Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 1-(2-Methoxyanilino)anthraquinone

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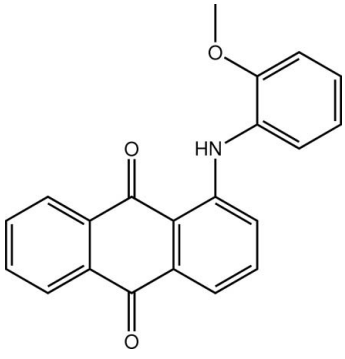
Received 23 March 2010; accepted 10 April 2010

Key indicators: single-crystal X-ray study; $T$ = 110 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.052; $wR$ factor = 0.161; data-to-parameter ratio = 19.7.

In the title compound, $C_{21}H_{15}NO_3$, the dihedral angle formed between the aromatic ring systems is 71.50 (3)°. The methoxy group is coplanar with the benzene ring to which it is connected, the C—O—C—C torsion angle being 6.37 (17)°. The observed conformation is stabilized by an intramolecular N—H···O hydrogen bond, generating an $S$(6) ring.

## Related literature

For background to anthraquinone derivatives, see: Matsui (1998); Rao & Choudhary (1990).




## Experimental

### Crystal data

$C_{21}H_{15}NO_3$
$M_r$ = 329.34
Monoclinic, $P2_1/c$
$a$ = 11.4222 (3) Å
$b$ = 7.9878 (2) Å
$c$ = 16.9332 (4) Å
$\beta$ = 100.9851 (12)°
$V$ = 1516.65 (7) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 110 K
0.40 × 0.30 × 0.14 mm

### Data collection

Bruker–Nonius X8 APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2006)
$T_{min}$ = 0.962, $T_{max}$ = 0.987
32405 measured reflections
5620 independent reflections
3863 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.031

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.161
$S$ = 1.05
5620 reflections
286 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.49 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O1 | 0.932 (19) | 1.886 (18) | 2.6279 (13) | 135.0 (17) |

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *XL* (Bruker, 2004); molecular graphics: *XL*; software used to prepare material for publication: *XL*.

This research was supported by the China Scholarship Council (No. 2007102249). We also wish to thank Dr Harold S. Freeman and Dr Paul Boyle at North Carolina State University for their help.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2648).

## References

Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Bruker (2004). *XL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2006). *SADABS*, *APEX2* and *SAINT*. Madison, Wisconsin, USA.
Matsui, M. (1998). *Dyes Pigments*, **40**, 21–26.
Rao, B. V. & Choudhary, V. (1990). *J. Soc. Dyers Colour.* **106**, 388–394.

# supplementary materials

*Acta Cryst.* (2010). E**66**, o1117 [ **doi:10.1107/S1600536810013310** ]

# 1-(2-Methoxyanilino)anthraquinone

**L. Lu and L. He**

## Comment

Anthraquinone and its derivatives are important compounds in the fields of dyes and pigments (Matsui 1998; Rao & Choudhary, 1990). Here, we report the crystal structure of the title compound, (I), Fig. 1. The dihedral angle formed between the aromatic systems is 71.50 (3)°. The methoxy group is co-planar with the benzene ring to which it is connected with the C21–O3–C16–C17 torsion angle being 6.37 (17) °. The observed conformation is stabilised by an intramolecular N–H···O hydrogen bond, Table 1.

## Experimental

The crystal was obtained by dissolving (I) in methyl acetate (50 ml) and leaving the resulting solution, which was covered with Parafilm plastic containing pin holes, to evaporate at room temperature.

## Refinement

The hydrogen atoms were refined freely: N–H = 0.932 (19) Å, and C–H = 0.937 (16)–1.051 (17) Å.

## Figures

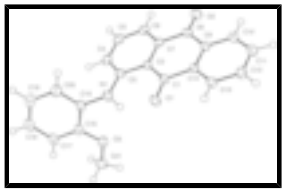


Fig. 1. The molecular structure of (I) showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level.

