# organic compounds

# 1-Phenylethane-1,2-diyl 1,1′-biphenyl-2,2′-dicarboxylate

**Hoong-Kun Fun,**[a]***‡ Ching Kheng Quah**[a]**§ and Dongdong Wu**[b]

[a]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and [b]School of Chemistry and Chemical Engineering, Nanjing University, Nanjing, 210093, People's Republic of China

Correspondence e-mail: hkfun@usm.my

In the title compound, $C_{22}H_{16}O_4$, the 7-phenyl ring is inclined at dihedral angles of 36.73 (9) and 69.37 (9)° with respect to the biphenyl benzene rings. The two benzene rings of the biphenyl unit form a dihedral angle of 55.99 (8)°. There are no significant hydrogen bonds observed in the crystal of this compound.

## Related literature

For a related structure, references to other similar structures and chemical and biological background, see: Fun *et al.* (2012). For the preparation, see: Wu *et al.* (2012).
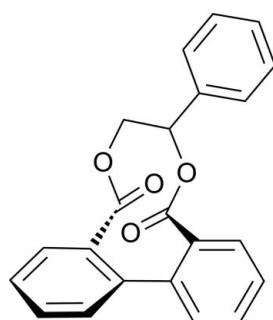
## Experimental

### Crystal data

| | |
|---|---|
| $C_{22}H_{16}O_4$ | $V$ = 3429.5 (4) Å$^3$ |
| $M_r$ = 344.35 | $Z$ = 8 |
| Orthorhombic, $Pbca$ | Mo $K\alpha$ radiation |
| $a$ = 21.2454 (15) Å | $\mu$ = 0.09 mm$^{-1}$ |
| $b$ = 13.2363 (7) Å | $T$ = 296 K |
| $c$ = 12.1954 (7) Å | 0.27 × 0.22 × 0.08 mm |

### Data collection

| | |
|---|---|
| Bruker SMART APEXII DUO CCD diffractometer | 67362 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2009) | 5014 independent reflections |
| $T_{min}$ = 0.976, $T_{max}$ = 0.993 | 2961 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.075 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.044 | 235 parameters |
| $wR(F^2)$ = 0.113 | H-atom parameters constrained |
| $S$ = 0.99 | $\Delta\rho_{max}$ = 0.16 e Å$^{-3}$ |
| 5014 reflections | $\Delta\rho_{min}$ = −0.16 e Å$^{-3}$ |

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

## References

Bruker (2009). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Fun, H.-K., Quah, C. K. & Wu, D. (2012). *Acta Cryst.* E**68**, accepted [IS5123].

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

Wu, D., Wang, L., Xu, K., Song, J., Fun, H-K., Xu, J. & Zhang, Y. (2012). *Chem. Commun.* **48**, 1168–1170.

‡ Thomson Reuters ResearcherID: A-3561-2009.
§ Thomson Reuters ResearcherID: A-5525-2009.

# 1-Phenylethane-1,2-diyl 1,1′-biphenyl-2,2′-dicarboxylate

## Hoong-Kun Fun, Ching Kheng Quah and Dongdong Wu

### S1. Comment

As part of our ongoing synthetic and structural studies of bis-lactones containing a biaryl motif (Wu *et al.*, 2012; Fun *et al.* 2012), we now report the structure of the title compound, (I).

In the title compound, Fig. 1, the terminal benzene ring (C17-C22) inclines at dihedral angles of 36.73 (9) and 69.37 (9)° with the other two benzene rings (C1-C6 and C7-C12), respectively. The two benzene rings form a dihedral angle of 55.99 (8)°.

### S2. Experimental

The title compound was the major diastereoisomer of the photoreaction products of 9,10-phenanthrenedione with styrene via a photocycloaddition-photooxidation sequence. The compound was purified by flash column chromatography with ethyl acetate/petroleum ether (1:9) as eluents. Colourless plates of the title compound was obtained from slow evaporation of an acetone and petroleum ether solution (1:10).

