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6,6′-Dimethoxy-2,3,2′,5′-tetranitro-1,1′-biphenyl

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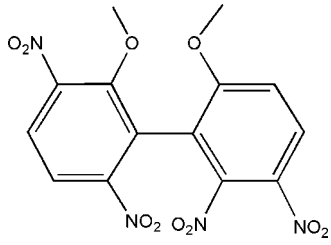
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.003 Å; R factor = 0.046; wR factor = 0.135; data-to-parameter ratio = 12.0.

The title compound, $C_{14}H_{10}N_4O_{10}$, was obtained by nitration of 6,6′-dimethoxy-2,2′-dinitro-1,1′-biphenyl in the presence of an excess of fuming nitric acid. In the molecule, the dihedral angle between the two benzene rings is 89.9 (2)°. In the crystal structure, molecules are connected by weak intermolecular C—H···O hydrogen bonds to form one-dimensional chains.

Related literature

For related literature, see: Agrawal & Tratnyek (1996); Fischer *et al.* (2007); Chen *et al.* (2001); Ramkishen *et al.* (2005); Shinichi & Yuichiro (2005); Unver *et al.* (2002); Yang *et al.* (2005); Zhang (2006).



Experimental

Crystal data

$C_{14}H_{10}N_4O_{10}$
M_r = 394.26
Triclinic, $P\overline{1}$
a = 8.1821 (11) Å
b = 10.2161 (13) Å
c = 10.6133 (14) Å
α = 95.118 (2)°
β = 90.579 (2)°
γ = 110.977 (2)°
V = 824.21 (19) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 291 (2) K
0.27 × 0.23 × 0.16 mm

Data collection

Bruker APEX II CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.913, T_{max} = 0.979
6347 measured reflections
3051 independent reflections
2173 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.135
S = 1.04
3051 reflections
255 parameters
48 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13B···O5^{i}	0.96	2.41	3.274 (4)	150
C14—H14A···O6^{ii}	0.96	2.60	3.165 (3)	118

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); 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: LH2441).

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supplementary materials

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6,6'-Dimethoxy-2,3,2',5'-tetranitro-1,1'-biphenyl

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Comment

Nitro compounds, specifically aromatic nitro compounds have been widely studied owing to their potential application in *e.g.* pathology (Ramkishen *et al.*, 2005), materials science (Shinichi & Yuichiro, 2005) and powder technology (Zhang, 2006). These compounds can also be reduced to obtain hydroxylamine, azo-, azoxy compounds and amines, which find applications in dyes, agrochemicals, pharmaceuticals and photographic chemicals (Agrawal & Tratnyek, 1996). In this paper, we report the synthesis and crystal structure of the title compound.

All bond lengths and angles in the title molecule (Fig. 1) are in the expected range (Unver *et al.*, 2002) and in good agreement with those reported previously (Yang *et al.*, 2005). Atoms N1/N2/O1/C1—C6/C14 lie in a plane with the largest deviation being 0.029Å for atom N2, and atoms N3/N4/O10/C7—C12 also lie in a plane, with the largest deviation being 0.0354Å for atom N4. The dihedral angle between the two benzene rings is 90.1°, which is considerably larger than found in other biphenyls (Fischer *et al.*, 2007), possibly due to the concomitant effects of steric hindrance of the methoxy and nitro groups. The dihedral angles formed between the benzene ring of C1—C6 and planes N1/O2/O3 and N2/O4/O5 are 24.3 and 70.4°, the dihedral angles formed between the benzene ring of C7—C12 and planes N3/O6/O7 and N4/O8/O9 are 15.7 and 43.0°, respectively. The H atom of the methoxy group forms weak C—H···O intermolecular hydrogen bonds with the nitro group O atom of the neighbouring molecule. The H13B···O5^{i} distance is 2.41 Å, which is considerable shorter than the sum of the van der Waals radii for O and H (2.70 Å). In the crystal structure, molecules are connected to form a one-dimension chain *via* weak C—H···O hydrogen bonds. In addition, there are also weak C—H···O hydrogen bonds between two one-dimension chains (Fig.2). The H14A···O6^{ii} distance is 2.60 Å. These weak intermolecular C—H···O hydrogen bonds play an important role in stabilizing the crystal structure (symmetry operation: (i) $1 + x,y,z$; (ii) $1 - x,1 - y,1 - z$).

