11514 measured reflections

 $R_{\rm int} = 0.033$ 

1 restraint

 $\Delta \rho_{\rm max} = 0.14 \text{ e} \text{ Å}^{-3}$ 

 $\Delta \rho_{\rm min} = -0.15 \text{ e} \text{ Å}^{-3}$ 

2850 independent reflections

1724 reflections with  $I > 2\sigma(I)$ 

H-atom parameters constrained

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# 7-Diethylamino-2-oxo-2H-chromene-3carbaldehyde

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Key indicators: single-crystal X-ray study; T = 295 K; mean  $\sigma$ (C–C) = 0.003 Å; disorder in main residue; R factor = 0.048; wR factor = 0.144; data-to-parameter ratio = 15.5.

In the title compound, C<sub>14</sub>H<sub>15</sub>NO<sub>3</sub>, all non-H atoms except for those of the methyl and the disordered ethyl groupare approximately co-planar, the largest deviation from the mean plane being 0.0223 (13) Å at the N atom. In the crystal, the packing of molecules through weak intermolecular C-H···O hydrogen-bonding interactions leads to the formation of layers parallel to bc plane. Within these layers, there exist slipped  $\pi$ - $\pi$  stacking interactions between symmetry-related fused rings [centroid–centroid distances = 3.527(3) and 3.554(3), slippage = 0.988 and 1.011 Å, respectively]. One ethyl group is disordered over two sets of sites with siteoccupation factors of 0.54 and 0.46.

#### **Related literature**

For background to the title compound, an organic intermediate and a fluorescent probe for cyanide and amino acids, see: Kim et al. (2010). For electronic and photonic applications of coumarins, see: Murray et al. (1982). For the synthesis, see: Wu et al. (2007).



#### **Experimental**

#### Crystal data

C <sub>14</sub> H <sub>15</sub> NO <sub>3</sub>	$V = 2517 (3) \text{ Å}^3$
$M_r = 245.27$	Z = 8
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
a = 25.488 (17)  Å	$\mu = 0.09 \text{ mm}^{-1}$
b = 7.844 (6) Å	T = 295  K
c = 12.599 (12)  Å	$0.41 \times 0.39 \times 0.21 \text{ mm}$
$\beta = 92.39 \ (3)^{\circ}$	

#### Data collection

Rigaku R-AXIS RAPID diffractometer Absorption correction: multi-scan (ABSCOR; Higashi, 1995)  $T_{\min} = 0.963, \ \tilde{T}_{\max} = 0.981$ 

#### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.048$  $wR(F^2) = 0.144$ S = 1.062850 reflections 184 parameters

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

$D - H \cdot \cdot \cdot A$	$D-\mathrm{H}$	$H \cdot \cdot \cdot A$	$D \cdot \cdot \cdot A$	$D - \mathbf{H} \cdot \cdot \cdot A$
C8-H8···O3 <sup>i</sup>	0.93	2.58	3.367 (4)	143
C9−H9···O1 <sup>ii</sup>	0.93	2.55	3.432 (3)	158
$C13-H13B\cdots O2^{iii}$	0.97	2.53	3.388 (3)	147
Symmetry codes: (i) $-x$	$+\frac{1}{2}, y + \frac{1}{2}, -z$	$+\frac{5}{2}$ ; (ii) x, -y, z	$+\frac{1}{2}$ ; (iii) $-x + \frac{1}{2}$ ,	$y + \frac{1}{2}, -z + \frac{3}{2}.$

Data collection: RAPID-AUTO (Rigaku, 1998); cell refinement: RAPID-AUTO; data reduction: CrystalStructure (Rigaku, 2002); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEPIII (Burnett & Johnson, 1996) and ORTEP-3 for Windows (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: DN2698).

#### References

- Burnett, M. N. & Johnson, C. K. (1996). ORTEPIII. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
- Farrugia, L. J. (1997). J. Appl. Cryst. 30, 565.
- Higashi, T. (1995). ABSCOR. Rigaku Corporation, Tokyo, Japan.
- Kim, G. J. & Kim, H. J. (2010). Tetrahedron Lett. 51, 2914-2916.
- Murray, R. D., Mendez, J. & Brown, S. A. (1982). The Natural Coumarins: Occurrence, Chemistry and Biochemistry, p. 227. New York: John Wiley and Sons
- Rigaku (1998). RAPID-AUTO. Rigaku Corporation, Tokyo, Japan.
- Rigaku (2002). CrystalStructure. Rigaku/MSC Inc., The Woodlands, Texas, USA.
- Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.
- Wu, J. S., Liu, W. M., Zhuang, X. Q., Wang, F., Wang, P. F., Tao, S. L., Zhang, X. H., Wu, S. K. & Lee, S. T. (2007). Org. Lett. 9, 33-36.

supplementary materials

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## 7-Diethylamino-2-oxo-2H-chromene-3-carbaldehyde

### H.-D. Li and B.-Z. Yin

#### Comment

Coumarins are an important class of naturally occurring and synthetic compounds, which have been extentively investigated for electronic and photonic applications (Murray *et al.*, 1982). Herein, we reported the crystal structure of the title compound, an important organic intermediate and a fluorescent probe for cyanide and amino acids (Kim *et al.*, 2010).

The molecule of title compound formed by two fused rings is mainly planar with the exception of the methyl and disordered ethyl group (Fig. 1). The weak intermolecular C—H···O hydrogen bonds (Table 1) link the molecules into layers parallel to the (100) plane. Futhermore, slipped  $\pi$ - $\pi$  stacking occurs between symetry related fused rings within the layers (Table 2)

#### Experimental

The title compound was prepared according to the literature (Wu *et al.*, 2007). Single crystals suitable for X-ray diffraction were prepared by recrystallization from mixture of dichloromethane and petroleum (60–90 °C).

#### Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93 to 0.97 Å) and were included in the refinement in the riding model with  $U_{iso}(H) = 1.2$  or 1.5  $U_{eq}(C_{methyl})$ .

One of the ethyl group is disordered over two positions with a site occupancy in the ratio 0.54/0.46. The refinement of the disordered moieties was carried out using the PART instruction and restraining them to have identical geometry with the SAME instruction available in SHELXL-97 (Sheldrick, 2008)

#### **Figures**



Fig. 1. The crystal structure of the title compound, with the atom numbering scheme. Displacement ellipsoids of non-H atoms are drawn at the 30% probalility level. H atoms are shown as small spheres of arbitrary radii. Only the major component of the disordered ethyl is represented for clarity.

