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(2*E*)-1-(4-Methylphenyl)-3-(4-nitrophenyl)prop-2-en-1-one

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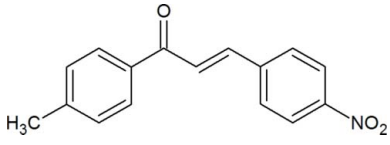
Key indicators: single-crystal X-ray study; T = 203 K; mean σ(C–C) = 0.005 Å; R factor = 0.055; wR factor = 0.162; data-to-parameter ratio = 12.4.

The title compound, $C_{16}H_{13}NO_3$, crystallizes with two nearly planar independent molecules in the asymmetric unit. The molecules exist as pseudo-inversion-related pairs and each of the independent molecules forms sheets approximately parallel to the *ab* plane which are alternately stacked along the *c* axis. The crystal structure is stabilized by C—H···O intermolecular hydrogen-bonding interactions.

Related literature

For related structures, see: Yathirajan *et al.* (2007); Harrison *et al.* (2006); Patil *et al.* (2006). For related literature, see: Dhar *et al.* (1981); Opletalova & Sedivy *et al.* (1999); Sarojini *et al.* (2006).



Experimental

Crystal data

$C_{16}H_{13}NO_3$
M_r = 267.27
Monoclinic, *Pc*
a = 5.97300 (1) Å
b = 15.0731 (5) Å
c = 14.6768 (4) Å
β = 95.785 (2)°
V = 1314.65 (6) Å^3
Z = 4
Mo *K*α radiation
μ = 0.09 mm^{-1}
T = 203 K
0.47 × 0.41 × 0.29 mm

Data collection

Oxford Diffraction Gemini R diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.955, T_{max} = 1.000 (expected range = 0.929–0.973)
37695 measured reflections
4496 independent reflections
2661 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.162
S = 1.25
4496 reflections
363 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6*A*—H6*A*···O2*B*^{i}	0.94	2.56	3.144 (4)	120
C6*B*—H6*B*···O2*A*^{ii}	0.94	2.57	3.409 (4)	148
C7*B*—H7*D*···O3*B*^{iii}	0.97	2.48	3.361 (5)	151
C16*A*—H16*A*···O1*B*^{iv}	0.94	2.57	3.401 (4)	148

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

Data collection: *CrysAlisPro* (Oxford Diffraction, 2007); cell refinement: *CrysAlisPro*; data reduction: *CrysAlisPro*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2427).

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supplementary materials

Acta Cryst. (2007). E**63**, o3680 [**doi:10.1107/S1600536807037063**]

(2*E*)-1-(4-Methylphenyl)-3-(4-nitrophenyl)prop-2-en-1-one

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Comment

Chalcone is an aromatic ketone that forms a central core for a variety of important biological compounds, which are known collectively as chalcones. Chalcones and the corresponding heterocyclic analogs are valuable intermediates in organic synthesis and show numerous biological effects. The non-linear optical (NLO) effects in organic molecules originates from a strong donor–acceptor intermolecular interaction, a delocalized π electron system and also the ability to crystallize in non-centro symmetric space groups. Chalcones are finding applications as organic non-linear optical materials due to their good SHG conversion efficiencies. Herein we report the synthesis and crystal structure of a new chalcone, the title compound.

The asymmetric unit of the title compound contains two independent molecules A and B both of which are shown in Fig. 1. The C9—C8—C1—C6 and C9—C10—C11—C12 torsion angles [(A) −0.8 (5), 6.4 (5)°; (B) 5.2 (4), −8.2 (5)°] indicate that the 4-methylphenyl and 4-nitrophenyl groups are slightly twisted with respect to the central O1/C8—C11 plane.

In the crystal structure, the independent molecues exist as a pseudo inversion-related pair with the centroids of the 4-methylphenyl and 4-nitrophenyl rings separated by a distance of 3.7550 (17) Å, indicating π-π stacking interaction. Crystal packing shows each of these independent molecules form sheets approximately parallel to the *ab* plane (Fig. 2). The sheets formed by these molecules are alternatively stacked along the *c* axis and are cross-linked by C—H···O intermolecular hydrogen-bonding interactions (Table 1).

