# 1,3-Dibenzyl-1*H*-anthra[1,2-*d*]-imidazole-2,6,11(3*H*)-trione

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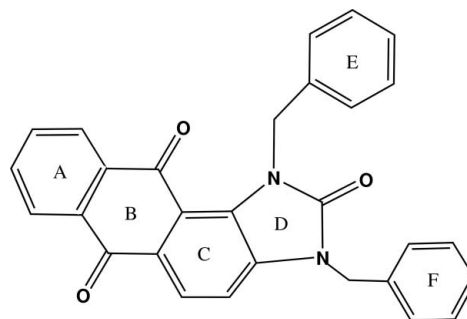Correspondence e-mail: kandri_rodi@yahoo.fr

The molecule of the title compound, $C_{29}H_{20}N_2O_3$, contains four fused rings, three are six-membered rings and one is the five-membered imidazole ring. The fused-ring system is linked to two benzyl groups. The four fused rings are folded around the O=C···C=O direction of the anthraquinone, with a dihedral angle of 16.36 (8)° between the two terminal rings (*A* and *D*). The imidazole ring (*D*) is almost perpendicular to the two benzyl groups (*E* and *F*) with dihedral angles of 86.69 (17) and 83.15 (13)°, respectively. In the crystal, adjacent molecules are linked by intermolecular C—H···O hydrogen bonding.

## Related literature

For background to the pharmacological activity of anthraquinone, see: Alves *et al.* (2004); Gatto *et al.* (1996); Krapcho *et al.* (1991). For information on its use as a synthetic dye, see: Naeimi & Namdari (2009). For related structures, see: Afrakssou *et al.* (2010); Guimarães *et al.* (2009). For puckering parameters, see: Cremer & Pople (1975).

## Experimental

### Crystal data

| | |
|---|---|
| $C_{29}H_{20}N_2O_3$ | $V = 2258.45$ (14) Å$^3$ |
| $M_r = 444.47$ | $Z = 4$ |
| Orthorhombic, $P2_12_12_1$ | Mo $K\alpha$ radiation |
| $a = 8.1389$ (3) Å | $\mu = 0.09$ mm$^{-1}$ |
| $b = 12.8748$ (4) Å | $T = 296$ K |
| $c = 21.5528$ (8) Å | $0.49 \times 0.18 \times 0.15$ mm |

### Data collection

| | |
|---|---|
| Bruker APEXII CCD diffractometer | 36228 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2009) | 2629 independent reflections |
| $T_{min} = 0.982$, $T_{max} = 0.987$ | 2137 reflections with $I > 2\sigma(I)$ |
| | $R_{int} = 0.047$ |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.039$ | 308 parameters |
| $wR(F^2) = 0.108$ | H-atom parameters constrained |
| $S = 1.05$ | $\Delta\rho_{max} = 0.23$ e Å$^{-3}$ |
| 2629 reflections | $\Delta\rho_{min} = -0.18$ e Å$^{-3}$ |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C13—H13···O1[i] | 0.93 | 2.39 | 3.312 (3) | 171 |
| C23—H23*A*···O2[ii] | 0.97 | 2.47 | 3.439 (4) | 174 |

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT-Plus* (Bruker, 2009); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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**supplementary materials**

## 1,3-Dibenzyl-1*H*-anthra[1,2-*d*]imidazole-2,6,11(3*H*)-trione

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### Comment

Anthraquinone-containing extracts from different plant sources such as senna, cascara, aloe, frangula, and rhubarb have been found to have wide variety of pharmacological activities such as antiinflammatory, wound healing, analgesic, antipyretic, antimicrobial, and antitumor activities (Alves *et al.*, 2004). Anthraquinone planarity allows an intercalation between base pairs of DNA in the β conformation, while its redox properties are linked to the production of radical species in biological systems. The chemical and biological activity of anthraquinone compounds depends on the different substituents of the planar ring system (Gatto *et al.*, 1996; Krapcho *et al.*, 1991). Anthraquinone dyes are used for coloration of cotton and cellulose fibers as well as of hydrophobic, synthetic materials (Naeimi *et al.*, 2009).