### 7-Diethylamino-2-oxo-2H-chromene-3-carbaldehyde

#### Crystal data

C <sub>14</sub> H <sub>15</sub> NO <sub>3</sub>
$M_r = 245.27$
Monoclinic, C2/c
Hall symbol: -C 2yc
<i>a</i> = 25.488 (17) Å
b = 7.844 (6) Å
<i>c</i> = 12.599 (12) Å
$\beta = 92.39 \ (3)^{\circ}$
$V = 2517 (3) \text{ Å}^3$
Z = 8

#### Data collection

2850 independent reflections
1724 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.033$
$\theta_{\text{max}} = 27.5^{\circ}, \ \theta_{\text{min}} = 3.2^{\circ}$
$h = -32 \rightarrow 32$
$k = -9 \rightarrow 10$
$l = -16 \rightarrow 16$

F(000) = 1040 $D_{\rm x} = 1.295 \text{ Mg m}^{-3}$ 

 $\theta = 3.2-27.5^{\circ}$  $\mu = 0.09 \text{ mm}^{-1}$ T = 295 KBlock, brown

 $0.41 \times 0.39 \times 0.21 \text{ mm}$ 

Mo K $\alpha$  radiation,  $\lambda = 0.71073$  Å Cell parameters from 6542 reflections

#### Refinement

Refinement on $F^2$	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.048$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.144$	H-atom parameters constrained
S = 1.06	$w = 1/[\sigma^2(F_o^2) + (0.0674P)^2 + 0.3544P]$ where $P = (F_o^2 + 2F_c^2)/3$
2850 reflections	$(\Delta/\sigma)_{\rm max} < 0.001$
184 parameters	$\Delta \rho_{max} = 0.14 \text{ e} \text{ Å}^{-3}$
1 restraint	$\Delta \rho_{\rm min} = -0.15 \text{ e } \text{\AA}^{-3}$

#### Special details

Experimental. (See detailed section in the paper)

