# organic compounds

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# 3'-(3-Hydroxyphenyl)-4-methylspiro-[benzo[e][1,4]diazepine-3,2'-oxirane]-2,5(1*H*,4*H*)-dione

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Key indicators: single-crystal X-ray study; T = 193 K; mean  $\sigma$ (C–C) = 0.003 Å; R factor = 0.033; wR factor = 0.107; data-to-parameter ratio = 8.2.

In the title compound,  $C_{17}H_{14}N_2O_4$ , the seven-membered ring adopts a boat conformation, and the two benzene rings make a dihedral angle of 45.22 (5)°. The crystal packing is stabilized by intermolecular N-H···O and O-H···O hydrogen bonds.

#### **Related literature**

For the biological activity of the title compound, see: Birkinshaw *et al.* (1963); Cutler *et al.* (1984); Heguy, *et al.* (1998). For the biosynthesis of cyclopenol, see: Nover & Luckner (1969).



#### **Experimental**

Crystal data	
$C_{17}H_{14}N_2O_4$	
$M_r = 310.30$	
Monoclinic, P2 <sub>1</sub>	

a = 7.0066 (2) Å b = 11.6160 (4) Å c = 9.1568 (2) Å  $\beta = 108.157 \ (1)^{\circ}$   $V = 708.15 \ (4) \ \text{\AA}^{3}$  Z = 2Mo  $K\alpha$  radiation

#### Data collection

Bruker SMART 1000 CCD areadetector diffractometer 6890 measured reflections

#### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.033$  $wR(F^2) = 0.107$ S = 0.991701 reflections 208 parameters

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

$D-H\cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - H \cdot \cdot \cdot A$
$N1 - H1 \cdots O2^{i}$ $D4 - H4A \cdots O1^{ii}$	0.86 0.82	2.13 1.95	2.893 (2) 2.7689 (17)	148 173

 $\mu = 0.11 \text{ mm}^{-1}$ 

 $0.55 \times 0.32 \times 0.22 \text{ mm}$ 

1701 independent reflections

1627 reflections with  $I > 2\sigma(I)$ 

H-atom parameters constrained

T = 193 K

 $R_{\rm int} = 0.021$ 

1 restraint

 $\Delta \rho_{\rm max} = 0.21 \text{ e} \text{ Å}^{-3}$ 

 $\Delta \rho_{\rm min} = -0.24 \text{ e} \text{ Å}^{-3}$ 

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5236).

#### References

- Birkinshaw, J. H., Luckner, M., Mohammed, Y. S., Mothes, K. & Stickings, C. E. (1963). *Biochem. J.* 89, 196–202.
- Bruker (2007). SAINT and SMART. Bruker AXS Inc., Madison, Wisconsin, USA.
- Cutler, H. G., Crumley, F. G., Cox, R. H., Wells, J. & Cole, R. J. (1984). *Plant Cell Physiol.* 25, 257–263.
- Farrugia, L. J. (1997). J. Appl. Cryst. 30, 565.
- Heguy, A., Cai, P., Meyn, P., Houck, D., Russo, S., Michitsch, R., Pearce, C. & Katz, B. (1998). Antivir. Chem. Chemother. 9, 149–155.
- Nover, L. & Luckner, M. (1969). Eur. J. Biochem. 10, 268-273.
- Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.

supplementary materials

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### 3'-(3-Hydroxyphenyl)-4-methylspiro[benzo[e][1,4]diazepine-3,2'-oxirane]-2,5(1H,4H)-dione

## J.-L. Liu, Z.-Y. Hu and Q.-Y. Xu

#### Comment

The title compund named cyclopenol is an benzodiazepine metabolite produced by a number of *Penicllium* species. Cyclopenol isolated from *Penicillium cyclopium* Westling (Birkinshaw *et al.*, 1963). It display intermediate in the biosynthesis of viridicatins, inhibitors of the TNF- $\alpha$ -induced replication of human HIV (Nover & Luckner, 1969; Heguy, *et al.*, 1998). It is of ecological significance due to its phytotoxic and antimicrobial properties (Cutler, *et al.*, 1984). In our study, we determined the crystal structure of the title compound. The seven membered ring adopts a boat conformation. The crystal packing is stabilized by intermolecular N—H···O and O—H···O hydrogen bondings (Table 1).

#### Experimental

The fungal F00734 was cultured using half sea-water Potato Dextrose Agar medium at 28 degrees celsius for 14 days. The fermentation (10 liters) was extracted with ethyl acetate (EtOAc). The EtOAc extract (5.0 g) which was subjected to column chromatography over RP-18, eluted with Methanol-H<sub>2</sub>O (30%, 50%, 70%, 100%; V/V) to yield 10 fractions. Fraction 5, eluted with methanol was further puried by Sephadex LH-20 chromatography. Then merged the components 1–15 tubes eluted with acetone, and further purified by silica-gel column chromatography to afford the title compound 1 (140.0 mg). F00734 is an high-yield strain of cyclopenol (2.8%).

#### Refinement

H atoms were positioned geometrically and were treated as riding on their parent atoms, with C—H distances of 0.93–0.98 Å, an N—H distance of 0.86 Å, and O—H distance of 0.82Å and  $U_{iso}(H)=1.2U_{eq}(N,C)$ .

#### Figures



Fig. 1. The molecular structure of the title compound with 50% probability ellipsoids.

# supplementary materials



Fig. 2. Partial packing diagram of the title compound, viewed along the *a* axis.

# 3'-(3-Hydroxyphenyl)-4-methylspiro[benzo[e][1,4]diazepine-3,2'- oxirane]-2,5(1H,4H)-dione

Crystal	data
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$C_{17}H_{14}N_2O_4$	F(000) = 324
$M_r = 310.30$	$D_{\rm x} = 1.455 {\rm ~Mg} {\rm ~m}^{-3}$
Monoclinic, P2 <sub>1</sub>	Mo <i>K</i> $\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2yb	Cell parameters from 1484 reflections
a = 7.0066 (2) Å	$\theta = 1.9 - 27.5^{\circ}$
b = 11.6160 (4)  Å	$\mu = 0.11 \text{ mm}^{-1}$
c = 9.1568 (2)  Å	T = 193  K
$\beta = 108.157 (1)^{\circ}$	Block, colourless
$V = 708.15 (4) \text{ Å}^3$	$0.55 \times 0.32 \times 0.22 \text{ mm}$
<i>Z</i> = 2	

#### Data collection

Bruker SMART 1000 CCD area-detector diffractometer	1627 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{\rm int} = 0.021$
graphite	$\theta_{\text{max}} = 27.5^{\circ}, \ \theta_{\text{min}} = 3.1^{\circ}$
$\phi$ and $\omega$ scans	$h = -8 \rightarrow 9$
6890 measured reflections	$k = -15 \rightarrow 15$
1701 independent reflections	$l = -11 \rightarrow 11$

### Refinement

Refinement on $F^2$	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.033$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.107$	H-atom parameters constrained
<i>S</i> = 0.99	$w = 1/[\sigma^{2}(F_{o}^{2}) + (0.1P)^{2}]$ where $P = (F_{o}^{2} + 2F_{c}^{2})/3$
1701 reflections	$(\Delta/\sigma)_{\rm max} = 0.009$

208 parameters	$\Delta \rho_{max} = 0.21 \text{ e } \text{\AA}^{-3}$
1 restraint	$\Delta \rho_{\rm min} = -0.24 \text{ e } \text{\AA}^{-3}$

#### 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  $F^2 > \sigma(F^2)$  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.

