

2,3-Dibromo-3-(5-nitro-2-furyl)-1-(4-nitrophenyl)propan-1-one

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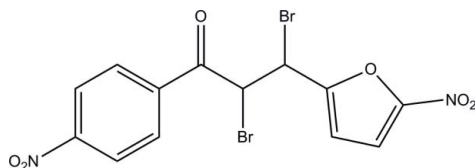
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.027; wR factor = 0.066; data-to-parameter ratio = 25.6.

In the title compound, $\text{C}_{13}\text{H}_8\text{Br}_2\text{N}_2\text{O}_6$, the 2-furyl ring is essentially planar, with a maximum deviation of 0.002 (2) Å. It is inclined at an angle of 33.94 (9)° to the benzene ring. Both nitro groups are slightly twisted away from their attached rings; the dihedral angles are 4.6 (2)° between the nitro group and the 2-furyl ring, and 13.72 (19)° between the nitro group and the benzene ring. In the crystal, molecules are linked into chains along [110] and $[\bar{1}\bar{1}0]$ via two pairs of intermolecular C—H...O hydrogen bonds, displaying $R_2^2(10)$ ring motifs.

Related literature

For general background to and the biological activity of nitrofurans, see: Holla *et al.* (1986, 1987, 1992). For the preparation of title compound, see: Rai *et al.* (2008). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986). For bond-length data, see: Allen *et al.* (1987). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For a related structure, see: Fun *et al.* (2010).



Experimental

Crystal data

$\text{C}_{13}\text{H}_8\text{Br}_2\text{N}_2\text{O}_6$
 $M_r = 448.03$
 Monoclinic, $P2_1/c$

$a = 12.1902$ (2) Å
 $b = 12.2006$ (2) Å
 $c = 9.9761$ (2) Å

$\beta = 96.282$ (1)°
 $V = 1474.81$ (5) Å³
 $Z = 4$
 Mo $K\alpha$ radiation

$\mu = 5.53$ mm⁻¹
 $T = 100$ K
 $0.48 \times 0.36 \times 0.30$ mm

Data collection

Bruker SMART APEXII CCD
 area-detector diffractometer
 Absorption correction: multi-scan
 (SADABS; Bruker, 2009)
 $T_{\min} = 0.176$, $T_{\max} = 0.291$

22940 measured reflections
 5315 independent reflections
 4546 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.027$
 $wR(F^2) = 0.066$
 $S = 1.02$
 5315 reflections

208 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.84$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.47$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---------------------------------------|-------|-------------|-------------|---------------|
| $\text{C}2-H2A\cdots\text{O}5^i$ | 0.93 | 2.48 | 3.211 (2) | 136 |
| $\text{C}12-H12A\cdots\text{O}3^{ii}$ | 0.93 | 2.43 | 3.317 (2) | 160 |

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

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; 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 and PLATON (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2362).

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§ Thomson Reuters ResearcherID: A-5525-2009.

supplementary materials

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2,3-Dibromo-3-(5-nitro-2-furyl)-1-(4-nitrophenyl)propan-1-one

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Comment

Nitrofurans are class of synthetic compounds characterized by the presence of 5-nitro-2-furyl group. The presence of nitro group in the position-5 of the molecule conferred antibacterial activity (Holla *et al.*, 1986). A number of nitrofurans have attained utility as antibacterial agents in humans and in veterinary medicine because of their broad spectrum of activity (Holla *et al.*, 1992; Holla *et al.*, 1987). 1-Aryl-3-(5-nitro-2-furyl)-2-propyn-1-ones were prepared by the hydrobromination of 2,3-dibromo-1-aryl-3-(5-nitro-2-furyl)-2-propan-1-ones in the presence of triethylamine in benzene medium. The dibromopropanones were in turn obtained by the bromination of 1-aryl-3-(5-nitro-2-furyl)-2-propen-1-ones. Acid-catalysed condensation of acetophenones with 5-nitrofuraldiacetate in acetic acid yielded the required 1-aryl-3-(5-nitro-2-furyl)-2-propen-1-ones called chalcones (Rai *et al.*, 2008).