**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.

O10.24299 (4)0.00447 (14)0.88750 (8)0.0556 (3)020.17217 (5)-0.12688 (18)0.82505 (10)0.0787 (4)030.12022 (6)-0.2463 (18)1.11710 (12)0.0874 (5)C10.19772 (6)-0.2463 (18)1.11710 (12)0.0874 (5)C10.19772 (6)-0.0872 (2)0.90386 (13)0.0562 (4)C20.18575 (6)-0.12332 (19)1.01323 (12)0.0533 (4)C30.21800 (6)-0.0707 (2)1.09396 (12)0.0546 (4)C40.26540 (6)0.01794 (19)1.07523 (11)0.0503 (4)C50.27674 (6)0.0510 (19)0.96975 (11)0.0478 (4)C60.32073 (6)0.1413 (2)0.94200 (12)0.0533 (4)C60.32073 (6)0.1413 (2)0.87100.064*C70.35790 (6)1.938 (2)1.02108 (13)0.0578 (4)C80.34057 (7)0.1572 (2)1.12833 (13)0.0653 (5)F80.37070.1974 (12)1.15318 (12)0.0613 (4)C90.30257 (7)0.0747 (2)1.15318 (12)0.0613 (4)F90.29630.05461.22430.074*C100.13764 (7)-2.25920.97190.081*C11A0.4515 (3)0.2676 (10)1.0761 (7)0.086 (2)0.46H11A0.44780.15661.12670.1032 (1.04H11A0.44780.25920.97190.03140.46H11A0.44790.45661.0754 (5)0.164*0.46 </th <th></th> <th>x</th> <th>У</th> <th>Ζ</th> <th><math>U_{\rm iso}</math>*/<math>U_{\rm eq}</math></th> <th>Occ. (&lt;1)</th>		x	У	Ζ	$U_{\rm iso}$ */ $U_{\rm eq}$	Occ. (<1)
O20.17217 (5)-0.12688 (18)0.82505 (10)0.0787 (4)O30.12022 (6)-0.24463 (18)1.11710 (12)0.0874 (5)N10.40226 (6)0.2780 (2)0.99386 (13)0.0562 (4)C10.19772 (6)-0.0872 (2)0.90386 (13)0.0552 (4)C20.18575 (6)-0.12332 (19)1.01323 (12)0.0533 (4)C30.21890 (6)-0.0707 (2)1.09396 (12)0.0544 (4)H30.2105-0.09401.16360.066*C40.26540 (6)0.01794 (19)1.07523 (11)0.0503 (4)C50.27674 (6)0.0510 (19)0.94207 (12)0.0548 (4)C60.32073 (6)0.1413 (2)0.94200 (12)0.0578 (4)C70.35790 (6)0.1938 (2)1.02108 (13)0.0578 (4)C80.34095 (7)0.1572 (2)1.12853 (13)0.0636 (5)H80.37070.19061.8260.074*C90.30257 (7)0.0747 (2)1.15318 (12)0.0613 (4)H90.29630.05461.22430.074*C11A0.4515 (3)0.2676 (10)1.0761 (7)0.868 (2)0.46H11A0.44780.17561.12670.103*0.46H11A0.44780.25991.03870.1030 (17)0.46H11A0.4513 (2)0.45161.1690.154*0.46H11A0.45130.25671.0751 (5)0.154*0.46H11A0.4390 (2)0.3468 (8)1.0751 (5)0.154*	01	0.24299 (4)	0.00447 (14)	0.88750 (8)	0.0556 (3)	
03   0.12022 (6)   -0.24463 (18)   1.11710 (12)   0.0874 (5)     N1   0.40226 (6)   0.2780 (2)   0.99586 (12)   0.0747 (5)     C1   0.19772 (6)   -0.0872 (2)   0.90386 (13)   0.0562 (4)     C2   0.18575 (6)   -0.12333 (19)   1.01323 (12)   0.0533 (4)     C3   0.21890 (6)   -0.0707 (2)   1.09396 (12)   0.0564 (4)     H3   0.2105   -0.0940   1.1636   0.666*     C4   0.26540 (6)   0.01794 (19)   1.07523 (11)   0.0503 (4)     C5   0.27674 (6)   0.0510 (19)   0.96975 (11)   0.064*     C6   0.32073 (6)   0.1938 (2)   1.12853 (13)   0.0578 (4)     C7   0.35790 (6)   0.1938 (2)   1.12853 (13)   0.0578 (4)     C8   0.34065 (7)   0.1972 (2)   1.18218 (12)   0.0613 (4)     H9   0.2963   0.0546   1.2243   0.076*     C10   0.13764 (7)   -0.2172 (2)   1.03121 (16)   0.0679 (5)     H10   0.1189   -0.2	02	0.17217 (5)	-0.12688 (18)	0.82505 (10)	0.0787 (4)	
N1   0.40226 (6)   0.2780 (2)   0.99586 (12)   0.0747 (5)     C1   0.19772 (6)   -0.0872 (2)   0.90386 (13)   0.0552 (4)     C2   0.18575 (6)   -0.12332 (19)   1.01323 (12)   0.0546 (4)     H3   0.2105   -0.0940   1.1636   0.066*     C4   0.26540 (6)   0.01794 (19)   1.07523 (11)   0.0503 (4)     C5   0.27674 (6)   0.05510 (19)   0.96975 (11)   0.064*     C6   0.32073 (6)   0.1413 (2)   0.91200 (12)   0.0533 (4)     C6   0.32073 (6)   0.1938 (2)   1.02108 (13)   0.0578 (4)     C7   0.35790 (6)   0.1938 (2)   1.02108 (13)   0.0578 (4)     C8   0.34695 (7)   0.1572 (2)   1.12853 (13)   0.0636 (5)     H8   0.330257 (7)   0.1572 (2)   1.1518 (12)   0.0613 (4)     H9   0.2963   0.0546   1.2243   0.074*     C10   0.13764 (7)   -0.2172 (2)   1.03121 (16)   0.0679 (5)     H10   0.13764 (7)   -0	03	0.12022 (6)	-0.24463 (18)	1.11710 (12)	0.0874 (5)	
C10.19772 (6)-0.0872 (2)0.90386 (13)0.0562 (4)C20.18575 (6)-0.12332 (19)1.01323 (12)0.0533 (4)C30.21890 (6)-0.0707 (2)1.09396 (12)0.0546 (4)H30.2105-0.09401.16360.0664C40.26540 (6)0.01794 (19)1.07523 (11)0.0503 (4)C50.27674 (6)0.05510 (19)0.96975 (11)0.04478 (4)C60.32073 (6)0.1413 (2)0.94200 (12)0.0533 (4)H60.32610.15520.87100.064*C70.35790 (6)0.1938 (2)1.21853 (13)0.0636 (5)H80.37070.19061.18260.074*C90.30257 (7)0.0747 (2)1.15118 (12)0.0613 (4)H90.29630.05461.22430.074*C100.13764 (7)-0.2172 (2)1.03121 (16)0.0679 (5)H100.1189-0.25920.97190.81*C11A0.44780.17561.12670.103*0.46H11B0.48360.25091.03870.1030 (17)0.46H11A0.44780.15061.07840.159*0.46H12D0.46070.44481.18050.154*0.46H12D0.43070.44481.16690.154*0.46H12D0.4300 (2)0.3468 (8)1.0753 (5)0.0750 (15)0.54H12D0.49070.44481.16690.154*0.46H12D0.49020.1394 <td>N1</td> <td>0.40226 (6)</td> <td>0.2780 (2)</td> <td>0.99586 (12)</td> <td>0.0747 (5)</td> <td></td>	N1	0.40226 (6)	0.2780 (2)	0.99586 (12)	0.0747 (5)	
