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# 2-(4-Methylphenyl)-1*H*-anthraceno-[1,2-*d*]imidazole-6,11-dione: a fluorescent chemosensor

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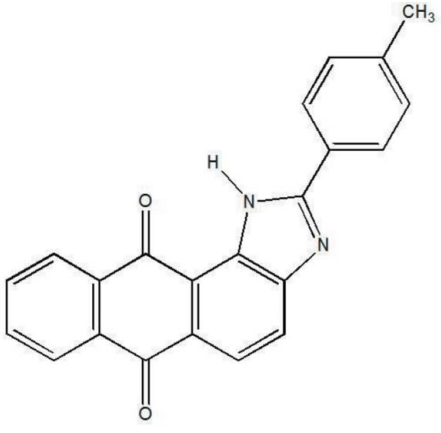
Key indicators: single-crystal X-ray study; $T$ = 295 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.060; $wR$ factor = 0.155; data-to-parameter ratio = 15.5.

In the title compound, $C_{22}H_{14}N_2O_2$, the five rings of the molecule are not coplanar. There is a significant twist between the four fused rings, which have a slightly arched conformation, and the pendant aromatic ring, as seen in the dihedral angle of 13.16 (8)° between the anthraquinonic ring system and the pendant aromatic ring plane.

## Related literature

For general background on organic fluorophores, see: Czarnik (1994); Friend *et al.* (1999); Joux & Lebaron (2000); Kasten (1999); Soukos *et al.* (2000); Zhu *et al.* (2008). For related structures and applications, see: Peng *et al.* (2005); Boiocchi *et al.* (2004); Yoshida *et al.* (2002).




## Experimental

### Crystal data

$C_{22}H_{14}N_2O_2$
$M_r$ = 338.35
Orthorhombic, *Pbca*
$a$ = 7.3850 (10) Å
$b$ = 14.0730 (4) Å
$c$ = 30.5630 (9) Å
$V$ = 3176.4 (4) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 295 K
0.14 × 0.14 × 0.07 mm

### Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
20847 measured reflections
3643 independent reflections
2282 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.066

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.155
$S$ = 1.05
3643 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2418).

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# supplementary materials

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# 2-(4-Methylphenyl)-1*H*-anthraceno[1,2-*d*]imidazole-6,11-dione: a fluorescent chemosensor

**T. T. Guimarães, E. N. Da Silva Júnior, C. E. M. Carvalho, C. A. De Simone and A. V. Pinto**

## Comment

Recently, much attention has been devoted to the study of organic fluorophores because of their potential use in analytical chemistry (Czarnik, 1994), optoeletronics (Friend *et al.*, 1999), dye technologies (Joux & Lebaron, 1988; Kasten, 1999), forensic chemistry (Soukos *et al.*, 2000), and in pharmaceutical analysis evaluations (Zhu *et al.*, 2008). In addition, specific and sensitive chemosensors for anions are of great importance in environmental science (Peng *et al.*, 2005). The N—H···F interaction is already well known (Boiocchi *et al.*, 2004) and can be exploited in the development of new molecules to function as fluorescent probes for fluoride. For instance, one such class of probe are the anthraimidazolic-derived quinones that can be deprotonated in the presence of anions to enhance their natural fluorescence by a supposed mechanism of photo-induced electron transfer (PET) or *via* a bathochromic shift of the absorption bands promoted by charge transfer (CT) (Peng *et al.*, 2005). Although many photophysical properties of fluorophores are well known in solution, only a few are known in solid-state (Yoshida *et al.*, 2002). In this paper we report the molecular structure of the 2-*p*-tolyl-1*H*-anthra[1,2-*d*]imidazole-6,11-dione, (I), a fluorescent probe synthesized in our laboratory.

In (I), the rings are not co-planar (Fig. 1). The anthraquinonic ring is almost planar with the greatest deviation from the least-squares plane of 0.102 (2) Å being exhibited by atom C7. The dihedral angle between the anthraquinonic ring [C2—C11] and the benzene ring [C12—C17] planes is 13.16 (8)°.