### S3. Refinement

All H atoms were positioned geometrically and refined using a riding model with C–H = 0.93-0.98 Å and $U_{iso}$(H) = 1.2 $U_{eq}$(C).
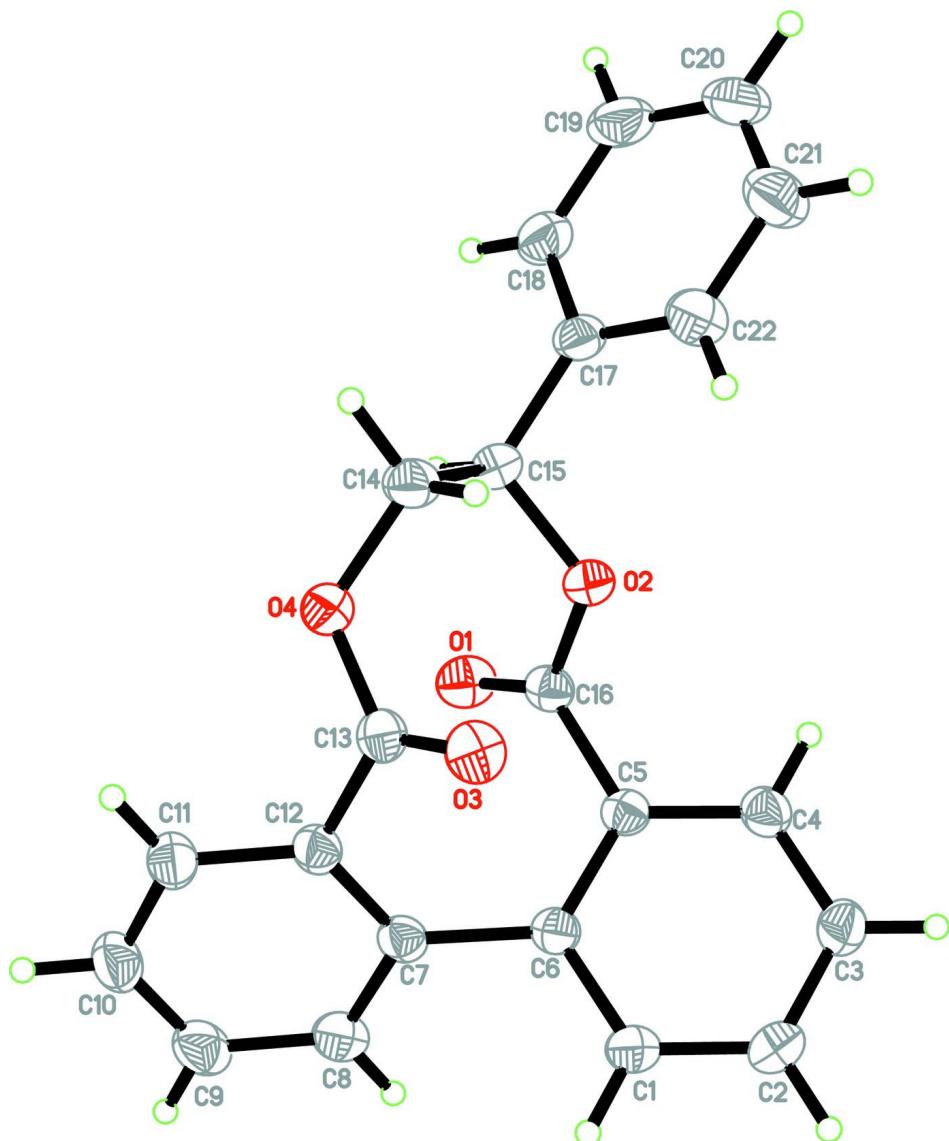
**Figure 1**

The molecular structure of the title compound showing 30% probability displacement ellipsoids for non-H atoms.

