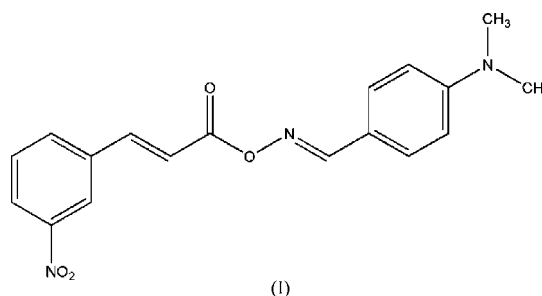


**(*E,E*)-4-(Dimethylamino)benzaldehyde
O-[3-(3-nitrophenyl)propenoyl]oxime**Shu-Ping Yang,^{a*} Li-Jun Han,^b
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yangshuping@hhit.edu.cn**Key indicators**Single-crystal X-ray study
T = 298 K
Mean $\sigma(\text{C}-\text{C}) = 0.007 \text{ \AA}$
R factor = 0.061
wR factor = 0.237
Data-to-parameter ratio = 12.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the title compound, $\text{C}_{18}\text{H}_{17}\text{N}_3\text{O}_4$, the molecule has a *trans* configuration; the dihedral angle between the benzene rings is $34.4(1)^\circ$. The molecules are linked into centrosymmetric dimers with edge-fused $[R_2^1(6)][R_2^2(10)][R_2^3(6)]$ rings by $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, and these dimers are linked by $\text{C}-\text{H}\cdots\text{O}$ weak interactions into a ribbon along [101]. Adjacent ribbons are linked into a three-dimensional network structure by $\pi-\pi$ stacking interactions.

Comment

Oxime ester derivatives have been shown to have a wide range of biological activities, including as herbicides (Koo *et al.*, 1997) and antitobacco mosaic virus agents (Yang *et al.*, 2005). We have recently reported the crystal structure of an oxime ester (Yang *et al.*, 2006). As part of our study of the molecular structures of oxime ester compounds, we report here the molecular structure of a new oxime ester, (I).



The molecule of (I) (Fig. 1), has a *trans* configuration, with the 4-dimethylaminophenyl and the 3-phenylpropenoyloxy groups located on opposite sides of the $\text{C}=\text{N}$ bond, and the 4-dimethylaminobenzaldehyde oxime and 3-nitrophenyl groups located on opposite sides of the $\text{C}=\text{C}$ bond. The dihedral angle between the benzene rings is $34.4(1)^\circ$. The $\text{O1}-\text{N1}$ distance agrees with the mean value for the $-\text{O}-\text{N}=\text{}$ distance in oximes (Allen *et al.*, 1987). Selected geometric parameters of compound (I) are shown in Table 1.

In the crystal structure of (I), the molecules are linked by $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds into centrosymmetric dimers with an array of three edge-fused $[R_2^1(6)][R_2^2(10)][R_2^3(6)]$ rings (Bernstein *et al.*, 1995), centered at $(\frac{1}{2}, \frac{1}{2}, 1)$. Atom O2 acts as a bifurcated acceptor, with atoms C3 and C9 both acting as hydrogen bond donors to atom O2 in the molecule at $(1-x, 1-y, 2-z)$. The resultant dimers are linked by further $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, forming ribbons in the [101] direction, alternating with $R_2^1(6)[R_2^2(10)R_2^3(14)]$ rings (García-Báez *et al.*, 2002) and $R_4^1(38)$ rings (Fig. 2 and Table 2). These ribbons are linked into a three-dimensional network structure by two $\pi-\pi$ stacking interactions [$\text{Cg1}\cdots\text{Cg2}^1 = 3.853 \text{ \AA}$ and $\text{Cg1}\cdots\text{Cg2}^{\text{ii}} =$

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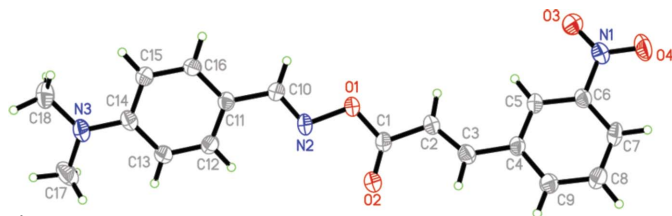


Figure 1
The molecular structure of compound (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level.

3.731 Å, where *Cg*1 is the center of ring C4–C9 and *Cg*2 is the center of ring C11–C16; symmetry codes: (i) $1 - x, -\frac{1}{2} + y, \frac{3}{2} - z$; (ii) $1 - x, \frac{1}{2} + y, \frac{3}{2} - z$] (Fig. 3).

Experimental

To a solution containing 4-dimethylaminobenzadehydroxime (1.64 g, 10 mmol) and anhydrous pyridine (10 ml), a solution of 3-(3-nitrophenyl)propenoyl chloride (2.11 g, 10 mmol) and anhydrous dichloromethane (10 ml) was slowly added over 30 min at 278–283 K with stirring. The reaction mixture was stirred continuously for 12 h at room temperature and then poured into ice water (200 ml). The solid obtained was filtered off, washed with water and dried at room temperature. Red crystals of (I) suitable for X-ray structure analysis were obtained by recrystallizing the crude product from ethanol (m.p. 453–455 K).

