Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N,*N*′-Bis[(*E*)-4-nitrobenzylidene]-4,4′-oxydianiline

Hee K. Lee and Soon W. Lee*

Department of Chemistry (BK21), Sungkyunkwan University, Natural Science Campus, Suwon 440-746, Republic of Korea
Correspondence e-mail: soonwlee@skku.edu

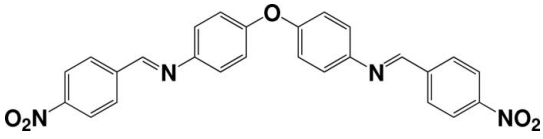
Received 20 August 2009; accepted 24 August 2009

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.114; data-to-parameter ratio = 10.0.

The title compound, $C_{26}H_{18}N_4O_5$, can be regarded as an extended ether with two terminal nitro groups. The two aryl rings bonded to the central O atom form a dihedral angle of 75.72 (6)°, and the terminal nitro groups are slightly twisted [by 6.4 (2) and 3.3 (3)°] from the benzene rings to which they are attached. The crystal packing exhibits weak intermolecular C—H···O hydrogen bonds and π–π interactions [centroid–centroid distances = 3.794 (3) Å].

Related literature

For applications of coordination polymers, see: Barnett & Champness (2003); Batten *et al.* (2009); Perry *et al.* (2009). For bis(pyridine)-, bis(furan)-, bis(thiophene)-, and (pyridine–amine)-type linking ligands as well as compounds that are structurally close to the title compound, see Yun *et al.* (2009) and references therein.



Experimental

Crystal data

$C_{26}H_{18}N_4O_5$
M_r = 466.44
Triclinic, $P\overline{1}$
a = 8.3322 (11) Å
b = 9.0716 (16) Å
c = 17.107 (2) Å
α = 74.714 (9)°
β = 78.885 (10)°
γ = 64.643 (10)°
V = 1122.4 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 K
0.52 × 0.32 × 0.26 mm

Data collection

Siemens P4 diffractometer
Absorption correction: none
4200 measured reflections
3909 independent reflections
2972 reflections with $I > 2\sigma(I)$
R_{int} = 0.015
3 standard reflections
every 97 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.114
S = 1.02
3909 reflections
389 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C19—H19···O1^{i}	0.956 (19)	2.57 (2)	3.375 (2)	142.4 (14)
C20—H20···O5^{ii}	1.016 (19)	2.48 (2)	3.323 (2)	139.7 (14)

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

Data collection: *XSCANS* (Siemens, 1995); cell refinement: *XSCANS*; data reduction: *XSCANS*; 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*.

This work was supported by the Korean Science and Engineering Foundation (KOSEF) grant funded by the Korean government (MEST) (grant No. 2009–007996).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2603).

References

Barnett, S. A. & Champness, N. R. (2003). *Coord. Chem. Rev.* **246**, 145–168.
Batten, S. R., Neville, S. M. & Turner, D. R. (2009). *Coordination Polymers: Design, Analysis and Application*. Cambridge: The Royal Society of Chemistry.
Perry IV, J. J., Perman, J. A. & Zaworotko, M. J. (2009). *Chem. Soc. Rev.* **38**, 1400–1417.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Siemens (1995). *XSCANS*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Yun, H. J., Lim, S. H. & Lee, S. W. (2009). *Polyhedron*, **28**, 614–620.

supplementary materials

Acta Cryst. (2009). E**65**, o2263 [**doi:10.1107/S1600536809033844**]

N,*N*'-Bis[(*E*)-4-nitrobenzylidene]-4,4'-oxydianiline

H. K. Lee and S. W. Lee

Comment

Coordination polymers gain continuous attention due to their desirable zeolite-like properties applicable to catalysis, non-linear optical activity, spin crossover, luminescence, long-range magnetism, adsorption-desorption, and gas storage (Barnett & Champness, 2003; Batten *et al.*, 2009; Perry IV *et al.*, 2009). Carefule choice of relevant linking ligands is one of the key factors for the successful preparation of such polymers. We have continually reported long bis(pyridine)-, bis(furan)-, bis(thiophene)-, and (pyridine–amine)-type linking ligands and their coordination polymers (Yun *et al.*, 2009). To an extension of our ongoing study of novel linking ligands and their coordination polymers, we prepared a long, potential linking ligand containing two terminal nitro groups.