**1-Phenylethane-1,2-diyl 1,1′-biphenyl-2,2′-dicarboxylate**

*Crystal data*

| | |
|---|---|
| $C_{22}H_{16}O_4$ | $F(000) = 1440$ |
| $M_r = 344.35$ | $D_x = 1.334$ Mg m$^{-3}$ |
| Orthorhombic, *Pbca* | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2ac 2ab | Cell parameters from 6139 reflections |
| $a = 21.2454$ (15) Å | $\theta = 2.5$–24.0° |
| $b = 13.2363$ (7) Å | $\mu = 0.09$ mm$^{-1}$ |
| $c = 12.1954$ (7) Å | $T = 296$ K |
| $V = 3429.5$ (4) Å$^3$ | Plate, colourless |
| $Z = 8$ | $0.27 \times 0.22 \times 0.08$ mm |

*Data collection*

| | |
|---|---|
| Bruker SMART APEXII DUO CCD diffractometer | 67362 measured reflections |
| Radiation source: fine-focus sealed tube | 5014 independent reflections |
| Graphite monochromator | 2961 reflections with $I > 2\sigma(I)$ |
| $\varphi$ and $\omega$ scans | $R_{int} = 0.075$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2009) | $\theta_{max} = 30.0°$, $\theta_{min} = 1.9°$ |
| | $h = -29 \rightarrow 29$ |
| | $k = -18 \rightarrow 18$ |
| $T_{min} = 0.976$, $T_{max} = 0.993$ | $l = -17 \rightarrow 17$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.044$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.113$ | |
| $S = 0.99$ | H-atom parameters constrained |
| 5014 reflections | $w = 1/[\sigma^2(F_o^2) + (0.0382P)^2 + 0.8815P]$ |
| 235 parameters | where $P = (F_o^2 + 2F_c^2)/3$ |
| 0 restraints | $(\Delta/\sigma)_{max} = 0.001$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{max} = 0.16$ e Å$^{-3}$ |
| | $\Delta\rho_{min} = -0.16$ e Å$^{-3}$ |

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on $F^2$, conventional R-factors R are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2sigma(F^2)$ 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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}*/U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.26894 (5) | 0.00729 (8) | −0.06424 (9) | 0.0525 (3) |
| O2 | 0.28774 (4) | 0.14794 (8) | 0.03621 (8) | 0.0431 (2) |
| O3 | 0.18085 (5) | 0.27892 (8) | −0.05404 (9) | 0.0517 (3) |
| O4 | 0.25786 (5) | 0.22593 (9) | −0.16930 (8) | 0.0494 (3) |
| C1 | 0.07994 (7) | 0.07069 (12) | 0.06878 (12) | 0.0481 (4) |
| H1A | 0.0415 | 0.0732 | 0.0323 | 0.058* |
| C2 | 0.08085 (7) | 0.06903 (14) | 0.18225 (13) | 0.0551 (4) |
| H2A | 0.0432 | 0.0708 | 0.2211 | 0.066* |
| C3 | 0.13733 (8) | 0.06473 (13) | 0.23800 (13) | 0.0525 (4) |
| H3A | 0.1378 | 0.0628 | 0.3142 | 0.063* |
| C4 | 0.19297 (7) | 0.06329 (12) | 0.18020 (12) | 0.0461 (4) |
| H4A | 0.2311 | 0.0611 | 0.2177 | 0.055* |
| C5 | 0.19263 (6) | 0.06515 (10) | 0.06611 (11) | 0.0375 (3) |
| C6 | 0.13535 (6) | 0.06867 (11) | 0.00836 (11) | 0.0382 (3) |
| C7 | 0.13142 (6) | 0.07071 (11) | −0.11413 (11) | 0.0397 (3) |
| C8 | 0.09627 (7) | −0.00380 (13) | −0.16669 (14) | 0.0492 (4) |