## Experimental

To an acetic acid solution (25 ml) of the 1,2-diaminoanthraquinone (238 mg, 1 mmol), *p*-methyl-benzaldehyde (132 mg, 1.1 mmol) and sodium acetate (107 mg, 1.3 mmol) were added. The mixture was left under agitation and reflux for 30 min. The reaction was leaked into cold water (50 ml) which precipitated a yellow solid that was filtered under vacuum. The new anthraimidazole derivate (I) was purified by column chromatography over silica-gel, using a dichloromethane/ethyl acetate (5:1) mixture as eluent and obtained as yellow crystals in 69.5% yield (235 mg, 0.70 mmol); m.p. 522 K. $^1$H NMR (300 MHz, $CDCl_3$) δ: 8.33–8.30 (m, 1H); 8.27–8.24 (m, 1H); 8.20 (d, *J* = 8.79 Hz, 1H); 8.08 (d, *J* = 7.91 Hz, 2H); 8.03 (d, *J* = 8.79 Hz, 1H); 7.83–7.75 (m, 2H); 7.37 (d, *J* = 7.91 Hz, 2H); 2.46 p.p.m. (s, 3H); N—H not obs. $^{13}$C NMR (300 MHz, $CDCl_3$): δ: 21.8, 117.82, 121.87, 125.40, 125.74, 126.37, 126.79, 126.91, 127.48, 128.35, 129.91, 129.91, 133.14, 133.23, 133.63, 133.94, 134.29, 141.94, 149.53, 156.78, 183.1, 183.1 p.p.m.

## Refinement

H atoms were located on stereochemical grounds and refined with fixed geometry, each riding on a carrier atom, with C—H = 0.93 - 0.98 Å and $U_{iso}$ = 1.5 (for methyl-H) and 1.2 (other H atoms) $U_{eq}$(carrier atom).

## Figures

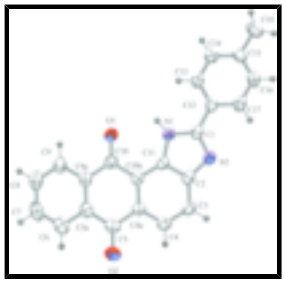


Fig. 1. Projection of (I), showing the atom labelling with 50% probability displacement ellipsoids.

## 2-(4-Methylphenyl)-1*H*-anthraceno[1,2-*d*]imidazole-6,11-dione

### *Crystal data*

| | |
|---|---|
| $C_{22}H_{14}N_2O_2$ | $F_{000}$ = 1408 |
| $M_r$ = 338.35 | $D_x$ = 1.415 Mg m$^{-3}$ |
| Orthorhombic, *Pbca* | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ac 2ab | Cell parameters from 14527 reflections |
| *a* = 7.3850 (10) Å | θ = 2.9–27.5º |
| *b* = 14.0730 (4) Å | μ = 0.09 mm$^{-1}$ |
| *c* = 30.5630 (9) Å | *T* = 295 K |
| *V* = 3176.4 (4) Å$^3$ | Prism, yellow |
| *Z* = 8 | 0.14 × 0.14 × 0.07 mm |

### *Data collection*

| | |
|---|---|
| Nonius KappaCCD diffractometer | 2282 reflections with $I > 2\sigma(I)$ |
| Radiation source: Enraf–Nonius FR590 | $R_{int}$ = 0.066 |
| Monochromator: horizonally mounted graphite crystal | $\theta_{max}$ = 27.5º |
| Detector resolution: 9 pixels mm$^{-1}$ | $\theta_{min}$ = 3.0º |
| CCD rotation images, thick slices scans | *h* = −9→7 |
| Absorption correction: none | *k* = −14→18 |
| 20847 measured reflections | *l* = −39→38 |
| 3643 independent reflections | |

