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# 2,5-Dichloro-4′-methoxybiphenyl

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**Key indicators**

Single-crystal X-ray study
$T$ = 90 K
Mean $\sigma$(C–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, $C_{13}H_{10}Cl_2O_1$, is 59.92 (9)°.

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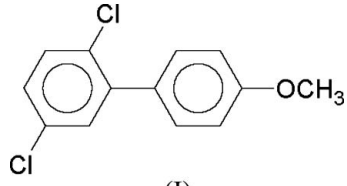
## Comment

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 angles 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)].




(I)

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.*, 1988*a*; Rømming *et al.*, 1974; Singh *et al.*, 1986), 82–83° (Lehmler *et al.*, 2005; Rissanen *et al.*, 1988*b*) 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*

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

*Data collection*

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

*Refinement*

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

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

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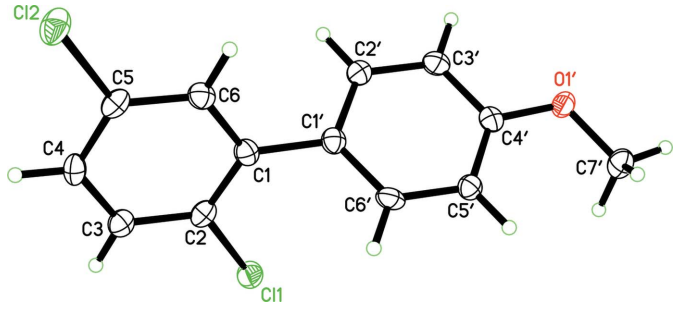


**Figure 1**
View of the title compound showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

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