Experimental

4-Nitrobenzaldehyde (1.81 g, 0.01 mol) in ethanol (50 ml) was mixed with 1-(4-methyl phenyl) ethanone (1.34 ml, 0.01 mol) and the mixture was treated with 10 ml of 10% KOH. The reaction mixture was then kept for constant stirring. The solid precipitate obtained was filtered, washed with ethanol and dried. The crystal growth was carried out in acetone solvent by the slow evaporation technique (m.p. 435 K). Analysis found: C 71.78, H 4.83, N 5.18%; $C_{16}H_{13}NO_3$ requires: C 71.90, H 4.90, N 5.24%.

Refinement

All H atoms were refined using a riding model with C—H = 0.94–0.97 Å, and U_{iso}(H) = 1.18–1.50U_{eq}(C). In the absence of significant anomalous scattering effects, Friedel pairs were averaged.

Figures

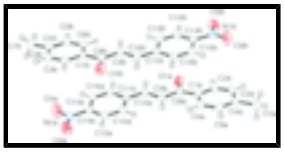

Fig. 1. A view of the two independent molecules (A and B) forming the asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

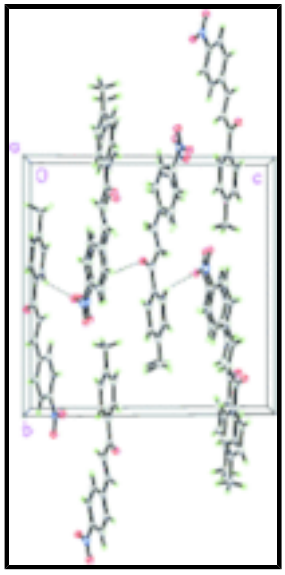

Fig. 2. The crystal packing of the title compound, viewed down the *a* axis. Dashed lines indicate C—H···O hydrogen bonds.

(2E)-1-(4-Methylphenyl)-3-(4-nitrophenyl)prop-2-en-1-one

Crystal data

$C_{16}H_{13}NO_3$	F_{000} = 560
M_r = 267.27	D_x = 1.350 Mg m^{-3}
Monoclinic, *Pc*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P -2yc	Cell parameters from 10389 reflections
a = 5.97300 (1) Å	θ = 4.6–32.4º
b = 15.0731 (5) Å	μ = 0.09 mm^{-1}
c = 14.6768 (4) Å	*T* = 203 K
β = 95.785 (2)º	Block, colourless
V = 1314.65 (6) Å^3	0.47 × 0.41 × 0.29 mm
Z = 4	

Data collection

Oxford Diffraction Gemini R diffractometer	4496 independent reflections
Radiation source: fine-focus sealed tube	2661 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.051
T = 203 K	θ_{max} = 32.5º
φ and ω scans	θ_{min} = 4.6º
Absorption correction: multi-scan (CrysAlisRED; Oxford Diffraction, 2007)	*h* = −8→9
T_{min} = 0.955, T_{max} = 1.000	*k* = −22→21
37695 measured reflections	*l* = −21→22

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.055$	$w = 1/[\sigma^2(F_o^2) + (0.0728P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.162$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.25$	$\Delta\rho_{max} = 0.23$ e Å^{-3}
4496 reflections	$\Delta\rho_{min} = -0.23$ e Å^{-3}
363 parameters	Extinction correction: none
2 restraints	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'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}
O1A	0.5810 (4)	0.15276 (19)	0.3609 (2)	0.0598 (7)
O2A	−0.5435 (4)	0.5503 (2)	0.1891 (2)	0.0638 (7)
O3A	−0.2876 (5)	0.6415 (2)	0.2422 (2)	0.0717 (9)
N1A	−0.3572 (5)	0.5665 (2)	0.22697 (19)	0.0434 (7)
C1A	0.3401 (6)	0.0319 (3)	0.3272 (2)	0.0377 (7)
C2A	0.5097 (5)	−0.0293 (3)	0.3529 (2)	0.0434 (8)
H2A	0.6549	−0.0089	0.3732	0.052*
C3A	0.4681 (6)	−0.1196 (3)	0.3492 (3)	0.0501 (9)
H3A	0.5850	−0.1594	0.3676	0.060*
C4A	0.2560 (5)	−0.1524 (2)	0.3185 (2)	0.0406 (8)
C5A	0.0874 (6)	−0.0926 (3)	0.2929 (2)	0.0452 (9)
H5A	−0.0568	−0.1136	0.2718	0.054*
C6A	0.1261 (5)	−0.0018 (2)	0.2977 (2)	0.0431 (8)
H6A	0.0072	0.0376	0.2809	0.052*
C7A	0.2110 (7)	−0.2512 (3)	0.3134 (3)	0.0546 (9)
H7A	0.0911	−0.2631	0.2654	0.082*