Experimental

6,6'-Dimethoxy-2,2'-dinitro-1,1'-biphenyl was prepared according to the reported procedure (Chen *et al.*, 2001). The title compound was synthesized by the nitration reaction of 6,6'-Dimethoxy-2,2'-dinitro-1,1'-biphenyl (0.5 mmol) in 20 ml fuming nitric acid at room temperature for 24 h. The resulting solution was poured into 50 ml ice water and the precipitation was collected by filtration and recrystallized from ethyl acetate as single crystals of the title compound, which were suitable for X-ray diffraction analysis.

Refinement

All H atoms were placed in calculated positions with C—H distances 0.93–0.96Å and included in the refinement in the riding-model approximation with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C) for methyl H atoms. Atoms O2—O9 were loosely restrained to be approximately isotropic.

Figures

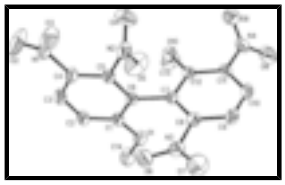

Fig. 1. The molecular structure of the title compound shown using 30% probability ellipsoids.

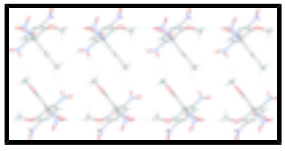

Fig. 2. Part of the title crystal structure with hydrogen bonds shown as dashed lines

6,6'-Dimethoxy-2,3,2',5'-tetranitro-1,1'-biphenyl

Crystal data

$C_{14}H_{10}N_4O_{10}$	$Z = 2$
$M_r = 394.26$	$F_{000} = 404$
Triclinic, $P\overline{1}$	$D_x = 1.589$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.1821$ (11) Å	Cell parameters from 1810 reflections
$b = 10.2161$ (13) Å	$\theta = 2.7$–23.5º
$c = 10.6133$ (14) Å	$\mu = 0.14$ mm^{-1}
$\alpha = 95.118$ (2)º	$T = 291$ (2) K
$\beta = 90.579$ (2)º	Block, yellow
$\gamma = 110.977$ (2)º	0.27 × 0.23 × 0.16 mm
$V = 824.21$ (19) Å^3	

Data collection

Bruker APEX II CCD area-detector diffractometer	3051 independent reflections
Radiation source: fine-focus sealed tube	2173 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.017$
$T = 291(2)$ K	$\theta_{max} = 25.5$º
φ and ω scans	$\theta_{min} = 2.7$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -9 \rightarrow 9$
$T_{min} = 0.913$, $T_{max} = 0.979$	$k = -12 \rightarrow 12$
6347 measured reflections	$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.046$	H-atom parameters constrained
$wR(F^2) = 0.135$	$w = 1/[\sigma^2(F_o^2) + (0.06P)^2 + 0.3203P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
3051 reflections	$\Delta\rho_{max} = 0.27$ e Å^{-3}
255 parameters	$\Delta\rho_{min} = -0.22$ e Å^{-3}
48 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.5521 (2)	0.38404 (17)	0.32635 (15)	0.0544 (5)
O2	0.1047 (4)	−0.2166 (3)	0.4665 (3)	0.1216 (11)
O3	−0.0829 (3)	−0.1796 (2)	0.3485 (2)	0.0847 (7)
O4	0.0530 (3)	−0.1066 (2)	0.1089 (2)	0.0836 (7)
O5	−0.0687 (3)	0.0425 (2)	0.1627 (3)	0.0909 (8)
O6	0.1341 (3)	0.3722 (2)	0.32138 (19)	0.0735 (6)
O7	0.0125 (3)	0.4502 (3)	0.1823 (2)	0.0864 (7)
O8	0.5697 (3)	0.3399 (2)	−0.2476 (2)	0.0972 (8)
O9	0.4681 (3)	0.1229 (2)	−0.2111 (2)	0.0861 (7)
O10	0.4716 (2)	0.13198 (17)	0.05720 (16)	0.0505 (4)

