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Methyl 2,2-bis(2,4-dinitrophenyl)-ethanoate

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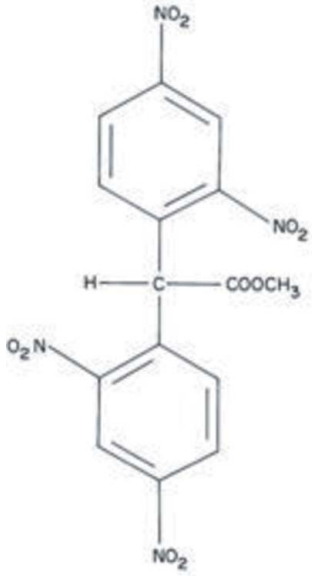
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.077; wR factor = 0.293; data-to-parameter ratio = 13.5.

In the title compound, $C_{15}H_{10}N_4O_{10}$, the dihedral angle between the aromatic rings is 89.05 (16)°. One O atom of one of the nitro groups is disordered over two sites in a 0.70:0.30 ratio. In the crystal, the molecules are linked by weak C—H···O interactions.

Related literature

For related structures, see: Chudek *et al.* (1989); Ertas *et al.* (1998). For background to the uses of ethyl/methyl 2,2-bis(2,4-dinitrophenyl)ethanoates, see: Hu (2005); Kawai & Watanabe (2002); Liu *et al.* (2009). For further synthetic details, see: McIvor & Miller (1965).



Experimental

Crystal data

$C_{15}H_{10}N_4O_{10}$
M_r = 406.27
Monoclinic, $P2_1/c$
a = 9.812 (5) Å
b = 10.974 (6) Å
c = 16.025 (9) Å
β = 91.589 (10)°
V = 1724.8 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 293 K
0.34 × 0.29 × 0.27 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2006)
T_{min} = 0.955, T_{max} = 0.965
13533 measured reflections
3525 independent reflections
1981 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.077
$wR(F^2)$ = 0.293
S = 0.98
3525 reflections
262 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.86 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O5^{i}	0.98	2.43	3.301 (5)	149
C7—H7···O10^{ii}	0.93	2.38	3.273 (5)	160
C15—H15*A*···O8^{iii}	0.96	2.59	3.255 (5)	127
C15—H15*B*···O3^{i}	0.96	2.41	3.216 (9)	141

Symmetry codes: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $x, -y-\frac{1}{2}, z+\frac{1}{2}$; (iii) $x+1, y, z$.

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP*-III (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97*.

The authors thank Dr Netaji of the IISc Bangalore for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6396).

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supplementary materials

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Methyl 2,2-bis(2,4-dinitrophenyl)ethanoate

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Comment

Ethyl / methyl 2,2-bis(2,4-dinitrophenyl)ethanoates have been used in many analytical detections (Kawai & Watanabe, 2002) and for the preparation of photo degradable aqueous inks (Hu, 2005) and tailor's chalk (Liu *et al.*, 2009). Articles have also appeared on the structure of ethyl 2,2-bis(2,4-dinitrophenyl) ethanoate (Chudek *et al.*, 1989, Ertas *et al.*, 1998).

Ethyl 2,2-bis(2,4-dinitrophenyl)ethanoate has been synthesized (yield 32–71%) by mixing equimolar amounts of 1-chloro-2,4-dinitrobenzene and ethyl 2,4-dinitrophenylacetate in the presence of tripropylamine in dimethylformamide medium (McIvor and Miller, 1965). The same authors have also prepared methyl 2,2-bis(2,4-dinitrophenyl)ethanoate (title molecule) only in 32% yield by adopting the same procedure. In this article we report an efficient new one pot synthesis to prepare title molecule (scheme) in good yield (65–70%) with high purity. The acetyl group of methyl 3-oxobutanoate has cleaved off during the formation of the title molecule.

The *ORTEP* diagram of title molecule is presented in Figure 1. The packing of the molecules features a number of C—H···O hydrogen bonds (Table 1).