### *Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.060 | H-atom parameters constrained |
| $wR(F^2)$ = 0.155 | $w = 1/[\sigma^2(F_o^2) + (0.0589P)^2 + 1.2992P]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |

| | |
|---|---|
| $S$ = 1.05 | $(\Delta/\sigma)_{max} < 0.001$ |
| 3643 reflections | $\Delta\rho_{max} = 0.18$ e Å$^{-3}$ |
| 235 parameters | $\Delta\rho_{min} = -0.20$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*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 | 0.7524 (2) | 0.58882 (10) | 0.24672 (5) | 0.0537 (4) |
| O2 | 0.4748 (2) | 0.25831 (11) | 0.30424 (6) | 0.0632 (5) |
| N1 | 0.6678 (2) | 0.53709 (11) | 0.16053 (6) | 0.0413 (4) |
| H1N | 0.7063 | 0.5904 | 0.1706 | 0.050* |
| N2 | 0.5832 (2) | 0.42641 (11) | 0.11186 (6) | 0.0454 (4) |
| C1 | 0.6423 (3) | 0.51458 (14) | 0.11723 (7) | 0.0420 (5) |
| C2 | 0.5674 (3) | 0.39056 (14) | 0.15381 (7) | 0.0420 (5) |
| C3 | 0.5055 (3) | 0.30226 (14) | 0.16831 (8) | 0.0480 (5) |
| H3 | 0.4709 | 0.2556 | 0.1484 | 0.058* |
| C4 | 0.4967 (3) | 0.28566 (14) | 0.21264 (8) | 0.0476 (5) |
| H4 | 0.4546 | 0.2272 | 0.2225 | 0.057* |
| C4A | 0.5494 (3) | 0.35426 (13) | 0.24325 (7) | 0.0406 (5) |
| C5 | 0.5310 (3) | 0.33481 (15) | 0.29076 (8) | 0.0454 (5) |
| C5A | 0.5811 (3) | 0.41206 (14) | 0.32185 (7) | 0.0440 (5) |
| C6 | 0.5545 (3) | 0.39803 (18) | 0.36653 (8) | 0.0567 (6) |
| H6 | 0.5056 | 0.3412 | 0.3766 | 0.068* |
| C7 | 0.6007 (3) | 0.46845 (19) | 0.39578 (8) | 0.0632 (7) |
| H7 | 0.5787 | 0.4597 | 0.4255 | 0.076* |
| C8 | 0.6794 (3) | 0.55197 (18) | 0.38151 (8) | 0.0621 (7) |
| H8 | 0.7133 | 0.5982 | 0.4016 | 0.075* |
| C9 | 0.7077 (3) | 0.56666 (16) | 0.33750 (8) | 0.0506 (6) |
| H9 | 0.7609 | 0.6228 | 0.3279 | 0.061* |
| C9A | 0.6566 (3) | 0.49753 (14) | 0.30745 (7) | 0.0420 (5) |
| C10 | 0.6808 (3) | 0.51561 (14) | 0.26033 (7) | 0.0399 (5) |
| C10A | 0.6161 (3) | 0.44294 (13) | 0.22942 (7) | 0.0380 (5) |
| C11 | 0.6208 (3) | 0.45918 (13) | 0.18450 (7) | 0.0381 (5) |
| C12 | 0.6719 (3) | 0.58162 (14) | 0.08136 (7) | 0.0428 (5) |

