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# 2-[(5′-Chloro-1,1′:3′,1″-terphenyl-4′-yl)-imino]acenaphthylen-1(2*H*)-one

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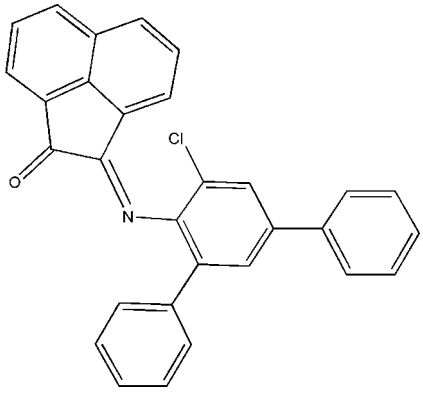
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.058; $wR$ factor = 0.121; data-to-parameter ratio = 15.0.

The title compound, $C_{30}H_{18}ClNO$, is a product of the condensation reaction of acenaphthylene-1,2-dione and 5′-chloro-1,1′:3′,1″-terphenyl-4′-amine. The acenaphthylene fragment and two terminal phenyl rings are rotated relative to the central benzene ring by 72.2 (3), 43.2 (3) and 41.2 (3)°, respectively. This molecular conformation is supported by weak C—H$\cdots\pi$ interactions. In the crystal, molecules form centrosymmetric dimers by the stacking interactions between two neighboring acenaphthylene fragments, with an interplanar distance of 3.365 (3) Å. The dimers are bound to each other by weak C—H$\cdots$N and C—H$\cdots\pi$ interactions, forming a three-dimensional framework.

## Related literature

For background to applications of Schiff bases, see: Lozier *et al.* (1975); Kargar *et al.* (2009); Yeap *et al.* (2009). For related structures, see: Higuchi *et al.* (2001); Manseong *et al.* (2006); Vitor *et al.* (2008).




## Experimental

### Crystal data

$C_{30}H_{18}ClNO$
$M_r$ = 443.90
Monoclinic, $P2_1/n$
$a$ = 12.4929 (6) Å
$b$ = 10.8699 (7) Å
$c$ = 16.0758 (8) Å
$\beta$ = 91.864 (5)°
$V$ = 2181.9 (2) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.20 mm$^{-1}$
$T$ = 100 K
0.32 × 0.28 × 0.25 mm

### Data collection

Agilent SuperNova (Dual, Cu at zero, Eos) diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
$T_{min}$ = 0.866, $T_{max}$ = 1.000
8827 measured reflections
4461 independent reflections
3151 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.041

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.121
$S$ = 1.09
4461 reflections
298 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.50 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.28 e Å$^{-3}$

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

*Cg*1 and *Cg*2 are the centroids of the C25–C30 and C19–C24 rings, respectively.

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| C24—H24$\cdots$N2$^{i}$ | 0.93 | 2.59 | 3.338 (3) | 138 |
| C4—H4$\cdots Cg1^{ii}$ | 0.93 | 2.74 | 3.551 (3) | 147 |
| C6—H6$\cdots Cg2^{iii}$ | 0.93 | 2.92 | 3.647 (3) | 136 |

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

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KQ2002).

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# supplementary materials

*Acta Cryst.* (2013). E**69**, o624–o625 [doi:10.1107/S1600536813008015]

## 2-[(5′-Chloro-1,1′:3′,1″-terphenyl-4′-yl)imino]acenaphthylen-1(2*H*)-one

**Zhengyin Du, Fushou Che, Yufei Yan and Wei Liu**

### Comment

Schiff bases often exhibit various biological activities, for example, anti-inflammatory, antibacterial, anticancer and antitoxic properties (Lozier *et al.*, 1975). They have also been used as versatile ligands in coordination chemistry (Kargar *et al.*, 2009; Yeap *et al.*, 2009). The present work describes the structure of a new Schiff base, $C_{30}H_{18}ClNO$, (**I**) obtained by the condensation reaction of acenaphthylene-1,2-dione and 5′-chloro-1,1′:3′,1″-terphenyl-4′-amine (Figure 1).