H7B	0.1665	−0.2717	0.3716	0.082*
H7C	0.3464	−0.2820	0.3001	0.082*
C8A	0.3919 (5)	0.1278 (2)	0.3334 (2)	0.0394 (7)
C9A	0.2096 (5)	0.1932 (3)	0.3060 (2)	0.0403 (8)
H9A	0.0735	0.1738	0.2746	0.048*
C10A	0.2392 (5)	0.2787 (2)	0.3258 (2)	0.0382 (7)
H10A	0.3773	0.2948	0.3579	0.046*
C11A	0.0756 (5)	0.3511 (2)	0.30221 (19)	0.0349 (7)
C12A	−0.1442 (5)	0.3358 (2)	0.2625 (2)	0.0400 (7)
H12A	−0.1949	0.2772	0.2523	0.048*
C13A	−0.2877 (5)	0.4058 (3)	0.2381 (2)	0.0408 (8)
H13A	−0.4348	0.3957	0.2110	0.049*
C14A	−0.2081 (5)	0.4915 (2)	0.2549 (2)	0.0371 (7)
C15A	0.0033 (5)	0.5092 (2)	0.2955 (2)	0.0407 (7)
H15A	0.0516	0.5679	0.3069	0.049*
C16A	0.1458 (5)	0.4373 (2)	0.3197 (2)	0.0404 (7)
H16A	0.2914	0.4479	0.3482	0.048*
O1B	−0.3940 (4)	0.40110 (19)	0.4712 (2)	0.0581 (7)
O2B	0.7162 (4)	−0.0017 (2)	0.6455 (2)	0.0614 (8)
O3B	0.4447 (5)	−0.0907 (2)	0.6053 (2)	0.0647 (8)
N1B	0.5230 (5)	−0.0162 (2)	0.61432 (18)	0.0430 (7)
C1B	−0.1587 (5)	0.5225 (2)	0.51618 (18)	0.0326 (6)
C2B	−0.3283 (6)	0.5826 (3)	0.4924 (2)	0.0404 (8)
H2B	−0.4714	0.5618	0.4695	0.048*
C3B	−0.2924 (5)	0.6731 (2)	0.5014 (2)	0.0444 (8)
H3B	−0.4124	0.7125	0.4862	0.053*
C4B	−0.0826 (5)	0.7064 (3)	0.5323 (2)	0.0399 (8)
C5B	0.0894 (5)	0.6454 (2)	0.5563 (2)	0.0416 (7)
H5B	0.2329	0.6662	0.5786	0.050*
C6B	0.0532 (5)	0.5552 (3)	0.5479 (2)	0.0391 (8)
H6B	0.1723	0.5155	0.5638	0.047*
C7B	−0.0428 (6)	0.8042 (3)	0.5426 (3)	0.0533 (9)
H7D	0.1068	0.8146	0.5730	0.080*
H7E	−0.1538	0.8296	0.5789	0.080*
H7F	−0.0557	0.8319	0.4826	0.080*
C8B	−0.2056 (5)	0.4258 (3)	0.5051 (2)	0.0378 (8)
C9B	−0.0307 (5)	0.3598 (3)	0.5351 (2)	0.0411 (8)
H9B	0.1033	0.3785	0.5688	0.049*
C10B	−0.0609 (5)	0.2744 (2)	0.5152 (2)	0.0375 (7)
H10B	−0.1970	0.2588	0.4812	0.045*
C11B	0.0964 (5)	0.2023 (2)	0.54079 (19)	0.0353 (7)
C12B	0.3171 (5)	0.2161 (2)	0.5814 (2)	0.0416 (8)
H12B	0.3699	0.2743	0.5926	0.050*
C13B	0.4571 (5)	0.1451 (2)	0.6050 (2)	0.0407 (7)
H13B	0.6043	0.1546	0.6324	0.049*
C14B	0.3778 (5)	0.0600 (2)	0.5879 (2)	0.0358 (7)
C15B	0.1615 (5)	0.0439 (3)	0.5465 (2)	0.0422 (8)
H15B	0.1097	−0.0143	0.5351	0.051*
C16B	0.0267 (5)	0.1153 (2)	0.5227 (2)	0.0399 (7)