N1	0.0619 (3)	−0.1446 (2)	0.3991 (2)	0.0620 (6)
N2	0.0430 (3)	−0.0071 (2)	0.1743 (2)	0.0520 (5)
N3	0.1122 (3)	0.3936 (2)	0.2140 (2)	0.0504 (5)
N4	0.4869 (3)	0.2450 (3)	−0.1846 (2)	0.0614 (6)
C1	0.4371 (3)	0.2571 (2)	0.3497 (2)	0.0416 (5)
C2	0.4469 (3)	0.1889 (3)	0.4556 (2)	0.0502 (6)
H2	0.5365	0.2319	0.5171	0.060*
C3	0.3246 (3)	0.0579 (3)	0.4698 (2)	0.0522 (6)
H3	0.3322	0.0127	0.5407	0.063*
C4	0.1917 (3)	−0.0063 (2)	0.3801 (2)	0.0446 (6)
C5	0.1809 (3)	0.0619 (2)	0.2745 (2)	0.0384 (5)
C6	0.3011 (3)	0.1926 (2)	0.25653 (19)	0.0364 (5)
C7	0.2998 (3)	0.2600 (2)	0.13651 (19)	0.0357 (5)
C8	0.2142 (3)	0.3520 (2)	0.1146 (2)	0.0406 (5)
C9	0.2197 (3)	0.4097 (3)	0.0016 (2)	0.0488 (6)
H9	0.1601	0.4704	−0.0098	0.059*
C10	0.3139 (3)	0.3768 (3)	−0.0940 (2)	0.0520 (7)
H10	0.3219	0.4173	−0.1699	0.062*
C11	0.3963 (3)	0.2837 (2)	−0.0768 (2)	0.0443 (6)
C12	0.3931 (3)	0.2246 (2)	0.0373 (2)	0.0395 (5)
C13	0.6577 (4)	0.1862 (3)	0.0691 (4)	0.0756 (9)
H13A	0.7046	0.2154	−0.0106	0.113*
H13B	0.6981	0.1144	0.0936	0.113*
H13C	0.6961	0.2655	0.1323	0.113*
C14	0.6954 (4)	0.4544 (3)	0.4180 (3)	0.0752 (9)
H14A	0.6497	0.4677	0.4991	0.113*
H14B	0.7652	0.5443	0.3916	0.113*
H14C	0.7665	0.3979	0.4240	0.113*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0564 (11)	0.0439 (9)	0.0475 (10)	−0.0004 (8)	−0.0195 (8)	0.0068 (8)
O2	0.113 (2)	0.0900 (17)	0.145 (2)	0.0020 (15)	−0.0259 (18)	0.0791 (18)
O3	0.0612 (14)	0.0777 (15)	0.0961 (17)	−0.0033 (11)	−0.0029 (12)	0.0326 (12)
O4	0.0737 (14)	0.0805 (15)	0.0690 (13)	0.0022 (12)	−0.0046 (11)	−0.0245 (12)
O5	0.0572 (13)	0.0830 (15)	0.129 (2)	0.0206 (12)	−0.0363 (13)	0.0153 (14)
O6	0.0964 (16)	0.0887 (15)	0.0536 (12)	0.0538 (13)	0.0126 (11)	0.0124 (11)
O7	0.0846 (15)	0.1112 (18)	0.0920 (16)	0.0701 (15)	−0.0017 (12)	0.0103 (13)
O8	0.121 (2)	0.0786 (15)	0.0592 (13)	−0.0054 (14)	0.0337 (13)	0.0081 (11)
O9	0.1195 (19)	0.0698 (15)	0.0668 (14)	0.0321 (14)	0.0249 (13)	0.0010 (11)
O10	0.0510 (10)	0.0455 (9)	0.0585 (11)	0.0205 (8)	0.0040 (8)	0.0098 (8)
N1	0.0672 (16)	0.0547 (14)	0.0580 (14)	0.0099 (12)	0.0050 (12)	0.0258 (11)
N2	0.0424 (12)	0.0499 (13)	0.0513 (13)	−0.0002 (10)	−0.0059 (10)	0.0142 (11)
N3	0.0488 (12)	0.0467 (12)	0.0558 (14)	0.0186 (10)	−0.0047 (10)	0.0013 (10)
N4	0.0704 (15)	0.0580 (15)	0.0388 (12)	0.0036 (12)	0.0053 (11)	0.0002 (11)
C1	0.0446 (13)	0.0403 (12)	0.0367 (12)	0.0116 (11)	−0.0051 (10)	0.0035 (10)
C2	0.0561 (15)	0.0540 (15)	0.0357 (13)	0.0148 (12)	−0.0126 (11)	0.0036 (11)