## 1-(2-Methoxyanilino)anthraquinone

*Crystal data*

| | |
|---|---|
| $C_{21}H_{15}NO_3$ | $F(000)$ = 688 |
| $M_r$ = 329.34 | $D_x$ = 1.442 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, λ = 0.71070 Å |
| Hall symbol: -P 2ybc | Cell parameters from 8857 reflections |
| $a$ = 11.4222 (3) Å | θ = 2.8–31.7° |
| $b$ = 7.9878 (2) Å | μ = 0.10 mm$^{-1}$ |
| $c$ = 16.9332 (4) Å | $T$ = 110 K |
| β = 100.9851 (12)° | Prism, red |
| $V$ = 1516.65 (7) Å$^3$ | 0.40 × 0.30 × 0.14 mm |

$Z = 4$

*Data collection*

| | |
|---|---|
| Bruker–Nonius X8 APEXII diffractometer | 5620 independent reflections |
| Radiation source: fine-focus sealed tube | 3863 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.031$ |
| φ scans | $\theta_{max} = 34.9°$, $\theta_{min} = 2.8°$ |
| Absorption correction: multi-scan (SADABS; Bruker, 2006) | $h = -17\rightarrow16$ |
| $T_{min} = 0.962$, $T_{max} = 0.987$ | $k = -12\rightarrow11$ |
| 32405 measured reflections | $l = -24\rightarrow25$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.052$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.161$ | All H-atom parameters refined |
| $S = 1.05$ | $w = 1/[\sigma^2(F_o^2) + (0.0934P)^2 + 0.1215P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 5620 reflections | $(\Delta/\sigma)_{max} = 0.001$ |
| 286 parameters | $\Delta\rho_{max} = 0.49$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.20$ 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 $F^2 > \sigma(F^2)$ 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 | 0.13993 (7) | 0.20278 (10) | 0.63675 (5) | 0.02712 (19) |
| O2 | −0.22023 (8) | −0.23872 (11) | 0.55875 (5) | 0.0302 (2) |
| O3 | 0.46774 (7) | −0.06574 (11) | 0.66601 (4) | 0.0286 (2) |
| N1 | 0.26972 (8) | −0.02097 (13) | 0.72798 (6) | 0.0258 (2) |
| H1 | 0.2651 (17) | 0.076 (2) | 0.6971 (11) | 0.058 (5)* |

