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# Dimethyl 3,3-dimethoxy-4,4′-methylene-di-2-naphthoate

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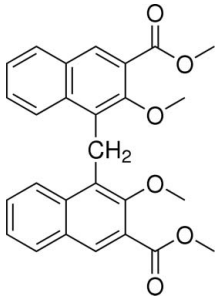
Key indicators: single-crystal X-ray study; $T$ = 153 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.036; $wR$ factor = 0.099; data-to-parameter ratio = 16.5.

In the title compound, $C_{27}H_{24}O_6$, the two naphthalene ring systems are nearly perpendicular to one another with a dihedral angle of 87.77 (2)°. The molecular structure is stabilized by several C—H···O intramolecular hydrogen bonds. In the crystal structure, inversion-related molecules are linked through $\pi$–$\pi$ interactions [centroid–centroid distance = 3.6311 (6) Å and perpendicular distance between unsubstituted aromatic rings = 3.476 Å] between the naphthalene ring systems and also by C—H···$\pi$ interactions. In addition, C—H···O intermolecular interactions are observed.

## Related literature

For synthesis, see: Georghiou *et al.* (1996). For related structures, see: Haynes *et al.* (2006) and Liu *et al.* (2006).



## Experimental

### Crystal data

$C_{27}H_{24}O_6$
$M_r$ = 444.46
Monoclinic, $P2_1/c$
$a$ = 12.9871 (4) Å
$b$ = 20.0999 (5) Å
$c$ = 8.7466 (3) Å
$\beta$ = 106.798 (1)°
$V$ = 2185.78 (11) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 153 (2) K
0.59 × 0.58 × 0.58 mm

### Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: none
21180 measured reflections
5007 independent reflections
4617 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.021

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.099
$S$ = 1.01
5007 reflections
303 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

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

*Cg*1 is the centroid of the C4–C9 ring and *Cg*2 is the centroid of the C15/C16/C21–C24 ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C8—H8···O4 | 0.95 | 2.19 | 3.0871 (13) | 158 |
| C11—H11*A*···O3 | 0.98 | 2.47 | 3.1107 (15) | 123 |
| C14—H14*A*···O1 | 0.99 | 2.42 | 2.8830 (13) | 108 |
| C14—H14*B*···O4 | 0.99 | 2.41 | 2.8768 (12) | 108 |
| C17—H17···O1 | 0.95 | 2.31 | 3.2206 (13) | 161 |
| C19—H19···O3$^{i}$ | 0.95 | 2.58 | 3.2069 (14) | 124 |
| C22—H22···O6$^{ii}$ | 0.95 | 2.53 | 3.4172 (13) | 156 |
| C25—H25*A*···O6 | 0.98 | 2.49 | 3.1471 (15) | 124 |
| C5—H5···*Cg*2$^{iii}$ | 0.95 | 2.82 | 3.6488 (12) | 146 |
| C11—H11*B*···*Cg*2$^{iv}$ | 0.98 | 2.78 | 3.5780 (13) | 139 |

Symmetry codes: (i) $-x, -y+1, -z$; (ii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (iii) $-x+1, -y+1, -z+1$; (iv) $-x, -y+1, -z+1$.

Data collection: *RAPID-AUTO* (Rigaku/MSC, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2414).

## References

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# supplementary materials

*Acta Cryst.* (2007). E**63**, o3508 [ **doi:10.1107/S1600536807033909** ]

# Dimethyl 3,3-dimethoxy-4,4'-methylenedi-2-naphthoate

**R. He, E. Gao, S.-J. Gu and D.-B. Qin**

## Comment

Pamoic acid or its derivatives or analogs are used in the pharmaceutical industry for the preparation of medicaments for the treatment of diseases characterized by deposits of amyloid aggregates. We report here the crystal structure of the title compound.

Bond lengths and angles in the title molecule (Fig. 1) are within normal ranges. Both naphthalene ring systems are slightly non-planar, with the dihedral angle between the two benzene rings being 5.06 (4)° for the C1—C10 ring system and 3.92 (3)° for the C15—C24 ring system. The two naphthalene ring systems are almost perpendicular, with a dihedral angle of 87.77 (2)°.