C3	0.0621 (16)	0.0576 (16)	0.0389 (13)	0.0216 (13)	−0.0024 (12)	0.0160 (11)
C4	0.0464 (13)	0.0432 (13)	0.0424 (13)	0.0120 (11)	0.0045 (10)	0.0125 (10)
C5	0.0385 (12)	0.0400 (12)	0.0364 (12)	0.0135 (10)	−0.0017 (9)	0.0049 (9)
C6	0.0381 (12)	0.0378 (12)	0.0325 (11)	0.0125 (10)	−0.0026 (9)	0.0047 (9)
C7	0.0355 (11)	0.0323 (11)	0.0336 (11)	0.0054 (9)	−0.0077 (9)	0.0037 (9)
C8	0.0371 (12)	0.0367 (12)	0.0429 (13)	0.0078 (10)	−0.0081 (10)	0.0022 (10)
C9	0.0527 (14)	0.0418 (13)	0.0497 (14)	0.0135 (11)	−0.0148 (12)	0.0105 (11)
C10	0.0598 (16)	0.0449 (14)	0.0420 (14)	0.0057 (12)	−0.0136 (12)	0.0145 (11)
C11	0.0472 (13)	0.0402 (12)	0.0342 (12)	0.0026 (11)	−0.0021 (10)	0.0014 (10)
C12	0.0400 (12)	0.0328 (11)	0.0399 (12)	0.0064 (10)	−0.0057 (10)	0.0039 (9)
C13	0.0544 (17)	0.0631 (18)	0.110 (3)	0.0250 (15)	−0.0126 (16)	−0.0002 (17)
C14	0.0695 (19)	0.0616 (18)	0.0679 (19)	−0.0081 (15)	−0.0308 (15)	0.0075 (15)

Geometric parameters (Å, °)

O1—C1	1.348 (3)	C3—C4	1.370 (3)
O1—C14	1.444 (3)	C3—H3	0.9300
O2—N1	1.203 (3)	C4—C5	1.389 (3)
O3—N1	1.212 (3)	C5—C6	1.377 (3)
O4—N2	1.206 (3)	C6—C7	1.503 (3)
O5—N2	1.204 (3)	C7—C8	1.391 (3)
O6—N3	1.203 (3)	C7—C12	1.402 (3)
O7—N3	1.216 (3)	C8—C9	1.377 (3)
O8—N4	1.225 (3)	C9—C10	1.370 (4)
O9—N4	1.208 (3)	C9—H9	0.9300
O10—C12	1.349 (3)	C10—C11	1.371 (3)
O10—C13	1.422 (3)	C10—H10	0.9300
N1—C4	1.465 (3)	C11—C12	1.397 (3)
N2—C5	1.474 (3)	C13—H13A	0.9600
N3—C8	1.478 (3)	C13—H13B	0.9600
N4—C11	1.471 (3)	C13—H13C	0.9600
C1—C2	1.391 (3)	C14—H14A	0.9600
C1—C6	1.410 (3)	C14—H14B	0.9600
C2—C3	1.376 (4)	C14—H14C	0.9600
C2—H2	0.9300		
C1—O1—C14	117.70 (19)	C1—C6—C7	120.03 (19)
C12—O10—C13	116.79 (19)	C8—C7—C12	117.51 (19)
O2—N1—O3	123.6 (2)	C8—C7—C6	126.4 (2)
O2—N1—C4	117.7 (2)	C12—C7—C6	116.11 (19)
O3—N1—C4	118.7 (2)	C9—C8—C7	122.9 (2)
O5—N2—O4	125.2 (2)	C9—C8—N3	116.4 (2)
O5—N2—C5	117.1 (2)	C7—C8—N3	120.8 (2)
O4—N2—C5	117.7 (2)	C10—C9—C8	119.3 (2)
O6—N3—O7	123.7 (2)	C10—C9—H9	120.4
O6—N3—C8	118.7 (2)	C8—C9—H9	120.4
O7—N3—C8	117.6 (2)	C9—C10—C11	119.4 (2)
O9—N4—O8	123.6 (2)	C9—C10—H10	120.3
O9—N4—C11	119.4 (2)	C11—C10—H10	120.3
O8—N4—C11	116.8 (2)	C10—C11—C12	122.2 (2)