| | | | | |
|---|---|---|---|---|
| C1 | 0.05822 (9) | 0.09907 (14) | 0.62187 (6) | 0.0203 (2) |
| C2 | 0.06875 (9) | −0.07113 (13) | 0.65401 (6) | 0.0192 (2) |
| C3 | 0.17497 (9) | −0.12548 (14) | 0.70664 (6) | 0.0216 (2) |
| C4 | 0.18047 (11) | −0.29225 (15) | 0.73478 (6) | 0.0263 (2) |
| H4 | 0.2586 (12) | −0.3278 (18) | 0.7699 (8) | 0.030 (4)* |
| C5 | 0.08556 (11) | −0.39923 (16) | 0.71402 (7) | 0.0279 (3) |
| H5 | 0.0911 (14) | −0.524 (2) | 0.7336 (10) | 0.043 (4)* |
| C6 | −0.02007 (11) | −0.34632 (15) | 0.66463 (6) | 0.0248 (2) |
| H6 | −0.0882 (13) | −0.4234 (19) | 0.6527 (9) | 0.034 (4)* |
| C7 | −0.02689 (9) | −0.18511 (14) | 0.63397 (6) | 0.0201 (2) |
| C8 | −0.13910 (9) | −0.13774 (14) | 0.57762 (6) | 0.0214 (2) |
| C9 | −0.14902 (9) | 0.03492 (14) | 0.54568 (6) | 0.0198 (2) |
| C10 | −0.25212 (10) | 0.08461 (15) | 0.49214 (6) | 0.0232 (2) |
| H10 | −0.3179 (11) | −0.0046 (17) | 0.4743 (7) | 0.020 (3)* |
| C11 | −0.26221 (10) | 0.24721 (15) | 0.46310 (6) | 0.0249 (2) |
| H11 | −0.3326 (12) | 0.2845 (18) | 0.4248 (8) | 0.029 (3)* |
| C12 | −0.17056 (10) | 0.36132 (15) | 0.48686 (6) | 0.0242 (2) |
| H12 | −0.1783 (13) | 0.481 (2) | 0.4670 (9) | 0.038 (4)* |
| C13 | −0.06699 (10) | 0.31181 (14) | 0.53857 (6) | 0.0222 (2) |
| H13 | −0.0034 (14) | 0.387 (2) | 0.5534 (9) | 0.037 (4)* |
| C14 | −0.05540 (9) | 0.14870 (13) | 0.56821 (5) | 0.0189 (2) |
| C15 | 0.37851 (10) | −0.06745 (14) | 0.77938 (6) | 0.0240 (2) |
| C16 | 0.48166 (10) | −0.08838 (14) | 0.74715 (6) | 0.0227 (2) |
| C17 | 0.58900 (10) | −0.12904 (15) | 0.79741 (7) | 0.0265 (2) |
| H17 | 0.6567 (14) | −0.143 (2) | 0.7741 (9) | 0.038 (4)* |
| C18 | 0.59215 (11) | −0.15392 (16) | 0.87909 (7) | 0.0297 (3) |
| H18 | 0.6648 (14) | −0.188 (2) | 0.9122 (10) | 0.043 (4)* |
| C19 | 0.49073 (12) | −0.13533 (17) | 0.91119 (7) | 0.0327 (3) |
| H19 | 0.4947 (14) | −0.153 (2) | 0.9695 (10) | 0.048 (5)* |
| C20 | 0.38352 (12) | −0.09066 (17) | 0.86123 (7) | 0.0315 (3) |
| H20 | 0.3124 (14) | −0.0724 (19) | 0.8831 (9) | 0.035 (4)* |
| C21 | 0.56705 (12) | −0.10204 (19) | 0.62942 (7) | 0.0329 (3) |
| H21A | 0.6315 (16) | −0.015 (2) | 0.6472 (11) | 0.048 (4)* |
| H21B | 0.5396 (15) | −0.094 (2) | 0.5726 (11) | 0.047 (4)* |
| H21C | 0.6026 (15) | −0.216 (2) | 0.6451 (10) | 0.048 (5)* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0201 (4) | 0.0221 (4) | 0.0365 (4) | −0.0035 (3) | −0.0012 (3) | 0.0040 (3) |
| O2 | 0.0269 (4) | 0.0259 (5) | 0.0363 (4) | −0.0078 (3) | 0.0020 (3) | −0.0011 (3) |
| O3 | 0.0257 (4) | 0.0362 (5) | 0.0235 (4) | 0.0020 (3) | 0.0038 (3) | 0.0023 (3) |
| N1 | 0.0191 (4) | 0.0260 (5) | 0.0305 (4) | 0.0014 (4) | 0.0001 (3) | 0.0068 (4) |
| C1 | 0.0180 (5) | 0.0207 (5) | 0.0221 (4) | −0.0002 (4) | 0.0040 (3) | 0.0001 (4) |
| C2 | 0.0193 (5) | 0.0189 (5) | 0.0204 (4) | 0.0014 (4) | 0.0059 (3) | 0.0007 (4) |
| C3 | 0.0204 (5) | 0.0232 (6) | 0.0224 (4) | 0.0015 (4) | 0.0064 (3) | 0.0015 (4) |
| C4 | 0.0272 (6) | 0.0256 (6) | 0.0262 (5) | 0.0045 (4) | 0.0058 (4) | 0.0066 (4) |