The molecular structure is stabilized by C—H···O hydrogen bonds (Table 1). The crystal structure is stabilized by π-π interactions between the naphthalene ring systems of the inversion related molecules, with a $Cg1\cdots Cg1^{i}$ distance of 3.6311 (6) Å [symmetry code: (i) $1-x, 1-y, 1-z$] where *Cg*1 is the C4—C9 ring centroid. In addition, weak C—H···O intermolecular hydrogen bonds and C—H···π interactions involving the C15/C16/C21—C24 ring (centroid *Cg*2) are observed (Table 1).

## Experimental

The title compound was prepared according to the reported procedure of Georghiou *et al.* (1996). Colourless single crystals suitable for X-ray diffraction were obtained by recrystallization from dichloromethane.

## Refinement

H atoms were placed in calculated positions with C—H = 0.95–0.99 Å, and refined in riding mode with $U_{iso}(H) = 1.2U_{eq}(C)$.

## Figures

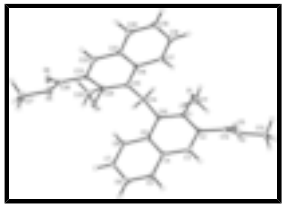


Fig. 1. The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atomic numbering.

## Dimethyl 3,3-dimethoxy-4,4'-methylenedi-2-naphthoate

*Crystal data*

$C_{27}H_{24}O_6$ $F_{000} = 936$

| | |
|---|---|
| $M_r$ = 444.46 | $D_x$ = 1.351 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 19190 reflections |
| $a$ = 12.9871 (4) Å | θ = 3.0–27.5º |
| $b$ = 20.0999 (5) Å | μ = 0.10 mm$^{-1}$ |
| $c$ = 8.7466 (3) Å | $T$ = 153 (2) K |
| β = 106.798 (1)º | Block, colourless |
| $V$ = 2185.78 (11) Å$^3$ | 0.59 × 0.58 × 0.58 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Rigaku R-AXIS RAPID diffractometer | 4617 reflections with $I > 2\sigma(I)$ |
| Radiation source: Rotating Anode | $R_{int}$ = 0.021 |
| Monochromator: graphite | $\theta_{max}$ = 27.5º |
| $T$ = 153(2) K | $\theta_{min}$ = 3.2º |
| ω scans | $h$ = −14→16 |
| Absorption correction: none | $k$ = −25→26 |
| 21180 measured reflections | $l$ = −11→11 |
| 5007 independent reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)]$ = 0.036 | $w = 1/[\sigma^2(F_o^2) + (0.056P)^2 + 0.7416P]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2)$ = 0.099 | $(\Delta/\sigma)_{max}$ = 0.001 |
| $S$ = 1.01 | $\Delta\rho_{max}$ = 0.33 e Å$^{-3}$ |
| 5007 reflections | $\Delta\rho_{min}$ = −0.20 e Å$^{-3}$ |
| 303 parameters | Extinction correction: SHELXL97,<br>$Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.0128 (11) |
| Secondary atom site location: difference Fourier map | |

*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 $F^2 > 2\text{sigma}(F^2)$ is used only for calculat-