O2 $0.4377 (2)$ $0.08072 (14)$ $0.31423 (17)$ $0.0269 (3)$ $O3$ $0.4521 (2)$ $0.40192 (14)$ $0.02123 (17)$ $0.0227 (3)$ $O1$ $0.6694 (2)$ $0.51497 (15)$ $0.29249 (19)$ $0.0291 (4)$ $O4$ $-0.0361 (2)$ $0.06229 (14)$ $-0.25108 (18)$ $0.0271 (4)$ $H4A$ $0.0758$ $0.0542$ $-0.2604$ $0.041*$ $N2$ $0.4837 (2)$ $0.24388 (15)$ $0.19567 (18)$ $0.0184 (3)$ $N1$ $0.4887 (2)$ $0.42631 (15)$ $0.42617 (18)$ $0.0205 (4)$ $H1$ $0.5578$ $0.4610$ $0.5087$ $0.225*$ $C8$ $0.3244 (3)$ $0.35791 (17)$ $0.4353 (2)$ $0.0186 (4)$ $C9$ $0.2804 (3)$ $0.24831 (18)$ $0.3691 (2)$ $0.0186 (4)$ $C7$ $0.2100 (3)$ $0.40240 (19)$ $0.5227 (2)$ $0.0216 (4)$ $H7$ $0.2433$ $0.4733$ $0.5712$ $0.026*$ $C4$ $0.1162 (3)$ $0.18798 (19)$ $0.3878 (2)$ $0.0236 (4)$ $H4$ $0.0858$ $0.1152$ $0.3445$ $0.028*$ $C3$ $0.4063 (3)$ $0.18510 (18)$ $0.2913 (2)$ $0.0212 (4)$ $C12$ $0.1144 (3)$ $0.22949 (19)$ $-0.1034 (2)$ $0.0216 (4)$ $H12$ $0.2423$ $0.1976$ $-0.0787$ $0.025*$ $C3$ $0.4063 (3)$ $0.1863 (2)$ $0.1544$ $0.038*$ $H10B$ $0.7499$ $0.2231$ $0.1592$ $0.038*$ $H10B$ $0.7499$ $0.2231$ $0.1592$ $0.028$		x	У	Ζ	$U_{\rm iso}*/U_{\rm eq}$
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N2 $0.4837 (2)$ $0.24388 (15)$ $0.19567 (18)$ $0.0184 (3)$ N1 $0.4887 (2)$ $0.42631 (15)$ $0.42617 (18)$ $0.0205 (4)$ H1 $0.5578$ $0.4610$ $0.5087$ $0.025*$ C8 $0.3244 (3)$ $0.35791 (17)$ $0.4353 (2)$ $0.0186 (4)$ C9 $0.2804 (3)$ $0.24831 (18)$ $0.3691 (2)$ $0.0186 (4)$ C7 $0.2100 (3)$ $0.40240 (19)$ $0.5227 (2)$ $0.0216 (4)$ H7 $0.2433$ $0.4733$ $0.5712$ $0.026*$ C4 $0.1162 (3)$ $0.18798 (19)$ $0.3878 (2)$ $0.0236 (4)$ H4 $0.0858$ $0.1152$ $0.3445$ $0.028*$ C3 $0.4063 (3)$ $0.18510 (18)$ $0.2913 (2)$ $0.0192 (4)$ C12 $0.1144 (3)$ $0.22949 (19)$ $-0.1034 (2)$ $0.025*$ C10 $0.6209 (3)$ $0.1863 (2)$ $0.1253 (2)$ $0.0257 (4)$ H10A $0.6350$ $0.1068$ $0.1554$ $0.038*$ H10B $0.7499$ $0.2231$ $0.1592$ $0.038*$ H10C $0.5671$ $0.1915$ $0.0154$ $0.038*$ C16 $-0.1031 (3)$ $0.3876 (2)$ $-0.0884 (2)$ $0.0214 (4)$ H14 $-0.2433 (3)$ $0.21769 (19)$ $-0.2334 (2)$ $0.0224 (4)$ H14 $-0.3541$ $0.1771$ $-0.2941$ $0.028*$ C6 $0.0469 (3)$ $0.3415 (2)$ $0.5941$ $0.030*$ C13 $-0.0508 (3)$ $0.16860 (19)$ $-0.1088 (2)$ $0.0208 (4)$	H4A	0.0758	0.0542	-0.2604	0.041*
N1 $0.4887 (2)$ $0.42631 (15)$ $0.42617 (18)$ $0.0205 (4)$ H1 $0.5578$ $0.4610$ $0.5087$ $0.025*$ C8 $0.3244 (3)$ $0.35791 (17)$ $0.4353 (2)$ $0.0186 (4)$ C9 $0.2804 (3)$ $0.24831 (18)$ $0.3691 (2)$ $0.0186 (4)$ C7 $0.2100 (3)$ $0.40240 (19)$ $0.5227 (2)$ $0.0216 (4)$ H7 $0.2433$ $0.4733$ $0.5712$ $0.026*$ C4 $0.1162 (3)$ $0.18798 (19)$ $0.3878 (2)$ $0.0236 (4)$ H4 $0.0858$ $0.1152$ $0.3445$ $0.028*$ C3 $0.4063 (3)$ $0.18510 (18)$ $0.2913 (2)$ $0.0192 (4)$ C12 $0.1144 (3)$ $0.22949 (19)$ $-0.1034 (2)$ $0.025*$ C10 $0.6209 (3)$ $0.1863 (2)$ $0.1253 (2)$ $0.0257 (4)$ H10A $0.6350$ $0.1068$ $0.1554$ $0.038*$ H10B $0.7499$ $0.2231$ $0.154$ $0.038*$ C16 $-0.1031 (3)$ $0.3876 (2)$ $-0.0884 (2)$ $0.0211 (4)$ H16 $-0.1207$ $0.4607$ $-0.0531$ $0.029*$ C11 $0.0875 (3)$ $0.33865 (18)$ $-0.0492 (2)$ $0.0214 (4)$ H14 $-0.3541$ $0.1771$ $-0.2941$ $0.028*$ C6 $0.0469 (3)$ $0.3415 (2)$ $0.578 (2)$ $0.0247 (4)$ H6 $-0.0307$ $0.3725$ $0.5941$ $0.030*$ C13 $-0.0508 (3)$ $0.16860 (19)$ $-0.1948 (2)$ $0.0208 (4)$	N2	0.4837 (2)	0.24388 (15)	0.19567 (18)	0.0184 (3)
H1 $0.5578$ $0.4610$ $0.5087$ $0.025^*$ C8 $0.3244$ (3) $0.35791$ (17) $0.4353$ (2) $0.0186$ (4)C9 $0.2804$ (3) $0.24831$ (18) $0.3691$ (2) $0.0186$ (4)C7 $0.2100$ (3) $0.40240$ (19) $0.5227$ (2) $0.0216$ (4)H7 $0.2433$ $0.4733$ $0.5712$ $0.026^*$ C4 $0.1162$ (3) $0.18798$ (19) $0.3878$ (2) $0.0236$ (4)H4 $0.0858$ $0.1152$ $0.3445$ $0.028^*$ C3 $0.4063$ (3) $0.18510$ (18) $0.2913$ (2) $0.0192$ (4)C12 $0.1144$ (3) $0.22949$ (19) $-0.1034$ (2) $0.0217$ (4)H12 $0.2423$ $0.1976$ $-0.0787$ $0.025^*$ C10 $0.6209$ (3) $0.1863$ (2) $0.1253$ (2) $0.0257$ (4)H10A $0.6350$ $0.1068$ $0.1554$ $0.038^*$ H10B $0.7499$ $0.2231$ $0.1592$ $0.038^*$ C16 $-0.1031$ (3) $0.3876$ (2) $-0.0884$ (2) $0.0241$ (4)H16 $-0.1207$ $0.4607$ $-0.0531$ $0.029^*$ C11 $0.0875$ (3) $0.33865$ (18) $-0.0492$ (2) $0.0201$ (4)C14 $-0.2433$ (3) $0.21769$ (19) $-0.2334$ (2) $0.0234$ (4)H14 $-0.3541$ $0.1771$ $-0.2941$ $0.028^*$ C6 $0.0469$ (3) $0.3415$ (2) $0.5378$ (2) $0.0247$ (4)H6 $-0.0307$ $0.3725$ $0.5941$ $0.030^*$ C13 $-0.0508$ (3) $0.16860$	N1	0.4887 (2)	0.42631 (15)	0.42617 (18)	0.0205 (4)
C8 $0.3244$ (3) $0.35791$ (17) $0.4353$ (2) $0.0186$ (4)C9 $0.2804$ (3) $0.24831$ (18) $0.3691$ (2) $0.0186$ (4)C7 $0.2100$ (3) $0.40240$ (19) $0.5227$ (2) $0.0216$ (4)H7 $0.2433$ $0.4733$ $0.5712$ $0.026^*$ C4 $0.1162$ (3) $0.18798$ (19) $0.3878$ (2) $0.0236$ (4)H4 $0.0858$ $0.1152$ $0.3445$ $0.028^*$ C3 $0.4063$ (3) $0.18510$ (18) $0.2913$ (2) $0.0192$ (4)C12 $0.1144$ (3) $0.22949$ (19) $-0.1034$ (2) $0.0212$ (4)H12 $0.2423$ $0.1976$ $-0.0787$ $0.025^*$ C10 $0.6209$ (3) $0.1863$ (2) $0.1253$ (2) $0.0257$ (4)H10A $0.6350$ $0.1068$ $0.1554$ $0.038^*$ H10B $0.7499$ $0.2231$ $0.1592$ $0.038^*$ C16 $-0.1031$ (3) $0.3876$ (2) $-0.0884$ (2) $0.0241$ (4)H16 $-0.1207$ $0.4607$ $-0.0531$ $0.029^*$ C11 $0.0875$ (3) $0.33865$ (18) $-0.0492$ (2) $0.0201$ (4)C14 $-0.2433$ (3) $0.21769$ (19) $-0.2334$ (2) $0.0247$ (4)H14 $-0.3541$ $0.1771$ $-0.2941$ $0.028^*$ C6 $0.0469$ (3) $0.3415$ (2) $0.5941$ $0.030^*$ C13 $-0.0508$ (3) $0.16860$ (19) $-0.1948$ (2) $0.0208$ (4)	H1	0.5578	0.4610	0.5087	0.025*
