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2,4,5-Trichlorobiphenyl

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Key indicators

Single-crystal X-ray study
T = 90 K
Mean σ(C–C) = 0.002 Å
R factor = 0.026
wR factor = 0.063
Data-to-parameter ratio = 17.5

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

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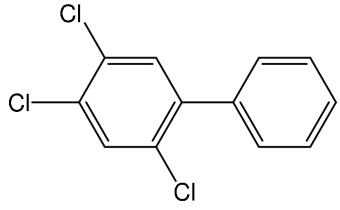
The dihedral angle between the benzene rings in the title compound, $C_{12}H_7Cl_3$, is 47.25 (4)°.

Comment

Polychlorinated biphenyls (PCBs) are a group of ubiquitous environmental pollutants (Robertson & Hansen, 2001). They are only slowly biodegraded, and they bioaccumulate and biomagnify. According to their substitution patterns, PCBs elicit a wide range of toxic responses in living organisms. Knowledge of three-dimensional structure, especially the dihedral angle which describes the deformation of the molecule from a planar conformation, helps to define the potential binding sites of PCB congeners and hence the hazards associated with their occurrence.



(I)

The title molecule, (I), has a solid-state dihedral angle of 47.25 (4)°. In contrast, the solid-state torsion angle between the two benzene rings of other mono-*ortho*-chloro-substituted biphenyls is in the range 50–52° (Miao *et al.*, 1996; Lehmler *et al.*, 2001). In solution, the calculated dihedral angle for (I) [calculated with *MM*2 using GB/SA water solvent continuum as implemented by *MACROMODEL* 5.0 (Still *et al.*, 1990)] is larger (57.7°) and is probably due to the alleviation of packing effects present in the solid state (Lehmler *et al.*, 2002). This raises the question whether the solid state or the calculated solution dihedral angle represents biologically relevant conformations of (I).

A partial answer to this question can be found in the crystallographic analysis of the binding of 4,4-hydroxy-3,3′,5,5′-tetrachlorobiphenyl to the estrogen receptor (Shevtsov *et al.*, 2003). The dihedral angle of the dihydroxy PCB bound to protein was 30°, while the calculated solution and the solid-state dihedral angle of the neat dihydroxy PCB were 42 and 0°, respectively (McKinney, 1988). This implies that the biologically relevant conformations of PCBs such as the title compound can be described as the range between the calculated solution and the solid-state dihedral angles, with the understanding that these torsion angles may be greatly influenced by the protein-binding sites in which they may reside.

Experimental

The title compound, (I), was synthesized in 52% yield by the Suzuki coupling of 2,4,5-trichloroiodobenzene with phenylboronic acid (Kania-Korwel *et al.*, 2004). White needles were obtained upon crystallization from methanol.

Crystal data

$C_{12}H_7Cl_3$
$M_r = 257.53$
Triclinic, $P\overline{1}$
$a = 3.85010\ (10)$ Å
$b = 11.4482\ (3)$ Å
$c = 13.0504\ (3)$ Å
$\alpha = 109.8409\ (10)^\circ$
$\beta = 92.9891\ (9)^\circ$
$\gamma = 99.2004\ (10)^\circ$
$V = 530.59\ (2)$ Å^3
$Z = 2$
$D_x = 1.612$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2350 reflections
$\theta = 1.0$–27.5°
$\mu = 0.82$ mm^{-1}
$T = 90.0\ (2)$ K
Block, colourless
$0.24 \times 0.15 \times 0.10$ mm

Data collection

Nonius KappaCCD diffractometer
ω scans
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
$T_{min} = 0.827$, $T_{max} = 0.923$
4668 measured reflections
2383 independent reflections
2065 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 27.4^\circ$
$h = -4 \rightarrow 4$
$k = -14 \rightarrow 14$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.063$
$S = 1.07$
2383 reflections
136 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0219P)^2 + 0.2643P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

Recollection of the first part of the first scan of area-detector data for this set showed no significant differences in integrated intensities. H atoms were placed in geometrically idealized positions and constrained using a riding model in which the C—H distance was fixed at 0.95 Å with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in Siemens *SHELXTL/PC* (Sheldrick, 1994); software used to prepare material for publication: *SHELX*97-2 (Sheldrick, 1997) and local programs.

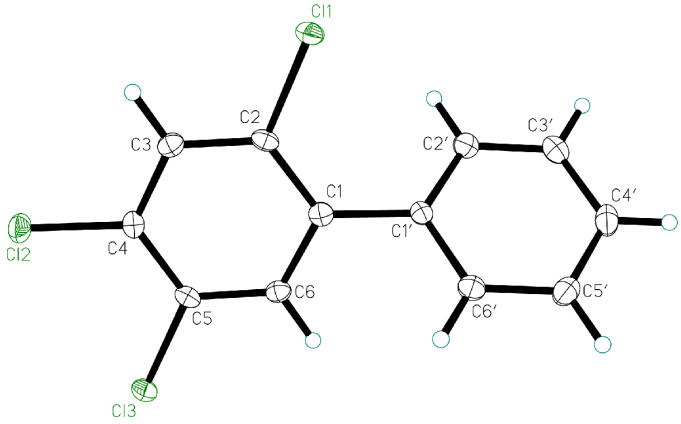


Figure 1
View of the title compound showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

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References

Kania-Korwel, I., Parkin, S., Robertson, L. W. & Lehmler, H.-J. (2004). *Chemosphere*, **56**, 735–744.
Lehmler, H.-J., Parkin, S. & Robertson, L. W. (2001). *Acta Cryst.* E**57**, o111–o112.
Lehmler, H.-J., Robertson, L. W., Parkin, S. & Brock, C. P. (2002). *Acta Cryst.* B**58**, 140–147.
McKinney, J. D. (1988). *Acta Cryst.* C**44**, 558–562.
Miao, X., Chu, S., Xu, X. & Jin, X. (1996). *Chin. Sci. Bull.* **42**, 1803–1806.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr and R. M. Sweet, pp. 307–326. New York: Academic Press.
Robertson, L. W. & Hansen, L. G. (2001). *Recent Advances in the Environmental Toxicology and Health Effects of PCBs*. Lexington: University Press of Kentucky.
Sheldrick, G. M. (1994). *SHELXTL/PC*. Version 5. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXL*97, *SHELXS*97 and *SHELX*97-2. University of Göttingen, Germany.
Shevtsov, S., Petrotchenko, E. V., Pedersen, L. C. & Negishi, M. (2003). *Environ. Health Perspect.* **111**, 884–888.
Still, W. C., Tempczyk, A., Hawley, R. C. & Hendrickson, T. (1990). *J. Am. Chem. Soc.* **112**, 6127–6129.