### Title

(E)-4-[(4-Nitrophenyl)diazenyl]phenyl anthracene-9-carboxylate




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# (*E*)-4-[(4-Nitrophenyl)diazenyl]phenyl anthracene-9-carboxylate

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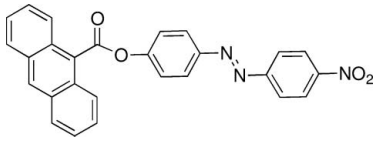
Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.043; $wR$ factor = 0.100; data-to-parameter ratio = 11.9.

In the title compound, $C_{27}H_{17}N_3O_4$, the azo group displays a *trans* conformation and the dihedral angles between the central benzene ring and the pendant anthracene and nitrobenzene rings are 82.94 (7) and 7.30 (9)°, respectively. In the crystal structure, weak C—H···O hydrogen bonds, likely associated with a dipole moment present on the molecule, help to consolidate the packing.

## Related literature

This structure is similar to the perviously reported compound (*E*)-2-{Ethyl[4-(4-nitrophenyldiazenyl)phenyl]amino}ethyl anthracene-9-carboxylate (Rodriguez, *et al.*, 2008). For general background, see: Atassi *et al.* (1998); Becke (1993).



## Experimental

### *Crystal data*

$C_{27}H_{17}N_3O_4$ $M_r$ = 447.44
Monoclinic, $P2_1/c$
$a$ = 13.525 (2) Å
$b$ = 8.6011 (14) Å
$c$ = 18.956 (3) Å
$\beta$ = 109.322 (3)°
$V$ = 2080.9 (6) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 173 (2) K
0.20 × 0.18 × 0.05 mm

### *Data collection*

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1999)
$T_{min}$ = 0.980, $T_{max}$ = 0.995
14511 measured reflections
3665 independent reflections
2752 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.038

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.100
$S$ = 1.03
3665 reflections
307 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C26—H26···O2$^{i}$ | 0.95 | 2.54 | 3.273 (3) | 134 |
| C17—H17···O4$^{ii}$ | 0.95 | 2.57 | 3.509 (3) | 169 |

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *XSHELL* (Bruker, 2001); 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: HB2827).

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# supplementary materials

*Acta Cryst.* (2008). E**64**, o2258 [ **doi:10.1107/S1600536808034958** ]

# (*E*)-4-[(4-Nitrophenyl)diazenyl]phenyl anthracene-9-carboxylate

**M. A. Rodriguez, J. L. Nichol, T. Zifer, A. L. Vance, B. M. Wong and F. Léonard**

## Comment

Atassi *et al.* (1998) has documented photoisomerization of the azobenzene in Disperse Red 1 (DR1) to a *cis* conformation under UV light, with decay back to the equilibrium *trans* species with removal of the UV light. In this manuscript we present another compound, (I), containing a *trans* azobenzene conformational state (Fig. 1). The displacement ellipsoids for most of the atoms are well defined. However, the O1 and O2 atoms at the termination of the nitroazobenzene unit do show subtle enlargement.

Figure 2 shows a packing arrangement and intermolecular interactions for (I). The nitroazobenzene portion is nearly planar as is the anthracene portion of the molecule. The anthracene is rotated from the nitroazobenzene through the carboxyl group. The title compound displays a head-to-toe configuration *via* weak C—H···O bonds as shown in Figure 2. Specifically, an O2 atom of one molecule makes a weak bond to H26 of the neighboring molecule with a bond length of 2.55 Å. The calculated dipole moment for a molecule of (I) is 7.6806 Debye using the B3LYP functional (Becke, 1993) with the 6–311 G(d,p) triple-zeta basis. This dipole moment likely drives the head-to-toe alignment of the molecules as illustrated in Figure 2.

