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2-(3,5-Dichlorophenyl)-1,4-benzoquinone

Hans-Joachim Lehmler,[a] Larry W. Robertson[a]* and Sean Parkin[b]

[a]Graduate Center for Toxicology, University of Kentucky, Lexington, KY 40536-0305, USA, and [b]Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055, USA

Correspondence e-mail: lwrobe01@uky.edu

Key indicators

Single-crystal X-ray study
T = 145 K
Mean σ(C–C) = 0.004 Å
R factor = 0.052
wR factor = 0.083
Data-to-parameter ratio = 13.0

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

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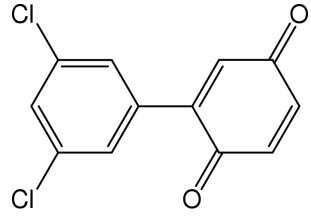
In the title compound, $C_{12}H_6Cl_5O_2$, the dihedral angle between the two rings is 37°. This dihedral angle is different from the calculated dihedral angle in aqueous solution (48°), a likely cause being the influence of crystal packing.

Comment

Polychlorinated biphenyls (PCBs) are large scale industrial chemicals used in dielectric fluids, transformers, capacitors, hydraulic fluids and as sealants (Robertson & Hansen, 2001; Hansen, 1999). Their resistance towards chemical and biological degradation has resulted in worldwide environmental contamination which causes concerns about possible human health effects. In particular, PCBs with few Cl atoms have measurable rates of cytochrome P-450 metabolism, resulting in the formation of PCB quinones (Srinivasan *et al.*, 2001; Oakley *et al.*, 1996). These quinones react readily with cellular nucleophiles, such as glutathione (Amaro *et al.*, 1996), deoxynucleotides (McLean *et al.*, 1996), DNA (Oakley *et al.*, 1996) and other cellular components (Amaro *et al.*, 1996). There is significant evidence in the literature that the chlorine substitution pattern and the degree of chlorination influences the reactivity of PCB quinones towards glutathione, DNA and possibly other cellular nucleophiles (Robertson & Hansen, 2001). One of many unanswered questions is whether the three-dimensional structure of the respective PCB quinone has any influence on the differences in reactivity observed in these studies. To the best of our knowledge, no crystal structures of PCB quinones have been reported, and improved knowledge about the three-dimensional structure of this interesting class of PCB metabolites is needed. We herein report the crystal structure of 2-(3,5-dichlorophenyl)-1,4-benzoquinone, (I), a possible quinone metabolite of 3,5-dichlorobiphenyl. The title compound shows a solid-state dihedral angle of 37.2 (3)° between the two rings. The dihedral angle in aqueous solution was calculated to be 48°. The differences in the solid-state dihedral angle and the calculated angle are probably due to crystal-packing effects (see Lehmler *et al.*, 2002, and references therein).



(I)

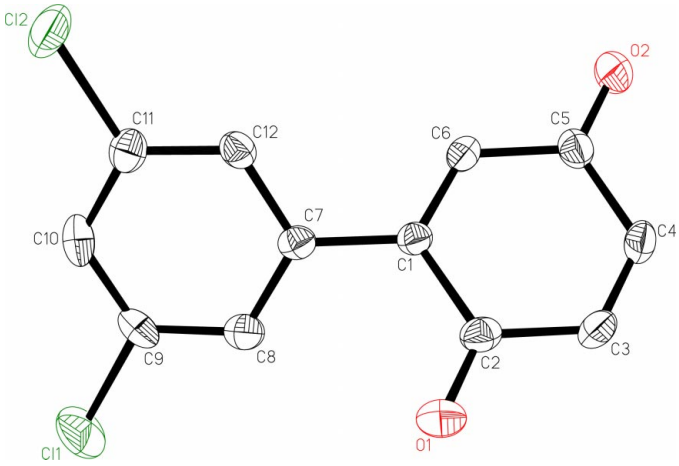


Figure 1
A view of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

Experimental

2-(3,5-Dichlorophenyl)-1,4-benzoquinone was synthesized as described previously (Srinivasan *et al.*, 2001; Amaro *et al.*, 1996). A brown–orange plate with irregular sides was obtained upon crystallization from acetone; m.p. = 436–437 K. The dihedral angle of the title compound was calculated with *MM2**, using GB/SA water solvent continuum, as implemented by *MACROMODEL*5.0 (Still *et al.*, 1990).

Crystal data

$C_{12}H_6Cl_2O_2$
M_r = 253.07
Monoclinic, $P2_1/c$
a = 18.1344 (14) Å
b = 6.6257 (5) Å
c = 9.0173 (7) Å
β = 95.903 (3)°
V = 1077.7 (2) Å^3
Z = 4
D_x = 1.560 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 40323 reflections
θ = 1.0–27.5°
μ = 0.58 mm^{-1}
T = 145 (2) K
Irregular plate, orange
0.40 × 0.25 × 0.01 mm

Data collection

Nonius KappaCCD diffractometer
ω scans at fixed χ = 55°
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.801, T_{max} = 0.994
3600 measured reflections
1891 independent reflections
1427 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 25.0°
$h = -21 \rightarrow 21$
$k = -7 \rightarrow 7$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.083
S = 1.10
1891 reflections
145 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.02P)^2 + 0.2379P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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 *SHELXTL* (Sheldrick, 1994); software used to prepare material for publication: *SHELX*97–2 (Sheldrick, 1997) and local procedures.

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