ing *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 | 0.08724 (6) | 0.39859 (4) | 0.27018 (9) | 0.02037 (17) |
| O2 | 0.25890 (7) | 0.35292 (4) | −0.02411 (9) | 0.02536 (18) |
| O3 | 0.14283 (7) | 0.29602 (4) | 0.07285 (9) | 0.02582 (18) |
| O4 | 0.27501 (6) | 0.52935 (4) | 0.87194 (8) | 0.01955 (16) |
| O5 | 0.42601 (7) | 0.69099 (5) | 0.89705 (11) | 0.0326 (2) |
| O6 | 0.30271 (7) | 0.66608 (4) | 1.02247 (10) | 0.0298 (2) |
| C1 | 0.19780 (8) | 0.39958 (5) | 0.33629 (12) | 0.0168 (2) |
| C2 | 0.26229 (8) | 0.37440 (5) | 0.24159 (12) | 0.0180 (2) |
| C3 | 0.37214 (8) | 0.38001 (5) | 0.29508 (12) | 0.0197 (2) |
| H3 | 0.4143 | 0.3669 | 0.2278 | 0.024* |
| C4 | 0.42325 (8) | 0.40517 (5) | 0.44938 (12) | 0.0184 (2) |
| C5 | 0.53713 (8) | 0.40633 (5) | 0.50967 (13) | 0.0226 (2) |
| H5 | 0.5795 | 0.3926 | 0.4431 | 0.027* |
| C6 | 0.58662 (9) | 0.42690 (6) | 0.66216 (14) | 0.0251 (2) |
| H6 | 0.6629 | 0.4274 | 0.7014 | 0.030* |
| C7 | 0.52378 (9) | 0.44744 (5) | 0.76095 (13) | 0.0235 (2) |
| H7 | 0.5582 | 0.4608 | 0.8677 | 0.028* |
| C8 | 0.41346 (8) | 0.44845 (5) | 0.70490 (12) | 0.0197 (2) |
| H8 | 0.3728 | 0.4629 | 0.7732 | 0.024* |
| C9 | 0.35920 (8) | 0.42820 (5) | 0.54631 (12) | 0.0165 (2) |
| C10 | 0.24400 (8) | 0.42940 (5) | 0.48266 (11) | 0.01613 (19) |
| C11 | 0.03374 (9) | 0.34490 (6) | 0.32574 (15) | 0.0265 (2) |
| H11A | 0.0530 | 0.3025 | 0.2859 | 0.032* |
| H11B | −0.0443 | 0.3513 | 0.2863 | 0.032* |
| H11C | 0.0561 | 0.3444 | 0.4428 | 0.032* |
| C12 | 0.21234 (8) | 0.33737 (5) | 0.09015 (12) | 0.0188 (2) |
| C13 | 0.22256 (10) | 0.31315 (6) | −0.16796 (13) | 0.0273 (2) |
| H13A | 0.2351 | 0.2660 | −0.1407 | 0.033* |
| H13B | 0.2625 | 0.3259 | −0.2429 | 0.033* |
| H13C | 0.1456 | 0.3207 | −0.2175 | 0.033* |
| C14 | 0.17457 (8) | 0.46359 (5) | 0.57397 (12) | 0.01689 (19) |
| H14A | 0.0979 | 0.4546 | 0.5187 | 0.020* |
| H14B | 0.1911 | 0.4441 | 0.6823 | 0.020* |
| C15 | 0.19164 (8) | 0.53865 (5) | 0.58891 (11) | 0.01617 (19) |
| C16 | 0.15427 (8) | 0.58152 (5) | 0.45237 (12) | 0.0166 (2) |
| C17 | 0.08944 (8) | 0.55826 (5) | 0.30175 (12) | 0.0196 (2) |
| H17 | 0.0715 | 0.5124 | 0.2881 | 0.024* |
| C18 | 0.05245 (9) | 0.60128 (6) | 0.17562 (13) | 0.0226 (2) |
| H18 | 0.0080 | 0.5849 | 0.0767 | 0.027* |
| C19 | 0.07947 (9) | 0.66946 (6) | 0.19073 (13) | 0.0247 (2) |
| H19 | 0.0548 | 0.6984 | 0.1018 | 0.030* |
| C20 | 0.14131 (9) | 0.69356 (5) | 0.33394 (13) | 0.0229 (2) |