The structure of (I) is similar in form to that of the previously reported ester (*E*)-2-{ethyl[4-(4-nitrophenyldiazenyl)phenyl]amino}ethyl anthracene-9-carboxylate (Rodriguez, *et al.*, 2008), with the subtle difference relating to the absence of the ethyl-amino ligand in (I). As with the aformentioned compound, intermolecular interactions for the title compound are exclusively C—H···O in nature (Table 2). An additional interaction which bridges molecules in the *a* axis direction is also shown in Figure 2. This weak hydrogen bond is between the terminal carboxyl oxygen O4 and the neighboring H17 atom. The hydrogen bond shows a length of 2.57 Å and symmetrically bonds the two H atoms of the anthracene of each molecule.

## Experimental

The title compound was synthesized from 9-anthracenecarboxylic acid and 4-(4-nitrophenyl)azophenol *via* a dicyclohexylcarbodiimide esterification in anhydrous dichloromethane. After filtration of insoluble side products and removal of solvent by rotary evaporation, the crude product was dissolved in dichloromethane and filtered through a silica gel plug. Evaporation of the solvent gave a red powder that was characterized by 1*H*-NMR, UV/Vis and FTIR. Red crystals of (I) were obtained by recrystallization from hot dichloromethane.

## Figures

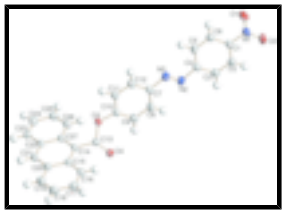

Fig. 1. The molecular structure of (I) with 50% probability displacement ellipsoids for non-H atoms.

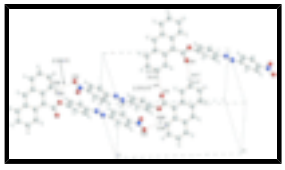

Fig. 2. A packing diagram of (I) illustrating weak C—H···O hydrogen-bond interactions associated with terminal oxygen atoms O2 and O4.

## (*E*)-4-[(4-Nitrophenyl)diazenyl]phenyl anthracene-9-carboxylate

*Crystal data*

| | |
|---|---|
| $C_{27}H_{17}N_3O_4$ | $F_{000}$ = 928 |
| $M_r$ = 447.44 | $D_x$ = 1.428 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 100 reflections |
| $a$ = 13.525 (2) Å | θ = 1.6–25.0º |
| $b$ = 8.6011 (14) Å | μ = 0.10 mm$^{-1}$ |
| $c$ = 18.956 (3) Å | $T$ = 173 (2) K |
| β = 109.322 (3)º | Plate, red |
| $V$ = 2080.9 (6) Å$^3$ | 0.20 × 0.18 × 0.05 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 3665 independent reflections |
| Radiation source: fine-focus sealed tube | 2752 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.038 |
| Detector resolution: 0 pixels mm$^{-1}$ | $\theta_{max}$ = 25.0º |
| $T$ = 173(2) K | $\theta_{min}$ = 1.6º |
| φ and ω scans | $h$ = −16→16 |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1999) | $k$ = −10→10 |
| $T_{min}$ = 0.980, $T_{max}$ = 0.995 | $l$ = −21→22 |
| 14511 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |

