0.0058 (12)
C7	0.0506 (17)	0.0634 (19)	0.074 (2)	-0.0191 (14)	-0.0030 (15)	-0.0121 (16)
C8	0.085 (2)	0.0442 (16)	0.0605 (17)	-0.0144 (14)	0.0043 (15)	-0.0192 (14)
C9	0.0667 (17)	0.0400 (15)	0.0549 (16)	-0.0186 (12)	0.0012 (13)	-0.0107 (12)
C10	0.0494 (14)	0.0359 (14)	0.0416 (13)	-0.0110 (11)	-0.0061 (11)	-0.0054 (11)
C11	0.0453 (13)	0.0386 (14)	0.0391 (13)	-0.0119 (10)	-0.0083 (11)	-0.0034 (11)
C12	0.0426 (13)	0.0404 (14)	0.0404 (13)	-0.0080 (10)	-0.0063 (10)	-0.0074 (11)
C13	0.0485 (14)	0.0494 (16)	0.0499 (15)	-0.0125 (12)	0.0041 (12)	-0.0104 (12)
C14	0.0724 (18)	0.0492 (17)	0.0573 (17)	-0.0080 (14)	0.0079 (14)	-0.0178 (14)

Geometric parameters (Å, °)

C15—O3	1.279 (4)	С3—Н3	0.9300
C15—N1	1.314 (4)	C4—C5	1.385 (3)
C15—H15	0.9300	C4—C11	1.499 (3)

NI-C16 1.441 (3) C5-H5 0.9300 C16-H16A 0.9600 C6-H6 0.9300 C16-H16B 0.9600 C8-C9 1.346 (3) C17-H17A 0.9600 C8-H8 0.9300 C17-H17B 0.9600 C9-C10 1.430 (3) C17-H17C 0.9600 C9-H9 0.9300 O1-C7 1.238 (3) C10-C12' 1.438 (3) O2-C7 1.255 (3) C10-C12' 1.438 (3) O2-C7 1.381 (3) C12-C10' 1.438 (3) C1-C2 1.381 (3) C12-C10' 1.438 (3) C1-C2 1.381 (3) C13-C14 1.353 (3) C2-H2 0.9300 C14-C8' 1.06(4) C3-C4 1.382 (3) C14-H14 0.9300 C2-H2 0.9300 C14-C5' 1.06 D1-C15-H15 1.88 C4-C5-H5 1.06 D1-C15-H15 1.88 C4-C5-H5 1.06 D1-C15-H15 1.88 C4-C5-H5 1.08 D1-C15-H15<	N1—C17	1.434 (4)	C5—C6	1.389 (3)
C16—H16A 0.9600 C8—C9 1.346 (3) C16—H16C 0.9600 C8—C14 ¹ 1.406 (4) C17—H17A 0.9600 C9—C10 1.430 (3) C17—H17B 0.9600 C9—C10 1.430 (3) C17—H17C 0.9600 C9—H19 0.9300 C17—H17C 0.9600 C9—H19 0.9300 O1—C7 1.238 (3) C10—C11 1.433 (3) O2—H2D 0.8200 C11—C12 1.438 (3) C1—C2 1.381 (3) C12—C13 1.428 (3) C1—C2 1.381 (3) C12—C10 ¹ 1.438 (3) C2—C3 1.392 (3) C14—H13 0.9300 C2—H2 0.9300 C14—C8 ¹ 1.406 (4) C3—C15—H1 1.25 (4) C4—C5—H5 119.6 N1—C15—H15 118.8 C4—C5—H5 119.6 N1—C15—H15 118.8 C4—C5—H5 119.6 C15—N1—C17 121.0 (3) C1—C6—C5 120.8 (2) C15—N1—C16 117.5 (2) C5—G—H6 119.6 C15—N1—C16 117.5 (2) C5—G—H6 119.6	N1—C16	1.441 (3)	С5—Н5	0.9300
C16—H16B 0.9600 C8—C9 1.346 (3) C16—H16C 0.9600 C8—C1 a^i 1.406 (4) C17—H17A 0.9600 C9—C10 1.430 (3) C17—H17B 0.9600 C9—H9 0.9300 C17—H17C 0.9600 C9—H9 0.9300 O1—C7 1.258 (3) C10—C12 1.438 (3) O2—C7 1.255 (3) C10—C12 1.438 (3) C1—C6 1.378 (3) C12—C13 1.428 (3) C1—C7 1.485 (3) C13—C14 1.353 (3) C2—H2 0.9300 C14—C4 ⁱ 1.406 (4) C3—C4 1.382 (3) C14—H14 0.9300 C3—C4 1.382 (3) C14—C4 ⁱ 1.406 (4) C3—C4 1.382 (3) C14—C4 ⁱ 1.406 (4) C3—C4 1.382 (3) C14—C5 1.205 (2) C15—N1 122.5 (4) C4—C5—C6 120.7 (2) C3—C15—N1 122.5 (4) C4—C5—C6 120.8 (2) C15—N1—C16 121.5 (3) C1—C6—C5 120.8 (2)	C16—H16A	0.9600	С6—Н6	0.9300
C16—H16C 0.9600 $C8-C14^i$ 1.406 (4) C17—H17A 0.9600 C9-C10 1.430 (3) C17—H17B 0.9600 C9-H9 0.9300 OL-C7 1.238 (3) C10-C11 1.403 (3) O2-C7 1.255 (3) C10-C12 1.401 (3) C1-C6 1.378 (3) C12-C13 1.428 (3) C1-C6 1.378 (3) C12-C14 1.353 (3) C1-C7 1.483 (3) C13-C14 1.353 (3) C2-C3 1.392 (3) C13-H13 0.9300 C2-C4 0.9300 C14-C5 ⁱ 1.406 (4) C3-C15-N1 1.225 (4) C4-C5-C6 1207 (2) O3-C15-N1 1.225 (4) C4-C5-C5 1208 (2) C15-N1-C17 121 0 (3) C1-C6-C5 1208 (2) C15-N1-C16 1175 (2) C5-C6-H6 119.6 N1-C16-H16A 109.5 01-C7-O2 122.7 (3) N1-C16-H16B 109.5 01-C7-O2 122.7 (3) N1-C16-H16B 109.5 C1-C6-H6 119.6 N1-C16-H16B 109.5 C1-C7-C1 119.7 (3)	C16—H16B	0.9600	C8—C9	1.346 (3)