| | | | | |
|---|---|---|---|---|
| C13 | 0.7054 (3) | 0.67704 (15) | 0.08847 (8) | 0.0504 (6) |
| H13 | 0.7151 | 0.6997 | 0.1170 | 0.060* |
| C14 | 0.7245 (3) | 0.73941 (16) | 0.05371 (8) | 0.0558 (6) |
| H14 | 0.7481 | 0.8032 | 0.0593 | 0.067* |
| C15 | 0.7090 (3) | 0.70857 (17) | 0.01088 (8) | 0.0526 (6) |
| C16 | 0.6790 (3) | 0.61297 (17) | 0.00396 (8) | 0.0595 (6) |
| H16 | 0.6702 | 0.5904 | −0.0246 | 0.071* |
| C17 | 0.6617 (3) | 0.55016 (16) | 0.03836 (8) | 0.0560 (6) |
| H17 | 0.6429 | 0.4860 | 0.0327 | 0.067* |
| C18 | 0.7200 (4) | 0.7767 (2) | −0.02702 (9) | 0.0722 (8) |
| H18A | 0.8401 | 0.8026 | −0.0287 | 0.108* |
| H18B | 0.6345 | 0.8273 | −0.0228 | 0.108* |
| H18C | 0.6926 | 0.7437 | −0.0537 | 0.108* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0679 (10) | 0.0417 (8) | 0.0517 (10) | −0.0081 (7) | −0.0037 (8) | −0.0011 (7) |
| O2 | 0.0776 (11) | 0.0491 (9) | 0.0630 (11) | −0.0064 (8) | 0.0067 (9) | 0.0101 (8) |
| N1 | 0.0463 (9) | 0.0352 (9) | 0.0424 (11) | −0.0031 (7) | −0.0018 (8) | −0.0024 (8) |
| N2 | 0.0500 (10) | 0.0411 (10) | 0.0452 (11) | 0.0008 (8) | 0.0006 (8) | −0.0064 (8) |
| C1 | 0.0414 (11) | 0.0418 (11) | 0.0427 (13) | 0.0036 (9) | −0.0024 (9) | −0.0058 (10) |
| C2 | 0.0402 (10) | 0.0403 (11) | 0.0456 (12) | 0.0030 (9) | −0.0003 (9) | −0.0045 (10) |
| C3 | 0.0529 (13) | 0.0362 (11) | 0.0550 (15) | −0.0020 (9) | 0.0011 (11) | −0.0098 (10) |
| C4 | 0.0491 (12) | 0.0351 (11) | 0.0586 (15) | −0.0019 (9) | 0.0037 (11) | −0.0012 (10) |
| C4A | 0.0379 (10) | 0.0360 (10) | 0.0478 (13) | 0.0042 (8) | 0.0018 (9) | 0.0012 (10) |
| C5 | 0.0398 (11) | 0.0414 (12) | 0.0550 (14) | 0.0047 (9) | 0.0035 (10) | 0.0074 (10) |
| C5A | 0.0382 (11) | 0.0488 (12) | 0.0452 (13) | 0.0075 (9) | −0.0030 (9) | 0.0022 (10) |
| C6 | 0.0529 (13) | 0.0672 (15) | 0.0499 (15) | 0.0062 (11) | 0.0004 (11) | 0.0078 (13) |
| C7 | 0.0656 (15) | 0.0835 (19) | 0.0405 (14) | 0.0123 (14) | −0.0019 (12) | 0.0012 (13) |
| C8 | 0.0679 (16) | 0.0670 (16) | 0.0515 (16) | 0.0107 (13) | −0.0098 (12) | −0.0144 (13) |
| C9 | 0.0547 (13) | 0.0490 (12) | 0.0482 (14) | 0.0087 (10) | −0.0067 (11) | −0.0057 (11) |
| C9A | 0.0400 (11) | 0.0428 (11) | 0.0432 (13) | 0.0098 (9) | −0.0037 (9) | −0.0006 (10) |
| C10 | 0.0391 (10) | 0.0338 (10) | 0.0468 (13) | 0.0044 (9) | −0.0032 (9) | 0.0005 (9) |
| C10A | 0.0344 (10) | 0.0369 (10) | 0.0426 (12) | 0.0051 (8) | 0.0004 (8) | −0.0027 (9) |
| C11 | 0.0369 (10) | 0.0341 (10) | 0.0435 (12) | 0.0013 (8) | −0.0002 (9) | −0.0029 (9) |
| C12 | 0.0431 (11) | 0.0441 (12) | 0.0412 (12) | 0.0005 (9) | 0.0005 (9) | −0.0028 (10) |
| C13 | 0.0598 (14) | 0.0479 (13) | 0.0434 (13) | −0.0037 (10) | −0.0031 (10) | −0.0052 (10) |
| C14 | 0.0656 (15) | 0.0490 (13) | 0.0526 (15) | −0.0101 (11) | −0.0020 (11) | 0.0014 (11) |
| C15 | 0.0445 (12) | 0.0649 (15) | 0.0484 (14) | −0.0049 (11) | 0.0024 (10) | 0.0066 (12) |
| C16 | 0.0709 (16) | 0.0690 (16) | 0.0387 (13) | −0.0046 (13) | 0.0007 (11) | −0.0036 (12) |
| C17 | 0.0713 (15) | 0.0505 (13) | 0.0463 (14) | −0.0040 (11) | 0.0021 (11) | −0.0087 (11) |
| C18 | 0.0713 (17) | 0.0866 (19) | 0.0587 (17) | −0.0103 (14) | −0.0009 (13) | 0.0207 (15) |

