organic compounds

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N,N'-Bis(2-methoxyphenyl)biphenyl-2,2'dicarboxamide

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Key indicators: single-crystal X-ray study; T = 113 K; mean σ (C–C) = 0.005 Å; R factor = 0.039; wR factor = 0.093; data-to-parameter ratio = 6.4.

In the title compound, $C_{28}H_{24}N_2O_4$, the dihedral angle between the two rings of the biphenyl unit is 75.34 (9)°. The outer aromatic rings form dihedral angles of 66.96 (1) and 85.69 (8)° with the rings to which they are attached. The molecular structure is stabilized by intramolecular $C-H\cdots O$ and $N-H\cdots O$ hydrogen bonds. In the crystal structure, intermolecular $N-H\cdots O$ interactions are observed.

Related literature

For the synthesis, see: Gao & Gao (2002). For related structures, see: Wang & Han (2004); Wang & Jiang (2004); Huang & Yang (2008).



Experimental

Crystal data $C_{28}H_{24}N_2O_4$ $M_r = 452.49$ Monoclinic, *Cc* a = 18.184 (4) Å

<i>b</i> = 16.304 (3) Å
c = 7.9998 (16) Å
$\beta = 108.90 \ (3)^{\circ}$
V = 2243.9 (8) Å ³

Z = 4Mo $K\alpha$ radiation $\mu = 0.09 \text{ mm}^{-1}$

Data collection

Rigaku Saturn CCD diffractometer
Absorption correction: multi-scan
(CrystalStructure; Rigaku/MSC,
2004)
$T_{\min} = 0.986, T_{\max} = 0.991$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.039$ $wR(F^2) = 0.093$ S = 1.061991 reflections 309 parameters

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

$D - H \cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdots A$
$N1 - H1N \cdots O3^{i}$	0.86	2.02	2.833 (3)	157
$N2 - H2N \cdots O2$	0.86	2.24	3.081 (4)	167
$N2 - H2N \cdots O4$	0.86	2.24	2.612 (3)	106
C22−H22···O3	0.93	2.30	2.885 (4)	120

T = 113 (2) K

 $R_{\rm int} = 0.054$

2 restraints

 $\Delta \rho_{\text{max}} = 0.17 \text{ e } \text{\AA}^-$

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

 $0.16 \times 0.14 \times 0.10 \text{ mm}$

6422 measured reflections 1991 independent reflections

1858 reflections with $I > 2\sigma(I)$

H-atom parameters constrained

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

Data collection: *RAPID-AUTO* (Rigaku/MSC, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; 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: GW2044).

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supporting information

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N,N'-Bis(2-methoxyphenyl)biphenyl-2,2'-dicarboxamide

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S1. Comment

The distortion of diphenyl spacer about central bond not only endows dpa a peculiar characterization to link metal ions or metal clusters into macrocycles or helical chains, but also makes diphenic acid (H2dpa) can deprotonate partially forming hydrogen bonds of carboxylic groups to meet both geometric and energetic requirements. We here report the crystal structure of the title compound.

The C8—C13 and C14—C19 planes form the dihedral angle of 75.34 (9)°, and C1—C6 ring are nearly perpendicular to C14—C19 ring, with a dihedral angle of 85.69 (8)°. The molecular structure is stabilized by C—H…O and N—H…O intramolecular hydrogen bonds. In addition, weak C—H…O intermolecular hydrogen bonds are observed.

S2. Experimental

The title compound was prepared according to the reported procedure of M. Z. Gao & Gao (2002). Colourless single crystals suitable for X-ray diffraction were obtained by recrystallization from dimethyl sulfoxide.

S3. Refinement

H atoms were placed in calculated positions with C—H = 0.93 Å, and N—H = 0.86 Å, and refined in riding mode with $U_{iso}(H) = 1.2U_{eq}(C,N)$.



Figure 1

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

N,*N*'-Bis(2-methoxyphenyl)biphenyl-2,2'-dicarboxamide

Crystal data	
$C_{28}H_{24}N_2O_4$	F(000) = 952
$M_r = 452.49$	$D_{\rm x} = 1.339 {\rm ~Mg} {\rm ~m}^{-3}$
Monoclinic, Cc	Mo <i>K</i> α radiation, $\lambda = 0.71073$ Å
a = 18.184 (4) Å	Cell parameters from 3190 reflections
b = 16.304 (3) Å	$\theta = 1.7 - 27.9^{\circ}$
c = 7.9998 (16) Å	$\mu=0.09~\mathrm{mm^{-1}}$
$\beta = 108.90 \ (3)^{\circ}$	T = 113 K
V = 2243.9 (8) Å ³	Block, colourless
Z = 4	$0.16 \times 0.14 \times 0.10 \text{ mm}$

Data collection

Rigaku Saturn diffractometer	6422 measured reflections 1991 independent reflections
Radiation source: rotating anode	1858 reflections with $I > 2\sigma(I)$
Confocal monochromator	$R_{\rm int} = 0.054$
ω scans	$\theta_{\text{max}} = 25.0^{\circ}, \ \theta_{\text{min}} = 1.7^{\circ}$
Absorption correction: multi-scan	$h = -21 \rightarrow 20$
(CrystalStructure; Rigaku/MSC, 2004)	$k = -17 \rightarrow 19$
$T_{\min} = 0.986, \ T_{\max} = 0.991$	$l = -9 \rightarrow 9$
Refinement	
Refinement on F^2	Secondary atom site location: difference Fourier
Least-squares matrix: full	map
$R[F^2 > 2\sigma(F^2)] = 0.039$	Hydrogen site location: inferred from
$wR(F^2) = 0.093$	neighbouring sites
S = 1.06	H-atom parameters constrained
1991 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0537P)^2]$
309 parameters	where $P = (F_o^2 + 2F_c^2)/3$
2 restraints	$(\Delta/\sigma)_{\rm max} = 0.007$
Primary atom site location: structure-invariant	$\Delta \rho_{\rm max} = 0.17 \text{ e } \text{\AA}^{-3}$
direct methods	$\Delta \rho_{\min} = -0.20 \text{ e} \text{ \AA}^{-3}$
RefinementRefinement on F^2 Least-squares matrix: full $R[F^2 > 2\sigma(F^2)] = 0.039$ $wR(F^2) = 0.093$ $S = 1.06$ 1991 reflections309 parameters2 restraintsPrimary atom site location: structure-invariant direct methods	Secondary atom site location: difference Fourier map Hydrogen site location: inferred from neighbouring sites H-atom parameters constrained $w = 1/[\sigma^2(F_o^2) + (0.0537P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{max} = 0.007$ $\Delta\rho_{max} = 0.17$ e Å ⁻³ $\Delta\rho_{min} = -0.20$ e Å ⁻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.

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

	x	У	Ζ	$U_{ m iso}$ */ $U_{ m eq}$	
01	-0.01240 (15)	0.26417 (14)	0.9137 (3)	0.0338 (6)	
O2	0.21854 (13)	0.17729 (12)	1.0081 (2)	0.0234 (5)	
03	0.45976 (12)	0.32159 (13)	1.0239 (2)	0.0239 (5)	
O4	0.31213 (13)	0.07137 (13)	0.8380 (3)	0.0273 (5)	
N1	0.09211 (15)	0.17216 (15)	0.8317 (3)	0.0222 (6)	
H1N	0.0615	0.1801	0.7258	0.027*	
N2	0.37809 (15)	0.21050 (14)	0.9645 (3)	0.0216 (6)	
H2N	0.3350	0.1932	0.9743	0.026*	
C1	0.00360 (19)	0.19053 (18)	0.9988 (4)	0.0229 (7)	
C2	-0.0328 (2)	0.16090 (19)	1.1154 (4)	0.0277 (7)	
H2	-0.0694	0.1928	1.1441	0.033*	
C3	-0.0139 (2)	0.0831 (2)	1.1889 (4)	0.0298 (8)	
Н3	-0.0378	0.0632	1.2674	0.036*	
C4	0.0399 (2)	0.0355 (2)	1.1457 (4)	0.0305 (8)	
H4	0.0512	-0.0170	1.1926	0.037*	
C5	0.07701 (19)	0.06580 (18)	1.0327 (3)	0.0258 (7)	