C17-H17A 0.9600 C8-H8 0.9300 C17-H17B 0.9600 C9-C10 1.430 (3) C17-H17C 0.9600 C9-H9 0.9300 01-C7 1.238 (3) C10-C11 1.430 (3) 02-H2D 0.8200 C11-C12 1.438 (3) 02-H2D 0.8200 C12-C13 1.428 (3) C1-C2 1.381 (3) C12-C10 ¹ 1.438 (3) C1-C2 1.381 (3) C12-C13 1.428 (3) C2-H2 0.9300 C14-C4 ¹ 1.436 (4) C3-C4 1.382 (3) C14-H14 0.9300 C3-C4 1.382 (3) C14-C4 ¹ 1.96 (4) C15-N1 122.5 (4) C4-C5-C6 120.7 (2) 03-C15-H15 118.8 C4-C5-H5 119.6 N1-C15 118.8 C4-C5-H5 119.6 C17-N1-C16 121.5 (3) C1-C6-H6 119.6 N1-C16-H16A 109.5 O2-C7-C1 117.6 (3) N1-C16-H16B 109.5 C14-C8-H8 119.6	C16—H16C	0.9600	C8—C14 ⁱ	1.406 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C17—H17A	0.9600	С8—Н8	0.9300
C17-H17C 0.9600 C9-H9 0.9300 O1-C7 1.238 (3) C10-C11 1.403 (3) 02-C7 1.235 (3) C10-C12 1.438 (3) 02-H2D 0.8200 C11-C12 1.438 (3) C1-C6 1.378 (3) C12-C13 1.428 (3) C1-C7 1.381 (3) C12-C13 1.438 (3) C2-C3 1.392 (3) C13-C14 0.9300 C2-H2 0.9300 C14-C8 ⁱ 1.406 (4) C3-C15-N1 1.22.5 (4) C4-C5-H5 119.6 N1-C15-H15 118.8 C4-C5-H5 119.6 N1-C15-H15 118.8 C4-C5-H5 119.6 C15-N1-C17 121.0 (3) C1-C6-C5 120.7 (2) C15-N1-C16 121.5 (3) C1-C6-C5 120.8 (2) C15-N1-C16 121.5 (3) C1-C6-C5 120.8 (3) N1-C16-H16A 109.5 01-C7-02 122.7 (3) N1-C16-H16B 109.5 02-C7-C1 117.6 (3) N1-C16-H16B 109.5 C9-C8-C14 ⁱ 120.8 (3) N1-C16-H16C 109.5 C9-C8-H8 119	С17—Н17В	0.9600	C9—C10	1.430 (3)
$01-C7$ 1.238 (3) $C10-C11$ 1.403 (3) $02-C7$ 1.255 (3) $C10-C12^i$ 1.438 (3) $02-H2D$ 0.8200 $C11-C12$ 1.401 (3) $C1-C6$ 1.378 (3) $C12-C13$ 1.428 (3) $C1-C2$ 1.381 (3) $C12-C10^i$ 1.438 (3) $C1-C7$ 1.485 (3) $C13-C14$ 1.353 (3) $C2-C3$ 1.392 (3) $C13-H13$ 0.9300 $C2-H2$ 0.9300 $C14-C8^i$ 1.406 (4) $C3-C4$ 1.382 (3) $C14-C5-C6$ 120.7 (2) $O3-C15-N1$ 122.5 (4) $C4-C5-H5$ 119.6 $N1-C15-H15$ 118.8 $C4-C5-H5$ 119.6 $N1-C15-H15$ 118.8 $C4-C5-H5$ 119.6 $C15-N1-C17$ 121.0 (3) $C1-C6-C5$ 120.8 (2) $C15-N1-C16$ 121.5 (3) $C1-C6-H6$ 119.6 $N1-C16-H16A$ 109.5 $01-C7-C1$ 119.7 (3) $N1-C16-H16B$ 109.5 $01-C7-C1$	С17—Н17С	0.9600	С9—Н9	0.9300
$02-C7$ $1.255 (3)$ $C10-C12^i$ $1.438 (3)$ $02-H2D$ 0.8200 $C11-C12$ $1.401 (3)$ $C1-C6$ $1.378 (3)$ $C12-C13$ $1.428 (3)$ $C1-C7$ $1.485 (3)$ $C12-C10^i$ $1.438 (3)$ $C1-C7$ $1.485 (3)$ $C13-C14$ $1.353 (3)$ $C2-H2$ 0.9300 $C14-C8^i$ $1.406 (4)$ $C3-C4$ $1.382 (3)$ $C14-H14$ 0.9300 $C3-C4$ $1.382 (3)$ $C14-C8^i$ $1.406 (4)$ $C3-C4$ $1.382 (3)$ $C14-C8^i$ $1.496 (4)$ $C3-C4$ $1.382 (3)$ $C14-C5-C6$ $120.7 (2)$ $O3-C15-M1$ $122.5 (4)$ $C4-C5-H5$ 119.6 $N1-C15-H15$ 118.8 $C4-C5-H5$ 119.6 $N1-C16-H16$ $102.5 (3)$ $C1-C6-H6$ 119.6 $N1-C16-H16B$ 109.5 $O1-C7-C1$ $117.6 (3)$ $N1-C16-H16B$ 109.5 $C9-C8-H8$ 119.6 $N1-C16-H16C$ 109.5 $C14-C8-H8$ <t< td=""><td>O1—C7</td><td>1.238 (3)</td><td>C10—C11</td><td>1.403 (3)</td></t<>	O1—C7	1.238 (3)	C10—C11	1.403 (3)
$02-H2D$ 0.8200 $C11-C12$ $1.401(3)$ $C1-C6$ $1.378(3)$ $C12-C13$ $1.428(3)$ $C1-C2$ $1.381(3)$ $C12-C10^1$ $1.438(3)$ $C1-C7$ $1.488(3)$ $C13-C14$ $1.353(3)$ $C2-C3$ $1.392(3)$ $C13-H13$ 0.9300 $C2-H2$ 0.9300 $C14-C8^1$ $1.406(4)$ $C3-C15-N1$ $122.5(4)$ $C4-C5-H5$ 19.6 $O3-C15-H15$ 118.8 $C4-C5-H5$ 19.6 $O3-C15-H15$ 118.8 $C6-C5-H5$ $120.8(2)$ $C15-N1-C17$ $121.0(3)$ $C1-C6-C5$ $120.8(2)$ $C15-N1-C16$ $117.5(2)$ $C5-C6-H6$ 19.6 $N1-C16-H16A$ 109.5 $O1-C7-O2$ $122.7(3)$ $N1-C16-H16B$ 109.5 $O2-C7-C1$ $119.7(3)$ $N1-C16-H16B$ 109.5 $O2-C7-C1$ $119.7(3)$ $N1-C16-H16C$ 109.5 $C14^{-1}C8-H8$ 119.6 $N1-C17-H17A$ 109.5 $C8-C9-H9$ 19.2 $N1-C17-H17B$ 109.5 $C14-C3-H18$ 19	O2—C7	1.255 (3)	C10-C12 ⁱ	1.438 (3)
