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The three-dimensional structure of 3,3′,4,4′-tetrachlorobiphenyl, a dioxin-like polychlorinated biphenyl (PCB)

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Abstract

The crystal structure of PCB 77 (3,3′,4,4′-tetrachlorobiphenyl, $C_{12}H_6Cl_4$), a dioxin-like PCB congener, is described. The dihedral angle of PCB 77 is 43.94(6)°, which is slightly larger than calculated or experimental dihedral angles of biphenyl derivatives in solution but smaller than experimental dihedral angles in the gas phase.

Keywords: Environmental contaminants; Dioxin-like PCBs; Dihedral angle; Crystal structure

1. Introduction

Polychlorinated biphenyls (PCBs) are a class of persistent organic chemicals that were manufactured on an industrial scale until the late 1970s (Hansen, 1999; Robertson and Hansen, 2001). Due to their high chemical stability, low flammability and other desirable physical properties, such as electrical insulation properties, they were used for technical applications such as hydraulic fluids, lubricants and as additives in paint, pesticides, sealants and plastics. In the United States, PCBs are still used as dielectric fluids in closed systems such as transformers and capacitors. Although their production is banned worldwide, PCBs continue to be a health concern due to their persistence in the environment, their tendency to bioaccumulate and to biomagnify, and their adverse effects in animal and epidemiological studies.

Technical PCB products are complex mixtures containing over 50 individual PCB congeners with different chemical structures and physicochemical properties. Depending on their three-dimensional structure, PCB congeners bind to different cellular target sites, and thus cause adverse effects by different mechanisms. For example, PCB congeners with *ortho*-chlorine substituents can bind to the constitutive androstane (CAR) (Denomme et al., 1983) and/or the pregnane X receptor (PXR) (Schuetz et al., 1998). Other *ortho* substituted PCB congeners interact with both the aryl hydrocarbon (Ah receptor) and the CAR receptor (Parkinson et al., 1983). PCB congeners with zero or one *ortho*-chlorine substituent can bind to the aryl hydrocarbon receptor (Ah receptor), thus mimicking the action of 2,3,7,8-tetrachlorodibenzo-*p*-dioxin (TCDD) (Goldstein et al., 1978; Safe, 1994). These dioxin-like PCB congeners, for example PCBs 77 and 126, are of particular regulatory interest because of their mammalian and human toxicity, which appears to be mediated primarily via the Ah receptor.

Efforts to elucidate the molecular structure of individual PCB congeners are highly desirable because of the relationship between their three-dimensional structure and their

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toxicity. Indeed, the crystal structures of several *ortho* substituted PCB congeners have been published (Singh and McKinney, 1979; Singh et al., 1986; Miao et al., 1997; Lehmler et al., 2001, 2005; Kania-Korwel et al., 2004; Vyas et al., 2006). However, despite the environmental importance of dioxin-like PCB congeners, no crystal structure of such a dioxin-like PCB congener has been reported to date. We herein report the first X-ray crystal structure of dioxin-like PCB congener, PCB 77 (3,3′,4,4′-tetrachlorobiphenyl).

2. Results and discussion

We were able to obtain crystals of PCB 77 suitable for crystal structure analysis by recrystallization from hot methanol. Crystal data and other relevant parameters are summarized in Table 1 and selected bond lengths and angles are given in Table 2. The molecular structure with the atom numbering scheme and a crystal packing diagram are shown in Figs. 1 and 2, respectively. PCB 77 crystallizes in an orthorhombic space group ($P2_1\ 2_1\ 2$) with $a = 11.1458(2)$ Å, $b = 13.5539(3)$ Å, $c = 3.7735(1)$ Å and with half a molecule per asymmetric unit. The closest Cl–Cl intermolecular interactions are 3.492(2) Å between Cl1 and a 2-fold screw related Cl2 (symmetry operation is $x - 0.5$, $0.5 - y$, $1 - z$).

The dihedral angle between the two phenyl rings of PCB congeners is an important determinant to describe the conformation of PCBs, and, therefore, their binding activity with cellular target molecules (McKinney and Singh, 1988; Lehmler et al., 2002). The experimental dihedral angle for PCB 77 in the solid state is 43.94(6)° (Fig. 1b). As shown in Table 3, this dihedral angle is larger than the dihedral angle of 3,3′,5′-trichloro-4-methoxybiphenyl (Lehmler et al., 2002) and of axially substituted biphenyls such as 4,4′-dichlorobiphenyl (Brock et al., 1978). This value is also larger than the dihedral angles reported for biphenyl in different solvents (reported dihedral angles of biphenyl in solution range from approximately 30° to 40°