The geometrical parameters of **I** are in good accordance with those found in the related compounds (Higuchi *et al.*, 2001; Manseong *et al.*, 2006; Vitor *et al.*, 2008). The acenaphthylene fragment and two terminal phenyl rings in **I** are rotated in relative to the central benzene ring by 72.2 (3), 43.2 (3) and 41.2 (3)°, respectively (Figure 2). The molecular conformation of **I** is supported by the weak intramolecular C20—H20···N2 (Table 1) and C2—H2···$\pi$(C13=C14) [H2···C13 2.76 Å, H2···C14 2.80 Å] hydrogen bonding interactions (Figure 2).

In the crystal, the molecules form centrosymmetric dimers by the stacking interactions between two neighboring acenaphthylene fragments, with the interplane distance of 3.365 (3) Å. The dimers are bound to each other by the weak C24—H24···N2$^{i}$, C4—H4···Cg1$^{ii}$ (Cg1 is the centroid of the C25/C26/C27/C28/C29/C30 ring) and C6—H6···Cg2$^{iii}$ (Cg2 is the centroid of the C19/C20/C21/C22/C23/C24 ring) hydrogen bonding interactions (Table 1) into 3-dimensional framework. Symmetry codes: (i) –*x*+1/2, *y*+1/2, –*z*+1/2; (ii) *x*–1/2, –*y*+1/2, *z*–1/2; (iii) –*x*+1, –*y*+1, –*z*+1.

### Experimental

Formic acid (1 mL) was added to a stirred solution of acenaphthenequinone (1.2 mmol) and 2-chloro-4,6-diphenylaniline (1.2 mmol) in methanol (20 mL). The mixture was refluxed for 24 h, then cooled, and the precipitate was separated by filtration. The solid was recrystallized from dichloromethane/cyclohexane (*v*/*v* = 8:1), washed with cold ethanol and dried under vacuum to give the title compound **I**. Yield is 0.15 g (83%). Crystals of **I** suitable for X-ray structure determination were grown from a cyclohexane/dichloromethane (1:2, *v*/*v*) solution. Anal. Calcd. for $C_{30}H_{18}ClNO$: C, 81.17; H, 4.09; N,3.16. Found: C, 81.11; H, 4.19; N, 3.12.

### Refinement

All hydrogen atoms were placed in the calculated positions with C—H = 0.93 Å and refined in the riding model with fixed isotropic displacement parameters [$U_{iso}$(H) = 1.2$U_{eq}$(C)].

### Computing details

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO* (Agilent, 2012); data reduction: *CrysAlis PRO* (Agilent, 2012); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

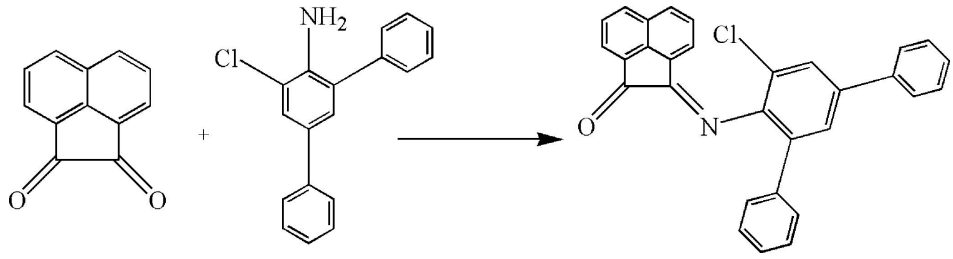


**Figure 1**

A condensation reaction of acenaphthylene-1,2-dione and 5′-chloro-1,1′:3′,1″-terphenyl-4′-amine.

