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3-Methylanilinium hydrogen phthalate

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ (C–C) = 0.005 Å; R factor = 0.066; wR factor = 0.165; data-to-parameter ratio = 13.3.

The asymmetric unit of the title salt, $C_7H_{10}N^+ \cdot C_8H_5O_4^-$, consists of two 3-methylphenylammonium cations and two hydrogen phthalate anions. There are strong intramolecular $O-H \cdot \cdot \cdot O$ hydrogen bonds in the virtually planar (r.m.s. deviations = 0.054 Å) phthalate anions. In the crystal, the cations and anions are connected *via* an extensive sytem of $N-H \cdot \cdot \cdot O$ hydrogen bonds into a corrugated layer extended parallel to (001).

Related literature

The title compound was investigated as part of work looking for new ferroelectric compounds. For background to ferroelectric compounds consisting of organic cations and inorganic anions, see: Fu *et al.* (2011); Ye *et al.* (2010). For a related structure, see: Kadirvelraj *et al.* (1996).



a = 7.9325 (16) Å

b = 17.931 (4) Å

c = 19.575 (4) Å

Experimental

Crystal data $C_7H_{10}N^+ \cdot C_8H_5O_4^ M_r = 273.28$ Monoclinic, $P2_1/n$ $\beta = 93.37 (3)^{\circ}$ $V = 2779.5 (10) \text{ Å}^3$ Z = 8Mo $K\alpha$ radiation

Data collection

Rigaku Mercury2 diffractometer Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005) $T_{\rm min} = 0.963, T_{\rm max} = 0.971$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.066$ $wR(F^2) = 0.165$ S = 1.034906 reflections

Table 1

Hydrogen-bond geometry (Å, °).

$D - H \cdots A$	$D-\mathrm{H}$	$H \cdot \cdot \cdot A$	$D{\cdots}A$	$D - \mathbf{H} \cdot \cdot \cdot A$
$N2-H2A\cdotsO5^{i}$	0.89	1.87	2.739 (3)	166
$N2 - H2B \cdot \cdot \cdot O2^{ii}$	0.89	1.93	2.815 (3)	178
$N2 - H2C \cdots O8$	0.89	1.90	2.789 (3)	178
$N1 - H1A \cdots O6^{i}$	0.89	1.94	2.826 (3)	177
$N1 - H1B \cdot \cdot \cdot O1^{i}$	0.89	1.91	2.784 (3)	166
$N1 - H1C \cdots O4^{iii}$	0.89	1.90	2.788 (3)	172
O3−H3···O2	0.82	1.58	2.392 (3)	173
O7−H7···O6	0.82	1.57	2.392 (3)	180
Symmetry codes: $x - 1, y + 1, z$.	(i) $-x + \frac{1}{2}, y$	$+\frac{1}{2}, -z+\frac{1}{2};$	(ii) $-x + \frac{3}{2}, y + \frac{1}{2}$	$-z + \frac{1}{2};$ (iii)

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2431).

References

Fu, D. W., Zhang, W., Cai, H. L., Zhang, Y., Ge, J. Z., Xiong, R. G. & Huang, S. P. (2011). J. Am. Chem. Soc. 133, 12780–12786.

Kadirvelraj, R., Umarji, A. M., Robinson, W. T., Bhattacharya, S. & Row, T. N. G. (1996). Chem. Mater. 8, 2313–2323.

Rigaku (2005). CrystalClear. Rigaku Corporation, Tokyo, Japan.

Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122

Ye, H.-Y., Cai, H.-L., Ge, J.-Z. & Xiong, R.-G. (2010). J. Appl. Cryst. 43, 1031– 1035.

 $\mu = 0.10 \text{ mm}^{-1}$

 $0.36 \times 0.32 \times 0.28 \text{ mm}$

22962 measured reflections

4906 independent reflections

2489 reflections with $I > 2\sigma(I)$

H-atom parameters constrained

T = 293 K

 $R_{\rm int} = 0.090$

368 parameters

 $\Delta \rho_{\text{max}} = 0.18 \text{ e } \text{\AA}^{-3}$ $\Delta \rho_{\text{min}} = -0.21 \text{ e } \text{\AA}^{-3}$

supporting information

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3-Methylanilinium hydrogen phthalate

Ming-Liang Liu

S1. Comment

Recently much attention has been devoted to simple molecular-ionic compounds containing inorganic ions and organic ions owing to the tunability of their special structural features and their potential ferroelectric properties (Fu *et al.*, 2011; Ye *et al.*, 2010;).

In our laboratory, the title compound has been synthesized and its crystal structure is herein reported. The title salt, $C_7H_{10}N^+$. $C_8H_5O_4^-$ has an asymmetric unit that consists of two 3-methylphenylamonium cations and two phthalate anions (Fig 1). In the crystal structure, there are some O—H—O intramolecular hydrogen bonds in the phthalate anions, the phthalate anion is almostly planar. The 3-methylphenylamonium cations and phthalate anions are associated by N—H···O hydrogen-bonding interaction (Fig. 2, Table 1).

The dielectric constant of the compound as a function of temperature indicates that the permittivity is basically temperature-independent ($\varepsilon = C/(T-T_0)$), suggesting that this compound is not ferroelectric or there may be no distinct phase transition occurring within the measured temperature range (below the melting point).

S2. Experimental

3.21 g (0.03 mol) of 3-methylaniline was dissolved in 30 ml ethanol to which 4.98 g (0.03 mol) of phthalic acid was added to afford the solution without any precipitation under stirring at the ambient temperature. Single crystals suitable for X-ray structure analysis were obtained by slow evaporation of the solution after 3 days.

S3. Refinement

H atoms were placed in calculated positions (N—H = 0.89 Å; O—H = 0.82 Å; C—H = 0.93 Å for Csp^2 atoms and C—H = 0.96 Å for Csp^3 atoms) with U_{iso} values $U_{iso} = 1.2Ueq(Csp^2,O)$ and $U_{iso} = 1.5Ueq(Csp^3,N)$ and allowed to ride.



Figure 1

The structure of the title compound, showing the atomic numbering scheme with 30% probability displacement ellipsoids.



Figure 2

Crystal structure of the title compound with view along the *a* axis. Dashed lines indicate hydrogen bonds.

3-methylanilinium 2-carboxybenzoate

Crystal data

C₇H₁₀N⁺·C₈H₅O₄⁻ $M_r = 273.28$ Monoclinic, $P2_1/n$ Hall symbol: -P 2yn a = 7.9325 (16) Å b = 17.931 (4) Å c = 19.575 (4) Å $\beta = 93.37$ (3)° V = 2779.5 (10) Å³ Z = 8

Data collection

Rigaku Mercury2 diffractometer Radiation source: fine-focus sealed tube Graphite monochromator F(000) = 1152 $D_x = 1.306 \text{ Mg m}^{-3}$ Melting point: 413 K Mo Ka radiation, $\lambda = 0.71073 \text{ Å}$ Cell parameters from 4906 reflections $\theta = 3.4-25.0^{\circ}$ $\mu = 0.10 \text{ mm}^{-1}$ T = 293 KBlock, colourless $0.36 \times 0.32 \times 0.28 \text{ mm}$

Detector resolution: 13.6612 pixels mm⁻¹ ω scans Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)

$T_{\min} = 0.963, \ T_{\max} = 0.971$	$\theta_{\text{max}} = 25.0^{\circ}, \theta_{\text{min}} = 3.1^{\circ}$
22962 measured reflections	$h = -9 \rightarrow 9$
4906 independent reflections	$k = -21 \rightarrow 21$
2489 reflections with $I > 2\sigma(I)$	$l = -23 \rightarrow 23$
$R_{\rm int} = 0.090$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from
Least-squares matrix: full	neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.066$	H-atom parameters constrained
$wR(F^2) = 0.165$	$w = 1/[\sigma^2(F_o^2) + (0.0672P)^2]$
<i>S</i> = 1.03	where $P = (F_o^2 + 2F_c^2)/3$
4906 reflections	$(\Delta/\sigma)_{\rm max} = 0.003$
368 parameters	$\Delta \rho_{\rm max} = 0.18 \text{ e} \text{ Å}^{-3}$
0 restraints	$\Delta \rho_{\rm min} = -0.21 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: <i>SHELXL97</i> (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/sin(2\theta)]^{-1/4}$
Secondary atom site location: difference Fourier	Extinction coefficient: 0.0038 (9)
map	

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 $F^2 > 2$ 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.

	x	У	Ζ	$U_{ m iso}$ */ $U_{ m eq}$
N2	0.4142 (3)	0.70027 (13)	0.16189 (12)	0.0493 (7)
H2A	0.3797	0.7446	0.1761	0.074*
H2B	0.4874	0.6809	0.1932	0.074*
H2C	0.3258	0.6700	0.1556	0.074*
N1	-0.0859 (3)	0.85234 (13)	0.15519 (12)	0.0471 (7)
H1A	-0.0165	0.8742	0.1865	0.071*
H1B	-0.1163	0.8078	0.1704	0.071*
H1C	-0.1773	0.8805	0.1473	0.071*
O2	0.8571 (3)	0.14134 (13)	0.23666 (12)	0.0671 (7)
O6	0.3588 (3)	0.41675 (12)	0.24495 (12)	0.0680 (7)
O3	0.8400 (3)	0.02633 (13)	0.17473 (13)	0.0627 (7)
Н3	0.8455	0.0637	0.1989	0.094*
O4	0.6480 (3)	-0.04790 (12)	0.13023 (12)	0.0701 (7)
01	0.6943 (3)	0.22617 (13)	0.27712 (13)	0.0703 (7)
O5	0.2074 (3)	0.32453 (13)	0.27620 (13)	0.0780 (8)
07	0.3337 (3)	0.53387 (12)	0.18671 (13)	0.0626 (7)
H7	0.3424	0.4936	0.2065	0.094*
O8	0.1401 (3)	0.60431 (12)	0.13895 (12)	0.0676 (7)
C10	0.0608 (3)	0.41746 (16)	0.21047 (14)	0.0378 (7)