| | | | | |
|---|---|---|---|---|
| H20 | 0.1590 | 0.7395 | 0.3442 | 0.028* |
| C21 | 0.17943 (8) | 0.65081 (5) | 0.46755 (12) | 0.0179 (2) |
| C22 | 0.24206 (8) | 0.67646 (5) | 0.61591 (12) | 0.0192 (2) |
| H22 | 0.2636 | 0.7218 | 0.6244 | 0.023* |
| C23 | 0.27166 (8) | 0.63584 (5) | 0.74749 (12) | 0.0178 (2) |
| C24 | 0.24304 (8) | 0.56738 (5) | 0.73454 (11) | 0.01641 (19) |
| C25 | 0.19433 (9) | 0.52489 (6) | 0.95462 (13) | 0.0262 (2) |
| H25A | 0.1782 | 0.5695 | 0.9866 | 0.031* |
| H25B | 0.2210 | 0.4970 | 1.0498 | 0.031* |
| H25C | 0.1288 | 0.5051 | 0.8839 | 0.031* |
| C26 | 0.33310 (9) | 0.66448 (5) | 0.90516 (13) | 0.0205 (2) |
| C27 | 0.48928 (11) | 0.72350 (7) | 1.04184 (18) | 0.0421 (3) |
| H27A | 0.4460 | 0.7583 | 1.0722 | 0.051* |
| H27B | 0.5534 | 0.7435 | 1.0231 | 0.051* |
| H27C | 0.5112 | 0.6907 | 1.1280 | 0.051* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0163 (4) | 0.0186 (4) | 0.0240 (4) | −0.0002 (3) | 0.0023 (3) | −0.0011 (3) |
| O2 | 0.0339 (4) | 0.0249 (4) | 0.0193 (4) | −0.0056 (3) | 0.0107 (3) | −0.0059 (3) |
| O3 | 0.0295 (4) | 0.0255 (4) | 0.0205 (4) | −0.0067 (3) | 0.0042 (3) | −0.0030 (3) |
| O4 | 0.0234 (4) | 0.0196 (4) | 0.0162 (3) | 0.0032 (3) | 0.0066 (3) | 0.0020 (3) |
| O5 | 0.0227 (4) | 0.0363 (5) | 0.0373 (5) | −0.0077 (3) | 0.0063 (3) | −0.0119 (4) |
| O6 | 0.0398 (5) | 0.0280 (4) | 0.0219 (4) | −0.0035 (3) | 0.0092 (3) | −0.0062 (3) |
| C1 | 0.0170 (5) | 0.0138 (4) | 0.0187 (5) | 0.0009 (3) | 0.0038 (4) | 0.0012 (3) |
| C2 | 0.0222 (5) | 0.0144 (4) | 0.0169 (4) | 0.0007 (4) | 0.0050 (4) | −0.0004 (3) |
| C3 | 0.0220 (5) | 0.0181 (5) | 0.0209 (5) | 0.0014 (4) | 0.0090 (4) | −0.0018 (4) |
| C4 | 0.0187 (5) | 0.0163 (4) | 0.0206 (5) | 0.0009 (4) | 0.0062 (4) | 0.0001 (4) |
| C5 | 0.0191 (5) | 0.0242 (5) | 0.0256 (5) | 0.0014 (4) | 0.0082 (4) | −0.0023 (4) |
| C6 | 0.0164 (5) | 0.0291 (6) | 0.0278 (5) | 0.0004 (4) | 0.0035 (4) | −0.0014 (4) |
| C7 | 0.0228 (5) | 0.0246 (5) | 0.0201 (5) | 0.0008 (4) | 0.0015 (4) | −0.0023 (4) |
| C8 | 0.0216 (5) | 0.0185 (5) | 0.0186 (5) | 0.0029 (4) | 0.0051 (4) | −0.0010 (4) |
| C9 | 0.0180 (5) | 0.0130 (4) | 0.0183 (5) | 0.0010 (3) | 0.0050 (4) | 0.0007 (3) |
| C10 | 0.0185 (5) | 0.0127 (4) | 0.0176 (4) | 0.0010 (3) | 0.0059 (4) | 0.0010 (3) |
| C11 | 0.0212 (5) | 0.0240 (5) | 0.0354 (6) | −0.0051 (4) | 0.0101 (4) | −0.0036 (4) |
| C12 | 0.0216 (5) | 0.0162 (5) | 0.0173 (5) | 0.0034 (4) | 0.0037 (4) | 0.0006 (3) |
| C13 | 0.0348 (6) | 0.0291 (6) | 0.0182 (5) | −0.0013 (5) | 0.0077 (4) | −0.0067 (4) |
| C14 | 0.0176 (5) | 0.0156 (4) | 0.0185 (4) | 0.0002 (3) | 0.0067 (4) | −0.0009 (3) |
| C15 | 0.0155 (4) | 0.0156 (4) | 0.0189 (5) | 0.0019 (3) | 0.0075 (4) | 0.0000 (3) |
| C16 | 0.0149 (4) | 0.0184 (5) | 0.0183 (5) | 0.0031 (3) | 0.0075 (4) | 0.0005 (4) |
| C17 | 0.0185 (5) | 0.0200 (5) | 0.0209 (5) | 0.0022 (4) | 0.0066 (4) | −0.0014 (4) |
