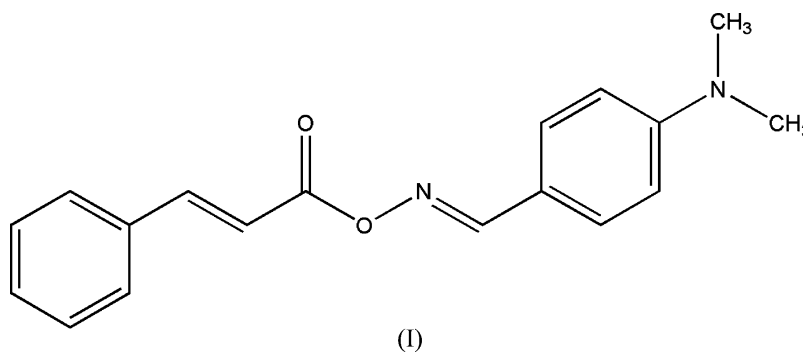


**(*E,E*)-4-(Dimethylamino)benzaldehyde
O-(3-phenylpropenoyl)oxime**Shu-Ping Yang,^{a*} Li-Jun Han,^b
Da-Qi Wang^c and Hai-Tao Xia^a^aDepartment of Chemical Engineering, Huaihai Institute of Technology, Lianyungang 222005, People's Republic of China, ^bDepartment of Mathematics and Science, Huaihai Institute of Technology, Lianyungang 222005, People's Republic of China, and ^cCollege of Chemistry and Chemical Engineering, Liaocheng University, Shandong 252059, People's Republic of ChinaCorrespondence e-mail:
yangshuping@hhit.edu.cn**Key indicators**Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$
 R factor = 0.055
 wR factor = 0.143
Data-to-parameter ratio = 14.0For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the title compound, $\text{C}_{18}\text{H}_{18}\text{N}_2\text{O}_2$, the molecules are linked into a chain of $R_2^1(6)$ rings by weak intermolecular $\text{C}-\text{H}\cdots\text{O}$ interactions; these chains are linked by $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{N}$ weak interactions, resulting in the formation of a three-dimensional network.

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Oxime ester derivatives exhibit a large number of biological activities, such as herbicidal (Suk *et al.*, 1997) and anti-TMV activity (Yang *et al.*, 2005; Ma *et al.*, 1999). The crystal structures of various oxime ester derivatives (Brito-Arias *et al.*, 2004; Ohba *et al.*, 2005) have been described. We report here the molecular structure of a new oxime ester, (*E,E*)-4-dimethylaminobenzaldehyde *O*-(3-phenylpropenoyl)oxime, (I).



In the molecule of (I) (Fig. 1), the 4-dimethylaminobenzaldehyde and 3-phenylpropenoyloxy groups are situated on opposite sides of the $\text{C}=\text{N}$ bond, and the 4-dimethylaminobenzaldehyde oxime and phenyl groups are situated on opposite sides of the $\text{C}=\text{C}$ bond, resulting in a *trans* configuration (*E,E*). The dihedral angle between the benzene rings is $34.83(5)^\circ$. The $\text{O1}-\text{N1}$ bond length corresponds with the mean value for the $-\text{O}-\text{N}=\text{}$ distance in oximes (Allen *et al.*, 1987). All other distances are also typical of their types (Table 1).

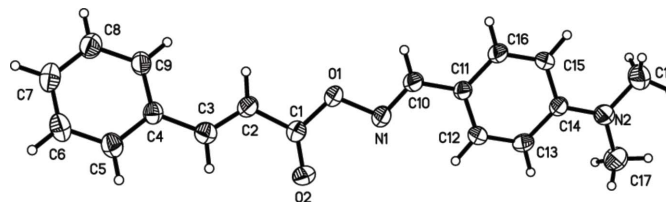


Figure 1
The molecular structure of compound (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