C1-C6 1.378 (3) C12-C13 1.428 (3) C1-C2 1.381 (3) C12-C10 ⁱ 1.438 (3) C1-C7 1.485 (3) C13-C14 1.353 (3) C2-C3 1.392 (3) C13-H13 0.9300 C2-H2 0.9300 C14-C8 ⁱ 1.406 (4) C3-C4 1.382 (3) C14-H14 0.9300 O3-C15-N1 122.5 (4) C4-CS-C6 120.7 (2) O3-C15-H15 118.8 C6-CS-H5 119.6 N1-C15-H15 118.8 C6-CS-H5 19.6 C15-N1-C16 121.5 (3) C1-C6-C5 120.8 (2) C17-N1-C16 117.5 (2) CS-C6-H6 119.6 N1-C16-H16A 109.5 O1-C7-O2 122.7 (3) N1-C16-H16B 109.5 O2-C7-C1 119.7 (3) H16A-C16-H16B 109.5 C9-C8-C14 ⁱ 120.8 (3) N1-C17-H17B 109.5 C14-C8-H8 119.6 N1-C17-H17B 109.5 C10-C9-H9 122 N1-C17-H17B 109.5 C12-C11-C1	O2—H2D	0.8200	C11—C12	1.401 (3)
C1-C2 1.381 (3) C12-C10 ⁱ 1.488 (3) C1-C7 1.485 (3) C13-C14 1.353 (3) C2-C3 1.392 (3) C13-H13 0.9300 C2-H2 0.9300 C14-C8 ⁱ 1.406 (4) C3-C4 1.382 (3) C14-H14 0.9300 O3-C15-N1 122.5 (4) C4-C5-C6 120.7 (2) O3-C15-H15 118.8 C4-C5-H5 119.6 N1-C15-H15 118.8 C6-C5-H5 120.8 (2) C15-N1-C16 121.5 (3) C1-C6-H6 119.6 C15-N1-C16 121.5 (3) C1-C6-H6 119.6 N1-C16-H16A 109.5 O1-C7-O2 122.7 (3) N1-C16-H16B 109.5 O2-C7-C1 117.6 (3) N1-C16-H16B 109.5 C9-C8-H8 119.6 N1-C16-H16C 109.5 C9-C8-H8 119.6 N1-C16-H16C 109.5 C8-C9-H9 119.2 N1-C1-H17B 109.5 C8-C9-H9 119.2 N1-C17-H17A 109.5 C8-C9-H9 119.2 N1-C17-H17B 109.5 C14-C10-C19 122.0 (2) <td>C1—C6</td> <td>1.378 (3)</td> <td>C12—C13</td> <td>1.428 (3)</td>	C1—C6	1.378 (3)	C12—C13	1.428 (3)
C1-C71.485 (3)C13-C141.353 (3)C2-C31.392 (3)C13-H130.9300C2-H20.9300C14-C8 ⁱ 1.406 (4)C3-C41.382 (3)C14-H140.9300O3-C15-N1122.5 (4)C4-C5-C6120.7 (2)O3-C15-H15118.8C4-C5-H5119.6N1-C15-H15118.8C4-C5-H5119.6C15-N1-C16121.6 (3)C1-C6-C5120.8 (2)C15-N1-C16121.5 (3)C1-C6-H6119.6C17-N1-C1617.5 (2)C5-C6-H6119.6N1-C16-H16B109.5O1-C7-O2122.7 (3)N1-C16-H16B109.5O2-C7-C1117.6 (3)N1-C16-H16B109.5C9-C8-H8119.6N1-C16-H16C109.5C9-C8-H8119.6N1-C17-H17A109.5C8-C9-H9119.2N1-C17-H17B109.5C11-C10-C9121.5 (2)N1-C17-H17B109.5C11-C10-C9122.0 (2)H17A-C17-H17C109.5C11-C10-C9122.0 (2)H17A-C17-H17C109.5C10-C12 ⁱ 119.9 (2)C6-C1-C7119.4 (2)C12-C10-C12 ⁱ 119.9 (2)C6-C1-C7119.4 (2)C11-C12-C13122.3 (2)C1-C2-H2119.9C13-C12-C10 ⁱ 122.3 (2)C1-C2-C3120.2 (2)C11-C12-C13122.3 (2)C1-C2-C3120.2 (2)C11-C12-C10 ⁱ 120.2 (2)C1-C2-H2119.9C13-C12-C10 ⁱ 120.2 (2)C1-C2-H2119.9C13-C12-C10 ⁱ 120.2 (2)<	C1—C2	1.381 (3)	C12—C10 ⁱ	1.438 (3)
$C2-C3$ $I.392 (3)$ $C13-H13$ 0.9300 $C2-H2$ 0.9300 $C14-C8^{i}$ $I.406 (4)$ $C3-C4$ $I.382 (3)$ $C14-H14$ 0.9300 $O3-C15-N1$ $I22.5 (4)$ $C4-C5-C6$ $I20.7 (2)$ $O3-C15-H15$ $I18.8$ $C4-C5-H5$ $I19.6$ $N1-C15-H15$ $I18.8$ $C6-C5-H5$ $I19.6$ $N1-C15-H15$ $I12.15 (3)$ $C1-C6-C5$ $I20.8 (2)$ $C15-N1-C16$ $I21.5 (3)$ $C1-C6-H6$ $I19.6$ $N1-C16-H16A$ 109.5 $O1-C7-O2$ $I22.7 (3)$ $N1-C16-H16B$ 109.5 $O1-C7-O2$ $I22.7 (3)$ $N1-C16-H16B$ 109.5 $O1-C7-C1$ $I17.6 (3)$ $N1-C16-H16B$ 109.5 $O2-C7-C1$ $I17.6 (3)$ $N1-C16-H16B$ 109.5 $C9-C8-H8$ $I19.6$ $N1-C16-H16C$ 109.5 $C14-C8-H8$ $I19.6$ $N1-C17-H17B$ 109.5 $C8-C9-C10$ $I21.5 (2)$ $N1-C17-H17B$ 109.5 $C10-C9-H9$ 119.2 $N1-C17-H17B$ 109.5 $C10-C10-C12^{i}$ $119.9 (2)$ $H17A-C17-H17B$ 109.5 $C10-C10-C12^{i}$ $119.9 (2)$ $H17A-C17-H17C$ 109.5 $C12-C10-C12^{i}$ $119.9 (2)$ $H17A-C17-H17C$ 109.5 $C12-C10-C12^{i}$ $119.9 (2)$ $C7-O2-H2D$ 109.5 $C12-C10-C12^{i}$ $119.9 (2)$ $C1-C2-C1$ $119.4 (2)$ $C10-C1-C12^{i}$ $122.2 (2)$ $C1-C2-C1$ $119.9 (2)$ $C14-C13-C12$ $122.0 (2)$ $C1-C2-C1-C7$ $119.9 ($	C1—C7	1.485 (3)	C13—C14	1.353 (3)
