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# 9,9-Dimethyl-12-phenyl-8,9-dihydro-12*H*-benzo[*a*]xanthen-11(10*H*)-one

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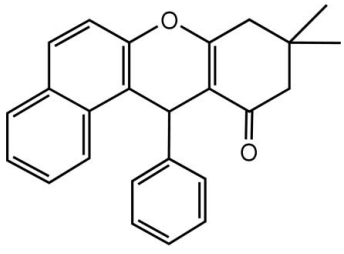
Key indicators: single-crystal X-ray study; $T$ = 113 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.040; $wR$ factor = 0.114; data-to-parameter ratio = 17.5.

The title compound, $C_{25}H_{22}O_2$, was synthesized *via* the three-component coupling of benzaldehyde, 2-naphthol and 5,5-dimethylcyclohexane-1,3-dione. In the crystal structure, centrosymmetrically related molecules are linked into dimers by pairs of intermolecular C—H···O hydrogen bonds. The dimers are further connected into a three-dimensional network by $\pi$–$\pi$ aromatic stacking interactions involving the naphthalene ring system, with centroid–centroid separations of 3.695 (7) Å.

## Related literature

For the biological and pharmacological activity of xanthenes and benzoxanthenes, see: Ion *et al.* (1998); Lambert *et al.* (1997); Poupelin *et al.* (1978); Saint-Ruf *et al.* (1975). For reference structural data, see: Allen *et al.* (1987).



## Experimental

### Crystal data

$C_{25}H_{22}O_2$ $M_r$ = 354.43
Triclinic, $P\overline{1}$
$a$ = 9.1881 (18) Å
$b$ = 9.2317 (18) Å
$c$ = 12.866 (3) Å
$\alpha$ = 72.78 (3)°
$\beta$ = 80.82 (3)°
$\gamma$ = 62.17 (2)°
$V$ = 921.6 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 113 K
0.20 × 0.18 × 0.14 mm

### Data collection

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min}$ = 0.984, $T_{max}$ = 0.989
8318 measured reflections
4294 independent reflections
2797 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.114
$S$ = 0.97
4294 reflections
246 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.26 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C8—H8···O2$^{i}$ | 0.95 | 2.49 | 3.366 (2) | 154 |

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

Data collection: *CrystalClear* (Rigaku/MSC, 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: RZ2384).

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# supporting information

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## 9,9-Dimethyl-12-phenyl-8,9-dihydro-12*H*-benzo[*a*]xanthen-11(10*H*)-one

**Yong Zhang, Hong-Jun Zang and Bo-Wen Cheng**

### S1. Comment

Xanthenes and benzoxanthenes are important biologically active heterocycles They possess anti-inflammatory (Poupelin *et al.*, 1978) and antiviral (Lambert *et al.*, 1997) activities and are utilized as antagonists for paralyzing action of zoxazolamine (Saint-Ruf *et al.*, 1975) and in photodynamic therapy (Ion *et al.*, 1998). So far, no crystallographic studies have been performed on benzoxanthenes. We report herein the crystal structure of the title compound.

In the molecule of the title compound (Fig. 1), bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. The pyran ring adopts a boat conformation, with atoms O1 and C11 displaced by 0.1568 (9) and 0.3301 (12) Å from the C1/C10/C12/C17 plane, while the cyclohexene ring displays an envelope conformation, with atom C15 displaced by 0.6705 (13) Å from the C12/C13/C14/C16/C17 plane. In the crystal packing (Fig. 2), centrosymmetrically related molecules are connected into dimers by intermolecular C—H···O hydrogen bonds (Table 1). The dimers are further linked into a three-dimensional network by $\pi\cdots\pi$ aromatic stacking interactions involving the naphthalene ring system, with centroid-to-centroid separations of 3.695 (7) Å.

### S2. Experimental

$NaHSO_4$ (0.2 mmol) was added to benzaldehyde (1 mmol), 2-naphthol (1 mmol), 5,5 -dimethylcyclohexane-1,3-dione (1.1 mmol) and [BMIM]$BF_4$ (1 ml; $BMIM^+$ is 1-n-butyl-3-methylimidazolium), and the mixture was stirred at 80 °C for 1 h. After completion of the reaction as indicated by TLC, the system was cooled to room temperature. The mixture was washed with water (10 ml) and extracted with ethyl acetate (3×15 ml). The combined organic layers were dried over anhydrous sodium sulfate, filtered, and evaporated to dryness. The product was purified by column chromatography on silica gel. Single crystals of the title compound suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution at room temperature.

