

2,6-Bis(4,6-dimethoxypyrimidin-2-yloxy)-
benzoic acidDeepak Chopra,^{a*} T.P. Mohan,^b
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Key indicators

Single-crystal X-ray study
 $T = 290\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.065
 wR factor = 0.158
Data-to-parameter ratio = 13.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.The title compound, $\text{C}_{19}\text{H}_{18}\text{N}_4\text{O}_8$, belonging to the pyrimidin-
yloxybenzoic acid family, exhibits herbicidal properties. The
crystal structure is stabilized by $\text{C}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{N}$
intermolecular hydrogen bonds.Received 8 September 2005
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Comment

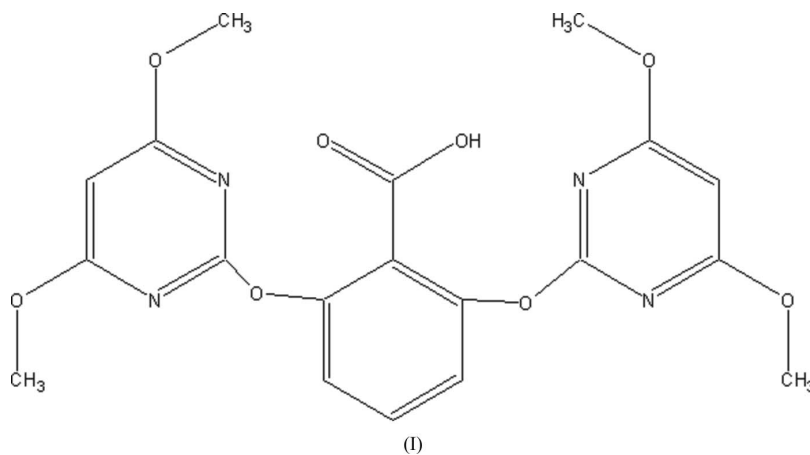
An important aspect in the rational design of bioactive mol-
ecules involves relating chemical structure to biological
activity (Lewis *et al.*, 1991). The conformation of the molecule
is found to influence the levels of biological activity. Corre-
lation of the results obtained from X-ray crystallography with
biological activity has aided in the chemical design of a few
active agrochemicals. The activity of a series of triazolyl
ketone herbicides (Anderson *et al.*, 1983) has been investi-
gated along with the fungicidal activities of *N*-phenylsuccin-
amides (Zenei *et al.*, 1988). In this paper, we report the
structure of the title compound, (I), which is a selective,
systemic post-emergence herbicide used for the control of a
wide range of weeds.

Fig. 1 shows an *ORTEP*-3 (Farrugia, 1997) view of the compound. The methoxy groups are displaced from each other to minimize steric repulsions between the non-bonded H atoms, but lie nearly in the plane of the pyrimidine ring. The pyrimidine rings ($\text{C}1/\text{N}1/\text{C}3-\text{C}5/\text{N}2$ and $\text{C}22/\text{N}3/\text{C}10-\text{C}12/\text{N}4$) make dihedral angles of $85.2(1)^\circ$ and $60.9(1)^\circ$, respectively, with the plane of the benzene ring. The H atom of the carboxylic group is not involved in the formation of classical carboxylic acid dimers. Instead it forms a hydrogen bond (Table 2 and Fig. 2) with the pyrimidinyl N atom, forming ring dimers [Etter's symbol $R_2^2(16)$; Bernstein *et al.*, 1995]. Atom O7 is also involved in the formation of dimeric motifs *via* $\text{C}-\text{H}\cdots\text{O}$ interactions [Etter's symbol $R_2^2(20)$].

Experimental

Compound (I) was supplied by Rallis India Limited. Crystals were grown by slow evaporation of a solution in methanol at 278 K.

Crystal data

$C_{19}H_{18}N_4O_8$ $Z = 2$
 $M_r = 430.37$ $D_x = 1.420 \text{ Mg m}^{-3}$
 Triclinic, $P\bar{1}$ Mo $K\alpha$ radiation
 Cell parameters from 765 reflections
 $a = 7.7779 (12) \text{ \AA}$ $\theta = 1.4\text{--}25.4^\circ$
 $b = 8.2973 (13) \text{ \AA}$ $\mu = 0.11 \text{ mm}^{-1}$
 $c = 16.883 (3) \text{ \AA}$ $T = 290 (2) \text{ K}$
 $\alpha = 87.899 (3)^\circ$ Plate, colorless
 $\beta = 79.054 (3)^\circ$ $0.40 \times 0.30 \times 0.04 \text{ mm}$
 $\gamma = 70.276 (3)^\circ$
 $V = 1006.5 (3) \text{ \AA}^3$