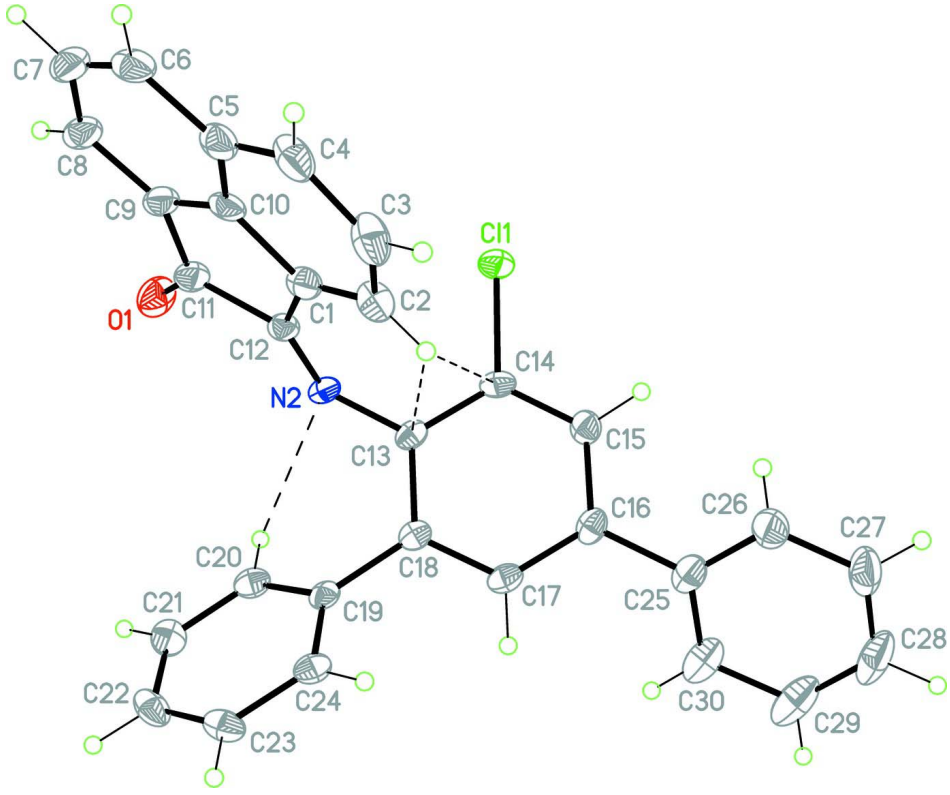


**Figure 2**

Molecular structure of **I**. Displacement ellipsoids are shown at the 40% probability level. H atoms are presented as small spheres of arbitrary radius. The dashed lines indicate the intramolecular C—H···N and C—H···$\pi$(C=C) hydrogen bonds.

### 2-[(5′-Chloro-1,1′:3′,1″-terphenyl-4′-yl)imino]acenaphthylen-1(2*H*)-one

*Crystal data*

$C_{30}H_{18}ClNO$
$M_r = 443.90$
Monoclinic, $P2_1/n$
$a = 12.4929$ (6) Å
$b = 10.8699$ (7) Å
$c = 16.0758$ (8) Å
$\beta = 91.864$ (5)°
$V = 2181.9$ (2) Å$^3$
$Z = 4$

$F(000) = 920$
$D_x = 1.351$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.7107$ Å
Cell parameters from 2796 reflections
$\theta = 3.1$–28.4°
$\mu = 0.20$ mm$^{-1}$
$T = 100$ K
Block, clear light-yellow
0.32 × 0.28 × 0.25 mm

*Data collection*

Agilent SuperNova (Dual, Cu at zero, Eos) diffractometer
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 16.0733 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
$T_{min}$ = 0.866, $T_{max}$ = 1.000
8827 measured reflections
4461 independent reflections
3151 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.041
$\theta_{max}$ = 26.4°, $\theta_{min}$ = 3.2°
$h$ = −15→15
$k$ = −13→11
$l$ = −19→20

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.121
$S$ = 1.09
4461 reflections
298 parameters
0 restraints
Primary 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
$w = 1/[\sigma^2(F_o^2) + (0.031P)^2 + 0.7817P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.50 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.28 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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.04696 (5) | 0.31870 (6) | 0.48276 (4) | 0.02604 (18) |
| O1 | 0.41337 (15) | 0.16285 (19) | 0.45458 (12) | 0.0333 (5) |
| N2 | 0.23922 (15) | 0.29536 (19) | 0.37546 (11) | 0.0179 (5) |
| C1 | 0.29301 (19) | 0.4619 (3) | 0.47857 (15) | 0.0226 (6) |
| C2 | 0.2362 (2) | 0.5671 (3) | 0.46784 (16) | 0.0255 (6) |
| H2 | 0.1824 | 0.5737 | 0.4267 | 0.031* |
| C3 | 0.2617 (2) | 0.6671 (3) | 0.52178 (18) | 0.0335 (7) |
| H3 | 0.2249 | 0.7408 | 0.5143 | 0.040* |
| C4 | 0.3393 (2) | 0.6593 (3) | 0.58509 (17) | 0.0334 (7) |
| H4 | 0.3515 | 0.7262 | 0.6201 | 0.040* |
| C5 | 0.3989 (2) | 0.5525 (3) | 0.59681 (16) | 0.0276 (7) |
| C6 | 0.4832 (2) | 0.5294 (3) | 0.65685 (16) | 0.0330 (7) |
| H6 | 0.5019 | 0.5901 | 0.6954 | 0.040* |
| C7 | 0.5368 (2) | 0.4199 (3) | 0.65874 (16) | 0.0352 (8) |
| H7 | 0.5911 | 0.4087 | 0.6990 | 0.042* |
| C8 | 0.5140 (2) | 0.3233 (3) | 0.60276 (15) | 0.0317 (7) |