C2 $0.18575 (6)$ $-0.1232 (19)$ $1.01323 (12)$ $0.0533 (4)$ C3 $0.21890 (6)$ $-0.0707 (2)$ $1.09396 (12)$ $0.0546 (4)$ H3 $0.2105$ $-0.0940$ $1.1636$ $0.066*$ C4 $0.26540 (6)$ $0.01794 (19)$ $1.07523 (11)$ $0.0503 (4)$ C5 $0.27674 (6)$ $0.05510 (19)$ $0.96975 (11)$ $0.0478 (4)$ C6 $0.32073 (6)$ $0.1413 (2)$ $0.94200 (12)$ $0.0533 (4)$ H6 $0.3261$ $0.1652$ $0.8710$ $0.064*$ C7 $0.35790 (6)$ $0.1572 (2)$ $1.12853 (13)$ $0.0636 (5)$ H8 $0.3707$ $0.1972 (2)$ $1.12853 (13)$ $0.0636 (5)$ H8 $0.3707$ $0.1906$ $1.1826$ $0.074*$ C9 $0.30257 (7)$ $0.0747 (2)$ $1.15318 (12)$ $0.0613 (4)$ H9 $0.2963$ $0.0546$ $1.2243$ $0.074*$ C10 $0.13764 (7)$ $-0.2172 (2)$ $1.03121 (16)$ $0.0679 (5)$ H10 $0.1189$ $-0.2592$ $0.9719$ $0.081*$ C11A $0.4515 (3)$ $0.2676 (10)$ $1.0761 (7)$ $0.866 (2)$ $0.46$ H11B $0.4836$ $0.2509$ $1.0387$ $0.103*$ $0.46$ H11A $0.4478$ $0.1756$ $1.1267$ $0.1030 (17)$ $0.46$ H11A $0.4478$ $0.1568$ $0.154*$ $0.46$ H12B $0.4807$ $0.4448$ $1.1303 (5)$ $0.1304 (7)$ $0.46$ H12A $0.4501$ $0.3488 (8)$ $1.0753 (5)$ $0.154*$ </td <td>C1</td> <td>0.19772 (6)</td> <td>-0.0872 (2)</td> <td>0.90386 (13)</td> <td>0.0562 (4)</td> <td></td>	C1	0.19772 (6)	-0.0872 (2)	0.90386 (13)	0.0562 (4)	
C30.21890 (6)-0.0707 (2)1.09396 (12)0.0546 (4)H30.2105-0.09401.16360.066*C40.26540 (6)0.01794 (19)1.07523 (11)0.0503 (4)C50.27674 (6)0.05510 (19)0.96975 (11)0.0478 (4)C60.32073 (6)0.1413 (2)0.94200 (12)0.0533 (4)H60.32610.16520.87100.0636 (5)C70.35790 (6)0.1938 (2)1.02108 (13)0.0578 (4)C80.34695 (7)0.1572 (2)1.12853 (13)0.0636 (5)H80.37070.19061.18260.707*C90.30257 (7)0.0747 (2)1.15318 (12)0.0613 (4)H90.29630.05461.22430.074*C100.13764 (7)-0.2172 (2)1.03121 (16)0.679 (5)H100.1189-0.25920.97190.081*C11A0.4515 (3)0.2676 (10)1.0761 (7)0.806 (2)0.46H11A0.44780.17561.12670.103*0.46H11B0.48360.25091.03870.1030.46H12A0.4513 (2)0.4378 (8)1.1303 (5)0.1030 (17)0.46H12A0.45390.52661.07840.154*0.46H12B0.48070.44481.18050.154*0.46H12A0.4390 (2)0.3468 (8)1.0753 (5)0.0750 (15)0.54H11D0.45700.44481.18050.154*0.46H12E0.5	C2	0.18575 (6)	-0.12332 (19)	1.01323 (12)	0.0533 (4)	
H30.2105-0.09401.16360.066*C40.26540 (6)0.01794 (19)1.07523 (11)0.0503 (4)C50.27674 (6)0.05510 (19)0.96975 (11)0.0478 (4)C60.32073 (6)0.1413 (2)0.94200 (12)0.0533 (4)C70.35790 (6)0.1938 (2)1.02108 (13)0.0578 (4)C80.34695 (7)0.1572 (2)1.12853 (13)0.0636 (5)H80.37070.19061.18260.076*C90.30257 (7)0.0747 (2)1.15318 (12)0.0613 (4)H90.29630.05461.22430.074*C100.13764 (7)-0.2172 (2)1.03121 (16)0.0679 (5)H100.1189-0.25920.97190.081*C11A0.4515 (3)0.2676 (10)1.0761 (7)0.086 (2)0.46H11B0.48360.25091.0333 (5)0.1030 (17)0.46H12A0.4513 (2)0.4378 (8)1.1303 (5)0.1030 (17)0.46H12B0.48070.44481.18050.154*0.46H12B0.48070.44481.18050.154*0.46H12D0.45700.238351.13700.090*0.54H11D0.45700.2488 (8)1.1068 (5)0.125 (2)0.54H12D0.46020.11301.13540.188*0.54H12D0.46020.11301.13540.188*0.54H12D0.46020.11301.13550.188*0.54H12D	C3	0.21890 (6)	-0.0707 (2)	1.09396 (12)	0.0546 (4)	
C4 $0.26540$ (6) $0.01794$ (19) $1.07523$ (11) $0.0503$ (4)C5 $0.27674$ (6) $0.05510$ (19) $0.96975$ (11) $0.0478$ (4)C6 $0.32073$ (6) $0.1413$ (2) $0.94200$ (12) $0.0533$ (4)H6 $0.3261$ $0.1652$ $0.8710$ $0.064*$ C7 $0.35790$ (6) $0.1938$ (2) $1.02108$ (13) $0.0678$ (4)C8 $0.34695$ (7) $0.1572$ (2) $1.12853$ (13) $0.0636$ (5)H8 $0.3707$ $0.1906$ $1.1826$ $0.076*$ C9 $0.30257$ (7) $0.0747$ (2) $1.15318$ (12) $0.0613$ (4)H9 $0.2963$ $0.0546$ $1.2243$ $0.074*$ C10 $0.13764$ (7) $-0.2172$ (2) $1.03121$ (16) $0.0679$ (5)H10 $0.1189$ $-0.2592$ $0.9719$ $0.081*$ C11A $0.4515$ (3) $0.2676$ (10) $1.0367$ $0.103*$ $0.46$ H11A $0.4478$ $0.1756$ $1.1267$ $0.103*$ $0.46$ H11B $0.4836$ $0.2509$ $1.0387$ $0.1030$ (17) $0.46$ H12A $0.4437$ $0.5266$ $1.0784$ $0.154*$ $0.46$ H12B $0.4807$ $0.4448$ $1.1805$ $0.154*$ $0.46$ C11B $0.4390$ (2) $0.3468$ (8) $1.0753$ (5) $0.750$ (15) $0.54$ H11D $0.4570$ $0.4445$ $1.0469$ $0.909*$ $0.54$ H12C $0.4966$ $1.0734$ $1.0455$ $0.188*$ $0.54$ H12D $0.4502$ $0.1304$ $1.$	Н3	0.2105	-0.0940	1.1636	0.066*	
C50.27674 (6)0.05510 (19)0.96975 (11)0.0478 (4)C60.32073 (6)0.1413 (2)0.94200 (12)0.0533 (4)H60.32610.16520.87100.064*C70.35790 (6)0.1938 (2)1.02108 (13)0.0578 (4)C80.34695 (7)0.1572 (2)1.12853 (13)0.0636 (5)H80.37070.19061.18260.076*C90.30257 (7)0.0747 (2)1.15318 (12)0.0613 (4)H90.29630.05461.22430.074*C100.13764 (7)-0.2172 (2)1.03121 (16)0.0679 (5)H100.1189-0.25920.97190.081*C11A0.4515 (3)0.2676 (10)1.0761 (7)0.086 (2)0.46H11A0.44780.17561.12670.103*0.46H11A0.44780.17561.12670.103*0.46H12A0.45390.52661.07840.154*0.46H12A0.45390.52661.07840.154*0.46H12A0.4390 (2)0.3468 (8)1.0753 (5)0.750 (15)0.54H11D0.45700.44451.46690.909*0.54H11D0.45700.44451.04690.909*0.54H12D0.46020.13841.04690.909*0.54H12D0.46020.1361.13540.188*0.54H12D0.46020.1360.154*0.540.54H12D0.46020.1369 (3	C4	0.26540 (6)	0.01794 (19)	1.07523 (11)	0.0503 (4)	
