Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,4-Bis(2-bromophenyl)-1,3-bis(3-nitrobenzoyl)cyclobutane

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.038
wR factor = 0.091
Data-to-parameter ratio = 15.7

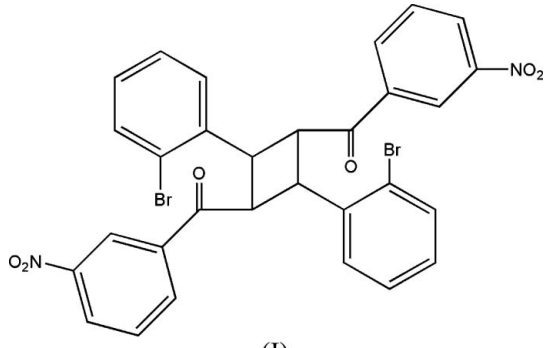
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 26 May 2006
Accepted 31 May 2006

The molecule of the title compound, $C_{30}H_{20}Br_2N_2O_6$, has a centre of symmetry at the centroid of the planar cyclobutane ring.

Comment

Recently, we have reported the structures of two chalcone derivatives (Qiu, Liu & Zhu, 2006; Qiu, Yang *et al.*, 2006). As an extension of our work on the structural characterization of chalcone derivatives, the title compound, (I), is reported here.



(I)

The asymmetric unit of (I) consists of one half-molecule (Fig. 1). All bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The molecule has a centre of symmetry at the centroid of the planar cyclobutane ring. The dihedral angle between the C1–C6 and C10–C15 benzene rings is 13.8 (2)°.

In the crystal structure of (I), the molecules stack along the *a* axis, with no short molecular contacts (<3.2 Å) (Fig. 2).

Experimental

The reagents were commercial products and were used without further purification. An aqueous solution of potassium hydroxide

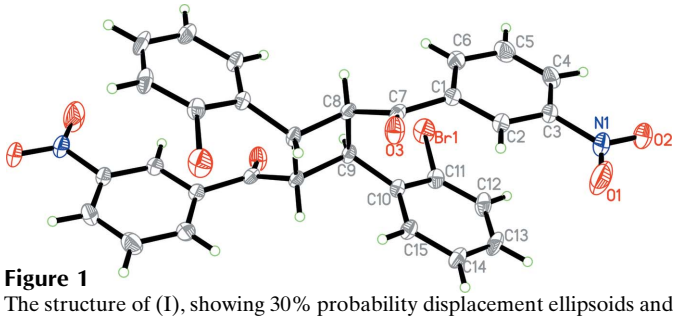


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Unlabelled atoms are related to labelled atoms by $1-x, 1-y, 1-z$.

(20%, 1 ml) was added with overnight stirring to a solution of 2-bromobenzaldehyde (1 mmol, 0.19 g) and 1-(3-nitrophenyl)ethanone (1 mmol, 0.17 g) in ethanol (15 ml) at room temperature. The reaction mixture was then poured on to ice and neutralized with hydrochloric acid (5%), yielding a yellow solid. This was dissolved in acetone (12 ml) and stirred for about 10 min to give a clear yellow solution. After allowing the solution to stand in air for 10 d, yellow block-shaped crystals of (I) were formed at the bottom of the vessel on slow evaporation of the solvent. These were collected, washed three times with acetone and dried in a vacuum desiccator using $CaCl_2$. The title compound was isolated in 58% yield.

Crystal data

$C_{30}H_{20}Br_2N_2O_6$
M_r = 664.30
Monoclinic, $P2_1/c$
a = 7.3293 (15) Å
b = 15.793 (3) Å
c = 11.571 (2) Å
β = 97.80 (3)°
V = 1327.0 (5) Å^3
Z = 2
D_x = 1.663 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 3.10 mm^{-1}
T = 298 (2) K
Block, yellow
0.28 × 0.15 × 0.09 mm

Data collection

Bruker SMART APEX area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.575, T_{max} = 0.754
7881 measured reflections
2976 independent reflections
1891 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 27.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.091
S = 1.01
2976 reflections
189 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0387P)^2 + 0.2379P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.006
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

Atoms H8 and H9 were located in a difference map and refined freely; C8—H8 = 0.98 (2) and C9—H9 = 0.91 (3) Å. Other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å and 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); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2001); software used to prepare material for publication: *SHELXTL*.

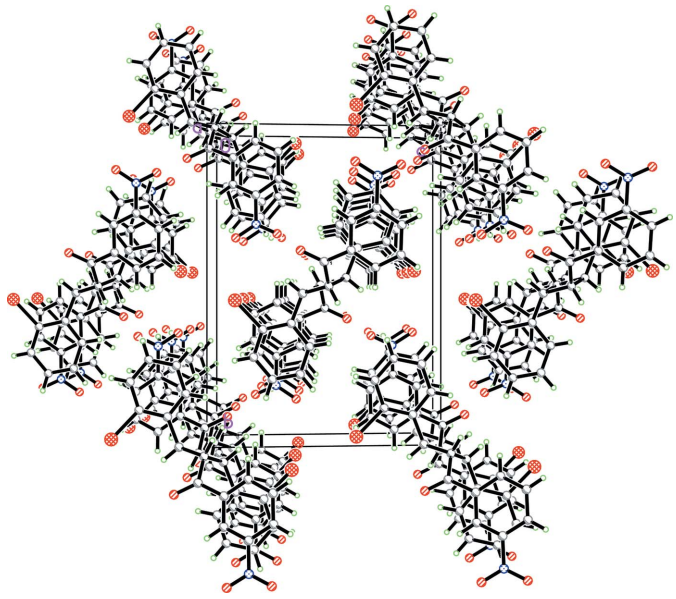


Figure 2
The crystal packing of (I), viewed along the *a* axis.

The authors thank the Education Office of Anhui Province, China, for research grant No. 2006kj158B, and Fuyang Normal College, China, for research grant No. LQ007.

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