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

C1 0.5594 (4) 0.13815 (16) 0.20140 (14) 0.0399 (8) C15 0.0443 (4) 0.48752 (16) 0.17754 (14) 0.0401 (7) C2 0.0006 (4) 0.84311 (18) 0.09148 (15) 0.0401 (7) C22 0.0006 (4) 0.37315 (18) 0.21255 (16) 0.0522 (9) D11 -0.0827 (4) 0.37315 (18) 0.21255 (16) 0.0522 (9) P12 0.4205 0.2266 0.2266 0.0624 (8) C7 0.6849 (4) 0.01263 (19) 0.15662 (16) 0.04469 (8) C8 0.7121 (4) 0.7078 (18) 0.0216 (16) 0.0446 (8) C3 0.0200 (4) 0.77319 (18) 0.06485 (17) 0.0517 (9) P12 -0.0179 0.7314 0.0876 (10) 0.0624 (10) D33 0.0200 (4) 0.77319 (18) 0.04618 (18) 0.617 (10) C12 -0.2372 (4) 0.3946 (2) 0.1856 (18) 0.617 (10) D43 0.1568 (14) 0.6518 (10) 0.6674 (10) 0.658 (10) C12 -0.237					
C15 0.0443 (4) 0.48752 (16) 0.17754 (14) 0.0402 (7) C6 0.5481 (4) 0.06991 (16) 0.16526 (15) 0.0441 (7) C22 0.0006 (4) 0.84311 (18) 0.09148 (15) 0.0443 (8) C9 0.2169 (4) 0.37315 (18) 0.21255 (16) 0.0522 (9) H11 -0.0725 0.3266 0.2333 0.063* C2 0.4145 (4) 0.18156 (18) 0.20308 (16) 0.0458 (8) C12 0.4205 0.2266 0.2266 0.064* C7 0.6849 (4) 0.01263 (19) 0.15662 (16) 0.0468 (8) C23 0.0200 (4) 0.77319 (18) 0.0485 (17) 0.0517 (9) H23 -0.0179 0.7314 0.06876 0.0662* C12 -0.3299 0.3631 0.1877 0.062* C12 -0.3299 0.3631 0.1877 0.074* C30 0.5465 (4) 0.64590 (19) 0.05128 (10) 0.0514 (10) H3A 0.1686 0.994 0.0838	C1	0.5594 (4)	0.13815 (16)	0.20140 (14)	0.0399 (8)
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H11 -0.0725 0.3266 0.2333 0.063^* C2 0.4145 (4) 0.18156 (18) 0.20308 (16) 0.0514 (9)H2 0.4205 0.2266 0.2266 0.062^* C7 0.6849 (4) 0.01263 (19) 0.1562 (16) 0.04480 (8)C29 0.4959 (4) 0.70911 (18) 0.09736 (16) 0.04460 (8)C3 0.0200 (4) 0.77319 (18) 0.06485 (17) 0.0517 (9)H23 -0.0179 0.7314 0.06485 (17) 0.0517 (9)H23 -0.0179 0.7314 0.0876 0.062^* C3 0.2629 (4) 0.1606 (2) 0.17137 (18) 0.0626 (10)H3A 0.1686 0.1912 0.1732 0.075^* C12 -0.2372 (4) 0.3946 (2) 0.18566 (18) 0.0617 (10)H12 -0.3299 0.3631 0.1877 0.074^* C30 0.5465 (4) 0.64590 (19) 0.06421 (17) 0.0558 (9)H30 0.5298 0.5994 0.0838 0.067^* C28 0.5197 (4) 0.77878 (19) 0.0716 (2) 0.0651 (10)H28 0.4882 0.8211 0.0951 0.0732 (11)C14 -0.1122 (4) 0.50854 (19) 0.15125 (16) 0.0567 (9)H14 -0.1270 0.5547 0.1300 0.068^* C13 -0.2539 (4) 0.44986 (2) 0.15549 (18) 0.0662 (10)H14 -0.1270 0.5547 0.1379 0.079^* C5 0.3929 (4)<	C11	-0.0827 (4)	0.37315 (18)	0.21255 (16)	0.0522 (9)
C2 0.4145 (4) 0.18156 (18) 0.20308 (16) 0.0514 (9)H2 0.4205 0.2266 0.2266 $0.062*$ C7 0.6849 (4) 0.01263 (19) 0.15662 (16) 0.0480 (8)C29 0.4259 (4) 0.70911 (18) 0.0736 (16) 0.0469 (8)C3 0.0200 (4) 0.77319 (18) 0.24167 (16) 0.0461 (8)C3 0.02200 (4) 0.77319 (18) 0.06485 (17) 0.0517 (9)H23 -0.0179 0.7314 0.06876 $0.062*$ C3 0.2629 (4) 0.1606 (2) 0.17137 (18) 0.06262 (10)H3A 0.1686 0.1912 0.1732 $0.075*$ C12 -0.2372 (4) 0.3946 (2) 0.18566 (18) 0.0617 (10)H12 -0.3299 0.3631 0.1877 $0.074*$ C30 0.5465 (4) 0.64590 (19) 0.06421 (17) 0.0558 (9)H30 0.5298 0.5994 0.0838 $0.067*$ C28 0.5197 (4) 0.77878 (19) 0.0716 (2) 0.0651 (10)H28 0.4882 0.8211 0.0951 $0.076*$ C25 0.6213 (5) 0.6503 (3) 0.0026 (2) 0.0732 (11)C14 -0.1142 (4) 0.50854 (19) 0.15549 (18) 0.06662 (10)H14 -0.1270 0.5547 0.1300 $0.68*$ C13 -0.2539 (4) 0.4634 (2) 0.15549 (18) 0.06662 (10)H13 -0.3591 0.4796 0.1379 $0.079*$ C5	H11	-0.0725	0.3266	0.2333	0.063*
H2 0.4205 0.2266 0.2266 0.0266 C7 $0.6849(4)$ $0.01263(19)$ $0.15662(16)$ $0.0480(8)$ C29 $0.4959(4)$ $0.70911(18)$ $0.09736(16)$ $0.0469(8)$ C3 $0.7021(4)$ $0.17078(18)$ $0.24167(16)$ $0.0461(8)$ C23 $0.0200(4)$ $0.77319(18)$ $0.24167(16)$ 0.062^* C3 $0.2629(4)$ $0.1606(2)$ $0.17137(18)$ $0.0626(10)$ H3A 0.1686 0.1912 0.1732 0.075^* C12 $-0.2372(4)$ $0.3946(2)$ $0.18566(18)$ $0.0617(10)$ H12 -0.3299 0.3631 0.1877 0.074^* C30 $0.5465(4)$ $0.64590(19)$ $0.06421(17)$ $0.0558(9)$ H30 0.5298 0.5994 0.0838 0.067^* C28 $0.5197(4)$ $0.77878(19)$ $0.0716(2)$ $0.0651(10)$ H28 0.4882 0.8211 0.0951 $0.073e(11)$ C14 $-0.1142(4)$ $0.5084(19)$ $0.15125(16)$ $0.0567(9)$ H14 -0.1270 0.5547 0.1300 0.068^* C5 $0.329(4)$ $0.4634(2)$ $0.1549(18)$ $0.0662(10)$ H13 -0.3591 0.4796 0.1379 0.079^* C5 $0.3929(4)$ $0.4985(18)$ $0.1338(17)$ $0.0555(9)$ H5 0.3842 0.0051 0.1099 0.067^* C1 $0.0550(4)$ $0.9060(2)$ $0.06061(19)$ $0.0663(10)$ H2 $0.0510(6)$ $-0.02783(19)$ $0.0888($	C2	0.4145 (4)	0.18156 (18)	0.20308 (16)	0.0514 (9)
C7 $0.6849 (4)$ $0.01263 (19)$ $0.15662 (16)$ $0.0480 (8)$ C29 $0.4959 (4)$ $0.70911 (18)$ $0.09736 (16)$ $0.0469 (8)$ C8 $0.7121 (4)$ $0.17078 (18)$ $0.24167 (16)$ $0.0461 (8)$ C3 $0.0200 (4)$ $0.77319 (18)$ $0.06485 (17)$ $0.0517 (9)$ H23 -0.0179 0.7314 $0.0685 (17)$ 0.062^* C3 $0.2629 (4)$ $0.1606 (2)$ $0.17137 (18)$ $0.0626 (10)$ H3A 0.1686 0.1912 0.1732 0.075^* C12 $-0.3272 (4)$ $0.3946 (2)$ $0.1856 (18)$ $0.0617 (10)$ H12 -0.3299 0.3631 0.1877 0.074^* C30 $0.5465 (4)$ $0.44990 (19)$ $0.06421 (17)$ $0.0558 (9)$ H30 0.5298 0.5994 0.0838 0.067^* C28 $0.5197 (4)$ $0.77878 (19)$ $0.0716 (2)$ $0.0651 (10)$ H28 0.4882 0.8211 0.0951 0.078^* C25 $0.6213 (5)$ $0.6503 (3)$ $0.0026 (2)$ $0.0732 (11)$ C14 -0.11270 0.5547 0.1300 0.068^* C13 $-0.2539 (4)$ $0.4634 (2)$ 0.1379 0.079^* C5 $0.3929 (4)$ $0.4985 (18)$ $0.1338 (17)$ $0.0555 (9)$ H5 0.3842 0.0051 0.1099 0.067^* C21 $0.0560 (4)$ $0.9060 (2)$ $0.66661 (19)$ $0.6663 (10)$ H14 -0.1270 $0.8296 (3)$ $-0.02783 (19)$ $0.888 (13)$ H1	H2	0.4205	0.2266	0.2266	0.062*
C29 0.4959 (4) 0.70911 (18) 0.09736 (16) 0.0469 (8)C8 0.7121 (4) 0.70718 (18) 0.24167 (16) 0.0461 (8)C23 0.0200 (4) 0.77319 (18) 0.06485 (17) 0.0517 H23 -0.0179 0.7314 0.0876 $0.062*$ C3 0.2629 (4) 0.1606 (2) 0.17137 (18) 0.0626 (10)H3A 0.1686 0.1912 0.1732 $0.075*$ C12 -0.2372 (4) 0.3946 (2) 0.18566 (18) 0.0617 (10)H12 -0.3299 0.3631 0.1877 $0.074*$ C30 0.5465 (4) 0.64590 (19) 0.06421 (17) 0.0558 (9)H30 0.5298 0.5994 0.0838 $0.067*$ C28 0.5197 (4) 0.77878 (19) 0.0716 (2) 0.0651 (10)H28 0.4882 0.8211 0.0951 $0.078*$ C25 0.6213 (5) 0.6503 (3) 0.0026 (2) 0.0732 (11)C14 -0.1142 (4) 0.50854 (19) 0.15125 (16) 0.0662 (10)H14 -0.1270 0.5547 0.1379 $0.079*$ C5 0.3929 (4) 0.4985 (18) 0.13383 (17) 0.0555 (9)H5 0.3842 0.0051 0.1099 $0.067*$ C19 0.1539 (5) 0.8296 (3) -0.02783 (19) 0.0682 (11)C4 0.2521 (4) 0.0941 (2) 0.13703 (19) 0.0672 (11)C4 0.2521 (4) 0.0790 (112) 0.0888 (13)H19 0.2068 <td>C7</td> <td>0.6849 (4)</td> <td>0.01263 (19)</td> <td>0.15662 (16)</td> <td>0.0480 (8)</td>	C7	0.6849 (4)	0.01263 (19)	0.15662 (16)	0.0480 (8)