$C2-H2$ 0.9300 $C14C8^i$ 1.406 (4) $C3-C4$ 1.382 (3) $C14H14$ 0.9300 $O3-C15-N1$ 122.5 (4) $C4C5C6$ 120.7 (2) $O3-C15-H15$ 118.8 $C4C5H5$ 119.6 $N1-C15-H15$ 118.8 $C6C5-H5$ 120.8 (2) $C15-N1-C17$ 121.0 (3) $C1-C6H6$ 119.6 $C17-N1-C16$ 117.5 (2) $C5-C6-H6$ 119.6 $O1-C7-O2$ 122.7 (3) $O1-C7-O2$ 122.7 (3) $N1-C16-H16A$ 109.5 $O1-C7-C1$ 119.7 (3) $N1-C16-H16B$ 109.5 $O2-C7-C1$ 117.6 (3) $N1-C16-H16B$ 109.5 $C9-C8-C14^i$ 120.8 (3) $N1-C16-H16C$ 109.5 $C9-C8-H8$ 119.6 $N1-C17-H17B$ 109.5 $C14^{-1}-C8-H8$ 119.6 $N1-C17-H17B$ 109.5 $C1-C9-H19$ 119.2 $N1-C17-H17B$ 109.5 $C1-C9-H19$ 119.2 $N1-C17-H17B$ 109.5 $C1-C9-H19$ 119.2 $N1-C17-H17B$ 109.5 $C1-C1-C10-C9$ 122.0 (2) $N1-C17-H17C$ 109.5 $C1-C1-C10-C12^i$ 118.1 (2) $C7-O2-H2D$ 109.5 $C12-C11-C10$ 119.9 (2) $C1-C2-C1$ 118.9 (2) $C12-C11-C10$ 119.9 (2) $C1-C2-C1$ 118.9 (2) $C12-C11-C10$ 119.3 (2) $C-C1-C7$ 121.6 (2) $C12-C11-C10$ 119.3 (2) $C-C2-C1$ 118.9 (2) $C12-C11-C10$ 119.9 (2) $C1-C2-C12$ 118.9 (2) $C12-C11-C10$ 119.3 (2) $C-C2-C12$ 118.9 (2) $C12-C11-$	C2—C3	1.392 (3)	С13—Н13	0.9300
C3—C4 1.382 (3) C14—H14 0.9300 O3—C15—N1 122.5 (4) C4—C5—C6 120.7 (2) O3—C15—N1 122.5 (4) C4—C5—C6 120.7 (2) O3—C15—H15 118.8 C4—C5—H5 119.6 N1—C15—H15 118.8 C6—C5—H5 120.8 (2) C15—N1—C17 121.0 (3) C1—C6—H6 119.6 C17—N1—C16 121.5 (3) C1—C6—H6 119.6 N1—C16—H16A 109.5 O1—C7—O2 122.7 (3) N1—C16—H16B 109.5 O2—C7—C1 117.6 (3) N1—C16—H16B 109.5 C9—C8—C14 ⁱ 120.8 (3) H16A—C16—H16C 109.5 C9—C8—H8 119.6 N1—C17—H17A 109.5 C14—C8—H8 119.6 N1—C17—H17A 109.5 C14—C8—H8 119.2 N1—C17—H17B 109.5 C11—C10—C9 122.0 (2) N1—C17—H17B 109.5 C11—C10—C12 ⁱ 119.9 (2) N1—C17—H17C 109.5 C12—C11—C10 119.9 (2) N1—C17—H17C 109.5 C12—C11—C10 119.9 (2) C6—C1—C1 118.4 (2)	С2—Н2	0.9300	C14—C8 ⁱ	1.406 (4)
$03-C15-N1$ $122.5 (4)$ $C4-C5-C6$ $120.7 (2)$ $03-C15-H15$ 118.8 $C4-C5-H5$ 119.6 $N1-C15-H15$ 118.8 $C6-C5-H5$ 119.6 $C15-N1-C17$ $121.0 (3)$ $C1-C6-C5$ $120.8 (2)$ $C15-N1-C16$ $121.5 (3)$ $C1-C6-H6$ 119.6 $C17-N1-C16$ $117.5 (2)$ $C5-C6-H6$ 119.6 $N1-C16-H16A$ 109.5 $01-C7-02$ $122.7 (3)$ $N1-C16-H16B$ 109.5 $02-C7-C1$ $117.6 (3)$ $N1-C16-H16B$ 109.5 $02-C7-C1$ $117.6 (3)$ $N1-C16-H16C$ 109.5 $C9-C8-H8$ 119.6 $N1-C16-H16C$ 109.5 $C9-C8-H8$ 119.6 $N1-C17-H17A$ 109.5 $C8-C9-C10$ $121.5 (2)$ $N1-C17-H17A$ 109.5 $C8-C9-H9$ 119.2 $N1-C17-H17B$ 109.5 $C1-C10-C9$ $122.0 (2)$ $N1-C17-H17C$ 109.5 $C1-C10-C12^{1}$ $119.9 (2)$ $N1-C17-H17C$ 109.5 $C1-C10-C12^{1}$ $119.9 (2)$ $N1-C17-H17C$ 109.5 $C1-C10-C12^{1}$ $119.9 (2)$ $C6-C1-C2$ $118.9 (2)$ $C12-C11-C10$ $119.9 (2)$ $C6-C1-C7$ $119.4 (2)$ $C10-C11-C4$ $120.8 (2)$ $C1-C2-H2$ 119.9 $C13-C12-C10^{1}$ $122.0 (2)$ $C1-C2-H2$ 119.9 $C13-C12-C10^{1}$ $117.5 (2)$ $C3-C2-H2$ 119.9 $C13-C12-C10^{1}$ $117.5 (2)$ $C3-C2-H2$ 119.9 $C13-C12-C10^{1}$ $117.5 (2)$ $C3-C2-H2$ 119.9 <	C3—C4	1.382 (3)	C14—H14	0.9300
$03-C15-H15$ 118.8 $C4-C5-H5$ 119.6 $NI-C15-H15$ 118.8 $C6-C5-H5$ 120.8 (2) $C15-N1-C17$ 121.0 (3) $C1-C6-H5$ 120.8 (2) $C15-N1-C16$ 121.5 (3) $C1-C6-H6$ 119.6 $C17-N1-C16$ 117.5 (2) $C5-C6-H6$ 119.6 $N1-C16-H16A$ 109.5 $01-C7-O2$ 122.7 (3) $N1-C16-H16B$ 109.5 $02-C7-C1$ 117.6 (3) $N1-C16-H16B$ 109.5 $02-C7-C1$ 117.6 (3) $N1-C16-H16C$ 109.5 $C9-C8-C14^{14}$ 120.8 (3) $N1-C16-H16C$ 109.5 $C9-C8-H8$ 119.6 $N1-C17-H17A$ 109.5 $C8-C9-C10$ 121.5 (2) $N1-C17-H17B$ 109.5 $C10-C9-H9$ 119.2 $N1-C17-H17B$ 109.5 $C11-C10-C9$ 122.0 (2) $N1-C17-H17C$ 109.5 $C11-C10-C12^{1}$ 118.1 (2) $C7-O2-H2D$ 109.5 $C11-C10-C12^{1}$ 118.1 (2) $C7-O2-H2D$ 109.5 $C12-C11-C10$ 119.9 (2) $C6-C1-C2$ 118.9 (2) $C12-C11-C14$ 119.3 (2) $C6-C1-C7$ 119.4 (2) $C10-C12^{1}$ 118.1 (2) $C1-C2-H2$ 119.9 $C13-C12-C10^{1}$ 122.3 (2) $C1-C2-C13$ 122.2 (2) $C11-C12-C10^{1}$ 120.2 (2) $C1-C2-C1-C7$ 121.6 (2) $C11-C12-C10^{1}$ 120.2 (2) $C1-C2-H2$ 119.9 $C13-C12-C10^{1}$ 122.0 (2) $C1-C2-H2$ 119.9 $C13-C12-C10^{1}$ 120.2 (2)	O3—C15—N1	122.5 (4)	C4—C5—C6	120.7 (2)