C6 $0.32073(6)$ $0.1413(2)$ $0.94200(12)$ $0.0533(4)$ H6 $0.3261$ $0.1652$ $0.8710$ $0.064*$ C7 $0.35790(6)$ $0.1938(2)$ $1.02108(13)$ $0.0578(4)$ C8 $0.34695(7)$ $0.1572(2)$ $1.12853(13)$ $0.0636(5)$ H8 $0.3707$ $0.1906$ $1.1826$ $0.076*$ C9 $0.30257(7)$ $0.0747(2)$ $1.15318(12)$ $0.0613(4)$ H9 $0.2963$ $0.0546$ $1.2243$ $0.074*$ C10 $0.13764(7)$ $-0.2172(2)$ $1.03121(16)$ $0.6679(5)$ H10 $0.1189$ $-0.2592$ $0.9719$ $0.081^*$ C11A $0.4515(3)$ $0.2676(10)$ $1.0761(7)$ $0.086(2)$ $0.46$ H11B $0.4336$ $0.2509$ $1.0387$ $0.103^*$ $0.46$ H11B $0.4336$ $0.2509$ $1.0387$ $0.103(17)$ $0.46$ H12A $0.4513(2)$ $0.4378(8)$ $1.1303(5)$ $0.1530(17)$ $0.46$ H12B $0.4807$ $0.4448$ $1.1805$ $0.154^*$ $0.46$ H12B $0.4309(2)$ $0.3468(8)$ $1.0753(5)$ $0.0750(15)$ $0.54$ H11D $0.4570$ $0.2088(8)$ $1.1068(5)$ $0.154^*$ $0.46$ H11D $0.4570$ $0.2088(8)$ $1.068(5)$ $0.154^*$ $0.54$ H12B $0.490(2)$ $0.3468(8)$ $1.0753(5)$ $0.750(15)$ $0.54$ H11D $0.4570$ $0.2088(8)$ $1.168(5)$ $0.154^*$ $0.54$ <td>C5</td> <td>0.27674 (6)</td> <td>0.05510 (19)</td> <td>0.96975 (11)</td> <td>0.0478 (4)</td> <td></td>	C5	0.27674 (6)	0.05510 (19)	0.96975 (11)	0.0478 (4)	
H60.32610.16520.87100.064*C70.35790 (6)0.1938 (2)1.02108 (13)0.0578 (4)C80.34695 (7)0.1572 (2)1.12853 (13)0.0636 (5)H80.37070.19061.18260.076*C90.30257 (7)0.0747 (2)1.15318 (12)0.0613 (4)H90.29630.05461.22430.077*C100.13764 (7)-0.2172 (2)1.03121 (16)0.0679 (5)H100.1189-0.25920.97190.886 (2)0.46H11A0.4515 (3)0.2676 (10)1.0761 (7)0.086 (2)0.46H11B0.48360.25091.03870.103*0.46H12A0.4513 (2)0.4378 (8)1.1303 (5)0.1030 (17)0.46H12B0.48070.44481.18050.154*0.46H12B0.48070.3468 (8)1.0753 (5)0.0750 (15)0.54H11C0.42040.38351.13700.090*0.54H11D0.45700.44451.04690.090*0.54H11D0.45700.25271.15950.188*0.54H12E0.50310.25271.15950.188*0.54H12F0.49660.17341.04550.188*0.54H13A0.43740.41160.88470.089*.54H13B0.38060.35330.84950.89*.54H13A0.46920.13940.85630.152 (8).11025 (8) <td>C6</td> <td>0.32073 (6)</td> <td>0.1413 (2)</td> <td>0.94200 (12)</td> <td>0.0533 (4)</td> <td></td>	C6	0.32073 (6)	0.1413 (2)	0.94200 (12)	0.0533 (4)	
C7 $0.35790(6)$ $0.1938(2)$ $1.02108(13)$ $0.0578(4)$ $C8$ $0.34695(7)$ $0.1572(2)$ $1.12853(13)$ $0.0636(5)$ $H8$ $0.3707$ $0.1906$ $1.1826$ $0.076*$ $C9$ $0.30257(7)$ $0.0747(2)$ $1.15318(12)$ $0.0613(4)$ $H9$ $0.2963$ $0.0546$ $1.2243$ $0.074*$ $C10$ $0.13764(7)$ $-0.2172(2)$ $1.03121(16)$ $0.0679(5)$ $H10$ $0.1189$ $-0.2592$ $0.9719$ $0.81*$ $C11A$ $0.4515(3)$ $0.2676(10)$ $1.767(7)$ $0.088(2)$ $0.46$ $H11A$ $0.4515(3)$ $0.2676(10)$ $1.0761(7)$ $0.038(2)$ $0.46$ $H11A$ $0.44178$ $0.1756$ $1.1267$ $0.103*$ $0.46$ $H11B$ $0.4836$ $0.2509$ $1.0387$ $0.1030(17)$ $0.46$ $H12A$ $0.4539$ $0.5266$ $1.0784$ $0.154*$ $0.46$ $H12B$ $0.4807$ $0.4448$ $1.1805$ $0.154*$ $0.46$ $H12C$ $0.4193$ $0.4510$ $1.1669$ $0.090*$ $0.54$ $H11C$ $0.4570$ $0.4445$ $1.4049$ $0.909*$ $0.54$ $H11D$ $0.4570$ $0.2527$ $1.1370$ $0.909*$ $0.54$ $H12E$ $0.5031$ $0.2527$ $1.1595$ $0.188*$ $0.54$ $H12E$ $0.5031$ $0.2527$ $1.1595$ $0.188*$ $0.54$ $H12E$ $0.5031$ $0.2527$ $1.1595$ $0.188*$ $0.54$ $H12E$ $0.5031$ <	Н6	0.3261	0.1652	0.8710	0.064*	
C8   0.34695 (7)   0.1572 (2)   1.12853 (13)   0.0636 (5)     H8   0.3707   0.1906   1.1826   0.076*     C9   0.30257 (7)   0.0747 (2)   1.15318 (12)   0.0613 (4)     H9   0.2963   0.0546   1.2243   0.074*     C10   0.13764 (7)   -0.2172 (2)   1.03121 (16)   0.0679 (5)     H10   0.1189   -0.2592   0.9719   0.081 *     C11A   0.4515 (3)   0.2676 (10)   1.0761 (7)   0.086 (2)   0.46     H11B   0.4438   0.1756   1.1267   0.103*   0.46     H11B   0.4438   0.2509   1.0387   0.1030 (17)   0.46     H12A   0.4513 (2)   0.4378 (8)   1.1303 (5)   0.154*   0.46     H12B   0.4807   0.4448   1.1805   0.154*   0.46     H12B   0.4807   0.4448   1.1805   0.154*   0.46     H12C   0.4193   0.4510   1.1669   0.090*   0.54     H11C<	C7	0.35790 (6)	0.1938 (2)	1.02108 (13)	0.0578 (4)	
H80.37070.19061.18260.076*C90.30257 (7)0.0747 (2)1.15318 (12)0.6613 (4)H90.29630.05461.22430.074*C100.13764 (7)-0.2172 (2)1.03121 (16)0.0679 (5)H100.1189-0.25920.97190.081*C11A0.4515 (3)0.2676 (10)1.0761 (7)0.086 (2)0.46H11B0.44780.17561.12670.103*0.46H11B0.48360.25091.03870.1030 (17)0.46H12A0.4513 (2)0.4378 (8)1.1303 (5)0.1030 (17)0.46H12B0.48070.52661.07840.154*0.46H12C0.41930.45101.16690.154*0.46H12C0.4390 (2)0.3468 (8)1.0753 (5)0.0750 (15)0.54H11D0.45700.44451.04690.900*0.54H11D0.45700.2488 (8)1.1068 (5)0.125 (2)0.54H12D0.46020.11301.13540.188*0.54H12E0.50310.25271.15950.188*0.54H12F0.49660.17341.04550.188*0.54H13A0.43740.41160.88470.689*.54H13B0.38060.35330.84950.089*.54H13A0.4352 (9)0.1696 (3)0.8251 (2)0.125 (8).54	C8	0.34695 (7)	0.1572 (2)	1.12853 (13)	0.0636 (5)	