C6 $0.05817 (18)$ $0.14248 (18)$ $0.9576 (3)$ $0.0210 (7)$ C7 $0.16777 (18)$ $0.18877 (17)$ $0.8643 (3)$ $0.0188 (6)$ C8 $0.18756 (18)$ $0.22120 (18)$ $0.7085 (3)$ $0.0221 (7)$ C9 $0.16253 (18)$ $0.1798 (18)$ $0.5469 (4)$ $0.0219 (7)$ H9 0.1304 0.1342 0.5336 0.026^* C10 $0.18522 (19)$ $0.20637 (19)$ $0.4066 (3)$ $0.0251 (7)$ H10 0.1695 0.1779 0.3000 0.300^* C11 $0.2317 (2)$ $0.27591 (19)$ $0.4260 (4)$ $0.0275 (7)$ H11 0.2471 0.2940 0.3321 0.033^* C12 $0.25501 (19)$ $0.31821 (19)$ $0.5843 (4)$ $0.0225 (7)$ H12 $0.2333 (17)$ $0.29096 (18)$ $0.7281 (3)$ $0.0190 (6)$ C14 $0.25474 (18)$ $0.34128 (17)$ $0.8956 (3)$ $0.0204 (6)$ C15 $0.1978 (2)$ $0.39160 (18)$ $0.9223 (4)$ $0.0270 (7)$ H15 0.1475 0.3901 0.8428 0.032^* C16 $0.2152 (2)$ $0.4441 (2)$ $1.0670 (4)$ $0.0307 (8)$ H16 0.1763 0.4766 1.0847 0.037^* C17 $0.2397 (2)$ $0.4481 (219)$ $1.1841 (4)$ $0.0290 (8)$ H17 0.3015 0.4837 1.2800 0.035^* C18 $0.34668 (19)$ $0.3987 (18)$ $1.1576 (4)$ $0.0214 (7)$ H18 0.3972 0.4021 1.2355 0.029^*	Н5	0.1148	0.0345	1.0072	0.031*
$C7$ $0.16777 (18)$ $0.18877 (17)$ $0.8643 (3)$ $0.0188 (6)$ $C8$ $0.18756 (18)$ $0.22120 (18)$ $0.7085 (3)$ $0.0201 (7)$ $C9$ $0.16253 (18)$ $0.17982 (18)$ $0.5469 (4)$ $0.0219 (7)$ $H9$ 0.1304 0.1342 0.5336 $0.02c4^*$ $C10$ $0.18522 (19)$ $0.20637 (19)$ $0.4066 (3)$ $0.0251 (7)$ $H10$ 0.1695 0.1779 0.3000 0.030^* $C11$ $0.2317 (2)$ $0.27591 (19)$ $0.4260 (4)$ $0.0275 (7)$ $H11$ 0.2471 0.2940 0.3321 0.033^* $C12$ $0.25501 (19)$ $0.31821 (19)$ $0.5843 (4)$ $0.0225 (7)$ $H12$ 0.2853 0.3651 0.5956 0.030^* $C13$ $0.2333 (17)$ $0.29096 (18)$ $0.7281 (3)$ $0.0190 (6)$ $C14$ $0.25474 (18)$ $0.34128 (17)$ $0.8950 (3)$ $0.0204 (6)$ $C15$ $0.1978 (2)$ $0.39160 (18)$ $0.9223 (4)$ 0.037^* $C16$ $0.2152 (2)$ $0.4441 (2)$ $1.0670 (4)$ $0.0307 (8)$ $H15$ 0.1475 0.3901 0.8428 0.032^* $C16$ $0.2197 (2)$ $0.44812 (19)$ $1.1841 (4)$ $0.02210 (7)$ $H17$ 0.3075 0.4837 1.2800 0.035^* $C18$ $0.34668 (19)$ $0.39879 (18)$ $1.1576 (4)$ $0.0214 (7)$ $H18$ 0.3972 0.4021 1.2355 0.029^* $C19$ $0.32979 (19)$ $0.34399 (18)$ $1.0156 ($	C6	0.05817 (18)	0.14248 (18)	0.9576 (3)	0.0210(7)
C8 $0.18756(18)$ $0.22120(18)$ $0.7085(3)$ $0.0201(7)$ C9 $0.16233(18)$ $0.17982(18)$ $0.5469(4)$ $0.0219(7)$ H9 0.1304 0.1342 0.5336 0.026^{+} C10 $0.18522(19)$ $0.20637(19)$ $0.4066(3)$ $0.0251(7)$ H10 0.1695 0.1779 0.3000 0.030^{*} C11 $0.2317(2)$ $0.27591(19)$ $0.4260(4)$ $0.0275(7)$ H11 0.2471 0.2940 0.3321 0.033^{*} C12 $0.2550(19)$ $0.31821(19)$ $0.5843(4)$ $0.0225(7)$ H12 0.2853 0.3651 0.5956 0.030^{*} C13 $0.23333(17)$ $0.29096(18)$ $0.7281(3)$ $0.0190(6)$ C14 $0.25474(18)$ $0.34128(17)$ $0.8950(3)$ $0.0224(6)$ C15 $0.1978(2)$ $0.39160(18)$ $0.9223(4)$ $0.0270(7)$ H15 0.1475 0.3901 0.8428 0.032^{*} C16 $0.2152(2)$ $0.4441(2)$ $1.0670(4)$ $0.037(8)$ H16 0.1763 0.4766 1.0847 0.037^{*} C17 $0.2897(2)$ $0.44812(19)$ $1.181(4)$ $0.0290(8)$ H17 0.3015 0.4837 1.2800 0.035^{*} C18 $0.34668(19)$ $0.39879(18)$ $1.1576(4)$ $0.0294(7)$ H18 0.3972 0.4021 1.2355 0.0294^{*} C19 $0.32979(19)$ $0.34399(18)$ $1.0156(3)$ $0.0211(6)$ C20 $0.3954(18)$ $0.1519(18)$ <td>C7</td> <td>0.16777 (18)</td> <td>0.18877 (17)</td> <td>0.8643 (3)</td> <td>0.0188 (6)</td>	C7	0.16777 (18)	0.18877 (17)	0.8643 (3)	0.0188 (6)
C9 0.16253 (18) 0.17982 (18) 0.5469 (4) 0.0219 (7)H9 0.1304 0.1342 0.5336 $0.02c^{4}$ C10 0.18522 (19) 0.20637 (19) 0.4066 (3) 0.0251 (7)H10 0.1695 0.1779 0.3000 0.030^{*} C11 0.2317 (2) 0.27591 (19) 0.4260 (4) 0.0275 (7)H11 0.2471 0.2940 0.3321 0.033^{*} C12 0.25501 (19) 0.31821 (19) 0.5843 (4) 0.0225 (7)H12 0.2853 0.3651 0.5956 0.030^{*} C13 0.23333 (17) 0.29096 (18) 0.7281 (3) 0.0190 (6)C14 0.25474 (18) 0.34128 (17) 0.8950 (3) 0.0204 (6)C15 0.1978 (2) 0.39160 (18) 0.9223 (4) 0.037^{*} C16 0.2152 (2) 0.4441 (2) 1.0670 (4) 0.0307 (8)H16 0.1763 0.4766 1.0847 0.037^{*} C17 0.2897 (2) 0.44812 (19) 1.1841 (4) 0.0290 (8)H17 0.3015 0.4837 1.2800 0.035^{*} C18 0.34668 (19) 0.39879 (18) 1.1576 (4) 0.0244 (7)H18 0.3972 0.4021 1.2355 0.029^{*} C19 0.32979 (19) 0.34399 (18) 1.0156 (3) 0.0211 (7)C21 0.4521 (18) 0.2191 (7) 1.0011 (3) 0.0212 (7)C22 0.5013 (2) 0.16379 (2) 0.9756 0.038^{*}	C8	0.18756 (18)	0.22120 (18)	0.7085 (3)	0.0201 (7)
H90.13040.13420.53360.026*C100.18522 (19)0.20637 (19)0.4066 (3)0.0251 (7)H100.16950.17790.30000.300*C110.2317 (2)0.27591 (19)0.4260 (4)0.0275 (7)H110.24710.29400.33210.033*C120.25501 (19)0.31821 (19)0.5843 (4)0.0252 (7)H120.28530.36510.59560.030*C130.23333 (17)0.2096 (18)0.7281 (3)0.0190 (6)C140.25474 (18)0.34128 (17)0.8950 (3)0.0244 (6)C150.1978 (2)0.39010.84280.032*C160.2152 (2)0.4441 (2)1.0670 (4)0.0307 (8)H160.17630.47661.08470.037*C170.2897 (2)0.44812 (19)1.1841 (4)0.0290 (8)H170.30150.48371.28000.035*C180.34668 (19)0.39879 (18)1.0156 (3)0.0211 (6)C200.39544 (18)0.29130 (17)1.0011 (3)0.0210 (7)C210.42452 (18)0.15199 (18)0.9115 (3)0.0212 (7)C220.5013 (2)0.1627 (2)0.9232 (4)0.0317 (8)H220.52760.20990.97560.038*C230.5398 (2)0.1035 (2)0.8573 (5)0.042*C240.5015 (2)0.0217 (2)0.7829 (5)0.0354 (8)H240.5271 -0.0048 0.73050.042*C25 <td>С9</td> <td>0.16253 (18)</td> <td>0.17982 (18)</td> <td>0.5469 (4)</td> <td>0.0219 (7)</td>	С9	0.16253 (18)	0.17982 (18)	0.5469 (4)	0.0219 (7)
C10 $0.18522 (19)$ $0.20637 (19)$ $0.4066 (3)$ $0.0251 (7)$ H10 0.1695 0.1779 0.3000 0.030^* C11 $0.2317 (2)$ $0.27591 (19)$ $0.4260 (4)$ $0.0275 (7)$ H11 0.2471 0.2940 0.3321 0.033^* C12 $0.25501 (19)$ $0.31821 (19)$ $0.5843 (4)$ $0.0252 (7)$ H12 0.2853 0.3651 0.5956 0.030^* C13 $0.23333 (17)$ $0.29096 (18)$ $0.7281 (3)$ $0.0190 (6)$ C14 $0.25474 (18)$ $0.34128 (17)$ $0.8950 (3)$ $0.0204 (6)$ C15 $0.1978 (2)$ $0.3916 (18)$ $0.9223 (4)$ $0.0270 (7)$ H15 0.1475 $0.3901 (0.18)$ 0.8428 0.032^* C16 $0.2152 (2)$ $0.4441 (2)$ $1.0670 (4)$ $0.0307 (8)$ H16 0.1763 0.4766 1.0847 0.037^* C17 $0.2897 (2)$ $0.44812 (19)$ $1.1841 (4)$ $0.0290 (8)$ H17 0.3015 0.4837 1.2800 0.035^* C18 $0.34668 (19)$ $0.39879 (18)$ $1.1576 (4)$ $0.0244 (7)$ H18 0.3972 0.4021 1.2355 0.029^* C19 $0.32979 (19)$ $0.34399 (18)$ $1.0156 (3)$ $0.0210 (7)$ C21 $0.42452 (18)$ $0.15199 (18)$ $0.9115 (3)$ $0.0210 (7)$ C22 $0.5013 (2)$ $0.1627 (2)$ $0.9232 (4)$ $0.0317 (8)$ H22 0.5276 0.2099 0.9756 0.038^* C23<	Н9	0.1304	0.1342	0.5336	0.026*