The present work is a continuation of the preparation of new derivatives of anthra[1,2-*d*]imidazole-2,6,11–trione for biological applications (Afrakssou *et al.*, (2010), Guimarães *et al.* (2009)). The reactivity of benzyl bromide towards 1*H*-anthra [2,1-*d*]imidazole-2,6,11(3*H*)-trione under phase-transfer catalysis conditions using tetra *n*-butyl ammonium bromide (TBAB) as catalyst and potassium carbonate as base leads to 1,3-dibenzyl-1*H*-anthra[2,1-*d*]imidazole-2,6,11(3*H*)-trione with good yield (Scheme 1).

All rings forming the molecule are planar except for the anthraquinone (B) which adopts a twisted conformation (Fig. 1), as indicated by Cremer & Pople (1975) with puckering parameters Q = 0.242 (2) Å, θ = 104.7 (5) ° and φ = 137.6 (5)°. The fused five and six-membered rings (C, D) are planar and built with A ring (sheme 1) a dihedral angle of 16.36 (8) °. The imidazole ring (D) is almost perpendicular to the two benzyl groups (E, F) with dihedral angles of 86.69 (17) ° and 83.15 (13) ° respectively. In the crystal, adjacent molecules are linked by intermolecular C—H⋯O hydrogen bonding (Table 1). The structure is further stabilized by π-π interactions between rings A and D with a centroid to centroid distance of 3.411 (2) Å and an interplanar distance of 3.395 (2)Å resulting in slight offset of 5.32°.

### Experimental

To a solution of 1*H*-anthra [2, 1 - d] imidazole-2, 6, 11(3*H*)-trione (0.5 g, 0.18 mmol), potassium carbonate (0.78 g, 0.56 mmol) and tetra n-butylammonium bromide (0.06 g, 0.018 mmol) in DMF (15 ml)) was added Benzyl bromide (0.56 ml, 0.47 mmol). Stirring was continued at room temperature for 24 h. The mixture was filtered and the solvent removed. The residue was extracted with water. The organic compound was chromatographed on a column of silica gel with ethyl acetate-hexane (1/1) as eluent. Orange crystals were isolated when the solvent was allowed to evaporate.

### Refinement

H atoms were located in a difference map and treated as riding with C—H = 0.93 Å for all H atoms with $U_{iso}$(H) = 1.2 $U_{eq}$ aromatic and methylene. In the absence of significant anomalous scattering, the absolute structure could not be reliably determined and thus the Friedel pairs were merged and any references to the Flack parameter were removed. The reflections

# supplementary materials

(0 0 2) and (0 1 1) were omitted because the difference between their calculated and observed intensities are very large. They are affected by the beamstop.
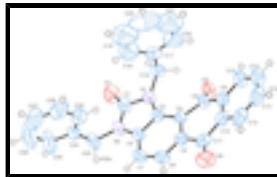
**Figures**



Fig. 1. Molecular plot the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small circles.