The molecular structure of the title compound with the atom-numbering scheme is shown in Fig. 1. The overall structure can be regarded as a long ether possessing two terminal nitro (NO_2) groups. Two bis(pyridine)-type linking ligands containing an intervening oxydianilne fragment, which are structurally close to the title compound, were recently reported by our research group: [(3-py)—CHN—C_6H_4—O—C_6H_4—NCH—(3-py)] and [(4-py)—CHN—C_6H_4—O—C_6H_4—NCH—(4-py)] (Yun *et al.*, 2009), which, however, were not structurally characterized. In the title compound, the dihedral angle between two aryl rings (C8–13 and C14–C19) bonded to the central oxygen (O13) is 75.72 (6)°. Terminal nitro groups are not co-planar with the phenyl rings to which they are attached, with the dihedral angle 6.4 (2) (N1, O1, O2) or 3.3 (3)° (N2, O4, O5). These bonding parameters might indicate the flexibility of the title compound. The crystal packing exhibits weak intermolecular C—H···O hydrogen bonds (Table 1) and π–π interactions proved by centroid-to-centroid distances of 3.794 (3) Å.

Experimental

4-Nitrobenzaldehyde (1.12 g, 7.41 mmol) and 4,4-oxydianiline (0.67 g, 3.31 mmol) were dissolved in methanol (80 ml), to which formic acid (0.15 ml) was added. The resulting mixture was stirred at room temperature for 1 h. Dichloromethane (50 ml) was then added to the mixture, which was further stirred for 24 h. The resulting solution was filtered to give a yellow solid, which was washed with hexane (20 ml × 2). X-ray quality crystals were obtained from dichloromethane/hexane. Yield: 92%. mp: 457–459 K. IR (KBr, cm^{-1}): 3427, 3099, 2846, 2441, 1595, 1517, 1490, 1340, 1240, 1104, 850.

Refinement

All H atoms were located on a Fourier difference map and refined isotropically.

Figures

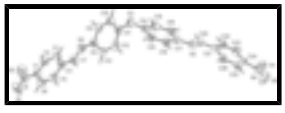


Fig. 1. Molecular structure of the title compound showing 50% probability displacement ellipsoids.

N,*N*'-Bis[(*E*)-4-nitrobenzylidene]-4,4'-oxydianiline

Crystal data

$C_{26}H_{18}N_4O_5$	$Z = 2$
$M_r = 466.44$	$F_{000} = 484$
Triclinic, $P\overline{1}$	$D_x = 1.380$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 8.3322$ (11) Å	Cell parameters from 23 reflections
$b = 9.0716$ (16) Å	$\theta = 5.2$–12.5º
$c = 17.107$ (2) Å	$\mu = 0.10$ mm^{-1}
$\alpha = 74.714$ (9)º	$T = 293$ K
$\beta = 78.885$ (10)º	Block, yellow
$\gamma = 64.643$ (10)º	0.52 × 0.32 × 0.26 mm
$V = 1122.4$ (3) Å^3	

Data collection

Siemens P4 diffractometer	$R_{int} = 0.015$
Radiation source: sealed tube	$\theta_{max} = 25.0$º
Monochromator: graphite	$\theta_{min} = 2.5$º
$T = 293$ K	$h = 0 \rightarrow 9$
ω scans	$k = -9 \rightarrow 10$
Absorption correction: none	$l = -19 \rightarrow 20$
4200 measured reflections	3 standard reflections
3909 independent reflections	every 97 reflections
2972 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)] = 0.041$	$w = 1/[\sigma^2(F_o^2) + (0.0503P)^2 + 0.1958P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.114$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.02$	$\Delta\rho_{max} = 0.14$ e Å^{-3}
3909 reflections	$\Delta\rho_{min} = -0.19$ e Å^{-3}
389 parameters	Extinction correction: SHELXTL (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: 0.0142 (18)
Secondary atom site location: difference Fourier map	