H10 0.1695 0.1779 0.3000 0.030^{*} C11 $0.2317 (2)$ $0.27591 (19)$ $0.4260 (4)$ $0.0275 (7)$ H11 0.2471 0.2940 0.3321 0.033^{*} C12 $0.25501 (19)$ $0.31821 (19)$ $0.5843 (4)$ $0.0252 (7)$ H12 0.2853 0.3651 0.5956 0.030^{*} C13 $0.23333 (17)$ $0.29096 (18)$ $0.7281 (3)$ $0.0190 (6)$ C14 $0.25474 (18)$ $0.34128 (17)$ $0.8950 (3)$ $0.0204 (6)$ C15 $0.1978 (2)$ $0.39160 (18)$ $0.9223 (4)$ 0.037^{*} C16 $0.2152 (2)$ $0.4441 (2)$ $1.0670 (4)$ $0.0307 (8)$ H16 0.1763 0.4766 1.0847 0.037^{*} C17 $0.2897 (2)$ $0.44481 (19)$ $1.1841 (4)$ $0.0290 (8)$ H17 0.3015 0.4837 1.2800 0.035^{*} C18 $0.34668 (19)$ $0.39879 (18)$ $1.1576 (4)$ $0.0214 (7)$ H18 0.3972 0.4021 1.2355 0.029^{*} C19 $0.32979 (19)$ $0.34399 (18)$ $1.0156 (3)$ $0.0211 (6)$ C20 $0.39544 (18)$ $0.29130 (17)$ $1.0011 (3)$ $0.0210 (7)$ C21 $0.44452 (18)$ $0.15199 (18)$ $0.9115 (3)$ $0.0212 (7)$ C22 $0.5013 (2)$ $0.1627 (2)$ $0.9232 (4)$ $0.0317 (8)$ H22 0.5918 0.1111 0.8674 0.049^{*} C23 $0.5398 (2)$ $0.0252 (2)$ $0.7773 (4)$ $0.0334 (8)$	C10	0.18522 (19)	0.20637 (19)	0.4066 (3)	0.0251 (7)
C11 0.2317 (2) 0.27591 (19) 0.4260 (4) 0.0275 (7)H11 0.2471 0.2940 0.3321 $0.033*$ C12 0.25501 (19) 0.31821 (19) 0.5843 (4) 0.0252 (7)H12 0.2853 0.3651 0.5956 $0.030*$ C13 0.23333 (17) 0.29096 (18) 0.7281 (3) 0.0190 (6)C14 0.25474 (18) 0.34128 (17) 0.8950 (3) 0.0204 (6)C15 0.1978 (2) 0.39160 (18) 0.9223 (4) 0.0270 (7)H15 0.1475 0.3901 0.8428 $0.032*$ C16 0.2152 (2) 0.4441 (2) 1.0670 (4) $0.037*$ C17 0.2897 (2) 0.44812 (19) 1.1841 (4) 0.0290 (8)H17 0.3015 0.4837 1.2800 $0.035*$ C18 0.34668 (19) 0.39879 (18) 1.1576 (4) 0.0214 (7)H18 0.3972 0.4021 1.2355 $0.029*$ C19 0.32979 (19) 0.34399 (18) 1.0156 (3) 0.0211 (6)C20 0.39544 (18) 0.29130 (17) 1.0011 (3) 0.0212 (7)C21 0.44452 (18) 0.15199 (18) 0.9115 (3) 0.0212 (7)C22 0.5013 (2) 0.1627 (2) 0.8573 (5) 0.0407 (9)H22 0.5276 0.2099 0.9756 $0.038*$ C23 0.5398 (2) 0.1035 (2) 0.8573 (5) 0.4047 (9)H23 0.5918 0.1111 0.8674 0.4047 (8)H24 <td>H10</td> <td>0.1695</td> <td>0.1779</td> <td>0.3000</td> <td>0.030*</td>	H10	0.1695	0.1779	0.3000	0.030*
H11 0.2471 0.2940 0.3321 $0.033*$ C12 $0.25501 (19)$ $0.31821 (19)$ $0.5843 (4)$ $0.0252 (7)$ H12 0.2853 0.3651 0.5956 $0.030*$ C13 $0.23333 (17)$ $0.29096 (18)$ $0.7281 (3)$ $0.0190 (6)$ C14 $0.25474 (18)$ $0.34128 (17)$ $0.8950 (3)$ $0.0204 (6)$ C15 $0.1978 (2)$ $0.39160 (18)$ $0.9223 (4)$ $0.0270 (7)$ H15 0.1475 0.3901 0.8428 $0.032*$ C16 $0.2152 (2)$ $0.4441 (2)$ $1.0670 (4)$ $0.0307 (8)$ H16 0.1763 0.4766 1.0847 $0.037*$ C17 $0.2897 (2)$ $0.44812 (19)$ $1.1841 (4)$ $0.0290 (8)$ H17 0.3015 0.4837 1.2800 $0.035*$ C18 $0.34668 (19)$ $0.39879 (18)$ $1.1576 (4)$ $0.0244 (7)$ H18 0.3972 0.4021 1.2355 $0.029*$ C19 $0.32979 (19)$ $0.34399 (18)$ $1.0156 (3)$ $0.0211 (6)$ C20 $0.39544 (18)$ $0.29130 (17)$ $1.0011 (3)$ $0.0210 (7)$ C12 $0.42452 (18)$ $0.15199 (17)$ $0.0317 (8)$ H22 0.5276 0.2099 0.9756 $0.038*$ C23 $0.5398 (2)$ $0.1035 (2)$ $0.8573 (5)$ $0.0407 (9)$ H23 0.5918 0.1111 0.8674 $0.049*$ C24 0.5271 -0.0048 $0.7730 (4)$ $0.0354 (8)$ H24 0.5271 -0.0048 0.787	C11	0.2317 (2)	0.27591 (19)	0.4260 (4)	0.0275 (7)
C12 $0.25501(19)$ $0.31821(19)$ $0.5843(4)$ $0.0252(7)$ H12 0.2853 0.3651 0.5956 $0.030*$ C13 $0.2333(17)$ $0.29096(18)$ $0.7281(3)$ $0.0190(6)$ C14 $0.25474(18)$ $0.34128(17)$ $0.8950(3)$ $0.0204(6)$ C15 $0.1978(2)$ $0.39160(18)$ $0.9223(4)$ $0.0270(7)$ H15 0.1475 0.3901 0.8428 $0.032*$ C16 $0.2152(2)$ $0.4441(2)$ $1.0670(4)$ $0.0307(8)$ H16 0.1763 0.4766 1.0847 $0.037*$ C17 $0.2897(2)$ $0.44812(19)$ $1.1841(4)$ $0.0290(8)$ H17 0.3015 0.4837 1.2800 $0.035*$ C18 $0.34668(19)$ $0.39879(18)$ $1.1576(4)$ $0.0214(7)$ H18 0.3972 0.4021 1.2355 $0.029*$ C19 $0.32979(19)$ $0.34399(18)$ $1.0156(3)$ $0.211(6)$ C20 $0.39544(18)$ $0.29130(17)$ $1.0011(3)$ $0.2010(7)$ C12 $0.42452(18)$ $0.15199(18)$ $0.9115(3)$ $0.0212(7)$ C21 $0.42452(18)$ $0.15199(18)$ $0.915(3)$ $0.0217(8)$ H22 0.5276 0.2099 0.9756 $0.038*$ C23 0.5918 0.1111 0.8674 $0.494*$ C24 $0.5015(2)$ $0.0318(2)$ $0.7773(4)$ $0.0354(8)$ H24 0.5271 -0.0048 0.7305 $0.424*$ C25 $0.4250(2)$ $0.0217(2)$ $0.7829(5)$ <td< td=""><td>H11</td><td>0.2471</td><td>0.2940</td><td>0.3321</td><td>0.033*</td></td<>	H11	0.2471	0.2940	0.3321	0.033*
H12 0.2853 0.3651 0.5956 0.030^* C13 $0.23333 (17)$ $0.29096 (18)$ $0.7281 (3)$ $0.0190 (6)$ C14 $0.25474 (18)$ $0.34128 (17)$ $0.8950 (3)$ $0.0204 (6)$ C15 $0.1978 (2)$ $0.39160 (18)$ $0.9223 (4)$ $0.0270 (7)$ H15 0.1475 0.3901 0.8428 0.032^* C16 $0.2152 (2)$ $0.4441 (2)$ $1.0670 (4)$ $0.0307 (8)$ H16 0.1763 0.4766 1.0847 0.037^* C17 $0.2897 (2)$ $0.4481 (219)$ $1.1841 (4)$ $0.0290 (8)$ H17 0.3015 0.4837 1.2800 0.035^* C18 $0.34668 (19)$ $0.39879 (18)$ $1.1576 (4)$ $0.0244 (7)$ H18 0.3972 0.4021 1.2355 0.029^* C19 $0.32979 (19)$ $0.34399 (18)$ $1.0156 (3)$ $0.0211 (6)$ C20 $0.39544 (18)$ $0.29130 (17)$ $1.0011 (3)$ $0.0210 (7)$ C21 $0.42452 (18)$ $0.15199 (18)$ $0.9115 (3)$ $0.0212 (7)$ C22 $0.5013 (2)$ $0.1627 (2)$ $0.9232 (4)$ $0.0317 (8)$ H22 0.5276 0.2099 0.9756 0.038^* C23 0.5918 0.1111 0.8674 0.049^* C24 $0.5015 (2)$ $0.0338 (2)$ $0.7773 (4)$ $0.0354 (8)$ H24 0.5271 -0.0048 0.7305 0.042^* C25 $0.4250 (2)$ $0.0217 (2)$ $0.7669 (4)$ $0.0225 (7)$ C28 $0.2734 $	C12	0.25501 (19)	0.31821 (19)	0.5843 (4)	0.0252 (7)
C13 $0.23333 (17)$ $0.29096 (18)$ $0.7281 (3)$ $0.0190 (6)$ C14 $0.25474 (18)$ $0.34128 (17)$ $0.8950 (3)$ $0.0204 (6)$ C15 $0.1978 (2)$ $0.39160 (18)$ $0.9223 (4)$ $0.0270 (7)$ H15 0.1475 0.3901 0.8428 $0.032*$ C16 $0.2152 (2)$ $0.4441 (2)$ $1.0670 (4)$ $0.0307 (8)$ H16 0.1763 0.4766 1.0847 $0.037*$ C17 $0.2897 (2)$ $0.44812 (19)$ $1.1841 (4)$ $0.0290 (8)$ H17 0.3015 0.4837 1.2800 $0.035*$ C18 $0.34668 (19)$ $0.39879 (18)$ $1.1576 (4)$ $0.0244 (7)$ H18 0.3972 0.4021 1.2355 $0.029*$ C19 $0.32979 (19)$ $0.34399 (18)$ $1.0156 (3)$ $0.0211 (6)$ C20 $0.39544 (18)$ $0.29130 (17)$ $1.0011 (3)$ $0.0210 (7)$ C21 $0.42452 (18)$ $0.15199 (18)$ $0.9115 (3)$ $0.0212 (7)$ C22 $0.5013 (2)$ $0.1627 (2)$ $0.9232 (4)$ $0.0317 (8)$ H22 0.5276 0.2099 0.9756 $0.038*$ C23 0.5918 0.1111 0.8674 $0.049*$ C24 $0.5015 (2)$ $0.0217 (2)$ $0.7669 (4)$ $0.0225 (8)$ H24 0.5271 -0.0048 0.7305 $0.442*$ C25 $0.4250 (2)$ $0.0217 (2)$ $0.7669 (4)$ $0.0225 (7)$ C26 $0.38714 (18)$ $0.07931 (18)$ $0.8372 (3)$ $0.0225 (7)$ C26	H12	0.2853	0.3651	0.5956	0.030*