| | | | | |
|------|------------|----------------|----------------|------------|
| H8A | 0.0757 | −0.0524 | −0.1250 | 0.059* |
| C9 | 0.09149 (8) | −0.00670 (14) | −0.27979 (15) | 0.0587 (5) |
| H9A | 0.0677 | −0.0569 | −0.3134 | 0.070* |
| C10 | 0.12184 (8) | 0.06460 (15) | −0.34267 (14) | 0.0602 (5) |
| H10A | 0.1185 | 0.0625 | −0.4187 | 0.072* |
| C11 | 0.15715 (7) | 0.13905 (14) | −0.29305 (12) | 0.0511 (4) |
| H11A | 0.1781 | 0.1866 | −0.3357 | 0.061* |
| C12 | 0.16148 (6) | 0.14330 (11) | −0.17924 (11) | 0.0404 (3) |
| C13 | 0.19893 (7) | 0.22471 (12) | −0.12604 (12) | 0.0417 (3) |
| C14 | 0.30724 (7) | 0.26949 (13) | −0.10300 (13) | 0.0508 (4) |
| H14A | 0.2900 | 0.3201 | −0.0539 | 0.061* |
| H14B | 0.3386 | 0.3014 | −0.1493 | 0.061* |
| C15 | 0.33672 (6) | 0.18389 (12) | −0.03764 (12) | 0.0433 (3) |
| H15A | 0.3492 | 0.1293 | −0.0874 | 0.052* |
| C16 | 0.25324 (6) | 0.06640 (11) | 0.00485 (12) | 0.0384 (3) |
| C17 | 0.39237 (6) | 0.21678 (12) | 0.02917 (12) | 0.0446 (3) |
| C18 | 0.45246 (7) | 0.18547 (15) | 0.00219 (14) | 0.0592 (4) |
| H18A | 0.4587 | 0.1439 | −0.0583 | 0.071* |
| C19 | 0.50365 (8) | 0.21590 (18) | 0.06533 (17) | 0.0737 (6) |
| H19A | 0.5441 | 0.1957 | 0.0460 | 0.088* |
| C20 | 0.49468 (9) | 0.27522 (16) | 0.15542 (18) | 0.0722 (6) |
| H20A | 0.5288 | 0.2936 | 0.1989 | 0.087* |
| C21 | 0.43562 (10) | 0.30752 (16) | 0.18154 (16) | 0.0706 (5) |
| H21A | 0.4298 | 0.3491 | 0.2422 | 0.085* |
| C22 | 0.38446 (8) | 0.27928 (14) | 0.11904 (14) | 0.0584 (4) |
| H22A | 0.3445 | 0.3024 | 0.1374 | 0.070* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|------|-----------|------------|------------|------------|------------|------------|
| O1 | 0.0485 (6) | 0.0438 (6) | 0.0653 (7) | 0.0023 (5) | 0.0063 (5) | −0.0075 (5) |
| O2 | 0.0387 (5) | 0.0468 (6) | 0.0439 (5) | −0.0077 (4) | 0.0023 (4) | 0.0004 (5) |
| O3 | 0.0564 (6) | 0.0452 (6) | 0.0536 (6) | 0.0025 (5) | −0.0006 (5) | −0.0029 (5) |