N1C15H15118.8C6C5H5119.6C15N1C17121.0 (3)C1C6C5120.8 (2)C15N1C16121.5 (3)C1C6H6119.6C17N1C1617.5 (2)C5C6H6119.6N1C16H16A109.5O1C7O2122.7 (3)N1C16H16B109.5O2C7C1117.6 (3)N1C16H16B109.5C9C8C14 ⁱ 120.8 (3)N1C16H16C109.5C9C8H8119.6N1C16H16C109.5C9C8H8119.6N1C17H17A109.5C8C9C10121.5 (2)N1C17H17B109.5C10C9H9119.2N1C17H17B109.5C11C10C12 ⁱ 119.9 (2)N1C17H17C109.5C11C10C12 ⁱ 119.9 (2)N1C17H17C109.5C12C11C14119.9 (2)C6C1C2118.9 (2)C12C11C14119.9 (2)C6C1C2118.9 (2)C12C11C14120.8 (2)C2C1C7121.6 (2)C11C12C13122.3 (2)C1C2C3120.2 (2)C11C12C13122.3 (2)C1C2C3120.2 (2)C11C12C13122.3 (2)C1C2H2119.9C13C12C10 ⁱ 117.5 (2)C3C2-H2119.9C13C12C10 ⁱ 117.5 (2)C3C2-H2119.9C14C13H13119.0C4C3-H3119.4C12C13H13119.0C2C3-H3119.4C12C13H13119.0C2C3-H3119.4C12C13H13 </td <td>O3—C15—H15</td> <td>118.8</td> <td>С4—С5—Н5</td> <td>119.6</td>	O3—C15—H15	118.8	С4—С5—Н5	119.6
C15N1C17121.0 (3)C1C6C5120.8 (2)C15N1C16121.5 (3)C1C6H6119.6C17N1C16117.5 (2)C5C6H6119.6N1C16H16A109.5O1C7O2122.7 (3)N1C16H16B109.5O2C7C1117.6 (3)N1C16H16B109.5C9C8C14 ⁱ 120.8 (3)N1C16H16C109.5C9C8H8119.6N1C16H16C109.5C9C8H8119.6N1C16H16C109.5C14 ⁱ -C8H8119.6N1C17H17A109.5C8C9C10121.5 (2)N1C17H17B109.5C8C9H9119.2N1C17H17B109.5C11C10C12 ⁱ 119.9 (2)N1C17H17C109.5C11C10C12 ⁱ 119.9 (2)N1-C17H17C109.5C12C11C10119.9 (2)H17AC17H17C109.5C12C11C10119.9 (2)C7O2H2D109.5C12C11C14119.3 (2)C6C1C2118.9 (2)C12C11C14120.8 (2)C2C1-C7121.6 (2)C11C12C13122.3 (2)C1C2C3120.2 (2)C11C12C10 ⁱ 120.2 (2)C1C2H2119.9C13C12C10 ⁱ 119.0C4C3H2119.9C13C12C10 ⁱ 112.5 (2)C1C2H2119.9C14C13H13119.0C4C3H3119.4C12C13H13119.0C2C1C3121.2 (2)C14C13H13119.0C2C2H3119.4C13-	N1—C15—H15	118.8	С6—С5—Н5	119.6
C15—N1—C16121.5 (3)C1—C6—H6119.6C17—N1—C16117.5 (2)C5—C6—H6119.6N1—C16—H16A109.5O1—C7—O2122.7 (3)N1—C16—H16B109.5O1—C7—C1119.7 (3)H16A—C16—H16B109.5O2—C7—C1117.6 (3)N1—C16—H16C109.5C9—C8—C14 ⁱ 120.8 (3)H16A—C16—H16C109.5C9—C8—H8119.6N1—C17—H17A109.5C8—C9—C10121.5 (2)N1—C17—H17B109.5C8—C9—H9119.2H17A—C17—H17B109.5C11—C10—C9122.0 (2)H17A—C17—H17C109.5C11—C10—C12 ⁱ 119.9 (2)H17B—C17—H17C109.5C12—C11—C10119.9 (2)H17B—C17—H17C109.5C12—C11—C10119.9 (2)C7—O2—H2D109.5C12—C11—C10119.9 (2)C6—C1—C2118.9 (2)C12—C11—C14119.3 (2)C6—C1—C7121.6 (2)C11—C12—C13122.3 (2)C1—C2—C3120.2 (2)C11—C12—C10 ⁱ 117.5 (2)C3—C2—H2119.9C13—C12—C10 ⁱ 117.5 (2)C3—C2—H2119.9C13—C12—C10 ⁱ 117.5 (2)C3—C2—H3119.4C12—C13—H13119.0C4—C3—H3119.4C12—C13—H13119.0C2—C3—H3119.4C13—C14—H14120.0	C15—N1—C17	121.0 (3)	C1—C6—C5	120.8 (2)
C17N1C16117.5 (2)C5C6H6119.6N1C16H16A109.5O1C7O2122.7 (3)N1C16H16B109.5O2C7C1119.7 (3)H16AC16H16B109.5O2C7C1117.6 (3)N1C16H16C109.5C9C8C14^i120.8 (3)H16AC16H16C109.5C9C8H8119.6N1C17H17A109.5C8C9C10121.5 (2)N1C17H17B109.5C8C9H9119.2H17AC17H17B109.5C10C9H9122.0 (2)N1C17H17C109.5C11C10C9122.0 (2)H17AC17H17C109.5C11C10C12^i119.9 (2)C6C1C2118.9 (2)C12C11C4119.3 (2)C6C1C2119.9 (2)C10C11C4120.8 (2)C2C1C7121.6 (2)C11C12C10^i122.3 (2)C1C2C3120.2 (2)C11C12C10^i120.2 (2)C1C2C3120.2 (2)C11C12C10^i120.2 (2)C1C2H219.9C13C12C10^i120.2 (2)C1C2H219.9C14C13C12122.0 (2)C4C3C2121.2 (2)C14C13H13119.0C4C3C2121.2 (2)C14C13H13119.0C4C3H3119.4C12C13H13119.0C2C3H3119.4C12C13H13119.0C2C3H3119.4C13C14C8^i120.0 (2)C3C4C5118.1 (2)C13C14H14120.0	C15—N1—C16	121.5 (3)	С1—С6—Н6	119.6