C8 0.7121 0.17078 0.24167 0.6 0.0461 (8) C23 0.0200 0.77319 0.77319 0.6485 0.0517 0.0517 9 H23 -0.0179 0.7314 0.06485 0.062^* 0.062^* C3 0.2629 0.1606 0.17137 0.0626 0.062^* C12 -0.2372 0.3946 0.1732 0.075^* C12 -0.3299 0.3631 0.1877 0.074^* C30 0.5465 0.64590 0.9944 0.8388 0.067^* C28 0.5197 0.5298 0.5994 0.0838 0.067^* C28 0.5197 0.77878 0.9951 0.078^* C24 0.6213 0.05245 0.6213 0.0756 C25 0.6213 0.5594 0.15125 0.0667^* C25 0.6213 0.5594 0.15125 0.0757^* C13 -0.2539 0.4634 0.1379 0.079^* C5 0.3929 0.4634 0.1379 0.079^* C5 0.3929 0.4951 0.1379 0.0667^* C21 0.0560 0.9951 0.0667^* C21 0.0560 0.9951 0.0668^* C13 -0.2539 0.4796 0.1379 0.079^* C5 0.3929 0.4796 0.1379 0.067^* C5 0.3929 0.3625 0.06084 0.1019 H14 0.1497 0.9951 0.0668 C14 0.2527 0.8806	C29	0.4959 (4)	0.70911 (18)	0.09736 (16)	0.0469 (8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C8	0.7121 (4)	0.17078 (18)	0.24167 (16)	0.0461 (8)
H23 -0.0179 0.7314 0.0876 $0.062*$ C3 0.2629 (4) 0.1606 (2) 0.17137 (18) 0.0626 (10)H3A 0.1686 0.1912 0.1732 $0.075*$ C12 -0.2372 (4) 0.3946 (2) 0.18566 (18) 0.0617 (10)H12 -0.3299 0.3631 0.18577 $0.074*$ C30 0.5465 (4) 0.64590 (19) 0.06421 (17) 0.0558 (9)H30 0.5298 0.5994 0.0838 $0.067*$ C28 0.5197 (4) 0.77878 (19) 0.0716 (2) 0.0651 (10)H28 0.4882 0.8211 0.0951 $0.078*$ C25 0.6213 (5) 0.6503 (3) 0.0026 (2) 0.0732 (11)C14 -0.1142 (4) 0.50854 (19) 0.15125 (16) 0.0567 (9)H14 -0.2739 (4) 0.4796 0.1379 $0.079*$ C5 0.3929 (4) 0.44985 (18) 0.13383 (17) 0.0555 (9)H5 0.3842 0.0051 0.1099 $0.667*$ C21 0.0560 (4) 0.9606 (2) 0.06061 (19) 0.0663 (10)H21 0.0413 0.9527 0.0800 $0.080*$ C19 0.1539 (5) 0.8296 (3) -0.02783 (19) 0.0838 (13)H19 0.2068 0.8255 -0.0688 $0.101*$ C18 0.0977 (4) 0.7677 (2) 0.0001 (2) 0.08080 (13)C20 0.1342 (5) 0.8988 (3) -0.0019 $0.113*$ C26 0.6419 (5) 0.7202	C23	0.0200 (4)	0.77319 (18)	0.06485 (17)	0.0517 (9)
C3 0.2629 (4) 0.1606 (2) 0.17137 (18) 0.0626 (10)H3A 0.1686 0.1912 0.1732 0.075^* C12 -0.2372 (4) 0.3946 (2) 0.18566 (18) 0.0617 (10)H12 -0.3299 0.3631 0.1877 0.074^* C30 0.5465 (4) 0.64590 (19) 0.06421 (17) 0.0558 (9)H30 0.5298 0.5994 0.0838 0.067^* C28 0.5197 (4) 0.77878 (19) 0.0716 (2) 0.0651 (10)H28 0.4882 0.8211 0.0951 0.078^* C25 0.6213 (5) 0.6503 (3) 0.0026 (2) 0.0732 (11)C14 -0.1142 (4) 0.50854 (19) 0.15125 (16) 0.0567 (9)H14 -0.1270 0.5547 0.1300 0.668^* C13 -0.2539 (4) 0.4634 (2) 0.15549 (18) 0.0662 (10)H13 -0.3591 0.4796 0.1379 0.079^* C5 0.3929 (4) 0.4985 (18) 0.13383 (17) 0.0555 (9)H5 0.3842 0.0051 0.1099 0.667^* C21 0.0560 (4) 0.9060 (2) 0.06061 (19) 0.0663 (10)H21 0.0413 0.9527 0.0880 0.080^* C19 0.1539 (5) 0.8296 (3) -0.02783 (19) 0.0838 (13)H19 0.2068 0.8255 -0.0688 0.101^* C4 0.2521 (4) 0.9941 (2) 0.13703 (19) 0.0672 (11)H4 0.1497 <td< td=""><td>H23</td><td>-0.0179</td><td>0.7314</td><td>0.0876</td><td>0.062*</td></td<>	H23	-0.0179	0.7314	0.0876	0.062*
H3A 0.1686 0.1912 0.1732 $0.075*$ C12 $-0.2372 (4)$ $0.3946 (2)$ $0.18566 (18)$ $0.0617 (10)$ H12 -0.3299 0.3631 0.1877 $0.074*$ C30 $0.5465 (4)$ $0.64590 (19)$ $0.06421 (17)$ $0.0558 (9)$ H30 0.5298 0.59944 0.0838 $0.067*$ C28 $0.5197 (4)$ $0.77878 (19)$ $0.0716 (2)$ $0.0651 (10)$ H28 0.4882 0.8211 0.0951 $0.078*$ C25 $0.6213 (5)$ $0.6503 (3)$ $0.0026 (2)$ $0.0732 (11)$ C14 $-0.1142 (4)$ $0.50854 (19)$ $0.15125 (16)$ $0.0567 (9)$ H14 -0.1270 0.5547 0.1300 $0.668*$ C13 $-0.2539 (4)$ $0.4634 (2)$ $0.15549 (18)$ $0.0662 (10)$ H13 -0.3591 0.4796 0.1379 $0.079*$ C5 $0.3929 (4)$ $0.04985 (18)$ $0.13383 (17)$ $0.0555 (9)$ H5 0.3842 0.0051 0.1099 $0.067*$ C21 $0.0560 (4)$ $0.9060 (2)$ $0.06061 (19)$ $0.0633 (10)$ H21 0.0413 0.9527 0.0800 $0.080*$ C19 $0.1539 (5)$ $0.8296 (3)$ $-0.02783 (19)$ $0.081*$ C18 $0.0977 (4)$ $0.7657 (2)$ $0.0029 (2)$ $0.0682 (11)$ C4 $0.2521 (4)$ 0.0948 -0.0218 $0.106*$ C27 $0.5930 (5)$ $0.7842 (3)$ $0.00088 (3)$ $0.0940 (15)$ H20 0.1736 0.9408	C3	0.2629 (4)	0.1606 (2)	0.17137 (18)	0.0626 (10)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H3A	0.1686	0.1912	0.1732	0.075*
H12 -0.3299 0.3631 0.1877 $0.074*$ C30 0.5465 (4) 0.64590 (19) 0.06421 (17) 0.0558 (9)H30 0.5298 0.5994 0.0838 $0.067*$ C28 0.5197 (4) 0.77878 (19) 0.0716 (2) 0.06511 (0)H28 0.4882 0.8211 0.0951 $0.078*$ C25 0.6213 (5) 0.6503 (3) 0.0026 (2) 0.0732 (11)C14 -0.1142 (4) 0.50854 (19) 0.15125 (16) 0.0567 (9)H14 -0.270 0.5547 0.1300 $0.068*$ C13 -0.2539 (4) 0.4634 (2) 0.15549 (18) 0.0662 (10)H13 -0.3591 0.4796 0.1379 $0.079*$ C5 0.3929 (4) 0.04985 (18) 0.13383 (17) 0.0555 (9)H5 0.3842 0.0051 0.1099 $0.067*$ C21 0.0560 (4) 0.9060 (2) 0.06061 (19) 0.06838 (13)H19 0.2068 0.8255 -0.0688 $0.101*$ C4 0.2521 (4) 0.941 (2) 0.13703 (19) 0.0622 (11)C4 0.2521 (4) 0.9408 -0.0218 $0.106*$ C27 0.5930 (5) 0.7842 (3) 0.0088 (3) 0.0940 (15)H20 0.1736 0.9408 -0.0218 $0.106*$ C27 0.5930 (5) 0.7842 (3) 0.0088 (3) 0.0940 (15)H20 0.1736 0.9408 -0.0218 $0.106*$ C27 0.5930 (5) 0.7842 (3)	C12	-0.2372(4)	0.3946 (2)	0.18566 (18)	0.0617 (10)
C30 0.5465 (4) 0.64590 (19) 0.06421 (17) 0.0558 (9)H30 0.5298 0.5994 0.0838 $0.067*$ C28 0.5197 (4) 0.77878 (19) 0.0716 (2) 0.06511 (10)H28 0.4882 0.8211 0.0951 $0.078*$ C25 0.6213 (5) 0.6503 (3) 0.0026 (2) 0.0732 (11)C14 -0.1142 (4) 0.50854 (19) 0.15125 (16) 0.0567 (9)H14 -0.270 0.5547 0.1300 $0.068*$ C13 -0.2539 (4) 0.4634 (2) 0.15549 (18) 0.0662 (10)H13 -0.3591 0.4796 0.1379 $0.079*$ C5 0.3929 (4) 0.04985 (18) 0.13383 (17) 0.0555 (9)H5 0.3842 0.0051 0.1099 $0.067*$ C21 0.0560 (4) 0.9960 (2) 0.06601 (19) 0.0633 (10)H21 0.0413 0.9527 0.0800 $0.80*$ C19 0.1539 (5) 0.8296 (3) -0.02783 (19) 0.0838 (13)H19 0.2068 0.8255 -0.0688 $0.101*$ C18 0.0977 (4) 0.7657 (2) 0.0029 (2) 0.0682 (11)C4 0.2521 (4) 0.9408 -0.0218 $0.106*$ C27 0.5930 (5) 0.7842 (3) 0.0088 (3) 0.0940 (15)H20 0.1736 0.9408 -0.0218 $0.106*$ C26 0.6419 (5) 0.7202 (3) -0.0240 (2) 0.9000 (14)H26 0.6907 0.7248	H12	-0.3299	0.3631	0.1877	0.074*