Crystal data

$C_{18}H_{17}N_3O_4$	$Z = 4$
$M_r = 339.35$	$D_x = 1.359 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 18.031 (12) \text{ \AA}$	$\mu = 0.10 \text{ mm}^{-1}$
$b = 7.332 (5) \text{ \AA}$	$T = 298 (2) \text{ K}$
$c = 12.714 (9) \text{ \AA}$	Block, red
$\beta = 99.338 (11)^\circ$	$0.46 \times 0.43 \times 0.25 \text{ mm}$
$V = 1659 (2) \text{ \AA}^3$	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	8286 measured reflections
φ and ω scans	2921 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1142 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.956, T_{\max} = 0.976$	$R_{\text{int}} = 0.069$
	$\theta_{\text{max}} = 25.0^\circ$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.061$	$w = 1/[\sigma^2(F_o^2) + 0.7102P]$
$wR(F^2) = 0.237$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2921 reflections	$\Delta\rho_{\text{max}} = 0.21 \text{ e \AA}^{-3}$
226 parameters	$\Delta\rho_{\text{min}} = -0.22 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

N2–C10	1.245 (6)	N2–O1	1.442 (5)
C10–N2–O1	110.3 (4)	C2–C3–C4	130.2 (5)
C3–C2–C1	119.7 (5)	N2–C10–C11	120.0 (5)
N2–O1–C1–C2	178.2 (4)	O1–N2–C10–C11	178.9 (4)
C1–C2–C3–C4	179.7 (5)		

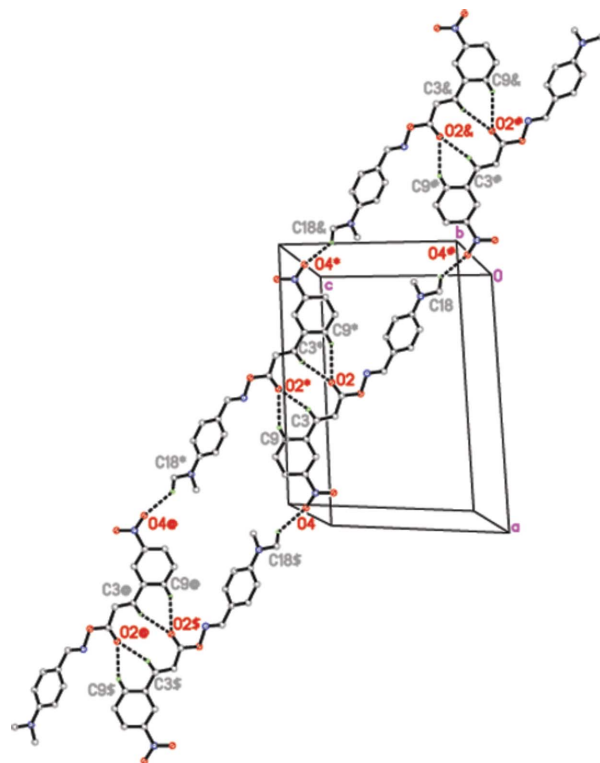


Figure 2

Part of the crystal structure of (I), showing the formation of a ribbon along the [101] direction. For the sake of clarity, H atoms not involved in the motif shown have been omitted [symmetry codes: (*) $-x + 1, -y + 1, -z + 2$; (#) $x - 1, y, z - 1$; (&) $-x, 1 - y, 1 - z$; (\$) $1 + x, y, 1 + z$; (@) $2 - x, 1 - y, 3 - z$]. Dashed lines indicate hydrogen bonds.

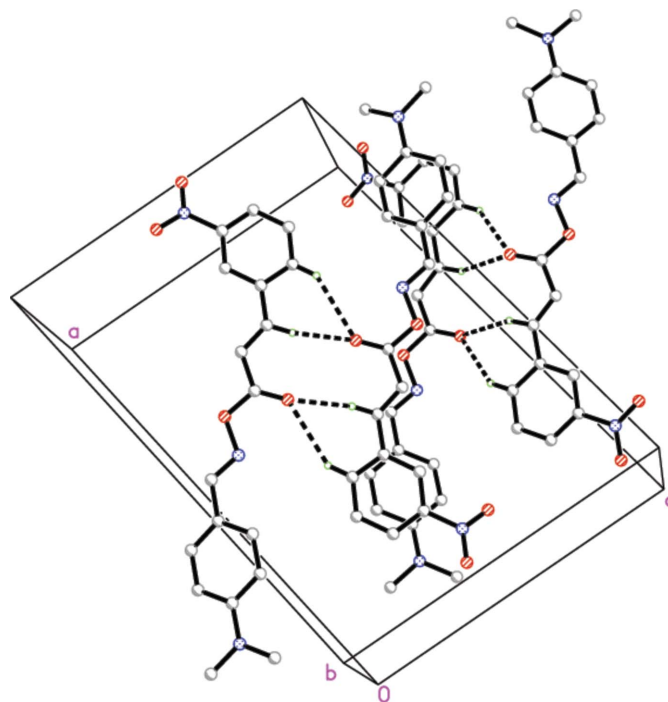


Figure 3

Part of the crystal structure of (I), showing adjacent ribbons linked by weak π – π interactions. For the sake of clarity, H atoms not involved in the motif shown have been omitted. Dashed lines indicate hydrogen bonds.

Table 2
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C18—H18B \cdots O4 ⁱ	0.96	2.65	3.340 (7)	129
C3—H3 \cdots O2 ⁱⁱ	0.93	2.51	3.341 (7)	149
C9—H9 \cdots O2 ⁱⁱ	0.93	2.67	3.481 (6)	146

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

All H atoms were positioned geometrically and refined as riding on their parent atoms, with C—H = 0.96 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms, and C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for all other H atoms.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

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