N1C16H16A109.5O1C7O2122.7 (3)N1C16H16B109.5O1C7C1119.7 (3)H16AC16H16B109.5O2C7C1117.6 (3)N1C16H16C109.5C9C8C14 ⁱ 120.8 (3)H16AC16H16C109.5C9C8H8119.6H16BC16H16C109.5C14 ⁱ -C8H8119.6N1C17H17A109.5C8C9C10121.5 (2)N1C17H17B109.5C8C9H9119.2H17AC17H17B109.5C10C9H9122.0 (2)H17AC17H17C109.5C11C10C12 ⁱ 119.9 (2)N1C17H17C109.5C10C12 ⁱ 119.9 (2)C6C1C2118.9 (2)C12C11C10119.9 (2)C6C1C2118.9 (2)C12C11C10119.9 (2)C6C1C7121.6 (2)C11C12C13122.3 (2)C1C7121.6 (2)C11C12C13122.3 (2)C1C2H2119.9C13C12C10 ⁱ 117.5 (2)C3C2H2119.9C14C13H13119.0C4C3C2121.2 (2)C14C13H13119.0C4C3H3119.4C12C13H13119.0C2C3H3119.4C13C14C8 ⁱ 120.0 (2)C3C4C5118.1 (2)C13C14H14120.0	C17—N1—C16	117.5 (2)	С5—С6—Н6	119.6
N1C16H16B109.5 $01C7C1$ 119.7 (3)H16AC16H16B109.5 $02C7C1$ 117.6 (3)N1C16H16C109.5 $C9C8C14^{i}$ 120.8 (3)H16AC16H16C109.5 $C9C8H8$ 119.6 H16BC16H16C109.5 $C14^{i}-C8H8$ 119.6 N1C17H17A109.5 $C8C9C10$ 121.5 (2)N1C17H17B109.5 $C10C9H9$ 119.2 H17AC17H17B109.5 $C11C10C12^{i}$ 119.9 (2)H17AC17H17C109.5 $C11C10C12^{i}$ 119.9 (2)H17BC17H17C109.5 $C9C10C12^{i}$ 118.1 (2)C7O2H2D109.5 $C12C11C10$ 119.9 (2)C6C1C2118.9 (2) $C12C11C4$ 119.3 (2)C6C1C7119.4 (2) $C10C11C4$ 120.8 (2)C1C2C3120.2 (2) $C11C12C10^{i}$ 120.2 (2)C1C2H2119.9 $C13C12C10^{i}$ 117.5 (2)C3C2H2119.9 $C14C13C12$ 120.2 (2)C4C3H3119.4 $C12C13H13$ 119.0 C4C3H3119.4 $C12C13H13$ 119.0 C2C3H3119.4 $C13C14C8^{i}$ 120.0 (2)C3C4C5118.1 (2) $C13C14H14$ 120.0	N1—C16—H16A	109.5	O1—C7—O2	122.7 (3)
H16A—C16—H16B109.5 $02-C7-C1$ 117.6 (3)N1—C16—H16C109.5 $C9-C8-C14^{i}$ 120.8 (3)H16A—C16—H16C109.5 $C9-C8-H8$ 119.6N1-C17—H17A109.5 $C14^{i}-C8-H8$ 119.6N1-C17—H17B109.5 $C8-C9-C10$ 121.5 (2)N1-C17—H17B109.5 $C8-C9-H9$ 119.2H17A-C17—H17B109.5 $C10-C9-H9$ 119.2N1-C17—H17C109.5 $C11-C10-C9$ 122.0 (2)H17A-C17—H17C109.5 $C11-C10-C12^{i}$ 119.9 (2)H17B-C17—H17C109.5 $C12-C11-C10$ 119.9 (2)C7-O2-H2D109.5 $C12-C11-C10$ 119.9 (2)C6-C1-C2118.9 (2) $C12-C11-C4$ 119.3 (2)C6-C1-C7119.4 (2) $C10-C11-C4$ 120.8 (2)C2-C1-C7121.6 (2) $C11-C12-C10^{i}$ 120.2 (2)C1-C2-H2119.9 $C13-C12-C10^{i}$ 117.5 (2)C3-C2-H2119.9 $C14-C13-C12$ 122.0 (2)C4-C3-H3119.4 $C12-C13-H13$ 119.0C2-C3-H3119.4 $C12-C13-H13$ 119.0C2-C3-H3119.4 $C13-C14-C8^{i}$ 120.0 (2)C3-C4-C5118.1 (2) $C13-C14-H14$ 120.0	N1—C16—H16B	109.5	O1—C7—C1	119.7 (3)
N1C16H16C109.5C9C8C14 ⁱ 120.8 (3)H16AC16H16C109.5C9C8H8119.6H16BC16H16C109.5C14 ⁱ C8H8119.6N1C17H17A109.5C8C9C10121.5 (2)N1C17H17B109.5C8C9H9119.2H17AC17H17B109.5C10C9H9122.0 (2)H17AC17H17C109.5C11C10C12 ⁱ 119.9 (2)H17AC17H17C109.5C12C11C10119.9 (2)C702H2D109.5C12C11C10119.9 (2)C6C1C2118.9 (2)C12C11C4120.8 (2)C2C1C7121.6 (2)C11C12C13122.3 (2)C1C2C3120.2 (2)C11C12C10 ⁱ 120.2 (2)C1C2H2119.9C13C12C10 ⁱ 120.2 (2)C1C2H2119.9C14C13C12122.0 (2)C4C3C2121.2 (2)C14C13H13119.0C4C3H3119.4C12C13H13119.0C2C3H3119.4C12C13H13119.0C2C3H3119.4C12C13H13119.0C3C4C5118.1 (2)C13C14C8 ⁱ 120.0 (2)	H16A—C16—H16B	109.5	O2—C7—C1	117.6 (3)
H16A—C16—H16C109.5C9—C8—H8119.6H16B—C16—H16C109.5 $C14^i$ —C8—H8119.6N1—C17—H17A109.5C8—C9—C10121.5 (2)N1—C17—H17B109.5C10—C9—H9119.2H17A—C17—H17B109.5C11—C10—C9122.0 (2)H17A—C17—H17C109.5C11—C10—C12^i119.9 (2)H17B—C17—H17C109.5C12—C11—C10119.9 (2)C7—O2—H2D109.5C12—C11—C10119.9 (2)C6—C1—C2118.9 (2)C12—C11—C4119.3 (2)C6—C1—C7119.4 (2)C10—C11—C4120.8 (2)C2—C1—C7121.6 (2)C11—C12—C10 ⁱ 122.2 (2)C1—C2—C3120.2 (2)C11—C12—C10 ⁱ 120.2 (2)C1—C2—H2119.9C13—C12—C10 ⁱ 117.5 (2)C3—C2—H2119.9C14—C13—H13119.0C4—C3—H3119.4C12—C13—H13119.0C2—C3—H3119.4C13—C14—C8 ⁱ 120.0 (2)C3—C4—C5118.1 (2)C13—C14—H14120.0	N1—C16—H16C	109.5	C9—C8—C14 ⁱ	120.8 (3)