C9   0.30257 (7)   0.0747 (2)   1.15318 (12)   0.0613 (4)     H9   0.2963   0.0546   1.2243   0.074*     C10   0.13764 (7)   -0.2172 (2)   1.03121 (16)   0.0679 (5)     H10   0.1189   -0.2592   0.9719   0.081*     C11A   0.4515 (3)   0.2676 (10)   1.0761 (7)   0.086 (2)   0.46     H11A   0.4478   0.1756   1.1267   0.103*   0.46     H11B   0.4836   0.2509   1.0387   0.1030 (17)   0.46     H12A   0.4513 (2)   0.4378 (8)   1.1303 (5)   0.1030 (17)   0.46     H12A   0.4539   0.5266   1.0784   0.154*   0.46     H12B   0.4807   0.4448   1.805   0.154*   0.46     H12C   0.4193   0.4510   1.1669   0.154*   0.46     H12C   0.4193   0.4510   1.1669   0.909*   0.54     H11C   0.4204   0.3835   1.1370   0.909*   0.54	H8	0.3707	0.1906	1.1826	0.076*	
H90.29630.05461.22430.074*C100.13764 (7)-0.2172 (2)1.03121 (16)0.0679 (5)H100.1189-0.25920.97190.081*C11A0.4515 (3)0.2676 (10)1.0761 (7)0.086 (2)0.46H11A0.44780.17561.12670.103*0.46H11B0.48360.25091.03870.1030 (17)0.46H12A0.4513 (2)0.4378 (8)1.1303 (5)0.1030 (17)0.46H12B0.48070.44481.18050.154*0.46H12C0.41930.45101.16690.154*0.46H11C0.42040.38351.13700.090*0.54H11D0.45700.44451.04690.909*0.54H12D0.46020.11301.13540.188*0.54H12D0.46020.11301.13540.188*0.54H12E0.50310.25271.15950.188*0.54H12F0.49660.17341.04550.188*0.54H13A0.43740.41160.88577 (15)0.0742 (5)1.4354H13B0.38060.35330.84950.089*1.134*H14A0.46220.13940.85630.154*1.154*	С9	0.30257 (7)	0.0747 (2)	1.15318 (12)	0.0613 (4)	
C10   0.13764 (7)   -0.2172 (2)   1.03121 (16)   0.0679 (5)     H10   0.1189   -0.2592   0.9719   0.081*     C11A   0.4515 (3)   0.2676 (10)   1.0761 (7)   0.086 (2)   0.46     H11A   0.4478   0.1756   1.1267   0.103*   0.46     H11B   0.4836   0.2509   1.0387   0.1030 (17)   0.46     C12A   0.4513 (2)   0.4378 (8)   1.1303 (5)   0.1030 (17)   0.46     H12A   0.4539   0.5266   1.0784   0.154*   0.46     H12B   0.4807   0.4448   1.1805   0.154*   0.46     H12C   0.4193   0.4510   1.1669   0.154*   0.46     C11B   0.4390 (2)   0.3468 (8)   1.0753 (5)   0.0750 (15)   0.54     H11C   0.4204   0.3835   1.1370   0.090*   0.54     H11D   0.4570   0.4445   1.0469   0.909*   0.54     H12D   0.4602   0.1130   1.1354	Н9	0.2963	0.0546	1.2243	0.074*	
H100.1189-0.25920.97190.081*C11A0.4515 (3)0.2676 (10)1.0761 (7)0.086 (2)0.46H11A0.44780.17561.12670.103*0.46H11B0.48360.25091.03870.103*0.46C12A0.4513 (2)0.4378 (8)1.1303 (5)0.1030 (17)0.46H12B0.45390.52661.07840.154*0.46H12C0.41930.45101.16690.154*0.46C11B0.4390 (2)0.3468 (8)1.0753 (5)0.0750 (15)0.54H11C0.42040.38351.13700.090*0.54H11D0.45700.44451.04690.090*0.54H12E0.50310.25271.15950.188*0.54H12F0.49660.17341.04550.188*0.54H12F0.49660.17340.88577 (15)0.0742 (5)1.54H13A0.43740.41160.88470.089*1.413H13B0.38060.35330.84950.089*1.14A	C10	0.13764 (7)	-0.2172 (2)	1.03121 (16)	0.0679 (5)	
C11A   0.4515 (3)   0.2676 (10)   1.0761 (7)   0.086 (2)   0.46     H11A   0.4478   0.1756   1.1267   0.103*   0.46     H11B   0.4836   0.2509   1.0387   0.103*   0.46     C12A   0.4513 (2)   0.4378 (8)   1.1303 (5)   0.1030 (17)   0.46     H12A   0.4539   0.5266   1.0784   0.154*   0.46     H12B   0.4807   0.4448   1.1805   0.154*   0.46     H12C   0.4193   0.4510   1.1669   0.154*   0.46     C11B   0.4390 (2)   0.3468 (8)   1.0753 (5)   0.0750 (15)   0.54     H11C   0.4204   0.3835   1.1370   0.090*   0.54     H11D   0.4570   0.4445   1.0469   0.090*   0.54     H12B   0.4602   0.1130   1.1354   0.188*   0.54     H12D   0.4602   0.1130   1.1354   0.188*   0.54     H12F   0.4966   0.1734	H10	0.1189	-0.2592	0.9719	0.081*	
H11A0.44780.17561.12670.103*0.46H11B0.48360.25091.03870.103*0.46C12A0.4513 (2)0.4378 (8)1.1303 (5)0.1030 (17)0.46H12A0.45390.52661.07840.154*0.46H12B0.48070.44481.18050.154*0.46H12C0.41930.45101.16690.154*0.46C11B0.4390 (2)0.3468 (8)1.0753 (5)0.0750 (15)0.54H11C0.42040.38351.13700.090*0.54H11D0.45700.44451.04690.900*0.54H12D0.46020.11301.13540.188*0.54H12E0.50310.25271.15950.188*0.54H12F0.49660.17341.04550.188*0.54H12F0.49660.3169 (3)0.88577 (15)0.0742 (5)H13A0.43740.41160.88470.089*1H13B0.38060.35330.84950.089*1H14A0.46920.13940.85630.154*1	C11A	0.4515 (3)	0.2676 (10)	1.0761 (7)	0.086 (2)	0.46
H11B0.48360.25091.03870.103*0.46C12A0.4513 (2)0.4378 (8)1.1303 (5)0.1030 (17)0.46H12A0.45390.52661.07840.154*0.46H12B0.48070.44481.18050.154*0.46H12C0.41930.45101.16690.154*0.46C11B0.4390 (2)0.3468 (8)1.0753 (5)0.0750 (15)0.54H11C0.42040.38351.13700.090*0.54H11D0.45700.44451.04690.090*0.54C12B0.4784 (2)0.2088 (8)1.1068 (5)0.125 (2)0.54H12C0.50310.25271.15950.188*0.54H12F0.49660.17341.04550.188*0.54H12F0.49060.3169 (3)0.88577 (15)0.0742 (5)H13A0.43740.41160.88470.089*1H13B0.38060.35330.84950.089*1H14A0.46920.13940.85630.154*1	H11A	0.4478	0.1756	1.1267	0.103*	0.46
C12A 0.4513 (2) 0.4378 (8) 1.1303 (5) 0.1030 (17) 0.46   H12A 0.4539 0.5266 1.0784 0.154* 0.46   H12B 0.4807 0.4448 1.1805 0.154* 0.46   H12C 0.4193 0.4510 1.1669 0.154* 0.46   C11B 0.4390 (2) 0.3468 (8) 1.0753 (5) 0.0750 (15) 0.54   H11C 0.4204 0.3835 1.1370 0.090* 0.54   H11D 0.4570 0.4445 1.0469 0.090* 0.54   H12D 0.4784 (2) 0.2088 (8) 1.1068 (5) 0.125 (2) 0.54   H12D 0.4602 0.1130 1.1354 0.188* 0.54   H12F 0.4966 0.1734 1.0455 0.188* 0.54   H12F 0.4966 0.1734 1.0455 0.188* 0.54   C13 0.41299 (8) 0.3169 (3) 0.88577 (15) 0.0742 (5)   H13A 0.4374 0.4116 0.8847 0.089* 1   H13B 0.3806 0.3533	H11B	0.4836	0.2509	1.0387	0.103*	0.46