| C18 | 0.0196 (5) | 0.0288 (6) | 0.0187 (5) | 0.0030 (4) | 0.0042 (4) | −0.0001 (4) |
| C19 | 0.0238 (5) | 0.0269 (5) | 0.0231 (5) | 0.0041 (4) | 0.0061 (4) | 0.0084 (4) |
| C20 | 0.0225 (5) | 0.0204 (5) | 0.0268 (5) | 0.0015 (4) | 0.0084 (4) | 0.0061 (4) |
| C21 | 0.0164 (4) | 0.0188 (5) | 0.0204 (5) | 0.0024 (4) | 0.0082 (4) | 0.0020 (4) |
| C22 | 0.0194 (5) | 0.0163 (4) | 0.0237 (5) | 0.0003 (4) | 0.0090 (4) | −0.0003 (4) |
| C23 | 0.0167 (4) | 0.0179 (5) | 0.0197 (5) | 0.0012 (3) | 0.0068 (4) | −0.0023 (4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C24 | 0.0162 (4) | 0.0166 (4) | 0.0176 (4) | 0.0029 (3) | 0.0067 (4) | 0.0007 (3) |
| C25 | 0.0307 (6) | 0.0294 (6) | 0.0218 (5) | −0.0025 (4) | 0.0126 (4) | 0.0014 (4) |
| C26 | 0.0214 (5) | 0.0146 (4) | 0.0238 (5) | 0.0028 (4) | 0.0037 (4) | −0.0018 (4) |
| C27 | 0.0305 (6) | 0.0385 (7) | 0.0486 (8) | −0.0085 (5) | −0.0023 (6) | −0.0164 (6) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C1 | 1.3843 (12) | C11—H11C | 0.98 |
| O1—C11 | 1.4419 (13) | C13—H13A | 0.98 |
| O2—C12 | 1.3459 (13) | C13—H13B | 0.98 |
| O2—C13 | 1.4497 (12) | C13—H13C | 0.98 |
| O3—C12 | 1.2040 (13) | C14—C15 | 1.5250 (13) |
| O4—C24 | 1.3829 (11) | C14—H14A | 0.99 |
| O4—C25 | 1.4377 (13) | C14—H14B | 0.99 |
| O5—C26 | 1.3396 (14) | C15—C24 | 1.3821 (13) |
| O5—C27 | 1.4507 (15) | C15—C16 | 1.4385 (13) |
| O6—C26 | 1.2015 (13) | C16—C17 | 1.4219 (14) |
| C1—C10 | 1.3836 (13) | C16—C21 | 1.4280 (14) |
| C1—C2 | 1.4299 (14) | C17—C18 | 1.3745 (14) |
| C2—C3 | 1.3715 (14) | C17—H17 | 0.95 |
| C2—C12 | 1.4943 (13) | C18—C19 | 1.4114 (16) |
| C3—C4 | 1.4142 (14) | C18—H18 | 0.95 |
| C3—H3 | 0.95 | C19—C20 | 1.3665 (16) |
| C4—C5 | 1.4196 (14) | C19—H19 | 0.95 |
| C4—C9 | 1.4257 (14) | C20—C21 | 1.4194 (14) |
| C5—C6 | 1.3665 (15) | C20—H20 | 0.95 |
| C5—H5 | 0.95 | C21—C22 | 1.4146 (14) |
| C6—C7 | 1.4108 (16) | C22—C23 | 1.3724 (14) |
| C6—H6 | 0.95 | C22—H22 | 0.95 |
| C7—C8 | 1.3738 (15) | C23—C24 | 1.4213 (14) |
| C7—H7 | 0.95 | C23—C26 | 1.4946 (14) |
| C8—C9 | 1.4217 (14) | C25—H25A | 0.98 |
| C8—H8 | 0.95 | C25—H25B | 0.98 |
| C9—C10 | 1.4379 (13) | C25—H25C | 0.98 |
| C10—C14 | 1.5295 (13) | C27—H27A | 0.98 |
| C11—H11A | 0.98 | C27—H27B | 0.98 |
| C11—H11B | 0.98 | C27—H27C | 0.98 |
| C1—O1—C11 | 114.37 (8) | C15—C14—H14A | 108.9 |
| C12—O2—C13 | 114.39 (8) | C10—C14—H14A | 108.9 |
| C24—O4—C25 | 113.09 (8) | C15—C14—H14B | 108.9 |
| C26—O5—C27 | 115.13 (10) | C10—C14—H14B | 108.9 |
| C10—C1—O1 | 120.85 (9) | H14A—C14—H14B | 107.7 |
| C10—C1—C2 | 121.29 (9) | C24—C15—C16 | 118.17 (9) |
| O1—C1—C2 | 117.60 (9) | C24—C15—C14 | 120.79 (9) |
| C3—C2—C1 | 119.93 (9) | C16—C15—C14 | 121.04 (9) |
| C3—C2—C12 | 119.05 (9) | C17—C16—C21 | 117.72 (9) |
| C1—C2—C12 | 120.86 (9) | C17—C16—C15 | 122.66 (9) |
| C2—C3—C4 | 120.66 (9) | C21—C16—C15 | 119.59 (9) |
| C2—C3—H3 | 119.7 | C18—C17—C16 | 120.86 (10) |