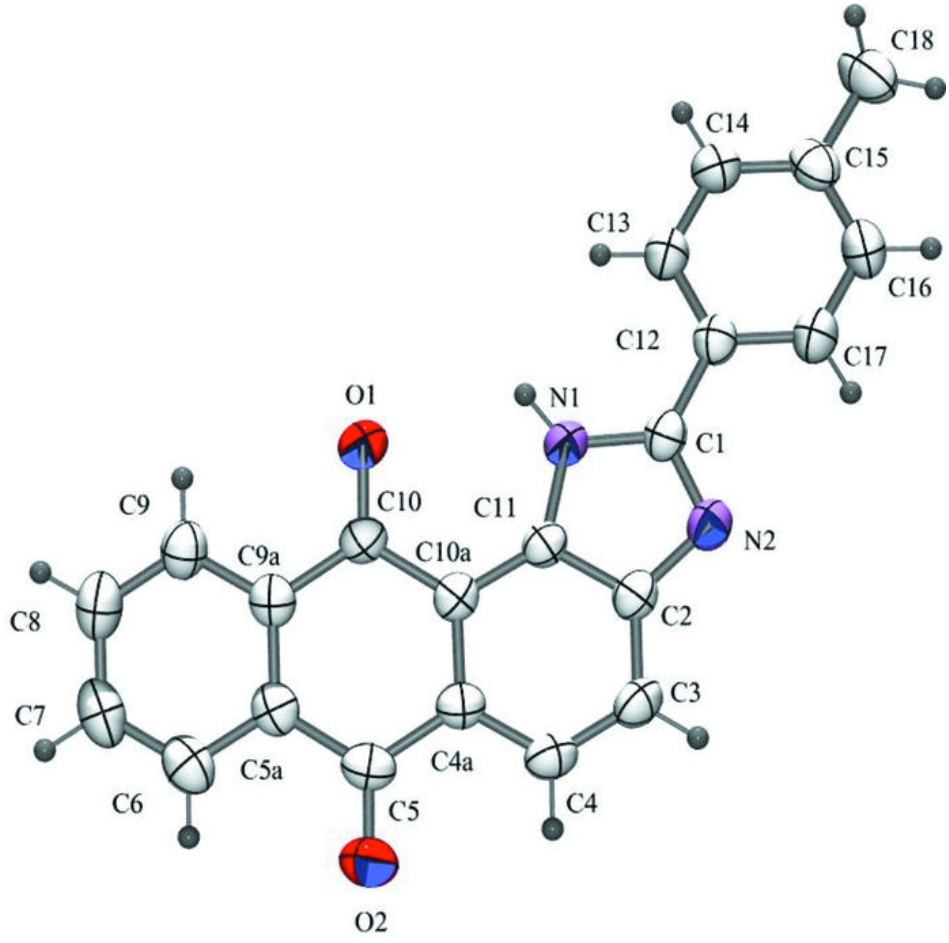
*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C10 | 1.231 (2) | C7—H7 | 0.9300 |
| O2—C5 | 1.225 (2) | C8—C9 | 1.377 (3) |
| N1—C11 | 1.364 (2) | C8—H8 | 0.9300 |