### S3. Refinement

All H atoms were included in the refinement in the riding model approximation, with C–H = 0.95–1.00 Å, and with $U_{iso}$(H) = 1.2 $U_{eq}$(C) or 1.5 $U_{eq}$(C) for methyl H atoms.

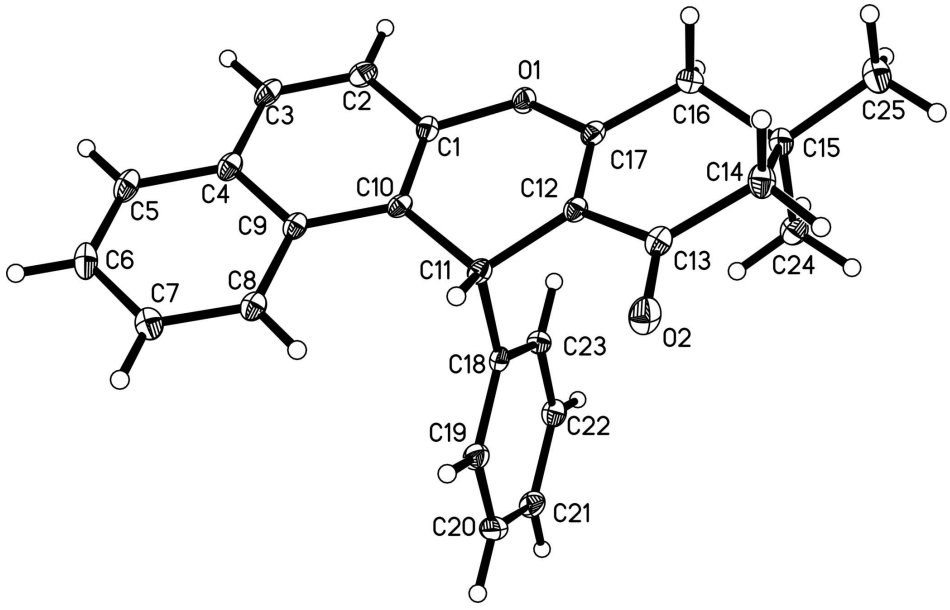


**Figure 1**

The molecular structure of the title compound, showing the atom-numbering scheme. Dispacement ellipsoids are drawn at the 30% probability level.

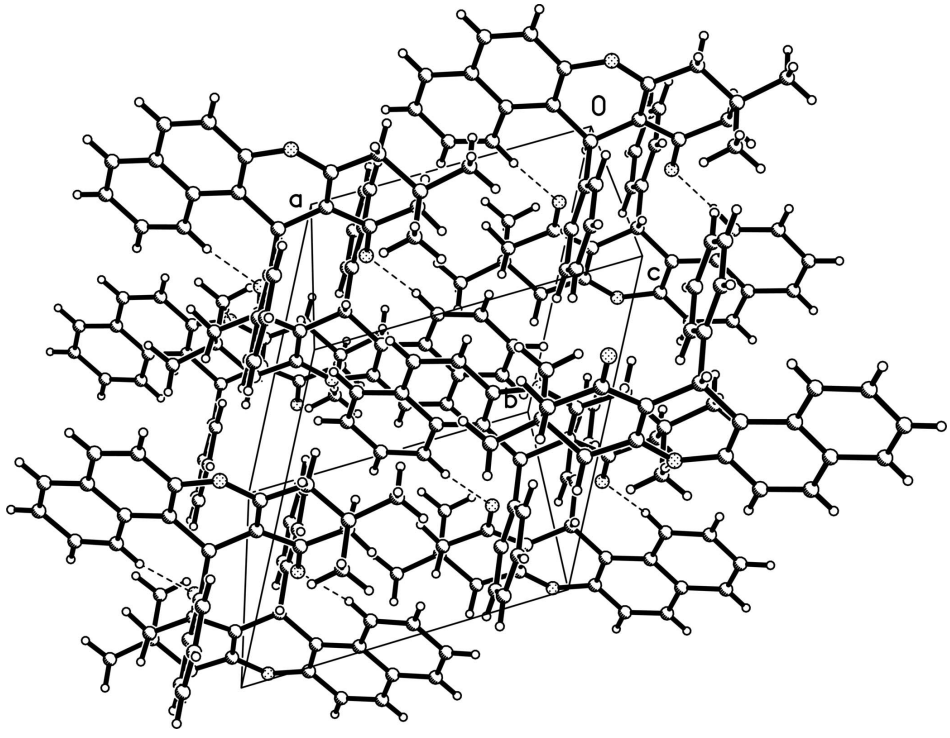


**Figure 2**

Packing diagram of the title compound, showing hydrogen-bonding interactions as dashed lines, H atoms are shown as small spheres of arbitary radii.