| | | | | |
|---|---|---|---|---|
| H8 | 0.5527 | 0.2502 | 0.6045 | 0.038* |
| C9 | 0.4309 (2) | 0.3422 (3) | 0.54485 (15) | 0.0249 (6) |
| C10 | 0.3752 (2) | 0.4534 (3) | 0.54261 (15) | 0.0250 (6) |
| C11 | 0.3865 (2) | 0.2656 (3) | 0.47682 (15) | 0.0247 (6) |
| C12 | 0.29469 (18) | 0.3418 (2) | 0.43510 (14) | 0.0186 (6) |
| C13 | 0.15077 (18) | 0.3582 (2) | 0.33866 (14) | 0.0176 (5) |
| C14 | 0.05499 (19) | 0.3719 (2) | 0.38076 (14) | 0.0195 (6) |
| C15 | −0.03509 (19) | 0.4241 (2) | 0.34434 (15) | 0.0213 (6) |
| H15 | −0.0974 | 0.4306 | 0.3741 | 0.026* |
| C16 | −0.03305 (19) | 0.4674 (2) | 0.26273 (15) | 0.0208 (6) |
| C17 | 0.06207 (18) | 0.4559 (2) | 0.22035 (15) | 0.0195 (6) |
| H17 | 0.0645 | 0.4862 | 0.1663 | 0.023* |
| C18 | 0.15357 (18) | 0.4010 (2) | 0.25532 (14) | 0.0169 (5) |
| C19 | 0.25352 (18) | 0.3931 (2) | 0.20691 (14) | 0.0176 (5) |
| C20 | 0.31803 (19) | 0.2884 (2) | 0.20722 (14) | 0.0211 (6) |
| H20 | 0.2982 | 0.2193 | 0.2372 | 0.025* |
| C21 | 0.4119 (2) | 0.2865 (3) | 0.16287 (15) | 0.0250 (6) |
| H21 | 0.4542 | 0.2160 | 0.1632 | 0.030* |
| C22 | 0.4425 (2) | 0.3883 (3) | 0.11853 (15) | 0.0265 (6) |
| H22 | 0.5062 | 0.3874 | 0.0902 | 0.032* |
| C23 | 0.3783 (2) | 0.4918 (3) | 0.11635 (15) | 0.0247 (6) |
| H23 | 0.3984 | 0.5603 | 0.0859 | 0.030* |
| C24 | 0.28386 (19) | 0.4937 (2) | 0.15946 (14) | 0.0209 (6) |
| H24 | 0.2403 | 0.5631 | 0.1566 | 0.025* |
| C25 | −0.1326 (2) | 0.5199 (3) | 0.22308 (17) | 0.0258 (6) |
| C26 | −0.2001 (2) | 0.5956 (3) | 0.26780 (18) | 0.0335 (7) |
| H26 | −0.1807 | 0.6176 | 0.3221 | 0.040* |
| C27 | −0.2959 (2) | 0.6385 (3) | 0.2324 (2) | 0.0415 (8) |
| H27 | −0.3399 | 0.6897 | 0.2625 | 0.050* |
| C28 | −0.3251 (2) | 0.6047 (3) | 0.1522 (2) | 0.0447 (9) |
| H28 | −0.3900 | 0.6316 | 0.1287 | 0.054* |
| C29 | −0.2592 (2) | 0.5316 (3) | 0.1070 (2) | 0.0434 (9) |
| H29 | −0.2794 | 0.5096 | 0.0529 | 0.052* |
| C30 | −0.1619 (2) | 0.4899 (3) | 0.14165 (18) | 0.0338 (7) |
| H30 | −0.1167 | 0.4420 | 0.1101 | 0.041* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0262 (3) | 0.0333 (4) | 0.0187 (3) | −0.0013 (3) | 0.0026 (2) | 0.0074 (3) |