| O4 | 0.0434 (5) | 0.0608 (7) | 0.0440 (6) | −0.0064 (5) | −0.0021 (4) | 0.0075 (5) |
| C1 | 0.0363 (7) | 0.0583 (10) | 0.0498 (9) | −0.0033 (7) | −0.0002 (6) | 0.0030 (8) |
| C2 | 0.0455 (8) | 0.0677 (12) | 0.0521 (10) | −0.0073 (8) | 0.0113 (7) | 0.0018 (8) |
| C3 | 0.0584 (9) | 0.0594 (10) | 0.0398 (8) | −0.0107 (8) | 0.0029 (7) | 0.0032 (7) |
| C4 | 0.0472 (8) | 0.0479 (9) | 0.0432 (8) | −0.0070 (7) | −0.0058 (6) | 0.0062 (7) |
| C5 | 0.0382 (7) | 0.0333 (7) | 0.0410 (7) | −0.0027 (6) | −0.0011 (6) | 0.0038 (6) |
| C6 | 0.0365 (7) | 0.0378 (7) | 0.0405 (7) | −0.0013 (6) | −0.0019 (6) | 0.0027 (6) |
| C7 | 0.0333 (6) | 0.0443 (8) | 0.0416 (7) | 0.0052 (6) | −0.0023 (6) | −0.0020 (6) |
| C8 | 0.0420 (7) | 0.0500 (9) | 0.0557 (9) | 0.0000 (7) | −0.0016 (7) | −0.0073 (8) |
| C9 | 0.0511 (9) | 0.0685 (12) | 0.0566 (10) | 0.0000 (9) | −0.0052 (8) | −0.0228 (9) |
| C10 | 0.0563 (9) | 0.0838 (14) | 0.0405 (8) | 0.0066 (10) | −0.0045 (7) | −0.0124 (9) |
| C11 | 0.0483 (8) | 0.0649 (11) | 0.0400 (8) | 0.0051 (8) | −0.0009 (7) | 0.0021 (8) |
| C12 | 0.0361 (6) | 0.0463 (8) | 0.0387 (7) | 0.0056 (6) | −0.0028 (6) | 0.0005 (6) |
| C13 | 0.0427 (7) | 0.0434 (8) | 0.0391 (7) | 0.0019 (6) | −0.0035 (6) | 0.0107 (7) |
| C14 | 0.0436 (8) | 0.0549 (10) | 0.0539 (9) | −0.0118 (7) | −0.0041 (7) | 0.0081 (8) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C15 | 0.0376 (7) | 0.0486 (8) | 0.0437 (8) | −0.0068 (6) | 0.0042 (6) | 0.0024 (7) |
| C16 | 0.0365 (6) | 0.0354 (7) | 0.0433 (7) | 0.0013 (6) | −0.0053 (6) | 0.0055 (6) |
| C17 | 0.0389 (7) | 0.0483 (9) | 0.0467 (8) | −0.0072 (7) | 0.0008 (6) | 0.0089 (7) |
| C18 | 0.0435 (8) | 0.0797 (13) | 0.0544 (10) | −0.0010 (8) | 0.0062 (7) | 0.0063 (9) |
| C19 | 0.0367 (8) | 0.1048 (17) | 0.0796 (14) | −0.0100 (10) | 0.0000 (9) | 0.0220 (13) |
| C20 | 0.0571 (10) | 0.0842 (14) | 0.0752 (13) | −0.0311 (10) | −0.0176 (10) | 0.0184 (11) |
