

Phenyl(2,4,5-triphenylcyclopenta-1,4-dien-1-yl)methanone

David B. Cordes, Guoxiong Hua, Alexandra M. Z. Slawin* and J. Derek Woollins

School of Chemistry, University of St Andrews, Fife KY16 9ST, Scotland
Correspondence e-mail: amzs@st-andrews.ac.uk

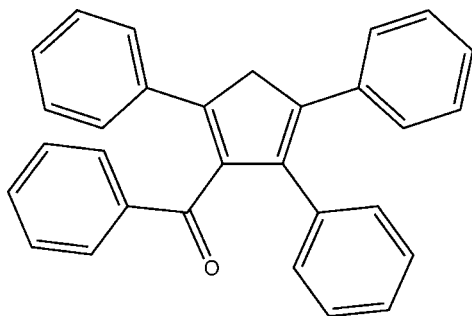
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Key indicators: single-crystal X-ray study; $T = 93$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.081; wR factor = 0.225; data-to-parameter ratio = 15.1.

The title compound, $\text{C}_{30}\text{H}_{22}\text{O}$, does not form face-to-face $\pi-\pi$ interactions despite the presence of four phenyl rings within the compound. Instead weak $\text{C}-\text{H}\cdots\pi$ interactions occur between adjacent molecules, with $\text{C}\cdots\text{C}$ contact distances in the range 3.633 (4)–3.974 (4) Å. The ketone O atom also takes part in a weak $\text{C}-\text{H}\cdots\text{O}$ interaction. The three pendant phenyl rings are twisted relative to the central cyclopentadiene ring by 17.82 (17), 29.63 (14) and 61.57 (9)°, while the phenylmethanone is nearly orthogonal, the angle between planes being 87.77 (9)°.

Related literature

For a previous preparation of the title compound, see: Lund (2005). The crystal studied was obtained by reaction of Woollins' reagent [2,4-bis(phenyl)-1,3-diselenadiphosphetane-2,4-diselenide] with quinoxaline-2,3-dithiol. For a review of the chemistry of Woollins' reagent, see: Hua & Woollins (2009). There are no structurally closely-related compounds in the literature; however, for some of the closest related, see: Evrard *et al.* (1971); Wender *et al.* (2006).



Experimental

Crystal data

| | |
|--------------------------------------|-----------------------------------|
| $\text{C}_{30}\text{H}_{22}\text{O}$ | $V = 4153.3$ (16) Å ³ |
| $M_r = 398.48$ | $Z = 8$ |
| Monoclinic, $C2/c$ | Mo $K\alpha$ radiation |
| $a = 25.946$ (6) Å | $\mu = 0.08$ mm ⁻¹ |
| $b = 6.1573$ (14) Å | $T = 93$ K |
| $c = 26.602$ (6) Å | $0.30 \times 0.20 \times 0.06$ mm |
| $\beta = 102.236$ (7)° | |

Data collection

| | |
|---|--|
| Rigaku Mercury CCD diffractometer | 13266 measured reflections |
| Absorption correction: multi-scan (<i>CrystalClear</i> ; Rigaku, 2010) | 4252 independent reflections |
| $T_{\min} = 0.978$, $T_{\max} = 0.996$ | 2479 reflections with $I > 2\sigma(I)$ |
| | $R_{\text{int}} = 0.120$ |

Refinement

| | |
|---------------------------------|---|
| $R[F^2 > 2\sigma(F^2)] = 0.081$ | 281 parameters |
| $wR(F^2) = 0.225$ | H-atom parameters constrained |
| $S = 1.04$ | $\Delta\rho_{\text{max}} = 0.29$ e Å ⁻³ |
| 4252 reflections | $\Delta\rho_{\text{min}} = -0.39$ e Å ⁻³ |

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 and Cg2 are the centroids of the $\text{C6}-\text{C11}$ and $\text{C25}-\text{C30}$ rings, respectively.