## 9,9-Dimethyl-12-phenyl-8,9-dihydro-12*H*-benzo[*a*]xanthen- 11(10*H*)-one

*Crystal data*

$C_{25}H_{22}O_2$
$M_r = 354.43$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.1881\ (18)$ Å
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$c = 12.866\ (3)$ Å
$\alpha = 72.78\ (3)°$
$\beta = 80.82\ (3)°$
$\gamma = 62.17\ (2)°$
$V = 921.6\ (3)$ Å$^3$
$Z = 2$
$F(000) = 376$
$D_x = 1.277$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2907 reflections
$\theta = 2.5–27.9°$
$\mu = 0.08$ mm$^{-1}$
$T = 113$ K
Prism, colourless
0.20 × 0.18 × 0.14 mm

*Data collection*

Rigaku Saturn CCD area-detector diffractometer
Radiation source: rotating anode
Confocal monochromator
Detector resolution: 7.31 pixels mm$^{-1}$
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min} = 0.984$, $T_{max} = 0.989$
8318 measured reflections
4294 independent reflections
2797 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 27.9°$, $\theta_{min} = 2.5°$
$h = -12\rightarrow11$
$k = -12\rightarrow12$
$l = -16\rightarrow13$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.114$
$S = 0.97$
4294 reflections
246 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
$w = 1/[\sigma^2(F_o^2) + (0.0691P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å$^{-3}$
$\Delta\rho_{min} = -0.26$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.80464 (10) | 0.56824 (10) | 0.17827 (6) | 0.0210 (2) |
| O2 | 1.16069 (10) | 0.04959 (11) | 0.40301 (7) | 0.0304 (3) |
| C1 | 0.66568 (14) | 0.56096 (15) | 0.23792 (9) | 0.0183 (3) |

