Crystal structure of 2-phenyl-1,4-benzoquinone, $C_{12}H_8O_2$

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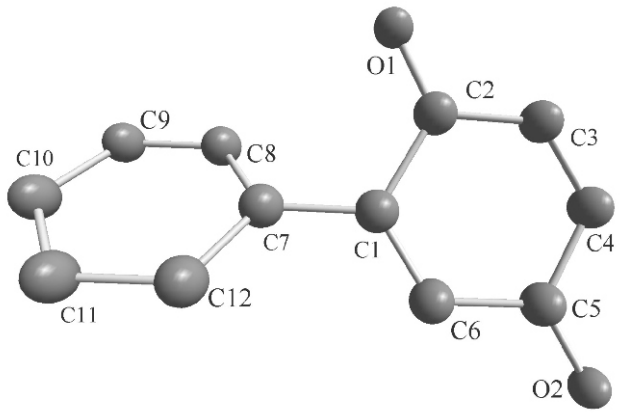

Abstract

$C_{12}H_8O_2$, orthorhombic, *Pbca* (no. 61), $a = 6.763(1)$ Å, $b = 7.152(1)$ Å, $c = 38.224(6)$ Å, $V = 1849.0$ Å^3, $Z = 8$, $R_{gt}(F) = 0.042$, $wR_{ref}(F^2) = 0.107$, $T = 296$ K.

Source of material

The title compound was prepared as described in literature [1] and recrystallized from dichloromethane-petroleum ether solution at room temperature to give the desired crystals suitable for diffraction experiment.

Discussion

Compounds containing the quinone group have been found to exhibit a wide range of pharmacological properties [2,3] and have also been used as reoxidants for palladium-catalyzed reactions [4,5]. Among them, compounds functionalized at the quinone moiety with aryl groups constitute a common structural moiety. These compounds have been synthesized by a few general methods such as oxidation of the corresponding aromatics [6,7]. In the title crystal structure, the benzene ring and quinone ring are not coplanar with a dihedral angle of 40.4°. All the bond distances and angles are within normal ranges. There exist O–H···O hydrogen bonds between the adjacent molecules, which construct the chain structure.

Table 1. Data collection and handling.

Crystal:	yellow block, size 0.18 × 0.23 × 0.25 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	0.90 cm^{-1}
Diffractometer, scan mode:	Bruker SMART APEX-II CCD, φ/ω
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	10528, 1719
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1373
$N(param)_{refined}$:	127
Programs:	SHELXS-97, SHELXL-97, SHELXTL [8]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(3)	8*c*	0.6555	0.6323	0.4539	0.070
H(4)	8*c*	0.9288	0.6882	0.4848	0.071
H(6)	8*c*	1.2682	0.5681	0.3982	0.058
H(8)	8*c*	0.7615	0.6674	0.3355	0.054
H(9)	8*c*	0.7810	0.5981	0.2769	0.062
H(10)	8*c*	1.0166	0.3933	0.2564	0.066
H(11)	8*c*	1.2430	0.2676	0.2946	0.071
H(12)	8*c*	1.2298	0.3392	0.3533	0.062

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	8*c*	0.9843(2)	0.5533(2)	0.38885(4)	0.0356(8)	0.0399(9)	0.0394(9)	0.0022(7)	0.0029(7)	0.0005(7)
C(2)	8*c*	0.7866(3)	0.5608(3)	0.40632(5)	0.040(1)	0.049(1)	0.050(1)	0.0008(8)	0.0051(8)	0.0006(8)
C(3)	8*c*	0.7781(3)	0.6188(3)	0.44317(5)	0.053(1)	0.069(1)	0.053(1)	0.003(1)	0.0169(9)	–0.004(1)
C(4)	8*c*	0.9396(3)	0.6521(3)	0.46150(5)	0.068(1)	0.071(1)	0.038(1)	0.001(1)	0.0092(9)	–0.0076(9)
C(5)	8*c*	1.1347(3)	0.6331(3)	0.44564(5)	0.053(1)	0.078(1)	0.042(1)	–0.002(1)	–0.0033(9)	–0.0060(9)
C(6)	8*c*	1.1445(3)	0.5816(3)	0.40850(4)	0.0378(9)	0.065(1)	0.042(1)	0.0027(8)	0.0027(7)	–0.0034(8)
C(7)	8*c*	0.9927(2)	0.5092(2)	0.35106(4)	0.0347(8)	0.0388(8)	0.0391(9)	–0.0003(7)	0.0011(7)	0.0000(7)
C(8)	8*c*	0.8591(2)	0.5865(2)	0.32752(4)	0.0421(9)	0.0455(9)	0.047(1)	0.0050(8)	–0.0028(8)	–0.0017(8)
C(9)	8*c*	0.8703(3)	0.5443(3)	0.29237(5)	0.055(1)	0.056(1)	0.045(1)	–0.0034(9)	–0.0112(8)	0.0032(8)
C(10)	8*c*	1.0118(3)	0.4236(3)	0.28007(5)	0.069(1)	0.055(1)	0.040(1)	–0.009(1)	0.0038(9)	–0.0077(8)
C(11)	8*c*	1.1456(3)	0.3481(3)	0.30283(5)	0.064(1)	0.059(1)	0.054(1)	0.015(1)	0.014(1)	–0.0071(9)
C(12)	8*c*	1.1372(3)	0.3907(3)	0.33810(5)	0.052(1)	0.058(1)	0.046(1)	0.0169(9)	0.0021(8)	0.0004(8)
O(1)	8*c*	0.6363(2)	0.5139(2)	0.39095(4)	0.0387(7)	0.102(1)	0.0647(9)	–0.0105(8)	0.0043(6)	–0.0076(8)
O(2)	8*c*	1.2844(2)	0.6639(3)	0.46238(4)	0.062(1)	0.173(2)	0.0573(9)	–0.008(1)	–0.0148(8)	–0.031(1)

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