In the title molecule (Fig. 1), the 2-furyl (O2/C10-C13) ring is essentially planar (maximum deviation = 0.002 (2) Å for atoms C11, C12 and C13) and is inclined at an angle of 33.94 (9) ° with the phenyl ring (C1-C6). Both nitro groups (N1/O3/O4 and N2/O5/O6) are slightly twisted away from the attached rings [the dihedral angles are 4.6 (2)° between nitro group and 2-fury ring and 13.72 (19)° between nitro group and phenyl ring]. Bond lengths (Allen *et al.*, 1987) and angles are within normal ranges and comparable to a related structure (Fun *et al.*, 2010).

In the crystal packing (Fig. 2), the molecules are linked into one-dimensional chains along [110] and [1-10] via pairs of intermolecular C2–H2A···O5 and C12–H12A···O3 hydrogen bonds, displaying R₂²(10) ring motifs (Bernstein *et al.*, 1995).

Experimental

1-(*p*-Nitrophenyl)-3-(5-nitro-2-furyl)-2-propen-1-one (0.01 mol) was dissolved in glacial acetic acid (25 ml) by gentle warming. A solution of bromine in glacial acetic acid (30% [w/v]) was added to it with constant stirring till yellow color of the bromine persisted. The reaction mixture was kept aside at room temperature for overnight. Crystals of dibromopropanones separated out were collected by filtration and washed with ethanol and dried. It was then recrystallized from glacial acetic acid. Crystals suitable for X-ray analysis were obtained from 1:2 mixtures of DMF and ethanol by slow evaporation.

Refinement

All H atoms were positioned geometrically and refined using a riding model with C–H = 0.93–0.98 Å and $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$. The highest residual electron density peak is located at 0.70 Å from Br1 and the deepest hole is located at 0.53 Å from Br2.

Figures

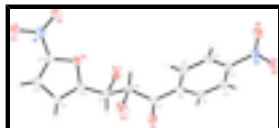


Fig. 1. The molecular structure of the title compound showing 50% probability displacement ellipsoids for non-H atoms and the atom-numbering scheme.

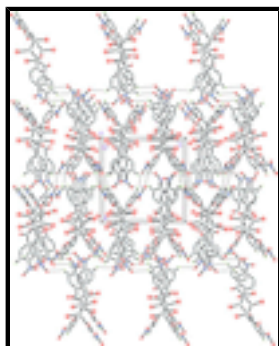


Fig. 2. The crystal structure of the title compound, viewed along the *c* axis. H atoms not involved in hydrogen bonds (dashed lines) have been omitted for clarity.

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Crystal data

$C_{13}H_8Br_2N_2O_6$

$M_r = 448.03$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 12.1902(2) \text{ \AA}$

$b = 12.2006(2) \text{ \AA}$

$c = 9.9761(2) \text{ \AA}$

$\beta = 96.282(1)^\circ$

$V = 1474.81(5) \text{ \AA}^3$

$Z = 4$

$F(000) = 872$

$D_x = 2.018 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 9181 reflections

$\theta = 2.7\text{--}35.0^\circ$

$\mu = 5.53 \text{ mm}^{-1}$

$T = 100 \text{ K}$

Block, light yellow

$0.48 \times 0.36 \times 0.30 \text{ mm}$

Data collection

Bruker SMART APEXII CCD area-detector diffractometer

Radiation source: fine-focus sealed tube graphite

φ and ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2009)

$T_{\min} = 0.176$, $T_{\max} = 0.291$

22940 measured reflections

5315 independent reflections

4546 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

$\theta_{\max} = 32.5^\circ$, $\theta_{\min} = 2.7^\circ$

$h = -18 \rightarrow 17$

$k = -18 \rightarrow 18$

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2

Primary atom site location: structure-invariant direct methods

| | |
|---------------------------------|--|
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.027$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.066$ | H-atom parameters constrained |
| $S = 1.02$ | $w = 1/[\sigma^2(F_o^2) + (0.0329P)^2 + 0.6835P]$ |
| 5315 reflections | where $P = (F_o^2 + 2F_c^2)/3$ |
| 208 parameters | $(\Delta/\sigma)_{\max} = 0.003$ |
| 0 restraints | $\Delta\rho_{\max} = 0.84 \text{ e } \text{\AA}^{-3}$ |
| | $\Delta\rho_{\min} = -0.47 \text{ e } \text{\AA}^{-3}$ |