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	1.7461 (2)	−1.5786 (2)	0.74989 (10)	0.1006 (6)
O2	1.8293 (3)	−1.6837 (2)	0.64341 (12)	0.1072 (6)
O3	0.66294 (17)	−0.41925 (15)	0.27173 (8)	0.0675 (4)
O4	0.8910 (2)	0.87019 (18)	−0.12942 (11)	0.0838 (5)
O5	0.7292 (3)	0.9709 (2)	−0.02700 (11)	0.1184 (7)
N1	1.7396 (2)	−1.5702 (2)	0.67832 (12)	0.0737 (5)
N2	1.2107 (2)	−0.96099 (19)	0.43282 (10)	0.0631 (4)
N3	0.6330 (2)	0.22173 (17)	0.13724 (9)	0.0556 (4)
N4	0.7983 (2)	0.86027 (19)	−0.06546 (11)	0.0667 (4)
C1	1.6151 (2)	−1.4143 (2)	0.63208 (11)	0.0561 (4)
C2	1.5930 (3)	−1.4084 (3)	0.55334 (13)	0.0697 (5)
C3	1.4715 (3)	−1.2638 (3)	0.51122 (13)	0.0692 (5)
C4	1.3747 (2)	−1.1275 (2)	0.54727 (11)	0.0567 (4)
C5	1.4043 (3)	−1.1372 (3)	0.62583 (12)	0.0666 (5)
C6	1.5244 (3)	−1.2814 (3)	0.66859 (12)	0.0646 (5)
C7	1.2366 (3)	−0.9765 (3)	0.50481 (13)	0.0640 (5)
C8	1.0753 (2)	−0.8152 (2)	0.39338 (11)	0.0557 (4)
C9	1.0170 (3)	−0.8290 (2)	0.32617 (11)	0.0614 (5)
C10	0.8827 (3)	−0.6950 (2)	0.28467 (12)	0.0603 (5)
C11	0.8091 (2)	−0.5460 (2)	0.30985 (11)	0.0554 (4)
C12	0.8703 (3)	−0.5267 (2)	0.37428 (12)	0.0640 (5)
C13	1.0025 (3)	−0.6607 (2)	0.41617 (13)	0.0650 (5)
C14	0.6656 (2)	−0.2624 (2)	0.24132 (10)	0.0527 (4)
C15	0.5020 (2)	−0.1291 (2)	0.23764 (11)	0.0570 (4)
C16	0.4942 (2)	0.0295 (2)	0.20338 (11)	0.0560 (4)
C17	0.6481 (2)	0.0556 (2)	0.17089 (9)	0.0504 (4)
C18	0.8120 (2)	−0.0792 (2)	0.17666 (11)	0.0565 (4)
C19	0.8211 (2)	−0.2388 (2)	0.21218 (11)	0.0569 (4)
C20	0.7171 (2)	0.2500 (2)	0.06917 (11)	0.0534 (4)
C21	0.7241 (2)	0.4137 (2)	0.03302 (10)	0.0495 (4)
C22	0.8183 (3)	0.4350 (2)	−0.04281 (11)	0.0580 (5)
C23	0.8408 (3)	0.5821 (2)	−0.07591 (12)	0.0588 (5)
C24	0.7657 (2)	0.70731 (19)	−0.03286 (11)	0.0527 (4)