C14 0.25474 (18) 0.34128 (17) 0.8950 (3) 0.0204 (6)C15 0.1978 (2) 0.39160 (18) 0.9223 (4) 0.0270 (7)H15 0.1475 0.3901 0.8428 0.032^* C16 0.2152 (2) 0.4441 (2) 1.0670 (4) 0.0307 (8)H16 0.1763 0.4766 1.0847 0.037^* C17 0.2897 (2) 0.44812 (19) 1.1841 (4) 0.0290 (8)H17 0.3015 0.4837 1.2800 0.035^* C18 0.34668 (19) 0.39879 (18) 1.1576 (4) 0.0244 (7)H18 0.3972 0.4021 1.2355 0.029^* C19 0.32979 (19) 0.34399 (18) 1.0156 (3) 0.0211 (6)C20 0.39544 (18) 0.29130 (17) 1.0011 (3) 0.0210 (7)C21 0.42452 (18) 0.15199 (18) 0.9115 (3) 0.0212 (7)C22 0.5013 (2) 0.1627 (2) 0.9232 (4) 0.0317 (8)H22 0.5276 0.2099 0.9756 0.038^* C23 0.5398 (2) 0.1035 (2) 0.8573 (5) 0.0407 (9)H23 0.5918 0.1111 0.8674 0.049^* C24 0.5015 (2) 0.0217 (2) 0.7669 (4) 0.0275 (8)H24 0.5271 -0.0048 0.7305 $0.042*$ C25 0.4250 (2) 0.0217 (2) 0.7669 (4) 0.0225 (7)C28 0.2734 (2) -0.0051 (2) 0.7829 (5) 0.03366 (9)H25	C13	0.23333 (17)	0.29096 (18)	0.7281 (3)	0.0190 (6)
C15 0.1978 (2) 0.39160 (18) 0.9223 (4) 0.0270 (7)H15 0.1475 0.3901 0.8428 $0.032*$ C16 0.2152 (2) 0.4441 (2) 1.0670 (4) 0.0307 (8)H16 0.1763 0.4766 1.0847 $0.037*$ C17 0.2897 (2) 0.44812 (19) 1.1841 (4) 0.0290 (8)H17 0.3015 0.4837 1.2800 $0.035*$ C18 0.34668 (19) 0.39879 (18) 1.1576 (4) 0.0244 (7)H18 0.3972 0.4021 1.2355 $0.029*$ C19 0.32979 (19) 0.34399 (18) 1.0156 (3) 0.0211 (6)C20 0.39544 (18) 0.29130 (17) 1.0011 (3) 0.0210 (7)C21 0.42452 (18) 0.15199 (18) 0.9115 (3) 0.0212 (7)C22 0.5013 (2) 0.1627 (2) 0.9232 (4) 0.0317 (8)H22 0.5276 0.2099 0.9756 $0.038*$ C23 0.5398 (2) 0.1035 (2) 0.8573 (5) 0.0407 (9)H23 0.5918 0.1111 0.8674 $0.049*$ C24 0.5015 (2) 0.0338 (2) 0.773 (4) 0.0354 (8)H24 0.5271 -0.0048 0.7305 $0.042*$ C25 0.4250 (2) 0.0217 (2) 0.7829 (5) 0.0366 (9)H28 0.2714 (18) 0.07931 (18) 0.8372 (3) 0.0225 (7)C28 0.2734 (2) -0.0051 (2) 0.7829 (5) 0.0366 (9)H28B 0.2	C14	0.25474 (18)	0.34128 (17)	0.8950 (3)	0.0204 (6)
H15 0.1475 0.3901 0.8428 0.032^* C16 $0.2152 (2)$ $0.4441 (2)$ $1.0670 (4)$ $0.0307 (8)$ H16 0.1763 0.4766 1.0847 0.037^* C17 $0.2897 (2)$ $0.44812 (19)$ $1.1841 (4)$ $0.0290 (8)$ H17 0.3015 0.4837 1.2800 0.035^* C18 $0.34668 (19)$ $0.39879 (18)$ $1.1576 (4)$ $0.0244 (7)$ H18 0.3972 0.4021 1.2355 0.029^* C19 $0.32979 (19)$ $0.34399 (18)$ $1.0156 (3)$ $0.0211 (6)$ C20 $0.39544 (18)$ $0.29130 (17)$ $1.0011 (3)$ $0.0210 (7)$ C21 $0.42452 (18)$ $0.15199 (18)$ $0.9115 (3)$ $0.0212 (7)$ C22 $0.5013 (2)$ $0.1627 (2)$ $0.9232 (4)$ $0.0317 (8)$ H22 0.5276 0.2099 0.9756 0.038^* C23 0.5918 0.1111 0.8674 0.049^* C24 $0.5015 (2)$ $0.0217 (2)$ $0.7669 (4)$ $0.0275 (8)$ H24 0.5271 -0.0048 0.7305 0.042^* C25 $0.4250 (2)$ $0.0217 (2)$ $0.7669 (4)$ $0.0225 (7)$ C28 $0.2734 (2)$ $-0.0051 (2)$ $0.7829 (5)$ $0.0366 (9)$ H28A 0.2719 -0.0168 0.6642 0.055^* H28B 0.2214 -0.0019 0.7873 0.055^* H28B 0.2214 -0.0019 0.7873 0.055^* H27C -0.0684 0.3234 1.05	C15	0.1978 (2)	0.39160 (18)	0.9223 (4)	0.0270 (7)
C16 $0.2152 (2)$ $0.4441 (2)$ $1.0670 (4)$ $0.0307 (8)$ H16 0.1763 0.4766 1.0847 $0.037*$ C17 $0.2897 (2)$ $0.44812 (19)$ $1.1841 (4)$ $0.0290 (8)$ H17 0.3015 0.4837 1.2800 $0.035*$ C18 $0.34668 (19)$ $0.39879 (18)$ $1.1576 (4)$ $0.0244 (7)$ H18 0.3972 0.4021 1.2355 $0.029*$ C19 $0.32979 (19)$ $0.34399 (18)$ $1.0156 (3)$ $0.211 (6)$ C20 $0.39544 (18)$ $0.29130 (17)$ $1.0011 (3)$ $0.0210 (7)$ C21 $0.42452 (18)$ $0.15199 (18)$ $0.9115 (3)$ $0.0212 (7)$ C22 $0.5013 (2)$ $0.1627 (2)$ $0.9232 (4)$ $0.0317 (8)$ H22 0.5276 0.2099 0.9756 $0.038*$ C23 $0.5398 (2)$ $0.1035 (2)$ $0.8573 (5)$ $0.0407 (9)$ H23 0.5918 0.1111 0.8674 $0.049*$ C24 $0.5015 (2)$ $0.0217 (2)$ $0.7669 (4)$ $0.0275 (8)$ H24 0.5271 -0.0048 0.7305 $0.042*$ C25 $0.4250 (2)$ $0.0217 (2)$ $0.7669 (4)$ $0.0225 (7)$ C28 $0.2734 (2)$ $-0.0051 (2)$ $0.7829 (5)$ $0.0366 (9)$ H28A 0.2719 -0.0168 0.6642 $0.055*$ H28B 0.2214 -0.019 0.7873 $0.055*$ H28B 0.2214 -0.0168 0.8601 $0.055*$ H27A -0.1234 0.2746	H15	0.1475	0.3901	0.8428	0.032*
H16 0.1763 0.4766 1.0847 0.037^* C17 $0.2897 (2)$ $0.44812 (19)$ $1.1841 (4)$ $0.0290 (8)$ H17 0.3015 0.4837 1.2800 0.035^* C18 $0.34668 (19)$ $0.39879 (18)$ $1.1576 (4)$ $0.0244 (7)$ H18 0.3972 0.4021 1.2355 0.029^* C19 $0.32979 (19)$ $0.34399 (18)$ $1.0156 (3)$ $0.0211 (6)$ C20 $0.39544 (18)$ $0.29130 (17)$ $1.0011 (3)$ $0.0210 (7)$ C21 $0.42452 (18)$ $0.15199 (18)$ $0.9115 (3)$ $0.0212 (7)$ C22 $0.5013 (2)$ $0.1627 (2)$ $0.9232 (4)$ $0.0317 (8)$ H22 0.5276 0.2099 0.9756 0.038^* C23 $0.5398 (2)$ $0.1035 (2)$ $0.8573 (5)$ $0.0407 (9)$ H23 0.5918 0.1111 0.8674 0.049^* C24 $0.5015 (2)$ $0.0217 (2)$ $0.7669 (4)$ $0.0275 (8)$ H24 0.5271 -0.0048 0.7305 0.042^* C25 $0.4250 (2)$ $0.0217 (2)$ $0.7669 (4)$ $0.0275 (8)$ H25 0.3988 -0.0252 0.7127 0.033^* C26 $0.38714 (18)$ $0.07931 (18)$ $0.8372 (3)$ $0.0225 (7)$ C28 $0.2734 (2)$ $-0.0051 (2)$ 0.7873 0.055^* H28B 0.2214 -0.0019 0.7873 0.055^* H28B 0.2214 -0.0019 0.7873 0.055^* H27C $-0.0779 (3)$ 0.3085	C16	0.2152 (2)	0.4441 (2)	1.0670 (4)	0.0307 (8)
C17 $0.2897(2)$ $0.44812(19)$ $1.1841(4)$ $0.0290(8)$ H17 0.3015 0.4837 1.2800 $0.035*$ C18 $0.34668(19)$ $0.39879(18)$ $1.1576(4)$ $0.0244(7)$ H18 0.3972 0.4021 1.2355 $0.029*$ C19 $0.32979(19)$ $0.34399(18)$ $1.0156(3)$ $0.0211(6)$ C20 $0.39544(18)$ $0.29130(17)$ $1.0011(3)$ $0.0210(7)$ C21 $0.42452(18)$ $0.15199(18)$ $0.9115(3)$ $0.0212(7)$ C22 $0.5013(2)$ $0.1627(2)$ $0.9232(4)$ $0.0317(8)$ H22 0.5276 0.2099 0.9756 $0.038*$ C23 $0.5398(2)$ $0.1035(2)$ $0.8573(5)$ $0.0407(9)$ H23 0.5918 0.1111 0.8674 $0.049*$ C24 $0.5015(2)$ $0.0217(2)$ $0.7669(4)$ $0.0275(8)$ H24 0.5271 -0.0048 0.7305 $0.042*$ C25 $0.4250(2)$ $0.0217(2)$ $0.7669(4)$ $0.0275(8)$ H25 0.3988 -0.0252 0.7127 $0.033*$ C26 $0.38714(18)$ $0.07931(18)$ $0.8372(3)$ $0.0225(7)$ C28 $0.2734(2)$ $-0.0051(2)$ 0.7873 $0.055*$ H28B 0.2214 -0.0019 0.7873 $0.055*$ H28B 0.2214 -0.0019 0.7873 $0.055*$ H27A -0.1234 0.2746 0.8892 $0.069*$ H27B -0.0856 0.3371 0.8578 $0.069*$ <	H16	0.1763	0.4766	1.0847	0.037*