| C21 | 0.0758 (12) | 0.0676 (13) | 0.0682 (12) | −0.0184 (10) | −0.0152 (10) | −0.0050 (10) |
| C22 | 0.0521 (9) | 0.0604 (11) | 0.0626 (11) | −0.0031 (8) | −0.0051 (8) | −0.0048 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C16 | 1.1972 (17) | C9—H9A | 0.9300 |
| O2—C16 | 1.3596 (17) | C10—C11 | 1.378 (2) |
| O2—C15 | 1.4562 (16) | C10—H10A | 0.9300 |
| O3—C13 | 1.1973 (17) | C11—C12 | 1.392 (2) |
| O4—C13 | 1.3586 (17) | C11—H11A | 0.9300 |
| O4—C14 | 1.4446 (18) | C12—C13 | 1.488 (2) |
| C1—C2 | 1.384 (2) | C14—C15 | 1.520 (2) |
| C1—C6 | 1.3891 (19) | C14—H14A | 0.9700 |
| C1—H1A | 0.9300 | C14—H14B | 0.9700 |
| C2—C3 | 1.380 (2) | C15—C17 | 1.5003 (19) |
| C2—H2A | 0.9300 | C15—H15A | 0.9800 |
| C3—C4 | 1.376 (2) | C17—C18 | 1.382 (2) |
| C3—H3A | 0.9300 | C17—C22 | 1.383 (2) |
| C4—C5 | 1.3916 (19) | C18—C19 | 1.392 (2) |
| C4—H4A | 0.9300 | C18—H18A | 0.9300 |
| C5—C6 | 1.4068 (18) | C19—C20 | 1.364 (3) |
| C5—C16 | 1.4888 (19) | C19—H19A | 0.9300 |
| C6—C7 | 1.4965 (19) | C20—C21 | 1.363 (3) |
| C7—C8 | 1.393 (2) | C20—H20A | 0.9300 |
| C7—C12 | 1.400 (2) | C21—C22 | 1.379 (2) |
| C8—C9 | 1.384 (2) | C21—H21A | 0.9300 |
| C8—H8A | 0.9300 | C22—H22A | 0.9300 |
| C9—C10 | 1.376 (3) | | |
| | | | |
| C16—O2—C15 | 118.08 (11) | C7—C12—C13 | 119.56 (12) |
| C13—O4—C14 | 117.17 (12) | O3—C13—O4 | 124.98 (14) |
| C2—C1—C6 | 121.21 (14) | O3—C13—C12 | 125.60 (13) |
| C2—C1—H1A | 119.4 | O4—C13—C12 | 109.39 (13) |
| C6—C1—H1A | 119.4 | O4—C14—C15 | 107.18 (13) |
| C3—C2—C1 | 120.35 (14) | O4—C14—H14A | 110.3 |
| C3—C2—H2A | 119.8 | C15—C14—H14A | 110.3 |
| C1—C2—H2A | 119.8 | O4—C14—H14B | 110.3 |
| C4—C3—C2 | 119.66 (14) | C15—C14—H14B | 110.3 |
| C4—C3—H3A | 120.2 | H14A—C14—H14B | 108.5 |
| C2—C3—H3A | 120.2 | O2—C15—C17 | 108.79 (11) |
| C3—C4—C5 | 120.49 (14) | O2—C15—C14 | 105.86 (11) |
| C3—C4—H4A | 119.8 | C17—C15—C14 | 113.15 (13) |