| | | | | |
|---|---|---|---|---|
| C2 | 0.51931 (15) | 0.71327 (15) | 0.21330 (10) | 0.0233 (3) |
| H2 | 0.5195 | 0.8081 | 0.1582 | 0.028* |
| C3 | 0.37777 (14) | 0.72247 (16) | 0.26954 (10) | 0.0248 (3) |
| H3 | 0.2786 | 0.8242 | 0.2530 | 0.030* |
| C4 | 0.37678 (14) | 0.58228 (16) | 0.35227 (10) | 0.0210 (3) |
| C5 | 0.23201 (15) | 0.59156 (17) | 0.41469 (10) | 0.0258 (3) |
| H5 | 0.1328 | 0.6938 | 0.4003 | 0.031* |
| C6 | 0.23318 (15) | 0.45569 (18) | 0.49505 (10) | 0.0268 (3) |
| H6 | 0.1352 | 0.4639 | 0.5361 | 0.032* |
| C7 | 0.37922 (15) | 0.30371 (17) | 0.51717 (10) | 0.0240 (3) |
| H7 | 0.3792 | 0.2096 | 0.5731 | 0.029* |
| C8 | 0.52136 (14) | 0.28998 (16) | 0.45884 (9) | 0.0203 (3) |
| H8 | 0.6188 | 0.1862 | 0.4748 | 0.024* |
| C9 | 0.52538 (14) | 0.42815 (15) | 0.37510 (9) | 0.0175 (3) |
| C10 | 0.67273 (13) | 0.41870 (14) | 0.31377 (9) | 0.0165 (2) |
| C11 | 0.83294 (13) | 0.25608 (14) | 0.32854 (9) | 0.0165 (3) |
| H11 | 0.8452 | 0.1939 | 0.4073 | 0.020* |
| C12 | 0.97420 (13) | 0.30107 (15) | 0.29088 (9) | 0.0171 (3) |
| C13 | 1.13999 (14) | 0.17861 (16) | 0.33168 (9) | 0.0193 (3) |
| C14 | 1.28077 (15) | 0.22110 (17) | 0.28404 (10) | 0.0244 (3) |
| H14A | 1.3836 | 0.1144 | 0.2888 | 0.029* |
| H14B | 1.2938 | 0.2853 | 0.3284 | 0.029* |
| C15 | 1.25745 (14) | 0.32512 (16) | 0.16526 (9) | 0.0205 (3) |
| C16 | 1.09217 (14) | 0.48479 (15) | 0.15974 (10) | 0.0221 (3) |
| H16A | 1.1030 | 0.5620 | 0.1941 | 0.027* |
| H16B | 1.0646 | 0.5445 | 0.0825 | 0.027* |
| C17 | 0.95571 (14) | 0.44364 (15) | 0.21571 (9) | 0.0183 (3) |
| C18 | 0.83235 (13) | 0.14387 (14) | 0.26191 (9) | 0.0167 (3) |
| C19 | 0.82901 (15) | −0.01023 (15) | 0.31132 (10) | 0.0225 (3) |
| H19 | 0.8283 | −0.0485 | 0.3885 | 0.027* |
| C20 | 0.82669 (16) | −0.10895 (16) | 0.24890 (11) | 0.0283 (3) |
| H20 | 0.8240 | −0.2139 | 0.2838 | 0.034* |
| C21 | 0.82820 (15) | −0.05570 (17) | 0.13675 (11) | 0.0263 (3) |
| H21 | 0.8265 | −0.1235 | 0.0944 | 0.032* |
| C22 | 0.83223 (15) | 0.09814 (16) | 0.08610 (10) | 0.0233 (3) |
| H22 | 0.8335 | 0.1358 | 0.0089 | 0.028* |
| C23 | 0.83433 (14) | 0.19590 (15) | 0.14836 (9) | 0.0197 (3) |
| H23 | 0.8372 | 0.3007 | 0.1132 | 0.024* |
| C24 | 1.25856 (16) | 0.21964 (16) | 0.09293 (10) | 0.0247 (3) |
| H24A | 1.2394 | 0.2881 | 0.0175 | 0.037* |
| H24B | 1.1714 | 0.1834 | 0.1179 | 0.037* |
| H24C | 1.3655 | 0.1198 | 0.0971 | 0.037* |
| C25 | 1.39520 (16) | 0.37858 (19) | 0.12682 (11) | 0.0319 (3) |
| H25A | 1.5017 | 0.2776 | 0.1341 | 0.048* |
| H25B | 1.3928 | 0.4495 | 0.1713 | 0.048* |
| H25C | 1.3796 | 0.4430 | 0.0504 | 0.048* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0171 (4) | 0.0158 (4) | 0.0237 (5) | −0.0045 (3) | −0.0001 (3) | −0.0013 (3) |
| O2 | 0.0233 (5) | 0.0274 (5) | 0.0263 (5) | −0.0047 (4) | −0.0044 (4) | 0.0036 (4) |
| C1 | 0.0162 (6) | 0.0188 (6) | 0.0185 (6) | −0.0062 (5) | 0.0009 (5) | −0.0064 (5) |