Data collection

Bruker SMART CCD area-detector 4089 independent reflections
 diffractometer 2777 reflections with $I > 2\sigma(I)$
 φ and ω scans $R_{int} = 0.023$
 Absorption correction: multi-scan $\theta_{max} = 27.4^\circ$
 (SADABS; Sheldrick, 1996) $h = -10 \rightarrow 9$
 $T_{min} = 0.947, T_{max} = 0.996$ $k = -10 \rightarrow 10$
 8103 measured reflections $l = -21 \rightarrow 21$

Refinement

Refinement on F^2 H atoms treated by a mixture of
 $R[F^2 > 2\sigma(F^2)] = 0.065$ independent and constrained
 $wR(F^2) = 0.158$ refinement
 $S = 1.14$ $w = 1/[\sigma^2(F_o^2) + (0.072P)^2]$
 4089 reflections where $P = (F_o^2 + 2F_c^2)/3$
 308 parameters $(\Delta/\sigma)_{max} < 0.001$
 $\Delta\rho_{max} = 0.22 \text{ e \AA}^{-3}$
 $\Delta\rho_{min} = -0.19 \text{ e \AA}^{-3}$

Table 1 Selected geometric parameters (\AA , $^\circ$).

O10—C22	1.357 (3)	O1—C1	1.353 (3)
O10—C19	1.394 (3)	O1—C16	1.403 (3)
O6—C21	1.312 (3)	O7—C21	1.206 (3)
C16—O1—C1—N1	1.7 (3)	C15—O5—C12—N4	178.7 (3)
C22—O10—C19—C23	121.8 (2)	C8—O3—C5—N2	-6.4 (4)
C1—O1—C16—C17	-91.0 (3)	C7—O2—C3—N1	-2.0 (4)
C14—O4—C10—N3	0.0 (4)	C19—O10—C22—N3	-0.6 (3)
C19—C20—C21—O7	129.3 (3)		

Table 2 Hydrogen-bond geometry (\AA , $^\circ$).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
C11—H11 \cdots O7 ⁱ	0.93 (3)	2.43 (3)	3.332 (3)	164 (2)
O6—H100 \cdots N4 ⁱⁱ	0.92 (4)	1.77 (4)	2.675 (2)	168 (4)

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

The H atoms bonded to the C atoms of the methyl groups were positioned geometrically and allowed to ride on the parent atom, with $C\text{--}H = 0.96 \text{ \AA}$ and $U_{iso} = 1.5U_{eq}(C_{methyl})$. The remaining H atoms were located in difference Fourier maps and refined isotropically.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SIR92 (Altomare, 1993); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and CAMERON (Watkin, 1993); software used to prepare material for publication: PLATON (Spek, 2003).

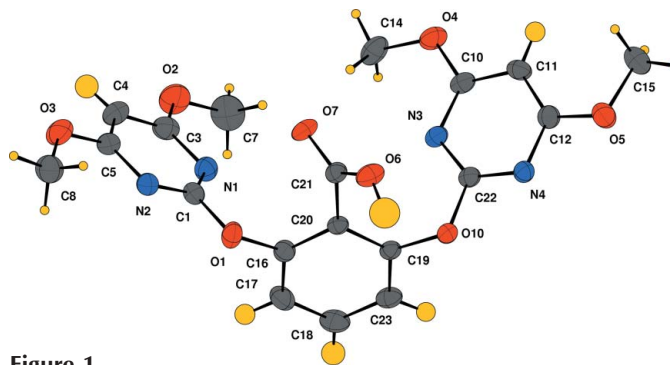


Figure 1 Molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

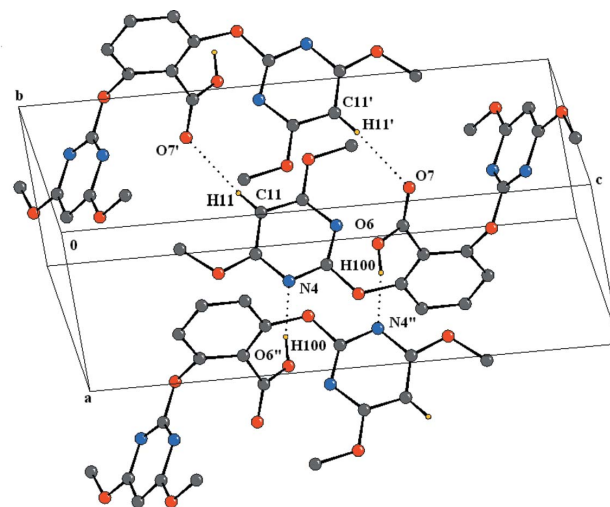


Figure 2 Packing diagram of (I). Dotted lines indicate O—H \cdots N and C—H \cdots O interactions. H atoms have been omitted for clarity, except for those involved in the hydrogen bonds. The symbols ' and '' are the symmetry codes $(1 - x, -y, 1 - z)$ and $(-x, 1 - y, 1 - z)$, respectively.

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