C25	0.6657 (3)	0.6929 (2)	0.04074 (11)	0.0606 (5)
C26	0.6447 (3)	0.5455 (2)	0.07374 (11)	0.0567 (4)
H2	1.657 (3)	−1.501 (3)	0.5313 (12)	0.079 (6)*
H3	1.454 (3)	−1.258 (3)	0.4561 (14)	0.089 (7)*
H5	1.332 (3)	−1.034 (3)	0.6515 (13)	0.089 (7)*
H6	1.542 (3)	−1.293 (2)	0.7242 (13)	0.077 (6)*
H7	1.167 (3)	−0.892 (3)	0.5362 (14)	0.099 (8)*
H9	1.073 (3)	−0.939 (2)	0.3098 (11)	0.072 (6)*
H10	0.839 (3)	−0.707 (2)	0.2398 (12)	0.077 (6)*
H12	0.822 (3)	−0.421 (3)	0.3907 (12)	0.075 (6)*
H13	1.044 (2)	−0.650 (2)	0.4595 (12)	0.063 (5)*
H15	0.397 (3)	−0.151 (2)	0.2596 (11)	0.071 (6)*
H16	0.381 (3)	0.125 (2)	0.2019 (11)	0.071 (6)*
H18	0.923 (3)	−0.061 (2)	0.1556 (11)	0.063 (5)*
H19	0.934 (3)	−0.331 (2)	0.2162 (11)	0.064 (5)*
H20	0.784 (3)	0.161 (2)	0.0355 (11)	0.066 (5)*
H22	0.876 (3)	0.342 (2)	−0.0724 (11)	0.071 (6)*
H23	0.904 (3)	0.597 (2)	−0.1244 (12)	0.075 (6)*
H25	0.616 (3)	0.777 (2)	0.0689 (12)	0.071 (6)*
H26	0.577 (3)	0.528 (2)	0.1242 (12)	0.069 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0832 (11)	0.1146 (13)	0.0768 (11)	−0.0193 (10)	−0.0332 (9)	0.0079 (9)
O2	0.1096 (14)	0.0678 (10)	0.1184 (14)	−0.0056 (10)	−0.0316 (11)	−0.0138 (10)
O3	0.0578 (8)	0.0524 (7)	0.0882 (9)	−0.0272 (6)	−0.0217 (7)	0.0123 (6)
O4	0.0881 (11)	0.0700 (9)	0.0968 (11)	−0.0467 (8)	−0.0059 (9)	0.0018 (8)
O5	0.200 (2)	0.0732 (10)	0.1070 (13)	−0.0782 (13)	0.0012 (13)	−0.0290 (10)
N1	0.0614 (11)	0.0742 (12)	0.0796 (13)	−0.0268 (9)	−0.0185 (9)	0.0020 (10)
N2	0.0586 (9)	0.0617 (9)	0.0639 (10)	−0.0236 (8)	−0.0106 (8)	−0.0018 (7)
N3	0.0617 (9)	0.0480 (8)	0.0558 (9)	−0.0231 (7)	−0.0096 (7)	−0.0031 (6)
N4	0.0812 (12)	0.0512 (9)	0.0746 (11)	−0.0319 (9)	−0.0258 (9)	−0.0009 (8)
C1	0.0512 (10)	0.0583 (10)	0.0584 (11)	−0.0253 (9)	−0.0112 (8)	−0.0007 (8)
C2	0.0724 (13)	0.0627 (12)	0.0707 (13)	−0.0205 (11)	−0.0128 (10)	−0.0147 (10)
C3	0.0763 (13)	0.0713 (13)	0.0579 (12)	−0.0268 (11)	−0.0163 (10)	−0.0073 (10)
C4	0.0542 (10)	0.0590 (10)	0.0568 (10)	−0.0278 (9)	−0.0060 (8)	−0.0018 (8)
C5	0.0674 (12)	0.0655 (12)	0.0615 (12)	−0.0217 (10)	−0.0082 (10)	−0.0108 (9)
C6	0.0667 (12)	0.0721 (13)	0.0549 (11)	−0.0286 (10)	−0.0128 (9)	−0.0061 (9)
C7	0.0611 (12)	0.0633 (12)	0.0619 (12)	−0.0249 (10)	−0.0042 (9)	−0.0045 (10)
C8	0.0493 (10)	0.0543 (10)	0.0570 (10)	−0.0224 (8)	−0.0051 (8)	0.0020 (8)
C9	0.0598 (11)	0.0569 (11)	0.0606 (11)	−0.0197 (9)	−0.0048 (9)	−0.0074 (9)
C10	0.0596 (11)	0.0620 (11)	0.0575 (11)	−0.0259 (9)	−0.0091 (9)	−0.0037 (9)
C11	0.0492 (10)	0.0511 (10)	0.0598 (10)	−0.0242 (8)	−0.0069 (8)	0.0071 (8)
C12	0.0705 (13)	0.0498 (10)	0.0674 (12)	−0.0228 (9)	−0.0100 (10)	−0.0047 (9)
C13	0.0733 (13)	0.0614 (12)	0.0618 (12)	−0.0294 (10)	−0.0179 (10)	−0.0022 (9)
C14	0.0561 (10)	0.0483 (9)	0.0528 (10)	−0.0247 (8)	−0.0109 (8)	0.0019 (7)
C15	0.0475 (10)	0.0582 (11)	0.0636 (11)	−0.0237 (9)	−0.0086 (8)	−0.0025 (8)

