

Centrosymmetric π -stacked dimers in
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Key indicators

Single-crystal X-ray study

T = 120 K

Mean $\sigma(\text{C}–\text{C}) = 0.002 \text{ \AA}$

R factor = 0.055

wR factor = 0.126

Data-to-parameter ratio = 15.0

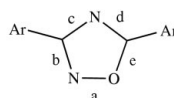
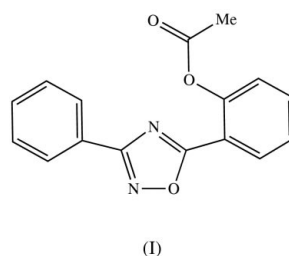
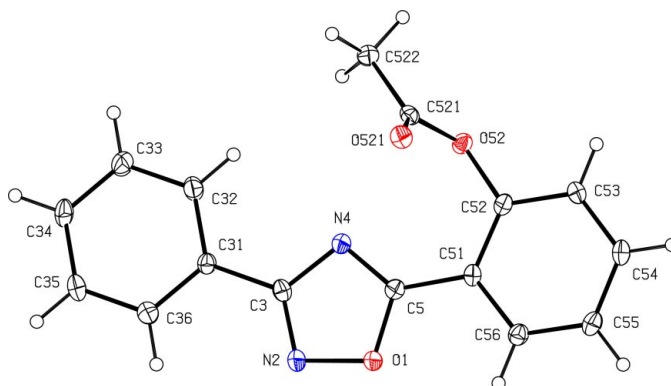
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.In molecules of the title compound, $\text{C}_{16}\text{H}_{12}\text{N}_2\text{O}_3$, the three independent rings are nearly coplanar; the molecules are linked into centrosymmetric dimers by a π – π stacking interaction.

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Comment

The title compound, (I), was prepared as part of a study of the fluorescence spectra of 5-(2-ROC₆H₄)-3-phenyl-1,2,4-oxadiazole compounds in solution (Brinn *et al.*, 1991). The structure was determined in order to ascertain the intermolecular interactions present in the solid state.Within the molecule of (I) (Fig. 1), the bond distances in the heterocyclic ring (Table 1) are very similar to those observed in other simply substituted 1,2,4-oxadiazoles (Viterbo *et al.*, 1980; Pfoertner & Daly, 1987; Wilkins *et al.*, 1987; Ebersson *et*

al., 1994; Bokach *et al.*, 2003), while the bond angles in this ring show considerable variation about the mean value of 108° expected for a regular planar pentagon. The bond distances in the heterocyclic ring are suggestive of considerable bond fixation, and this can be explored in more detail by means of the corresponding bond orders calculated using the recent recalibration by Kotelevskii & Prezhdo (2001) of the original equation relating bond order to bond length (Gordy, 1947). For the bonds marked *a–e* (see scheme), the bond orders calculated in this way are 1.149, 1.883, 1.445, 1.889 and 1.296, respectively, indicative of a modest degree of heteroaromatic delocalization, but with the heterodiene form dominant. With the exception of the acetyloxy substituent, the molecule is almost planar; the dihedral angles made by the aryl rings C31–C36 and C51–C56 with the heterocyclic ring are $5.9(2)$ and $2.5(2)^\circ$, respectively.

While there are no hydrogen bonds of the C–H...O, C–H...N or C–H... π (arene) types within the structure, the molecules are, however, weakly linked into centrosymmetric dimers by a single π – π stacking interaction. The heterocyclic ring of the molecule at (*x*, *y*, *z*) and the substituted aryl ring C51–C56 of the molecule at ($1-x$, $1-y$, $1-z$) are almost parallel, as noted above; the centroid separation is $3.583(2)$ Å and the interplanar spacing is *ca* 3.25 Å, corresponding to a centroid offset of *ca* 1.51 Å (Fig. 2). The unsubstituted aryl ring C31–C36, although unencumbered by any other substituent, does not participate in the supramolecular aggregation.

Experimental

Compound (I) was synthesized according to a published procedure (Brinn *et al.*, 1991).

Crystal data

$C_{16}H_{12}N_2O_3$	$D_x = 1.418 \text{ Mg m}^{-3}$
$M_r = 280.28$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 2875 reflections
$a = 14.5489(8) \text{ \AA}$	$\theta = 3.3\text{--}27.5^\circ$
$b = 5.4293(3) \text{ \AA}$	$\mu = 0.10 \text{ mm}^{-1}$
$c = 17.2806(13) \text{ \AA}$	$T = 120(2) \text{ K}$
$\beta = 105.955(2)^\circ$	Plate, colourless
$V = 1312.42(14) \text{ \AA}^3$	$0.20 \times 0.08 \times 0.01 \text{ mm}$
$Z = 4$	

Data collection

Nonius KappaCCD diffractometer	2875 independent reflections
φ scans, and ω scans with κ offsets	1649 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (DENZO-SMN; Otwinowski & Minor, 1997)	$R_{\text{int}} = 0.115$
$T_{\text{min}} = 0.951$, $T_{\text{max}} = 0.999$	$\theta_{\text{max}} = 27.5^\circ$
8160 measured reflections	$h = -16 \rightarrow 18$
	$k = -6 \rightarrow 5$
	$l = -18 \rightarrow 22$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0465P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.055$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.126$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 0.97$	$\Delta\rho_{\text{max}} = 0.26 \text{ e \AA}^{-3}$
2875 reflections	$\Delta\rho_{\text{min}} = -0.27 \text{ e \AA}^{-3}$
192 parameters	Extinction correction: SHELXL97
H-atom parameters constrained	Extinction coefficient: 0.016(3)

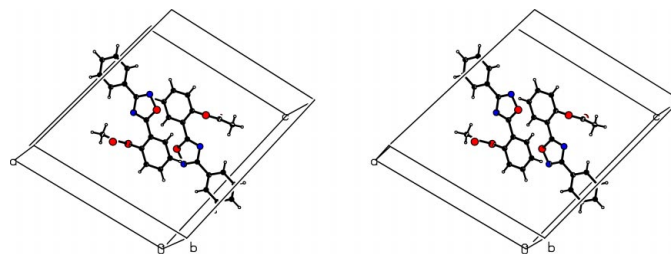


Figure 2

Stereoview of part of the crystal structure of (I), showing formation of a centrosymmetric π -stacked dimer.

Table 1

Selected geometric parameters (Å, °).

O1–N2	1.415(2)	N4–C5	1.302(2)
N2–C3	1.303(3)	C5–O1	1.351(2)
C3–N4	1.379(3)		
C5–O1–N2	106.44(12)	C3–N4–C5	102.65(14)
O1–N2–C3	103.13(15)	N4–C5–O1	112.81(11)
N2–C3–N4	114.97(18)		

All H atoms were located in difference maps and then treated as riding atoms with C–H distances of 0.95 (aromatic) and 0.98 Å (methyl). The $U_{\text{iso}}(\text{H})$ values were constrained to be $1.2U_{\text{eq}}(\text{C})$ for aromatic H and $1.5U_{\text{eq}}(\text{C})$ for methyl H atoms.

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC X-ray Crystallographic Service, University of Southampton, England. The authors thank the staff for all their help and advice. JNL thanks NCR Self-Service, Dundee, for grants which have provided computing facilities for this work.

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