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cyrosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

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

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|---------------|---------------|----------------------------------|
| Br1 | 1.041889 (15) | 0.421114 (15) | 0.681600 (19) | 0.03228 (5) |
| Br2 | 0.885347 (14) | 0.105613 (13) | 0.491276 (17) | 0.02690 (5) |
| O1 | 1.09576 (10) | 0.14526 (11) | 0.72205 (13) | 0.0308 (3) |
| O2 | 0.79177 (9) | 0.35369 (9) | 0.44313 (11) | 0.0231 (2) |
| O3 | 0.57672 (11) | 0.52110 (12) | 0.31188 (15) | 0.0376 (3) |
| O4 | 0.71217 (11) | 0.44726 (12) | 0.21746 (13) | 0.0343 (3) |
| O5 | 1.58062 (10) | 0.13853 (11) | 0.42438 (14) | 0.0334 (3) |
| O6 | 1.51706 (11) | 0.26900 (12) | 0.29087 (14) | 0.0335 (3) |
| N1 | 0.66040 (12) | 0.46327 (12) | 0.31406 (15) | 0.0274 (3) |
| N2 | 1.50858 (11) | 0.20428 (12) | 0.38341 (14) | 0.0251 (3) |
| C1 | 1.28637 (13) | 0.12333 (13) | 0.59042 (16) | 0.0235 (3) |
| H1A | 1.2691 | 0.0664 | 0.6464 | 0.028* |
| C2 | 1.38425 (14) | 0.12046 (13) | 0.53263 (17) | 0.0246 (3) |
| H2A | 1.4337 | 0.0628 | 0.5493 | 0.030* |
| C3 | 1.40608 (12) | 0.20650 (13) | 0.44904 (16) | 0.0219 (3) |
| C4 | 1.33605 (14) | 0.29473 (13) | 0.42338 (17) | 0.0253 (3) |
| H4A | 1.3540 | 0.3515 | 0.3676 | 0.030* |
| C5 | 1.23848 (14) | 0.29687 (13) | 0.48241 (16) | 0.0252 (3) |
| H5A | 1.1900 | 0.3555 | 0.4665 | 0.030* |
| C6 | 1.21302 (13) | 0.21085 (13) | 0.56577 (15) | 0.0218 (3) |