| O1 | 0.0344 (11) | 0.0298 (12) | 0.0354 (11) | 0.0085 (10) | −0.0043 (8) | 0.0040 (9) |
| N2 | 0.0197 (10) | 0.0197 (12) | 0.0139 (10) | −0.0025 (10) | −0.0030 (8) | 0.0026 (9) |
| C1 | 0.0201 (12) | 0.0284 (16) | 0.0193 (13) | −0.0087 (13) | 0.0024 (10) | −0.0033 (11) |
| C2 | 0.0239 (13) | 0.0242 (16) | 0.0285 (14) | −0.0040 (13) | 0.0047 (11) | −0.0062 (12) |
| C3 | 0.0247 (14) | 0.0299 (18) | 0.0461 (18) | −0.0004 (14) | 0.0070 (12) | −0.0112 (14) |
| C4 | 0.0246 (14) | 0.041 (2) | 0.0352 (16) | −0.0075 (15) | 0.0095 (12) | −0.0183 (14) |
| C5 | 0.0208 (13) | 0.0387 (19) | 0.0235 (14) | −0.0099 (14) | 0.0055 (11) | −0.0036 (13) |
| C6 | 0.0295 (15) | 0.050 (2) | 0.0195 (14) | −0.0194 (16) | 0.0031 (11) | −0.0103 (14) |
| C7 | 0.0259 (15) | 0.058 (2) | 0.0209 (14) | −0.0123 (16) | −0.0051 (11) | 0.0032 (14) |
| C8 | 0.0264 (14) | 0.048 (2) | 0.0201 (13) | −0.0138 (15) | −0.0022 (10) | 0.0100 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C9 | 0.0231 (13) | 0.0350 (18) | 0.0165 (12) | −0.0062 (14) | −0.0005 (10) | 0.0046 (12) |
| C10 | 0.0212 (13) | 0.0396 (18) | 0.0145 (12) | −0.0137 (14) | 0.0059 (10) | −0.0023 (12) |
| C11 | 0.0251 (14) | 0.0293 (17) | 0.0197 (13) | −0.0020 (14) | 0.0009 (10) | 0.0075 (12) |
| C12 | 0.0188 (12) | 0.0219 (15) | 0.0150 (12) | −0.0035 (12) | 0.0013 (9) | 0.0020 (11) |
| C13 | 0.0212 (12) | 0.0141 (13) | 0.0170 (12) | −0.0008 (11) | −0.0048 (9) | −0.0020 (10) |
| C14 | 0.0250 (13) | 0.0184 (15) | 0.0150 (12) | −0.0048 (12) | −0.0005 (10) | 0.0031 (10) |
| C15 | 0.0174 (12) | 0.0217 (15) | 0.0248 (13) | −0.0032 (12) | 0.0014 (10) | 0.0031 (11) |
| C16 | 0.0165 (12) | 0.0186 (15) | 0.0268 (14) | −0.0040 (12) | −0.0043 (10) | 0.0020 (11) |
| C17 | 0.0235 (13) | 0.0180 (14) | 0.0167 (12) | −0.0036 (12) | −0.0039 (10) | 0.0014 (11) |
| C18 | 0.0201 (12) | 0.0135 (13) | 0.0168 (12) | −0.0033 (11) | −0.0028 (9) | −0.0026 (10) |
| C19 | 0.0186 (12) | 0.0204 (14) | 0.0134 (11) | −0.0007 (12) | −0.0050 (9) | −0.0044 (10) |
| C20 | 0.0266 (13) | 0.0191 (15) | 0.0174 (12) | −0.0025 (12) | −0.0036 (10) | −0.0020 (11) |