| | |
|---|---|
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.043$ | H-atom parameters constrained |
| $wR(F^2) = 0.100$ | $w = 1/[\sigma^2(F_o^2) + (0.0388P)^2 + 0.7361P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.03$ | $(\Delta/\sigma)_{max} = 0.001$ |
| 3665 reflections | $\Delta\rho_{max} = 0.39$ e Å$^{-3}$ |
| 307 parameters | $\Delta\rho_{min} = -0.16$ 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 least-square (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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.69229 (14) | 1.52655 (19) | 0.65761 (9) | 0.0352 (4) |
| N2 | 0.44775 (13) | 1.12430 (19) | 0.43308 (9) | 0.0350 (4) |
| N3 | 0.48826 (13) | 1.08369 (18) | 0.38663 (9) | 0.0333 (4) |
| O1 | 0.78660 (13) | 1.5368 (2) | 0.66951 (9) | 0.0581 (5) |
| O2 | 0.64573 (13) | 1.60250 (18) | 0.69126 (8) | 0.0486 (4) |
| O3 | 0.26778 (10) | 0.69438 (15) | 0.15211 (7) | 0.0304 (3) |
| O4 | 0.10043 (11) | 0.77469 (17) | 0.12517 (8) | 0.0416 (4) |
| C1 | 0.63159 (15) | 1.4180 (2) | 0.59981 (10) | 0.0272 (4) |
| C2 | 0.52768 (15) | 1.3952 (2) | 0.59086 (11) | 0.0322 (5) |
| H2 | 0.4957 | 1.4476 | 0.6218 | 0.039* |
| C3 | 0.47087 (16) | 1.2945 (2) | 0.53590 (11) | 0.0334 (5) |
| H3 | 0.3993 | 1.2749 | 0.5295 | 0.040* |
| C4 | 0.51755 (15) | 1.2218 (2) | 0.49006 (10) | 0.0289 (5) |
| C5 | 0.62352 (16) | 1.2433 (2) | 0.50109 (11) | 0.0307 (5) |
| H5 | 0.6556 | 1.1907 | 0.4703 | 0.037* |
| C6 | 0.68173 (16) | 1.3411 (2) | 0.55702 (11) | 0.0304 (5) |
| H6 | 0.7545 | 1.3555 | 0.5660 | 0.037* |
| C7 | 0.42162 (15) | 0.9862 (2) | 0.32817 (10) | 0.0298 (5) |
| C8 | 0.31857 (16) | 0.9475 (2) | 0.31890 (11) | 0.0326 (5) |
| H8 | 0.2860 | 0.9874 | 0.3524 | 0.039* |
| C9 | 0.26266 (16) | 0.8502 (2) | 0.26061 (11) | 0.0316 (5) |
| H9 | 0.1924 | 0.8218 | 0.2543 | 0.038* |