| | | | |
|---|---|---|---|
| C5—C4—H4A | 119.8 | O2—C15—H15A | 109.6 |
| C4—C5—C6 | 120.37 (13) | C17—C15—H15A | 109.6 |
| C4—C5—C16 | 119.83 (12) | C14—C15—H15A | 109.6 |
| C6—C5—C16 | 119.77 (12) | O1—C16—O2 | 124.52 (13) |
| C1—C6—C5 | 117.92 (13) | O1—C16—C5 | 125.93 (13) |
| C1—C6—C7 | 118.80 (12) | O2—C16—C5 | 109.50 (12) |
| C5—C6—C7 | 123.27 (12) | C18—C17—C22 | 118.70 (15) |
| C8—C7—C12 | 117.99 (13) | C18—C17—C15 | 120.77 (15) |
| C8—C7—C6 | 118.44 (13) | C22—C17—C15 | 120.53 (14) |
| C12—C7—C6 | 123.57 (13) | C17—C18—C19 | 120.21 (18) |
| C9—C8—C7 | 121.17 (16) | C17—C18—H18A | 119.9 |
| C9—C8—H8A | 119.4 | C19—C18—H18A | 119.9 |
| C7—C8—H8A | 119.4 | C20—C19—C18 | 120.20 (18) |
| C10—C9—C8 | 120.13 (16) | C20—C19—H19A | 119.9 |
| C10—C9—H9A | 119.9 | C18—C19—H19A | 119.9 |
| C8—C9—H9A | 119.9 | C21—C20—C19 | 119.83 (17) |
| C9—C10—C11 | 120.04 (15) | C21—C20—H20A | 120.1 |
| C9—C10—H10A | 120.0 | C19—C20—H20A | 120.1 |
| C11—C10—H10A | 120.0 | C20—C21—C22 | 120.74 (19) |
| C10—C11—C12 | 120.17 (16) | C20—C21—H21A | 119.6 |
| C10—C11—H11A | 119.9 | C22—C21—H21A | 119.6 |
| C12—C11—H11A | 119.9 | C21—C22—C17 | 120.28 (17) |
| C11—C12—C7 | 120.49 (14) | C21—C22—H22A | 119.9 |
| C11—C12—C13 | 119.94 (14) | C17—C22—H22A | 119.9 |
| | | | |
| C6—C1—C2—C3 | −0.4 (3) | C11—C12—C13—O3 | 129.03 (16) |
| C1—C2—C3—C4 | 0.8 (3) | C7—C12—C13—O3 | −51.7 (2) |
| C2—C3—C4—C5 | −0.6 (3) | C11—C12—C13—O4 | −53.03 (17) |
| C3—C4—C5—C6 | 0.1 (2) | C7—C12—C13—O4 | 126.21 (13) |
| C3—C4—C5—C16 | 178.33 (15) | C13—O4—C14—C15 | 92.18 (15) |
| C2—C1—C6—C5 | −0.2 (2) | C16—O2—C15—C17 | −141.79 (12) |
| C2—C1—C6—C7 | −179.94 (15) | C16—O2—C15—C14 | 96.32 (14) |
| C4—C5—C6—C1 | 0.3 (2) | O4—C14—C15—O2 | −65.31 (15) |
| C16—C5—C6—C1 | −177.94 (14) | O4—C14—C15—C17 | 175.64 (12) |
| C4—C5—C6—C7 | −179.93 (14) | C15—O2—C16—O1 | 18.96 (19) |
| C16—C5—C6—C7 | 1.8 (2) | C15—O2—C16—C5 | −158.71 (11) |
| C1—C6—C7—C8 | −56.42 (19) | C4—C5—C16—O1 | 124.59 (16) |
| C5—C6—C7—C8 | 123.83 (15) | C6—C5—C16—O1 | −57.1 (2) |
| C1—C6—C7—C12 | 123.92 (16) | C4—C5—C16—O2 | −57.78 (17) |
| C5—C6—C7—C12 | −55.8 (2) | C6—C5—C16—O2 | 120.49 (14) |
| C12—C7—C8—C9 | 0.5 (2) | O2—C15—C17—C18 | 132.03 (15) |
| C6—C7—C8—C9 | −179.19 (14) | C14—C15—C17—C18 | −110.62 (17) |
| C7—C8—C9—C10 | 0.2 (3) | O2—C15—C17—C22 | −48.06 (19) |
| C8—C9—C10—C11 | 0.1 (3) | C14—C15—C17—C22 | 69.29 (19) |
| C9—C10—C11—C12 | −1.0 (2) | C22—C17—C18—C19 | 0.6 (3) |
| C10—C11—C12—C7 | 1.6 (2) | C15—C17—C18—C19 | −179.52 (16) |
| C10—C11—C12—C13 | −179.13 (14) | C17—C18—C19—C20 | 1.3 (3) |
| C8—C7—C12—C11 | −1.4 (2) | C18—C19—C20—C21 | −2.2 (3) |

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| C6—C7—C12—C11 | 178.28 (13) | C19—C20—C21—C22 | 1.3 (3) |
| C8—C7—C12—C13 | 179.39 (13) | C20—C21—C22—C17 | 0.6 (3) |
| C6—C7—C12—C13 | −1.0 (2) | C18—C17—C22—C21 | −1.5 (3) |
| C14—O4—C13—O3 | 21.5 (2) | C15—C17—C22—C21 | 178.61 (16) |
| C14—O4—C13—C12 | −156.50 (12) | | |