Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,2′,3,3′,6-Pentachlorobiphenyl (PCB 84)

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.032
wR factor = 0.078
Data-to-parameter ratio = 18.6

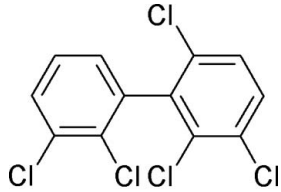
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 22 July 2005
Accepted 15 August 2005
Online 20 August 2005

The dihedral angle between the benzene rings in the title compound, $C_{12}H_5Cl_5$, is 81.5 (2)°.

Comment

Polychlorinated biphenyls (PCBs) are a class of persistent and ubiquitous environmental contaminants that have been manufactured for a large number of technical applications, for example for use in transformers and capacitors (Robertson & Hansen, 2001). Laboratory and epidemiological studies have implicated PCBs in a range of adverse health effects, such as cancer, heart disease, developmental toxicity and neurotoxicity. The mechanisms by which PCBs cause these adverse health effects are only poorly understood, partly because environmental PCBs are complex mixtures containing many of the 209 possible PCB congeners, and many open questions remain.



(I)

PCB congeners with multiple *ortho* chlorine substituents have been implicated in developmental and neurotoxicity (Lehmler *et al.*, 2005; Robertson & Hansen, 2001). The toxicity of *ortho*-substituted PCB derivatives is likely due to interaction of these PCB derivatives with cellular target sites, for example the ryanodine receptor. Their binding to these target sites requires a suitable three-dimensional structure, which is determined by the substitution pattern (Kodavanti *et al.*, 1995) and the torsion angle between the two phenyl rings (Lehmler, Parkin & Robertson, 2002). Unfortunately, only a few crystal structures of PCBs (Kania-Korwel *et al.*, 2004; Lehmler, Parkin & Robertson, 2001; Miao *et al.*, 1997; Rømming *et al.*, 1974; Singh *et al.*, 1986), PCB metabolites (Lehmler, Robertson & Parkin, 2001, 2002; Lehmler, Robertson *et al.*, 2002; McKinney & Singh, 1988) and related PCB derivatives (Lehmler, Parkin & Robertson, 2002; Rissanen *et al.*, 1988*a*,*b*) have been reported. This presents an obstacle for the development of three-dimensional quantitative structure–activity relationships for the binding of PCBs and derivatives to receptors involved in the developmental and neurotoxicity of PCBs.

We report here the crystal structure of 2,2′,3,3′,6-pentachlorobiphenyl (PCB 84), (I), a neurotoxic PCB congener with

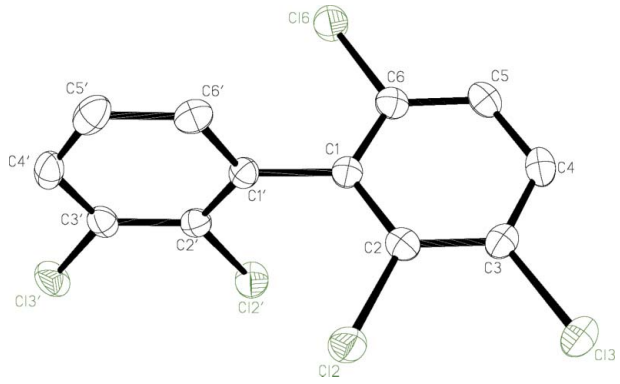


Figure 1
A view of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

three *ortho* chlorine substituents (Lehmler *et al.*, 2005). The dihedral angle between the benzene rings in (I) is 81.5 (2)°. This value is smaller than the calculated dihedral angle of 90° in an aqueous solution [calculated with *MM2* using GB/SA water solvent continuum, as implemented by *MACROMODEL* (version 5.0; Still *et al.*, 1990)]. Similar differences in the solid-state *versus* the calculated dihedral angle have been reported for other PCB congeners (Kania-Korwel *et al.*, 2004; Lehmler, Parkin & Robertson, 2001). These differences are probably due to crystal-packing effects, *i.e.* optimization of the crystal packing at the cost of a higher energy conformation (and therefore smaller dihedral angle) is energetically favourable (Lehmler, Robertson *et al.*, 2002). Our finding suggests that even highly *ortho*-substituted PCB congeners with limited or no conformational freedom around the single bond between the two benzene rings can adopt a range of conformations which, in a biological system, may be greatly influenced by the protein-binding sites in which PCBs may reside.

Experimental

Compound (I) was synthesized using the method described previously by Lehmler *et al.* (2005). Colourless broken laths were obtained upon crystallization from methanol.

Crystal data

$C_{12}H_5Cl_5$
M_r = 326.41
Monoclinic, $P2_1/c$
a = 7.7015 (3) Å
b = 7.8357 (3) Å
c = 21.1617 (7) Å
β = 99.9257 (17)°
V = 1257.92 (8) Å^3
Z = 4
D_x = 1.724 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10705 reflections
θ = 1.0–27.5°
μ = 1.12 mm^{-1}
T = 173 (1) K
Broken lath, colourless
0.28 × 0.20 × 0.06 mm

Data collection

Nonius KappaCCD diffractometer
ω scans
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.744, T_{max} = 0.936
10705 measured reflections
2861 independent reflections
2356 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 27.4°
$h = -9 \rightarrow 9$
$k = -10 \rightarrow 10$
$l = -27 \rightarrow 27$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.078
S = 1.04
2861 reflections
154 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.034P)^2 + 0.5413P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

After their location in a difference map, all H atoms were positioned geometrically (C—H = 0.95 Å) and allowed to ride on their attached atoms, with U_{iso}(H) = 1.2U_{eq}(C). Crystal decay was determined by remeasuring a portion of the first data-collection scan under otherwise identical conditions and comparing the average reflection intensities.

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/PC* (Sheldrick, 1994); software used to prepare material for publication: *SHELX97-2* (Sheldrick, 1997) and local programs.

This research was supported by grants ES07380 and ES012475 from the National Institute of Environmental Health Sciences, NIH.

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