| C2 | 0.0242 (6) | 0.0158 (6) | 0.0233 (7) | −0.0037 (5) | −0.0038 (5) | −0.0030 (5) |
| C3 | 0.0182 (6) | 0.0192 (6) | 0.0289 (7) | 0.0009 (5) | −0.0049 (5) | −0.0085 (5) |
| C4 | 0.0170 (6) | 0.0229 (6) | 0.0214 (6) | −0.0044 (5) | −0.0020 (5) | −0.0100 (5) |
| C5 | 0.0158 (6) | 0.0306 (7) | 0.0279 (7) | −0.0033 (5) | −0.0016 (5) | −0.0143 (6) |
| C6 | 0.0182 (6) | 0.0419 (8) | 0.0238 (7) | −0.0136 (6) | 0.0041 (5) | −0.0150 (6) |
| C7 | 0.0244 (6) | 0.0313 (7) | 0.0197 (6) | −0.0144 (6) | 0.0003 (5) | −0.0081 (5) |
| C8 | 0.0186 (6) | 0.0233 (6) | 0.0190 (6) | −0.0076 (5) | −0.0012 (5) | −0.0081 (5) |
| C9 | 0.0157 (5) | 0.0200 (6) | 0.0162 (6) | −0.0051 (5) | −0.0014 (4) | −0.0079 (5) |
| C10 | 0.0159 (5) | 0.0159 (5) | 0.0167 (6) | −0.0043 (5) | −0.0021 (4) | −0.0067 (5) |
| C11 | 0.0161 (5) | 0.0141 (5) | 0.0160 (6) | −0.0040 (4) | −0.0015 (4) | −0.0033 (4) |
| C12 | 0.0151 (5) | 0.0180 (6) | 0.0171 (6) | −0.0053 (5) | −0.0008 (4) | −0.0065 (5) |
| C13 | 0.0181 (6) | 0.0227 (6) | 0.0148 (6) | −0.0058 (5) | −0.0019 (5) | −0.0064 (5) |
| C14 | 0.0181 (6) | 0.0323 (7) | 0.0221 (7) | −0.0098 (5) | −0.0034 (5) | −0.0070 (5) |
| C15 | 0.0173 (6) | 0.0239 (6) | 0.0207 (7) | −0.0090 (5) | 0.0001 (5) | −0.0069 (5) |
| C16 | 0.0223 (6) | 0.0199 (6) | 0.0255 (7) | −0.0108 (5) | 0.0012 (5) | −0.0062 (5) |
| C17 | 0.0166 (6) | 0.0184 (6) | 0.0194 (6) | −0.0057 (5) | −0.0012 (4) | −0.0073 (5) |
| C18 | 0.0123 (5) | 0.0163 (5) | 0.0195 (6) | −0.0042 (4) | 0.0009 (4) | −0.0060 (5) |
| C19 | 0.0248 (6) | 0.0190 (6) | 0.0205 (6) | −0.0087 (5) | 0.0036 (5) | −0.0044 (5) |
| C20 | 0.0333 (7) | 0.0208 (6) | 0.0329 (8) | −0.0146 (6) | 0.0086 (6) | −0.0105 (6) |
| C21 | 0.0259 (7) | 0.0263 (7) | 0.0317 (8) | −0.0119 (5) | 0.0041 (5) | −0.0164 (6) |
| C22 | 0.0226 (6) | 0.0264 (7) | 0.0208 (6) | −0.0098 (5) | 0.0001 (5) | −0.0081 (5) |
| C23 | 0.0196 (6) | 0.0181 (6) | 0.0207 (6) | −0.0083 (5) | 0.0003 (5) | −0.0044 (5) |
| C24 | 0.0261 (6) | 0.0259 (7) | 0.0205 (7) | −0.0100 (5) | 0.0017 (5) | −0.0079 (5) |
| C25 | 0.0240 (7) | 0.0409 (8) | 0.0344 (8) | −0.0176 (6) | 0.0018 (6) | −0.0104 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C17 | 1.3697 (15) | C14—C15 | 1.5321 (17) |
| O1—C1 | 1.4002 (14) | C14—H14A | 0.9900 |
| O2—C13 | 1.2224 (15) | C14—H14B | 0.9900 |
| C1—C10 | 1.3651 (16) | C15—C25 | 1.5262 (17) |
| C1—C2 | 1.4116 (17) | C15—C24 | 1.5293 (18) |
| C2—C3 | 1.3620 (17) | C15—C16 | 1.5382 (17) |
| C2—H2 | 0.9500 | C16—C17 | 1.4932 (17) |
| C3—C4 | 1.4144 (18) | C16—H16A | 0.9900 |
| C3—H3 | 0.9500 | C16—H16B | 0.9900 |
| C4—C5 | 1.4195 (17) | C18—C19 | 1.3886 (17) |
| C4—C9 | 1.4287 (17) | C18—C23 | 1.3964 (17) |
| C5—C6 | 1.3659 (19) | C19—C20 | 1.3902 (19) |
| C5—H5 | 0.9500 | C19—H19 | 0.9500 |
| C6—C7 | 1.4062 (19) | C20—C21 | 1.3800 (19) |
| C6—H6 | 0.9500 | C20—H20 | 0.9500 |

