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

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In the title molecule, $C_{23}H_{17}ClN_2O_6$, all bond lengths and angles are within normal ranges. The crystal packing is stabilized by weak intermolecular C—H···O hydrogen bonds with H···O distances less than 2.5 Å.

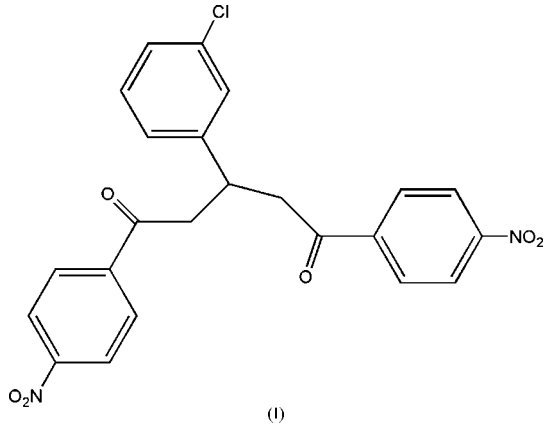
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.042
wR factor = 0.123
Data-to-parameter ratio = 18.1

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

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 study of multi-ring compounds (Qiu, Liu, & Zhu, 2006; Qiu, Liu, Zhu & Ma, 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*),

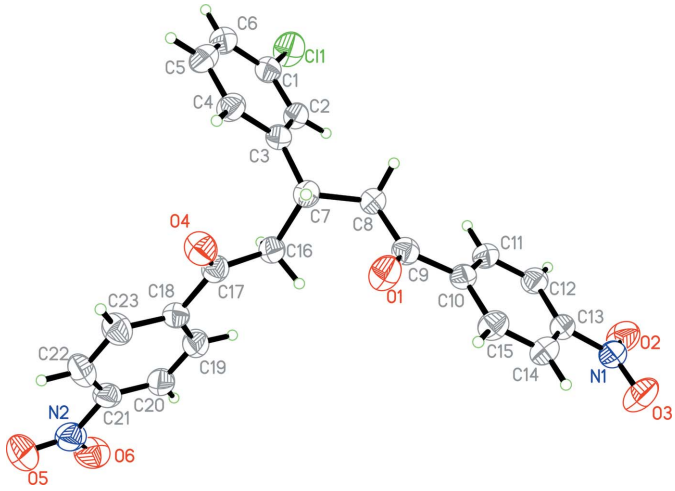


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

C10–C15 (*B*) and C18–C23 (*C*), make the following dihedral angles: *A*/*B* 10.3 (1)°, *A*/*C* 81.8 (1)° and *B*/*C* 86.7 (1)°. The crystal packing (Fig. 2) is stabilized by weak intermolecular C—H···O hydrogen bonds (Table 1).

Experimental

The title compound was synthesized by the reaction of equivalent amounts of (*E*)-3-(3-chlorophenyl)-1-(4-nitrophenyl)prop-2-en-1-one (0.1 mmol), isonicotinohydrazide (0.1 mmol) and 1-(4-nitrophenyl)ethanone (0.1 mmol) in an ethanol solution (30 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
Monoclinic, $P2_1/n$
a = 7.2164 (14) Å
b = 28.246 (6) Å
c = 10.378 (2) Å
β = 90.37 (3)°
V = 2115.3 (7) Å^3
Z = 4
D_x = 1.422 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 298 (2) K
Plate, brown
0.43 × 0.26 × 0.08 mm

Data collection

Bruker SMART APEX area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.928, T_{max} = 0.979
19219 measured reflections
5317 independent reflections
1609 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
θ_{max} = 28.8°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.123
S = 0.70
5317 reflections
293 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0629P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 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
C12—H12···O1^{i}	0.93	2.41	3.214 (3)	144
C16—H16A···O6^{ii}	0.97	2.49	3.407 (3)	157

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

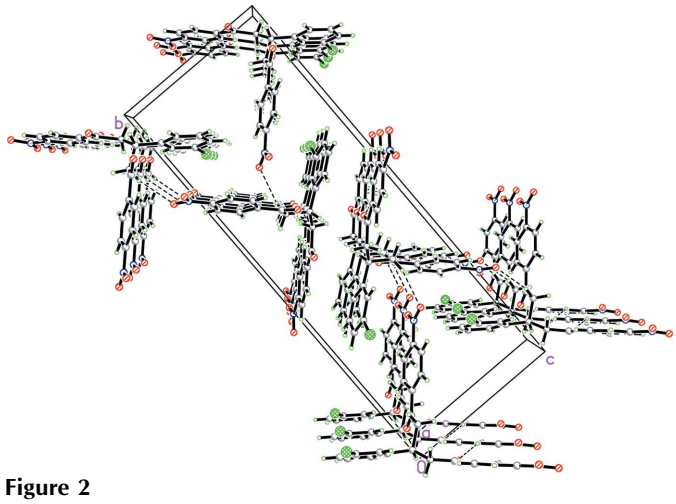


Figure 2
The molecular packing of (I), viewed along the *a* axis. Dashed lines indicate intermolecular hydrogen bonds.

All H atoms were placed in geometrically idealized positions, with C—H distances of 0.93–0.97 Å, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

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*.

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