| C5 | 0.0342 (6) | 0.0232 (6) | 0.0277 (5) | 0.0009 (5) | 0.0090 (4) | 0.0060 (4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C6 | 0.0298 (6) | 0.0206 (6) | 0.0256 (5) | −0.0033 (5) | 0.0089 (4) | 0.0015 (4) |
| C7 | 0.0217 (5) | 0.0199 (5) | 0.0201 (4) | −0.0002 (4) | 0.0075 (3) | −0.0013 (4) |
| C8 | 0.0213 (5) | 0.0209 (5) | 0.0230 (4) | −0.0018 (4) | 0.0066 (3) | −0.0025 (4) |
| C9 | 0.0194 (5) | 0.0204 (5) | 0.0204 (4) | −0.0006 (4) | 0.0054 (3) | −0.0027 (4) |
| C10 | 0.0196 (5) | 0.0252 (6) | 0.0244 (4) | −0.0006 (4) | 0.0034 (4) | −0.0027 (4) |
| C11 | 0.0208 (5) | 0.0280 (6) | 0.0250 (4) | 0.0025 (4) | 0.0018 (4) | −0.0017 (4) |
| C12 | 0.0233 (5) | 0.0218 (6) | 0.0269 (5) | 0.0032 (4) | 0.0037 (4) | 0.0007 (4) |
| C13 | 0.0203 (5) | 0.0206 (5) | 0.0254 (4) | −0.0011 (4) | 0.0038 (4) | −0.0013 (4) |
| C14 | 0.0172 (5) | 0.0195 (5) | 0.0204 (4) | 0.0004 (4) | 0.0042 (3) | −0.0013 (4) |
| C15 | 0.0217 (5) | 0.0235 (6) | 0.0251 (4) | 0.0016 (4) | 0.0002 (4) | 0.0023 (4) |
| C16 | 0.0231 (5) | 0.0193 (5) | 0.0243 (4) | 0.0002 (4) | 0.0014 (4) | −0.0006 (4) |
| C17 | 0.0207 (5) | 0.0243 (6) | 0.0323 (5) | 0.0000 (4) | −0.0007 (4) | −0.0004 (4) |
| C18 | 0.0280 (6) | 0.0256 (6) | 0.0305 (5) | 0.0007 (5) | −0.0069 (4) | −0.0006 (4) |
| C19 | 0.0383 (7) | 0.0342 (7) | 0.0232 (5) | 0.0031 (5) | −0.0002 (4) | 0.0014 (4) |
| C20 | 0.0312 (6) | 0.0365 (7) | 0.0270 (5) | 0.0047 (5) | 0.0059 (4) | 0.0031 (5) |
| C21 | 0.0300 (6) | 0.0394 (8) | 0.0307 (5) | −0.0020 (6) | 0.0094 (5) | −0.0037 (5) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C1 | 1.2374 (13) | C10—C11 | 1.3858 (17) |
| O2—C8 | 1.2241 (13) | C10—H10 | 1.038 (13) |
| O3—C16 | 1.3647 (13) | C11—C12 | 1.3886 (16) |
| O3—C21 | 1.4222 (15) | C11—H11 | 0.978 (14) |
| N1—C3 | 1.3600 (15) | C12—C13 | 1.3884 (14) |
| N1—C15 | 1.4238 (13) | C12—H12 | 1.009 (16) |
| N1—H1 | 0.932 (19) | C13—C14 | 1.3934 (15) |
| C1—C2 | 1.4608 (15) | C13—H13 | 0.937 (16) |
| C1—C14 | 1.4892 (14) | C15—C20 | 1.3887 (16) |
| C2—C7 | 1.4128 (15) | C15—C16 | 1.3996 (16) |
| C2—C3 | 1.4293 (14) | C16—C17 | 1.3912 (15) |
| C3—C4 | 1.4122 (16) | C17—C18 | 1.3910 (16) |
| C4—C5 | 1.3726 (17) | C17—H17 | 0.940 (16) |
| C4—H4 | 1.014 (14) | C18—C19 | 1.3782 (19) |
| C5—C6 | 1.3961 (16) | C18—H18 | 0.948 (16) |
| C5—H5 | 1.051 (17) | C19—C20 | 1.3956 (17) |
| C6—C7 | 1.3851 (16) | C19—H19 | 0.990 (17) |
| C6—H6 | 0.983 (15) | C20—H20 | 0.966 (16) |
| C7—C8 | 1.4933 (14) | C21—H21A | 1.016 (18) |
| C8—C9 | 1.4779 (16) | C21—H21B | 0.955 (18) |
| C9—C14 | 1.3998 (14) | C21—H21C | 1.013 (18) |
| C9—C10 | 1.3998 (14) | | |
| C16—O3—C21 | 117.52 (9) | C10—C11—H11 | 121.5 (8) |
| C3—N1—C15 | 124.05 (10) | C12—C11—H11 | 118.1 (8) |
| C3—N1—H1 | 113.9 (12) | C13—C12—C11 | 120.03 (11) |
| C15—N1—H1 | 120.7 (12) | C13—C12—H12 | 119.3 (9) |
| O1—C1—C2 | 122.81 (9) | C11—C12—H12 | 120.6 (9) |
| O1—C1—C14 | 118.80 (10) | C12—C13—C14 | 120.30 (10) |
| C2—C1—C14 | 118.38 (9) | C12—C13—H13 | 120.7 (10) |
| C7—C2—C3 | 118.67 (9) | C14—C13—H13 | 119.0 (10) |