H16B—C16—H16C109.5 $C14^{i}$ —C8—H8119.6N1—C17—H17A109.5C8—C9—C10121.5 (2)N1—C17—H17B109.5C8—C9—H9119.2H17A—C17—H17B109.5C10—C9—H9119.2N1—C17—H17C109.5C11—C10—C9122.0 (2)H17A—C17—H17C109.5C11—C10—C12^{i}119.9 (2)H17B—C17—H17C109.5C9—C10—C12^{i}118.1 (2)C7—O2—H2D109.5C9—C10—C12^{i}119.9 (2)C6—C1—C2118.9 (2)C12—C11—C10119.9 (2)C6—C1—C7119.4 (2)C10—C11—C4120.8 (2)C1—C2—C3120.2 (2)C11—C12—C10^{i}120.2 (2)C1—C2—H2119.9C13—C12—C10^{i}117.5 (2)C3—C2—H2119.9C14—C13—C12122.0 (2)C4—C3—C2121.2 (2)C14—C13—H13119.0C4—C3—H3119.4C12—C13—H13119.0C2—C3—H3119.4C13—C14—C8^{i}120.0 (2)C3—C4—C5118.1 (2)C13—C14—H14120.0	H16A—C16—H16C	109.5	С9—С8—Н8	119.6
N1—C17—H17A109.5C8—C9—C10121.5 (2)N1—C17—H17B109.5C8—C9—H9119.2H17A—C17—H17B109.5C10—C9—H9119.2N1—C17—H17C109.5C11—C10—C9122.0 (2)H17A—C17—H17C109.5C11—C10—C12 ⁱ 119.9 (2)H17B—C17—H17C109.5C9—C10—C12 ⁱ 118.1 (2)C7—O2—H2D109.5C12—C11—C10119.9 (2)C6—C1—C2118.9 (2)C12—C11—C4119.3 (2)C6—C1—C7119.4 (2)C10—C11—C4120.8 (2)C2—C1—C7121.6 (2)C11—C12—C10 ⁱ 120.2 (2)C1—C2—H2119.9C13—C12—C10 ⁱ 117.5 (2)C3—C2—H2119.9C14—C13—H13119.0C4—C3—H3119.4C12—C13—H13119.0C2—C3—H3119.4C13—C14—C8 ⁱ 120.0 (2)C3—C4—C5118.1 (2)C13—C14—H14120.0	H16B—C16—H16C	109.5	C14 ⁱ —C8—H8	119.6
N1—C17—H17B109.5C8—C9—H9119.2H17A—C17—H17B109.5C10—C9—H9119.2N1—C17—H17C109.5C11—C10—C9122.0 (2)H17A—C17—H17C109.5C11—C10—C12 ⁱ 119.9 (2)H17B—C17—H17C109.5C9—C10—C12 ⁱ 118.1 (2)C7—O2—H2D109.5C12—C11—C10119.9 (2)C6—C1—C2118.9 (2)C12—C11—C4119.3 (2)C6—C1—C7119.4 (2)C10—C11—C4120.8 (2)C2—C1—C7121.6 (2)C11—C12—C13122.3 (2)C1—C2—H2119.9C13—C12—C10 ⁱ 120.2 (2)C1—C2—H2119.9C14—C13—C12122.0 (2)C4—C3—H2119.4C12—C13—H13119.0C4—C3—H3119.4C12—C13—H13119.0C2—C3—H3119.4C13—C14—C8 ⁱ 120.0 (2)C3—C4—C5118.1 (2)C13—C14—H14120.0	N1—C17—H17A	109.5	C8—C9—C10	121.5 (2)
H17A-C17-H17B109.5C10-C9-H9119.2N1-C17-H17C109.5C11-C10-C9122.0 (2)H17A-C17-H17C109.5C11-C10-C12 ⁱ 119.9 (2)H17B-C17-H17C109.5C9-C10-C12 ⁱ 118.1 (2)C7-O2-H2D109.5C12-C11-C10119.9 (2)C6-C1-C2118.9 (2)C12-C11-C419.3 (2)C6-C1-C7119.4 (2)C10-C11-C4120.8 (2)C2-C1-C7121.6 (2)C11-C12-C13122.3 (2)C1-C2-H2119.9C13-C12-C10 ⁱ 117.5 (2)C3-C2-H2121.2 (2)C14-C13-C12122.0 (2)C4-C3-H3119.4C12-C13-H13119.0C2-C3-H3119.4C13-C14-C8 ⁱ 120.0 (2)C3-C4-C5118.1 (2)C13-C14-H14120.0	N1—C17—H17B	109.5	С8—С9—Н9	119.2
N1—C17—H17C109.5C11—C10—C9122.0 (2)H17A—C17—H17C109.5C11—C10—C12 ⁱ 119.9 (2)H17B—C17—H17C109.5C9—C10—C12 ⁱ 118.1 (2)C7—O2—H2D109.5C12—C11—C10119.9 (2)C6—C1—C2118.9 (2)C12—C11—C4119.3 (2)C6—C1—C7119.4 (2)C10—C11—C4120.8 (2)C2—C1—C7121.6 (2)C11—C12—C13122.3 (2)C1—C2—C3120.2 (2)C11—C12—C10 ⁱ 117.5 (2)C3—C2—H2119.9C13—C12—C10 ⁱ 117.5 (2)C4—C3—C2121.2 (2)C14—C13—H13119.0C4—C3—H3119.4C12—C13—H13119.0C2—C3—H3119.4C13—C14—C8 ⁱ 120.0 (2)C3—C4—C5118.1 (2)C13—C14—H14120.0	H17A—C17—H17B	109.5	С10—С9—Н9	119.2
H17A—C17—H17C109.5 $C11$ —C10—C12 ⁱ 119.9 (2)H17B—C17—H17C109.5 $C9$ —C10—C12 ⁱ 118.1 (2)C7—O2—H2D109.5 $C12$ —C11—C10119.9 (2)C6—C1—C2118.9 (2) $C12$ —C11—C4119.3 (2)C6—C1—C7119.4 (2) $C10$ —C11—C4120.8 (2)C2—C1—C7121.6 (2) $C11$ —C12—C13122.3 (2)C1—C2—C3120.2 (2) $C11$ —C12—C10 ⁱ 120.2 (2)C1—C2—H2119.9 $C13$ —C12—C10 ⁱ 117.5 (2)C3—C2—H2121.2 (2) $C14$ —C13—H13119.0C4—C3—H3119.4 $C12$ —C13—H13119.0C2—C3—H3119.4 $C13$ —C14—C8 ⁱ 120.0 (2)C3—C4—C5118.1 (2) $C13$ —C14—H14120.0	N1—C17—H17C	109.5	C11—C10—C9	122.0 (2)
H17B—C17—H17C109.5 $C9$ —C10—C12 ⁱ 118.1 (2)C7—O2—H2D109.5C12—C11—C10119.9 (2)C6—C1—C2118.9 (2)C12—C11—C4119.3 (2)C6—C1—C7119.4 (2)C10—C11—C4120.8 (2)C2—C1—C7121.6 (2)C11—C12—C13122.3 (2)C1—C2—C3120.2 (2)C11—C12—C10 ⁱ 120.2 (2)C1—C2—H2119.9C13—C12—C10 ⁱ 117.5 (2)C3—C2—H2121.2 (2)C14—C13—H13119.0C4—C3—H3119.4C12—C13—H13119.0C2—C3—H3119.4C13—C14—C8 ⁱ 120.0 (2)C3—C4—C5118.1 (2)C13—C14—H14120.0	H17A—C17—H17C	109.5	C11—C10—C12 ⁱ	119.9 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H17B—C17—H17C	109.5	C9—C10—C12 ⁱ	118.1 (2)