| C21 | 0.0273 (14) | 0.0236 (16) | 0.0239 (14) | 0.0030 (13) | −0.0003 (11) | −0.0086 (12) |
| C22 | 0.0242 (14) | 0.0339 (18) | 0.0218 (14) | −0.0070 (14) | 0.0071 (11) | −0.0105 (12) |
| C23 | 0.0313 (14) | 0.0247 (16) | 0.0183 (13) | −0.0079 (14) | 0.0039 (10) | −0.0023 (11) |
| C24 | 0.0269 (13) | 0.0205 (15) | 0.0151 (12) | −0.0011 (12) | −0.0037 (10) | −0.0019 (11) |
| C25 | 0.0197 (13) | 0.0257 (16) | 0.0318 (15) | −0.0054 (13) | −0.0030 (11) | 0.0104 (12) |
| C26 | 0.0249 (14) | 0.0405 (19) | 0.0354 (16) | 0.0011 (15) | 0.0070 (12) | 0.0145 (14) |
| C27 | 0.0211 (14) | 0.047 (2) | 0.058 (2) | 0.0073 (15) | 0.0114 (14) | 0.0223 (17) |
| C28 | 0.0195 (14) | 0.045 (2) | 0.069 (2) | −0.0037 (16) | −0.0114 (15) | 0.0275 (19) |
| C29 | 0.0426 (18) | 0.033 (2) | 0.052 (2) | −0.0058 (17) | −0.0250 (15) | 0.0092 (16) |
| C30 | 0.0345 (16) | 0.0253 (17) | 0.0405 (17) | −0.0008 (15) | −0.0146 (13) | 0.0026 (14) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C14 | 1.745 (2) | C15—C16 | 1.395 (3) |
| O1—C11 | 1.223 (3) | C16—C17 | 1.394 (3) |
| N2—C12 | 1.269 (3) | C16—C25 | 1.492 (3) |
| N2—C13 | 1.412 (3) | C17—H17 | 0.9300 |
| C1—C2 | 1.354 (4) | C17—C18 | 1.392 (3) |
| C1—C10 | 1.433 (3) | C18—C19 | 1.495 (3) |
| C1—C12 | 1.481 (4) | C19—C20 | 1.395 (3) |
| C2—H2 | 0.9300 | C19—C24 | 1.393 (3) |
| C2—C3 | 1.420 (4) | C20—H20 | 0.9300 |
| C3—H3 | 0.9300 | C20—C21 | 1.392 (3) |
| C3—C4 | 1.385 (4) | C21—H21 | 0.9300 |
| C4—H4 | 0.9300 | C21—C22 | 1.378 (4) |
| C4—C5 | 1.389 (4) | C22—H22 | 0.9300 |
| C5—C6 | 1.427 (4) | C22—C23 | 1.381 (4) |
| C5—C10 | 1.411 (4) | C23—H23 | 0.9300 |
| C6—H6 | 0.9300 | C23—C24 | 1.388 (3) |
| C6—C7 | 1.366 (4) | C24—H24 | 0.9300 |
| C7—H7 | 0.9300 | C25—C26 | 1.394 (4) |
| C7—C8 | 1.407 (4) | C25—C30 | 1.387 (4) |
| C8—H8 | 0.9300 | C26—H26 | 0.9300 |
| C8—C9 | 1.387 (3) | C26—C27 | 1.389 (4) |
| C9—C10 | 1.394 (4) | C27—H27 | 0.9300 |
| C9—C11 | 1.469 (4) | C27—C28 | 1.378 (5) |
| C11—C12 | 1.550 (4) | C28—H28 | 0.9300 |
| C13—C14 | 1.402 (3) | C28—C29 | 1.370 (5) |

