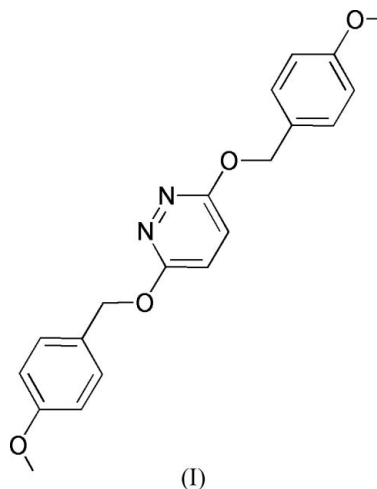


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of ChinaCorrespondence e-mail:
chshengyao@mail.nankai.edu.cn**Key indicators**Single-crystal X-ray study
 $T = 294$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.040
 wR factor = 0.115
Data-to-parameter ratio = 15.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**3,6-Bis(4-methoxybenzyloxy)pyridazine**

In the crystal structure of the title compound, $\text{C}_{20}\text{H}_{20}\text{N}_2\text{O}_4$, the molecules are linked by a weak intermolecular $\text{C}-\text{H} \cdots \text{N}$ hydrogen bond. The molecule has crystallographic twofold rotation symmetry.

Comment

Derivatives of pyridazine are very interesting because of their varied bioactivities, for example, acaricidal (Fuchs *et al.*, 1977), bactericidal (Douglass, 1977), anti-HIV (Bussolari, & Panzica, 1999), insecticidal (Ito *et al.*, 1983), antiviral (Galtier *et al.*, 2003), plant-growth regulating (Okamoto *et al.*, 1982) and herbicidal activities (Tsukamoto *et al.*, 2003; Kadotani *et al.*, 2004). In addition, maleic hydrazide, pyrazon and norflurazon are widely used as herbicides. This led us to direct our attention to the synthesis and structure determination of pyridazine derivatives. In a search for novel herbicides, we have synthesized a series of derivatives of pyridazine to study the relationship between their structure and their herbicidal activity. We report here the crystal structure of the title compound, (I).



The molecular structure of (I) is shown in Fig. 1. The molecule has crystallographic twofold rotation symmetry. The dihedral angle between the benzene and pyridazine rings is $27.37(8)^\circ$. The $\text{C}2-\text{O}1-\text{C}3-\text{C}4$ torsion angle is $177.4(1)^\circ$ (Table 1).

In the crystal structure, the molecules are linked by a weak intermolecular $\text{C}-\text{H} \cdots \text{N}$ hydrogen bond (Table 2 and Fig. 2).

Experimental

The title compound was synthesized according to the reported procedure of Yang *et al.* (2002), by refluxing 3,6-difluoropyridazine

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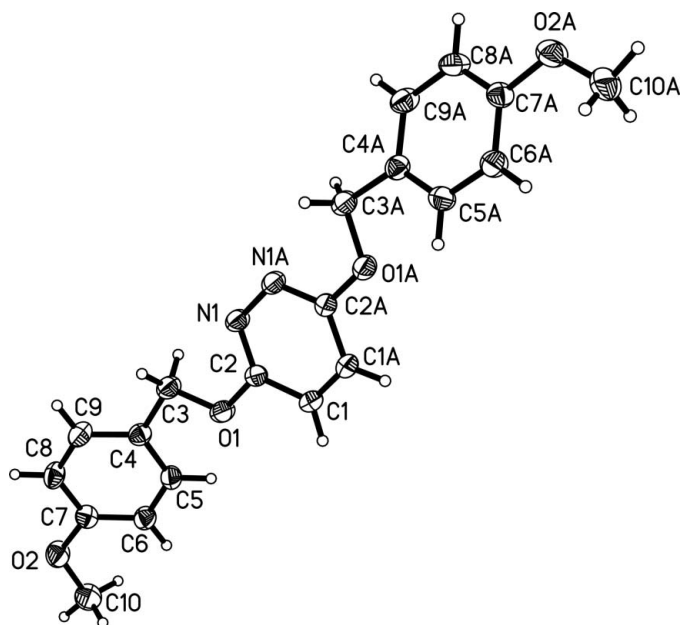


Figure 1
The structure of (I), showing 40% probability displacement ellipsoids and the atom-numbering scheme. The suffix A corresponds to symmetry code (i) in Table 1.