C6—C1—C2118.9 (2)C12—C11—C4119.3 (2)C6—C1—C7119.4 (2)C10—C11—C4120.8 (2)C2—C1—C7121.6 (2)C11—C12—C13122.3 (2)C1—C2—C3120.2 (2)C11—C12—C10 ⁱ 120.2 (2)C1—C2—H2119.9C13—C12—C10 ⁱ 117.5 (2)C3—C2—H2119.9C14—C13—C12122.0 (2)C4—C3—C2121.2 (2)C14—C13—H13119.0C4—C3—H3119.4C12—C13—H13119.0C2—C3—H3119.4C13—C14—C8 ⁱ 120.0 (2)C3—C4—C5118.1 (2)C13—C14—H14120.0	C7—O2—H2D	109.5	C12-C11-C10	119.9 (2)
C6—C1—C7119.4 (2)C10—C11—C4120.8 (2)C2—C1—C7121.6 (2)C11—C12—C13122.3 (2)C1—C2—C3120.2 (2)C11—C12—C10 ⁱ 120.2 (2)C1—C2—H2119.9C13—C12—C10 ⁱ 117.5 (2)C3—C2—H2119.9C14—C13—C12122.0 (2)C4—C3—C2121.2 (2)C14—C13—H13119.0C4—C3—H3119.4C12—C13—H13119.0C2—C3—H3119.4C13—C14—C8 ⁱ 120.0 (2)C3—C4—C5118.1 (2)C13—C14—H14120.0	C6—C1—C2	118.9 (2)	C12—C11—C4	119.3 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C6—C1—C7	119.4 (2)	C10-C11-C4	120.8 (2)
$C1-C2-C3$ $120.2 (2)$ $C11-C12-C10^i$ $120.2 (2)$ $C1-C2-H2$ 119.9 $C13-C12-C10^i$ $117.5 (2)$ $C3-C2-H2$ 119.9 $C14-C13-C12$ $122.0 (2)$ $C4-C3-C2$ $121.2 (2)$ $C14-C13-H13$ 119.0 $C4-C3-H3$ 119.4 $C12-C13-H13$ 119.0 $C2-C3-H3$ 119.4 $C13-C14-C8^i$ $120.0 (2)$ $C3-C4-C5$ $118.1 (2)$ $C13-C14-H14$ 120.0	C2—C1—C7	121.6 (2)	C11—C12—C13	122.3 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C1—C2—C3	120.2 (2)	C11—C12—C10 ⁱ	120.2 (2)
C3—C2—H2 119.9 C14—C13—C12 122.0 (2) C4—C3—C2 121.2 (2) C14—C13—H13 119.0 C4—C3—H3 119.4 C12—C13—H13 119.0 C2—C3—H3 119.4 C13—C14—C8 ⁱ 120.0 (2) C3—C4—C5 118.1 (2) C13—C14—H14 120.0	С1—С2—Н2	119.9	C13—C12—C10 ⁱ	117.5 (2)
C4—C3—C2 121.2 (2) C14—C13—H13 119.0 C4—C3—H3 119.4 C12—C13—H13 119.0 C2—C3—H3 119.4 C13—C14—C8 ⁱ 120.0 (2) C3—C4—C5 118.1 (2) C13—C14—H14 120.0	С3—С2—Н2	119.9	C14—C13—C12	122.0 (2)
C4—C3—H3119.4C12—C13—H13119.0C2—C3—H3119.4C13—C14—C8 ⁱ 120.0 (2)C3—C4—C5118.1 (2)C13—C14—H14120.0	C4—C3—C2	121.2 (2)	C14—C13—H13	119.0
C2—C3—H3 119.4 C13—C14—C8 ⁱ 120.0 (2) C3—C4—C5 118.1 (2) C13—C14—H14 120.0	С4—С3—Н3	119.4	C12—C13—H13	119.0
C3-C4-C5 118.1 (2) C13-C14-H14 120.0	С2—С3—Н3	119.4	C13—C14—C8 ⁱ	120.0 (2)
	C3—C4—C5	118.1 (2)	C13—C14—H14	120.0

supplementary materials

C3—C4—C11	121.9 (2)	C8 ⁱ —C14—H14	120.0
C5—C4—C11	119.9 (2)		
O3—C15—N1—C17	3.6 (5)	C8—C9—C10—C11	-178.9 (2)
O3—C15—N1—C16	-177.4 (4)	C8—C9—C10—C12 ⁱ	0.9 (4)
C6—C1—C2—C3	-1.1 (4)	C9—C10—C11—C12	-179.8 (2)
C7—C1—C2—C3	179.7 (2)	C12 ⁱ —C10—C11—C12	0.4 (4)
C1—C2—C3—C4	0.5 (4)	C9—C10—C11—C4	2.2 (3)
C2—C3—C4—C5	0.3 (4)	C12 ⁱ —C10—C11—C4	-177.6 (2)
C2—C3—C4—C11	-178.8 (2)	C3—C4—C11—C12	106.8 (3)
C3—C4—C5—C6	-0.5 (4)	C5-C4-C11-C12	-72.3 (3)
C11—C4—C5—C6	178.6 (2)	C3-C4-C11-C10	-75.2 (3)
C2—C1—C6—C5	0.9 (4)	C5-C4-C11-C10	105.7 (3)
C7—C1—C6—C5	-179.9 (2)	C10-C11-C12-C13	178.1 (2)
C4—C5—C6—C1	-0.1 (4)	C4—C11—C12—C13	-3.9 (3)
C6—C1—C7—O1	-2.6 (4)	C10-C11-C12-C10 ⁱ	-0.4 (4)
C2-C1-C7-O1	176.6 (3)	C4—C11—C12—C10 ⁱ	177.6 (2)
C6—C1—C7—O2	176.5 (3)	C11-C12-C13-C14	-179.8 (2)
C2—C1—C7—O2	-4.3 (4)	C10 ⁱ —C12—C13—C14	-1.3 (4)
C14 ⁱ —C8—C9—C10	0.3 (4)	C12-C13-C14-C8 ⁱ	0.1 (4)
Symmetry codes: (i) $-x+1$, $-y+1$, $-z$.			

Hydrogen-bond geometry (Å, °)

D—H···A	<i>D</i> —Н	$H \cdots A$	$D \cdots A$	D—H···A
O2—H2D···O3 ⁱⁱ	0.82	1.79	2.603 (4)	170
С5—Н5…ОЗ'	0.93	2.63	3.478 (5)	152
C16—H16A···Cg1	0.96	2.91	3.485 (3)	120
Symmetry codes: (ii) $-x, -y, -z+1$.				



Fig. 1

Fig. 2