O1—C1—C2	124.6 (2)	C10—C11—N4	117.5 (2)
O1—C1—C6	115.30 (19)	C12—C11—N4	120.4 (2)
C2—C1—C6	120.1 (2)	O10—C12—C11	123.7 (2)
C3—C2—C1	120.3 (2)	O10—C12—C7	117.54 (19)
C3—C2—H2	119.9	C11—C12—C7	118.7 (2)
C1—C2—H2	119.9	O10—C13—H13A	109.5
C4—C3—C2	120.4 (2)	O10—C13—H13B	109.5
C4—C3—H3	119.8	H13A—C13—H13B	109.5
C2—C3—H3	119.8	O10—C13—H13C	109.5
C3—C4—C5	119.5 (2)	H13A—C13—H13C	109.5
C3—C4—N1	119.0 (2)	H13B—C13—H13C	109.5
C5—C4—N1	121.5 (2)	O1—C14—H14A	109.5
C6—C5—C4	121.9 (2)	O1—C14—H14B	109.5
C6—C5—N2	117.51 (18)	H14A—C14—H14B	109.5
C4—C5—N2	120.5 (2)	O1—C14—H14C	109.5
C5—C6—C1	117.90 (19)	H14A—C14—H14C	109.5
C5—C6—C7	121.83 (18)	H14B—C14—H14C	109.5
C14—O1—C1—C2	−0.1 (4)	C5—C6—C7—C12	−86.7 (3)
C14—O1—C1—C6	−179.3 (2)	C1—C6—C7—C12	87.5 (3)
O1—C1—C2—C3	−178.8 (2)	C12—C7—C8—C9	−0.9 (3)
C6—C1—C2—C3	0.3 (4)	C6—C7—C8—C9	179.9 (2)
C1—C2—C3—C4	−0.3 (4)	C12—C7—C8—N3	179.59 (18)
C2—C3—C4—C5	−0.1 (4)	C6—C7—C8—N3	0.3 (3)
C2—C3—C4—N1	−178.9 (2)	O6—N3—C8—C9	−163.8 (2)
O2—N1—C4—C3	−24.1 (4)	O7—N3—C8—C9	14.9 (3)
O3—N1—C4—C3	154.7 (3)	O6—N3—C8—C7	15.8 (3)
O2—N1—C4—C5	157.1 (3)	O7—N3—C8—C7	−165.5 (2)
O3—N1—C4—C5	−24.1 (4)	C7—C8—C9—C10	−0.4 (3)
C3—C4—C5—C6	0.5 (4)	N3—C8—C9—C10	179.2 (2)
N1—C4—C5—C6	179.3 (2)	C8—C9—C10—C11	2.0 (3)
C3—C4—C5—N2	177.7 (2)	C9—C10—C11—C12	−2.4 (3)
N1—C4—C5—N2	−3.5 (4)	C9—C10—C11—N4	176.4 (2)
O5—N2—C5—C6	−70.8 (3)	O9—N4—C11—C10	−134.9 (3)
O4—N2—C5—C6	107.7 (3)	O8—N4—C11—C10	40.7 (3)
O5—N2—C5—C4	111.9 (3)	O9—N4—C11—C12	43.9 (3)
O4—N2—C5—C4	−69.7 (3)	O8—N4—C11—C12	−140.5 (3)
C4—C5—C6—C1	−0.4 (3)	C13—O10—C12—C11	72.0 (3)
N2—C5—C6—C1	−177.7 (2)	C13—O10—C12—C7	−109.6 (3)
C4—C5—C6—C7	173.9 (2)	C10—C11—C12—O10	179.5 (2)
N2—C5—C6—C7	−3.5 (3)	N4—C11—C12—O10	0.7 (3)
O1—C1—C6—C5	179.2 (2)	C10—C11—C12—C7	1.2 (3)
C2—C1—C6—C5	0.0 (3)	N4—C11—C12—C7	−177.63 (19)
O1—C1—C6—C7	4.8 (3)	C8—C7—C12—O10	−177.95 (18)
C2—C1—C6—C7	−174.4 (2)	C6—C7—C12—O10	1.4 (3)
C5—C6—C7—C8	92.6 (3)	C8—C7—C12—C11	0.5 (3)
C1—C6—C7—C8	−93.3 (3)	C6—C7—C12—C11	179.82 (19)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13B···O5^{i}	0.96	2.41	3.274 (4)	150
C14—H14A···O6^{ii}	0.96	2.60	3.165 (3)	118