Experimental

1-Chloro-2,4-dinitrobenzene (2 g, 0.01 mol) in absolute ethanol was mixed with methyl 3-oxobutanoate (1.2 g, 0.01 mol) in absolute ethanol. Triethylamine (5 g, 0.05 mol) was then added and the mixture was shaken well for 5 to 6 h. On standing pale yellow crystals come out from the solution after 15 days. The crystals were filtered and washed well with distilled water and dried. The dried crystals were powdered and washed with copious amount of ether to remove the unreacted reactants and then with little absolute alcohol. The crystals obtained after washing were recrystallized either from ethylacetate or chloroform to yield colourless blocks of the title compound (yield 65–70%: m.pt. 428 K).

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

$F^2 > 2\sigma(F^2)$ 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.

Figures

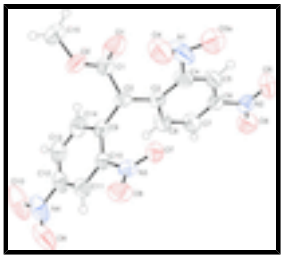


Fig. 1. The molecular structure of (I) showing 50% displacement ellipsoids.

Methyl 2,2-bis(2,4-dinitrophenyl)ethanoate

Crystal data

$C_{15}H_{10}N_4O_{10}$	$F(000) = 832$
$M_r = 406.27$	$D_x = 1.565$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 9.812$ (5) Å	Cell parameters from 567 reflections
$b = 10.974$ (6) Å	$\theta = 2.5$–$26.0°$
$c = 16.025$ (9) Å	$\mu = 0.14$ mm^{-1}
$\beta = 91.589$ (10)°	$T = 293$ K
$V = 1724.8$ (16) Å^3	Block, colorless
$Z = 4$	0.34 × 0.29 × 0.27 mm

Data collection

Bruker SMART APEX CCD diffractometer	3525 independent reflections
Radiation source: fine-focus sealed tube	1981 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.046$
Detector resolution: 0.3 pixels mm^{-1}	$\theta_{max} = 26.4°$, $\theta_{min} = 2.1°$
ω scans	$h = -12 \rightarrow 12$
Absorption correction: multi-scan (*SADABS*; Bruker, 2006)	$k = -13 \rightarrow 13$
$T_{min} = 0.955$, $T_{max} = 0.965$	$l = -20 \rightarrow 20$
13533 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full with fixed elements per cycle	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.077$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.293$	H-atom parameters constrained

S = 0.98	$w = 1/[\sigma^2(F_o^2) + (0.2P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
3525 reflections	$(\Delta/\sigma)_{max} = 0.012$
262 parameters	$\Delta\rho_{max} = 0.86$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.52$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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}	Occ. (<1)
O1	0.5549 (3)	0.1001 (4)	0.33068 (19)	0.1017 (12)	
O2	0.5029 (2)	0.1801 (3)	0.20813 (16)	0.0676 (8)	
O3	0.5184 (7)	0.3122 (6)	0.4951 (5)	0.136 (2)*	0.7
O3A	0.4078 (11)	0.3806 (10)	0.5064 (7)	0.086 (3)*	0.3
O4	0.4263 (4)	0.3497 (3)	0.38083 (18)	0.0951 (10)	
O5	0.2382 (4)	0.1011 (2)	0.69206 (16)	0.0784 (9)	
O6	0.1291 (3)	−0.0550 (3)	0.64934 (17)	0.0822 (9)	
O7	0.0686 (2)	0.2483 (2)	0.30932 (14)	0.0568 (6)	
O8	−0.0449 (3)	0.2648 (3)	0.19403 (17)	0.0695 (8)	
O9	−0.0984 (4)	−0.1013 (3)	0.03896 (17)	0.0908 (10)	
O10	0.0800 (5)	−0.2084 (3)	0.0167 (2)	0.1186 (14)	
N1	0.4152 (5)	0.3015 (4)	0.4429 (2)	0.1069 (15)	
N2	0.1982 (3)	0.0338 (3)	0.63757 (17)	0.0529 (7)	
N3	0.0397 (3)	0.2146 (2)	0.23940 (17)	0.0455 (7)	