Table 1
Crystal data and structure refinement for 3,3′,4,4′-tetrachlorobiphenyl

Empirical formula	$C_{12}H_6C_{l4}$
Formula weight	291.97
Temperature	120.0(2) K
Wavelength	1.54178 Å
Crystal system, space group	Orthorhombic, $P\ 2_1\ 2_1\ 2$
Unit cell dimensions	
a	11.1458(2) Å
b	13.5539(3) Å
c	3.7735(1) Å
Volume	570.06(2) Å^3
Z, calculated density	2, 1.701 Mg/m^3
Absorption coefficient	9.137 mm^{-1}
F(000)	292
Crystal size	0.18 × 0.08 × 0.08 mm
Theta range for data collection	5.14–67.49°
Limiting indices	$-13 < h < 9$, $-15 < k < 16$, $-4 < l < 2$
Reflections collected/unique	2102/852 [R(int) = 0.0298]
Completeness to $\theta = 67.49$	96%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.529 and 0.315
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	852/0/75
Goodness-of-fit on F^2	1.108
Final R indices [$I > 2\Sigma(I)$]	$R1 = 0.0253$, $wR2 = 0.0652$
R indices (all data)	$R1 = 0.0254$, $wR2 = 0.0653$
Extinction coefficient	0.0076(12)
Largest diff. peak and hole	0.301 and −0.280 e A^{-3}

Table 2
Selected bond lengths (Å) and angles (°) for 3,3′,4,4′-tetrachlorobiphenyl

C-atoms	Bond lengths (A)	C-atoms	Bond angles (°)
Cl(1)–C(3)	1.733(2)	C(6)–C(1)–C(2)	118.6(2)
Cl(2)–C(4)	1.731(2)	C(6)–C(l)–C(l′)	120.9(2)
C(1)–C(6)	1.389(3)	C(2)–C(l)–C(l′)	120.5(2)
C(1)–C(2)	1.397(3)	C(3)–C(2)–C(1)	120.4(2)
C(l)–C(1)	1.484(4)	C(3)–C(2)–H(2)	119.8
C(2)–C(3)	1.380(3)	C(1)–C(2)–H(2)	119.8
		C(2)–C(3)–C(4)	120.6(2)
C(3)–C(4)	1.387(4)	C(2)–C(3)–Cl(1)	118.95(2)
C(4)–C(5)	1.394(3)	C(4)–C(3)–Cl(1)	120.49(2)
C(5)–C(6)	1.383(4)	C(3)–C(4)–C(5)	119.5(2)
		C(3)–C(4)–Cl(2)121.29(2)	121.29(2)
		C(5)–C(4)–Cl(2)119.2(2)	119.2(2)
		C(6)–C(5)–C(4)	119.6(2)
		C(6)–C(5)–H(5)	120.2
		C(4)–C(5)–H(5)	120.2
		C(5)–C(6)–C(1)	121.3(2)
		C(5)–C(6)–H(6)	119.4
		C(1)–C(6)–H(6)	119.4

Symmetry transformations used to generate equivalent atoms: #1 $-x + 1$, $-y + 1$, z.

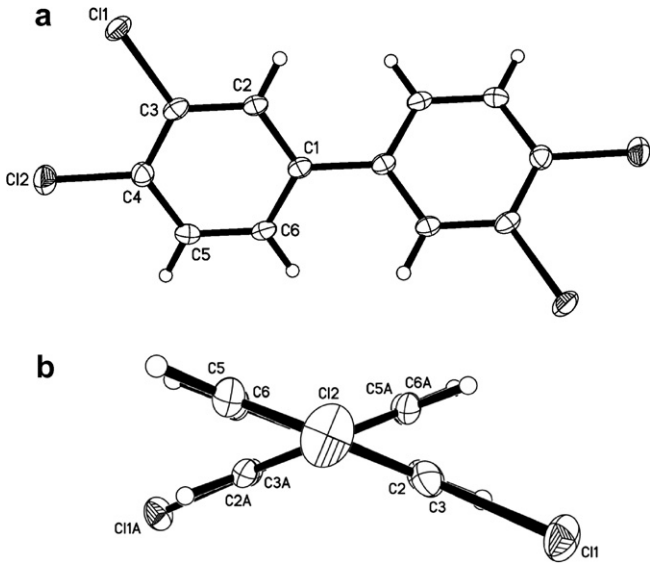
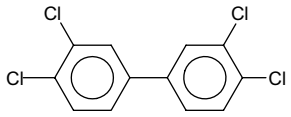
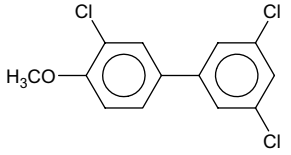
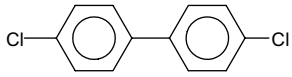
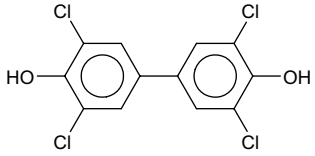


Fig. 1. (a) Molecular structure of PCB 77 showing the atom-labelling scheme and (b) view of PCB 77 along the C1–C1′ axis illustrating the non-planar conformation of the molecule. Displacement ellipsoids are drawn at the 50% probability level. Unlabeled atoms are at the symmetry position ($1 - x$; $1 - y$; z).