H12A0.45390.52661.07840.154*0.46H12B0.48070.44481.18050.154*0.46H12C0.41930.45101.16690.154*0.46C11B0.4390 (2)0.3468 (8)1.0753 (5)0.0750 (15)0.54H11C0.42040.38351.13700.090*0.54H11D0.45700.44451.04690.090*0.54H12D0.46020.11301.13540.188*0.54H12E0.50310.25271.15950.188*0.54H12F0.49660.17341.04550.188*0.54H13A0.43740.41160.88470.089*.54H13B0.38060.35330.84950.089*.54H14A0.46920.13940.85630.154*.54	C12A	0.4513 (2)	0.4378 (8)	1.1303 (5)	0.1030 (17)	0.46
H12B0.48070.44481.18050.154*0.46H12C0.41930.45101.16690.154*0.46C11B0.4390 (2)0.3468 (8)1.0753 (5)0.0750 (15)0.54H11C0.42040.38351.13700.090*0.54H11D0.45700.44451.04690.090*0.54C12B0.4784 (2)0.2088 (8)1.1068 (5)0.125 (2)0.54H12D0.46020.11301.13540.188*0.54H12E0.50310.25271.15950.188*0.54H12F0.49660.17341.04550.188*0.54C130.41299 (8)0.3169 (3)0.88577 (15)0.0742 (5)H13A0.43740.41160.88470.089*.H13B0.38060.35330.84950.089*.C140.43552 (9)0.1696 (3)0.8251 (2)0.1025 (8).H14A0.46920.13940.85630.154*.	H12A	0.4539	0.5266	1.0784	0.154*	0.46
H12C0.41930.45101.16690.154*0.46C11B0.4390 (2)0.3468 (8)1.0753 (5)0.0750 (15)0.54H11C0.42040.38351.13700.090*0.54H11D0.45700.44451.04690.090*0.54C12B0.4784 (2)0.2088 (8)1.1068 (5)0.125 (2)0.54H12D0.46020.11301.13540.188*0.54H12E0.50310.25271.15950.188*0.54H12F0.49660.17341.04550.188*0.54C130.41299 (8)0.3169 (3)0.88577 (15)0.0742 (5)H13A0.43740.41160.88470.089*H13B0.38060.35330.84950.089*C140.43552 (9)0.1696 (3)0.8251 (2)0.1025 (8)H14A0.46920.13940.85630.154*	H12B	0.4807	0.4448	1.1805	0.154*	0.46
C11B0.4390 (2)0.3468 (8)1.0753 (5)0.0750 (15)0.54H11C0.42040.38351.13700.090*0.54H11D0.45700.44451.04690.090*0.54C12B0.4784 (2)0.2088 (8)1.1068 (5)0.125 (2)0.54H12D0.46020.11301.13540.188*0.54H12E0.50310.25271.15950.188*0.54H12F0.49660.17341.04550.188*0.54C130.41299 (8)0.3169 (3)0.88577 (15)0.0742 (5)H13A0.43740.41160.88470.089*1138H13B0.38060.35330.84950.089*1144H14A0.46920.13940.85630.154*1154*	H12C	0.4193	0.4510	1.1669	0.154*	0.46
H11C0.42040.38351.13700.090*0.54H11D0.45700.44451.04690.090*0.54C12B0.4784 (2)0.2088 (8)1.1068 (5)0.125 (2)0.54H12D0.46020.11301.13540.188*0.54H12E0.50310.25271.15950.188*0.54H12F0.49660.17341.04550.188*0.54C130.41299 (8)0.3169 (3)0.88577 (15)0.0742 (5)H13A0.43740.41160.88470.089*H13B0.38060.35330.84950.089*C140.43552 (9)0.1696 (3)0.8251 (2)0.1025 (8)H14A0.46920.13940.85630.154*	C11B	0.4390 (2)	0.3468 (8)	1.0753 (5)	0.0750 (15)	0.54
H11D0.45700.44451.04690.090*0.54C12B0.4784 (2)0.2088 (8)1.1068 (5)0.125 (2)0.54H12D0.46020.11301.13540.188*0.54H12E0.50310.25271.15950.188*0.54H12F0.49660.17341.04550.188*0.54C130.41299 (8)0.3169 (3)0.88577 (15)0.0742 (5)H13A0.43740.41160.88470.089*H13B0.38060.35330.84950.089*C140.43552 (9)0.1696 (3)0.8251 (2)0.1025 (8)H14A0.46920.13940.85630.154*	H11C	0.4204	0.3835	1.1370	0.090*	0.54
C12B0.4784 (2)0.2088 (8)1.1068 (5)0.125 (2)0.54H12D0.46020.11301.13540.188*0.54H12E0.50310.25271.15950.188*0.54H12F0.49660.17341.04550.188*0.54C130.41299 (8)0.3169 (3)0.88577 (15)0.0742 (5)H13A0.43740.41160.88470.089*H13B0.38060.35330.84950.089*C140.43552 (9)0.1696 (3)0.8251 (2)0.1025 (8)H14A0.46920.13940.85630.154*	H11D	0.4570	0.4445	1.0469	0.090*	0.54
H12D0.46020.11301.13540.188*0.54H12E0.50310.25271.15950.188*0.54H12F0.49660.17341.04550.188*0.54C130.41299 (8)0.3169 (3)0.88577 (15)0.0742 (5)H13A0.43740.41160.88470.089*H13B0.38060.35330.84950.089*C140.43552 (9)0.1696 (3)0.8251 (2)0.1025 (8)H14A0.46920.13940.85630.154*	C12B	0.4784 (2)	0.2088 (8)	1.1068 (5)	0.125 (2)	0.54
H12E0.50310.25271.15950.188*0.54H12F0.49660.17341.04550.188*0.54C130.41299 (8)0.3169 (3)0.88577 (15)0.0742 (5)H13A0.43740.41160.88470.089*H13B0.38060.35330.84950.089*C140.43552 (9)0.1696 (3)0.8251 (2)0.1025 (8)H14A0.46920.13940.85630.154*	H12D	0.4602	0.1130	1.1354	0.188*	0.54
H12F0.49660.17341.04550.188*0.54C130.41299 (8)0.3169 (3)0.88577 (15)0.0742 (5)H13A0.43740.41160.88470.089*H13B0.38060.35330.84950.089*C140.43552 (9)0.1696 (3)0.8251 (2)0.1025 (8)H14A0.46920.13940.85630.154*	H12E	0.5031	0.2527	1.1595	0.188*	0.54
C130.41299 (8)0.3169 (3)0.88577 (15)0.0742 (5)H13A0.43740.41160.88470.089*H13B0.38060.35330.84950.089*C140.43552 (9)0.1696 (3)0.8251 (2)0.1025 (8)H14A0.46920.13940.85630.154*	H12F	0.4966	0.1734	1.0455	0.188*	0.54
H13A0.43740.41160.88470.089*H13B0.38060.35330.84950.089*C140.43552 (9)0.1696 (3)0.8251 (2)0.1025 (8)H14A0.46920.13940.85630.154*	C13	0.41299 (8)	0.3169 (3)	0.88577 (15)	0.0742 (5)	
H13B0.38060.35330.84950.089*C140.43552 (9)0.1696 (3)0.8251 (2)0.1025 (8)H14A0.46920.13940.85630.154*	H13A	0.4374	0.4116	0.8847	0.089*	
C140.43552 (9)0.1696 (3)0.8251 (2)0.1025 (8)H14A0.46920.13940.85630.154*	H13B	0.3806	0.3533	0.8495	0.089*	
H14A 0.4692 0.1394 0.8563 0.154*	C14	0.43552 (9)	0.1696 (3)	0.8251 (2)	0.1025 (8)	
	H14A	0.4692	0.1394	0.8563	0.154*	