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| | | | | |
|------|--------------|--------------|--------------|------------|
| C7 | 1.10791 (13) | 0.20769 (14) | 0.62976 (16) | 0.0239 (3) |
| C8 | 1.01418 (13) | 0.28532 (13) | 0.57771 (16) | 0.0227 (3) |
| H8A | 1.0158 | 0.2995 | 0.4812 | 0.027* |
| C9 | 0.90304 (13) | 0.23822 (13) | 0.60376 (16) | 0.0222 (3) |
| H9A | 0.9064 | 0.2168 | 0.6988 | 0.027* |
| C10 | 0.80678 (13) | 0.31058 (13) | 0.57093 (15) | 0.0222 (3) |
| C11 | 0.72425 (13) | 0.34199 (13) | 0.64346 (16) | 0.0245 (3) |
| H11A | 0.7166 | 0.3234 | 0.7324 | 0.029* |
| C12 | 0.65187 (14) | 0.40878 (14) | 0.55717 (17) | 0.0258 (3) |
| H12A | 0.5873 | 0.4425 | 0.5773 | 0.031* |
| C13 | 0.69716 (13) | 0.41271 (13) | 0.43947 (16) | 0.0233 (3) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|-------------|--------------|--------------|-------------|--------------|
| Br1 | 0.03186 (10) | 0.03185 (9) | 0.03482 (10) | -0.00803 (6) | 0.01125 (7) | -0.01036 (7) |
| Br2 | 0.02422 (8) | 0.02524 (8) | 0.03086 (9) | 0.00128 (5) | 0.00126 (6) | -0.00446 (6) |
| O1 | 0.0231 (6) | 0.0417 (7) | 0.0277 (6) | -0.0014 (5) | 0.0023 (5) | 0.0128 (5) |
| O2 | 0.0209 (5) | 0.0286 (5) | 0.0210 (5) | 0.0039 (4) | 0.0068 (4) | 0.0037 (4) |
| O3 | 0.0334 (7) | 0.0421 (7) | 0.0381 (7) | 0.0164 (6) | 0.0073 (6) | 0.0102 (6) |
| O4 | 0.0344 (7) | 0.0457 (7) | 0.0241 (6) | 0.0072 (6) | 0.0086 (5) | 0.0075 (5) |
| O5 | 0.0231 (6) | 0.0371 (6) | 0.0404 (7) | 0.0058 (5) | 0.0059 (5) | 0.0039 (5) |
| O6 | 0.0285 (6) | 0.0407 (7) | 0.0329 (6) | 0.0017 (5) | 0.0104 (5) | 0.0080 (5) |
| N1 | 0.0259 (7) | 0.0302 (7) | 0.0265 (7) | 0.0032 (5) | 0.0049 (5) | 0.0045 (5) |
| N2 | 0.0208 (6) | 0.0291 (6) | 0.0255 (6) | -0.0010 (5) | 0.0034 (5) | -0.0026 (5) |
| C1 | 0.0233 (7) | 0.0232 (6) | 0.0238 (7) | -0.0010 (5) | 0.0013 (6) | 0.0015 (5) |
| C2 | 0.0238 (7) | 0.0234 (7) | 0.0265 (7) | 0.0020 (5) | 0.0026 (6) | 0.0003 (6) |
| C3 | 0.0193 (6) | 0.0252 (7) | 0.0215 (7) | -0.0010 (5) | 0.0027 (5) | -0.0026 (5) |
| C4 | 0.0254 (7) | 0.0276 (7) | 0.0237 (7) | 0.0019 (6) | 0.0057 (6) | 0.0033 (6) |
| C5 | 0.0254 (7) | 0.0277 (7) | 0.0228 (7) | 0.0044 (6) | 0.0045 (6) | 0.0045 (6) |
| C6 | 0.0196 (7) | 0.0271 (7) | 0.0187 (6) | -0.0002 (5) | 0.0019 (5) | 0.0009 (5) |
| C7 | 0.0204 (7) | 0.0302 (7) | 0.0207 (7) | -0.0005 (5) | 0.0009 (5) | 0.0017 (5) |
| C8 | 0.0212 (7) | 0.0270 (7) | 0.0205 (6) | -0.0004 (5) | 0.0051 (5) | -0.0008 (5) |
| C9 | 0.0202 (7) | 0.0256 (7) | 0.0212 (7) | 0.0007 (5) | 0.0037 (5) | -0.0003 (5) |
| C10 | 0.0212 (7) | 0.0263 (7) | 0.0198 (7) | 0.0017 (5) | 0.0054 (5) | 0.0016 (5) |
| C11 | 0.0233 (7) | 0.0294 (7) | 0.0218 (7) | 0.0016 (6) | 0.0073 (6) | -0.0006 (6) |
| C12 | 0.0243 (7) | 0.0282 (7) | 0.0262 (7) | 0.0049 (6) | 0.0080 (6) | -0.0013 (6) |
| C13 | 0.0217 (7) | 0.0251 (7) | 0.0238 (7) | 0.0038 (5) | 0.0054 (5) | 0.0015 (5) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|--------|-------------|--------|-----------|
| Br1—C8 | 1.9639 (16) | C3—C4 | 1.380 (2) |
| Br2—C9 | 1.9674 (16) | C4—C5 | 1.384 (2) |
| O1—C7 | 1.216 (2) | C4—H4A | 0.9300 |
| O2—C13 | 1.3567 (19) | C5—C6 | 1.395 (2) |
| O2—C10 | 1.3728 (18) | C5—H5A | 0.9300 |
| O3—N1 | 1.2385 (19) | C6—C7 | 1.493 (2) |
| O4—N1 | 1.2240 (19) | C7—C8 | 1.531 (2) |
| O5—N2 | 1.2260 (19) | C8—C9 | 1.520 (2) |