Table 3
Comparison of the space group and solid state dihedral angle of selected chlorinated biphenyl derivatives without ortho substituent

Entry	Molecular structures of biphenyl	Space group	Solid state dihedral angle (°)	Reference
1		Orthorhombic, $P\ 2_1\ 2_1\ 2$	43.94(06)	Present work
2		Monoclinic, $P2_1/c$	41.31(07)	Lehmler et al. (2002)
3		Monoclinic, $P2_1/n$	39.42	Brock et al. (1978)
4		Monoclinic, $2_1/c$	Coplanar	McKinney and Singh (1988)

depending on the solvent and the experimental approach used for its determination (Akiyama et al., 1986)), and the calculated dihedral angle of 41.2°. However, the solid state dihedral angle of PCB 77 is smaller compared to experimental gas phase dihedral angles of biphenyl, 4-chlorobiphenyl and 4,4′-dichlorobiphenyl, which are approximately 44–45° (Almenningen et al., 1985a, 1985b).

To date 3,3′,5,5′-tetrachloro-4,4′-dihydroxybiphenyl is the only reported crystal structure of a non-ortho substituted PCB derivative (McKinney and Singh, 1988). This compound is a metabolite of PCB 77 (Koga et al., 1989; Doi et al., 2006) and has a strong affinity to both human estrogen sulfotransferase (Shevtsov et al., 2003) and thyroxine (McKinney et al., 1987). 3,3′,5,5′-Tetrachloro-4,4′-dihydroxybiphenyl, like chlorinated dioxins (Cantrell et al., 1969, 1989; Boer and North, 1972; Boer et al., 1972; Koester et al., 1988), is essentially coplanar in the solid state, and thus adopts a conformation that is significantly different from that of PCB 77. The tendency of this dihydroxylated PCB derivative to adopt a more planar conformation in the solid state is due to the stabilizing intermolecular interactions resulting, in part, from a stacking arrangement of the benzene rings (McKinney and Singh, 1988). Although some stacking interactions are also present in PCB 77, the hypothetical energy gain resulting from the packing of coplanar PCB 77 molecules does not offset the increase in intramolecular energy associated with such a coplanar conformation. Therefore, in contrast to 3,3′,5,5′-tetrachloro-4,4′-dihydroxybiphenyl, PCB 77 does not adopt a coplanar conformation in its crystal structure.

The comparison of the solid state structure of PCB 77 and the structurally related 3,3′,5,5′-tetrachloro-4,4′-dihydroxybiphenyl shows that intermolecular interactions may be important determinants of the three-dimensional structure of PCBs. It has been proposed that similar intermolecular interactions are also important in the binding interactions of PCB congeners with target molecules such as the Ah receptor (McKinney and Singh, 1988; Lehmler et al., 2002). PCB molecules are likely to adopt a conformation that allows an energetically favourable binding to the target site due to the unrestricted rotation between two phenyl rings (i.e., the C1–C1′ bond). For example, crystallographic analysis of the binding of 3,3′,5,5′-tetrachloro-4,4′-dihydroxybiphenyl to human estrogen sulfotransferase shows the dihedral angle of the bound dihydroxy PCB was 30° (Shevtsov et al., 2003). For comparison, the solid state dihedral angle is significantly smaller at 0°, whereas the calculated dihedral angle is larger. This example suggests that the biologically relevant conformations of PCB congeners, such as PCB 77, and PCB metabolites, such as 3,3′,5,5′-tetrachloro-4,4′-dihydroxybiphenyl, exist over a range of dihedral angles, with the understanding that the dihedral angles may be greatly influenced by the protein-binding sites in which they were accommodated. Further studies are needed to determine the actual structure of PCB and other dioxin-like PCB congers in the binding site of their target molecules.

3. Conclusions

We herein report the crystal structure of PCB 77, a dioxin-like PCB congener. The dihedral angle between two phenyl rings of PCB 77 is 43.94(6)°, which is comparable to calculated or experimental dihedral angles of

biphenyl and other PCB congeners in solution or in the gas phase. Overall, this X-ray crystallographic determination provides the first highly accurate picture of the molecular geometry of a dioxin-like PCB congener in a specific solid state environment and gives some insight into the crystal packing arrangement which may help to understand the intermolecular forces of importance for the interaction of PCB 77 with biological binding sites.