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|--|--------------|--------------------|-------------|----------------------|
| $\text{C1}-\text{H1B}\cdots\text{O1}^{\text{i}}$ | 0.99 | 2.64 | 3.229 (3) | 118 (2) |
| $\text{C10}-\text{H10}\cdots\text{Cg1}^{\text{ii}}$ | 0.95 | 2.80 | 3.527 (3) | 134 (2) |
| $\text{C20}-\text{H20}\cdots\text{Cg2}^{\text{iii}}$ | 0.95 | 2.80 | 3.605 (3) | 143 (2) |
| $\text{C28}-\text{H28}\cdots\text{Cg1}^{\text{iv}}$ | 0.95 | 2.88 | 3.612 (3) | 134 (2) |

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

Data collection: *CrystalClear* (Rigaku, 2010); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2426).

References

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supplementary materials

Acta Cryst. (2011). E67, o1718 [doi:10.1107/S1600536811022902]

Phenyl(2,4,5-triphenylcyclopenta-1,4-dien-1-yl)methanone

D. B. Cordes, G. Hua, A. M. Z. Slawin and J. D. Woollins

Comment

The previously known title compound (Lund, 2005) has been prepared by the reaction of Woollins' reagent with quinoxaline-2,3-dithiol. In a similar manner to the two somewhat related structures (Evrard *et al.*, 1971 and Wender *et al.*, 2006) no face-to-face π -interactions are observed, adjacent molecules instead interacting *via* a series of CH \cdots π interactions. The ketone oxygen makes intermolecular CH \cdots O contacts at a distance of 2.64 Å.

Experimental

A mixture of 0.194 g of quinoxaline-2,3-dithiol (1.0 mmol) and Woollins' reagent (0.54 g, 1.0 mmol) in 20 ml of dry toluene was refluxed for 7 h. The red suspension disappeared and a deep red solution formed. Following cooling to room temperature and removal of solvent *in vacuo* the residue was purified by silica gel column chromatography (1:1 hexane/dichloromethane eluent) to give the title compound as a brown solid (0.060 g, 13%). Crystals suitable for X-ray structure determination were obtained from the diffusion of hexane into a dichloromethane solution of the title compound. Selected IR (KBr, cm^{-1}): 1658(s, C=O), 1596(m), 1490(m), 1443(m), 1243(s), 754(s), 6932(*versus*). ^1H NMR (CD_2Cl_2 , δ), 8.13–8.00 (m, 2H, ArH), 7.93–7.83 (m, 3H, ArH), 7.61–6.92 (m, 15H, ArH), 4.24 (s, 2H, CH_2) p.p.m.. ^{13}C NMR (CD_2Cl_2 , δ), 168.5 (C=O), 144.0, 135.8, 134.4, 133.4, 132.6, 130.7, 129.8, 129.4, 129.2, 129.0, 128.9, 128.8, 128.5, 128.3, 128.1, 127.9, 127.6, 127.4, 127.2, 127.0, 126.6, 46.0 p.p.m.. MS (Cl^+ , m/z), 399 [$M+\text{H}$] $^+$. Accurate mass measurement [Cl^+ , m/z]: 399.1737 [$M+\text{H}$] $^+$, calculated mass for $\text{C}_{30}\text{H}_{23}\text{O}$: 399.1743.

Refinement

All the crystals chosen appeared to be poorly diffracting at higher angles, with low values of $I/\sigma(I)$, and missing independent data in the experimentally measured range. All H atoms were included in calculated positions (C—H distances are 0.99 Å for methylene H atoms and 0.95 Å for phenyl H atoms) and refined as riding atoms with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{parent atom})$.

Figures

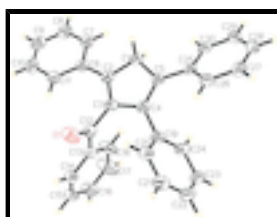


Fig. 1. The structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

phenyl(2,4,5-triphenylcyclopenta-1,4-dien-1-yl)methanone

Crystal data

| | |
|---------------------------------|---|
| $C_{30}H_{22}O$ | $F(000) = 1680$ |
| $M_r = 398.48$ | $D_x = 1.275 \text{ Mg m}^{-3}$ |
| Monoclinic, $C2/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| Hall symbol: $-C 2yc$ | Cell parameters from 3958 reflections |
| $a = 25.946 (6) \text{ \AA}$ | $\theta = 6.3\text{--}54.9^\circ$ |
| $b = 6.1573 (14) \text{ \AA}$ | $\mu = 0.08 \text{ mm}^{-1}$ |
| $c = 26.602 (6) \text{ \AA}$ | $T = 93 \text{ K}$ |
| $\beta = 102.236 (7)^\circ$ | Prism, colourless |
| $V = 4153.3 (16) \text{ \AA}^3$ | $0.30 \times 0.20 \times 0.06 \text{ mm}$ |
| $Z = 8$ | |