H30 0.5298 0.5994 0.0838 0.067^* C28 0.5197 (4) 0.77878 (19) 0.0716 (2) 0.0651 (10)H28 0.4882 0.8211 0.0951 0.078^* C25 0.6213 (5) 0.6503 (3) 0.0026 (2) 0.0732 (11)C14 -0.1142 (4) 0.50854 (19) 0.15125 (16) 0.0567 (9)H14 -0.2539 (4) 0.4634 (2) 0.15549 (18) 0.0668^* C13 -0.2539 (4) 0.4634 (2) 0.15549 (18) 0.0662 (10)H13 -0.3591 0.4796 0.1379 0.079^* C5 0.3929 (4) 0.04985 (18) 0.13383 (17) 0.05556 (9)H5 0.3842 0.0051 0.1099 0.667^* C21 0.0560 (4) 0.9060 (2) 0.06061 (19) 0.0683 (10)H21 0.0413 0.9527 0.0800 0.080^* C19 0.1539 (5) 0.8296 (3) -0.02783 (19) 0.0838 (13)H19 0.2068 0.8255 -0.0688 0.101^* C4 0.2521 (4) 0.9414 (2) 0.13703 (19) 0.0672 (11)H4 0.1497 0.790 0.1159 0.081^* C27 0.5930 (5) 0.7842 (3) 0.0088 (3) 0.0940 (15)H20 0.1736 0.9408 -0.0218 0.106^* C24 0.6775 (6) 0.5823 (3) -0.0240 (2) 0.9000 (14)H26 0.6907 0.7248 -0.0290 0.176^* H24B 0.7864 $0.$	C30	0.5465 (4)	0.64590 (19)	0.06421 (17)	0.0558 (9)
C28 $0.5197 (4)$ $0.77878 (19)$ $0.0716 (2)$ $0.0651 (10)$ H28 0.4882 0.8211 0.0951 $0.078*$ C25 $0.6213 (5)$ $0.6503 (3)$ $0.0026 (2)$ $0.0732 (11)$ C14 $-0.1142 (4)$ $0.50854 (19)$ $0.15125 (16)$ $0.0567 (9)$ H14 -0.1270 0.5547 0.1300 $0.068*$ C13 $-0.2539 (4)$ $0.4634 (2)$ $0.15549 (18)$ $0.0662 (10)$ H13 -0.3591 0.4796 0.1379 $0.079*$ C5 $0.3929 (4)$ $0.04985 (18)$ $0.13383 (17)$ $0.0555 (9)$ H5 0.3842 0.0051 0.1099 $0.0663 (10)$ C21 $0.0560 (4)$ $0.9060 (2)$ $0.06061 (19)$ $0.0663 (10)$ H21 0.0413 0.9527 0.0800 $0.080*$ C19 $0.1539 (5)$ $0.8296 (3)$ $-0.02783 (19)$ $0.0682 (11)$ C4 $0.2521 (4)$ $0.941 (2)$ $0.13703 (19)$ $0.0672 (11)$ H4 0.1497 0.0790 0.1159 $0.081*$ C20 $0.1342 (5)$ $0.898 (3)$ $0.0001 (2)$ $0.0880 (13)$ L20 0.1736 0.9408 -0.0218 $0.106*$ C27 $0.5930 (5)$ $0.7842 (3)$ $0.0088 (3)$ $0.0940 (15)$ H24 0.6977 0.7248 -0.0218 $0.106*$ C24 $0.6775 (6)$ $0.5423 (3)$ $-0.0240 (2)$ $0.1177 (18)$ H24A 0.5976 $0.5428 (-0.0290$ $0.176*$ H24B 0.7864 $0.5936 (-0.0152$	H30	0.5298	0.5994	0.0838	0.067*
H28 0.4882 0.8211 0.0951 0.078^{*} C25 0.6213 (5) 0.6503 (3) 0.0026 (2) 0.0732 (11)C14 -0.1142 (4) 0.50854 (19) 0.15125 (16) 0.0567 (9)H14 -0.1270 0.5547 0.1300 0.068^{*} C13 -0.2539 (4) 0.4634 (2) 0.15549 (18) 0.0662 (10)H13 -0.3591 0.4796 0.1379 0.079^{*} C5 0.3929 (4) 0.04985 (18) 0.13383 (17) 0.0555 (9)H5 0.3842 0.0051 0.1099 0.067^{*} C21 0.0560 (4) 0.9060 (2) 0.06061 (19) 0.0638 (10)H21 0.0413 0.9527 0.0800 0.080^{*} C19 0.1539 (5) 0.8296 (3) -0.02783 (19) 0.0682 (11)H19 0.2068 0.8255 -0.0688 0.101^{*} C18 0.0977 (4) 0.7657 (2) 0.0029 (2) 0.0682 (11)C4 0.2521 (4) 0.0941 (2) 0.13703 (19) 0.0682 (11)H4 0.1497 0.0790 0.1159 0.081^{*} C20 0.1342 (5) 0.8988 (3) 0.0001 (2) 0.0880 (13)H20 0.1736 0.9408 -0.0218 0.106^{*} C27 0.5930 (5) 0.7842 (3) 0.0088 (3) 0.0940 (15)H27 0.6089 0.8306 -0.0109 0.113^{*} C26 0.6419 (5) 0.7202 (3) -0.0240 (2) 0.1076^{*} H24A 0.5	C28	0.5197 (4)	0.77878 (19)	0.0716 (2)	0.0651 (10)
C25 $0.6213 (5)$ $0.6503 (3)$ $0.0026 (2)$ $0.0732 (11)$ C14 $-0.1142 (4)$ $0.50854 (19)$ $0.15125 (16)$ $0.0567 (9)$ H14 -0.1270 0.5547 0.1300 $0.068*$ C13 $-0.2539 (4)$ $0.4634 (2)$ $0.15549 (18)$ $0.0662 (10)$ H13 -0.3591 0.4796 0.1379 $0.079*$ C5 $0.3929 (4)$ $0.04985 (18)$ $0.13383 (17)$ $0.0555 (9)$ H5 0.3842 0.0051 0.1099 $0.067*$ C21 $0.0560 (4)$ $0.9060 (2)$ $0.06061 (19)$ $0.0663 (10)$ H21 0.0413 0.9527 0.8000 $0.80*$ C19 $0.1539 (5)$ $0.8296 (3)$ $-0.02783 (19)$ $0.838 (13)$ H19 0.2068 0.8255 -0.0688 $0.101*$ C4 $0.2521 (4)$ $0.0941 (2)$ $0.13703 (19)$ $0.0672 (11)$ H4 0.1497 0.0790 0.1159 $0.081*$ C20 $0.1342 (5)$ $0.8988 (3)$ $0.0001 (2)$ $0.0880 (13)$ H20 0.1736 0.9408 -0.0218 $0.106*$ C27 $0.5930 (5)$ $0.7242 (3)$ $-0.0240 (2)$ $0.9090 (14)$ H26 0.6907 0.7248 -0.0659 $0.108*$ C24 $0.6775 (6)$ $0.5823 (3)$ $-0.0342 (2)$ $0.1177 (18)$ H24A 0.5976 0.5428 -0.0290 $0.176*$ H24B 0.7864 0.5670 -0.0152 $0.176*$ H24B 0.7864 0.5670 -0.0819 <	H28	0.4882	0.8211	0.0951	0.078*
C14 -0.1142 (4) 0.50854 (19) 0.15125 (16) 0.0567 (9)H14 -0.1270 0.5547 0.1300 $0.068*$ C13 -0.2539 (4) 0.4634 (2) 0.15549 (18) 0.0662 (10)H13 -0.3591 0.4796 0.1379 $0.079*$ C5 0.3929 (4) 0.04985 (18) 0.13383 (17) 0.0555 (9)H5 0.3842 0.0051 0.1099 $0.067*$ C21 0.0560 (4) 0.9060 (2) 0.06061 (19) 0.0663 (10)H21 0.0413 0.9527 0.0800 $0.080*$ C19 0.1539 (5) 0.8296 (3) -0.02783 (19) 0.0838 (13)H19 0.2068 0.8255 -0.0688 $0.101*$ C18 0.0977 (4) 0.7657 (2) 0.0029 (2) 0.0682 (11)C4 0.2521 (4) 0.0941 (2) 0.13703 (19) 0.0672 (11)H4 0.1497 0.0790 0.1159 $0.081*$ C20 0.1342 (5) 0.8988 (3) 0.0001 (2) 0.0880 (13)H20 0.1736 0.9408 -0.0218 $0.106*$ C27 0.5930 (5) 0.7242 (3) 0.0088 (3) 0.0940 (15)H26 0.6097 0.7248 -0.0240 (2) 0.1090 (14)H26 0.6907 0.7248 -0.0290 $0.176*$ H24B 0.7864 0.5670 -0.0152 $0.176*$ H24B 0.7864 0.5936 -0.0819 $0.176*$ H24C 0.6846 0.5936 -0.0819 <td< td=""><td>C25</td><td>0.6213 (5)</td><td>0.6503 (3)</td><td>0.0026 (2)</td><td>0.0732 (11)</td></td<>	C25	0.6213 (5)	0.6503 (3)	0.0026 (2)	0.0732 (11)
H14 -0.1270 0.5547 0.1300 0.068^* C13 -0.2539 (4) 0.4634 (2) 0.15549 (18) 0.0662 (10)H13 -0.3591 0.4796 0.1379 0.079^* C5 0.3929 (4) 0.04985 (18) 0.13383 (17) 0.0555 (9)H5 0.3842 0.0051 0.1099 0.067^* C21 0.0560 (4) 0.9060 (2) 0.06061 (19) 0.0663 (10)H21 0.0413 0.9527 0.0800 0.080^* C19 0.1539 (5) 0.8296 (3) -0.02783 (19) 0.0838 (13)H19 0.2068 0.8255 -0.0688 0.101^* C18 0.0977 (4) 0.7657 (2) 0.0029 (2) 0.0682 (11)C4 0.2521 (4) 0.0941 (2) 0.13703 (19) 0.0672 (11)H4 0.1497 0.0790 0.1159 0.081^* C20 0.1342 (5) 0.8988 (3) 0.0001 (2) 0.0880 (13)H20 0.1736 0.9408 -0.0218 0.106^* C27 0.5930 (5) 0.7842 (3) 0.0088 (3) 0.0940 (15)H27 0.6089 0.8306 -0.0109 0.113^* C26 0.6419 (5) 0.7223 (3) -0.0240 (2) 0.10900 (14)H26 0.6907 0.7248 -0.0290 0.176^* H24B 0.7864 0.5670 -0.0152 0.176^* H24B 0.7864 0.5670 -0.0152 0.176^* H24B 0.7864 0.5676 -0.0819 <td< td=""><td>C14</td><td>-0.1142 (4)</td><td>0.50854 (19)</td><td>0.15125 (16)</td><td>0.0567 (9)</td></td<>	C14	-0.1142 (4)	0.50854 (19)	0.15125 (16)	0.0567 (9)
C13 $-0.2539 (4)$ $0.4634 (2)$ $0.15549 (18)$ $0.0662 (10)$ H13 -0.3591 0.4796 0.1379 $0.079*$ C5 $0.3929 (4)$ $0.04985 (18)$ $0.13383 (17)$ $0.0555 (9)$ H5 0.3842 0.0051 0.1099 $0.067*$ C21 $0.0560 (4)$ $0.9060 (2)$ $0.06061 (19)$ $0.0663 (10)$ H21 0.0413 0.9527 0.0800 $0.080*$ C19 $0.1539 (5)$ $0.8296 (3)$ $-0.02783 (19)$ $0.0838 (13)$ H19 0.2068 0.8255 -0.0688 $0.101*$ C18 $0.0977 (4)$ $0.7657 (2)$ $0.0029 (2)$ $0.0662 (11)$ C4 $0.2521 (4)$ $0.0941 (2)$ $0.13703 (19)$ $0.0672 (11)$ H4 0.1497 0.0790 0.1159 $0.081*$ C20 $0.1342 (5)$ $0.8988 (3)$ $0.0001 (2)$ $0.0880 (13)$ H20 0.1736 0.9408 -0.0218 $0.106*$ C27 $0.5930 (5)$ $0.7842 (3)$ $0.0088 (3)$ $0.0940 (15)$ H27 0.6089 0.8306 -0.0109 $0.113*$ C26 $0.6419 (5)$ $0.7202 (3)$ $-0.0240 (2)$ $0.9000 (14)$ H26 0.6907 0.7248 -0.0290 $0.176*$ H24B 0.7864 0.5670 $-0.0342 (2)$ $0.1177 (18)$ H24A 0.5976 0.5428 -0.0290 $0.176*$ H24B 0.7864 0.5670 -0.0152 $0.176*$ H24B 0.78464 0.5936 -0.0819	H14	-0.1270	0.5547	0.1300	0.068*