C16	0.0490 (10)	0.0518 (10)	0.0607 (11)	−0.0156 (8)	−0.0112 (8)	−0.0043 (8)
C17	0.0575 (10)	0.0481 (9)	0.0454 (9)	−0.0227 (8)	−0.0089 (8)	−0.0033 (7)
C18	0.0519 (10)	0.0543 (10)	0.0615 (11)	−0.0248 (9)	−0.0053 (8)	−0.0024 (8)
C19	0.0484 (10)	0.0509 (10)	0.0634 (11)	−0.0176 (8)	−0.0083 (8)	−0.0003 (8)
C20	0.0603 (11)	0.0473 (9)	0.0549 (10)	−0.0230 (8)	−0.0103 (8)	−0.0080 (8)
C21	0.0536 (10)	0.0456 (9)	0.0499 (9)	−0.0201 (8)	−0.0122 (7)	−0.0048 (7)
C22	0.0698 (12)	0.0462 (10)	0.0567 (11)	−0.0224 (9)	−0.0026 (9)	−0.0119 (8)
C23	0.0635 (11)	0.0524 (10)	0.0573 (11)	−0.0245 (9)	−0.0026 (9)	−0.0057 (8)
C24	0.0592 (10)	0.0431 (9)	0.0589 (10)	−0.0221 (8)	−0.0202 (8)	−0.0018 (7)
C25	0.0757 (13)	0.0463 (10)	0.0595 (11)	−0.0190 (9)	−0.0140 (10)	−0.0137 (8)
C26	0.0651 (11)	0.0524 (10)	0.0507 (10)	−0.0219 (9)	−0.0066 (9)	−0.0091 (8)

Geometric parameters (Å, °)

O1—N1	1.217 (2)	C10—C11	1.373 (3)
O2—N1	1.211 (2)	C10—H10	0.96 (2)
O3—C14	1.388 (2)	C11—C12	1.379 (3)
O3—C11	1.394 (2)	C12—C13	1.379 (3)
O4—N4	1.218 (2)	C12—H12	0.97 (2)
O5—N4	1.216 (2)	C13—H13	0.920 (19)
N1—C1	1.474 (2)	C14—C19	1.380 (2)
N2—C7	1.252 (3)	C14—C15	1.381 (2)
N2—C8	1.422 (2)	C15—C16	1.381 (2)
N3—C20	1.262 (2)	C15—H15	0.97 (2)
N3—C17	1.424 (2)	C16—C17	1.387 (2)
N4—C24	1.472 (2)	C16—H16	0.97 (2)
C1—C6	1.360 (3)	C17—C18	1.389 (2)
C1—C2	1.378 (3)	C18—C19	1.389 (2)
C2—C3	1.382 (3)	C18—H18	0.990 (19)
C2—H2	0.92 (2)	C19—H19	0.956 (19)
C3—C4	1.384 (3)	C20—C21	1.472 (2)
C3—H3	0.97 (2)	C20—H20	1.016 (19)
C4—C5	1.386 (3)	C21—C26	1.392 (2)
C4—C7	1.475 (3)	C21—C22	1.393 (2)
C5—C6	1.380 (3)	C22—C23	1.383 (3)
C5—H5	1.03 (2)	C22—H22	0.99 (2)
C6—H6	0.96 (2)	C23—C24	1.371 (3)
C7—H7	0.96 (2)	C23—H23	0.90 (2)
C8—C9	1.385 (3)	C24—C25	1.378 (3)
C8—C13	1.397 (3)	C25—C26	1.378 (3)
C9—C10	1.386 (3)	C25—H25	0.92 (2)
C9—H9	0.99 (2)	C26—H26	0.953 (19)
C14—O3—C11	118.85 (13)	C13—C12—H12	119.3 (12)
O2—N1—O1	123.39 (19)	C12—C13—C8	120.5 (2)
O2—N1—C1	118.48 (19)	C12—C13—H13	120.5 (12)
O1—N1—C1	118.1 (2)	C8—C13—H13	119.0 (12)
C7—N2—C8	120.80 (18)	C19—C14—C15	120.83 (16)
C20—N3—C17	118.44 (15)	C19—C14—O3	122.74 (16)
O5—N4—O4	123.56 (17)	C15—C14—O3	116.35 (15)