Data collection

| | |
|---|--|
| Rigaku Mercury CCD diffractometer | 4252 independent reflections |
| Radiation source: rotating anode confocal | 2479 reflections with $I > 2\sigma(I)$ |
| Detector resolution: $14.7059 \text{ pixels mm}^{-1}$ | $R_{\text{int}} = 0.120$ |
| ω and φ scans | $\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 3.1^\circ$ |
| Absorption correction: multi-scan (<i>CrystalClear</i> ; Rigaku, 2010) | $h = -33 \rightarrow 26$ |
| $T_{\text{min}} = 0.978$, $T_{\text{max}} = 0.996$ | $k = -7 \rightarrow 7$ |
| 13266 measured reflections | $l = -28 \rightarrow 33$ |

Refinement

| | |
|---------------------------------|--|
| Refinement on F^2 | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.081$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.225$ | H-atom parameters constrained |
| $S = 1.04$ | $w = 1/[\sigma^2(F_o^2) + (0.1072P)^2]$ |
| 4252 reflections | where $P = (F_o^2 + 2F_c^2)/3$ |
| 281 parameters | $(\Delta/\sigma)_{\text{max}} < 0.001$ |
| 0 restraints | $\Delta\rho_{\text{max}} = 0.29 \text{ e \AA}^{-3}$ |
| | $\Delta\rho_{\text{min}} = -0.39 \text{ e \AA}^{-3}$ |

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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|------------|---------------|----------------------------------|
| O1 | 0.36026 (8) | 0.0838 (4) | 0.13591 (8) | 0.0494 (6) |
| C1 | 0.41982 (10) | 0.7166 (5) | 0.21370 (9) | 0.0300 (7) |
| H1A | 0.4480 | 0.6866 | 0.2443 | 0.036* |
| H1B | 0.4032 | 0.8577 | 0.2185 | 0.036* |
| C2 | 0.37945 (10) | 0.5375 (4) | 0.20539 (9) | 0.0279 (7) |
| C3 | 0.37812 (10) | 0.4503 (4) | 0.15812 (9) | 0.0289 (7) |
| C4 | 0.41591 (10) | 0.5655 (4) | 0.13312 (9) | 0.0283 (7) |
| C5 | 0.44176 (10) | 0.7189 (4) | 0.16562 (9) | 0.0269 (6) |
| C6 | 0.34825 (10) | 0.4843 (5) | 0.24389 (10) | 0.0304 (7) |
| C7 | 0.34567 (11) | 0.6341 (5) | 0.28290 (10) | 0.0368 (7) |
| H7 | 0.3645 | 0.7672 | 0.2842 | 0.044* |
| C8 | 0.31633 (12) | 0.5923 (6) | 0.31959 (11) | 0.0454 (8) |
| H8 | 0.3153 | 0.6964 | 0.3457 | 0.054* |
| C9 | 0.28875 (12) | 0.4015 (6) | 0.31855 (11) | 0.0452 (8) |
| H9 | 0.2681 | 0.3746 | 0.3434 | 0.054* |
| C10 | 0.29138 (11) | 0.2480 (5) | 0.28080 (12) | 0.0434 (8) |
| H10 | 0.2730 | 0.1144 | 0.2803 | 0.052* |
| C11 | 0.32083 (10) | 0.2887 (5) | 0.24366 (11) | 0.0350 (7) |
| H11 | 0.3223 | 0.1828 | 0.2180 | 0.042* |
| C12 | 0.34422 (11) | 0.2708 (5) | 0.13193 (10) | 0.0315 (7) |
| C13 | 0.29162 (11) | 0.3222 (5) | 0.09964 (10) | 0.0313 (7) |
| C14 | 0.26130 (11) | 0.1535 (5) | 0.07379 (10) | 0.0374 (7) |
| H14 | 0.2746 | 0.0093 | 0.0765 | 0.045* |
| C15 | 0.21138 (11) | 0.1970 (5) | 0.04388 (11) | 0.0416 (8) |
| H15 | 0.1906 | 0.0819 | 0.0265 | 0.050* |
| C16 | 0.19237 (12) | 0.4045 (6) | 0.03957 (12) | 0.0516 (9) |
| H16 | 0.1584 | 0.4337 | 0.0191 | 0.062* |
| C17 | 0.22223 (14) | 0.5704 (6) | 0.06479 (16) | 0.0740 (13) |
| H17 | 0.2090 | 0.7148 | 0.0615 | 0.089* |
| C18 | 0.27205 (12) | 0.5288 (5) | 0.09539 (12) | 0.0522 (10) |
| H18 | 0.2923 | 0.6443 | 0.1132 | 0.063* |
| C19 | 0.42011 (10) | 0.5280 (5) | 0.07848 (9) | 0.0291 (7) |
| C20 | 0.43588 (10) | 0.3314 (5) | 0.06182 (10) | 0.0341 (7) |
| H20 | 0.4437 | 0.2132 | 0.0852 | 0.041* |
| C21 | 0.44040 (11) | 0.3058 (5) | 0.01114 (11) | 0.0397 (8) |
| H21 | 0.4518 | 0.1709 | 0.0000 | 0.048* |
| C22 | 0.42837 (11) | 0.4765 (5) | -0.02322 (11) | 0.0398 (8) |
| H22 | 0.4315 | 0.4583 | -0.0579 | 0.048* |