H13 -0.3591 0.4796 0.1379 $0.079*$ C5 $0.3929 (4)$ $0.04985 (18)$ $0.13383 (17)$ $0.0555 (9)$ H5 0.3842 0.0051 0.1099 $0.067*$ C21 $0.0560 (4)$ $0.9060 (2)$ $0.06061 (19)$ $0.0663 (10)$ H21 0.0413 0.9527 0.0800 $0.080*$ C19 $0.1539 (5)$ $0.8296 (3)$ $-0.02783 (19)$ $0.0838 (13)$ H19 0.2068 0.8255 -0.0688 $0.101*$ C18 $0.0977 (4)$ $0.7657 (2)$ $0.0029 (2)$ $0.0682 (11)$ C4 $0.2521 (4)$ $0.0941 (2)$ $0.13703 (19)$ $0.0672 (11)$ H4 0.1497 0.0790 0.1159 $0.081*$ C20 $0.1342 (5)$ $0.8988 (3)$ $0.0001 (2)$ $0.0880 (13)$ H20 0.1736 0.9408 -0.0218 $0.106*$ C27 $0.5930 (5)$ $0.7842 (3)$ $0.0088 (3)$ $0.0940 (15)$ H27 0.6089 0.8306 -0.0109 $0.113*$ C26 $0.6419 (5)$ $0.7202 (3)$ $-0.0240 (2)$ $0.9000 (14)$ H26 0.6907 0.7248 -0.0290 $0.176*$ H24B 0.7864 0.5670 -0.0152 $0.176*$ H24B 0.7864 0.5670 -0.0819 $0.176*$ H24C 0.6846 0.5936 -0.0819 $0.176*$ H24C 0.6846 0.5936 $-0.0274 (2)$ $0.1080 (16)$	C13	-0.2539 (4)	0.4634 (2)	0.15549 (18)	0.0662 (10)
C5 $0.3929 (4)$ $0.04985 (18)$ $0.13383 (17)$ $0.0555 (9)$ H5 0.3842 0.0051 0.1099 0.067^* C21 $0.0560 (4)$ $0.9060 (2)$ $0.60601 (19)$ $0.0663 (10)$ H21 0.0413 0.9527 0.800 0.080^* C19 $0.1539 (5)$ $0.8296 (3)$ $-0.02783 (19)$ $0.0838 (13)$ H19 0.2068 0.8255 -0.0688 0.101^* C18 $0.0977 (4)$ $0.7657 (2)$ $0.0029 (2)$ $0.0682 (11)$ C4 $0.2521 (4)$ $0.0941 (2)$ $0.13703 (19)$ $0.0672 (11)$ H4 0.1497 0.0790 0.1159 0.081^* C20 $0.1342 (5)$ $0.8988 (3)$ $0.0001 (2)$ $0.0880 (13)$ H20 0.1736 0.9408 -0.0218 0.106^* C27 $0.5930 (5)$ $0.7202 (3)$ $-0.0240 (2)$ $0.0900 (14)$ H26 0.6097 0.7248 -0.0659 0.108^* C24 $0.6775 (6)$ $0.5823 (3)$ $-0.0342 (2)$ $0.1177 (18)$ H24A 0.5976 0.5428 -0.0290 0.176^* H24B 0.7864 0.5670 -0.0819 0.176^* H24B 0.7864 0.5670 -0.0819 0.176^* C16 $0.1788 (4)$ $0.54521 (18)$ $0.16718 (16)$ $0.0465 (8)$ C17 $0.1206 (5)$ $0.6898 (3)$ $-0.0274 (2)$ $0.1080 (16)$	H13	-0.3591	0.4796	0.1379	0.079*
H5 0.3842 0.0051 0.1099 0.067^* C21 0.0560 (4) 0.9060 (2) 0.06061 (19) 0.0663 (10)H21 0.0413 0.9527 0.0800 0.080^* C19 0.1539 (5) 0.8296 (3) -0.02783 (19) 0.0838 (13)H19 0.2068 0.8255 -0.0688 0.101^* C18 0.0977 (4) 0.7657 (2) 0.0029 (2) 0.0682 (11)C4 0.2521 (4) 0.0941 (2) 0.13703 (19) 0.0672 (11)H4 0.1497 0.0790 0.1159 0.081^* C20 0.1342 (5) 0.8988 (3) 0.0001 (2) 0.0880 (13)H20 0.1736 0.9408 -0.0218 0.106^* C27 0.5930 (5) 0.7842 (3) 0.0088 (3) 0.0940 (15)H27 0.6089 0.8306 -0.0109 0.113^* C26 0.6419 (5) 0.7202 (3) -0.0240 (2) 0.0900 (14)H26 0.6907 0.7248 -0.0659 0.108^* C24 0.6775 (6) 0.5823 (3) -0.0342 (2) 0.1177 (18)H24B 0.7864 0.5670 -0.0152 0.176^* H24B 0.7864 0.5670 -0.0819 0.176^* H24C 0.6846 0.5936 -0.0819 0.176^* C16 0.1788 (4) 0.54521 (18) 0.16718 (16) 0.0465 (8)C17 0.1206 (5) 0.6898 (3) -0.0274 (2) 0.1080 (16)	C5	0.3929 (4)	0.04985 (18)	0.13383 (17)	0.0555 (9)
C21 $0.0560(4)$ $0.9060(2)$ $0.06061(19)$ $0.0663(10)$ H21 0.0413 0.9527 0.0800 0.080^* C19 $0.1539(5)$ $0.8296(3)$ $-0.02783(19)$ $0.0838(13)$ H19 0.2068 0.8255 -0.0688 0.101^* C18 $0.0977(4)$ $0.7657(2)$ $0.0029(2)$ $0.0682(11)$ C4 $0.2521(4)$ $0.0941(2)$ $0.13703(19)$ $0.0672(11)$ H4 0.1497 0.0790 0.1159 0.081^* C20 $0.1342(5)$ $0.8988(3)$ $0.0001(2)$ $0.0880(13)$ H20 0.1736 0.9408 -0.0218 0.106^* C27 $0.5930(5)$ $0.7842(3)$ $0.0088(3)$ $0.0940(15)$ H27 0.6089 0.8306 -0.0109 0.113^* C26 $0.6419(5)$ $0.7202(3)$ $-0.0240(2)$ $0.0900(14)$ H26 0.6907 0.7248 -0.0659 0.108^* C24 $0.6775(6)$ $0.5823(3)$ $-0.0342(2)$ $0.1177(18)$ H24A 0.5976 0.5428 -0.0290 0.176^* H24B 0.7864 0.5670 -0.0819 0.176^* H24B 0.7864 0.5670 -0.0819 0.176^* H24C 0.6846 0.5936 -0.0819 0.176^* H24C 0.6846 0.5936 $-0.0274(2)$ $0.1080(16)$	Н5	0.3842	0.0051	0.1099	0.067*
H21 0.0413 0.9527 0.0800 0.080^* C19 $0.1539 (5)$ $0.8296 (3)$ $-0.02783 (19)$ $0.0838 (13)$ H19 0.2068 0.8255 -0.0688 0.101^* C18 $0.0977 (4)$ $0.7657 (2)$ $0.0029 (2)$ $0.0682 (11)$ C4 $0.2521 (4)$ $0.0941 (2)$ $0.13703 (19)$ $0.0672 (11)$ H4 0.1497 0.0790 0.1159 0.081^* C20 $0.1342 (5)$ $0.8988 (3)$ $0.0001 (2)$ $0.0880 (13)$ H20 0.1736 0.9408 -0.0218 0.106^* C27 $0.5930 (5)$ $0.7842 (3)$ $0.0088 (3)$ $0.0940 (15)$ H27 0.6089 0.8306 -0.0109 0.113^* C26 $0.6419 (5)$ $0.7202 (3)$ $-0.0240 (2)$ $0.0900 (14)$ H26 0.6907 0.7248 -0.0659 0.108^* C24 $0.6775 (6)$ $0.5823 (3)$ $-0.0342 (2)$ $0.1177 (18)$ H24A 0.5976 0.5428 -0.0290 0.176^* H24B 0.7864 0.5670 -0.0152 0.176^* H24B 0.7864 0.5670 -0.0819 0.176^* H24C 0.6846 0.5936 -0.0819 0.176^* C16 $0.1788 (4)$ $0.54521 (18)$ $0.16718 (16)$ $0.0465 (8)$ C17 $0.1206 (5)$ $0.6898 (3)$ $-0.0274 (2)$ $0.1080 (16)$	C21	0.0560 (4)	0.9060 (2)	0.06061 (19)	0.0663 (10)
C19 $0.1539 (5)$ $0.8296 (3)$ $-0.02783 (19)$ $0.0838 (13)$ H19 0.2068 0.8255 -0.0688 0.101^* C18 $0.0977 (4)$ $0.7657 (2)$ $0.0029 (2)$ $0.0682 (11)$ C4 $0.2521 (4)$ $0.0941 (2)$ $0.13703 (19)$ $0.0672 (11)$ H4 0.1497 0.0790 0.1159 0.081^* C20 $0.1342 (5)$ $0.8988 (3)$ $0.0001 (2)$ $0.0880 (13)$ H20 0.1736 0.9408 -0.0218 0.106^* C27 $0.5930 (5)$ $0.7842 (3)$ $0.0088 (3)$ $0.0940 (15)$ H27 0.6089 0.8306 -0.0109 0.113^* C26 $0.6419 (5)$ $0.7202 (3)$ $-0.0240 (2)$ $0.0900 (14)$ H26 0.6907 0.7248 -0.0659 0.108^* C24 $0.6775 (6)$ $0.5823 (3)$ -0.0290 0.176^* H24A 0.5976 0.5428 -0.0290 0.176^* H24B 0.7864 0.5670 -0.0819 0.176^* H24C 0.6846 0.5936 -0.0819 0.176^* H24C 0.6846 0.5936 -0.0819 0.176^* H24C 0.6846 0.5936 $-0.0274 (2)$ $0.1080 (16)$	H21	0.0413	0.9527	0.0800	0.080*
H19 0.2068 0.8255 -0.0688 0.101^* C18 $0.0977 (4)$ $0.7657 (2)$ $0.0029 (2)$ $0.0682 (11)$ C4 $0.2521 (4)$ $0.0941 (2)$ $0.13703 (19)$ $0.0672 (11)$ H4 0.1497 0.0790 0.1159 0.081^* C20 $0.1342 (5)$ $0.8988 (3)$ $0.0001 (2)$ $0.0880 (13)$ H20 0.1736 0.9408 -0.0218 0.106^* C27 $0.5930 (5)$ $0.7842 (3)$ $0.0088 (3)$ $0.0940 (15)$ H27 0.6089 0.8306 -0.0109 0.113^* C26 $0.6419 (5)$ $0.7202 (3)$ $-0.0240 (2)$ $0.0900 (14)$ H26 0.6907 0.7248 -0.0659 0.108^* C24 $0.6775 (6)$ $0.5823 (3)$ -0.0290 0.176^* H24B 0.7864 0.5670 -0.0152 0.176^* H24B 0.7864 0.5670 -0.0819 0.176^* H24C 0.6846 0.5936 -0.0819 0.176^* H24C $0.6946 (15) (18) (16) (16) (166) (16) (16) (16) (16) (1$	C19	0.1539 (5)	0.8296 (3)	-0.02783 (19)	0.0838 (13)