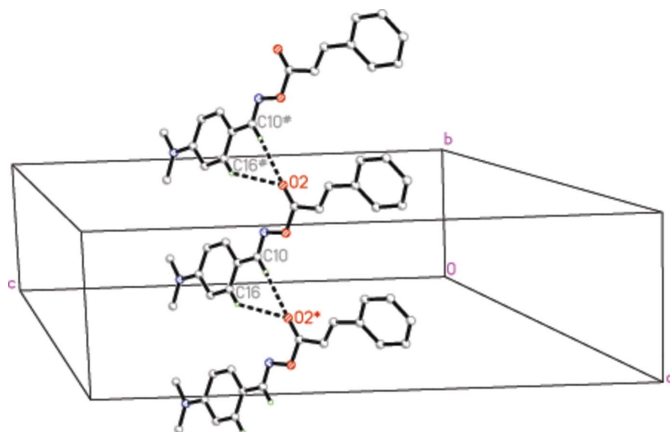


Figure 2
Part of the crystal structure of (I), showing the formation of a $C(6)C(8)[R_2^1(6)]$ chain of rings along b axis. For the sake of clarity, H atoms not involved in the motif shown have been omitted. [Symmetry codes: (*) $x, 1 + y, z$; (#) $x, -1 + y, z$.] Dashed lines indicate hydrogen bonds.

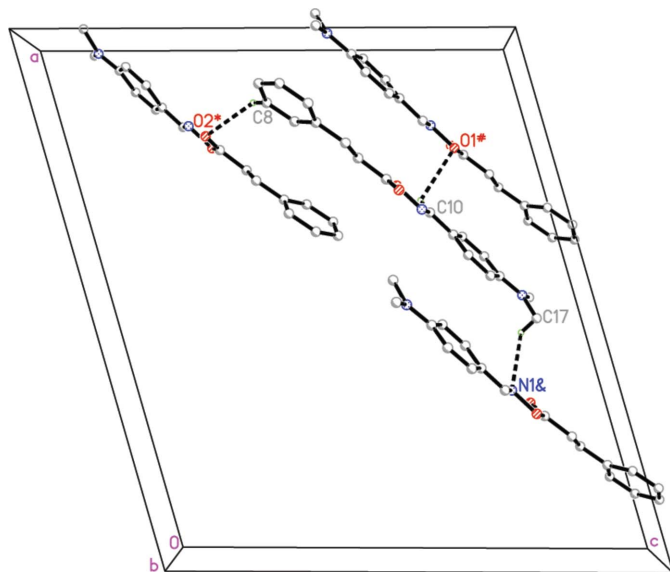


Figure 3
Part of the crystal structure of (I), viewed down the b axis, showing molecular chains linked by two weak $C-H \cdots O$ and one $C-H \cdots N$ interactions [symmetry codes: (*) $\frac{1}{2} - x, -\frac{1}{2} + y, \frac{1}{2} - z$; (#) $\frac{1}{2} - x, \frac{3}{2} - y, 1 - z$, (&) $-x, 2 - y, 1 - z$]. Dashed lines indicate hydrogen bonds.

In the crystal structure of (I), molecules are linked into a $C(6)C(8)[R_2^1(6)]$ chain of rings (Bernstein *et al.*, 1995) along the b axis through two weak intermolecular $C-H \cdots O$ interactions ($C10-H10 \cdots O2^{ii}$ and $C16-H16 \cdots O2^{ii}$; Fig. 2 and Table 2). Atom O2 acts as a bifurcated acceptor, and atoms C10 and C16 in the molecule at (x, y, z) act as hydrazone-bond donors to atom O2 in the molecule at $(x, -1 + y, z)$. Neighboring chains of molecules are connected by two $C-H \cdots O$ [$C8-H8 \cdots O2^{i}$ and $C10-H10 \cdots O1^{ii}$; symmetry codes: (i) $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$; (ii) $-x + \frac{1}{2}, -y + \frac{3}{2}, -z + 1$], and one $C-H \cdots N$ [$C17-H17 \cdots N1^{iv}$; symmetry code: (iv) $-x, -y + 2, -z + 1$] weak intermolecular interactions (Fig. 3 and Table 2), resulting in a three-dimensional network structure (Fig. 4).