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

Fig. 1

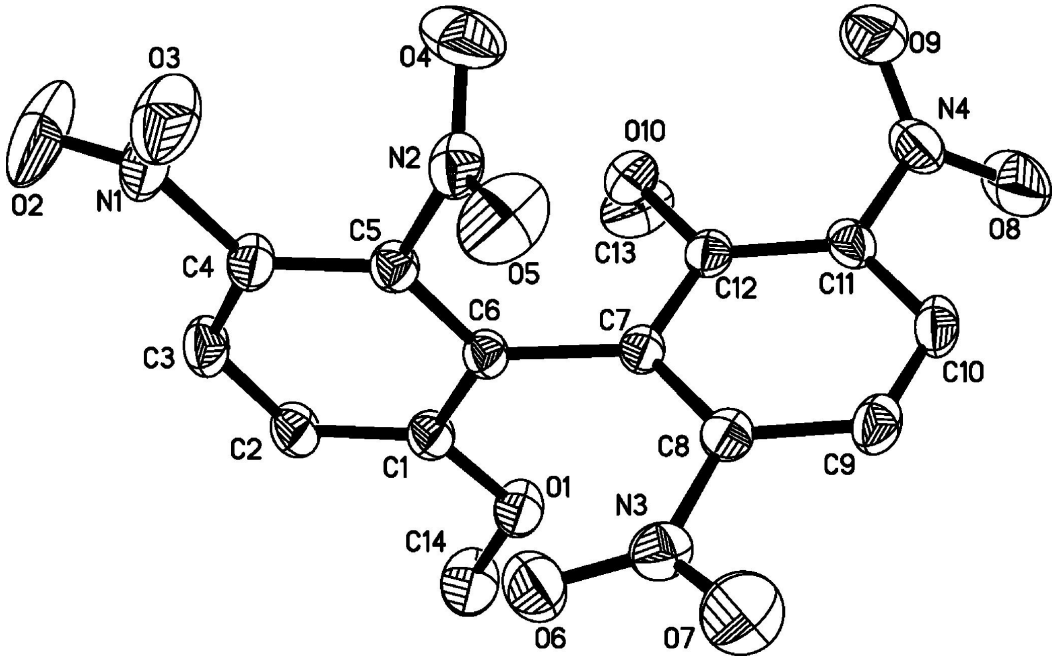
O3
O4
O9
N4
O10
N2
O2
N1
O8
C5
C13
C4
O5
C12
C11
C6
C7
C3
C10
C2
C8
C1
C9
O1
N3
C14
O6
O7

Fig. 2