H16B	−0.1182	0.1053	0.4932	0.048*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.0407 (13)	0.0393 (16)	0.0947 (19)	−0.0026 (11)	−0.0155 (12)	−0.0039 (13)
O2A	0.0416 (15)	0.062 (2)	0.0841 (18)	0.0046 (12)	−0.0106 (12)	0.0084 (15)
O3A	0.0562 (16)	0.0420 (18)	0.112 (2)	0.0054 (14)	−0.0137 (15)	0.0037 (17)
N1A	0.0383 (15)	0.0412 (19)	0.0508 (15)	0.0056 (13)	0.0050 (12)	0.0063 (13)
C1A	0.0336 (16)	0.039 (2)	0.0403 (15)	−0.0015 (14)	0.0033 (12)	−0.0021 (14)
C2A	0.0300 (16)	0.039 (2)	0.0592 (19)	0.0030 (14)	−0.0058 (13)	−0.0014 (16)
C3A	0.0412 (19)	0.043 (2)	0.064 (2)	0.0060 (17)	−0.0044 (15)	0.0048 (18)
C4A	0.0415 (18)	0.035 (2)	0.0452 (16)	0.0005 (14)	0.0045 (13)	0.0006 (13)
C5A	0.0380 (18)	0.041 (2)	0.0547 (18)	−0.0036 (16)	−0.0031 (14)	−0.0006 (17)
C6A	0.0342 (17)	0.035 (2)	0.0581 (19)	0.0046 (14)	−0.0037 (13)	−0.0031 (15)
C7A	0.063 (2)	0.037 (2)	0.064 (2)	−0.0034 (19)	0.0048 (17)	0.0001 (17)
C8A	0.0384 (16)	0.0322 (19)	0.0460 (16)	0.0023 (14)	−0.0042 (12)	0.0004 (13)
C9A	0.0396 (18)	0.033 (2)	0.0454 (17)	−0.0021 (15)	−0.0077 (13)	−0.0009 (14)
C10A	0.0397 (16)	0.0355 (19)	0.0385 (14)	0.0016 (14)	−0.0003 (11)	−0.0018 (13)
C11A	0.0342 (16)	0.0344 (19)	0.0361 (14)	0.0011 (13)	0.0035 (11)	0.0015 (13)
C12A	0.0357 (16)	0.036 (2)	0.0477 (16)	−0.0062 (14)	0.0012 (12)	−0.0008 (14)
C13A	0.0304 (16)	0.043 (2)	0.0489 (17)	−0.0010 (15)	0.0036 (13)	−0.0004 (15)
C14A	0.0365 (17)	0.036 (2)	0.0387 (15)	0.0028 (14)	0.0059 (12)	0.0025 (12)
C15A	0.0383 (17)	0.0344 (19)	0.0497 (17)	−0.0026 (14)	0.0053 (13)	0.0016 (14)
C16A	0.0380 (16)	0.039 (2)	0.0434 (15)	−0.0029 (14)	−0.0007 (12)	−0.0038 (14)