| | | | |
|---|---|---|---|
| N1—C1 | 1.374 (3) | C9—C9A | 1.390 (3) |
| N1—H1N | 0.8600 | C9—H9 | 0.9300 |
| N2—C1 | 1.325 (2) | C9A—C10 | 1.473 (3) |
| N2—C2 | 1.383 (3) | C10—C10A | 1.472 (3) |
| C1—C12 | 1.463 (3) | C10A—C11 | 1.392 (3) |
| C2—C3 | 1.396 (3) | C12—C13 | 1.383 (3) |
| C2—C11 | 1.403 (3) | C12—C17 | 1.389 (3) |
| C3—C4 | 1.376 (3) | C13—C14 | 1.385 (3) |
| C3—H3 | 0.9300 | C13—H13 | 0.9300 |
| C4—C4A | 1.399 (3) | C14—C15 | 1.384 (3) |
| C4—H4 | 0.9300 | C14—H14 | 0.9300 |
| C4A—C10A | 1.407 (3) | C15—C16 | 1.380 (3) |
| C4A—C5 | 1.484 (3) | C15—C18 | 1.506 (3) |
| C5—C5A | 1.491 (3) | C16—C17 | 1.380 (3) |
| C5A—C6 | 1.393 (3) | C16—H16 | 0.9300 |
| C5A—C9A | 1.397 (3) | C17—H17 | 0.9300 |
| C6—C7 | 1.378 (3) | C18—H18A | 0.9600 |
| C6—H6 | 0.9300 | C18—H18B | 0.9600 |
| C7—C8 | 1.382 (3) | C18—H18C | 0.9600 |
| C11—N1—C1 | 107.29 (16) | C9—C9A—C5A | 120.2 (2) |
| C11—N1—H1N | 126.4 | C9—C9A—C10 | 119.47 (19) |
| C1—N1—H1N | 126.4 | C5A—C9A—C10 | 120.34 (19) |
| C1—N2—C2 | 104.75 (17) | O1—C10—C10A | 120.28 (19) |
| N2—C1—N1 | 112.35 (18) | O1—C10—C9A | 121.81 (19) |
| N2—C1—C12 | 124.07 (19) | C10A—C10—C9A | 117.91 (18) |
| N1—C1—C12 | 123.55 (18) | C11—C10A—C4A | 116.79 (18) |
| N2—C2—C3 | 130.29 (19) | C11—C10A—C10 | 120.72 (18) |
| N2—C2—C11 | 110.19 (17) | C4A—C10A—C10 | 122.48 (19) |
| C3—C2—C11 | 119.5 (2) | N1—C11—C10A | 131.92 (18) |
| C4—C3—C2 | 118.6 (2) | N1—C11—C2 | 105.41 (18) |
| C4—C3—H3 | 120.7 | C10A—C11—C2 | 122.65 (18) |
| C2—C3—H3 | 120.7 | C13—C12—C17 | 117.9 (2) |
| C3—C4—C4A | 121.86 (19) | C13—C12—C1 | 122.37 (19) |
| C3—C4—H4 | 119.1 | C17—C12—C1 | 119.70 (19) |
| C4A—C4—H4 | 119.1 | C12—C13—C14 | 120.9 (2) |
| C4—C4A—C10A | 120.6 (2) | C12—C13—H13 | 119.6 |
| C4—C4A—C5 | 120.09 (18) | C14—C13—H13 | 119.6 |
| C10A—C4A—C5 | 119.33 (18) | C15—C14—C13 | 121.2 (2) |
| O2—C5—C4A | 121.5 (2) | C15—C14—H14 | 119.4 |
| O2—C5—C5A | 120.7 (2) | C13—C14—H14 | 119.4 |
| C4A—C5—C5A | 117.81 (18) | C16—C15—C14 | 117.6 (2) |
| C6—C5A—C9A | 119.1 (2) | C16—C15—C18 | 120.8 (2) |
| C6—C5A—C5 | 119.1 (2) | C14—C15—C18 | 121.6 (2) |
| C9A—C5A—C5 | 121.8 (2) | C17—C16—C15 | 121.5 (2) |
| C7—C6—C5A | 119.9 (2) | C17—C16—H16 | 119.2 |
| C7—C6—H6 | 120.0 | C15—C16—H16 | 119.2 |
| C5A—C6—H6 | 120.0 | C16—C17—C12 | 120.8 (2) |
| C6—C7—C8 | 120.8 (2) | C16—C17—H17 | 119.6 |
| C6—C7—H7 | 119.6 | C12—C17—H17 | 119.6 |