C9 $0.2804 (3)$ $0.24831 (18)$ $0.3691 (2)$ $0.0186 (4)$ C7 $0.2100 (3)$ $0.40240 (19)$ $0.5227 (2)$ $0.0216 (4)$ H7 $0.2433$ $0.4733$ $0.5712$ $0.026*$ C4 $0.1162 (3)$ $0.18798 (19)$ $0.3878 (2)$ $0.0236 (4)$ H4 $0.0858$ $0.1152$ $0.3445$ $0.028*$ C3 $0.4063 (3)$ $0.18510 (18)$ $0.2913 (2)$ $0.0192 (4)$ C12 $0.1144 (3)$ $0.22949 (19)$ $-0.1034 (2)$ $0.0212 (4)$ H12 $0.2423$ $0.1976$ $-0.0787$ $0.025*$ C10 $0.6209 (3)$ $0.1863 (2)$ $0.1253 (2)$ $0.0257 (4)$ H10A $0.6350$ $0.1068$ $0.1554$ $0.038*$ H10B $0.7499$ $0.2231$ $0.1592$ $0.038*$ C16 $-0.1031 (3)$ $0.3876 (2)$ $-0.0884 (2)$ $0.0241 (4)$ H16 $-0.1207$ $0.4607$ $-0.09231 (2)$ $0.0201 (4)$ C14 $-0.2433 (3)$ $0.21769 (19)$ $-0.2334 (2)$ $0.0234 (4)$ H14 $-0.3541$ $0.1771$ $-0.2941$ $0.028*$ C6 $0.0469 (3)$ $0.3415 (2)$ $0.5941$ $0.030*$ C13 $-0.0508 (3)$ $0.16860 (19)$ $-0.1948 (2)$ $0.0208 (4)$	C8	0.3244 (3)	0.35791 (17)	0.4353 (2)	0.0186 (4)
C7 $0.2100 (3)$ $0.40240 (19)$ $0.5227 (2)$ $0.0216 (4)$ H7 $0.2433$ $0.4733$ $0.5712$ $0.026^*$ C4 $0.1162 (3)$ $0.18798 (19)$ $0.3878 (2)$ $0.0236 (4)$ H4 $0.0858$ $0.1152$ $0.3445$ $0.028^*$ C3 $0.4063 (3)$ $0.18510 (18)$ $0.2913 (2)$ $0.0192 (4)$ C12 $0.1144 (3)$ $0.22949 (19)$ $-0.1034 (2)$ $0.0212 (4)$ H12 $0.2423$ $0.1976$ $-0.0787$ $0.025^*$ C10 $0.6209 (3)$ $0.1863 (2)$ $0.1253 (2)$ $0.0257 (4)$ H10A $0.6350$ $0.1068$ $0.1554$ $0.038^*$ H10B $0.7499$ $0.2231$ $0.1592$ $0.0241 (4)$ H16 $-0.1031 (3)$ $0.3876 (2)$ $-0.0884 (2)$ $0.0241 (4)$ H16 $-0.1207$ $0.4607$ $-0.0492 (2)$ $0.0201 (4)$ C14 $-0.2433 (3)$ $0.21769 (19)$ $-0.2334 (2)$ $0.0234 (4)$ H14 $-0.3541$ $0.1771$ $-0.2941$ $0.028^*$ C6 $0.0469 (3)$ $0.3415 (2)$ $0.5378 (2)$ $0.0247 (4)$ H6 $-0.0307$ $0.3725$ $0.5941$ $0.030^*$ C13 $-0.0508 (3)$ $0.16860 (19)$ $-0.1948 (2)$ $0.0208 (4)$	С9	0.2804 (3)	0.24831 (18)	0.3691 (2)	0.0186 (4)
H7 $0.2433$ $0.4733$ $0.5712$ $0.026^*$ C4 $0.1162$ (3) $0.18798$ (19) $0.3878$ (2) $0.0236$ (4)H4 $0.0858$ $0.1152$ $0.3445$ $0.028^*$ C3 $0.4063$ (3) $0.18510$ (18) $0.2913$ (2) $0.0192$ (4)C12 $0.1144$ (3) $0.22949$ (19) $-0.1034$ (2) $0.0212$ (4)H12 $0.2423$ $0.1976$ $-0.0787$ $0.025^*$ C10 $0.6209$ (3) $0.1863$ (2) $0.1253$ (2) $0.0257$ (4)H10A $0.6350$ $0.1068$ $0.1554$ $0.038^*$ H10B $0.7499$ $0.2231$ $0.1592$ $0.038^*$ C16 $-0.1031$ (3) $0.3876$ (2) $-0.0884$ (2) $0.0241$ (4)H16 $-0.1207$ $0.4607$ $-0.0531$ $0.029^*$ C11 $0.0875$ (3) $0.33865$ (18) $-0.0492$ (2) $0.0211$ (4)H14 $-0.3541$ $0.1771$ $-0.2941$ $0.028^*$ C6 $0.0469$ (3) $0.3415$ (2) $0.5378$ (2) $0.0247$ (4)H6 $-0.0307$ $0.3725$ $0.5941$ $0.308^*$ C13 $-0.0508$ (3) $0.16860$ (19) $-0.1948$ (2) $0.0208$ (4)	C7	0.2100 (3)	0.40240 (19)	0.5227 (2)	0.0216 (4)
C4 $0.1162 (3)$ $0.18798 (19)$ $0.3878 (2)$ $0.0236 (4)$ H4 $0.0858$ $0.1152$ $0.3445$ $0.028*$ C3 $0.4063 (3)$ $0.18510 (18)$ $0.2913 (2)$ $0.0192 (4)$ C12 $0.1144 (3)$ $0.22949 (19)$ $-0.1034 (2)$ $0.0212 (4)$ H12 $0.2423$ $0.1976$ $-0.0787$ $0.025*$ C10 $0.6209 (3)$ $0.1863 (2)$ $0.1253 (2)$ $0.0257 (4)$ H10A $0.6350$ $0.1068$ $0.1554$ $0.038*$ H10B $0.7499$ $0.2231$ $0.1592$ $0.038*$ H10C $0.5671$ $0.1915$ $0.0154$ $0.038*$ C16 $-0.1031 (3)$ $0.3876 (2)$ $-0.0884 (2)$ $0.0211 (4)$ H16 $-0.1207$ $0.4607$ $-0.0531$ $0.029*$ C11 $0.0875 (3)$ $0.33865 (18)$ $-0.0492 (2)$ $0.0214 (4)$ H14 $-0.2433 (3)$ $0.21769 (19)$ $-0.2334 (2)$ $0.0234 (4)$ H14 $-0.3541$ $0.1771$ $-0.2941$ $0.028*$ C6 $0.0469 (3)$ $0.3415 (2)$ $0.5378 (2)$ $0.0247 (4)$ H6 $-0.0307$ $0.3725$ $0.5941$ $0.030*$ C13 $-0.0508 (3)$ $0.16860 (19)$ $-0.1948 (2)$ $0.0208 (4)$	H7	0.2433	0.4733	0.5712	0.026*
H4 $0.0858$ $0.1152$ $0.3445$ $0.028*$ C3 $0.4063$ (3) $0.18510$ (18) $0.2913$ (2) $0.0192$ (4)C12 $0.1144$ (3) $0.22949$ (19) $-0.1034$ (2) $0.0212$ (4)H12 $0.2423$ $0.1976$ $-0.0787$ $0.025*$ C10 $0.6209$ (3) $0.1863$ (2) $0.1253$ (2) $0.0257$ (4)H10A $0.6350$ $0.1068$ $0.1554$ $0.038*$ H10B $0.7499$ $0.2231$ $0.1592$ $0.038*$ H10C $0.5671$ $0.1915$ $0.0154$ $0.038*$ C16 $-0.1031$ (3) $0.3876$ (2) $-0.0884$ (2) $0.0241$ (4)H16 $-0.1207$ $0.4607$ $-0.0492$ (2) $0.0201$ (4)C14 $-0.2433$ (3) $0.21769$ (19) $-0.2334$ (2) $0.0234$ (4)H14 $-0.3541$ $0.1771$ $-0.2941$ $0.028*$ C6 $0.0469$ (3) $0.3415$ (2) $0.5941$ $0.030*$ C13 $-0.0508$ (3) $0.16860$ (19) $-0.1948$ (2) $0.0208$ (4)	C4	0.1162 (3)	0.18798 (19)	0.3878 (2)	0.0236 (4)
C3 $0.4063 (3)$ $0.18510 (18)$ $0.2913 (2)$ $0.0192 (4)$ C12 $0.1144 (3)$ $0.22949 (19)$ $-0.1034 (2)$ $0.0212 (4)$ H12 $0.2423$ $0.1976$ $-0.0787$ $0.025*$ C10 $0.6209 (3)$ $0.1863 (2)$ $0.1253 (2)$ $0.0257 (4)$ H10A $0.6350$ $0.1068$ $0.1554$ $0.038*$ H10B $0.7499$ $0.2231$ $0.1592$ $0.038*$ H10C $0.5671$ $0.1915$ $0.0154$ $0.029*$ C16 $-0.1031 (3)$ $0.3876 (2)$ $-0.0884 (2)$ $0.0241 (4)$ H16 $-0.1207$ $0.4607$ $-0.0531$ $0.029*$ C11 $0.0875 (3)$ $0.33865 (18)$ $-0.0492 (2)$ $0.0201 (4)$ C14 $-0.2433 (3)$ $0.21769 (19)$ $-0.2334 (2)$ $0.028*$ C6 $0.0469 (3)$ $0.3415 (2)$ $0.5718 (2)$ $0.0247 (4)$ H6 $-0.0307$ $0.3725$ $0.5941$ $0.030*$ C13 $-0.0508 (3)$ $0.16860 (19)$ $-0.1948 (2)$ $0.0208 (4)$	H4	0.0858	0.1152	0.3445	0.028*
C12 $0.1144(3)$ $0.22949(19)$ $-0.1034(2)$ $0.0212(4)$ H12 $0.2423$ $0.1976$ $-0.0787$ $0.025*$ C10 $0.6209(3)$ $0.1863(2)$ $0.1253(2)$ $0.0257(4)$ H10A $0.6350$ $0.1068$ $0.1554$ $0.038*$ H10B $0.7499$ $0.2231$ $0.1592$ $0.038*$ H10C $0.5671$ $0.1915$ $0.0154$ $0.038*$ C16 $-0.1031(3)$ $0.3876(2)$ $-0.0884(2)$ $0.0241(4)$ H16 $-0.1207$ $0.4607$ $-0.0531$ $0.029*$ C11 $0.0875(3)$ $0.33865(18)$ $-0.0492(2)$ $0.0201(4)$ C14 $-0.2433(3)$ $0.21769(19)$ $-0.2334(2)$ $0.0234(4)$ H14 $-0.3541$ $0.1771$ $-0.2941$ $0.028*$ C6 $0.0469(3)$ $0.3415(2)$ $0.5378(2)$ $0.0247(4)$ H6 $-0.0307$ $0.3725$ $0.5941$ $0.030*$ C13 $-0.0508(3)$ $0.16860(19)$ $-0.1948(2)$ $0.0208(4)$	C3	0.4063 (3)	0.18510 (18)	0.2913 (2)	0.0192 (4)