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|---|---|---|---|
| C13—C18 | 1.420 (3) | C29—H29 | 0.9300 |
| C14—C15 | 1.374 (3) | C29—C30 | 1.396 (4) |
| C15—H15 | 0.9300 | C30—H30 | 0.9300 |

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| C12—N2—C13 | 121.6 (2) | C15—C16—C25 | 119.4 (2) |
| C2—C1—C10 | 120.5 (2) | C17—C16—C15 | 118.1 (2) |
| C2—C1—C12 | 134.4 (2) | C17—C16—C25 | 122.5 (2) |
| C10—C1—C12 | 105.1 (2) | C16—C17—H17 | 118.6 |
| C1—C2—H2 | 121.2 | C18—C17—C16 | 122.9 (2) |
| C1—C2—C3 | 117.5 (2) | C18—C17—H17 | 118.6 |
| C3—C2—H2 | 121.2 | C13—C18—C19 | 121.3 (2) |
| C2—C3—H3 | 118.7 | C17—C18—C13 | 118.4 (2) |
| C4—C3—C2 | 122.7 (3) | C17—C18—C19 | 120.2 (2) |
| C4—C3—H3 | 118.7 | C20—C19—C18 | 122.5 (2) |
| C3—C4—H4 | 119.6 | C24—C19—C18 | 119.1 (2) |
| C3—C4—C5 | 120.7 (3) | C24—C19—C20 | 118.4 (2) |
| C5—C4—H4 | 119.6 | C19—C20—H20 | 119.8 |
| C4—C5—C6 | 128.3 (3) | C21—C20—C19 | 120.4 (2) |
| C4—C5—C10 | 117.0 (2) | C21—C20—H20 | 119.8 |
| C10—C5—C6 | 114.8 (3) | C20—C21—H21 | 119.8 |
| C5—C6—H6 | 119.4 | C22—C21—C20 | 120.4 (3) |
| C7—C6—C5 | 121.3 (3) | C22—C21—H21 | 119.8 |
| C7—C6—H6 | 119.4 | C21—C22—H22 | 120.1 |
| C6—C7—H7 | 118.4 | C21—C22—C23 | 119.8 (2) |
| C6—C7—C8 | 123.2 (3) | C23—C22—H22 | 120.1 |
| C8—C7—H7 | 118.4 | C22—C23—H23 | 119.9 |
| C7—C8—H8 | 121.6 | C22—C23—C24 | 120.2 (3) |
| C9—C8—C7 | 116.8 (3) | C24—C23—H23 | 119.9 |
| C9—C8—H8 | 121.6 | C19—C24—H24 | 119.6 |
| C8—C9—C10 | 120.5 (3) | C23—C24—C19 | 120.8 (3) |
| C8—C9—C11 | 132.2 (3) | C23—C24—H24 | 119.6 |
| C10—C9—C11 | 107.2 (2) | C26—C25—C16 | 121.0 (2) |
| C5—C10—C1 | 121.7 (3) | C30—C25—C16 | 120.3 (3) |
| C9—C10—C1 | 114.8 (2) | C30—C25—C26 | 118.7 (3) |
| C9—C10—C5 | 123.5 (2) | C25—C26—H26 | 119.5 |
| O1—C11—C9 | 129.4 (3) | C27—C26—C25 | 120.9 (3) |
| O1—C11—C12 | 124.6 (2) | C27—C26—H26 | 119.5 |
| C9—C11—C12 | 106.0 (2) | C26—C27—H27 | 120.2 |
| N2—C12—C1 | 133.7 (2) | C28—C27—C26 | 119.5 (3) |
| N2—C12—C11 | 119.5 (2) | C28—C27—H27 | 120.2 |
| C1—C12—C11 | 106.8 (2) | C27—C28—H28 | 119.8 |
| N2—C13—C18 | 120.7 (2) | C29—C28—C27 | 120.3 (3) |
| C14—C13—N2 | 121.2 (2) | C29—C28—H28 | 119.8 |
| C14—C13—C18 | 117.9 (2) | C28—C29—H29 | 119.8 |
| C13—C14—Cl1 | 119.65 (18) | C28—C29—C30 | 120.5 (3) |
| C15—C14—Cl1 | 117.78 (19) | C30—C29—H29 | 119.8 |
| C15—C14—C13 | 122.6 (2) | C25—C30—C29 | 120.0 (3) |
| C14—C15—H15 | 120.0 | C25—C30—H30 | 120.0 |
| C14—C15—C16 | 120.0 (2) | C29—C30—H30 | 120.0 |