H17 0.3015 0.4837 1.2800 0.035^* C18 $0.34668 (19)$ $0.39879 (18)$ $1.1576 (4)$ $0.0244 (7)$ H18 0.3972 0.4021 1.2355 0.029^* C19 $0.32979 (19)$ $0.34399 (18)$ $1.0156 (3)$ $0.0211 (6)$ C20 $0.39544 (18)$ $0.29130 (17)$ $1.0011 (3)$ $0.0210 (7)$ C21 $0.42452 (18)$ $0.15199 (18)$ $0.9115 (3)$ $0.0212 (7)$ C22 $0.5013 (2)$ $0.1627 (2)$ $0.9232 (4)$ $0.0317 (8)$ H22 0.5276 0.2099 0.9756 0.038^* C23 $0.5398 (2)$ $0.1035 (2)$ $0.8573 (5)$ $0.0407 (9)$ H23 0.5918 0.1111 0.8674 0.049^* C24 $0.5015 (2)$ $0.0217 (2)$ $0.7773 (4)$ $0.0354 (8)$ H24 0.5271 -0.0048 0.7305 0.042^* C25 $0.4250 (2)$ $0.0217 (2)$ $0.7669 (4)$ $0.0275 (8)$ H25 0.3988 -0.0252 0.7127 0.033^* C26 $0.38714 (18)$ $0.07931 (18)$ $0.8372 (3)$ $0.0225 (7)$ C28 $0.2734 (2)$ -0.0019 0.7873 0.055^* H28B 0.2214 -0.0019 0.7873 0.055^* H28B 0.2214 -0.0019 0.7873 0.055^* H28B 0.2214 -0.0480 0.8601 0.055^* H27A -0.1234 0.2746 0.8892 0.069^* H27B -0.0856 0.3571 0.8578 <td>C17</td> <td>0.2897 (2)</td> <td>0.44812 (19)</td> <td>1.1841 (4)</td> <td>0.0290 (8)</td>	C17	0.2897 (2)	0.44812 (19)	1.1841 (4)	0.0290 (8)
C18 $0.34668 (19)$ $0.39879 (18)$ $1.1576 (4)$ $0.0244 (7)$ H18 0.3972 0.4021 1.2355 $0.029*$ C19 $0.32979 (19)$ $0.34399 (18)$ $1.0156 (3)$ $0.0211 (6)$ C20 $0.39544 (18)$ $0.29130 (17)$ $1.0011 (3)$ $0.0210 (7)$ C21 $0.42452 (18)$ $0.15199 (18)$ $0.9115 (3)$ $0.0212 (7)$ C22 $0.5013 (2)$ $0.1627 (2)$ $0.9232 (4)$ $0.0317 (8)$ H22 0.5276 0.2099 0.9756 $0.038*$ C23 $0.5398 (2)$ $0.1035 (2)$ $0.8573 (5)$ $0.0407 (9)$ H23 0.5918 0.1111 0.8674 $0.049*$ C24 $0.5015 (2)$ $0.0338 (2)$ $0.7773 (4)$ $0.0354 (8)$ H24 0.5271 -0.0048 0.7305 $0.042*$ C25 $0.4250 (2)$ $0.0217 (2)$ $0.7669 (4)$ $0.0275 (8)$ H25 0.3988 -0.0252 0.7127 $0.033*$ C26 $0.38714 (18)$ $0.07931 (18)$ $0.8372 (3)$ $0.0225 (7)$ C28 $0.2734 (2)$ $-0.0051 (2)$ $0.7829 (5)$ $0.0366 (9)$ H28A 0.2719 -0.0168 0.6642 $0.055*$ H28B 0.2214 -0.0019 0.7873 $0.055*$ H28B 0.2214 -0.0019 0.8601 $0.055*$ H27A -0.1234 0.2746 0.8892 $0.069*$ H27B -0.0856 0.3571 0.8578 $0.069*$	H17	0.3015	0.4837	1.2800	0.035*
H18 0.3972 0.4021 1.2355 0.029^* C19 $0.32979(19)$ $0.34399(18)$ $1.0156(3)$ $0.0211(6)$ C20 $0.39544(18)$ $0.29130(17)$ $1.0011(3)$ $0.0210(7)$ C21 $0.42452(18)$ $0.15199(18)$ $0.9115(3)$ $0.0212(7)$ C22 $0.5013(2)$ $0.1627(2)$ $0.9232(4)$ $0.0317(8)$ H22 0.5276 0.2099 0.9756 0.038^* C23 $0.5398(2)$ $0.1035(2)$ $0.8573(5)$ $0.0407(9)$ H23 0.5918 0.1111 0.8674 0.049^* C24 $0.5015(2)$ $0.0338(2)$ $0.7773(4)$ $0.0354(8)$ H24 0.5271 -0.0048 0.7305 0.042^* C25 $0.4250(2)$ $0.0217(2)$ $0.7669(4)$ $0.0275(8)$ H25 0.3988 -0.0252 0.7127 0.033^* C26 $0.38714(18)$ $0.07931(18)$ $0.8372(3)$ $0.0225(7)$ C28 $0.2734(2)$ $-0.0051(2)$ $0.7829(5)$ $0.0366(9)$ H28A 0.2719 -0.0168 0.6642 0.055^* H28B 0.2214 -0.0019 0.7873 0.055^* H28B 0.2214 0.2746 0.8892 0.069^* H27A -0.1234 0.2746 0.8878 0.069^* H27B -0.0856 0.3571 0.8578 0.069^*	C18	0.34668 (19)	0.39879 (18)	1.1576 (4)	0.0244 (7)
C19 $0.32979(19)$ $0.34399(18)$ $1.0156(3)$ $0.0211(6)$ C20 $0.39544(18)$ $0.29130(17)$ $1.0011(3)$ $0.0210(7)$ C21 $0.42452(18)$ $0.15199(18)$ $0.9115(3)$ $0.0212(7)$ C22 $0.5013(2)$ $0.1627(2)$ $0.9232(4)$ $0.0317(8)$ H22 0.5276 0.2099 0.9756 $0.038*$ C23 $0.5398(2)$ $0.1035(2)$ $0.8573(5)$ $0.0407(9)$ H23 0.5918 0.1111 0.8674 $0.049*$ C24 $0.5015(2)$ $0.0338(2)$ $0.7773(4)$ $0.0354(8)$ H24 0.5271 -0.0048 0.7305 $0.042*$ C25 $0.4250(2)$ $0.0217(2)$ $0.7669(4)$ $0.0275(8)$ H25 0.3988 -0.0252 0.7127 $0.033*$ C26 $0.38714(18)$ $0.07931(18)$ $0.8372(3)$ $0.0225(7)$ C28 $0.2734(2)$ $-0.0051(2)$ 0.7873 $0.055*$ H28B 0.2214 -0.0019 0.7873 $0.055*$ H28B 0.2214 -0.0480 0.8601 $0.055*$ H27C $-0.079(3)$ $0.3085(2)$ $0.9290(5)$ $0.0448(10)$	H18	0.3972	0.4021	1.2355	0.029*
C20 0.39544 (18) 0.29130 (17) 1.0011 (3) 0.0210 (7)C21 0.42452 (18) 0.15199 (18) 0.9115 (3) 0.0212 (7)C22 0.5013 (2) 0.1627 (2) 0.9232 (4) 0.0317 (8)H22 0.5276 0.2099 0.9756 $0.038*$ C23 0.5398 (2) 0.1035 (2) 0.8573 (5) 0.0407 (9)H23 0.5918 0.1111 0.8674 $0.049*$ C24 0.5015 (2) 0.0338 (2) 0.7773 (4) 0.0354 (8)H24 0.5271 -0.0048 0.7305 $0.042*$ C25 0.4250 (2) 0.0217 (2) 0.7669 (4) 0.0275 (8)H25 0.3988 -0.0252 0.7127 $0.033*$ C26 0.38714 (18) 0.07931 (18) 0.8372 (3) 0.0225 (7)C28 0.2734 (2) -0.0051 (2) 0.7829 (5) 0.0366 (9)H28A 0.2719 -0.0168 0.6642 $0.055*$ H28B 0.2214 -0.0019 0.7873 $0.055*$ H28C 0.3011 -0.0480 0.8601 $0.055*$ H27A -0.1234 0.2746 0.8892 $0.069*$ H27B -0.0856 0.3571 0.8578 $0.069*$ H27C -0.0684 0.3234 1.0502 $0.069*$	C19	0.32979 (19)	0.34399 (18)	1.0156 (3)	0.0211 (6)
C21 $0.42452 (18)$ $0.15199 (18)$ $0.9115 (3)$ $0.0212 (7)$ C22 $0.5013 (2)$ $0.1627 (2)$ $0.9232 (4)$ $0.0317 (8)$ H22 0.5276 0.2099 0.9756 $0.038*$ C23 $0.5398 (2)$ $0.1035 (2)$ $0.8573 (5)$ $0.0407 (9)$ H23 0.5918 0.1111 0.8674 $0.049*$ C24 $0.5015 (2)$ $0.0338 (2)$ $0.7773 (4)$ $0.0354 (8)$ H24 0.5271 -0.0048 0.7305 $0.042*$ C25 $0.4250 (2)$ $0.217 (2)$ $0.7669 (4)$ $0.0275 (8)$ H25 0.3988 -0.0252 0.7127 $0.033*$ C26 $0.38714 (18)$ $0.07931 (18)$ $0.8372 (3)$ $0.0225 (7)$ C28 $0.2734 (2)$ $-0.0051 (2)$ $0.7829 (5)$ $0.0366 (9)$ H28A 0.2719 -0.0168 0.6642 $0.055*$ H28B 0.2214 -0.0019 0.7873 $0.055*$ H28C 0.3011 -0.0480 0.8601 $0.055*$ C27 $-0.0779 (3)$ $0.3085 (2)$ $0.9290 (5)$ $0.0458 (10)$ H27A -0.1234 0.2746 0.8892 $0.069*$ H27B -0.0856 0.3571 0.8578 $0.069*$	C20	0.39544 (18)	0.29130 (17)	1.0011 (3)	0.0210 (7)
C22 $0.5013 (2)$ $0.1627 (2)$ $0.9232 (4)$ $0.0317 (8)$ H22 0.5276 0.2099 0.9756 $0.038*$ C23 $0.5398 (2)$ $0.1035 (2)$ $0.8573 (5)$ $0.0407 (9)$ H23 0.5918 0.1111 0.8674 $0.049*$ C24 $0.5015 (2)$ $0.0338 (2)$ $0.7773 (4)$ $0.0354 (8)$ H24 0.5271 -0.0048 0.7305 $0.042*$ C25 $0.4250 (2)$ $0.0217 (2)$ $0.7669 (4)$ $0.0275 (8)$ H25 0.3988 -0.0252 0.7127 $0.033*$ C26 $0.38714 (18)$ $0.07931 (18)$ $0.8372 (3)$ $0.0225 (7)$ C28 $0.2734 (2)$ $-0.0051 (2)$ $0.7829 (5)$ $0.0366 (9)$ H28A 0.2719 -0.0168 0.6642 $0.055*$ H28B 0.2214 -0.0019 0.7873 $0.055*$ H28C 0.3011 -0.0480 0.8601 $0.055*$ C27 $-0.0779 (3)$ $0.3085 (2)$ $0.9290 (5)$ $0.04458 (10)$ H27A -0.1234 0.2746 0.8892 $0.069*$ H27B -0.0856 0.3571 0.8578 $0.069*$ H27C -0.0684 0.3234 1.0502 $0.069*$	C21	0.42452 (18)	0.15199 (18)	0.9115 (3)	0.0212 (7)