C18 $0.0977(4)$ $0.7657(2)$ $0.0029(2)$ $0.0682(11)$ C4 $0.2521(4)$ $0.0941(2)$ $0.13703(19)$ $0.0672(11)$ H4 0.1497 0.0790 0.1159 $0.081*$ C20 $0.1342(5)$ $0.8988(3)$ $0.0001(2)$ $0.0880(13)$ H20 0.1736 0.9408 -0.0218 $0.106*$ C27 $0.5930(5)$ $0.7842(3)$ $0.0088(3)$ $0.0940(15)$ H27 0.6089 0.8306 -0.0109 $0.113*$ C26 $0.6419(5)$ $0.7202(3)$ $-0.0240(2)$ $0.0900(14)$ H26 0.6907 0.7248 -0.0659 $0.108*$ C24 $0.6775(6)$ $0.5823(3)$ $-0.0342(2)$ $0.1177(18)$ H24A 0.5976 0.5428 -0.0290 $0.176*$ H24B 0.7864 0.5670 -0.0819 $0.176*$ H24C 0.6846 0.5936 -0.0819 $0.176*$ H24C 0.6846 0.5936 -0.0819 $0.176*$ H24C 0.6846 0.5936 $-0.0214(2)$ $0.0465(8)$ C16 $0.1788(4)$ $0.54521(18)$ $0.16718(16)$ $0.0465(8)$ C17 $0.1206(5)$ $0.6898(3)$ $-0.0274(2)$ $0.1080(16)$	H19	0.2068	0.8255	-0.0688	0.101*
C40.2521 (4)0.0941 (2)0.13703 (19)0.0672 (11)H40.14970.07900.11590.081*C200.1342 (5)0.8988 (3)0.0001 (2)0.0880 (13)H200.17360.9408-0.02180.106*C270.5930 (5)0.7842 (3)0.0088 (3)0.0940 (15)H270.60890.8306-0.01090.113*C260.6419 (5)0.7202 (3)-0.0240 (2)0.0900 (14)H260.69070.7248-0.06590.108*C240.6775 (6)0.5823 (3)-0.0342 (2)0.1177 (18)H24A0.59760.5428-0.02900.176*H24B0.78640.5670-0.01520.176*H24C0.68460.5936-0.08190.176*C160.1788 (4)0.54521 (18)0.16718 (16)0.0465 (8)C170.1206 (5)0.6898 (3)-0.0274 (2)0.1080 (16)	C18	0.0977 (4)	0.7657 (2)	0.0029 (2)	0.0682 (11)
H40.14970.07900.11590.081*C200.1342 (5)0.8988 (3)0.0001 (2)0.0880 (13)H200.17360.9408-0.02180.106*C270.5930 (5)0.7842 (3)0.0088 (3)0.0940 (15)H270.60890.8306-0.01090.113*C260.6419 (5)0.7202 (3)-0.0240 (2)0.0900 (14)H260.69070.7248-0.06590.108*C240.6775 (6)0.5823 (3)-0.0342 (2)0.1177 (18)H24A0.59760.5428-0.02900.176*H24B0.78640.5670-0.01520.176*H24C0.68460.5936-0.08190.176*C160.1788 (4)0.54521 (18)0.16718 (16)0.0465 (8)C170.1206 (5)0.6898 (3)-0.0274 (2)0.1080 (16	C4	0.2521 (4)	0.0941 (2)	0.13703 (19)	0.0672 (11)
C20 $0.1342 (5)$ $0.8988 (3)$ $0.0001 (2)$ $0.0880 (13)$ H20 0.1736 0.9408 -0.0218 $0.106*$ C27 $0.5930 (5)$ $0.7842 (3)$ $0.0088 (3)$ $0.0940 (15)$ H27 0.6089 0.8306 -0.0109 $0.113*$ C26 $0.6419 (5)$ $0.7202 (3)$ $-0.0240 (2)$ $0.0900 (14)$ H26 0.6907 0.7248 -0.0659 $0.108*$ C24 $0.6775 (6)$ $0.5823 (3)$ $-0.0342 (2)$ $0.1177 (18)$ H24A 0.5976 0.5428 -0.0290 $0.176*$ H24B 0.7864 0.5670 -0.0819 $0.176*$ H24C 0.6846 0.5936 -0.0819 $0.176*$ C16 $0.1788 (4)$ $0.54521 (18)$ $0.16718 (16)$ $0.0465 (8)$ C17 $0.1206 (5)$ $0.6898 (3)$ $-0.0274 (2)$ $0.1080 (16)$	H4	0.1497	0.0790	0.1159	0.081*
H20 0.1736 0.9408 -0.0218 0.106^* C27 $0.5930 (5)$ $0.7842 (3)$ $0.0088 (3)$ $0.0940 (15)$ H27 0.6089 0.8306 -0.0109 0.113^* C26 $0.6419 (5)$ $0.7202 (3)$ $-0.0240 (2)$ $0.0900 (14)$ H26 0.6907 0.7248 -0.0659 0.108^* C24 $0.6775 (6)$ $0.5823 (3)$ $-0.0342 (2)$ $0.1177 (18)$ H24A 0.5976 0.5428 -0.0290 0.176^* H24B 0.7864 0.5670 -0.0819 0.176^* H24C 0.6846 0.5936 -0.0819 0.176^* C16 $0.1788 (4)$ $0.54521 (18)$ $0.16718 (16)$ $0.0465 (8)$ C17 $0.1206 (5)$ $0.6898 (3)$ $-0.0274 (2)$ $0.1080 (16)$	C20	0.1342 (5)	0.8988 (3)	0.0001 (2)	0.0880 (13)
C27 $0.5930(5)$ $0.7842(3)$ $0.0088(3)$ $0.0940(15)$ H27 0.6089 0.8306 -0.0109 $0.113*$ C26 $0.6419(5)$ $0.7202(3)$ $-0.0240(2)$ $0.0900(14)$ H26 0.6907 0.7248 -0.0659 $0.108*$ C24 $0.6775(6)$ $0.5823(3)$ $-0.0342(2)$ $0.1177(18)$ H24A 0.5976 0.5428 -0.0290 $0.176*$ H24B 0.7864 0.5670 -0.0152 $0.176*$ H24C 0.6846 0.5936 -0.0819 $0.176*$ C16 $0.1788(4)$ $0.54521(18)$ $0.16718(16)$ $0.0465(8)$ C17 $0.1206(5)$ $0.6898(3)$ $-0.0274(2)$ $0.1080(16)$	H20	0.1736	0.9408	-0.0218	0.106*
H27 0.6089 0.8306 -0.0109 0.113^* C26 $0.6419 (5)$ $0.7202 (3)$ $-0.0240 (2)$ $0.0900 (14)$ H26 0.6907 0.7248 -0.0659 0.108^* C24 $0.6775 (6)$ $0.5823 (3)$ $-0.0342 (2)$ $0.1177 (18)$ H24A 0.5976 0.5428 -0.0290 0.176^* H24B 0.7864 0.5670 -0.0152 0.176^* H24C 0.6846 0.5936 -0.0819 0.176^* C16 $0.1788 (4)$ $0.54521 (18)$ $0.16718 (16)$ $0.0465 (8)$ C17 $0.1206 (5)$ $0.6898 (3)$ $-0.0274 (2)$ $0.1080 (16)$	C27	0.5930 (5)	0.7842 (3)	0.0088 (3)	0.0940 (15)
C26 $0.6419(5)$ $0.7202(3)$ $-0.0240(2)$ $0.0900(14)$ H26 0.6907 0.7248 -0.0659 $0.108*$ C24 $0.6775(6)$ $0.5823(3)$ $-0.0342(2)$ $0.1177(18)$ H24A 0.5976 0.5428 -0.0290 $0.176*$ H24B 0.7864 0.5670 -0.0152 $0.176*$ H24C 0.6846 0.5936 -0.0819 $0.176*$ C16 $0.1788(4)$ $0.54521(18)$ $0.16718(16)$ $0.0465(8)$ C17 $0.1206(5)$ $0.6898(3)$ $-0.0274(2)$ $0.1080(16)$	H27	0.6089	0.8306	-0.0109	0.113*
H26 0.6907 0.7248 -0.0659 $0.108*$ C24 $0.6775 (6)$ $0.5823 (3)$ $-0.0342 (2)$ $0.1177 (18)$ H24A 0.5976 0.5428 -0.0290 $0.176*$ H24B 0.7864 0.5670 -0.0152 $0.176*$ H24C 0.6846 0.5936 -0.0819 $0.176*$ C16 $0.1788 (4)$ $0.54521 (18)$ $0.16718 (16)$ $0.0465 (8)$ C17 $0.1206 (5)$ $0.6898 (3)$ $-0.0274 (2)$ $0.1080 (16)$	C26	0.6419 (5)	0.7202 (3)	-0.0240 (2)	0.0900 (14)
C240.6775 (6)0.5823 (3)-0.0342 (2)0.1177 (18)H24A0.59760.5428-0.02900.176*H24B0.78640.5670-0.01520.176*H24C0.68460.5936-0.08190.176*C160.1788 (4)0.54521 (18)0.16718 (16)0.0465 (8)C170.1206 (5)0.6898 (3)-0.0274 (2)0.1080 (16)	H26	0.6907	0.7248	-0.0659	0.108*
H24A0.59760.5428-0.02900.176*H24B0.78640.5670-0.01520.176*H24C0.68460.5936-0.08190.176*C160.1788 (4)0.54521 (18)0.16718 (16)0.0465 (8)C170.1206 (5)0.6898 (3)-0.0274 (2)0.1080 (16)	C24	0.6775 (6)	0.5823 (3)	-0.0342(2)	0.1177 (18)
H24B0.78640.5670-0.01520.176*H24C0.68460.5936-0.08190.176*C160.1788 (4)0.54521 (18)0.16718 (16)0.0465 (8)C170.1206 (5)0.6898 (3)-0.0274 (2)0.1080 (16)	H24A	0.5976	0.5428	-0.0290	0.176*
H24C0.68460.5936-0.08190.176*C160.1788 (4)0.54521 (18)0.16718 (16)0.0465 (8)C170.1206 (5)0.6898 (3)-0.0274 (2)0.1080 (16)	H24B	0.7864	0.5670	-0.0152	0.176*
C160.1788 (4)0.54521 (18)0.16718 (16)0.0465 (8)C170.1206 (5)0.6898 (3)-0.0274 (2)0.1080 (16)	H24C	0.6846	0.5936	-0.0819	0.176*
C17 0.1206 (5) 0.6898 (3) -0.0274 (2) 0.1080 (16	C16	0.1788 (4)	0.54521 (18)	0.16718 (16)	0.0465 (8)
	C17	0.1206 (5)	0.6898 (3)	-0.0274 (2)	0.1080 (16)