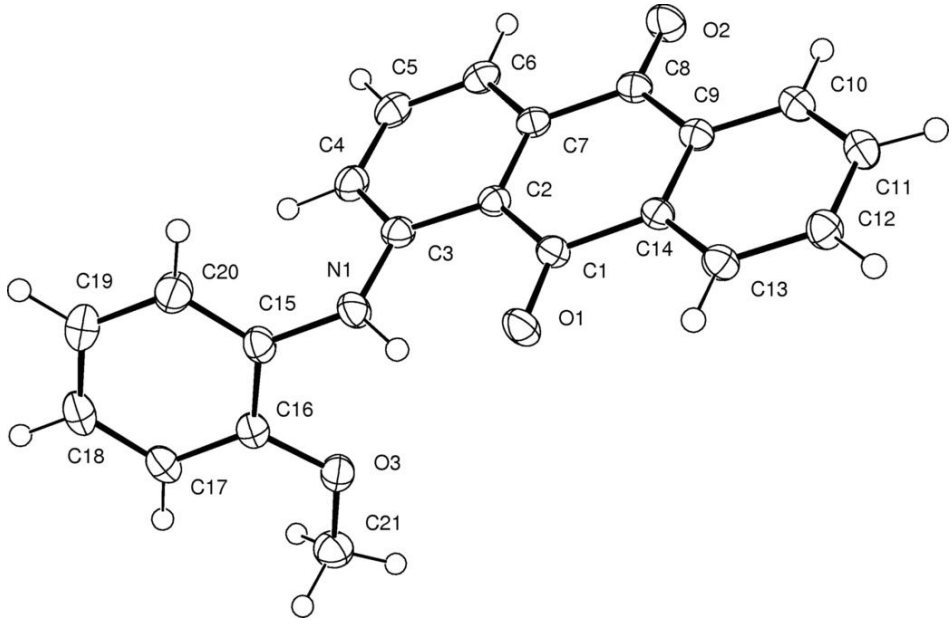
| | | | |
|---|---|---|---|
| C7—C2—C1 | 120.35 (9) | C13—C14—C9 | 119.59 (9) |
| C3—C2—C1 | 120.99 (9) | C13—C14—C1 | 118.73 (9) |
| N1—C3—C4 | 120.49 (10) | C9—C14—C1 | 121.67 (9) |
| N1—C3—C2 | 121.15 (10) | C20—C15—C16 | 119.71 (10) |
| C4—C3—C2 | 118.35 (10) | C20—C15—N1 | 120.68 (11) |
| C5—C4—C3 | 121.24 (10) | C16—C15—N1 | 119.61 (9) |
| C5—C4—H4 | 122.7 (8) | O3—C16—C17 | 124.53 (11) |
| C3—C4—H4 | 116.1 (8) | O3—C16—C15 | 115.56 (9) |
| C4—C5—C6 | 121.01 (11) | C17—C16—C15 | 119.91 (10) |
| C4—C5—H5 | 120.9 (9) | C18—C17—C16 | 119.63 (11) |
| C6—C5—H5 | 118.0 (9) | C18—C17—H17 | 122.3 (9) |
| C7—C6—C5 | 119.11 (11) | C16—C17—H17 | 118.0 (9) |
| C7—C6—H6 | 121.3 (9) | C19—C18—C17 | 120.82 (10) |
| C5—C6—H6 | 119.6 (9) | C19—C18—H18 | 120.3 (10) |
| C6—C7—C2 | 121.56 (9) | C17—C18—H18 | 118.9 (10) |
| C6—C7—C8 | 117.08 (10) | C18—C19—C20 | 119.67 (11) |
| C2—C7—C8 | 121.36 (9) | C18—C19—H19 | 119.7 (10) |
| O2—C8—C9 | 121.19 (10) | C20—C19—H19 | 120.6 (10) |
| O2—C8—C7 | 120.98 (10) | C15—C20—C19 | 120.24 (12) |
| C9—C8—C7 | 117.83 (9) | C15—C20—H20 | 119.0 (9) |
| C14—C9—C10 | 119.81 (10) | C19—C20—H20 | 120.7 (9) |
| C14—C9—C8 | 120.32 (9) | O3—C21—H21A | 108.9 (10) |
| C10—C9—C8 | 119.87 (10) | O3—C21—H21B | 106.8 (10) |
| C11—C10—C9 | 119.89 (10) | H21A—C21—H21B | 109.4 (15) |
| C11—C10—H10 | 122.2 (7) | O3—C21—H21C | 112.5 (10) |
| C9—C10—H10 | 117.8 (7) | H21A—C21—H21C | 107.9 (13) |
| C10—C11—C12 | 120.35 (10) | H21B—C21—H21C | 111.3 (14) |
| O1—C1—C2—C7 | −179.01 (10) | C8—C9—C10—C11 | 179.05 (9) |
| C14—C1—C2—C7 | 0.30 (14) | C9—C10—C11—C12 | −0.04 (16) |
| O1—C1—C2—C3 | 1.50 (16) | C10—C11—C12—C13 | 1.45 (17) |
| C14—C1—C2—C3 | −179.20 (9) | C11—C12—C13—C14 | −1.36 (16) |