H220.52760.20990.97560.038*C230.5398 (2)0.1035 (2)0.8573 (5)0.0407 (9)H230.59180.11110.86740.049*C240.5015 (2)0.0338 (2)0.7773 (4)0.0354 (8)H240.5271-0.00480.73050.042*C250.4250 (2)0.0217 (2)0.7669 (4)0.0275 (8)H250.3988-0.02520.71270.033*C260.38714 (18)0.07931 (18)0.8372 (3)0.0225 (7)C280.2734 (2)-0.0051 (2)0.7829 (5)0.0366 (9)H28A0.2719-0.01680.66420.055*H28B0.2214-0.00190.78730.055*H28C0.3011-0.04800.86010.055*C27-0.0779 (3)0.3085 (2)0.9290 (5)0.0458 (10)H27A-0.12340.27460.88920.069*H27B-0.08560.35710.85780.069*H27C-0.06840.32341.05020.069*	C22	0.5013 (2)	0.1627 (2)	0.9232 (4)	0.0317 (8)
C23 $0.5398(2)$ $0.1035(2)$ $0.8573(5)$ $0.0407(9)$ H23 0.5918 0.1111 0.8674 $0.049*$ C24 $0.5015(2)$ $0.0338(2)$ $0.7773(4)$ $0.0354(8)$ H24 0.5271 -0.0048 0.7305 $0.042*$ C25 $0.4250(2)$ $0.0217(2)$ $0.7669(4)$ $0.0275(8)$ H25 0.3988 -0.0252 0.7127 $0.033*$ C26 $0.38714(18)$ $0.07931(18)$ $0.8372(3)$ $0.0225(7)$ C28 $0.2734(2)$ $-0.0051(2)$ $0.7829(5)$ $0.0366(9)$ H28A 0.2719 -0.0168 0.6642 $0.055*$ H28B 0.2214 -0.0019 0.7873 $0.055*$ H28C 0.3011 -0.0480 0.8601 $0.55*$ C27 $-0.0779(3)$ $0.3085(2)$ $0.9290(5)$ $0.0458(10)$ H27A -0.1234 0.2746 0.8892 $0.669*$ H27B -0.0856 0.3571 0.8578 $0.069*$	H22	0.5276	0.2099	0.9756	0.038*
H23 0.5918 0.1111 0.8674 0.049^* C24 $0.5015(2)$ $0.0338(2)$ $0.7773(4)$ $0.0354(8)$ H24 0.5271 -0.0048 0.7305 0.042^* C25 $0.4250(2)$ $0.0217(2)$ $0.7669(4)$ $0.0275(8)$ H25 0.3988 -0.0252 0.7127 0.033^* C26 $0.38714(18)$ $0.07931(18)$ $0.8372(3)$ $0.0225(7)$ C28 $0.2734(2)$ $-0.0051(2)$ $0.7829(5)$ $0.0366(9)$ H28A 0.2719 -0.0168 0.6642 0.055^* H28B 0.2214 -0.0019 0.7873 0.055^* H28C 0.3011 -0.0480 0.8601 0.055^* C27 $-0.0779(3)$ $0.3085(2)$ $0.9290(5)$ $0.0458(10)$ H27A -0.1234 0.2746 0.8892 0.069^* H27B -0.0856 0.3571 0.8578 0.069^*	C23	0.5398 (2)	0.1035 (2)	0.8573 (5)	0.0407 (9)
C24 $0.5015(2)$ $0.0338(2)$ $0.7773(4)$ $0.0354(8)$ H24 0.5271 -0.0048 0.7305 $0.042*$ C25 $0.4250(2)$ $0.0217(2)$ $0.7669(4)$ $0.0275(8)$ H25 0.3988 -0.0252 0.7127 $0.033*$ C26 $0.38714(18)$ $0.07931(18)$ $0.8372(3)$ $0.0225(7)$ C28 $0.2734(2)$ $-0.0051(2)$ $0.7829(5)$ $0.0366(9)$ H28A 0.2719 -0.0168 0.6642 $0.055*$ H28B 0.2214 -0.0019 0.7873 $0.055*$ H28C 0.3011 -0.0480 0.8601 $0.055*$ C27 $-0.0779(3)$ $0.3085(2)$ $0.9290(5)$ $0.0448(10)$ H27A -0.1234 0.2746 0.8892 $0.069*$ H27B -0.0856 0.3571 0.8578 $0.069*$ H27C -0.0684 0.3234 1.0502 $0.069*$	H23	0.5918	0.1111	0.8674	0.049*
H24 0.5271 -0.0048 0.7305 $0.042*$ C25 $0.4250(2)$ $0.0217(2)$ $0.7669(4)$ $0.0275(8)$ H25 0.3988 -0.0252 0.7127 $0.033*$ C26 $0.38714(18)$ $0.07931(18)$ $0.8372(3)$ $0.0225(7)$ C28 $0.2734(2)$ $-0.0051(2)$ $0.7829(5)$ $0.0366(9)$ H28A 0.2719 -0.0168 0.6642 $0.055*$ H28B 0.2214 -0.0019 0.7873 $0.055*$ H28C 0.3011 -0.0480 0.8601 $0.055*$ C27 $-0.0779(3)$ $0.3085(2)$ $0.9290(5)$ $0.0458(10)$ H27A -0.1234 0.2746 0.8892 $0.069*$ H27B -0.0856 0.3571 0.8578 $0.069*$	C24	0.5015 (2)	0.0338 (2)	0.7773 (4)	0.0354 (8)
C25 $0.4250(2)$ $0.0217(2)$ $0.7669(4)$ $0.0275(8)$ H25 0.3988 -0.0252 0.7127 0.033^* C26 $0.38714(18)$ $0.07931(18)$ $0.8372(3)$ $0.0225(7)$ C28 $0.2734(2)$ $-0.0051(2)$ $0.7829(5)$ $0.0366(9)$ H28A 0.2719 -0.0168 0.6642 0.055^* H28B 0.2214 -0.0019 0.7873 0.055^* H28C 0.3011 -0.0480 0.8601 0.055^* C27 $-0.0779(3)$ $0.3085(2)$ $0.9290(5)$ $0.0458(10)$ H27A -0.1234 0.2746 0.8892 0.069^* H27B -0.0856 0.3571 0.8578 0.069^*	H24	0.5271	-0.0048	0.7305	0.042*
H25 0.3988 -0.0252 0.7127 0.033^* C26 $0.38714 (18)$ $0.07931 (18)$ $0.8372 (3)$ $0.0225 (7)$ C28 $0.2734 (2)$ $-0.0051 (2)$ $0.7829 (5)$ $0.0366 (9)$ H28A 0.2719 -0.0168 0.6642 0.055^* H28B 0.2214 -0.0019 0.7873 0.055^* H28C 0.3011 -0.0480 0.8601 0.055^* C27 $-0.0779 (3)$ $0.3085 (2)$ $0.9290 (5)$ $0.0458 (10)$ H27A -0.1234 0.2746 0.8892 0.069^* H27B -0.0856 0.3571 0.8578 0.069^* H27C -0.0684 0.3234 1.0502 0.069^*	C25	0.4250 (2)	0.0217 (2)	0.7669 (4)	0.0275 (8)
C26 $0.38714(18)$ $0.07931(18)$ $0.8372(3)$ $0.0225(7)$ C28 $0.2734(2)$ $-0.0051(2)$ $0.7829(5)$ $0.0366(9)$ H28A 0.2719 -0.0168 0.6642 $0.055*$ H28B 0.2214 -0.0019 0.7873 $0.055*$ H28C 0.3011 -0.0480 0.8601 $0.055*$ C27 $-0.0779(3)$ $0.3085(2)$ $0.9290(5)$ $0.0458(10)$ H27A -0.1234 0.2746 0.8892 $0.069*$ H27B -0.0856 0.3571 0.8578 $0.069*$	H25	0.3988	-0.0252	0.7127	0.033*
C280.2734 (2)-0.0051 (2)0.7829 (5)0.0366 (9)H28A0.2719-0.01680.66420.055*H28B0.2214-0.00190.78730.055*H28C0.3011-0.04800.86010.055*C27-0.0779 (3)0.3085 (2)0.9290 (5)0.0458 (10)H27A-0.12340.27460.88920.069*H27B-0.08560.35710.85780.069*H27C-0.06840.32341.05020.069*	C26	0.38714 (18)	0.07931 (18)	0.8372 (3)	0.0225 (7)
H28A0.2719-0.01680.66420.055*H28B0.2214-0.00190.78730.055*H28C0.3011-0.04800.86010.055*C27-0.0779 (3)0.3085 (2)0.9290 (5)0.0458 (10)H27A-0.12340.27460.88920.069*H27B-0.08560.35710.85780.069*H27C-0.06840.32341.05020.069*	C28	0.2734 (2)	-0.0051 (2)	0.7829 (5)	0.0366 (9)
H28B0.2214-0.00190.78730.055*H28C0.3011-0.04800.86010.055*C27-0.0779 (3)0.3085 (2)0.9290 (5)0.0458 (10)H27A-0.12340.27460.88920.069*H27B-0.08560.35710.85780.069*H27C-0.06840.32341.05020.069*	H28A	0.2719	-0.0168	0.6642	0.055*
H28C0.3011-0.04800.86010.055*C27-0.0779 (3)0.3085 (2)0.9290 (5)0.0458 (10)H27A-0.12340.27460.88920.069*H27B-0.08560.35710.85780.069*H27C-0.06840.32341.05020.069*	H28B	0.2214	-0.0019	0.7873	0.055*
C27-0.0779 (3)0.3085 (2)0.9290 (5)0.0458 (10)H27A-0.12340.27460.88920.069*H27B-0.08560.35710.85780.069*H27C-0.06840.32341.05020.069*	H28C	0.3011	-0.0480	0.8601	0.055*
H27A-0.12340.27460.88920.069*H27B-0.08560.35710.85780.069*H27C-0.06840.32341.05020.069*	C27	-0.0779 (3)	0.3085 (2)	0.9290 (5)	0.0458 (10)
H27B-0.08560.35710.85780.069*H27C-0.06840.32341.05020.069*	H27A	-0.1234	0.2746	0.8892	0.069*
H27C -0.0684 0.3234 1.0502 0.069*	H27B	-0.0856	0.3571	0.8578	0.069*
	H27C	-0.0684	0.3234	1.0502	0.069*