O1B	0.0446 (14)	0.0446 (16)	0.0805 (17)	−0.0035 (11)	−0.0155 (11)	−0.0055 (13)
O2B	0.0337 (14)	0.059 (2)	0.0889 (18)	0.0037 (11)	−0.0074 (12)	0.0012 (15)
O3B	0.0501 (15)	0.0375 (17)	0.103 (2)	0.0023 (13)	−0.0084 (14)	0.0014 (15)
N1B	0.0379 (16)	0.0441 (19)	0.0466 (14)	0.0029 (13)	0.0023 (11)	0.0020 (13)
C1B	0.0334 (15)	0.0319 (18)	0.0324 (13)	0.0010 (12)	0.0033 (11)	0.0017 (11)
C2B	0.0330 (16)	0.040 (2)	0.0464 (16)	−0.0027 (14)	−0.0040 (12)	0.0011 (15)
C3B	0.0374 (17)	0.039 (2)	0.0555 (18)	0.0049 (14)	−0.0016 (13)	0.0005 (15)
C4B	0.0392 (17)	0.038 (2)	0.0431 (16)	−0.0012 (14)	0.0075 (13)	0.0024 (14)
C5B	0.0294 (15)	0.044 (2)	0.0506 (17)	0.0007 (14)	−0.0016 (12)	−0.0020 (15)
C6B	0.0310 (16)	0.039 (2)	0.0463 (17)	−0.0012 (14)	0.0000 (12)	−0.0025 (15)
C7B	0.051 (2)	0.034 (2)	0.074 (2)	−0.0020 (17)	0.0044 (16)	−0.0014 (17)
C8B	0.0429 (18)	0.036 (2)	0.0335 (14)	−0.0028 (14)	−0.0014 (12)	−0.0014 (13)
C9B	0.0372 (17)	0.040 (2)	0.0441 (16)	0.0010 (14)	−0.0043 (12)	−0.0034 (14)
C10B	0.0359 (16)	0.036 (2)	0.0399 (15)	−0.0008 (14)	0.0022 (12)	0.0054 (14)
C11B	0.0387 (16)	0.0319 (18)	0.0354 (14)	0.0000 (13)	0.0040 (11)	0.0009 (12)
C12B	0.0387 (17)	0.0340 (18)	0.0518 (18)	−0.0049 (14)	0.0035 (13)	−0.0021 (14)
C13B	0.0352 (16)	0.041 (2)	0.0452 (16)	−0.0061 (14)	−0.0004 (12)	−0.0043 (14)
C14B	0.0323 (16)	0.0385 (19)	0.0364 (14)	0.0010 (14)	0.0022 (12)	0.0000 (13)
C15B	0.0373 (18)	0.037 (2)	0.0509 (18)	−0.0033 (14)	−0.0028 (13)	−0.0052 (15)
C16B	0.0334 (16)	0.037 (2)	0.0480 (16)	−0.0073 (14)	−0.0030 (12)	−0.0027 (14)