N4	0.0206 (4)	−0.1288 (3)	0.05241 (18)	0.0742 (11)
C1	0.4734 (4)	0.1400 (4)	0.2825 (2)	0.0544 (9)
C2	0.3221 (3)	0.1506 (3)	0.29780 (19)	0.0424 (8)
H2	0.2969	0.2361	0.2889	0.051*
C3	0.2927 (3)	0.1203 (3)	0.38819 (19)	0.0420 (8)
C4	0.3366 (4)	0.1903 (3)	0.4556 (2)	0.0557 (9)
C5	0.3089 (4)	0.1621 (3)	0.5366 (2)	0.0565 (10)
H5	0.3412	0.2108	0.5804	0.068*
C6	0.2338 (3)	0.0622 (3)	0.55141 (19)	0.0444 (8)
C7	0.1878 (4)	−0.0127 (3)	0.4884 (2)	0.0555 (9)
H7	0.1371	−0.0819	0.4999	0.067*
C8	0.2183 (4)	0.0169 (3)	0.4073 (2)	0.0548 (9)
H8	0.1881	−0.0339	0.3642	0.066*
C9	0.2407 (3)	0.0761 (3)	0.23477 (18)	0.0420 (7)
C10	0.1093 (3)	0.1079 (3)	0.20720 (18)	0.0399 (7)
C11	0.0366 (4)	0.0419 (3)	0.14770 (19)	0.0485 (8)
H11	−0.0506	0.0654	0.1302	0.058*
C12	0.0968 (4)	−0.0586 (3)	0.1154 (2)	0.0547 (10)
C13	0.2250 (5)	−0.0943 (3)	0.1401 (2)	0.0610 (11)
H13	0.2645	−0.1632	0.1171	0.073*
C14	0.2945 (4)	−0.0269 (3)	0.1994 (2)	0.0586 (10)
H14	0.3815	−0.0517	0.2164	0.07*
C15	0.6420 (4)	0.1669 (5)	0.1825 (3)	0.0790 (13)
H15A	0.7002	0.2184	0.2163	0.119*
H15B	0.6483	0.19	0.125	0.119*
H15C	0.67	0.0836	0.1892	0.119*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0536 (16)	0.175 (3)	0.0770 (19)	0.039 (2)	0.0044 (14)	0.038 (2)
O2	0.0451 (13)	0.099 (2)	0.0595 (15)	−0.0030 (14)	0.0116 (11)	0.0197 (14)
O4	0.130 (3)	0.091 (2)	0.0644 (17)	−0.057 (2)	0.0008 (17)	0.0107 (15)
O5	0.114 (2)	0.0730 (19)	0.0486 (14)	0.0012 (17)	0.0103 (14)	−0.0108 (13)
O6	0.0809 (19)	0.104 (2)	0.0625 (16)	−0.0308 (17)	0.0112 (14)	0.0161 (15)
O7	0.0572 (14)	0.0635 (15)	0.0499 (12)	0.0047 (12)	0.0041 (11)	−0.0124 (11)
O8	0.0556 (15)	0.0680 (17)	0.0838 (17)	0.0205 (13)	−0.0170 (13)	−0.0031 (14)
O9	0.142 (3)	0.0722 (19)	0.0568 (15)	−0.0440 (19)	−0.0298 (16)	0.0104 (13)
O10	0.233 (4)	0.0577 (18)	0.0638 (18)	0.013 (2)	−0.018 (2)	−0.0165 (15)
N1	0.144 (3)	0.124 (3)	0.0516 (19)	−0.089 (3)	−0.020 (2)	0.010 (2)
N2	0.0522 (17)	0.0567 (18)	0.0501 (15)	0.0065 (14)	0.0086 (13)	0.0082 (13)
N3	0.0356 (13)	0.0472 (16)	0.0535 (15)	−0.0013 (12)	0.0002 (11)	−0.0005 (12)
N4	0.136 (3)	0.0434 (17)	0.0423 (16)	−0.0151 (19)	−0.0114 (17)	0.0084 (13)
C1	0.0470 (19)	0.065 (2)	0.0512 (19)	0.0017 (18)	−0.0009 (16)	0.0027 (17)
C2	0.0379 (16)	0.0461 (18)	0.0433 (16)	−0.0005 (14)	0.0026 (13)	0.0064 (14)
C3	0.0373 (16)	0.0432 (18)	0.0455 (16)	0.0003 (14)	0.0018 (13)	0.0016 (14)
C4	0.060 (2)	0.058 (2)	0.0494 (18)	−0.0170 (18)	−0.0038 (16)	0.0050 (16)
C5	0.064 (2)	0.062 (2)	0.0436 (18)	−0.0139 (19)	−0.0057 (16)	−0.0023 (16)