| | | | |
|---|---|---|---|
| C4—C3—H3 | 119.7 | C18—C17—H17 | 119.6 |
| C3—C4—C5 | 120.78 (9) | C16—C17—H17 | 119.6 |
| C3—C4—C9 | 119.34 (9) | C17—C18—C19 | 121.06 (10) |
| C5—C4—C9 | 119.86 (9) | C17—C18—H18 | 119.5 |
| C6—C5—C4 | 120.88 (10) | C19—C18—H18 | 119.5 |
| C6—C5—H5 | 119.6 | C20—C19—C18 | 119.62 (10) |
| C4—C5—H5 | 119.6 | C20—C19—H19 | 120.2 |
| C5—C6—C7 | 119.61 (10) | C18—C19—H19 | 120.2 |
| C5—C6—H6 | 120.2 | C19—C20—C21 | 120.86 (10) |
| C7—C6—H6 | 120.2 | C19—C20—H20 | 119.6 |
| C8—C7—C6 | 120.93 (10) | C21—C20—H20 | 119.6 |
| C8—C7—H7 | 119.5 | C22—C21—C20 | 120.39 (9) |
| C6—C7—H7 | 119.5 | C22—C21—C16 | 119.75 (9) |
| C7—C8—C9 | 121.04 (9) | C20—C21—C16 | 119.86 (9) |
| C7—C8—H8 | 119.5 | C23—C22—C21 | 119.99 (9) |
| C9—C8—H8 | 119.5 | C23—C22—H22 | 120.0 |
| C8—C9—C4 | 117.60 (9) | C21—C22—H22 | 120.0 |
| C8—C9—C10 | 122.67 (9) | C22—C23—C24 | 120.38 (9) |
| C4—C9—C10 | 119.72 (9) | C22—C23—C26 | 119.35 (9) |
| C1—C10—C9 | 118.39 (9) | C24—C23—C26 | 120.26 (9) |
| C1—C10—C14 | 120.95 (9) | C15—C24—O4 | 120.91 (9) |
| C9—C10—C14 | 120.66 (8) | C15—C24—C23 | 121.57 (9) |
| O1—C11—H11A | 109.5 | O4—C24—C23 | 117.38 (9) |
| O1—C11—H11B | 109.5 | O4—C25—H25A | 109.5 |
| H11A—C11—H11B | 109.5 | O4—C25—H25B | 109.5 |
| O1—C11—H11C | 109.5 | H25A—C25—H25B | 109.5 |
| H11A—C11—H11C | 109.5 | O4—C25—H25C | 109.5 |
| H11B—C11—H11C | 109.5 | H25A—C25—H25C | 109.5 |
| O3—C12—O2 | 123.26 (9) | H25B—C25—H25C | 109.5 |
| O3—C12—C2 | 124.95 (9) | O6—C26—O5 | 123.90 (10) |
| O2—C12—C2 | 111.68 (9) | O6—C26—C23 | 125.36 (10) |
| O2—C13—H13A | 109.5 | O5—C26—C23 | 110.69 (9) |
| O2—C13—H13B | 109.5 | O5—C27—H27A | 109.5 |
| H13A—C13—H13B | 109.5 | O5—C27—H27B | 109.5 |
| O2—C13—H13C | 109.5 | H27A—C27—H27B | 109.5 |
| H13A—C13—H13C | 109.5 | O5—C27—H27C | 109.5 |
| H13B—C13—H13C | 109.5 | H27A—C27—H27C | 109.5 |
| C15—C14—C10 | 113.34 (8) | H27B—C27—H27C | 109.5 |
| C11—O1—C1—C10 | −84.36 (11) | C10—C14—C15—C24 | −109.68 (10) |
| C11—O1—C1—C2 | 101.37 (10) | C10—C14—C15—C16 | 70.68 (11) |
| C10—C1—C2—C3 | −0.43 (15) | C24—C15—C16—C17 | −172.29 (9) |
| O1—C1—C2—C3 | 173.81 (9) | C14—C15—C16—C17 | 7.37 (14) |
| C10—C1—C2—C12 | 174.96 (9) | C24—C15—C16—C21 | 5.58 (13) |
| O1—C1—C2—C12 | −10.80 (13) | C14—C15—C16—C21 | −174.77 (9) |
| C1—C2—C3—C4 | 5.60 (15) | C21—C16—C17—C18 | −0.05 (14) |
| C12—C2—C3—C4 | −169.88 (9) | C15—C16—C17—C18 | 177.86 (9) |
| C2—C3—C4—C5 | 175.19 (10) | C16—C17—C18—C19 | 1.32 (16) |
| C2—C3—C4—C9 | −3.41 (15) | C17—C18—C19—C20 | −1.53 (17) |
| C3—C4—C5—C6 | −176.06 (10) | C18—C19—C20—C21 | 0.45 (16) |