Geometric parameters (Å, °)

O1A—C8A	1.220 (4)	O1B—C8B	1.240 (4)

O2A—N1A	1.218 (4)	O2B—N1B	1.217 (4)
O3A—N1A	1.217 (4)	O3B—N1B	1.219 (4)
N1A—C14A	1.472 (4)	N1B—C14B	1.468 (5)
C1A—C2A	1.394 (5)	C1B—C2B	1.378 (5)
C1A—C6A	1.403 (5)	C1B—C6B	1.394 (5)
C1A—C8A	1.479 (5)	C1B—C8B	1.490 (5)
C2A—C3A	1.383 (5)	C2B—C3B	1.385 (5)
C2A—H2A	0.94	C2B—H2B	0.94
C3A—C4A	1.392 (5)	C3B—C4B	1.384 (5)
C3A—H3A	0.94	C3B—H3B	0.94
C4A—C5A	1.376 (5)	C4B—C5B	1.397 (5)
C4A—C7A	1.513 (5)	C4B—C7B	1.499 (5)
C5A—C6A	1.388 (5)	C5B—C6B	1.380 (5)
C5A—H5A	0.94	C5B—H5B	0.94
C6A—H6A	0.94	C6B—H6B	0.94
C7A—H7A	0.97	C7B—H7D	0.97
C7A—H7B	0.97	C7B—H7E	0.97
C7A—H7C	0.97	C7B—H7F	0.97
C8A—C9A	1.494 (5)	C8B—C9B	1.476 (5)
C9A—C10A	1.328 (5)	C9B—C10B	1.329 (5)
C9A—H9A	0.94	C9B—H9B	0.94
C10A—C11A	1.482 (5)	C10B—C11B	1.461 (5)
C10A—H10A	0.94	C10B—H10B	0.94
C11A—C16A	1.382 (5)	C11B—C16B	1.394 (5)
C11A—C12A	1.401 (4)	C11B—C12B	1.407 (5)
C12A—C13A	1.384 (5)	C12B—C13B	1.380 (5)
C12A—H12A	0.94	C12B—H12B	0.94
C13A—C14A	1.390 (5)	C13B—C14B	1.381 (5)
C13A—H13A	0.94	C13B—H13B	0.94
C14A—C15A	1.367 (5)	C14B—C15B	1.393 (5)
C15A—C16A	1.401 (5)	C15B—C16B	1.367 (5)
C15A—H15A	0.94	C15B—H15B	0.94
C16A—H16A	0.94	C16B—H16B	0.94
O2A—N1A—O3A	123.4 (3)	O2B—N1B—O3B	123.0 (3)
O2A—N1A—C14A	118.2 (3)	O2B—N1B—C14B	118.1 (3)
O3A—N1A—C14A	118.4 (3)	O3B—N1B—C14B	118.9 (3)
C2A—C1A—C6A	117.3 (3)	C2B—C1B—C6B	118.1 (3)
C2A—C1A—C8A	119.2 (3)	C2B—C1B—C8B	119.4 (3)
C6A—C1A—C8A	123.5 (3)	C6B—C1B—C8B	122.5 (3)
C3A—C2A—C1A	121.2 (3)	C1B—C2B—C3B	121.4 (3)
C3A—C2A—H2A	119.4	C1B—C2B—H2B	119.3
C1A—C2A—H2A	119.4	C3B—C2B—H2B	119.3
C2A—C3A—C4A	121.1 (3)	C2B—C3B—C4B	121.0 (3)
C2A—C3A—H3A	119.5	C2B—C3B—H3B	119.5
C4A—C3A—H3A	119.5	C4B—C3B—H3B	119.5
C5A—C4A—C3A	118.2 (3)	C3B—C4B—C5B	117.6 (3)
C5A—C4A—C7A	120.6 (3)	C3B—C4B—C7B	121.3 (3)
C3A—C4A—C7A	121.1 (3)	C5B—C4B—C7B	121.1 (3)
C4A—C5A—C6A	121.2 (3)	C6B—C5B—C4B	121.4 (3)