| C15—N1—C3—C4 | −0.72 (17) | C12—C13—C14—C9 | −0.14 (16) |
| C15—N1—C3—C2 | −179.32 (10) | C12—C13—C14—C1 | 178.47 (9) |
| C7—C2—C3—N1 | −179.95 (10) | C10—C9—C14—C13 | 1.55 (15) |
| C1—C2—C3—N1 | −0.44 (16) | C8—C9—C14—C13 | −178.96 (9) |
| C7—C2—C3—C4 | 1.43 (15) | C10—C9—C14—C1 | −177.02 (9) |
| C1—C2—C3—C4 | −179.07 (9) | C8—C9—C14—C1 | 2.46 (15) |
| N1—C3—C4—C5 | 179.81 (11) | O1—C1—C14—C13 | −1.90 (15) |
| C2—C3—C4—C5 | −1.55 (16) | C2—C1—C14—C13 | 178.77 (9) |
| C3—C4—C5—C6 | −0.36 (18) | O1—C1—C14—C9 | 176.69 (10) |
| C4—C5—C6—C7 | 2.38 (17) | C2—C1—C14—C9 | −2.64 (15) |
| C5—C6—C7—C2 | −2.49 (16) | C3—N1—C15—C20 | −71.76 (16) |
| C5—C6—C7—C8 | 176.51 (9) | C3—N1—C15—C16 | 108.85 (13) |
| C3—C2—C7—C6 | 0.58 (15) | C21—O3—C16—C17 | 6.37 (17) |
| C1—C2—C7—C6 | −178.92 (9) | C21—O3—C16—C15 | −173.84 (11) |
| C3—C2—C7—C8 | −178.37 (9) | C20—C15—C16—O3 | 178.95 (11) |
| C1—C2—C7—C8 | 2.13 (15) | N1—C15—C16—O3 | −1.66 (16) |
| C6—C7—C8—O2 | −1.10 (15) | C20—C15—C16—C17 | −1.25 (18) |
| C2—C7—C8—O2 | 177.90 (10) | N1—C15—C16—C17 | 178.14 (11) |

| | | | |
|---|---|---|---|
| C6—C7—C8—C9 | 178.70 (9) | O3—C16—C17—C18 | −178.15 (11) |
| C2—C7—C8—C9 | −2.30 (14) | C15—C16—C17—C18 | 2.07 (18) |
| O2—C8—C9—C14 | 179.78 (10) | C16—C17—C18—C19 | −1.38 (19) |
| C7—C8—C9—C14 | −0.03 (14) | C17—C18—C19—C20 | −0.1 (2) |
| O2—C8—C9—C10 | −0.74 (15) | C16—C15—C20—C19 | −0.27 (19) |
| C7—C8—C9—C10 | 179.46 (9) | N1—C15—C20—C19 | −179.65 (12) |
| C14—C9—C10—C11 | −1.46 (16) | C18—C19—C20—C15 | 1.0 (2) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O1 | 0.932 (19) | 1.886 (18) | 2.6279 (13) | 135.0 (17) |

**Fig. 1**


O2
C5
C6
C8
C9
C10
C4
C7
C11
C2
C12
C3
C14
C1
C13
N1
C19
C20
C15
O1
C16
C18
O3
C17
C21