Atomic displacement parameters $(Å^2)$

	U^{11}	U ²²	U ³³	U^{12}	U^{13}	U^{23}
01	0.0436 (16)	0.0284 (13)	0.0359 (11)	0.0087 (11)	0.0218 (11)	0.0078 (9)
02	0.0200 (12)	0.0303 (12)	0.0181 (10)	-0.0008 (9)	0.0038 (9)	0.0020 (8)

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O3	0.0182 (13)	0.0273 (12)	0.0252 (10)	-0.0060 (9)	0.0054 (10)	-0.0002 (8)
O4	0.0194 (12)	0.0223 (12)	0.0408 (11)	-0.0041 (9)	0.0104 (10)	-0.0049 (9)
N1	0.0164 (14)	0.0333 (15)	0.0163 (11)	-0.0017 (11)	0.0045 (11)	0.0036 (9)
N2	0.0172 (14)	0.0205 (14)	0.0279 (13)	0.0000 (10)	0.0084 (11)	-0.0017 (10)
C1	0.0267 (18)	0.0191 (15)	0.0228 (14)	-0.0017 (13)	0.0076 (13)	0.0001 (11)
C2	0.030 (2)	0.0306 (19)	0.0255 (14)	0.0003 (14)	0.0135 (15)	-0.0028 (12)
C3	0.039 (2)	0.0303 (19)	0.0251 (14)	-0.0089 (15)	0.0176 (16)	0.0009 (12)
C4	0.042 (2)	0.0234 (18)	0.0272 (16)	0.0002 (14)	0.0133 (16)	0.0033 (12)
C5	0.030 (2)	0.0248 (17)	0.0225 (14)	0.0023 (14)	0.0082 (14)	-0.0017 (12)
C6	0.0203 (17)	0.0250 (17)	0.0163 (12)	-0.0035 (12)	0.0042 (13)	-0.0008 (11)
C7	0.0183 (17)	0.0183 (15)	0.0201 (14)	0.0011 (12)	0.0066 (14)	-0.0023 (11)
C8	0.0134 (16)	0.0294 (18)	0.0170 (12)	0.0040 (12)	0.0045 (12)	0.0016 (11)
C9	0.0174 (17)	0.0245 (17)	0.0219 (14)	-0.0004 (13)	0.0036 (13)	-0.0011 (11)
C10	0.0213 (19)	0.0347 (18)	0.0182 (13)	0.0025 (14)	0.0050 (13)	-0.0018 (11)
C11	0.028 (2)	0.0348 (19)	0.0219 (14)	0.0019 (14)	0.0117 (14)	0.0081 (12)
C12	0.0236 (19)	0.0249 (17)	0.0278 (15)	-0.0002 (13)	0.0094 (14)	0.0035 (12)
C13	0.0123 (16)	0.0232 (16)	0.0209 (13)	0.0025 (11)	0.0045 (12)	0.0027 (11)
C14	0.0205 (17)	0.0175 (15)	0.0238 (14)	-0.0011 (12)	0.0079 (13)	0.0020 (11)
C15	0.0231 (18)	0.0254 (17)	0.0305 (15)	0.0006 (14)	0.0057 (14)	0.0010 (12)
C16	0.032 (2)	0.0278 (19)	0.0365 (17)	0.0041 (14)	0.0167 (17)	-0.0022 (13)
C17	0.037 (2)	0.0222 (17)	0.0277 (15)	-0.0017 (14)	0.0105 (15)	-0.0026 (12)
C18	0.0267 (19)	0.0206 (17)	0.0239 (14)	-0.0020 (13)	0.0054 (13)	-0.0010 (11)
C19	0.0221 (17)	0.0192 (16)	0.0234 (14)	0.0007 (12)	0.0091 (14)	0.0030 (11)
C20	0.0223 (19)	0.0250 (17)	0.0143 (13)	-0.0018 (13)	0.0041 (13)	0.0012 (10)
C21	0.0207 (18)	0.0212 (16)	0.0222 (14)	0.0009 (12)	0.0076 (14)	-0.0005 (11)
C22	0.0246 (19)	0.0289 (18)	0.0423 (17)	-0.0024 (14)	0.0118 (16)	-0.0068 (14)
C23	0.0207 (19)	0.042 (2)	0.063 (2)	-0.0016 (15)	0.0182 (18)	-0.0110 (17)
C24	0.034 (2)	0.029 (2)	0.0465 (19)	0.0069 (15)	0.0177 (17)	-0.0012 (14)
C25	0.031 (2)	0.0201 (17)	0.0321 (16)	-0.0004 (13)	0.0110 (15)	-0.0015 (12)
C26	0.0204 (19)	0.0219 (16)	0.0241 (14)	-0.0011 (12)	0.0059 (13)	0.0019 (11)
C28	0.033 (2)	0.031 (2)	0.0477 (19)	-0.0132 (15)	0.0152 (17)	-0.0088 (14)
C27	0.062 (3)	0.037 (2)	0.049 (2)	0.0233 (19)	0.032 (2)	0.0113 (16)

Geometric parameters (Å, °)