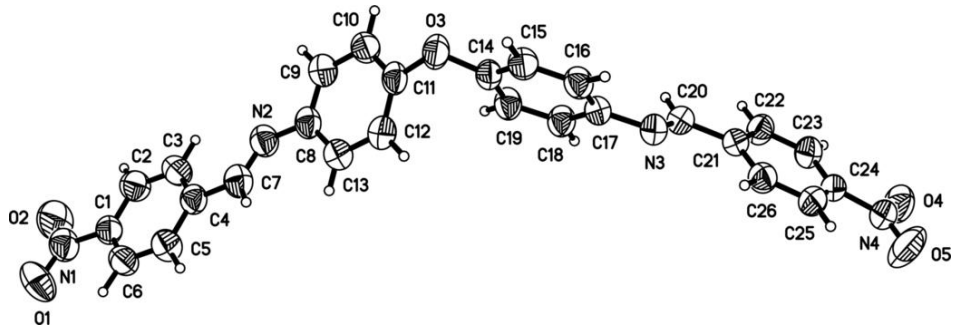
O5—N4—C24	117.74 (18)	C14—C15—C16	119.40 (17)
O4—N4—C24	118.69 (16)	C14—C15—H15	118.0 (11)
C6—C1—C2	122.07 (18)	C16—C15—H15	122.6 (11)
C6—C1—N1	119.08 (18)	C15—C16—C17	120.79 (17)
C2—C1—N1	118.85 (19)	C15—C16—H16	120.6 (12)
C1—C2—C3	118.6 (2)	C17—C16—H16	118.6 (12)
C1—C2—H2	119.0 (13)	C16—C17—C18	119.11 (15)
C3—C2—H2	122.4 (13)	C16—C17—N3	118.57 (15)
C2—C3—C4	120.64 (19)	C18—C17—N3	122.20 (16)
C2—C3—H3	119.7 (13)	C17—C18—C19	120.35 (17)
C4—C3—H3	119.6 (13)	C17—C18—H18	119.4 (10)
C3—C4—C5	118.88 (18)	C19—C18—H18	120.2 (10)
C3—C4—C7	121.08 (18)	C14—C19—C18	119.44 (17)
C5—C4—C7	119.99 (19)	C14—C19—H19	120.4 (11)
C6—C5—C4	120.9 (2)	C18—C19—H19	120.2 (11)
C6—C5—H5	121.3 (12)	N3—C20—C21	122.54 (17)
C4—C5—H5	117.8 (12)	N3—C20—H20	122.0 (10)
C1—C6—C5	118.84 (19)	C21—C20—H20	115.4 (10)
C1—C6—H6	118.9 (12)	C26—C21—C22	119.25 (16)
C5—C6—H6	122.2 (12)	C26—C21—C20	121.80 (16)
N2—C7—C4	121.7 (2)	C22—C21—C20	118.91 (16)
N2—C7—H7	122.5 (14)	C23—C22—C21	120.78 (17)
C4—C7—H7	115.8 (14)	C23—C22—H22	119.2 (11)
C9—C8—C13	118.62 (17)	C21—C22—H22	120.0 (11)
C9—C8—N2	116.51 (17)	C24—C23—C22	118.32 (18)
C13—C8—N2	124.84 (17)	C24—C23—H23	119.8 (13)
C8—C9—C10	120.91 (19)	C22—C23—H23	121.9 (13)
C8—C9—H9	117.4 (11)	C23—C24—C25	122.38 (16)
C10—C9—H9	121.7 (11)	C23—C24—N4	118.52 (17)
C11—C10—C9	119.33 (19)	C25—C24—N4	119.07 (16)
C11—C10—H10	120.1 (12)	C24—C25—C26	119.05 (17)
C9—C10—H10	120.6 (12)	C24—C25—H25	121.6 (12)
C10—C11—C12	120.95 (17)	C26—C25—H25	119.3 (12)
C10—C11—O3	117.62 (17)	C25—C26—C21	120.13 (18)
C12—C11—O3	121.29 (17)	C25—C26—H26	123.1 (12)
C11—C12—C13	119.60 (19)	C21—C26—H26	116.8 (12)
C11—C12—H12	121.1 (12)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C19—H19···O1^{i}	0.956 (19)	2.57 (2)	3.375 (2)	142.4 (14)
C20—H20···O5^{ii}	1.016 (19)	2.48 (2)	3.323 (2)	139.7 (14)

Symmetry codes: (i) −*x*+3, −*y*−2, −*z*+1; (ii) *x*, *y*−1, *z*.

Fig. 1


C10
O3
C14
C15
C16
C9
C11
C20
C22
N2
C12
C19
C18
C17
N3
C21
C23
C3
C2
C8
C13
C7
C24
O4
C1
C4
C26
C25
N4
O5
O2
C5
N1
C6
O1