**1,3-Dibenzyl-1***H***-anthra[1,2-*d*]imidazole-2,6,11(3***H***)-trione**

*Crystal data*

| | |
|---|---|
| $C_{29}H_{20}N_2O_3$ | $F(000) = 928$ |
| $M_r = 444.47$ | $D_x = 1.307$ Mg m$^{-3}$ |
| Orthorhombic, $P2_12_12_1$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: P 2ac 2ab | Cell parameters from 2629 reflections |
| $a = 8.1389$ (3) Å | $\theta = 2.5–26.4°$ |
| $b = 12.8748$ (4) Å | $\mu = 0.09$ mm$^{-1}$ |
| $c = 21.5528$ (8) Å | $T = 296$ K |
| $V = 2258.45$ (14) Å$^3$ | Flat, orange |
| $Z = 4$ | $0.49 \times 0.18 \times 0.15$ mm |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD diffractometer | 2629 independent reflections |
| Radiation source: fine-focus sealed tube | 2137 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.047$ |
| φ and ω scans | $\theta_{max} = 26.4°$, $\theta_{min} = 2.5°$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2009) | $h = -10 \rightarrow 10$ |
| $T_{min} = 0.982$, $T_{max} = 0.987$ | $k = -15 \rightarrow 16$ |
| 36228 measured reflections | $l = -26 \rightarrow 26$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.039$ | H-atom parameters constrained |
| $wR(F^2) = 0.108$ | $w = 1/[\sigma^2(F_o^2) + (0.0603P)^2 + 0.2421P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.05$ | $(\Delta/\sigma)_{max} < 0.001$ |

| | |
|---|---|
| 2629 reflections | $\Delta\rho_{max} = 0.23$ e Å$^{-3}$ |
| 308 parameters | $\Delta\rho_{min} = -0.18$ e Å$^{-3}$ |
| 0 restraints | Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.0123 (15) |

*Special details*

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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* | $U_{iso}*/U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.0570 (3) | 0.41604 (19) | 0.84012 (11) | 0.0512 (6) |
| C2 | 0.2441 (3) | 0.53761 (17) | 0.81399 (10) | 0.0420 (5) |
| C3 | 0.0919 (3) | 0.58851 (17) | 0.82177 (9) | 0.0375 (5) |
| C4 | 0.0807 (3) | 0.69572 (17) | 0.81222 (9) | 0.0387 (5) |
| C5 | 0.2294 (3) | 0.74849 (19) | 0.79858 (10) | 0.0439 (5) |
| C6 | 0.3764 (3) | 0.6961 (2) | 0.79119 (12) | 0.0508 (6) |
| H6 | 0.4711 | 0.7333 | 0.7818 | 0.061* |
| C7 | 0.3851 (3) | 0.5888 (2) | 0.79761 (11) | 0.0503 (6) |
| H7 | 0.4829 | 0.5532 | 0.7910 | 0.060* |
| C8 | −0.0748 (3) | 0.75336 (18) | 0.80889 (10) | 0.0425 (5) |
| C9 | −0.0669 (3) | 0.86723 (18) | 0.81962 (10) | 0.0471 (6) |
| C10 | 0.0803 (3) | 0.92029 (19) | 0.81274 (10) | 0.0507 (6) |
| C11 | 0.2320 (4) | 0.8639 (2) | 0.79481 (12) | 0.0546 (6) |
| C12 | 0.0849 (5) | 1.0278 (2) | 0.82132 (12) | 0.0674 (8) |
| H12 | 0.1826 | 1.0642 | 0.8158 | 0.081* |
| C13 | −0.0569 (5) | 1.0794 (2) | 0.83799 (13) | 0.0758 (9) |
| H13 | −0.0538 | 1.1507 | 0.8449 | 0.091* |
| C14 | −0.2029 (5) | 1.0266 (2) | 0.84455 (13) | 0.0730 (9) |
| H14 | −0.2975 | 1.0624 | 0.8558 | 0.088* |
| C15 | −0.2100 (4) | 0.9207 (2) | 0.83451 (13) | 0.0606 (7) |
| H15 | −0.3095 | 0.8855 | 0.8377 | 0.073* |
| C16 | −0.1814 (3) | 0.5233 (2) | 0.86850 (12) | 0.0506 (6) |
| H16A | −0.2310 | 0.4552 | 0.8728 | 0.061* |
| H16B | −0.2530 | 0.5651 | 0.8426 | 0.061* |
| C17 | −0.1677 (3) | 0.5729 (2) | 0.93142 (12) | 0.0590 (7) |
| C18 | −0.0688 (5) | 0.5290 (4) | 0.97586 (16) | 0.1043 (13) |