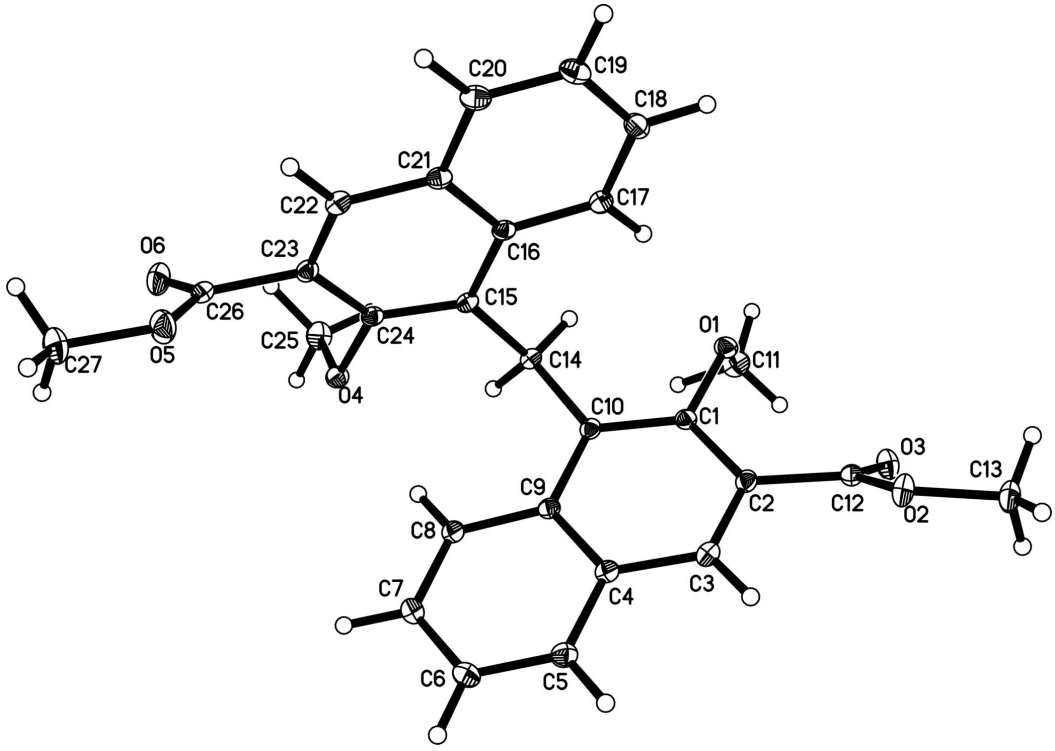
| | | | |
|---|---|---|---|
| C9—C4—C5—C6 | 2.54 (16) | C19—C20—C21—C22 | −179.06 (10) |
| C4—C5—C6—C7 | −0.18 (17) | C19—C20—C21—C16 | 0.81 (15) |
| C5—C6—C7—C8 | −1.44 (17) | C17—C16—C21—C22 | 178.87 (9) |
| C6—C7—C8—C9 | 0.66 (16) | C15—C16—C21—C22 | 0.89 (14) |
| C7—C8—C9—C4 | 1.67 (15) | C17—C16—C21—C20 | −1.01 (14) |
| C7—C8—C9—C10 | −179.14 (10) | C15—C16—C21—C20 | −178.98 (9) |
| C3—C4—C9—C8 | 175.39 (9) | C20—C21—C22—C23 | 175.03 (9) |
| C5—C4—C9—C8 | −3.22 (14) | C16—C21—C22—C23 | −4.84 (14) |
| C3—C4—C9—C10 | −3.82 (14) | C21—C22—C23—C24 | 2.27 (15) |
| C5—C4—C9—C10 | 177.56 (9) | C21—C22—C23—C26 | −176.94 (9) |
| O1—C1—C10—C9 | 179.26 (8) | C16—C15—C24—O4 | 176.06 (8) |
| C2—C1—C10—C9 | −6.68 (14) | C14—C15—C24—O4 | −3.59 (14) |
| O1—C1—C10—C14 | −1.45 (14) | C16—C15—C24—C23 | −8.33 (14) |
| C2—C1—C10—C14 | 172.60 (9) | C14—C15—C24—C23 | 172.02 (9) |
| C8—C9—C10—C1 | −170.44 (9) | C25—O4—C24—C15 | −90.58 (11) |
| C4—C9—C10—C1 | 8.74 (14) | C25—O4—C24—C23 | 93.63 (10) |
| C8—C9—C10—C14 | 10.28 (14) | C22—C23—C24—C15 | 4.53 (15) |
| C4—C9—C10—C14 | −170.55 (9) | C26—C23—C24—C15 | −176.27 (9) |
| C13—O2—C12—O3 | −3.15 (15) | C22—C23—C24—O4 | −179.71 (9) |