C6	0.0417 (17)	0.0492 (19)	0.0425 (16)	0.0015 (15)	0.0021 (13)	0.0025 (14)
C7	0.070 (2)	0.0450 (19)	0.0515 (19)	−0.0121 (18)	0.0027 (17)	0.0065 (16)
C8	0.072 (2)	0.046 (2)	0.0463 (18)	−0.0109 (18)	0.0038 (16)	0.0014 (15)
C9	0.0449 (17)	0.0445 (18)	0.0370 (15)	−0.0010 (15)	0.0097 (13)	0.0024 (13)
C10	0.0456 (17)	0.0385 (17)	0.0360 (15)	−0.0007 (14)	0.0049 (13)	0.0029 (12)
C11	0.059 (2)	0.0480 (19)	0.0385 (16)	−0.0071 (17)	−0.0011 (14)	0.0073 (14)
C12	0.084 (3)	0.0434 (19)	0.0364 (16)	−0.0099 (19)	0.0033 (16)	0.0040 (14)
C13	0.090 (3)	0.042 (2)	0.052 (2)	0.008 (2)	0.018 (2)	−0.0016 (16)
C14	0.063 (2)	0.053 (2)	0.060 (2)	0.0132 (19)	0.0123 (18)	−0.0016 (18)
C15	0.052 (2)	0.111 (4)	0.075 (3)	−0.007 (2)	0.016 (2)	−0.001 (3)

Geometric parameters (Å, °)

O1—C1	1.180 (4)	C3—C4	1.385 (5)
O2—C1	1.311 (4)	C3—C8	1.387 (5)
O2—C15	1.443 (5)	C4—C5	1.369 (5)
O3—N1	1.302 (7)	C5—C6	1.346 (5)
O3—O3A	1.336 (12)	C5—H5	0.9300
O3A—N1	1.341 (11)	C6—C7	1.369 (5)
O4—N1	1.134 (4)	C7—C8	1.380 (5)
O5—N2	1.201 (3)	C7—H7	0.9300
O6—N2	1.206 (3)	C8—H8	0.9300
O7—N3	1.206 (3)	C9—C14	1.376 (5)
O8—N3	1.220 (3)	C9—C10	1.396 (5)
O9—N4	1.219 (4)	C10—C11	1.380 (4)
O10—N4	1.204 (4)	C11—C12	1.360 (5)
N1—C4	1.460 (5)	C11—H11	0.9300
N2—C6	1.467 (4)	C12—C13	1.365 (6)
N3—C10	1.457 (4)	C13—C14	1.371 (5)
N4—C12	1.459 (5)	C13—H13	0.9300
C1—C2	1.516 (5)	C14—H14	0.9300
C2—C9	1.510 (4)	C15—H15A	0.9600
C2—C3	1.522 (4)	C15—H15B	0.9600
C2—H2	0.9800	C15—H15C	0.9600
C1—O2—C15	117.4 (3)	C4—C5—H5	120.8
N1—O3—O3A	61.1 (6)	C5—C6—C7	122.0 (3)
O3—O3A—N1	58.2 (6)	C5—C6—N2	119.0 (3)
O4—N1—O3	115.4 (5)	C7—C6—N2	119.0 (3)
O4—N1—O3A	111.8 (6)	C6—C7—C8	118.5 (3)
O3—N1—O3A	60.7 (6)	C6—C7—H7	120.7
O4—N1—C4	125.2 (3)	C8—C7—H7	120.7
O3—N1—C4	113.0 (5)	C7—C8—C3	121.9 (3)
O3A—N1—C4	113.3 (6)	C7—C8—H8	119.0
O5—N2—O6	123.9 (2)	C3—C8—H8	119.0
O5—N2—C6	118.2 (3)	C14—C9—C10	115.9 (3)
O6—N2—C6	117.9 (3)	C14—C9—C2	121.2 (3)
O7—N3—O8	123.7 (2)	C10—C9—C2	122.9 (3)
O7—N3—C10	118.4 (2)	C11—C10—C9	122.9 (3)
O8—N3—C10	118.0 (2)	C11—C10—N3	115.4 (3)