| H18 | −0.0091 | 0.4694 | 0.9667 | 0.125* |
| C19 | −0.0579 (8) | 0.5726 (6) | 1.0333 (2) | 0.155 (2) |
| H19 | 0.0095 | 0.5425 | 1.0631 | 0.186* |
| C20 | −0.1443 (10) | 0.6593 (6) | 1.0473 (2) | 0.164 (3) |
| H20 | −0.1352 | 0.6888 | 1.0866 | 0.197* |
| C21 | −0.2439 (9) | 0.7032 (4) | 1.0045 (3) | 0.152 (3) |
| H21 | −0.3042 | 0.7624 | 1.0140 | 0.183* |
| C22 | −0.2544 (6) | 0.6587 (3) | 0.94659 (17) | 0.1007 (13) |
| H22 | −0.3230 | 0.6886 | 0.9171 | 0.121* |
| C23 | 0.3437 (3) | 0.3524 (2) | 0.82695 (13) | 0.0583 (7) |
| H23A | 0.4241 | 0.3652 | 0.7946 | 0.070* |
| H23B | 0.2925 | 0.2859 | 0.8184 | 0.070* |
| C24 | 0.4309 (3) | 0.34610 (19) | 0.88834 (12) | 0.0522 (6) |
| C25 | 0.5405 (5) | 0.2681 (3) | 0.8964 (2) | 0.1062 (14) |
| H25 | 0.5582 | 0.2207 | 0.8645 | 0.127* |
| C26 | 0.6266 (7) | 0.2583 (5) | 0.9517 (3) | 0.143 (2) |
| H26 | 0.7019 | 0.2045 | 0.9563 | 0.172* |
| C27 | 0.6028 (6) | 0.3250 (4) | 0.9984 (2) | 0.1106 (15) |
| H27 | 0.6577 | 0.3162 | 1.0359 | 0.133* |
| C28 | 0.4987 (5) | 0.4050 (3) | 0.99050 (14) | 0.0869 (10) |
| H28 | 0.4856 | 0.4536 | 1.0221 | 0.104* |
| C29 | 0.4106 (4) | 0.4159 (2) | 0.93574 (13) | 0.0680 (8) |
| H29 | 0.3374 | 0.4709 | 0.9312 | 0.082* |
| N1 | −0.0211 (2) | 0.51260 (15) | 0.83808 (8) | 0.0440 (5) |
| N2 | 0.2183 (2) | 0.43334 (15) | 0.82446 (9) | 0.0484 (5) |
| O1 | −0.0047 (3) | 0.33329 (14) | 0.85284 (11) | 0.0743 (6) |
| O2 | 0.3554 (3) | 0.91046 (17) | 0.77953 (12) | 0.0851 (7) |