| | | | |
|---|---|---|---|
| C8—C7—H7 | 119.6 | C15—C18—H18A | 109.5 |
| C9—C8—C7 | 120.0 (2) | C15—C18—H18B | 109.5 |
| C9—C8—H8 | 120.0 | H18A—C18—H18B | 109.5 |
| C7—C8—H8 | 120.0 | C15—C18—H18C | 109.5 |
| C8—C9—C9A | 120.0 (2) | H18A—C18—H18C | 109.5 |
| C8—C9—H9 | 120.0 | H18B—C18—H18C | 109.5 |
| C9A—C9—H9 | 120.0 | | |
| C2—N2—C1—N1 | 0.8 (2) | C5A—C9A—C10—C10A | 2.6 (3) |
| C2—N2—C1—C12 | −177.41 (18) | C4—C4A—C10A—C11 | 2.0 (3) |
| C11—N1—C1—N2 | −0.6 (2) | C5—C4A—C10A—C11 | −176.46 (17) |
| C11—N1—C1—C12 | 177.64 (18) | C4—C4A—C10A—C10 | −177.16 (18) |
| C1—N2—C2—C3 | 177.6 (2) | C5—C4A—C10A—C10 | 4.4 (3) |
| C1—N2—C2—C11 | −0.7 (2) | O1—C10—C10A—C11 | −5.4 (3) |
| N2—C2—C3—C4 | −177.4 (2) | C9A—C10—C10A—C11 | 174.48 (17) |
| C11—C2—C3—C4 | 0.8 (3) | O1—C10—C10A—C4A | 173.70 (18) |
| C2—C3—C4—C4A | −0.6 (3) | C9A—C10—C10A—C4A | −6.4 (3) |
| C3—C4—C4A—C10A | −0.9 (3) | C1—N1—C11—C10A | −178.3 (2) |
| C3—C4—C4A—C5 | 177.60 (18) | C1—N1—C11—C2 | 0.1 (2) |
| C4—C4A—C5—O2 | 2.1 (3) | C4A—C10A—C11—N1 | 176.36 (19) |
| C10A—C4A—C5—O2 | −179.44 (19) | C10—C10A—C11—N1 | −4.5 (3) |
| C4—C4A—C5—C5A | −177.22 (18) | C4A—C10A—C11—C2 | −1.8 (3) |
| C10A—C4A—C5—C5A | 1.2 (3) | C10—C10A—C11—C2 | 177.34 (17) |
| O2—C5—C5A—C6 | −3.3 (3) | N2—C2—C11—N1 | 0.4 (2) |
| C4A—C5—C5A—C6 | 176.00 (18) | C3—C2—C11—N1 | −178.13 (17) |
| O2—C5—C5A—C9A | 175.73 (19) | N2—C2—C11—C10A | 179.00 (17) |
| C4A—C5—C5A—C9A | −5.0 (3) | C3—C2—C11—C10A | 0.5 (3) |
| C9A—C5A—C6—C7 | 0.7 (3) | N2—C1—C12—C13 | 169.3 (2) |
| C5—C5A—C6—C7 | 179.74 (19) | N1—C1—C12—C13 | −8.7 (3) |
| C5A—C6—C7—C8 | −2.3 (3) | N2—C1—C12—C17 | −8.8 (3) |
| C6—C7—C8—C9 | 1.9 (4) | N1—C1—C12—C17 | 173.16 (19) |
| C7—C8—C9—C9A | 0.1 (3) | C17—C12—C13—C14 | 1.2 (3) |
| C8—C9—C9A—C5A | −1.7 (3) | C1—C12—C13—C14 | −177.0 (2) |
| C8—C9—C9A—C10 | 177.59 (19) | C12—C13—C14—C15 | 0.7 (4) |
| C6—C5A—C9A—C9 | 1.3 (3) | C13—C14—C15—C16 | −1.8 (3) |
| C5—C5A—C9A—C9 | −177.70 (18) | C13—C14—C15—C18 | 176.8 (2) |
| C6—C5A—C9A—C10 | −178.00 (18) | C14—C15—C16—C17 | 1.1 (3) |
| C5—C5A—C9A—C10 | 3.0 (3) | C18—C15—C16—C17 | −177.5 (2) |
| C9—C9A—C10—O1 | 3.2 (3) | C15—C16—C17—C12 | 0.7 (4) |
| C5A—C9A—C10—O1 | −177.51 (18) | C13—C12—C17—C16 | −1.9 (3) |
| C9—C9A—C10—C10A | −176.75 (17) | C1—C12—C17—C16 | 176.3 (2) |

**Fig. 1**


C18
C14
C15
C13
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O1
N1
C1
C9
C10
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N2
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C10a
C8
C2
C3
C7
C5a
C4a
C6
C5
C4
O2