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|---|---|---|---|
| C16—C15—H15 | 120.0 | | |
| | | | |
| Cl1—C14—C15—C16 | −179.6 (2) | C12—C1—C2—C3 | −177.2 (3) |
| O1—C11—C12—N2 | 2.8 (4) | C12—C1—C10—C5 | 178.9 (2) |
| O1—C11—C12—C1 | −177.2 (2) | C12—C1—C10—C9 | 0.9 (3) |
| N2—C13—C14—Cl1 | 3.9 (3) | C13—N2—C12—C1 | −3.7 (4) |
| N2—C13—C14—C15 | −174.9 (2) | C13—N2—C12—C11 | 176.2 (2) |
| N2—C13—C18—C17 | 176.2 (2) | C13—C14—C15—C16 | −0.8 (4) |
| N2—C13—C18—C19 | −6.6 (4) | C13—C18—C19—C20 | 44.1 (3) |
| C1—C2—C3—C4 | −1.8 (4) | C13—C18—C19—C24 | −136.0 (2) |
| C2—C1—C10—C5 | 0.7 (4) | C14—C13—C18—C17 | 1.0 (4) |
| C2—C1—C10—C9 | −177.3 (2) | C14—C13—C18—C19 | 178.2 (2) |
| C2—C1—C12—N2 | −4.2 (5) | C14—C15—C16—C17 | 0.0 (4) |
| C2—C1—C12—C11 | 175.8 (3) | C14—C15—C16—C25 | 177.9 (2) |
| C2—C3—C4—C5 | 2.3 (4) | C15—C16—C17—C18 | 1.4 (4) |
| C3—C4—C5—C6 | 178.2 (3) | C15—C16—C25—C26 | 40.5 (4) |
| C3—C4—C5—C10 | −1.2 (4) | C15—C16—C25—C30 | −136.8 (3) |
| C4—C5—C6—C7 | −177.9 (3) | C16—C17—C18—C13 | −1.9 (4) |
| C4—C5—C10—C1 | −0.3 (4) | C16—C17—C18—C19 | −179.1 (2) |
| C4—C5—C10—C9 | 177.6 (2) | C16—C25—C26—C27 | −176.2 (3) |
| C5—C6—C7—C8 | 0.1 (4) | C16—C25—C30—C29 | 175.0 (3) |
| C6—C5—C10—C1 | −179.7 (2) | C17—C16—C25—C26 | −141.7 (3) |
| C6—C5—C10—C9 | −1.9 (4) | C17—C16—C25—C30 | 41.0 (4) |
| C6—C7—C8—C9 | −1.4 (4) | C17—C18—C19—C20 | −138.7 (2) |
| C7—C8—C9—C10 | 1.1 (4) | C17—C18—C19—C24 | 41.2 (3) |
| C7—C8—C9—C11 | 178.4 (3) | C18—C13—C14—Cl1 | 179.04 (18) |
| C8—C9—C10—C1 | 178.6 (2) | C18—C13—C14—C15 | 0.3 (4) |
| C8—C9—C10—C5 | 0.6 (4) | C18—C19—C20—C21 | −178.3 (2) |
| C8—C9—C11—O1 | 0.2 (5) | C18—C19—C24—C23 | 177.4 (2) |
| C8—C9—C11—C12 | −179.5 (3) | C19—C20—C21—C22 | 0.4 (4) |
| C9—C11—C12—N2 | −177.5 (2) | C20—C19—C24—C23 | −2.7 (3) |
| C9—C11—C12—C1 | 2.4 (2) | C20—C21—C22—C23 | −1.7 (4) |
| C10—C1—C2—C3 | 0.3 (4) | C21—C22—C23—C24 | 0.8 (4) |
| C10—C1—C12—N2 | 178.0 (3) | C22—C23—C24—C19 | 1.4 (4) |
| C10—C1—C12—C11 | −2.0 (2) | C24—C19—C20—C21 | 1.8 (3) |
| C10—C5—C6—C7 | 1.5 (4) | C25—C16—C17—C18 | −176.4 (2) |
| C10—C9—C11—O1 | 177.7 (3) | C25—C26—C27—C28 | 0.7 (4) |
| C10—C9—C11—C12 | −1.9 (3) | C26—C25—C30—C29 | −2.3 (4) |
| C11—C9—C10—C1 | 0.7 (3) | C26—C27—C28—C29 | −1.5 (5) |
| C11—C9—C10—C5 | −177.3 (2) | C27—C28—C29—C30 | 0.4 (5) |
| C12—N2—C13—C14 | −72.0 (3) | C28—C29—C30—C25 | 1.6 (5) |
| C12—N2—C13—C18 | 112.9 (3) | C30—C25—C26—C27 | 1.2 (4) |

*Hydrogen-bond geometry (Å, º)*

Cg1 and Cg2 are the centroids of the C25–C30 and C19–C24 rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C20—H20···N2 | 0.93 | 2.50 | 2.909 (3) | 107 |
| C24—H24···N2$^{i}$ | 0.93 | 2.59 | 3.338 (3) | 138 |

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|---|---|---|---|---|
| C4—H4···*Cg*1$^{ii}$ | 0.93 | 2.74 | 3.551 (3) | 147 |
| C6—H6···*Cg*2$^{iii}$ | 0.93 | 2.92 | 3.647 (3) | 136 |

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