| O3 | −0.2048 (2) | 0.71168 (14) | 0.79558 (9) | 0.0562 (5) |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0601 (15) | 0.0381 (13) | 0.0553 (13) | 0.0009 (12) | −0.0041 (12) | −0.0057 (10) |
| C2 | 0.0419 (12) | 0.0429 (12) | 0.0412 (11) | 0.0069 (10) | −0.0025 (10) | −0.0031 (9) |
| C3 | 0.0349 (11) | 0.0410 (11) | 0.0366 (10) | 0.0006 (10) | −0.0014 (9) | −0.0027 (9) |
| C4 | 0.0382 (11) | 0.0420 (12) | 0.0358 (10) | 0.0022 (10) | −0.0006 (9) | −0.0008 (9) |
| C5 | 0.0424 (13) | 0.0459 (13) | 0.0433 (12) | −0.0039 (11) | 0.0011 (10) | 0.0043 (10) |
| C6 | 0.0374 (12) | 0.0613 (16) | 0.0539 (13) | −0.0058 (12) | 0.0048 (11) | 0.0031 (12) |
| C7 | 0.0348 (12) | 0.0621 (15) | 0.0540 (13) | 0.0065 (12) | 0.0018 (10) | −0.0024 (12) |
| C8 | 0.0421 (12) | 0.0444 (12) | 0.0410 (11) | 0.0045 (11) | −0.0014 (10) | 0.0026 (9) |
| C9 | 0.0588 (14) | 0.0397 (12) | 0.0427 (12) | 0.0091 (12) | −0.0023 (12) | 0.0030 (9) |
| C10 | 0.0676 (16) | 0.0409 (12) | 0.0437 (12) | 0.0020 (13) | −0.0013 (12) | 0.0066 (10) |
| C11 | 0.0595 (16) | 0.0503 (14) | 0.0541 (14) | −0.0097 (13) | 0.0074 (12) | 0.0093 (12) |
| C12 | 0.103 (2) | 0.0414 (14) | 0.0578 (15) | −0.0049 (17) | −0.0003 (17) | 0.0088 (12) |
| C13 | 0.130 (3) | 0.0387 (13) | 0.0591 (16) | 0.016 (2) | 0.0005 (19) | 0.0022 (12) |
| C14 | 0.101 (3) | 0.0517 (16) | 0.0663 (17) | 0.0253 (18) | 0.0034 (17) | −0.0017 (13) |
| C15 | 0.0702 (17) | 0.0507 (14) | 0.0608 (15) | 0.0181 (14) | 0.0031 (14) | 0.0013 (12) |
| C16 | 0.0371 (12) | 0.0480 (13) | 0.0666 (14) | −0.0062 (11) | 0.0028 (11) | 0.0018 (11) |