H12 $0.2423$ $0.1976$ $-0.0787$ $0.025^*$ C10 $0.6209(3)$ $0.1863(2)$ $0.1253(2)$ $0.0257(4)$ H10A $0.6350$ $0.1068$ $0.1554$ $0.038^*$ H10B $0.7499$ $0.2231$ $0.1592$ $0.038^*$ H10C $0.5671$ $0.1915$ $0.0154$ $0.038^*$ C16 $-0.1031(3)$ $0.3876(2)$ $-0.0884(2)$ $0.0241(4)$ H16 $-0.1207$ $0.4607$ $-0.0531$ $0.029^*$ C11 $0.0875(3)$ $0.33865(18)$ $-0.0492(2)$ $0.0201(4)$ C14 $-0.2433(3)$ $0.21769(19)$ $-0.2334(2)$ $0.0234(4)$ H14 $-0.3541$ $0.1771$ $-0.2941$ $0.028^*$ C6 $0.0469(3)$ $0.3415(2)$ $0.5378(2)$ $0.0247(4)$ H6 $-0.0307$ $0.3725$ $0.5941$ $0.030^*$ C13 $-0.0508(3)$ $0.16860(19)$ $-0.1948(2)$ $0.0208(4)$	C12	0.1144 (3)	0.22949 (19)	-0.1034 (2)	0.0212 (4)
C10 $0.6209(3)$ $0.1863(2)$ $0.1253(2)$ $0.0257(4)$ H10A $0.6350$ $0.1068$ $0.1554$ $0.038*$ H10B $0.7499$ $0.2231$ $0.1592$ $0.038*$ H10C $0.5671$ $0.1915$ $0.0154$ $0.0241(4)$ H16 $-0.1031(3)$ $0.3876(2)$ $-0.0884(2)$ $0.0241(4)$ H16 $-0.1207$ $0.4607$ $-0.0531$ $0.029*$ C11 $0.0875(3)$ $0.33865(18)$ $-0.0492(2)$ $0.0201(4)$ C14 $-0.2433(3)$ $0.21769(19)$ $-0.2334(2)$ $0.0234(4)$ H14 $-0.3541$ $0.1771$ $-0.2941$ $0.028*$ C6 $0.0469(3)$ $0.3415(2)$ $0.5378(2)$ $0.0247(4)$ H6 $-0.0307$ $0.3725$ $0.5941$ $0.030*$ C13 $-0.0508(3)$ $0.16860(19)$ $-0.1948(2)$ $0.0208(4)$	H12	0.2423	0.1976	-0.0787	0.025*
H10A $0.6350$ $0.1068$ $0.1554$ $0.038*$ H10B $0.7499$ $0.2231$ $0.1592$ $0.038*$ H10C $0.5671$ $0.1915$ $0.0154$ $0.038*$ C16 $-0.1031$ (3) $0.3876$ (2) $-0.0884$ (2) $0.0241$ (4)H16 $-0.1207$ $0.4607$ $-0.0531$ $0.029*$ C11 $0.0875$ (3) $0.33865$ (18) $-0.0492$ (2) $0.0201$ (4)C14 $-0.2433$ (3) $0.21769$ (19) $-0.2334$ (2) $0.0234$ (4)H14 $-0.3541$ $0.1771$ $-0.2941$ $0.028*$ C6 $0.0469$ (3) $0.3415$ (2) $0.5378$ (2) $0.0247$ (4)H6 $-0.0307$ $0.3725$ $0.5941$ $0.030*$ C13 $-0.0508$ (3) $0.16860$ (19) $-0.1948$ (2) $0.0208$ (4)	C10	0.6209 (3)	0.1863 (2)	0.1253 (2)	0.0257 (4)
H10B $0.7499$ $0.2231$ $0.1592$ $0.038*$ H10C $0.5671$ $0.1915$ $0.0154$ $0.038*$ C16 $-0.1031(3)$ $0.3876(2)$ $-0.0884(2)$ $0.0241(4)$ H16 $-0.1207$ $0.4607$ $-0.0531$ $0.029*$ C11 $0.0875(3)$ $0.33865(18)$ $-0.0492(2)$ $0.0201(4)$ C14 $-0.2433(3)$ $0.21769(19)$ $-0.2334(2)$ $0.0234(4)$ H14 $-0.3541$ $0.1771$ $-0.2941$ $0.028*$ C6 $0.0469(3)$ $0.3415(2)$ $0.5378(2)$ $0.0247(4)$ H6 $-0.0307$ $0.3725$ $0.5941$ $0.030*$ C13 $-0.0508(3)$ $0.16860(19)$ $-0.1948(2)$ $0.0208(4)$	H10A	0.6350	0.1068	0.1554	0.038*
H10C $0.5671$ $0.1915$ $0.0154$ $0.038*$ C16 $-0.1031 (3)$ $0.3876 (2)$ $-0.0884 (2)$ $0.0241 (4)$ H16 $-0.1207$ $0.4607$ $-0.0531$ $0.029*$ C11 $0.0875 (3)$ $0.33865 (18)$ $-0.0492 (2)$ $0.0201 (4)$ C14 $-0.2433 (3)$ $0.21769 (19)$ $-0.2334 (2)$ $0.0234 (4)$ H14 $-0.3541$ $0.1771$ $-0.2941$ $0.028*$ C6 $0.0469 (3)$ $0.3415 (2)$ $0.5378 (2)$ $0.0247 (4)$ H6 $-0.0307$ $0.3725$ $0.5941$ $0.030*$ C13 $-0.0508 (3)$ $0.16860 (19)$ $-0.1948 (2)$ $0.0208 (4)$	H10B	0.7499	0.2231	0.1592	0.038*
C16 $-0.1031 (3)$ $0.3876 (2)$ $-0.0884 (2)$ $0.0241 (4)$ H16 $-0.1207$ $0.4607$ $-0.0531$ $0.029*$ C11 $0.0875 (3)$ $0.33865 (18)$ $-0.0492 (2)$ $0.0201 (4)$ C14 $-0.2433 (3)$ $0.21769 (19)$ $-0.2334 (2)$ $0.0234 (4)$ H14 $-0.3541$ $0.1771$ $-0.2941$ $0.028*$ C6 $0.0469 (3)$ $0.3415 (2)$ $0.5378 (2)$ $0.0247 (4)$ H6 $-0.0307$ $0.3725$ $0.5941$ $0.030*$ C13 $-0.0508 (3)$ $0.16860 (19)$ $-0.1948 (2)$ $0.0208 (4)$	H10C	0.5671	0.1915	0.0154	0.038*
H16 $-0.1207$ $0.4607$ $-0.0531$ $0.029*$ C11 $0.0875$ (3) $0.33865$ (18) $-0.0492$ (2) $0.0201$ (4)C14 $-0.2433$ (3) $0.21769$ (19) $-0.2334$ (2) $0.0234$ (4)H14 $-0.3541$ $0.1771$ $-0.2941$ $0.028*$ C6 $0.0469$ (3) $0.3415$ (2) $0.5378$ (2) $0.0247$ (4)H6 $-0.0307$ $0.3725$ $0.5941$ $0.030*$ C13 $-0.0508$ (3) $0.16860$ (19) $-0.1948$ (2) $0.0208$ (4)	C16	-0.1031 (3)	0.3876 (2)	-0.0884 (2)	0.0241 (4)
C11 $0.0875(3)$ $0.33865(18)$ $-0.0492(2)$ $0.0201(4)$ C14 $-0.2433(3)$ $0.21769(19)$ $-0.2334(2)$ $0.0234(4)$ H14 $-0.3541$ $0.1771$ $-0.2941$ $0.028*$ C6 $0.0469(3)$ $0.3415(2)$ $0.5378(2)$ $0.0247(4)$ H6 $-0.0307$ $0.3725$ $0.5941$ $0.030*$ C13 $-0.0508(3)$ $0.16860(19)$ $-0.1948(2)$ $0.0208(4)$ C17 $0.2579(3)$ $0.40891(18)$ $0.0485(2)$ $0.0108(4)$	H16	-0.1207	0.4607	-0.0531	0.029*
C14 $-0.2433(3)$ $0.21769(19)$ $-0.2334(2)$ $0.0234(4)$ H14 $-0.3541$ $0.1771$ $-0.2941$ $0.028*$ C6 $0.0469(3)$ $0.3415(2)$ $0.5378(2)$ $0.0247(4)$ H6 $-0.0307$ $0.3725$ $0.5941$ $0.030*$ C13 $-0.0508(3)$ $0.16860(19)$ $-0.1948(2)$ $0.0208(4)$ C17 $0.2579(3)$ $0.40891(18)$ $0.0485(2)$ $0.0108(4)$	C11	0.0875 (3)	0.33865 (18)	-0.0492 (2)	0.0201 (4)
H14 $-0.3541$ $0.1771$ $-0.2941$ $0.028*$ C6 $0.0469(3)$ $0.3415(2)$ $0.5378(2)$ $0.0247(4)$ H6 $-0.0307$ $0.3725$ $0.5941$ $0.030*$ C13 $-0.0508(3)$ $0.16860(19)$ $-0.1948(2)$ $0.0208(4)$ C17 $0.2579(3)$ $0.40891(18)$ $0.0485(2)$ $0.0108(4)$	C14	-0.2433 (3)	0.21769 (19)	-0.2334 (2)	0.0234 (4)
C6 $0.0469(3)$ $0.3415(2)$ $0.5378(2)$ $0.0247(4)$ H6 $-0.0307$ $0.3725$ $0.5941$ $0.030*$ C13 $-0.0508(3)$ $0.16860(19)$ $-0.1948(2)$ $0.0208(4)$ C17 $0.2579(3)$ $0.40891(18)$ $0.0485(2)$ $0.0108(4)$	H14	-0.3541	0.1771	-0.2941	0.028*
H6 $-0.0307$ $0.3725$ $0.5941$ $0.030*$ C13 $-0.0508(3)$ $0.16860(19)$ $-0.1948(2)$ $0.0208(4)$ C17 $0.2579(3)$ $0.40891(18)$ $0.0485(2)$ $0.0108(4)$	C6	0.0469 (3)	0.3415 (2)	0.5378 (2)	0.0247 (4)
C13 $-0.0508$ (3) $0.16860$ (19) $-0.1948$ (2) $0.0208$ (4)C17 $0.2579$ (3) $0.40891$ (18) $0.0485$ (2) $0.0108$ (4)	H6	-0.0307	0.3725	0.5941	0.030*
C17 0.2579 (3) 0.40801 (18) 0.0485 (2) 0.0109 (4)	C13	-0.0508 (3)	0.16860 (19)	-0.1948 (2)	0.0208 (4)
$C_{17} \qquad 0.2577(5) \qquad 0.40671(16) \qquad 0.0465(2) \qquad 0.0198(4)$	C17	0.2579 (3)	0.40891 (18)	0.0485 (2)	0.0198 (4)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters  $(A^2)$ 