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

# supplementary materials

H14B	0.4393	0.2024	0.7524	0.154*
H14C	0.4123	0.0735	0.8280	0.154*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
01	0.0602 (6)	0.0714 (7)	0.0356 (6)	-0.0004 (6)	0.0062 (4)	0.0006 (5)
02	0.0830 (8)	0.1019 (10)	0.0503 (7)	-0.0158 (7)	-0.0056 (6)	0.0026 (7)
03	0.0943 (10)	0.0941 (10)	0.0756 (9)	-0.0150 (8)	0.0259 (8)	0.0101 (7)
N1	0.0630 (8)	0.1053 (12)	0.0559 (9)	-0.0141 (8)	0.0021 (7)	0.0042 (8)
C1	0.0627 (9)	0.0599 (10)	0.0459 (9)	0.0078 (8)	0.0030(7)	0.0007 (7)
C2	0.0613 (9)	0.0508 (9)	0.0486 (9)	0.0078 (8)	0.0114 (7)	0.0042 (7)
C3	0.0697 (10)	0.0563 (9)	0.0387 (8)	0.0110 (8)	0.0125 (7)	0.0036 (7)
C4	0.0612 (9)	0.0544 (9)	0.0357 (8)	0.0106 (7)	0.0091 (6)	0.0020 (6)
C5	0.0565 (8)	0.0530 (9)	0.0342 (7)	0.0129 (7)	0.0044 (6)	-0.0019 (6)
C6	0.0602 (9)	0.0646 (10)	0.0358 (8)	0.0082 (8)	0.0089 (6)	0.0018 (7)
C7	0.0604 (9)	0.0651 (10)	0.0479 (9)	0.0078 (8)	0.0044 (7)	0.0016 (7)
C8	0.0707 (11)	0.0787 (12)	0.0408 (9)	0.0001 (9)	-0.0031 (7)	0.0005 (8)
C9	0.0784 (11)	0.0727 (11)	0.0329 (8)	0.0061 (9)	0.0046 (7)	0.0034 (7)
C10	0.0754 (11)	0.0657 (11)	0.0631 (12)	0.0018 (9)	0.0103 (9)	0.0037 (9)
C11A	0.069 (4)	0.099 (6)	0.091 (4)	0.013 (4)	0.007 (3)	0.022 (4)
C12A	0.093 (4)	0.121 (5)	0.094 (4)	-0.022 (3)	-0.009 (3)	-0.008 (4)
C11B	0.065 (3)	0.086 (4)	0.073 (3)	-0.015 (3)	-0.013 (2)	0.005 (3)
C12B	0.083 (3)	0.152 (5)	0.137 (5)	0.036 (3)	-0.040 (3)	0.021 (4)
C13	0.0713 (11)	0.0878 (13)	0.0643 (11)	-0.0101 (10)	0.0123 (9)	0.0046 (10)
C14	0.0940 (15)	0.1172 (19)	0.0991 (18)	0.0080 (14)	0.0368 (13)	-0.0051 (15)

# Geometric parameters (Å, °)

O1—C5	1.3774 (19)	С9—Н9	0.9300
O1—C1	1.382 (2)	C10—H10	0.9300
O2—C1	1.205 (2)	C11A—C12A	1.500 (8)
O3—C10	1.206 (2)	C11A—H11A	0.9700
N1—C7	1.358 (2)	C11A—H11B	0.9700
N1—C11B	1.446 (6)	C12A—H12A	0.9600
N1—C13	1.457 (3)	C12A—H12B	0.9600
N1—C11A	1.581 (8)	C12A—H12C	0.9600
C1—C2	1.452 (3)	C11B—C12B	1.517 (7)
C2—C3	1.359 (2)	C11B—H11C	0.9700
C2—C10	1.456 (3)	C11B—H11D	0.9700
C3—C4	1.402 (2)	C12B—H12D	0.9600
С3—Н3	0.9300	C12B—H12E	0.9600
C4—C5	1.402 (2)	C12B—H12F	0.9600
C4—C9	1.408 (2)	C13—C14	1.512 (3)
C5—C6	1.367 (2)	C13—H13A	0.9700
C6—C7	1.408 (2)	C13—H13B	0.9700
С6—Н6	0.9300	C14—H14A	0.9600
С7—С8	1.423 (2)	C14—H14B	0.9600
C8—C9	1.351 (2)	C14—H14C	0.9600

С8—Н8	0.9300		
C5	122.47 (12)	O3—C10—C2	125.00 (19)
C7—N1—C11B	122.7 (3)	O3—C10—H10	117.5
C7—N1—C13	121.03 (15)	С2—С10—Н10	117.5
C11B—N1—C13	116.1 (3)	C12A—C11A—N1	103.2 (5)
C7—N1—C11A	118.2 (3)	C12A—C11A—H11A	111.1
C13—N1—C11A	116.3 (3)	N1—C11A—H11A	111.1
O2—C1—O1	115.93 (15)	C12A—C11A—H11B	111.1
O2—C1—C2	127.14 (17)	N1-C11A-H11B	111.1
O1—C1—C2	116.93 (14)	H11A—C11A—H11B	109.1
C3—C2—C1	120.15 (16)	N1-C11B-C12B	108.5 (5)
C3—C2—C10	122.59 (16)	N1-C11B-H11C	110.0
C1—C2—C10	117.26 (16)	C12B—C11B—H11C	110.0
C2—C3—C4	121.88 (14)	N1-C11B-H11D	110.0
С2—С3—Н3	119.1	C12B—C11B—H11D	110.0
С4—С3—Н3	119.1	H11C—C11B—H11D	108.4
C3—C4—C5	118.13 (14)	C11B—C12B—H12D	109.5
C3—C4—C9	126.03 (14)	C11B—C12B—H12E	109.5
C5—C4—C9	115.84 (15)	H12D—C12B—H12E	109.5
C6—C5—O1	116.32 (13)	C11B—C12B—H12F	109.5
C6—C5—C4	123.28 (14)	H12D-C12B-H12F	109.5
O1—C5—C4	120.40 (15)	H12E—C12B—H12F	109.5
C5—C6—C7	119.92 (15)	N1-C13-C14	114.33 (19)
С5—С6—Н6	120.0	N1-C13-H13A	108.7
С7—С6—Н6	120.0	C14—C13—H13A	108.7
N1—C7—C6	121.26 (15)	N1—C13—H13B	108.7
N1—C7—C8	121.26 (16)	C14—C13—H13B	108.7
C6—C7—C8	117.48 (16)	H13A—C13—H13B	107.6
C9—C8—C7	120.99 (16)	C13—C14—H14A	109.5
С9—С8—Н8	119.5	C13—C14—H14B	109.5
С7—С8—Н8	119.5	H14A—C14—H14B	109.5
C8—C9—C4	122.47 (15)	C13—C14—H14C	109.5
С8—С9—Н9	118.8	H14A—C14—H14C	109.5
С4—С9—Н9	118.8	H14B—C14—H14C	109.5

#### Hydrogen-bond geometry (Å, °)

D—H···A	<i>D</i> —Н	H···A	$D \cdots A$	D—H···A
C8—H8···O3 <sup>i</sup>	0.93	2.58	3.367 (4)	143.
C9—H9…O1 <sup>ii</sup>	0.93	2.55	3.432 (3)	158.
C13—H13B····O2 <sup>iii</sup>	0.97	2.53	3.388 (3)	147.
	1/2 () 1/2	1/0 12/0		

Symmetry codes: (i) -x+1/2, y+1/2, -z+5/2; (ii) x, -y, z+1/2; (iii) -x+1/2, y+1/2, -z+3/2.

## Table 2

*Table 2*  $\pi$ - $\pi$  *stacking interactions (Å*, °)

Cg1 is the centroid of the O1—C5 ring. Cg2 is the centroid of the C4—C9 ring

# supplementary materials

CgI	CgJ	CgI…CgJ <sup>a</sup>	$CgI \cdots P(J)^{b}$	$CgJ \cdots P(I)^{c}$	Slippage
Cg1	Cg1 <sup>iv</sup>	3.527 (3)	-3.3856 (6)	-3.3856 (6)	0.988
Cg1	Cg2 <sup>iv</sup>	3.554 (3)	3.4110 (6)	3.4044 (6)	1.011

Symmetry codes: (iv)1/2-x,-1/2-y,2-z Notes:

a : Distance between centroids

b : Perpendicular distance of CgI on ring plan J

c : Perpendicular distance of CgJ on ring plan I Slippage = vertical displacement between ring centroids.



Fig. 1