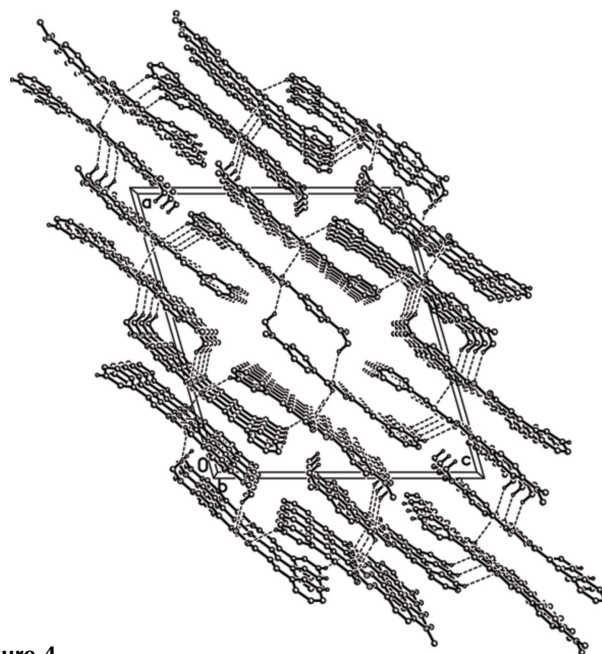


Figure 4
The packing of (I), viewed down the b axis. Dashed lines indicate hydrogen bonds.

Experimental

To a solution containing 4-(dimethylamino)benzadehydroxime (1.60 g, 10 mmol) and anhydrous pyridine (10 ml), a solution of 3-phenylpropenoyl chloride (1.75 g, 10 mmol) and anhydrous chloroform (10 ml) was slowly added at 278–283 K with stirring for 30 min. The reaction mixture was stirred continuously for 12 h at room temperature and then poured into ice–water (200 ml). The resulting solid was filtered, washed with water and dried at room temperature. Yellow crystals of (I) suitable for X-ray structure analysis were obtained by recrystallizing the crude product from ethanol (m.p. 415–416 K).

Crystal data

$C_{18}H_{18}N_2O_2$

$M_r = 294.34$

Monoclinic, $C2/c$

$a = 23.88$ (2) Å

$b = 6.406$ (6) Å

$c = 21.41$ (2) Å

$\beta = 106.092$ (14)°

$V = 3147$ (5) Å³

$Z = 8$

$D_x = 1.242$ Mg m⁻³

Mo $K\alpha$ radiation

$\mu = 0.08$ mm⁻¹

$T = 298$ (2) K

Plate, yellow

$0.58 \times 0.31 \times 0.09$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.954$, $T_{\max} = 0.993$

7760 measured reflections

2781 independent reflections

1160 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.070$

$\theta_{\max} = 25.0^\circ$

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.055$

$wR(F^2) = 0.143$

$S = 1.00$

2781 reflections

199 parameters

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0457P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.17$ e Å⁻³

$\Delta\rho_{\min} = -0.22$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

N1—C10	1.266 (4)	N1—O1	1.453 (3)
C10—N1—O1	108.7 (3)	C1—O1—N1	113.5 (2)
C10—N1—O1—C1	−178.2 (3)	N1—O1—C1—C2	−172.9 (2)
N1—O1—C1—O2	7.3 (5)		

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C8—H8...O2 ⁱ	0.93	3.12	3.961 (5)	151
C10—H10...O1 ⁱⁱ	0.93	3.14	3.737 (5)	123
C10—H10...O2 ⁱⁱⁱ	0.93	2.46	3.275 (5)	147
C16—H16...O2 ⁱⁱⁱ	0.93	2.78	3.530 (4)	139
C17—H17C...N1 ^{iv}	0.96	3.01	3.817 (5)	142

Symmetry codes: (i) $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$; (ii) $-x + \frac{1}{2}, -y + \frac{3}{2}, -z + 1$; (iii) $x, y - 1, z$; (iv) $-x, -y + 2, -z + 1$.

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