01—C1	1.364 (4)	C12—C13	1.403 (4)
O1—C27	1.431 (4)	C12—H12	0.9300
O2—C7	1.234 (3)	C13—C14	1.507 (4)
O3—C20	1.228 (4)	C14—C19	1.394 (4)
O4—C26	1.372 (4)	C14—C15	1.393 (4)
O4—C28	1.429 (4)	C15—C16	1.390 (4)
N1—C7	1.342 (4)	C15—H15	0.9300
N1—C6	1.425 (4)	C16—C17	1.377 (5)
N1—H1N	0.8600	C16—H16	0.9300
N2-C20	1.364 (4)	C17—C18	1.381 (5)
N2-C21	1.426 (4)	C17—H17	0.9300
N2—H2N	0.8600	C18—C19	1.398 (4)
C1—C6	1.385 (5)	C18—H18	0.9300

C1—C2	1.393 (4)	C19—C20	1.506 (4)
С2—С3	1.393 (5)	C21—C22	1.380 (5)
С2—Н2	0.9300	C21—C26	1.399 (4)
C3—C4	1.377 (5)	C22—C23	1.393 (5)
С3—Н3	0.9300	C22—H22	0.9300
C4—C5	1.383 (5)	C23—C24	1.377 (5)
C4—H4	0.9300	C23—H23	0.9300
С5—С6	1.381 (4)	C24—C25	1.381 (5)
С5—Н5	0.9300	C24—H24	0.9300
C7—C8	1.501 (4)	C25—C26	1.387 (4)
C8—C13	1.388 (4)	C25—H25	0.9300
C8—C9	1.397 (4)	C28—H28A	0.9600
C9-C10	1.397(1) 1.385(4)	C28—H28B	0.9600
С9—Н9	0.9300	C_{28} H28D	0.9600
C10-C11	1 392 (5)	C27—H27A	0.9600
C10 H10	0.0300	C27 H27B	0.9600
C11 $C12$	1.383(4)	$C_2 / - H_2 / B$	0.9600
	1.363 (4)	C27—H27C	0.9000
	0.9300		
C1 01 C27	11(0, (2))	C15 C14 C12	117.0(2)
C1 = 01 = C27	110.8(3)	C15 - C14 - C13	117.9(3)
$C_{20} - 04 - C_{28}$	118.1(2)	C16 - C15 - C14	120.8 (3)
C/-NI-C6	125.6 (2)	C16—C15—H15	119.6
C/—NI—HIN	117.2	C14—C15—H15	119.6
C6—NI—HIN	117.2	C17—C16—C15	120.3 (3)
C20—N2—C21	126.3 (3)	C17—C16—H16	119.9
C20—N2—H2N	116.9	C15—C16—H16	119.9
C21—N2—H2N	116.9	C16—C17—C18	119.3 (3)
01—C1—C6	115.6 (3)	C16—C17—H17	120.3
01—C1—C2	124.6 (3)	C18—C17—H17	120.3
C6—C1—C2	119.7 (3)	C17—C18—C19	121.2 (3)
C1—C2—C3	119.5 (3)	C17—C18—H18	119.4
C1—C2—H2	120.2	C19—C18—H18	119.4
С3—С2—Н2	120.2	C14—C19—C18	119.4 (3)
C4—C3—C2	120.3 (3)	C14—C19—C20	123.5 (3)
С4—С3—Н3	119.8	C18—C19—C20	117.1 (3)
С2—С3—Н3	119.8	O3—C20—N2	124.3 (3)
C3—C4—C5	120.0 (3)	O3—C20—C19	120.0 (3)
C3—C4—H4	120.0	N2—C20—C19	115.7 (3)
C5—C4—H4	120.0	C22—C21—C26	118.6 (3)
C6—C5—C4	120.2 (3)	C22—C21—N2	125.3 (3)
С6—С5—Н5	119.9	C26—C21—N2	116.1 (3)
С4—С5—Н5	119.9	C21—C22—C23	120.5 (3)
C5—C6—C1	120.3 (3)	C21—C22—H22	119.7
C5-C6-N1	120.8 (3)	C23—C22—H22	119.7
C1-C6-N1	118.9 (3)	C_{24} C_{23} C_{22}	120.5 (3)
02-C7-N1	124 1 (3)	C24—C23—H23	1197
02-C7-C8	121.3 (3)	C22—C23—H23	119 7
N1	114.6 (2)	C_{23} C_{24} C_{25}	119.6 (3)
	····· (-)		

C13—C8—C9	120.3 (3)	C23—C24—H24	120.2
C13—C8—C7	119.4 (2)	C25—C24—H24	120.2
C9—C8—C7	120.3 (3)	C24—C25—C26	120.1 (3)
C10—C9—C8	120.4 (3)	C24—C25—H25	120.0
С10—С9—Н9	119.8	C26—C25—H25	120.0
С8—С9—Н9	119.8	O4—C26—C25	124.3 (3)
C9—C10—C11	119.6 (3)	O4—C26—C21	115.1 (3)
C9—C10—H10	120.2	C25—C26—C21	120.6 (3)
C11—C10—H10	120.2	O4—C28—H28A	109.5
C12-C11-C10	120.2 (3)	04—C28—H28B	109.5
C12—C11—H11	119.9	H28A-C28-H28B	109.5
C10-C11-H11	119.9	04-C28-H28C	109.5
C_{11} C_{12} C_{13}	120.6 (3)	$H_{28} = C_{28} = H_{28} C_{28}$	109.5
$C_{11} = C_{12} = C_{13}$	110 7	$H_{28B} = C_{28} = H_{28C}$	109.5
$C_{12} = C_{12} = H_{12}$	110.7	01 C27 H27A	109.5
$C_{13}^{$	119.7	01 - 027 + 127R	109.5
$C_{8} = C_{13} = C_{14}$	119.0(3)	$U_{-}U_{2}$ $U_{-}H_{2}$ H_{2} $H_$	109.5
$C_{0} = C_{10} = C_{14}$	121.3(2) 110.6(2)	$H_2/A = C_2/=H_2/B$	109.5
C12 - C13 - C14	119.0 (3)	$U_{-}U_{2}$	109.5
C19 - C14 - C13	118.9 (3)	$H_2/A = C_2/=H_2/C$	109.5
C19 - C14 - C13	123.0 (3)	$H_2/B - C_2/-H_2/C$	109.5
C27 01 C1 C(1(0, 2, (2))	C9 C12 C14 C15	75.2(4)
$C_2 = 01 = C_1 = C_0$	109.2(3)	$C_{0} - C_{13} - C_{14} - C_{15}$	-73.3(4)
$C_2 = 0 = C_1 = C_2$	-8.3(4)	C12 - C13 - C14 - C15	99.9 (3)
01 - 01 - 02 - 03	1/7.3(3)	C19 - C14 - C15 - C16	0.3 (4)
C_{6} C_{1} C_{2} C_{3}	-0.2(4)	C13 - C14 - C15 - C16	-1/5.3(3)
C1—C2—C3—C4	-0.4 (5)	C14—C15—C16—C17	1.2 (5)
C2—C3—C4—C5	1.8 (5)	C15—C16—C17—C18	-0.8 (5)
C3—C4—C5—C6	-2.5 (4)	C16—C17—C18—C19	-1.0(5)
C4—C5—C6—C1	1.8 (4)	C15—C14—C19—C18	-2.0(4)
C4—C5—C6—N1	-175.7 (3)	C13—C14—C19—C18	173.3 (3)
O1—C1—C6—C5	-178.2 (3)	C15—C14—C19—C20	178.8 (3)
C2-C1-C6-C5	-0.5 (4)	C13—C14—C19—C20	-5.9 (4)
O1—C1—C6—N1	-0.6 (4)	C17—C18—C19—C14	2.4 (4)
C2-C1-C6-N1	177.1 (3)	C17—C18—C19—C20	-178.4 (3)
C7—N1—C6—C5	-65.1 (4)	C21—N2—C20—O3	-13.6 (4)
C7—N1—C6—C1	117.3 (3)	C21—N2—C20—C19	167.3 (2)
C6—N1—C7—O2	2.9 (5)	C14—C19—C20—O3	135.1 (3)
C6—N1—C7—C8	-178.7 (3)	C18—C19—C20—O3	-44.0 (4)
O2—C7—C8—C13	-50.2 (4)	C14—C19—C20—N2	-45.7 (4)
N1-C7-C8-C13	131.3 (3)	C18—C19—C20—N2	135.1 (3)
O2—C7—C8—C9	127.4 (3)	C20—N2—C21—C22	14.1 (4)
N1—C7—C8—C9	-51.1 (4)	C20—N2—C21—C26	-163.9(2)
C13—C8—C9—C10	2.1 (5)	C26—C21—C22—C23	2.0 (5)
C7—C8—C9—C10	-175.5 (3)	N2-C21-C22-C23	-175.9 (3)
C8—C9—C10—C11	-1.6 (5)	C21—C22—C23—C24	0.9 (5)
C9—C10—C11—C12	0.0 (5)	C22—C23—C24—C25	-1.8 (6)
C10-C11-C12-C13	1.1 (5)	C23—C24—C25—C26	-0.2(5)
C9—C8—C13—C12	-1.1 (4)	C28—O4—C26—C25	8.0 (4)

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C7—C8—C13—C12	176.6 (3)	C28—O4—C26—C21	-173.0 (3)
C9—C8—C13—C14	174.1 (3)	C24—C25—C26—O4	-177.9 (3)
C7—C8—C13—C14	-8.2 (4)	C24—C25—C26—C21	3.1 (4)
C11—C12—C13—C8	-0.5 (5)	C22—C21—C26—O4	176.9 (3)
C11—C12—C13—C14	-175.8 (3)	N2-C21-C26-O4	-4.9 (3)
C8—C13—C14—C19	109.4 (3)	C22—C21—C26—C25	-4.0 (4)
C12-C13-C14-C19	-75.4 (4)	N2-C21-C26-C25	174.2 (2)

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H…A	$D \cdots A$	D—H···A
N1—H1 <i>N</i> ···O3 ⁱ	0.86	2.02	2.833 (3)	157
N2—H2 <i>N</i> ···O2	0.86	2.24	3.081 (4)	167
N2—H2 <i>N</i> ···O4	0.86	2.24	2.612 (3)	106
С22—Н22…О3	0.93	2.30	2.885 (4)	120

Symmetry code: (i) x-1/2, -y+1/2, z-1/2.