supporting information

H17A	0.0371	0.6821	-0.0642	0.162*
H17B	0.1080	0.6525	0.0072	0.162*
H17C	0.2313	0.6861	-0.0444	0.162*

Atomic displacement parameters $(Å^2)$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N2	0.0534 (17)	0.0370 (15)	0.0571 (17)	0.0049 (13)	-0.0004 (14)	0.0010 (13)
N1	0.0494 (16)	0.0363 (15)	0.0553 (17)	-0.0015 (13)	-0.0004 (13)	0.0001 (13)
O2	0.0426 (14)	0.0666 (16)	0.0910 (18)	0.0052 (13)	-0.0060 (13)	-0.0292 (14)
06	0.0423 (14)	0.0593 (15)	0.101 (2)	-0.0084 (12)	-0.0082 (13)	0.0324 (14)
03	0.0503 (15)	0.0542 (16)	0.0834 (19)	0.0053 (12)	0.0017 (13)	-0.0211 (13)
O4	0.0704 (17)	0.0445 (15)	0.0935 (19)	0.0018 (13)	-0.0101 (14)	-0.0154 (14)
01	0.0647 (16)	0.0536 (15)	0.0921 (19)	0.0035 (13)	-0.0002 (13)	-0.0288 (14)
05	0.0611 (17)	0.0530 (16)	0.119 (2)	-0.0025 (13)	-0.0001 (15)	0.0312 (16)
O7	0.0471 (15)	0.0452 (14)	0.095 (2)	-0.0076 (12)	-0.0034 (13)	0.0204 (13)
08	0.0647 (17)	0.0446 (14)	0.0925 (19)	-0.0009 (12)	-0.0043 (13)	0.0181 (13)
C10	0.0354 (18)	0.0393 (18)	0.0392 (17)	-0.0020 (15)	0.0062 (14)	-0.0048 (14)
C1	0.0398 (19)	0.0389 (18)	0.0416 (18)	0.0002 (15)	0.0091 (15)	0.0057 (15)
C15	0.0421 (19)	0.0412 (19)	0.0380 (17)	0.0019 (16)	0.0075 (14)	-0.0056 (15)
C6	0.0393 (19)	0.0383 (18)	0.0429 (18)	0.0005 (15)	0.0036 (15)	0.0084 (15)
C22	0.0355 (18)	0.053 (2)	0.0440 (19)	0.0000 (16)	-0.0028 (15)	0.0059 (17)
C9	0.044 (2)	0.042 (2)	0.052 (2)	-0.0034 (17)	0.0049 (16)	0.0038 (16)
C11	0.048 (2)	0.052 (2)	0.057 (2)	-0.0032 (18)	0.0058 (17)	0.0013 (17)
C2	0.048 (2)	0.049 (2)	0.058 (2)	0.0047 (18)	0.0083 (17)	0.0028 (17)
C7	0.049 (2)	0.045 (2)	0.050 (2)	-0.0040 (18)	0.0025 (16)	0.0032 (17)
C29	0.0395 (19)	0.047 (2)	0.053 (2)	-0.0051 (16)	-0.0031 (16)	0.0107 (17)
C8	0.049 (2)	0.0370 (19)	0.052 (2)	0.0021 (17)	0.0058 (17)	-0.0005 (16)
C23	0.046 (2)	0.050 (2)	0.058 (2)	-0.0005 (17)	-0.0047 (17)	-0.0075 (18)
C3	0.040 (2)	0.069 (3)	0.080 (3)	0.010 (2)	0.0075 (18)	0.011 (2)
C12	0.041 (2)	0.072 (3)	0.072 (3)	-0.011 (2)	0.0047 (18)	-0.003 (2)
C30	0.059 (2)	0.051 (2)	0.058 (2)	-0.0056 (19)	0.0037 (18)	0.0004 (19)
C28	0.056 (2)	0.051 (2)	0.088 (3)	-0.0011 (19)	-0.001 (2)	0.023 (2)
C25	0.065 (3)	0.102 (3)	0.053 (2)	-0.008(2)	0.006 (2)	-0.007 (3)
C14	0.047 (2)	0.060 (2)	0.062 (2)	0.0070 (19)	-0.0002 (18)	0.0053 (18)
C13	0.036 (2)	0.087 (3)	0.074 (3)	0.009 (2)	-0.0050 (18)	0.000 (2)
C5	0.048 (2)	0.048 (2)	0.069 (2)	-0.0042 (18)	-0.0068 (18)	0.0001 (18)
C21	0.065 (3)	0.060 (2)	0.075 (3)	0.000 (2)	0.009 (2)	0.019 (2)
C19	0.065 (3)	0.139 (4)	0.048 (2)	0.017 (3)	0.013 (2)	0.016 (3)
C18	0.053 (2)	0.095 (3)	0.055 (2)	0.018 (2)	-0.008(2)	-0.020 (2)
C4	0.047 (2)	0.070 (3)	0.083 (3)	-0.003 (2)	-0.009 (2)	0.005 (2)
C20	0.081 (3)	0.105 (4)	0.080 (3)	0.006 (3)	0.018 (3)	0.035 (3)
C27	0.070 (3)	0.097 (4)	0.115 (4)	-0.007 (3)	0.006 (3)	0.065 (3)
C26	0.064 (3)	0.137 (4)	0.069 (3)	0.000 (3)	0.003 (2)	0.028 (3)
C24	0.109 (4)	0.149 (4)	0.099 (3)	-0.023 (3)	0.041 (3)	-0.058 (3)
C16	0.049 (2)	0.044 (2)	0.046 (2)	0.0031 (18)	0.0020 (17)	-0.0047 (16)
C17	0.103 (4)	0.128 (4)	0.092 (3)	0.027 (3)	-0.002 (3)	-0.054 (3)