(0.24 g, 2.06 mmol), 4-methoxybenzyl alcohol (0.29 g, 2.10 mmol) and sodium hydroxide (0.10 g, 2.50 mmol) in acetonitrile (15 ml) for about 2 h. After cooling, the reaction mixture was poured into water. The precipitate was filtered off and recrystallized from petroleum ether. Single crystals of (I) suitable for X-ray diffraction were obtained after slow evaporation of the mother liquor.

Crystal data

$C_{20}H_{20}N_2O_4$	$D_x = 1.327 \text{ Mg m}^{-3}$
$M_r = 352.38$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 1236 reflections
$a = 33.126 (9) \text{ \AA}$	$\theta = 3.6\text{--}24.3^\circ$
$b = 5.7499 (15) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$c = 9.258 (3) \text{ \AA}$	$T = 294 (2) \text{ K}$
$\beta = 90.305 (5)^\circ$	Prism, colourless
$V = 1763.4 (9) \text{ \AA}^3$	$0.24 \times 0.22 \times 0.18 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	1801 independent reflections
φ and ω scans	1051 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.039$
$T_{\text{min}} = 0.958$, $T_{\text{max}} = 0.981$	$\theta_{\text{max}} = 26.4^\circ$
4724 measured reflections	$h = -40 \rightarrow 40$
	$k = -7 \rightarrow 7$
	$l = -5 \rightarrow 11$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0535P)^2 + 0.2049P]$
$R[F^2 > 2\sigma(F^2)] = 0.040$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.115$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.02$	$\Delta\rho_{\text{max}} = 0.14 \text{ e \AA}^{-3}$
1801 reflections	$\Delta\rho_{\text{min}} = -0.13 \text{ e \AA}^{-3}$
120 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997)
H-atom parameters constrained	Extinction coefficient: 0.0041 (7)

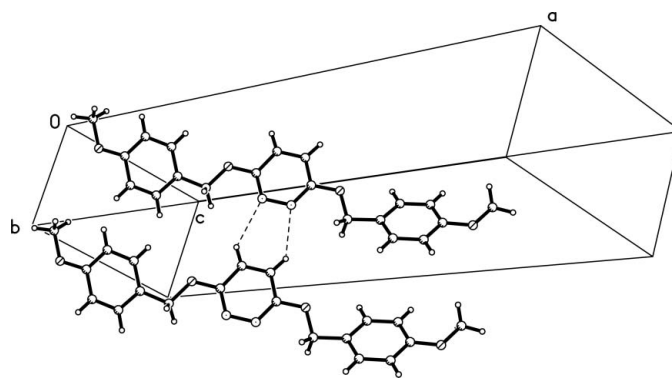


Figure 2
C—H...N hydrogen-bonded molecules in (I). Intermolecular hydrogen bonds are shown as dashed lines.

Table 1

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

N1—C2	1.3070 (19)	O1—C3	1.4356 (19)
N1—N1 ⁱ	1.377 (3)	O2—C7	1.3741 (19)
O1—C2	1.350 (2)	O2—C10	1.415 (2)
C2—O1—C3	117.92 (12)		
C2—O1—C3—C4	−177.40 (13)		

Symmetry code: (i) $-x, y, -z + \frac{1}{2}$.

Table 2

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

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
C1—H1 ⁱⁱ ...N1 ⁱⁱ	0.93	2.60	3.348 (2)	138

Symmetry code: (ii) $x, y - 1, z$.

H atoms were placed in calculated positions, with C—H = 0.93 or 0.97 \AA , and included in the final cycles of refinement using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{parent atom})$.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1999); software used to prepare material for publication: SHELXTL.

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