| | | | | |
|---|---|---|---|---|
| C10 | 0.31210 (15) | 0.7960 (2) | 0.21211 (10) | 0.0273 (4) |
| C11 | 0.41510 (15) | 0.8342 (2) | 0.22141 (11) | 0.0296 (5) |
| H11 | 0.4480 | 0.7949 | 0.1879 | 0.036* |
| C12 | 0.46943 (16) | 0.9293 (2) | 0.27953 (11) | 0.0318 (5) |
| H12 | 0.5401 | 0.9560 | 0.2862 | 0.038* |
| C13 | 0.16358 (15) | 0.6938 (2) | 0.11132 (11) | 0.0281 (4) |
| C14 | 0.14418 (14) | 0.5854 (2) | 0.04656 (10) | 0.0258 (4) |
| C15 | 0.09289 (14) | 0.6443 (2) | −0.02570 (11) | 0.0265 (4) |
| C16 | 0.05487 (14) | 0.8006 (2) | −0.04087 (12) | 0.0313 (5) |
| H16 | 0.0626 | 0.8699 | −0.0004 | 0.038* |
| C17 | 0.00814 (16) | 0.8515 (2) | −0.11171 (12) | 0.0383 (5) |
| H17 | −0.0159 | 0.9559 | −0.1201 | 0.046* |
| C18 | −0.00531 (17) | 0.7513 (3) | −0.17329 (12) | 0.0426 (6) |
| H18 | −0.0391 | 0.7882 | −0.2227 | 0.051* |
| C19 | 0.02967 (16) | 0.6035 (2) | −0.16205 (12) | 0.0381 (5) |
| H19 | 0.0206 | 0.5375 | −0.2039 | 0.046* |
| C20 | 0.07981 (14) | 0.5446 (2) | −0.08895 (11) | 0.0287 (5) |
| C21 | 0.11527 (14) | 0.3921 (2) | −0.07705 (11) | 0.0296 (5) |
| H21 | 0.1070 | 0.3269 | −0.1191 | 0.036* |
| C22 | 0.16242 (14) | 0.3316 (2) | −0.00585 (11) | 0.0256 (4) |
| C23 | 0.19358 (15) | 0.1725 (2) | 0.00493 (12) | 0.0309 (5) |
| H23 | 0.1821 | 0.1069 | −0.0373 | 0.037* |
| C24 | 0.23912 (15) | 0.1134 (2) | 0.07422 (12) | 0.0345 (5) |
| H24 | 0.2597 | 0.0073 | 0.0803 | 0.041* |
| C25 | 0.25608 (15) | 0.2095 (2) | 0.13743 (12) | 0.0339 (5) |
| H25 | 0.2886 | 0.1677 | 0.1860 | 0.041* |
| C26 | 0.22641 (15) | 0.3615 (2) | 0.12975 (11) | 0.0312 (5) |
| H26 | 0.2376 | 0.4236 | 0.1732 | 0.037* |
| C27 | 0.17899 (14) | 0.4293 (2) | 0.05797 (11) | 0.0260 (4) |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0431 (11) | 0.0312 (10) | 0.0275 (10) | −0.0035 (8) | 0.0066 (8) | −0.0032 (8) |
| N2 | 0.0409 (10) | 0.0305 (10) | 0.0359 (10) | 0.0027 (8) | 0.0158 (9) | 0.0012 (8) |
| N3 | 0.0388 (10) | 0.0277 (9) | 0.0353 (10) | 0.0021 (8) | 0.0148 (9) | 0.0029 (8) |
| O1 | 0.0400 (10) | 0.0717 (12) | 0.0571 (11) | −0.0170 (9) | 0.0088 (8) | −0.0273 (9) |
| O2 | 0.0602 (11) | 0.0453 (9) | 0.0393 (9) | 0.0034 (8) | 0.0155 (8) | −0.0165 (8) |
| O3 | 0.0253 (7) | 0.0304 (8) | 0.0328 (8) | −0.0026 (6) | 0.0060 (6) | −0.0102 (6) |
| O4 | 0.0307 (8) | 0.0404 (9) | 0.0486 (9) | 0.0042 (7) | 0.0062 (7) | −0.0176 (7) |
| C1 | 0.0340 (11) | 0.0229 (10) | 0.0210 (10) | −0.0012 (8) | 0.0040 (9) | 0.0008 (8) |
| C2 | 0.0352 (12) | 0.0302 (11) | 0.0306 (11) | 0.0052 (9) | 0.0102 (9) | −0.0003 (9) |
| C3 | 0.0295 (11) | 0.0335 (11) | 0.0348 (12) | −0.0004 (9) | 0.0074 (9) | 0.0016 (9) |
| C4 | 0.0348 (12) | 0.0224 (10) | 0.0241 (10) | −0.0027 (9) | 0.0023 (9) | 0.0017 (8) |
| C5 | 0.0401 (12) | 0.0276 (11) | 0.0263 (11) | 0.0024 (9) | 0.0135 (9) | −0.0016 (9) |
| C6 | 0.0308 (11) | 0.0299 (11) | 0.0309 (11) | −0.0023 (9) | 0.0106 (9) | 0.0009 (9) |
| C7 | 0.0351 (12) | 0.0226 (10) | 0.0253 (11) | −0.0047 (9) | 0.0013 (9) | 0.0003 (8) |