# supplementary materials

H17	0.2200	0.4869	0.0695	0.024*
C15	-0.2672 (3)	0.3264 (2)	-0.1808 (2)	0.0252 (4)
H15	-0.3946	0.3592	-0.2075	0.030*
C2	0.4422 (3)	0.36451 (16)	0.1645 (2)	0.0180 (4)
C5	-0.0007 (3)	0.2341 (2)	0.4688 (2)	0.0267 (5)
H5	-0.1113	0.1937	0.4774	0.032*
C1	0.5463 (3)	0.44186 (18)	0.2995 (2)	0.0195 (4)

# Atomic displacement parameters $(Å^2)$

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O2	0.0382 (8)	0.0157 (7)	0.0268 (7)	0.0038 (6)	0.0100 (6)	0.0041 (6)
O3	0.0288 (7)	0.0214 (7)	0.0222 (7)	0.0002 (5)	0.0139 (5)	0.0024 (6)
01	0.0309 (8)	0.0236 (8)	0.0359 (8)	-0.0097 (6)	0.0149 (6)	-0.0027 (7)
O4	0.0268 (7)	0.0222 (8)	0.0341 (8)	-0.0028 (6)	0.0121 (6)	-0.0060 (6)
N2	0.0227 (7)	0.0155 (8)	0.0180 (7)	0.0029 (6)	0.0077 (6)	0.0006 (7)
N1	0.0236 (8)	0.0174 (8)	0.0189 (8)	-0.0052 (6)	0.0044 (6)	-0.0034 (6)
C8	0.0194 (9)	0.0184 (9)	0.0169 (8)	-0.0022 (7)	0.0042 (7)	0.0015 (7)
C9	0.0225 (8)	0.0181 (9)	0.0144 (8)	0.0006 (7)	0.0046 (7)	0.0022 (7)
C7	0.0273 (9)	0.0183 (9)	0.0180 (8)	0.0001 (7)	0.0052 (7)	-0.0012 (7)
C4	0.0251 (9)	0.0204 (10)	0.0234 (9)	-0.0063 (8)	0.0050 (7)	0.0004 (8)
C3	0.0220 (9)	0.0140 (9)	0.0188 (8)	0.0025 (7)	0.0021 (6)	0.0016 (7)
C12	0.0234 (9)	0.0216 (10)	0.0186 (8)	0.0041 (7)	0.0065 (7)	0.0022 (7)
C10	0.0248 (10)	0.0251 (11)	0.0290 (9)	0.0094 (8)	0.0113 (7)	-0.0007 (8)
C16	0.0289 (10)	0.0229 (10)	0.0216 (9)	0.0058 (8)	0.0096 (8)	0.0013 (8)
C11	0.0256 (9)	0.0208 (10)	0.0149 (8)	0.0012 (7)	0.0076 (7)	0.0007 (7)
C14	0.0204 (9)	0.0291 (12)	0.0213 (9)	-0.0014 (7)	0.0071 (7)	0.0018 (8)
C6	0.0277 (10)	0.0291 (11)	0.0202 (9)	0.0014 (8)	0.0117 (8)	0.0027 (8)
C13	0.0265 (9)	0.0187 (9)	0.0195 (8)	-0.0010 (8)	0.0105 (7)	0.0000 (7)
C17	0.0263 (10)	0.0163 (9)	0.0178 (8)	0.0017 (7)	0.0085 (7)	0.0028 (7)
C15	0.0234 (10)	0.0300 (12)	0.0230 (10)	0.0054 (8)	0.0082 (8)	0.0030 (8)
C2	0.0220 (9)	0.0143 (9)	0.0193 (8)	0.0005 (7)	0.0087 (7)	0.0016 (7)
C5	0.0263 (10)	0.0300 (12)	0.0252 (10)	-0.0084 (9)	0.0101 (8)	0.0025 (9)
C1	0.0200 (8)	0.0149 (9)	0.0238 (9)	0.0001 (6)	0.0069 (7)	-0.0002 (7)

# Geometric parameters (Å, °)

O2—C3	1.238 (3)	C12—C13	1.392 (3)
O3—C2	1.405 (2)	C12—C11	1.396 (3)
O3—C17	1.461 (2)	С12—Н12	0.9300
O1—C1	1.226 (3)	C10—H10A	0.9600
O4—C13	1.354 (3)	C10—H10B	0.9600
O4—H4A	0.8200	C10—H10C	0.9600
N2—C3	1.350 (3)	C16—C15	1.392 (3)
N2—C2	1.441 (2)	C16—C11	1.392 (3)
N2—C10	1.474 (2)	C16—H16	0.9300
N1—C1	1.354 (3)	C11—C17	1.492 (3)
N1—C8	1.422 (2)	C14—C15	1.380 (3)
N1—H1	0.8600	C14—C13	1.404 (3)