| | | | | | |
|---|---|---|---|---|---|
| C17 | 0.0514 (14) | 0.0671 (16) | 0.0586 (14) | −0.0085 (15) | 0.0149 (12) | 0.0018 (13) |
| C18 | 0.096 (3) | 0.151 (4) | 0.0661 (19) | 0.017 (3) | −0.009 (2) | −0.003 (2) |
| C19 | 0.145 (5) | 0.254 (8) | 0.064 (2) | 0.017 (6) | −0.012 (3) | −0.020 (3) |
| C20 | 0.203 (7) | 0.214 (7) | 0.076 (3) | −0.038 (6) | 0.041 (4) | −0.055 (4) |
| C21 | 0.209 (7) | 0.148 (5) | 0.100 (3) | 0.019 (5) | 0.060 (4) | −0.043 (4) |
| C22 | 0.124 (3) | 0.094 (3) | 0.084 (2) | 0.021 (3) | 0.032 (2) | −0.010 (2) |
| C23 | 0.0621 (16) | 0.0460 (13) | 0.0666 (16) | 0.0194 (13) | −0.0007 (14) | −0.0110 (12) |
| C24 | 0.0457 (13) | 0.0493 (13) | 0.0615 (14) | 0.0066 (12) | 0.0049 (12) | 0.0079 (11) |
| C25 | 0.119 (3) | 0.093 (3) | 0.106 (3) | 0.061 (3) | −0.024 (3) | −0.004 (2) |
| C26 | 0.148 (4) | 0.148 (4) | 0.133 (4) | 0.082 (4) | −0.040 (4) | 0.016 (4) |
| C27 | 0.092 (3) | 0.152 (4) | 0.087 (3) | 0.008 (3) | −0.027 (2) | 0.044 (3) |
| C28 | 0.093 (2) | 0.111 (3) | 0.0569 (17) | −0.014 (2) | −0.0090 (17) | 0.0104 (17) |
| C29 | 0.0717 (19) | 0.0707 (17) | 0.0618 (16) | 0.0085 (17) | −0.0029 (14) | 0.0048 (14) |
| N1 | 0.0427 (11) | 0.0397 (10) | 0.0497 (10) | −0.0022 (9) | 0.0009 (9) | −0.0037 (8) |
| N2 | 0.0468 (11) | 0.0403 (11) | 0.0582 (11) | 0.0097 (9) | −0.0025 (10) | −0.0058 (9) |
| O1 | 0.0786 (14) | 0.0369 (9) | 0.1073 (17) | −0.0058 (10) | 0.0062 (12) | −0.0017 (9) |
| O2 | 0.0745 (14) | 0.0620 (12) | 0.1188 (18) | −0.0200 (12) | 0.0288 (14) | 0.0139 (12) |
| O3 | 0.0412 (9) | 0.0526 (10) | 0.0749 (12) | 0.0058 (8) | −0.0080 (8) | 0.0012 (9) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—O1 | 1.209 (3) | C16—C17 | 1.503 (4) |
| C1—N2 | 1.374 (3) | C16—H16A | 0.9700 |
| C1—N1 | 1.397 (3) | C16—H16B | 0.9700 |
| C2—C7 | 1.370 (3) | C17—C22 | 1.351 (5) |
| C2—N2 | 1.377 (3) | C17—C18 | 1.373 (5) |
| C2—C3 | 1.412 (3) | C18—C19 | 1.362 (6) |
| C3—N1 | 1.387 (3) | C18—H18 | 0.9300 |
| C3—C4 | 1.398 (3) | C19—C20 | 1.353 (9) |
| C4—C5 | 1.418 (3) | C19—H19 | 0.9300 |
| C4—C8 | 1.469 (3) | C20—C21 | 1.353 (9) |
| C5—C6 | 1.383 (3) | C20—H20 | 0.9300 |
| C5—C11 | 1.488 (4) | C21—C22 | 1.375 (7) |
| C6—C7 | 1.390 (4) | C21—H21 | 0.9300 |
| C6—H6 | 0.9300 | C22—H22 | 0.9300 |
| C7—H7 | 0.9300 | C23—N2 | 1.460 (3) |
| C8—O3 | 1.220 (3) | C23—C24 | 1.504 (4) |
| C8—C9 | 1.486 (3) | C23—H23A | 0.9700 |
| C9—C10 | 1.387 (4) | C23—H23B | 0.9700 |
| C9—C15 | 1.391 (4) | C24—C25 | 1.354 (4) |
| C10—C12 | 1.396 (4) | C24—C29 | 1.371 (4) |
| C10—C11 | 1.483 (4) | C25—C26 | 1.389 (6) |
| C11—O2 | 1.215 (3) | C25—H25 | 0.9300 |
| C12—C13 | 1.380 (5) | C26—C27 | 1.338 (6) |
| C12—H12 | 0.9300 | C26—H26 | 0.9300 |
| C13—C14 | 1.376 (5) | C27—C28 | 1.344 (5) |
| C13—H13 | 0.9300 | C27—H27 | 0.9300 |
| C14—C15 | 1.382 (4) | C28—C29 | 1.388 (4) |
| C14—H14 | 0.9300 | C28—H28 | 0.9300 |