| | | | |
|-------------|--------------|-----------------|--------------|
| O6—N2 | 1.2277 (19) | C8—H8A | 0.9800 |
| N1—C13 | 1.423 (2) | C9—C10 | 1.476 (2) |
| N2—C3 | 1.473 (2) | C9—H9A | 0.9800 |
| C1—C2 | 1.381 (2) | C10—C11 | 1.357 (2) |
| C1—C6 | 1.397 (2) | C11—C12 | 1.420 (2) |
| C1—H1A | 0.9300 | C11—H11A | 0.9300 |
| C2—C3 | 1.384 (2) | C12—C13 | 1.352 (2) |
| C2—H2A | 0.9300 | C12—H12A | 0.9300 |
| C13—O2—C10 | 104.77 (12) | O1—C7—C8 | 119.74 (15) |
| O4—N1—O3 | 124.87 (15) | C6—C7—C8 | 118.86 (13) |
| O4—N1—C13 | 118.89 (14) | C9—C8—C7 | 110.75 (13) |
| O3—N1—C13 | 116.23 (14) | C9—C8—Br1 | 109.50 (10) |
| O5—N2—O6 | 123.74 (15) | C7—C8—Br1 | 105.31 (10) |
| O5—N2—C3 | 118.38 (14) | C9—C8—H8A | 110.4 |
| O6—N2—C3 | 117.88 (14) | C7—C8—H8A | 110.4 |
| C2—C1—C6 | 120.76 (15) | Br1—C8—H8A | 110.4 |
| C2—C1—H1A | 119.6 | C10—C9—C8 | 115.96 (13) |
| C6—C1—H1A | 119.6 | C10—C9—Br2 | 109.29 (11) |
| C1—C2—C3 | 117.64 (15) | C8—C9—Br2 | 104.92 (10) |
| C1—C2—H2A | 121.2 | C10—C9—H9A | 108.8 |
| C3—C2—H2A | 121.2 | C8—C9—H9A | 108.8 |
| C4—C3—C2 | 123.18 (15) | Br2—C9—H9A | 108.8 |
| C4—C3—N2 | 118.00 (14) | C11—C10—O2 | 110.84 (13) |
| C2—C3—N2 | 118.82 (14) | C11—C10—C9 | 131.93 (15) |
| C3—C4—C5 | 118.60 (15) | O2—C10—C9 | 117.20 (13) |
| C3—C4—H4A | 120.7 | C10—C11—C12 | 106.65 (14) |
| C5—C4—H4A | 120.7 | C10—C11—H11A | 126.7 |
| C4—C5—C6 | 119.81 (15) | C12—C11—H11A | 126.7 |
| C4—C5—H5A | 120.1 | C13—C12—C11 | 105.13 (14) |
| C6—C5—H5A | 120.1 | C13—C12—H12A | 127.4 |
| C5—C6—C1 | 120.00 (15) | C11—C12—H12A | 127.4 |
| C5—C6—C7 | 122.11 (14) | C12—C13—O2 | 112.62 (14) |
| C1—C6—C7 | 117.88 (14) | C12—C13—N1 | 131.29 (15) |
| O1—C7—C6 | 121.40 (15) | O2—C13—N1 | 116.03 (14) |
| C6—C1—C2—C3 | -0.6 (2) | C7—C8—C9—C10 | 173.89 (13) |
| C1—C2—C3—C4 | 1.2 (2) | Br1—C8—C9—C10 | 58.18 (16) |
| C1—C2—C3—N2 | -178.53 (14) | C7—C8—C9—Br2 | -65.45 (14) |
| O5—N2—C3—C4 | 166.33 (15) | Br1—C8—C9—Br2 | 178.84 (7) |
| O6—N2—C3—C4 | -13.4 (2) | C13—O2—C10—C11 | -0.01 (18) |
| O5—N2—C3—C2 | -13.9 (2) | C13—O2—C10—C9 | 178.03 (14) |
| O6—N2—C3—C2 | 166.39 (15) | C8—C9—C10—C11 | -128.74 (19) |
| C2—C3—C4—C5 | -0.9 (2) | Br2—C9—C10—C11 | 112.98 (18) |
| N2—C3—C4—C5 | 178.81 (14) | C8—C9—C10—O2 | 53.73 (19) |
| C3—C4—C5—C6 | 0.0 (2) | Br2—C9—C10—O2 | -64.55 (16) |
| C4—C5—C6—C1 | 0.6 (2) | O2—C10—C11—C12 | 0.22 (19) |
| C4—C5—C6—C7 | -178.69 (15) | C9—C10—C11—C12 | -177.43 (17) |
| C2—C1—C6—C5 | -0.3 (2) | C10—C11—C12—C13 | -0.34 (19) |
| C2—C1—C6—C7 | 179.02 (15) | C11—C12—C13—O2 | 0.35 (19) |