supplementary materials

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|-----|--------------|------------|---------------|------------|
| C23 | 0.41199 (11) | 0.6712 (5) | -0.00742 (10) | 0.0380 (8) |
| H23 | 0.4035 | 0.7875 | -0.0312 | 0.046* |
| C24 | 0.40768 (11) | 0.6993 (5) | 0.04363 (10) | 0.0358 (7) |
| H24 | 0.3963 | 0.8346 | 0.0546 | 0.043* |
| C25 | 0.48404 (10) | 0.8684 (4) | 0.15913 (9) | 0.0271 (7) |
| C26 | 0.52110 (10) | 0.8136 (5) | 0.12983 (10) | 0.0336 (7) |
| H26 | 0.5184 | 0.6775 | 0.1127 | 0.040* |
| C27 | 0.56144 (11) | 0.9533 (5) | 0.12544 (10) | 0.0381 (8) |
| H27 | 0.5859 | 0.9127 | 0.1051 | 0.046* |
| C28 | 0.56674 (11) | 1.1516 (5) | 0.15023 (11) | 0.0392 (8) |
| H28 | 0.5946 | 1.2473 | 0.1471 | 0.047* |
| C29 | 0.53077 (11) | 1.2092 (5) | 0.17984 (11) | 0.0373 (8) |
| H29 | 0.5341 | 1.3447 | 0.1973 | 0.045* |
| C30 | 0.49004 (11) | 1.0692 (5) | 0.18395 (9) | 0.0317 (7) |
| H30 | 0.4656 | 1.1110 | 0.2042 | 0.038* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| O1 | 0.0409 (12) | 0.0385 (14) | 0.0614 (14) | 0.0034 (10) | -0.0057 (11) | -0.0054 (11) |
| C1 | 0.0278 (15) | 0.0406 (18) | 0.0201 (14) | 0.0017 (12) | 0.0013 (11) | 0.0012 (11) |
| C2 | 0.0215 (14) | 0.0374 (18) | 0.0244 (15) | 0.0014 (11) | 0.0041 (11) | 0.0016 (11) |
| C3 | 0.0221 (14) | 0.0344 (17) | 0.0271 (15) | 0.0022 (11) | -0.0017 (11) | 0.0006 (12) |
| C4 | 0.0243 (14) | 0.0341 (17) | 0.0251 (14) | 0.0014 (11) | 0.0019 (11) | 0.0019 (12) |
| C5 | 0.0227 (14) | 0.0343 (17) | 0.0223 (14) | 0.0008 (11) | 0.0016 (11) | 0.0032 (11) |
| C6 | 0.0197 (14) | 0.0410 (18) | 0.0280 (15) | 0.0001 (12) | -0.0003 (11) | 0.0011 (12) |
| C7 | 0.0349 (17) | 0.048 (2) | 0.0280 (15) | -0.0041 (14) | 0.0078 (13) | -0.0019 (13) |
| C8 | 0.047 (2) | 0.057 (2) | 0.0338 (17) | -0.0068 (16) | 0.0134 (14) | -0.0049 (15) |
| C9 | 0.0383 (18) | 0.068 (2) | 0.0318 (17) | -0.0027 (16) | 0.0139 (14) | 0.0047 (16) |