| C8 | 0.0467 (13) | 0.0280 (11) | 0.0246 (11) | 0.0042 (9) | 0.0137 (10) | 0.0006 (9) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C9 | 0.0327 (12) | 0.0317 (11) | 0.0296 (11) | −0.0027 (9) | 0.0094 (9) | −0.0003 (9) |
| C10 | 0.0343 (11) | 0.0202 (10) | 0.0236 (10) | −0.0005 (8) | 0.0045 (9) | −0.0015 (8) |
| C11 | 0.0316 (11) | 0.0270 (10) | 0.0282 (11) | −0.0010 (9) | 0.0071 (9) | −0.0018 (9) |
| C12 | 0.0314 (11) | 0.0301 (11) | 0.0303 (11) | −0.0035 (9) | 0.0056 (9) | −0.0022 (9) |
| C13 | 0.0271 (11) | 0.0222 (10) | 0.0337 (11) | −0.0021 (8) | 0.0083 (9) | −0.0007 (9) |
| C14 | 0.0212 (10) | 0.0246 (10) | 0.0304 (11) | −0.0045 (8) | 0.0069 (8) | −0.0032 (8) |
| C15 | 0.0202 (10) | 0.0244 (10) | 0.0343 (11) | −0.0031 (8) | 0.0083 (9) | −0.0007 (9) |
| C16 | 0.0266 (11) | 0.0249 (10) | 0.0408 (13) | −0.0026 (8) | 0.0091 (9) | −0.0020 (9) |
| C17 | 0.0350 (12) | 0.0281 (11) | 0.0482 (14) | 0.0031 (9) | 0.0092 (11) | 0.0068 (10) |
| C18 | 0.0461 (14) | 0.0416 (13) | 0.0358 (13) | 0.0042 (11) | 0.0076 (11) | 0.0094 (10) |
| C19 | 0.0422 (13) | 0.0392 (13) | 0.0316 (12) | 0.0006 (10) | 0.0105 (10) | −0.0004 (10) |
| C20 | 0.0256 (10) | 0.0289 (11) | 0.0318 (11) | −0.0015 (8) | 0.0097 (9) | −0.0010 (9) |
| C21 | 0.0295 (11) | 0.0299 (11) | 0.0301 (11) | −0.0036 (9) | 0.0108 (9) | −0.0062 (9) |
| C22 | 0.0213 (10) | 0.0237 (10) | 0.0319 (11) | −0.0034 (8) | 0.0091 (9) | −0.0039 (8) |
| C23 | 0.0319 (11) | 0.0251 (10) | 0.0378 (12) | −0.0008 (9) | 0.0142 (10) | −0.0050 (9) |
| C24 | 0.0336 (12) | 0.0227 (10) | 0.0466 (14) | −0.0001 (9) | 0.0123 (10) | 0.0022 (10) |
| C25 | 0.0313 (11) | 0.0308 (11) | 0.0353 (12) | −0.0014 (9) | 0.0053 (9) | 0.0056 (9) |
| C26 | 0.0319 (11) | 0.0280 (11) | 0.0314 (12) | −0.0040 (9) | 0.0071 (9) | −0.0009 (9) |
| C27 | 0.0209 (10) | 0.0248 (10) | 0.0316 (11) | −0.0044 (8) | 0.0078 (8) | −0.0019 (8) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| N1—O1 | 1.223 (2) | C12—H12 | 0.9500 |
| N1—O2 | 1.223 (2) | C13—C14 | 1.494 (3) |
| N1—C1 | 1.467 (2) | C14—C15 | 1.409 (3) |
| N2—N3 | 1.231 (2) | C14—C27 | 1.416 (3) |
| N2—C4 | 1.445 (2) | C15—C16 | 1.434 (3) |
| N3—C7 | 1.443 (2) | C15—C20 | 1.437 (3) |
| O3—C13 | 1.365 (2) | C16—C17 | 1.354 (3) |
| O3—C10 | 1.402 (2) | C16—H16 | 0.9500 |
| O4—C13 | 1.196 (2) | C17—C18 | 1.413 (3) |
| C1—C2 | 1.373 (3) | C17—H17 | 0.9500 |
| C1—C6 | 1.385 (3) | C18—C19 | 1.349 (3) |
| C2—C3 | 1.377 (3) | C18—H18 | 0.9500 |
| C2—H2 | 0.9500 | C19—C20 | 1.420 (3) |
| C3—C4 | 1.381 (3) | C19—H19 | 0.9500 |
| C3—H3 | 0.9500 | C20—C21 | 1.389 (3) |
| C4—C5 | 1.391 (3) | C21—C22 | 1.389 (3) |
| C5—C6 | 1.378 (3) | C21—H21 | 0.9500 |
| C5—H5 | 0.9500 | C22—C23 | 1.426 (3) |
| C6—H6 | 0.9500 | C22—C27 | 1.429 (3) |
| C7—C12 | 1.379 (3) | C23—C24 | 1.352 (3) |
| C7—C8 | 1.387 (3) | C23—H23 | 0.9500 |
| C8—C9 | 1.393 (3) | C24—C25 | 1.411 (3) |
| C8—H8 | 0.9500 | C24—H24 | 0.9500 |
| C9—C10 | 1.384 (3) | C25—C26 | 1.361 (3) |
| C9—H9 | 0.9500 | C25—H25 | 0.9500 |
| C10—C11 | 1.385 (3) | C26—C27 | 1.423 (3) |
| C11—C12 | 1.374 (3) | C26—H26 | 0.9500 |

