

Acta Crystallographica Section E

**Structure Reports**

**Online**

ISSN 1600-5368

Editors: **W. Clegg** and **D. G. Watson**

## **2,5-Dichloro-4'-methoxybiphenyl**

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## 2,5-Dichloro-4'-methoxybiphenyl

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## Key indicators

Single-crystal X-ray study  
 $T = 90$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.049  
 $wR$  factor = 0.131  
Data-to-parameter ratio = 18.1

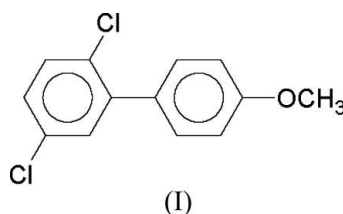
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The dihedral angle between the benzene rings in the title compound,  $\text{C}_{13}\text{H}_{10}\text{Cl}_2\text{O}$ , is  $59.92$  ( $9$ )°.

Received 14 August 2006  
Accepted 18 August 2006

## Comment

Polychlorinated biphenyls (PCBs) are an important class of persistent environmental contaminants (Robertson & Hansen, 2001). They are metabolized *in vivo* to hydroxylated and other metabolites. The three dimensional structure of PCBs and their metabolites is determined by the dihedral angle between the two benzene rings. The dihedral angle is thought to be an important determinant of the binding affinity of hydroxylated PCBs to various proteins (Lehmler *et al.*, 2002). We synthesized 2,5-dichloro-4'-methoxybiphenyl, a methylated analog of a hydroxylated PCB, as part of our ongoing research into the phase II metabolism of hydroxylated PCBs (Tampal *et al.*, 2002; van den Hurk *et al.*, 2002; Wang *et al.*, 2005; Wang *et al.*, 2006). The crystal structure of this PCB derivative showed a dihedral angle of  $59.92$  ( $9$ )°, which is slightly larger than the calculated dihedral angle of  $57.7$ ° in aqueous solution [calculated with *MM2* using GB/SA water solvent continuum as implemented by *MACROMODEL* 5.0 (Still *et al.*, 1990)].



According to our review of the literature, the experimental dihedral angles for mono-, di-, tri- and tetra-*ortho* Cl-substituted PCB derivatives are  $47$ – $51$ ° (Kania-Korwel *et al.*, 2004; Lehmler *et al.*, 2001; McKinney & Singh, 1988; Sluis *et al.*, 1990),  $59$ – $75$ ° (Vyas *et al.*, 2006; Miao *et al.*, 1997; Rissanen *et al.*, 1988a; Rømming *et al.*, 1974; Singh *et al.*, 1986),  $82$ – $83$ ° (Lehmler *et al.*, 2005; Rissanen *et al.*, 1988b) and  $84$ – $87$ ° (Pedersen, 1975; Shaikh *et al.*, 2006; Singh & McKinney, 1979), respectively. As a result of crystal packing effects, the calculated dihedral angles of these PCB derivatives (*viz.*,  $57.7$ °,  $73.0$ °,  $89.8$ ° and  $89.9$ ° for mono-, di-, tri- and tetra-*ortho* Cl-substituted PCB derivatives, respectively), in contrast to the title compound, are larger than the solid state dihedral angles. Overall, the title compound and other PCB derivatives may have some conformational flexibility when interacting with proteins, a fact that may be helpful in determining three-dimensional quantitative structure–activity relationships for a variety of phase II enzymes.

## Experimental

The title compound, (I), was synthesized in 75% yield by the Suzuki coupling of 4-methoxyphenylboronic acid and 2,5-dichlorobromobenzene (Kania-Korwel *et al.*, 2004). Colorless blocks were obtained upon crystallization from methanol.

### Crystal data

$C_{13}H_{10}Cl_2O$	$Z = 4$
$M_r = 253.11$	$D_x = 1.459 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 9.4758 (3) \text{ \AA}$	$\mu = 0.54 \text{ mm}^{-1}$
$b = 14.2682 (5) \text{ \AA}$	$T = 90.0 (2) \text{ K}$
$c = 9.5562 (3) \text{ \AA}$	Block, colourless
$\beta = 116.8711 (15)^\circ$	$0.18 \times 0.16 \times 0.12 \text{ mm}$
$V = 1152.52 (7) \text{ \AA}^3$	

### Data collection

Nonius KappaCCD diffractometer	5102 measured reflections
$\omega$ scans	2637 independent reflections
Absorption correction: multi-scan	1651 reflections with $I > 2\sigma(I)$
SCALEPACK (Otwinowski & Minor, 1997)	$R_{\text{int}} = 0.052$
$T_{\text{min}} = 0.91, T_{\text{max}} = 0.94$	$\theta_{\text{max}} = 27.5^\circ$

### Refinement

Refinement on $F^2$	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.049$	$w = 1/[\sigma^2(F_o^2) + (0.0666P)^2]$
$wR(F^2) = 0.131$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2637 reflections	$\Delta\rho_{\text{max}} = 0.61 \text{ e \AA}^{-3}$
146 parameters	$\Delta\rho_{\text{min}} = -0.43 \text{ e \AA}^{-3}$

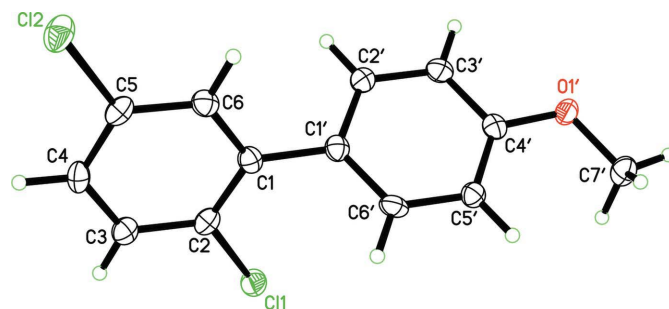
H atoms were positioned geometrically (C–H = 0.95–0.98 Å) and refined as riding, with  $U_{\text{iso}}(\text{H}) = 1.2$  or 1.5 times  $U_{\text{eq}}(\text{C})$ .

Data collection: COLLECT (Nonius, 1998); cell refinement: SCALEPACK (Otwinowski & Minor, 1997); data reduction: DENZO-SMN (Otwinowski & Minor, 1997); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: XP in SHELXTL (Sheldrick, 1994); software used to prepare material for publication: SHELX97-2 (Sheldrick, 1997) and local procedures.

This research was supported by grants ES05605, ES012475 and ES013661 from the National Institute of Environmental Health Sciences, NIH.

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**Figure 1**

View of the title compound showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

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