4. Experimental

4.1. Synthesis of 3,3′,4,4′-tetrachlorobiphenyl (Shaikh et al., 2006)

3,3′,4,4′-Tetrachlorobiphenyl was synthesized in 42% yield by copper bronze mediated symmetrical Ullmann coupling reaction (at 230 °C, 7 days) and purified by column chromatography over silica gel using a mixture of *n*-hexanes and ethyl acetate (10:1) as an eluent. Recrystallization from hot methanol was carried out to obtain the crystals suitable for X-ray analysis.

White solid m.p. = 174–176 °C, ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36 (dd, J = 2.2 and J = 8.3 Hz, 2 × H-6), 7.51 (d, J = 8.3 Hz, 2 × H-5), 7.61 (d, J = 2.2 Hz, 2 × H-2). ^{13}C NMR (400 MHz, $CDCl_3$): δ 126.15 (2 × C-6), 128.81 (2 × C-2), 130.97 (2 × C-5), 132.48 (2 × C-4), 133.25 (2 × C-3), 138.73 (2 × C-1). MS (EI): *m/z* (relative abundance %) 292 (M^+, 100), 256 (M^+−Cl, 5), 220 (M^+−2Cl, 40), 184 (M^+−3Cl, 10), 110 (12), 74 (5).

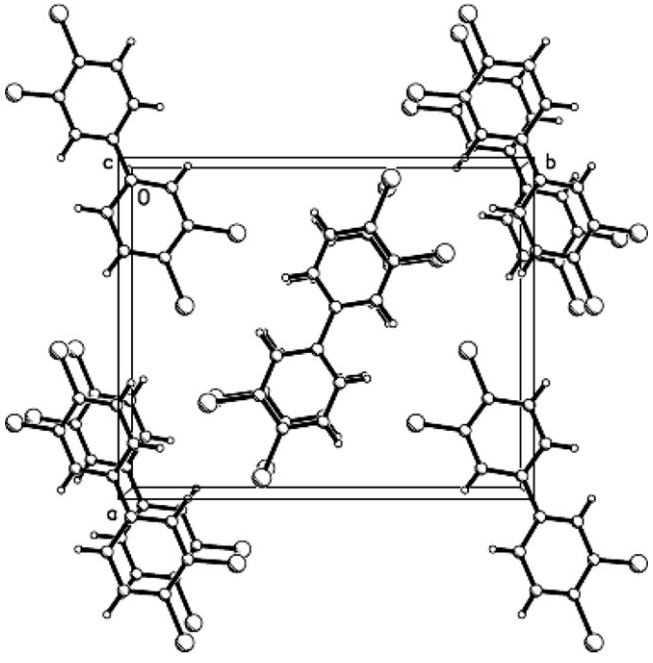


Fig. 2. View of the crystal packing of 3,3′,4,4′-tetrachlorobiphenyl molecules parallel to the *c*-axis. Large circles are Cl atoms.

4.2. Molecular orbital computation of dihedral angle of PCB 77 with the SCF-MO method

The conformation of PCB 77 was calculated using semi-empirical SCF-MO calculations with an Austin Model 1 (AM1) Hamiltonian (Dewar et al., 1985). This was contained in the Spartan 02 package and carried out on a Quad 2.5 GHz Power Mac G5 with a PCI express graphic card as described previously (Luthe et al., 2007). The use of symmetry constraints enhanced the convergence compared with completely unconstrained runs. The calculated value of the dihedral angle of PCB 77 of 41.2° is the average of the four torsion angles involving C1–C1′.

4.3. X-ray crystal structure analysis

X-ray diffraction data were collected at 120.0(2) K on a Bruker-Nonius X8 Proteum diffractometer with graded-multilayer focusing optics from a rod-shaped crystal. Raw data were integrated, scaled, merged and corrected for Lorentz-polarization effects using the APEX2 package (Bruker-Nonius, 2004). The structure was solved by direct methods (Sheldrick, 1997) and missing atoms were located in difference Fourier maps (Sheldrick, 1997). Refinement was carried out against F^2 by weighted full-matrix least-squares (Sheldrick, 1997). Hydrogen atoms were found in difference maps but subsequently placed at calculated positions and refined using a riding model. Non-hydrogen atoms were refined with anisotropic displacement parameters. Atomic scattering factors were those of SHELXL (Sheldrick, 1997), as taken from the International Tables for Crystallography (Hahn, 1992). Crystal data and relevant details of the structure determinations are summarized in Table 1 and selected geometrical parameters are given in Table 2.

Supplementary data

Crystallographic data for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Center as Supplementary Publication No. CCDC-640770. Copies of the data can be obtained free of charge on application to the CCDC, 12 Union Road, Cambridge CB2 1EZ, U.K. (fax: (+44)1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

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