| | | | |
|---|---|---|---|
| C11—H11 | 0.9500 | | |
| O1—N1—O2 | 123.42 (18) | O3—C13—C14 | 109.61 (15) |
| O1—N1—C1 | 118.41 (17) | C15—C14—C27 | 121.42 (17) |
| O2—N1—C1 | 118.17 (18) | C15—C14—C13 | 118.08 (16) |
| N3—N2—C4 | 111.35 (17) | C27—C14—C13 | 120.48 (17) |
| N2—N3—C7 | 113.66 (17) | C14—C15—C16 | 124.09 (18) |
| C13—O3—C10 | 123.10 (14) | C14—C15—C20 | 118.80 (17) |
| C2—C1—C6 | 122.62 (18) | C16—C15—C20 | 117.09 (17) |
| C2—C1—N1 | 118.71 (17) | C17—C16—C15 | 121.37 (19) |
| C6—C1—N1 | 118.67 (17) | C17—C16—H16 | 119.3 |
| C1—C2—C3 | 118.39 (19) | C15—C16—H16 | 119.3 |
| C1—C2—H2 | 120.8 | C16—C17—C18 | 120.84 (19) |
| C3—C2—H2 | 120.8 | C16—C17—H17 | 119.6 |
| C2—C3—C4 | 120.25 (19) | C18—C17—H17 | 119.6 |
| C2—C3—H3 | 119.9 | C19—C18—C17 | 120.1 (2) |
| C4—C3—H3 | 119.9 | C19—C18—H18 | 119.9 |
| C3—C4—C5 | 120.56 (18) | C17—C18—H18 | 119.9 |
| C3—C4—N2 | 114.30 (17) | C18—C19—C20 | 121.3 (2) |
| C5—C4—N2 | 125.14 (18) | C18—C19—H19 | 119.3 |
| C6—C5—C4 | 119.65 (18) | C20—C19—H19 | 119.3 |
| C6—C5—H5 | 120.2 | C21—C20—C19 | 121.55 (18) |
| C4—C5—H5 | 120.2 | C21—C20—C15 | 119.19 (18) |
| C5—C6—C1 | 118.43 (18) | C19—C20—C15 | 119.26 (18) |
| C5—C6—H6 | 120.8 | C22—C21—C20 | 122.30 (18) |
| C1—C6—H6 | 120.8 | C22—C21—H21 | 118.8 |
| C12—C7—C8 | 120.27 (18) | C20—C21—H21 | 118.8 |
| C12—C7—N3 | 114.06 (17) | C21—C22—C23 | 121.17 (17) |
| C8—C7—N3 | 125.67 (18) | C21—C22—C27 | 119.68 (17) |
| C7—C8—C9 | 120.27 (18) | C23—C22—C27 | 119.15 (18) |
| C7—C8—H8 | 119.9 | C24—C23—C22 | 121.19 (19) |
| C9—C8—H8 | 119.9 | C24—C23—H23 | 119.4 |
| C10—C9—C8 | 118.32 (19) | C22—C23—H23 | 119.4 |
| C10—C9—H9 | 120.8 | C23—C24—C25 | 119.90 (19) |
| C8—C9—H9 | 120.8 | C23—C24—H24 | 120.0 |
| C9—C10—C11 | 121.49 (18) | C25—C24—H24 | 120.0 |
| C9—C10—O3 | 125.30 (17) | C26—C25—C24 | 120.85 (19) |
| C11—C10—O3 | 113.16 (16) | C26—C25—H25 | 119.6 |
| C12—C11—C10 | 119.47 (18) | C24—C25—H25 | 119.6 |
| C12—C11—H11 | 120.3 | C25—C26—C27 | 121.29 (19) |
| C10—C11—H11 | 120.3 | C25—C26—H26 | 119.4 |
| C11—C12—C7 | 120.18 (19) | C27—C26—H26 | 119.4 |
| C11—C12—H12 | 119.9 | C14—C27—C26 | 123.82 (17) |
| C7—C12—H12 | 119.9 | C14—C27—C22 | 118.54 (17) |
| O4—C13—O3 | 123.49 (17) | C26—C27—C22 | 117.60 (17) |
| O4—C13—C14 | 126.81 (18) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| C26—H26···O2$^{i}$ | 0.95 | 2.54 | 3.273 (3) | 134 |
| C17—H17···O4$^{ii}$ | 0.95 | 2.57 | 3.509 (3) | 169 |