| | | | |
|---|---|---|---|
| C7—C8 | 1.3689 (17) | C21—C22 | 1.3916 (18) |
| C7—H7 | 0.9500 | C21—H21 | 0.9500 |
| C8—C9 | 1.4167 (17) | C22—C23 | 1.3805 (18) |
| C8—H8 | 0.9500 | C22—H22 | 0.9500 |
| C9—C10 | 1.4328 (16) | C23—H23 | 0.9500 |
| C10—C11 | 1.5210 (16) | C24—H24A | 0.9800 |
| C11—C12 | 1.5084 (16) | C24—H24B | 0.9800 |
| C11—C18 | 1.5298 (17) | C24—H24C | 0.9800 |
| C11—H11 | 1.0000 | C25—H25A | 0.9800 |
| C12—C17 | 1.3367 (16) | C25—H25B | 0.9800 |
| C12—C13 | 1.4730 (17) | C25—H25C | 0.9800 |
| C13—C14 | 1.5104 (17) | | |

| | | | |
|---|---|---|---|
| C17—O1—C1 | 117.38 (9) | C15—C14—H14B | 108.8 |
| C10—C1—O1 | 122.50 (10) | H14A—C14—H14B | 107.7 |
| C10—C1—C2 | 123.34 (11) | C25—C15—C24 | 109.07 (11) |
| O1—C1—C2 | 114.16 (10) | C25—C15—C14 | 110.56 (11) |
| C3—C2—C1 | 119.12 (11) | C24—C15—C14 | 109.76 (11) |
| C3—C2—H2 | 120.4 | C25—C15—C16 | 108.86 (11) |
| C1—C2—H2 | 120.4 | C24—C15—C16 | 111.11 (10) |
| C2—C3—C4 | 120.76 (11) | C14—C15—C16 | 107.46 (10) |
| C2—C3—H3 | 119.6 | C17—C16—C15 | 112.02 (10) |
| C4—C3—H3 | 119.6 | C17—C16—H16A | 109.2 |
| C3—C4—C5 | 121.59 (11) | C15—C16—H16A | 109.2 |
| C3—C4—C9 | 119.45 (11) | C17—C16—H16B | 109.2 |
| C5—C4—C9 | 118.96 (11) | C15—C16—H16B | 109.2 |
| C6—C5—C4 | 120.98 (12) | H16A—C16—H16B | 107.9 |
| C6—C5—H5 | 119.5 | C12—C17—O1 | 122.42 (11) |
| C4—C5—H5 | 119.5 | C12—C17—C16 | 125.56 (11) |
| C5—C6—C7 | 120.07 (12) | O1—C17—C16 | 111.98 (10) |
| C5—C6—H6 | 120.0 | C19—C18—C23 | 118.23 (12) |
| C7—C6—H6 | 120.0 | C19—C18—C11 | 121.73 (10) |
| C8—C7—C6 | 120.65 (12) | C23—C18—C11 | 120.04 (11) |
| C8—C7—H7 | 119.7 | C18—C19—C20 | 120.59 (12) |
| C6—C7—H7 | 119.7 | C18—C19—H19 | 119.7 |
| C7—C8—C9 | 121.00 (11) | C20—C19—H19 | 119.7 |
| C7—C8—H8 | 119.5 | C21—C20—C19 | 120.56 (12) |
| C9—C8—H8 | 119.5 | C21—C20—H20 | 119.7 |
| C8—C9—C4 | 118.34 (11) | C19—C20—H20 | 119.7 |
| C8—C9—C10 | 122.35 (10) | C20—C21—C22 | 119.49 (13) |
| C4—C9—C10 | 119.31 (11) | C20—C21—H21 | 120.3 |
| C1—C10—C9 | 117.94 (10) | C22—C21—H21 | 120.3 |
| C1—C10—C11 | 119.67 (10) | C23—C22—C21 | 119.78 (12) |
| C9—C10—C11 | 122.36 (10) | C23—C22—H22 | 120.1 |
| C12—C11—C10 | 108.68 (9) | C21—C22—H22 | 120.1 |
| C12—C11—C18 | 109.88 (10) | C22—C23—C18 | 121.36 (11) |
| C10—C11—C18 | 110.04 (10) | C22—C23—H23 | 119.3 |
| C12—C11—H11 | 109.4 | C18—C23—H23 | 119.3 |

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| C10—C11—H11 | 109.4 | C15—C24—H24A | 109.5 |
| C18—C11—H11 | 109.4 | C15—C24—H24B | 109.5 |
| C17—C12—C13 | 118.84 (11) | H24A—C24—H24B | 109.5 |
| C17—C12—C11 | 121.87 (10) | C15—C24—H24C | 109.5 |
| C13—C12—C11 | 119.12 (10) | H24A—C24—H24C | 109.5 |
| O2—C13—C12 | 120.62 (11) | H24B—C24—H24C | 109.5 |
| O2—C13—C14 | 121.87 (11) | C15—C25—H25A | 109.5 |
| C12—C13—C14 | 117.49 (10) | C15—C25—H25B | 109.5 |
| C13—C14—C15 | 113.72 (10) | H25A—C25—H25B | 109.5 |
| C13—C14—H14A | 108.8 | C15—C25—H25C | 109.5 |
| C15—C14—H14A | 108.8 | H25A—C25—H25C | 109.5 |
| C13—C14—H14B | 108.8 | H25B—C25—H25C | 109.5 |