Geometric parameters (Å, °)

N2—C29	1.462 (4)	C29—C30	1.377 (4)
N2—H2A	0.8900	C23—C18	1.399 (5)
N2—H2B	0.8900	С23—Н23	0.9300
N2—H2C	0.8900	C3—C4	1.368 (4)
N1—C22	1.468 (4)	С3—НЗА	0.9300
N1—H1A	0.8900	C12—C13	1.371 (5)
N1—H1B	0.8900	C12—H12	0.9300
N1—H1C	0.8900	C30—C25	1.377 (5)
O2—C8	1.275 (3)	С30—Н30	0.9300
О6—С9	1.271 (3)	C28—C27	1.394 (5)
O3—C7	1.284 (3)	C28—H28	0.9300
O3—H3	0.8200	C25—C26	1.372 (5)
O4—C7	1.230 (3)	C25—C24	1.496 (5)
O1—C8	1.225 (3)	C14—C13	1.379 (4)
О5—С9	1.223 (3)	C14—H14	0.9300
O7—C16	1.281 (3)	C13—H13	0.9300
O7—H7	0.8200	C5—C4	1.375 (4)
O8—C16	1.226 (3)	С5—Н5	0.9300
C10-C11	1.390 (4)	C21—C20	1.375 (5)
C10—C15	1.414 (4)	C21—H21	0.9300
С10—С9	1.509 (4)	C19—C20	1.367 (5)
C1—C2	1.390 (4)	C19—C18	1.381 (5)
C1—C6	1.413 (4)	C19—H19	0.9300
C1—C8	1.522 (4)	C18—C17	1.500 (5)
C15—C14	1.382 (4)	C4—H4	0.9300
C15—C16	1.508 (4)	C20—H20	0.9300
C6—C5	1.391 (4)	C27—C26	1.381 (6)
C6—C7	1.511 (4)	C27—H27	0.9300
C22—C21	1.364 (4)	C26—H26	0.9300
C22—C23	1.370 (4)	C24—H24A	0.9600
C11—C12	1.361 (4)	C24—H24B	0.9600
C11—H11	0.9300	C24—H24C	0.9600
C2—C3	1.373 (4)	C17—H17A	0.9600
С2—Н2	0.9300	C17—H17B	0.9600
C29—C28	1.364 (4)	C17—H17C	0.9600
C29—N2—H2A	109.5	C13—C12—H12	120.5
C29—N2—H2B	109.5	C29—C30—C25	121.2 (3)
H2A—N2—H2B	109.5	С29—С30—Н30	119.4
C29—N2—H2C	109.5	С25—С30—Н30	119.4
H2A—N2—H2C	109.5	C29—C28—C27	117.6 (4)
H2B—N2—H2C	109.5	C29—C28—H28	121.2
C22—N1—H1A	109.5	C27—C28—H28	121.2
C22—N1—H1B	109.5	C26—C25—C30	116.9 (4)
H1A—N1—H1B	109.5	C26—C25—C24	121.0 (4)
C22—N1—H1C	109.5	C30—C25—C24	122.1 (4)

	100 5	G10 G14 G15	100.0 (0)
HIA—NI—HIC	109.5	C13—C14—C15	122.3 (3)
H1B—N1—H1C	109.5	C13—C14—H14	118.8
С7—О3—Н3	109.5	C15—C14—H14	118.8
С16—О7—Н7	109.5	C12—C13—C14	119.7 (3)
C11—C10—C15	117.8 (3)	C12—C13—H13	120.1
C11—C10—C9	114.2 (3)	C14—C13—H13	120.1
C15—C10—C9	127.9 (3)	C4—C5—C6	122.1 (3)
C2—C1—C6	117.9 (3)	С4—С5—Н5	119.0
C2—C1—C8	114.0 (3)	С6—С5—Н5	119.0
C6—C1—C8	128.1 (3)	C22—C21—C20	118.5 (4)
C14—C15—C10	118.0 (3)	C22—C21—H21	120.7
C14—C15—C16	113.4 (3)	C20—C21—H21	120.7
C10—C15—C16	128.5 (3)	C20—C19—C18	122.1 (4)
C5—C6—C1	118.3 (3)	С20—С19—Н19	119.0
C5—C6—C7	113.4 (3)	С18—С19—Н19	119.0
C1—C6—C7	128.3 (3)	C19—C18—C23	117.9 (4)
$C_{21} - C_{22} - C_{23}$	122.8 (3)	C19 - C18 - C17	122.1 (4)
$C_{21} = C_{22} = N_1$	1175(3)	C_{23} C_{18} C_{17}	120.0(4)
C_{23} C_{22} N1	119.7 (3)	C_{3} C_{4} C_{5}	120.0(1) 119.8(3)
05-022 101	119.4 (3)	$C_3 - C_4 - H_4$	120.1
05 - C9 - C10	119.4 (3)	C5-C4-H4	120.1
$O_{5} = C_{7} = C_{10}$	120.8 (3)	C_{19} C_{20} C_{21}	120.1 110.8 (4)
$C_{12} = C_{10}$	120.0(3) 123.2(3)	$C_{19} = C_{20} = C_{21}$	119.8 (4)
C_{12} C_{11} U_{11}	125.2 (5)	$C_{19} = C_{20} = H_{20}$	120.1
	110.4	$C_{21} = C_{20} = H_{20}$	120.1
	118.4	$C_{20} = C_{27} = C_{28}$	119.7 (4)
$C_3 = C_2 = C_1$	122.6 (3)	$C_{20} = C_{27} = H_{27}$	120.1
$C_3 = C_2 = H_2$	118./	C28—C2/—H2/	120.1
C1—C2—H2	118.7	$C_{25} = C_{26} = C_{27}$	122.6 (4)
04-03	119.0 (3)	С25—С26—Н26	118.7
O4—C7—C6	119.5 (3)	C27—C26—H26	118.7
O3—C7—C6	121.4 (3)	C25—C24—H24A	109.5
C28—C29—C30	121.9 (3)	C25—C24—H24B	109.5
C28—C29—N2	119.8 (3)	H24A—C24—H24B	109.5
C30—C29—N2	118.3 (3)	C25—C24—H24C	109.5
O1—C8—O2	120.9 (3)	H24A—C24—H24C	109.5
O1—C8—C1	119.4 (3)	H24B—C24—H24C	109.5
O2—C8—C1	119.7 (3)	O8—C16—O7	118.8 (3)
C22—C23—C18	118.9 (3)	O8—C16—C15	119.5 (3)
С22—С23—Н23	120.6	O7—C16—C15	121.6 (3)
C18—C23—H23	120.6	C18—C17—H17A	109.5
C4—C3—C2	119.3 (3)	C18—C17—H17B	109.5
C4—C3—H3A	120.4	H17A—C17—H17B	109.5
С2—С3—НЗА	120.4	С18—С17—Н17С	109.5
C11—C12—C13	118.9 (3)	H17A—C17—H17C	109.5
C11—C12—H12	120.5	H17B—C17—H17C	109.5

D—H···A	<i>D</i> —Н	$H \cdots A$	$D \cdots A$	D—H··· A
N2—H2 <i>A</i> ···O5 ⁱ	0.89	1.87	2.739 (3)	166
N2—H2 <i>B</i> ···O2 ⁱⁱ	0.89	1.93	2.815 (3)	178
N2—H2 <i>C</i> ···O8	0.89	1.90	2.789 (3)	178
N1—H1 <i>A</i> ···O6 ⁱ	0.89	1.94	2.826 (3)	177
N1—H1 <i>B</i> …O1 ⁱ	0.89	1.91	2.784 (3)	166
N1—H1 <i>C</i> …O4 ⁱⁱⁱ	0.89	1.90	2.788 (3)	172
О3—Н3…О2	0.82	1.58	2.392 (3)	173
О7—Н7…О6	0.82	1.57	2.392 (3)	180

Hydrogen-bond geometry (Å, °)

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