Symmetry codes: (i) −*x*+1, −*y*+2, −*z*+1; (ii) −*x*, −*y*+2, −*z*.

**Fig. 1**

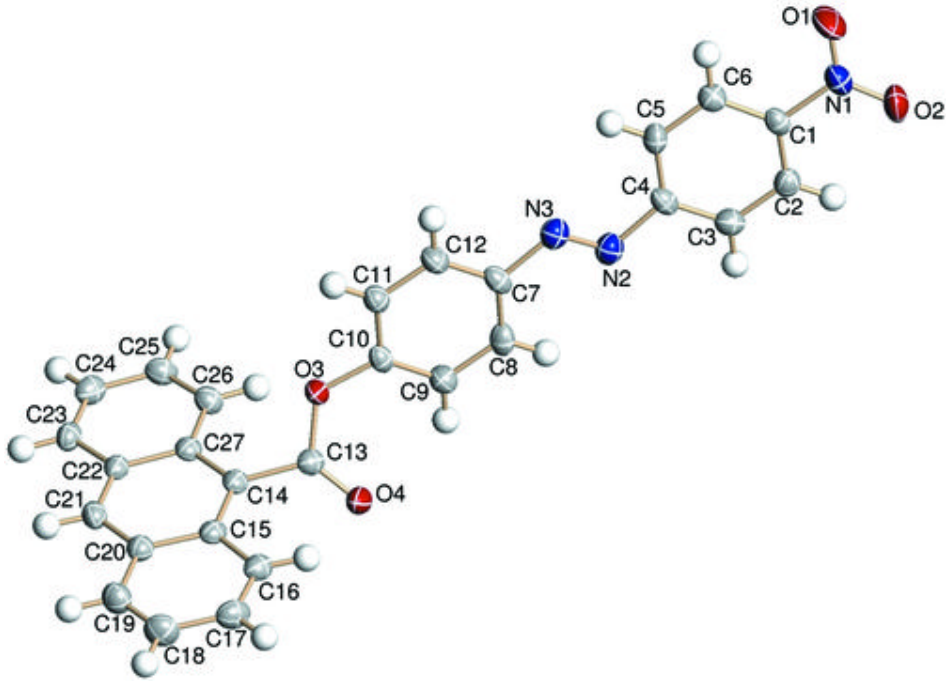
O1
C6
N1
O2
C5
C1
C4
C2
N3
C12
C3
N2
C11
C7
C10
C8
O3
C9
C25
C24
C26
C23
C27
C13
C22
C14
O4
C21
C15
C20
C16
C19
C17
C18

**Fig. 2**