C8=C9         1.402 (3)         C6=C5         1.391 (3)           C9-C3         1.489 (3)         C17-C2         1.486 (3)           C7-C6         1.387 (3)         C17-C2         1.486 (3)           C7-C6         1.387 (3)         C17-C1         0.9800           C7-L17         0.9300         C15-L115         0.9300           C4-C5         1.373 (3)         C2-C1         1.518 (3)           C3-OD-C17         62.43 (12)         C11-C16-H116         1202           C3-N2-C2         121.51 (17)         C16-C11-C17         117.10 (18)           C3-N2-C10         120.16 (17)         C12-C14-L114         120.1           C1-N1-C8         125.99 (16)         C15-C14-L114         120.1           C1-N1-C8         125.99 (16)         C15-C14-L114         120.1           C1-N1-C8         125.99 (17)         C1-C4-H14         120.1           C1-N1-H1         117.0         C7-C6-C5         119.99 (19)           C7-C8-C9         119.68 (18)         C7-C6-H6         120.0           C7-C8-C1         119.99 (19)         C1-C3-C12         122.98 (18)           C4-C9-C3         116.31 (19)         C12-C13-C14         117.11 (18)           C4-C9-C3         124.82 (17)<	C8—C7	1.397 (3)		C14—H14		0.9300
C9-C4       1.403 (3)       C6-H6       0.9300         C9-C3       1.489 (3)       C17-C2       1.486 (3)         C7-C6       1.337 (3)       C17-H17       0.9800         C4-C5       1.373 (3)       C2-C1       1.518 (3)         C4-H4       0.9300       C3-H5       0.9300         C2-O3-C17       62.43 (12)       C11-C16-H16       120.2         C13-O4-H4A       109.5       C16-C11-C17       117.10 (18)         C3-N2-C2       12.151 (17)       C16-C11-C17       117.10 (18)         C3-N2-C10       12.59 (16)       C15-C14-C13       119.7 (2)         C1-N1-C8       125.99 (16)       C15-C14-H14       120.1         C1-N1-C8       125.99 (16)       C15-C14-H14       120.1         C1-N1-H1       117.0       C13-C14-H114       120.1         C4-C9       11.953 (18)       C5-C6-H6       120.0         C7-C8-N1       11.633 (18)       C5-C6-H6       120.0         C7-C8-C8       11.633 (18)       C12-C13-C14       117.11 (18)         C4-C9-C3       11.633 (18)       C12-C13-C14       119.9 (2)         C8-C9-H3       12.483 (17)       O3-C17-C1       18.78 (16)         C6-C7-H7       119.8	C8—C9	1.402 (3)		C6—C5		1.391 (3)
C9-C3       1.489 (3)       C17-C2       1.486 (3)         C7-C6       1.387 (3)       C17-H17       0.9300         C4-C5       1.373 (3)       C2-C1       1.518 (3)         C4-H4       0.9300       C5-H5       0.9300         C13-O4-H4A       109.5       C16-C11-C12       120.2 (1)         C3-N2-C2       121.51 (17)       C16-C11-C17       112.29 (1)         C3-N2-C10       120.16 (17)       C12-C11-C17       122.59 (1)         C1-N1-C8       125.99 (16)       C15-C14-H14       120.1         C1-N1-H1       117.0       C13-C14-H14       120.1         C4-N3-C10       118.88 (17)       C15-C14-H14       120.1         C4-N1-H1       117.0       C13-C14-H14       120.1         C4-N1-H1       117.0       C13-C14-H14       120.1         C4-N1-H1       117.0       C13-C14-H14       120.0         C7-C8-N1       116.53 (18)       C5-C6-H6       120.0         C7-C8-N1       116.83 (18)       C12-C13-C14       H19.9 (19)         C4-C9-C3       116.83 (18)       C3-C17-C1       H28.8 (18)         C4-C9-C3       116.83 (18)       C3-C17-C1       H28.4 (18)         C6-C7-H7       H9.8       C2	C9—C4	1.403 (3)		С6—Н6		0.9300
C7-C6         1.387 (3)         C17-H17         0.9800           C7-H7         0.9300         C15-H15         0.9300           C4-C5         1.373 (3)         C2-C1         1.518 (3)           C4-H4         0.9300         C5-H5         0.9300           C3-O3-C17         62.43 (12)         C11-C16-H16         1.20.2           C13-O4-H4A         109.5         C16-C11-C17         117.10 (18)           C3-N2-C2         12.15 (17)         C16-C11-C17         117.10 (18)           C1-N1-C8         125.99 (16)         C15-C14-H14         120.1           C1-N1-C8         125.99 (16)         C15-C14-H14         120.1           C4-C9         119.68 (18)         C7-C6-C5         119.99 (19)           C7-C8-C9         119.68 (18)         C7-C6-H6         120.0           C7-C8-C8         118.82 (17)         O4-C13-C12         122.98 (18)           C4-C9-C3         118.33 (19)         O4-C13-C14         117.11 (18)           C4-C9-C3         118.43 (17)         O3-C17-C11         118.78 (16)           C5-C4-H7         119.8         O3-C17-C11         118.78 (16)           C6-C7-H7         119.8         C2-C17-C11         118.78 (16)           C5-C4-C9         1	С9—С3	1.489 (3)		C17—C2		1.486 (3)
C7-H7         0.9300         C15-H15         0.9300           C4-C5         1.373 (3)         C2-C1         1.518 (3)           C4-H4         0.9300         C5-H5         0.9300           C2-03-C17         C2.43 (12)         C11-C16-H16         120.2           C13-04-H4A         109.5         C16-C11-C12         120.29 (19)           C3-N2-C2         121.51 (17)         C16-C11-C17         122.59 (19)           C3-N2-C10         120.16 (7)         C12-C14-C13         119.7 (2)           C1-N1-C8         125.99 (16)         C15-C14-H14         120.1           C8-N1-H11         117.0         C13-C14-H14         120.1           C8-N1-H11         117.0         C13-C14-H14         120.1           C9-C8-N1         123.70 (17)         O4-C13-C12         122.98 (18)           C4-C9-C8         118.62 (18)         O4-C13-C14         119.9 (2)           C4-C9-C8         118.81 (19)         C12-C13-C14         119.9 (2)           C6-C7-C8         120.4 (2)         O3-C17-C2         56.95 (1)           C6-C7-C8         120.4 (2)         C3-C17-C11         118.78 (16)           C6-C7-C8         120.4 (2)         C2-C17-H17         114.1           C5-C4-C9         <	С7—С6	1.387 (3)		C17—H17		0.9800
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С7—Н7	0.9300		C15—H15		0.9300
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C4—C5	1.373 (3)		C2—C1		1.518 (3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C4—H4	0.9300		С5—Н5		0.9300
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C2—O3—C17	62.43 (12)		C11—C16—H16		120.2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C13—O4—H4A	109.5		C16—C11—C12		120.29 (19)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C3—N2—C2	121.51 (17)		C16—C11—C17		117.10 (18)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C3—N2—C10	120.16 (17)		C12—C11—C17		122.59 (17)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C2—N2—C10	118.28 (17)		C15—C14—C13		119.7 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C1—N1—C8	125.99 (16)		C15—C14—H14		120.1
C8-N1-H1       117.0       C7C6C5       119.99 (19)         C7-C8-C9       119.68 (18)       C7C6-H6       120.0         C7-C8-N1       116.53 (18)       C5C6-H6       120.0         C9-C8-N1       123.70 (17)       O4C13C12       122.98 (18)         C4-C9-C8       118.62 (18)       O4C13C14       117.11 (18)         C4-C9-C3       116.31 (19)       C12C13C14       119.9 (2)         C8-C9-C3       124.83 (17)       O3C17C2       56.95 (11)         C6-C7-L7       119.8       C2C17C11       118.78 (16)         C6-C7-H7       119.8       C2C17C11       126.41 (18)         C8-C7-H7       119.8       O3C17H17       114.1         C5-C4-C9       121.4 (2)       C2C17H17       114.1         C9-C4-H4       119.3       C11C17H17       114.1         C9-C4-H4       119.3       C11C17H15       119.6         O2-C3-C9       120.14 (19)       C16C15H15       119.6         O2-C3-C9       120.14 (19)       C16C15H15       119.6         O2-C3-C9       128.58 (18)       O3C2N2       114.81 (16)         C13C12-H12       120.1       N2C2-C1       115.22 (16)	C1—N1—H1	117.0		C13—C14—H14		120.1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C8—N1—H1	117.0		C7—C6—C5		119.99 (19)