| C10 | 0.0355 (18) | 0.053 (2) | 0.0419 (18) | -0.0084 (15) | 0.0078 (14) | 0.0089 (16) |
| C11 | 0.0307 (16) | 0.0411 (19) | 0.0337 (16) | -0.0035 (13) | 0.0079 (13) | -0.0009 (13) |
| C12 | 0.0314 (16) | 0.0336 (18) | 0.0300 (15) | 0.0018 (13) | 0.0079 (12) | 0.0020 (12) |
| C13 | 0.0323 (16) | 0.0339 (17) | 0.0270 (15) | 0.0001 (12) | 0.0044 (12) | -0.0020 (12) |
| C14 | 0.0387 (17) | 0.0398 (19) | 0.0317 (16) | -0.0051 (14) | 0.0031 (13) | -0.0001 (13) |
| C15 | 0.0395 (18) | 0.048 (2) | 0.0330 (17) | -0.0103 (15) | -0.0032 (13) | -0.0044 (14) |
| C16 | 0.0402 (19) | 0.054 (2) | 0.050 (2) | 0.0045 (16) | -0.0141 (15) | -0.0040 (17) |
| C17 | 0.055 (2) | 0.047 (2) | 0.097 (3) | 0.0130 (18) | -0.034 (2) | -0.014 (2) |
| C18 | 0.0411 (19) | 0.040 (2) | 0.063 (2) | 0.0018 (15) | -0.0173 (16) | -0.0145 (16) |
| C19 | 0.0254 (14) | 0.0352 (18) | 0.0242 (14) | -0.0018 (12) | -0.0003 (11) | -0.0022 (12) |
| C20 | 0.0331 (16) | 0.0387 (19) | 0.0277 (16) | 0.0003 (13) | 0.0001 (12) | -0.0043 (12) |
| C21 | 0.0349 (17) | 0.045 (2) | 0.0384 (18) | 0.0007 (14) | 0.0064 (14) | -0.0093 (14) |
| C22 | 0.0372 (17) | 0.054 (2) | 0.0269 (15) | -0.0033 (15) | 0.0041 (13) | -0.0038 (14) |
| C23 | 0.0385 (17) | 0.049 (2) | 0.0253 (16) | -0.0016 (14) | 0.0041 (13) | 0.0006 (13) |
| C24 | 0.0344 (16) | 0.0428 (19) | 0.0273 (16) | 0.0032 (13) | 0.0000 (12) | -0.0018 (13) |
| C25 | 0.0233 (14) | 0.0365 (17) | 0.0191 (14) | 0.0002 (12) | -0.0010 (11) | 0.0034 (11) |
| C26 | 0.0308 (16) | 0.0416 (19) | 0.0273 (15) | -0.0013 (13) | 0.0039 (12) | -0.0029 (12) |
| C27 | 0.0331 (17) | 0.050 (2) | 0.0319 (16) | -0.0055 (14) | 0.0086 (13) | 0.0022 (14) |
| C28 | 0.0299 (17) | 0.051 (2) | 0.0323 (17) | -0.0089 (14) | -0.0022 (13) | 0.0075 (14) |

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C29 | 0.0334 (17) | 0.0406 (19) | 0.0330 (16) | -0.0055 (13) | -0.0046 (13) | -0.0018 (13) |
| C30 | 0.0335 (16) | 0.0411 (19) | 0.0178 (13) | 0.0022 (13) | -0.0005 (11) | 0.0025 (12) |