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| C17—O1—C1—C10 | −15.68 (17) | C18—C11—C12—C13 | −81.65 (13) |
| C17—O1—C1—C2 | 163.81 (11) | C17—C12—C13—O2 | 177.56 (12) |
| C10—C1—C2—C3 | 2.0 (2) | C11—C12—C13—O2 | −7.11 (18) |
| O1—C1—C2—C3 | −177.51 (11) | C17—C12—C13—C14 | −0.99 (17) |
| C1—C2—C3—C4 | 0.5 (2) | C11—C12—C13—C14 | 174.34 (11) |
| C2—C3—C4—C5 | 177.48 (13) | O2—C13—C14—C15 | 150.16 (12) |
| C2—C3—C4—C9 | −1.5 (2) | C12—C13—C14—C15 | −31.31 (16) |
| C3—C4—C5—C6 | −179.36 (13) | C13—C14—C15—C25 | 174.07 (11) |
| C9—C4—C5—C6 | −0.4 (2) | C13—C14—C15—C24 | −65.56 (14) |
| C4—C5—C6—C7 | 0.1 (2) | C13—C14—C15—C16 | 55.38 (14) |
| C5—C6—C7—C8 | 0.0 (2) | C25—C15—C16—C17 | −169.02 (10) |
| C6—C7—C8—C9 | 0.19 (19) | C24—C15—C16—C17 | 70.84 (13) |
| C7—C8—C9—C4 | −0.50 (18) | C14—C15—C16—C17 | −49.25 (14) |
| C7—C8—C9—C10 | 178.98 (12) | C13—C12—C17—O1 | −176.11 (11) |
| C3—C4—C9—C8 | 179.59 (11) | C11—C12—C17—O1 | 8.69 (19) |
| C5—C4—C9—C8 | 0.59 (18) | C13—C12—C17—C16 | 6.36 (19) |
| C3—C4—C9—C10 | 0.09 (18) | C11—C12—C17—C16 | −168.84 (11) |
| C5—C4—C9—C10 | −178.91 (12) | C1—O1—C17—C12 | 14.15 (18) |
| O1—C1—C10—C9 | 176.12 (11) | C1—O1—C17—C16 | −168.01 (10) |
| C2—C1—C10—C9 | −3.32 (19) | C15—C16—C17—C12 | 20.60 (18) |
| O1—C1—C10—C11 | −5.42 (18) | C15—C16—C17—O1 | −157.15 (10) |
| C2—C1—C10—C11 | 175.13 (11) | C12—C11—C18—C19 | 127.33 (11) |
| C8—C9—C10—C1 | −177.25 (11) | C10—C11—C18—C19 | −113.03 (12) |
| C4—C9—C10—C1 | 2.23 (18) | C12—C11—C18—C23 | −53.01 (13) |
| C8—C9—C10—C11 | 4.34 (18) | C10—C11—C18—C23 | 66.63 (13) |
| C4—C9—C10—C11 | −176.19 (11) | C23—C18—C19—C20 | −0.39 (17) |
| C1—C10—C11—C12 | 24.78 (15) | C11—C18—C19—C20 | 179.28 (11) |
| C9—C10—C11—C12 | −156.83 (11) | C18—C19—C20—C21 | 0.21 (19) |
| C1—C10—C11—C18 | −95.58 (13) | C19—C20—C21—C22 | 0.06 (18) |
| C9—C10—C11—C18 | 82.81 (14) | C20—C21—C22—C23 | −0.13 (18) |
| C10—C11—C12—C17 | −26.92 (16) | C21—C22—C23—C18 | −0.05 (18) |
| C18—C11—C12—C17 | 93.53 (13) | C19—C18—C23—C22 | 0.31 (16) |
| C10—C11—C12—C13 | 157.90 (11) | C11—C18—C23—C22 | −179.36 (10) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C8—H8···O2$^{i}$ | 0.95 | 2.49 | 3.366 (2) | 154 |

Symmetry code: (i) −*x*+2, −*y*, −*z*+1.