supplementary materials

| | | | |
|--------------|--------------|----------------|--------------|
| C5—C6—C7—O1 | -165.16 (17) | C11—C12—C13—N1 | 177.30 (17) |
| C1—C6—C7—O1 | 15.6 (2) | C10—O2—C13—C12 | -0.22 (18) |
| C5—C6—C7—C8 | 14.6 (2) | C10—O2—C13—N1 | -177.67 (14) |
| C1—C6—C7—C8 | -164.68 (14) | O4—N1—C13—C12 | -173.83 (18) |
| O1—C7—C8—C9 | -26.5 (2) | O3—N1—C13—C12 | 6.2 (3) |
| C6—C7—C8—C9 | 153.73 (14) | O4—N1—C13—O2 | 3.0 (2) |
| O1—C7—C8—Br1 | 91.78 (16) | O3—N1—C13—O2 | -176.98 (15) |
| C6—C7—C8—Br1 | -87.98 (14) | | |

Hydrogen-bond geometry (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|------------------------------------|-------|-------------|-------------|---------------|
| C2—H2A \cdots O5 ⁱ | 0.93 | 2.48 | 3.211 (2) | 136 |
| C12—H12A \cdots O3 ⁱⁱ | 0.93 | 2.43 | 3.317 (2) | 160 |

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

Fig. 1

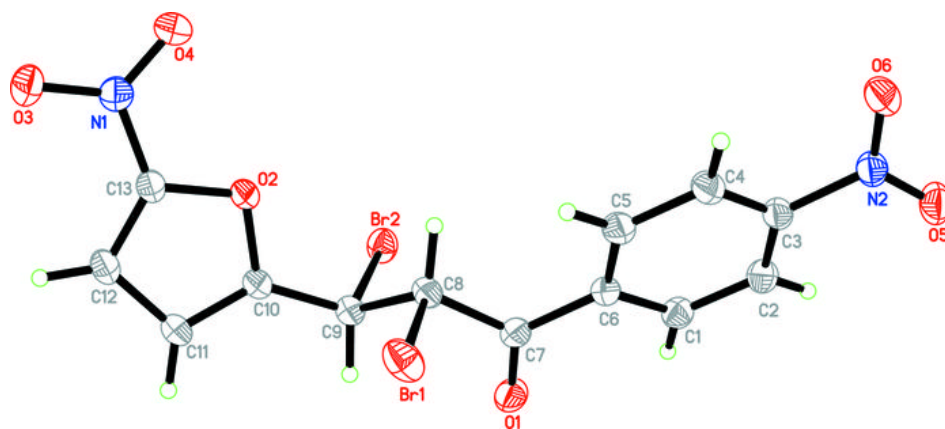


Fig. 2