Geometric parameters (Å, °)

| | | | |
|------------|-----------|-------------|-----------|
| O1—C12 | 1.221 (3) | C15—H15 | 0.9500 |
| C1—C2 | 1.504 (4) | C16—C17 | 1.369 (5) |
| C1—C5 | 1.506 (4) | C16—H16 | 0.9500 |
| C1—H1A | 0.9900 | C17—C18 | 1.398 (4) |
| C1—H1B | 0.9900 | C17—H17 | 0.9500 |
| C2—C3 | 1.361 (4) | C18—H18 | 0.9500 |
| C2—C6 | 1.471 (4) | C19—C20 | 1.381 (4) |
| C3—C4 | 1.478 (4) | C19—C24 | 1.396 (4) |
| C3—C12 | 1.490 (4) | C20—C21 | 1.387 (4) |
| C4—C5 | 1.358 (3) | C20—H20 | 0.9500 |
| C4—C19 | 1.498 (4) | C21—C22 | 1.384 (4) |
| C5—C25 | 1.470 (4) | C21—H21 | 0.9500 |
| C6—C11 | 1.398 (4) | C22—C23 | 1.367 (4) |
| C6—C7 | 1.401 (4) | C22—H22 | 0.9500 |
| C7—C8 | 1.383 (4) | C23—C24 | 1.397 (4) |
| C7—H7 | 0.9500 | C23—H23 | 0.9500 |
| C8—C9 | 1.372 (4) | C24—H24 | 0.9500 |
| C8—H8 | 0.9500 | C25—C30 | 1.395 (4) |
| C9—C10 | 1.392 (4) | C25—C26 | 1.401 (4) |
| C9—H9 | 0.9500 | C26—C27 | 1.379 (4) |
| C10—C11 | 1.394 (4) | C26—H26 | 0.9500 |
| C10—H10 | 0.9500 | C27—C28 | 1.380 (4) |
| C11—H11 | 0.9500 | C27—H27 | 0.9500 |
| C12—C13 | 1.484 (4) | C28—C29 | 1.389 (4) |
| C13—C18 | 1.366 (4) | C28—H28 | 0.9500 |
| C13—C14 | 1.393 (4) | C29—C30 | 1.386 (4) |
| C14—C15 | 1.395 (4) | C29—H29 | 0.9500 |
| C14—H14 | 0.9500 | C30—H30 | 0.9500 |
| C15—C16 | 1.366 (4) | | |
| C2—C1—C5 | 105.0 (2) | C14—C15—H15 | 119.9 |
| C2—C1—H1A | 110.7 | C15—C16—C17 | 120.0 (3) |
| C5—C1—H1A | 110.7 | C15—C16—H16 | 120.0 |
| C2—C1—H1B | 110.7 | C17—C16—H16 | 120.0 |
| C5—C1—H1B | 110.7 | C16—C17—C18 | 120.4 (3) |
| H1A—C1—H1B | 108.8 | C16—C17—H17 | 119.8 |
| C3—C2—C6 | 130.2 (3) | C18—C17—H17 | 119.8 |
| C3—C2—C1 | 107.8 (2) | C13—C18—C17 | 120.1 (3) |
| C6—C2—C1 | 122.0 (2) | C13—C18—H18 | 120.0 |
| C2—C3—C4 | 109.7 (2) | C17—C18—H18 | 120.0 |
| C2—C3—C12 | 128.4 (3) | C20—C19—C24 | 119.5 (3) |
| C4—C3—C12 | 121.9 (2) | C20—C19—C4 | 122.2 (2) |
| C5—C4—C3 | 109.4 (2) | C24—C19—C4 | 118.3 (2) |
| C5—C4—C19 | 126.7 (2) | C19—C20—C21 | 120.2 (3) |
| C3—C4—C19 | 123.7 (2) | C19—C20—H20 | 119.9 |