C7-C8-N1       116.53 (18)       C5-C6-H6       120.0         C9-C8-N1       123.70 (17)       04-C13-C12       122.98 (18)         C4-C9-C8       118.62 (18)       04-C13-C14       117.11 (18)         C4-C9-C3       116.31 (19)       C12-C13-C14       119.9 (2)         C8-C9-C3       124.83 (17)       03-C17-C2       56.95 (11)         C6-C7-C8       120.4 (2)       03-C17-C11       118.78 (16)         C6-C7-H7       119.8       C2-C17-C11       126.41 (18)         C8-C9-C4-H4       119.3       C11-C17-H17       114.1         C5-C4-H4       119.3       C14-C15-C16       120.80 (18)         02-C3-N2       121.27 (19)       C14-C15-C16       120.80 (18)         02-C3-C9       120.14 (19)       C16-C15-H15       119.6         N2-C3-C9       118.58 (18)       03-C2-N2       114.81 (16)         C13-C12-C11       119.76 (18)       03-C2-N2       114.81 (16)         C13-C12-C11       119.76 (18)       03-C2-C17       60.63 (12)         C13-C12-H12       120.1       N2-C2-C17       60.63 (12)         C13-C12-H12       120.1       N2-C2-C17       113.46 (16)         N2-C10-H10A       109.5       C4-C5-H5       120.1 <td>C7—C8—C9</td> <td>119.68 (18)</td> <td></td> <td>С7—С6—Н6</td> <td></td> <td>120.0</td>	C7—C8—C9	119.68 (18)		С7—С6—Н6		120.0
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C7—C8—N1	116.53 (18)		С5—С6—Н6		120.0
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C9—C8—N1	123.70 (17)		O4—C13—C12		122.98 (18)
C4-C9-C3       116.31 (19)       C12-C13-C14       119.9 (2)         C8-C9-C3       124.83 (17)       O3-C17-C2       56.95 (11)         C6-C7-C8       120.4 (2)       O3-C17-C11       118.78 (16)         C6-C7-H7       119.8       C2-C17-C11       126.41 (18)         C8-C7-H7       119.8       O3-C17-H17       114.1         C5-C4-C9       121.4 (2)       C2-C17-H17       114.1         C5-C4-H4       119.3       C11-C17-H17       114.1         C9-C4-H4       119.3       C14-C15-C16       120.80 (18)         O2-C3-N2       121.27 (19)       C14-C15-H15       119.6         O2-C3-C9       120.14 (19)       C16-C15-H15       119.6         O2-C3-C9       120.14 (19)       C16-C15-H15       119.6         O3-C2-C17       60.63 (12)       C11-C12-H12       120.1       N2-C2-C17       123.77 (17)         C11-C12-H12       120.1       O3-C2-C2       114.81 (16)       115.22 (16)       N2-C10-H10A       109.5       N2-C2-C1       113.46 (16)         N2-C10-H10A       109.5       C17-C2-C1       117.85 (17)       H10A-C10-H10B       109.5       C17-C2-C1       117.85 (17)         H10A-C10-H10C       109.5       C17-C2-C1       117.85 (19) </td <td>C4—C9—C8</td> <td>118.62 (18)</td> <td></td> <td>O4—C13—C14</td> <td></td> <td>117.11 (18)</td>	C4—C9—C8	118.62 (18)		O4—C13—C14		117.11 (18)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C4—C9—C3	116.31 (19)		C12—C13—C14		119.9 (2)
C6-C7-C8       120.4 (2)       O3-C17-C11       118.78 (16)         C6-C7-H7       119.8       C2-C17-C11       126.41 (18)         C8-C7-H7       119.8       O3-C17-H17       114.1         C5-C4-C9       121.4 (2)       C2-C17-H17       114.1         C5-C4-H4       119.3       C11-C17-H17       114.1         C9-C4-H4       119.3       C14-C15-C16       120.80 (18)         O2-C3-N2       121.27 (19)       C14-C15-H15       119.6         O2-C3-C9       120.14 (19)       C16-C15-H15       119.6         N2-C3-C9       118.58 (18)       O3-C2-N2       114.81 (16)         C13-C12-C11       119.76 (18)       O3-C2-C17       60.63 (12)         C13-C12-H12       120.1       N2-C2-C17       13.277 (17)         C11-C12-H12       120.1       N3-C2-C1       115.22 (16)         N2-C10-H10A       109.5       C17-C2-C1       117.85 (17)         H10A-C10-H10B       109.5       C4-C5-H5       120.1         H10A-C10-H10B       109.5       C4-C5-H5       120.1         H10A-C10-H10C       109.5       C4-C5-H5       120.1         H10A-C10-H10C       109.5       O1-C1-N1       122.65 (19)         C15-C16-C11	C8—C9—C3	124.83 (17)		O3—C17—C2		56.95 (11)
C6-C7-H7       119.8       C2-C17-C11       126.41 (18)         C8-C7-H7       119.8       O3-C17-H17       114.1         C5-C4-C9       121.4 (2)       C2-C17-H17       114.1         C5-C4-H4       119.3       C11-C17-H17       114.1         C9-C4-H4       119.3       C14-C15-C16       120.80 (18)         O2-C3-N2       121.27 (19)       C14-C15-H15       119.6         O2-C3-C9       120.14 (19)       C16-C15-H15       119.6         N2-C3-C9       118.58 (18)       O3-C2-N2       114.81 (16)         C13-C12-H12       120.1       N2-C2-C17       60.63 (12)         C13-C12-H12       120.1       N2-C2-C17       13.46 (16)         N2-C10-H10A       109.5       N2-C2-C1       113.46 (16)         N2-C10-H10A       109.5       C4-C5-C6       119.79 (19)         N2-C10-H10B       109.5       C4-C5-H5       120.1         H0A-C10-H10C       109.5       C4-C5-H5       120.1         H10A-C10-H10C       109.5       C4-C5-H5       120.1         H10A-C10-H10C       109.5       C4-C5-H5       120.1         H10B-C10-H10C       109.5       C4-C5-H5       120.1         H10B-C10-H10C       109.5	C6—C7—C8	120.4 (2)		O3—C17—C11		118.78 (16)
C8-C7-H7       119.8       O3-C17-H17       114.1         C5-C4-C9       121.4 (2)       C2-C17-H17       114.1         C5-C4-H4       119.3       C11-C17-H17       114.1         C9-C4-H4       119.3       C14-C15-C16       120.80 (18)         O2-C3-N2       121.27 (19)       C14-C15-H15       119.6         O2-C3-C9       120.14 (19)       C16-C15-H15       119.6         N2-C2-C17       60.63 (12)       C13-C12-C11       119.76 (18)       O3-C2-C2       114.81 (16)         C13-C12-C11       119.76 (18)       O3-C2-C17       60.63 (12)       C13-C12-H12       120.1       N2-C2-C17       123.77 (17)         C11-C12-H12       120.1       O3-C2-C1       115.22 (16)       N2-C10-H10A       109.5       N2-C2-C1       113.46 (16)         N2-C10-H10A       109.5       N2-C2-C1       113.46 (16)       N2-C10-H10B       109.5       C4-C5-H5       120.1         N10A-C10-H10B       109.5       C4-C5-H5       120.1       H14.97 (17)       114.1         H10A-C10-H10C       109.5       C4-C5-H5       120.1       H10A-C10-H10C       109.5       C4-C5-H5       120.1         H10B-C10-H10C       109.5       O1-C1-N1       122.65 (19)       C15-C16-C11	С6—С7—Н7	119.8		C2-C17-C11		126.41 (18)
C5-C4-C9       121.4 (2)       C2-C17-H17       114.1         C5-C4-H4       119.3       C11-C17-H17       114.1         C9-C4-H4       119.3       C14-C15-C16       120.80 (18)         O2-C3-N2       121.27 (19)       C14-C15-H15       119.6         O2-C3-C9       120.14 (19)       C16-C15-H15       119.6         N2-C3-C9       118.58 (18)       O3-C2-N2       114.81 (16)         C13-C12-C11       119.76 (18)       O3-C2-C17       60.63 (12)         C13-C12-H12       120.1       N2-C2-C17       123.77 (17)         C11-C12-H12       120.1       O3-C2-C1       115.22 (16)         N2-C10-H10A       109.5       N2-C2-C1       113.46 (16)         N2-C10-H10B       109.5       C4-C5-C6       119.79 (19)         N2-C10-H10B       109.5       C4-C5-H5       120.1         H10A-C10-H10C       109.5       C4-C5-H5       120.1         H10A-C10-H10C       109.5       C6-C5-H5       120.1         H10B-C10-H10C       109.5       C6-C5-H5       120.1         H10B-C10-H10C       109.5       01-C1-N1       122.65 (19)         C15-C16-C11       119.5 (2)       01-C1-C2       114.97 (17)         Hydroge	С8—С7—Н7	119.8		O3—C17—H17		114.1
C5-C4-H4119.3C11-C17-H17114.1C9-C4-H4119.3C14-C15-C16120.80 (18)O2-C3-N2121.27 (19)C14-C15-H15119.6O2-C3-C9120.14 (19)C16-C15-H15119.6N2-C3-C9118.58 (18)O3-C2-N2114.81 (16)C13-C12-C11119.76 (18)O3-C2-C1760.63 (12)C13-C12-H12120.1N2-C2-C17123.77 (17)C11-C12-H12120.1O3-C2-C1115.22 (16)N2-C10-H10A109.5N2-C2-C1113.46 (16)N2-C10-H10B109.5C17-C2-C1117.85 (17)H10A-C10-H10B109.5C4-C5-H5120.1H00A-C10-H10C109.5C4-C5-H5120.1H10B-C10-H10C109.5O1-C1-N1122.65 (19)C15-C16-C11119.5 (2)O1-C1-C2114.97 (17)Hydrogen-bond geometry (Å, °)N1-C1-C2114.97 (17)Hydrogen-bond geometry (Å, °)0.862.132.893 (2)D-H:-AD-HH:··AD···AD-H:··AN1-H1:··O2 <sup>1</sup> 0.821.952.7689 (17)0.821.952.7689 (17)173	C5—C4—C9	121.4 (2)		С2—С17—Н17		114.1
C9-C4-H4       119.3       C14-C15-C16       120.80 (18)         O2-C3-N2       121.27 (19)       C14-C15-H15       119.6         O2-C3-C9       120.14 (19)       C16-C15-H15       119.6         N2-C3-C9       118.58 (18)       O3-C2-N2       114.81 (16)         C13-C12-C11       119.76 (18)       O3-C2-C17       60.63 (12)         C13-C12-H12       120.1       N2-C2-C17       123.77 (17)         C11-C12-H12       120.1       O3-C2-C1       115.22 (16)         N2-C10-H10A       109.5       N2-C2-C1       113.46 (16)         N2-C10-H10B       109.5       C14-C5-C6       119.79 (19)         N2-C10-H10B       109.5       C4-C5-C6       119.79 (19)         N2-C10-H10C       109.5       C4-C5-H5       120.1         H10A-C10-H10C       109.5       C4-C5-H5       120.1         H10A-C10-H10C       109.5       O1-C1-N1       122.65 (19)         C15-C16-C11       119.5 (2)       O1-C1-C2       122.34 (19)         C15-C16-H16       120.2       N1-C1-C2       114.97 (17)         Hydrogen-bond geometry (Å, °)       D-H       H···A       D···A       D-H···A         D-H       H···A       D···A       D-H···A       NA <td>С5—С4—Н4</td> <td>119.3</td> <td></td> <td>C11—C17—H17</td> <td></td> <td>114.1</td>	С5—С4—Н4	119.3		C11—C17—H17		114.1