| | | | |
|---|---|---|---|
| C15—H15 | 0.9300 | C29—H29 | 0.9300 |
| C16—N1 | 1.467 (3) | | |
| O1—C1—N2 | 126.5 (2) | H16A—C16—H16B | 107.9 |
| O1—C1—N1 | 127.0 (2) | C22—C17—C18 | 118.3 (3) |
| N2—C1—N1 | 106.4 (2) | C22—C17—C16 | 121.8 (3) |
| C7—C2—N2 | 129.7 (2) | C18—C17—C16 | 119.9 (3) |
| C7—C2—C3 | 122.8 (2) | C19—C18—C17 | 120.2 (5) |
| N2—C2—C3 | 107.4 (2) | C19—C18—H18 | 119.9 |
| N1—C3—C4 | 133.6 (2) | C17—C18—H18 | 119.9 |
| N1—C3—C2 | 106.54 (18) | C20—C19—C18 | 120.6 (5) |
| C4—C3—C2 | 119.8 (2) | C20—C19—H19 | 119.7 |
| C3—C4—C5 | 116.6 (2) | C18—C19—H19 | 119.7 |
| C3—C4—C8 | 124.2 (2) | C21—C20—C19 | 120.2 (5) |
| C5—C4—C8 | 118.87 (18) | C21—C20—H20 | 119.9 |
| C6—C5—C4 | 121.9 (2) | C19—C20—H20 | 119.9 |
| C6—C5—C11 | 117.9 (2) | C20—C21—C22 | 118.9 (6) |
| C4—C5—C11 | 120.1 (2) | C20—C21—H21 | 120.6 |
| C5—C6—C7 | 121.2 (2) | C22—C21—H21 | 120.6 |
| C5—C6—H6 | 119.4 | C17—C22—C21 | 121.8 (5) |
| C7—C6—H6 | 119.4 | C17—C22—H22 | 119.1 |
| C2—C7—C6 | 117.5 (2) | C21—C22—H22 | 119.1 |
| C2—C7—H7 | 121.3 | N2—C23—C24 | 113.6 (2) |
| C6—C7—H7 | 121.3 | N2—C23—H23A | 108.8 |
| O3—C8—C4 | 122.4 (2) | C24—C23—H23A | 108.8 |
| O3—C8—C9 | 120.5 (2) | N2—C23—H23B | 108.8 |
| C4—C8—C9 | 117.0 (2) | C24—C23—H23B | 108.8 |
| C10—C9—C15 | 120.3 (2) | H23A—C23—H23B | 107.7 |
| C10—C9—C8 | 120.5 (2) | C25—C24—C29 | 118.0 (3) |
| C15—C9—C8 | 119.2 (2) | C25—C24—C23 | 117.6 (3) |
| C9—C10—C12 | 119.8 (3) | C29—C24—C23 | 124.3 (2) |
| C9—C10—C11 | 120.4 (2) | C24—C25—C26 | 120.7 (4) |
| C12—C10—C11 | 119.8 (3) | C24—C25—H25 | 119.7 |
| O2—C11—C10 | 121.1 (2) | C26—C25—H25 | 119.7 |
| O2—C11—C5 | 121.3 (3) | C27—C26—C25 | 120.9 (4) |
| C10—C11—C5 | 117.5 (2) | C27—C26—H26 | 119.5 |
| C13—C12—C10 | 119.3 (3) | C25—C26—H26 | 119.5 |
| C13—C12—H12 | 120.4 | C26—C27—C28 | 119.2 (4) |
| C10—C12—H12 | 120.4 | C26—C27—H27 | 120.4 |
| C14—C13—C12 | 120.8 (3) | C28—C27—H27 | 120.4 |
| C14—C13—H13 | 119.6 | C27—C28—C29 | 120.7 (4) |
| C12—C13—H13 | 119.6 | C27—C28—H28 | 119.6 |
| C13—C14—C15 | 120.5 (3) | C29—C28—H28 | 119.6 |
| C13—C14—H14 | 119.8 | C24—C29—C28 | 120.3 (3) |
| C15—C14—H14 | 119.8 | C24—C29—H29 | 119.8 |
| C14—C15—C9 | 119.3 (3) | C28—C29—H29 | 119.8 |
| C14—C15—H15 | 120.4 | C3—N1—C1 | 109.50 (19) |
| C9—C15—H15 | 120.4 | C3—N1—C16 | 129.55 (19) |
| N1—C16—C17 | 112.2 (2) | C1—N1—C16 | 118.3 (2) |
| N1—C16—H16A | 109.2 | C1—N2—C2 | 110.11 (19) |

| | | | | |
|---|---|---|---|---|
| C17—C16—H16A | 109.2 | C1—N2—C23 | 122.9 (2) |
| N1—C16—H16B | 109.2 | C2—N2—C23 | 126.6 (2) |
| C17—C16—H16B | 109.2 | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C13—H13···O1[i] | 0.93 | 2.39 | 3.312 (3) | 171. |
| C23—H23A···O2[ii] | 0.97 | 2.47 | 3.439 (4) | 174. |

Symmetry codes: (i) $x$, $y+1$, $z$; (ii) $-x+1$, $y-1/2$, $-z+3/2$.

**Fig. 1**