supplementary materials

| | | | |
|-------------|-----------|-------------|-----------|
| C4—C5—C25 | 129.9 (2) | C21—C20—H20 | 119.9 |
| C4—C5—C1 | 108.0 (2) | C22—C21—C20 | 120.1 (3) |
| C25—C5—C1 | 122.1 (2) | C22—C21—H21 | 119.9 |
| C11—C6—C7 | 117.8 (3) | C20—C21—H21 | 119.9 |
| C11—C6—C2 | 122.9 (3) | C23—C22—C21 | 120.3 (3) |
| C7—C6—C2 | 119.2 (3) | C23—C22—H22 | 119.9 |
| C8—C7—C6 | 121.3 (3) | C21—C22—H22 | 119.9 |
| C8—C7—H7 | 119.3 | C22—C23—C24 | 120.1 (3) |
| C6—C7—H7 | 119.3 | C22—C23—H23 | 120.0 |
| C9—C8—C7 | 120.5 (3) | C24—C23—H23 | 120.0 |
| C9—C8—H8 | 119.7 | C19—C24—C23 | 119.8 (3) |
| C7—C8—H8 | 119.7 | C19—C24—H24 | 120.1 |
| C8—C9—C10 | 119.4 (3) | C23—C24—H24 | 120.1 |
| C8—C9—H9 | 120.3 | C30—C25—C26 | 117.1 (2) |
| C10—C9—H9 | 120.3 | C30—C25—C5 | 120.7 (2) |
| C9—C10—C11 | 120.5 (3) | C26—C25—C5 | 122.1 (2) |
| C9—C10—H10 | 119.8 | C27—C26—C25 | 121.3 (3) |
| C11—C10—H10 | 119.8 | C27—C26—H26 | 119.4 |
| C10—C11—C6 | 120.5 (3) | C25—C26—H26 | 119.4 |
| C10—C11—H11 | 119.8 | C26—C27—C28 | 120.8 (3) |
| C6—C11—H11 | 119.8 | C26—C27—H27 | 119.6 |
| O1—C12—C13 | 120.4 (3) | C28—C27—H27 | 119.6 |
| O1—C12—C3 | 120.1 (2) | C27—C28—C29 | 119.1 (3) |
| C13—C12—C3 | 119.4 (2) | C27—C28—H28 | 120.5 |
| C18—C13—C14 | 119.5 (3) | C29—C28—H28 | 120.5 |
| C18—C13—C12 | 121.8 (2) | C30—C29—C28 | 120.1 (3) |
| C14—C13—C12 | 118.7 (3) | C30—C29—H29 | 120.0 |
| C13—C14—C15 | 119.8 (3) | C28—C29—H29 | 120.0 |
| C13—C14—H14 | 120.1 | C29—C30—C25 | 121.6 (3) |
| C15—C14—H14 | 120.1 | C29—C30—H30 | 119.2 |
| C16—C15—C14 | 120.2 (3) | C25—C30—H30 | 119.2 |
| C16—C15—H15 | 119.9 | | |

Hydrogen-bond geometry (\AA , $^\circ$)

Cg1 and Cg2 are the centroids of the C6—C11 and C25—C30 rings, respectively.

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-------------------------------------|-------|-------------|-------------|---------------|
| C1—H1B \cdots O1 ⁱ | 0.99 | 2.64 | 3.229 (3) | 118.(2) |
| C10—H10 \cdots Cg1 ⁱⁱ | 0.95 | 2.80 | 3.527 (3) | 134 (2) |
| C20—H20 \cdots Cg2 ⁱⁱⁱ | 0.95 | 2.80 | 3.605 (3) | 143 (2) |
| C28—H28 \cdots Cg1 ^{iv} | 0.95 | 2.88 | 3.612 (3) | 134 (2) |
| C10—H10 \cdots C10 ⁱⁱ | 0.95 | 3.06 | 3.908 (4) | 150 (2) |
| C20—H20 \cdots C30 ⁱⁱⁱ | 0.95 | 2.79 | 3.633 (4) | 148 (2) |
| C28—H28 \cdots C9 ^{iv} | 0.95 | 3.12 | 3.974 (4) | 151 (2) |

Symmetry codes: (i) $x, y+1, z$; (ii) $-x+1/2, y-1/2, -z+1/2$; (iii) $x, y-1, z$; (iv) $-x+1, y+1, -z+1/2$.

Fig. 1