O10—N4—O9	124.7 (3)	C9—C10—N3	121.8 (3)
O10—N4—C12	117.8 (3)	C12—C11—C10	117.8 (3)
O9—N4—C12	117.5 (3)	C12—C11—H11	121.1
O1—C1—O2	123.8 (3)	C10—C11—H11	121.1
O1—C1—C2	124.9 (3)	C11—C12—C13	121.9 (3)
O2—C1—C2	111.3 (3)	C11—C12—N4	118.1 (4)
C9—C2—C1	110.6 (3)	C13—C12—N4	120.0 (3)
C9—C2—C3	114.1 (3)	C12—C13—C14	118.8 (3)
C1—C2—C3	110.5 (3)	C12—C13—H13	120.6
C9—C2—H2	107.1	C14—C13—H13	120.6
C1—C2—H2	107.1	C13—C14—C9	122.7 (4)
C3—C2—H2	107.1	C13—C14—H14	118.7
C4—C3—C8	115.8 (3)	C9—C14—H14	118.7
C4—C3—C2	124.0 (3)	O2—C15—H15A	109.5
C8—C3—C2	120.2 (3)	O2—C15—H15B	109.5
C5—C4—C3	123.3 (3)	H15A—C15—H15B	109.5
C5—C4—N1	116.2 (3)	O2—C15—H15C	109.5
C3—C4—N1	120.5 (3)	H15A—C15—H15C	109.5
C6—C5—C4	118.4 (3)	H15B—C15—H15C	109.5
C6—C5—H5	120.8		
O3A—O3—N1—O4	101.8 (7)	O6—N2—C6—C7	−0.1 (4)
O3A—O3—N1—C4	−104.7 (7)	C5—C6—C7—C8	−0.9 (6)
O3—O3A—N1—O4	−107.8 (6)	N2—C6—C7—C8	178.0 (3)
O3—O3A—N1—C4	104.2 (6)	C6—C7—C8—C3	−0.6 (6)
C15—O2—C1—O1	4.1 (6)	C4—C3—C8—C7	1.3 (5)
C15—O2—C1—C2	−175.4 (3)	C2—C3—C8—C7	−179.0 (3)
O1—C1—C2—C9	−118.9 (4)	C1—C2—C9—C14	28.9 (4)
O2—C1—C2—C9	60.5 (4)	C3—C2—C9—C14	−96.4 (4)
O1—C1—C2—C3	8.4 (6)	C1—C2—C9—C10	−149.5 (3)
O2—C1—C2—C3	−172.2 (3)	C3—C2—C9—C10	85.2 (4)
C9—C2—C3—C4	−168.3 (3)	C14—C9—C10—C11	−0.5 (5)
C1—C2—C3—C4	66.4 (4)	C2—C9—C10—C11	177.9 (3)
C9—C2—C3—C8	12.1 (4)	C14—C9—C10—N3	179.9 (3)
C1—C2—C3—C8	−113.3 (4)	C2—C9—C10—N3	−1.6 (5)
C8—C3—C4—C5	−0.5 (6)	O7—N3—C10—C11	152.1 (3)
C2—C3—C4—C5	179.8 (3)	O8—N3—C10—C11	−27.7 (4)
C8—C3—C4—N1	−179.7 (4)	O7—N3—C10—C9	−28.3 (4)
C2—C3—C4—N1	0.6 (6)	O8—N3—C10—C9	151.9 (3)
O4—N1—C4—C5	−165.2 (5)	C9—C10—C11—C12	0.4 (5)
O3—N1—C4—C5	44.4 (6)	N3—C10—C11—C12	179.9 (3)
O3A—N1—C4—C5	−22.2 (7)	C10—C11—C12—C13	−0.2 (5)
O4—N1—C4—C3	14.1 (7)	C10—C11—C12—N4	−179.9 (3)
O3—N1—C4—C3	−136.3 (5)	O10—N4—C12—C11	171.1 (3)
O3A—N1—C4—C3	157.0 (6)	O9—N4—C12—C11	−8.0 (4)
C3—C4—C5—C6	−0.9 (6)	O10—N4—C12—C13	−8.7 (5)
N1—C4—C5—C6	178.4 (4)	O9—N4—C12—C13	172.2 (3)
C4—C5—C6—C7	1.6 (6)	C11—C12—C13—C14	0.2 (6)
C4—C5—C6—N2	−177.3 (3)	N4—C12—C13—C14	180.0 (3)
O5—N2—C6—C5	−0.3 (4)	C12—C13—C14—C9	−0.5 (6)