C4A—C5A—H5A	119.4	C6B—C5B—H5B	119.3
C6A—C5A—H5A	119.4	C4B—C5B—H5B	119.3
C5A—C6A—C1A	121.0 (3)	C5B—C6B—C1B	120.5 (3)
C5A—C6A—H6A	119.5	C5B—C6B—H6B	119.8
C1A—C6A—H6A	119.5	C1B—C6B—H6B	119.8
C4A—C7A—H7A	109.5	C4B—C7B—H7D	109.5
C4A—C7A—H7B	109.5	C4B—C7B—H7E	109.5
H7A—C7A—H7B	109.5	H7D—C7B—H7E	109.5
C4A—C7A—H7C	109.5	C4B—C7B—H7F	109.5
H7A—C7A—H7C	109.5	H7D—C7B—H7F	109.5
H7B—C7A—H7C	109.5	H7E—C7B—H7F	109.5
O1A—C8A—C1A	120.2 (3)	O1B—C8B—C9B	120.3 (3)
O1A—C8A—C9A	120.7 (3)	O1B—C8B—C1B	119.3 (3)
C1A—C8A—C9A	119.1 (3)	C9B—C8B—C1B	120.4 (3)
C10A—C9A—C8A	120.3 (3)	C10B—C9B—C8B	120.7 (3)
C10A—C9A—H9A	119.9	C10B—C9B—H9B	119.7
C8A—C9A—H9A	119.9	C8B—C9B—H9B	119.7
C9A—C10A—C11A	126.4 (3)	C9B—C10B—C11B	126.5 (3)
C9A—C10A—H10A	116.8	C9B—C10B—H10B	116.7
C11A—C10A—H10A	116.8	C11B—C10B—H10B	116.7
C16A—C11A—C12A	119.1 (3)	C16B—C11B—C12B	118.0 (3)
C16A—C11A—C10A	117.9 (3)	C16B—C11B—C10B	118.6 (3)
C12A—C11A—C10A	123.0 (3)	C12B—C11B—C10B	123.4 (3)
C13A—C12A—C11A	120.8 (3)	C13B—C12B—C11B	120.6 (3)
C13A—C12A—H12A	119.6	C13B—C12B—H12B	119.7
C11A—C12A—H12A	119.6	C11B—C12B—H12B	119.7
C12A—C13A—C14A	118.1 (3)	C14B—C13B—C12B	119.1 (3)
C12A—C13A—H13A	120.9	C14B—C13B—H13B	120.4
C14A—C13A—H13A	120.9	C12B—C13B—H13B	120.4
C15A—C14A—C13A	122.9 (3)	C13B—C14B—C15B	121.8 (3)
C15A—C14A—N1A	118.6 (3)	C13B—C14B—N1B	119.7 (3)
C13A—C14A—N1A	118.5 (3)	C15B—C14B—N1B	118.4 (3)
C14A—C15A—C16A	118.1 (3)	C16B—C15B—C14B	118.1 (3)
C14A—C15A—H15A	121.0	C16B—C15B—H15B	121.0
C16A—C15A—H15A	121.0	C14B—C15B—H15B	121.0
C11A—C16A—C15A	121.0 (3)	C15B—C16B—C11B	122.3 (3)
C11A—C16A—H16A	119.5	C15B—C16B—H16B	118.8
C15A—C16A—H16A	119.5	C11B—C16B—H16B	118.8
C6A—C1A—C2A—C3A	0.2 (5)	C6B—C1B—C2B—C3B	−1.4 (5)
C8A—C1A—C2A—C3A	179.3 (3)	C8B—C1B—C2B—C3B	−179.9 (3)
C1A—C2A—C3A—C4A	0.8 (5)	C1B—C2B—C3B—C4B	1.8 (5)
C2A—C3A—C4A—C5A	−0.7 (5)	C2B—C3B—C4B—C5B	−1.6 (5)
C2A—C3A—C4A—C7A	179.4 (3)	C2B—C3B—C4B—C7B	−179.7 (3)
C3A—C4A—C5A—C6A	−0.2 (5)	C3B—C4B—C5B—C6B	1.2 (5)
C7A—C4A—C5A—C6A	179.7 (3)	C7B—C4B—C5B—C6B	179.2 (3)
C4A—C5A—C6A—C1A	1.2 (5)	C4B—C5B—C6B—C1B	−0.9 (5)
C2A—C1A—C6A—C5A	−1.2 (5)	C2B—C1B—C6B—C5B	0.9 (5)
C8A—C1A—C6A—C5A	179.8 (3)	C8B—C1B—C6B—C5B	179.4 (3)
C2A—C1A—C8A—O1A	−0.1 (5)	C2B—C1B—C8B—O1B	2.9 (4)