| C13—O2—C12—C2 | 173.30 (9) | C26—C23—C24—O4 | −0.51 (13) |
| C3—C2—C12—O3 | 133.10 (11) | C27—O5—C26—O6 | −0.75 (16) |
| C1—C2—C12—O3 | −42.33 (15) | C27—O5—C26—C23 | 176.75 (10) |
| C3—C2—C12—O2 | −43.28 (13) | C22—C23—C26—O6 | 118.12 (12) |
| C1—C2—C12—O2 | 141.29 (9) | C24—C23—C26—O6 | −61.09 (14) |
| C1—C10—C14—C15 | −113.78 (10) | C22—C23—C26—O5 | −59.33 (12) |
| C9—C10—C14—C15 | 65.48 (12) | C24—C23—C26—O5 | 121.46 (10) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C8—H8···O4 | 0.95 | 2.19 | 3.0871 (13) | 158 |
| C11—H11A···O3 | 0.98 | 2.47 | 3.1107 (15) | 123 |
| C14—H14A···O1 | 0.99 | 2.42 | 2.8830 (13) | 108 |
| C14—H14B···O4 | 0.99 | 2.41 | 2.8768 (12) | 108 |
| C17—H17···O1 | 0.95 | 2.31 | 3.2206 (13) | 161 |
| C19—H19···O3$^{i}$ | 0.95 | 2.58 | 3.2069 (14) | 124 |
| C22—H22···O6$^{ii}$ | 0.95 | 2.53 | 3.4172 (13) | 156 |
| C25—H25A···O6 | 0.98 | 2.49 | 3.1471 (15) | 124 |
| C5—H5···Cg2$^{iii}$ | 0.95 | 2.82 | 3.6488 (12) | 146 |
| C11—H11B···Cg2$^{iv}$ | 0.98 | 2.78 | 3.5780 (13) | 139 |

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

**Fig. 1**


C20
C19
C18
C21
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C14
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C12
O2
C8
C7
C4
C3
C6
C5