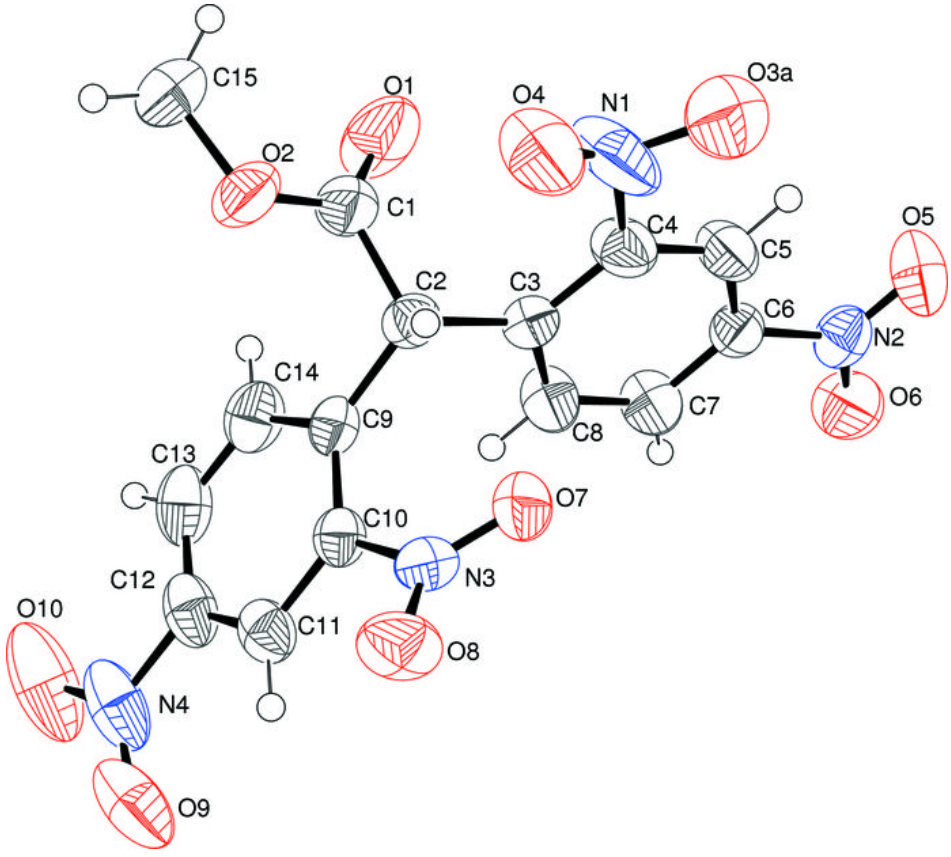
O6—N2—C6—C5	178.8 (3)	C10—C9—C14—C13	0.6 (5)
O5—N2—C6—C7	−179.2 (3)	C2—C9—C14—C13	−177.9 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O5^{i}	0.98	2.43	3.301 (5)	149
C7—H7···O10^{ii}	0.93	2.38	3.273 (5)	160
C15—H15A···O8^{iii}	0.96	2.59	3.255 (5)	127
C15—H15B···O3^{i}	0.96	2.41	3.216 (9)	141

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

Fig. 1


C15
O1
O4
N1
O3a
O2
C1
C4
C5
O5
C2
C3
C6
N2
C14
O6
C9
C7
C8
C13
O7
C10
C12
N3
O10
C11
O8
N4
O9