$02-C3-N2$ $121.27 (19)$ $C14-C15-H15$ $119.6$ $02-C3-C9$ $120.14 (19)$ $C16-C15-H15$ $119.6$ $N2-C3-C9$ $118.58 (18)$ $03-C2-N2$ $114.81 (16)$ $C13-C12-C11$ $119.76 (18)$ $03-C2-C17$ $60.63 (12)$ $C13-C12-H12$ $120.1$ $N2-C2-C17$ $123.77 (17)$ $C11-C12-H12$ $120.1$ $N2-C2-C17$ $123.77 (17)$ $C11-C12-H12$ $120.1$ $03-C2-C1$ $115.22 (16)$ $N2-C10-H10A$ $109.5$ $N2-C2-C1$ $113.46 (16)$ $N2-C10-H10B$ $109.5$ $C14-C5-C6$ $119.79 (19)$ $N2-C10-H10B$ $109.5$ $C4-C5-H5$ $120.1$ $N10A-C10-H10C$ $109.5$ $C4-C5-H5$ $120.1$ $N10A-C10-H10C$ $109.5$ $C4-C5-H5$ $120.1$ $H10B-C10-H10C$ $109.5$ $O1-C1-N1$ $122.65 (19)$ $C15-C16-C11$ $119.5 (2)$ $O1-C1-C2$ $122.34 (19)$ $C15-C16-H16$ $120.2$ $N1-C1-C2$ $114.97 (17)$ $D-H$ $H \cdots A$ $D \cdots A$ $D-H \cdots A$ $D-H$ <td>С9—С4—Н4</td> <td>119.3</td> <td></td> <td>C14—C15—C16</td> <td></td> <td>120.80 (18)</td>	С9—С4—Н4	119.3		C14—C15—C16		120.80 (18)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O2—C3—N2	121.27 (19)		C14—C15—H15		119.6
N2—C3—C9       118.58 (18)       O3—C2—N2       114.81 (16)         C13—C12—C11       119.76 (18)       O3—C2—C17       60.63 (12)         C13—C12—H12       120.1       N2—C2—C17       123.77 (17)         C11—C12—H12       120.1       O3—C2—C1       115.22 (16)         N2—C10—H10A       109.5       N2—C2—C1       113.46 (16)         N2—C10—H10B       109.5       C17—C2—C1       117.85 (17)         H10A—C10—H10B       109.5       C4—C5—C6       119.79 (19)         N2—C10—H10C       109.5       C4—C5—C6       119.79 (19)         N2—C10—H10C       109.5       C4—C5—H5       120.1         H10A—C10—H10C       109.5       C6—C5—H5       120.1         H10B—C10—H10C       109.5       O1—C1—N1       122.65 (19)         C15—C16—C11       119.5 (2)       O1—C1—C2       122.34 (19)         C15—C16—H16       120.2       N1—C1—C2       114.97 (17)         Hydrogen-bond geometry (Å, °)       D—H       H···A       D···A       D—H···A         N1—H1···O2 <sup>i</sup> 0.86       2.13       2.893 (2)       148         O4—H4A···O1 <sup>ii</sup> 0.82       1.95       2.7689 (17)       173	O2—C3—C9	120.14 (19)		C16—C15—H15		119.6
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N2—C3—C9	118.58 (18)		O3—C2—N2		114.81 (16)
C13—C12—H12       120.1       N2—C2—C17       123.77 (17)         C11—C12—H12       120.1       O3—C2—C1       115.22 (16)         N2—C10—H10A       109.5       N2—C2—C1       113.46 (16)         N2—C10—H10B       109.5       C17—C2—C1       117.85 (17)         H10A—C10—H10B       109.5       C4—C5—C6       119.79 (19)         N2—C10—H10C       109.5       C4—C5—H5       120.1         H10A—C10—H10C       109.5       C6—C5—H5       120.1         H10B—C10—H10C       109.5       O1—C1—N1       122.65 (19)         C15—C16—C11       119.5 (2)       O1—C1—C2       122.34 (19)         C15—C16—H16       120.2       N1—C1—C2       114.97 (17)         Hydrogen-bond geometry (Å, °)         D—H       H···A       D···A       D—H···A         N1—H1···O2 <sup>i</sup> 0.86       2.13       2.893 (2)       148         O4—H4A···O1 <sup>ii</sup> 0.82       1.95       2.7689 (17)       173	C13—C12—C11	119.76 (18)		O3—C2—C17		60.63 (12)
C11—C12—H12       120.1       O3—C2—C1       115.22 (16)         N2—C10—H10A       109.5       N2—C2—C1       113.46 (16)         N2—C10—H10B       109.5       C17—C2—C1       117.85 (17)         H10A—C10—H10B       109.5       C4—C5—C6       119.79 (19)         N2—C10—H10C       109.5       C4—C5—H5       120.1         H10A—C10—H10C       109.5       C6—C5—H5       120.1         H10B—C10—H10C       109.5       O1—C1—N1       122.65 (19)         C15—C16—C11       119.5 (2)       O1—C1—C2       122.34 (19)         C15—C16—H16       120.2       N1—C1—C2       114.97 (17)         Hydrogen-bond geometry (Å, °)       D—H       H···A       D···A       D—H···A         N1—H1···O2 <sup>i</sup> 0.86       2.13       2.893 (2)       148         O4—H4A···O1 <sup>ii</sup> 0.82       1.95       2.7689 (17)       173	C13—C12—H12	120.1		N2-C2-C17		123.77 (17)
N2—C10—H10A109.5N2—C2—C1113.46 (16)N2—C10—H10B109.5C17—C2—C1117.85 (17)H10A—C10—H10B109.5C4—C5—C6119.79 (19)N2—C10—H10C109.5C4—C5—H5120.1H10A—C10—H10C109.5C6—C5—H5120.1H10B—C10—H10C109.5O1—C1—N1122.65 (19)C15—C16—C11119.5 (2)O1—C1—C2122.34 (19)C15—C16—H16120.2N1—C1—C2114.97 (17)Hydrogen-bond geometry (Å, °)D—HH···AD···AD—H···AD—HM···AD—H···AN1—H1···O2 <sup>i</sup> 0.862.132.893 (2)148O4—H4A···O1 <sup>ii</sup> 0.821.952.7689 (17)173	C11—C12—H12	120.1		O3—C2—C1		115.22 (16)
N2—C10—H10B109.5C17—C2—C1117.85 (17)H10A—C10—H10B109.5C4—C5—C6119.79 (19)N2—C10—H10C109.5C4—C5—H5120.1H10A—C10—H10C109.5C6—C5—H5120.1H10B—C10—H10C109.5O1—C1—N1122.65 (19)C15—C16—C11119.5 (2)O1—C1—C2122.34 (19)C15—C16—H16120.2N1—C1—C2114.97 (17)Hydrogen-bond geometry (Å, °)D—HH···AD···AD—H···AD—HH···AD···AN1—H1···O2 <sup>i</sup> 0.862.132.893 (2)148O4—H4A···O1 <sup>ii</sup> 0.821.952.7689 (17)173	N2-C10-H10A	109.5		N2—C2—C1		113.46 (16)
H10A—C10—H10B109.5C4—C5—C6119.79 (19)N2—C10—H10C109.5C4—C5—H5120.1H10A—C10—H10C109.5C6—C5—H5120.1H10B—C10—H10C109.5O1—C1—N1122.65 (19)C15—C16—C11119.5 (2)O1—C1—C2122.34 (19)C15—C16—H16120.2N1—C1—C2114.97 (17)Hydrogen-bond geometry (Å, °)D—HH···AD—H···AD—HH···AN1—H1···O2 <sup>i</sup> 0.862.132.893 (2)O4—H4A···O1 <sup>ii</sup> 0.821.952.7689 (17)173	N2-C10-H10B	109.5		C17—C2—C1		117.85 (17)
N2—C10—H10C       109.5       C4—C5—H5       120.1         H10A—C10—H10C       109.5       C6—C5—H5       120.1         H10B—C10—H10C       109.5       O1—C1—N1       122.65 (19)         C15—C16—C11       119.5 (2)       O1—C1—C2       122.34 (19)         C15—C16—H16       120.2       N1—C1—C2       114.97 (17)         Hydrogen-bond geometry (Å, °)         D—H···A       D—H       H···A       D···A       D—H···A         N1—H1···O2 <sup>i</sup> 0.86       2.13       2.893 (2)       148         O4—H4A···O1 <sup>ii</sup> 0.82       1.95       2.7689 (17)       173	H10A—C10—H10B	109.5		C4—C5—C6		119.79 (19)
H10A—C10—H10C109.5C6—C5—H5120.1H10B—C10—H10C109.5O1—C1—N1122.65 (19)C15—C16—C11119.5 (2)O1—C1—C2122.34 (19)C15—C16—H16120.2N1—C1—C2114.97 (17)Hydrogen-bond geometry (Å, °) $D$ —H···AD—HH···AN1—H1···O2 <sup>i</sup> 0.862.13O4—H4A···O1 <sup>ii</sup> 0.821.952.7689 (17)	N2-C10-H10C	109.5		С4—С5—Н5		120.1
H10B—C10—H10C109.5O1—C1—N1122.65 (19)C15—C16—C11119.5 (2)O1—C1—C2122.34 (19)C15—C16—H16120.2N1—C1—C2114.97 (17)Hydrogen-bond geometry (Å, °)D—H···AD—HH···AD···AN1—H1···O2 <sup>i</sup> 0.862.132.893 (2)148O4—H4A···O1 <sup>ii</sup> 0.821.952.7689 (17)173	H10A—C10—H10C	109.5		С6—С5—Н5		120.1
C15—C16—C11       119.5 (2)       O1—C1—C2       122.34 (19)         C15—C16—H16       120.2       N1—C1—C2       114.97 (17)         Hydrogen-bond geometry (Å, °) $D$ —H       H···A $D$ ···A $D$ —H···A         N1—H1···O2 <sup>i</sup> 0.86       2.13       2.893 (2)       148         O4—H4A···O1 <sup>ii</sup> 0.82       1.95       2.7689 (17)       173	H10B-C10-H10C	109.5		01-C1-N1		122.65 (19)
C15—C16—H16       120.2       N1—C1—C2       114.97 (17)         Hydrogen-bond geometry (Å, °) $D$ —H       H···A $D$ ···A $D$ —H···A         N1—H1···O2 <sup>i</sup> 0.86       2.13       2.893 (2)       148         O4—H4A···O1 <sup>ii</sup> 0.82       1.95       2.7689 (17)       173	C15-C16-C11	119.5 (2)		O1—C1—C2		122.34 (19)
Hydrogen-bond geometry (Å, °) $D$ —H       H···A $D$ ···A $D$ —H···A         N1—H1···O2 <sup>i</sup> 0.86       2.13       2.893 (2)       148         O4—H4A···O1 <sup>ii</sup> 0.82       1.95       2.7689 (17)       173	C15—C16—H16	120.2		N1—C1—C2		114.97 (17)
D—H···A       D—H       H···A       D···A       D—H···A         N1—H1···O2 <sup>i</sup> 0.86       2.13       2.893 (2)       148         O4—H4A···O1 <sup>ii</sup> 0.82       1.95       2.7689 (17)       173	Hydrogen-bond geometry (Å, °)					
N1—H1···O2 <sup>i</sup> 0.862.132.893 (2)148O4—H4A···O1 <sup>ii</sup> 0.821.952.7689 (17)173	D—H···A		D—H	H···A	$D \cdots A$	D—H··· $A$
O4—H4A···O1 <sup>ii</sup> 0.82 1.95 2.7689 (17) 173	N1—H1····O2 <sup>i</sup>		0.86	2.13	2.893 (2)	148
	O4—H4A…O1 <sup>ii</sup>		0.82	1.95	2.7689 (17)	173

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







Fig. 2