Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-(2-Chlorophenyl)-1,5-bis(4-nitrophenyl)-pentane-1,5-dione

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Received 8 September 2006
Accepted 14 September 2006

Key indicators

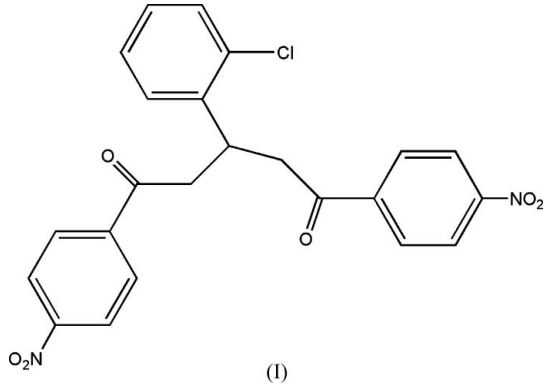
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.044
wR factor = 0.115
Data-to-parameter ratio = 16.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title molecule, $C_{23}H_{17}ClN_2O_6$, all bond lengths and angles are within normal ranges. The chloro-substituted benzene ring makes dihedral angles of 115.6 (2) and 109.6 (2)° with the two nitro-substituted benzene rings, and the dihedral angle between the two nitro-substituted benzene rings is 83.5 (2)°.

Comment

Multi-ring compounds play an important role in the development of chemistry related to sterilization and enzymatic reactions. In a continuation of our structural studies of multi-ring compounds (Qiu, Yang *et al.*, 2006; Qiu, Liu & Zhu, 2006), we report here the crystal structure of the title compound, (I) (Fig. 1)



(I)

All bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987). The three benzene rings, *viz*. C1–C6 (*A*), C10–C15 (*B*) and C18–C23 (*C*), make the following dihedral angles: *A*/*B* 115.6 (2)°, *A*/*C* 109.6 (2)° and *B*/*C* 83.5 (2)°.

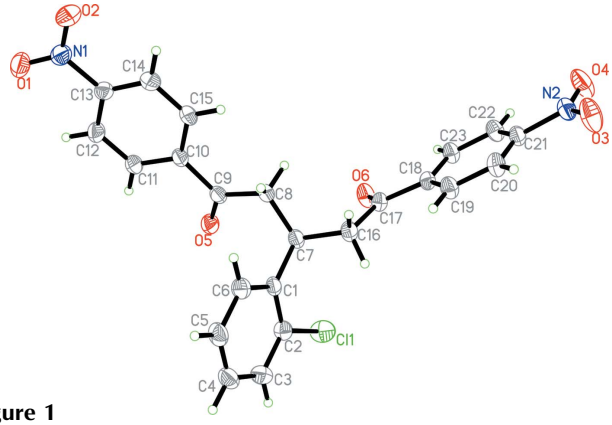


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

Experimental

The title compound was synthesized by the reaction of equivalent amounts of (*E*)-3-(2-chlorophenyl)-1-(4-nitrophenyl)prop-2-en-1-one (1 mmol), isonicotinohydrazide (1 mmol) and 1-(4-nitrophenyl)ethanone (1 mmol) in an ethanol solution (20 ml) for 3 h at 383–393 K. Single crystals suitable for X-ray diffraction analysis were obtained by evaporation of an ethanol solution.

Crystal data

$C_{23}H_{17}ClN_2O_6$
M_r = 452.84
Orthorhombic, $P2_12_12_1$
a = 5.7697 (7) Å
b = 14.545 (2) Å
c = 24.681 (3) Å
V = 2071.2 (5) Å^3
Z = 4
D_x = 1.452 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 298 (2) K
Block, brown
0.37 × 0.18 × 0.07 mm

Data collection

Bruker SMART APEX area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.949, T_{max} = 0.980
12428 measured reflections
4738 independent reflections
3298 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 27.6°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.115
S = 0.99
4738 reflections
293 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0582P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Absolute structure: Flack (1983), 1989 Friedel pairs
Flack parameter: −0.03 (7)

All H atoms, except H7, were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C). Atom H7, attached to C7, was refined isotropically, giving a C—H distance of 0.99 (2) Å.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

The authors thank the Education Office of Anhui Province, China, for research grant No. 2006kj158B.

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