C6A—C1A—C8A—O1A	179.0 (3)	C6B—C1B—C8B—O1B	−175.6 (3)
C2A—C1A—C8A—C9A	−179.8 (3)	C2B—C1B—C8B—C9B	−176.4 (3)
C6A—C1A—C8A—C9A	−0.8 (5)	C6B—C1B—C8B—C9B	5.2 (4)
O1A—C8A—C9A—C10A	−11.7 (5)	O1B—C8B—C9B—C10B	9.2 (5)
C1A—C8A—C9A—C10A	168.1 (3)	C1B—C8B—C9B—C10B	−171.5 (3)
C8A—C9A—C10A—C11A	179.2 (3)	C8B—C9B—C10B—C11B	−179.7 (3)
C9A—C10A—C11A—C16A	−173.0 (3)	C9B—C10B—C11B—C16B	173.0 (3)
C9A—C10A—C11A—C12A	6.4 (5)	C9B—C10B—C11B—C12B	−8.2 (5)
C16A—C11A—C12A—C13A	2.1 (4)	C16B—C11B—C12B—C13B	−1.9 (4)
C10A—C11A—C12A—C13A	−177.2 (3)	C10B—C11B—C12B—C13B	179.3 (3)
C11A—C12A—C13A—C14A	−0.5 (4)	C11B—C12B—C13B—C14B	0.2 (4)
C12A—C13A—C14A—C15A	−1.1 (5)	C12B—C13B—C14B—C15B	0.8 (5)
C12A—C13A—C14A—N1A	178.3 (3)	C12B—C13B—C14B—N1B	−178.7 (3)
O2A—N1A—C14A—C15A	178.5 (3)	O2B—N1B—C14B—C13B	−4.7 (4)
O3A—N1A—C14A—C15A	−1.0 (4)	O3B—N1B—C14B—C13B	174.3 (3)
O2A—N1A—C14A—C13A	−1.0 (4)	O2B—N1B—C14B—C15B	175.7 (3)
O3A—N1A—C14A—C13A	179.6 (3)	O3B—N1B—C14B—C15B	−5.3 (4)
C13A—C14A—C15A—C16A	1.1 (5)	C13B—C14B—C15B—C16B	−0.1 (5)
N1A—C14A—C15A—C16A	−178.3 (3)	N1B—C14B—C15B—C16B	179.5 (3)
C12A—C11A—C16A—C15A	−2.1 (4)	C14B—C15B—C16B—C11B	−1.7 (5)
C10A—C11A—C16A—C15A	177.3 (3)	C12B—C11B—C16B—C15B	2.7 (5)
C14A—C15A—C16A—C11A	0.6 (5)	C10B—C11B—C16B—C15B	−178.4 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6A—H6A···O2B^{i}	0.94	2.56	3.144 (4)	120
C6B—H6B···O2A^{ii}	0.94	2.57	3.409 (4)	148
C7B—H7D···O3B^{iii}	0.97	2.48	3.361 (5)	151
C16A—H16A···O1B^{iv}	0.94	2.57	3.401 (4)	148

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

Fig. 1

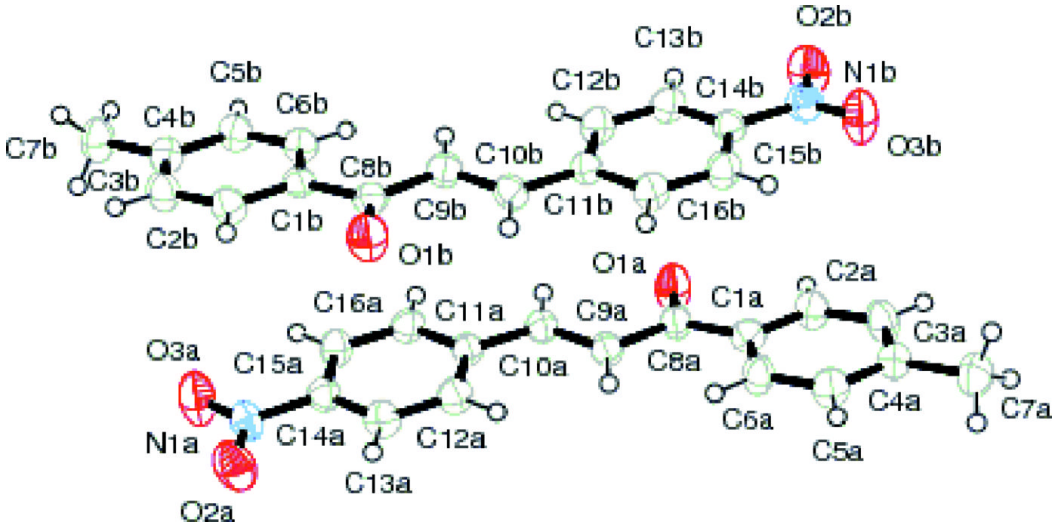
O2b
C13b
N1b
C12b
C14b
C5b
C6b
C4b
C7b
C15b
O3b
C3b
C8b
C10b
C1b
C9b
C11b
C16b
C2b
O1b
O1a
C2a
C16a
C11a
C9a
C1a
C3a
O3a
C15a
C10a
C8a
C4a
C7a
C6a
C14a
C12a
N1a
C5a
C13a
O2a

Fig. 2