Table 3. *Bond lengths and inter-bond angles*

C(1)–C(2)	1·389 Å	C(1)–C(2)–C(3)	120·4°
C(2)–C(3)	1·381	C(2)–C(3)–C(4)	119·5
C(3)–C(4)	1·391	C(3)–C(4)–C(5)	119·9
C(4)–C(5)	1·378	C(4)–C(5)–C(6)	120·6
C(5)–C(6)	1·399	C(5)–C(6)–C(1)	119·2
C(6)–C(1)	1·372	C(6)–C(1)–C(2)	120·4
C(1)–O(1)	1·380	C(6)–C(1)–O(1)	122·5
C(2)–O(2)	1·364	C(2)–C(1)–O(1)	117·1
O(1)–H–O(2′)	2·795	C(1)–C(2)–O(2)	121·0
O(2)–H–O(1′)	2·806	C(3)–C(2)–O(2)	118·6

+0·007, C(4) −0·002, C(5) −0·003, C(6) +0·006 Å. The two oxygen atoms are −0·014 and −0·056 Å respectively out of this plane, this slight distortion from rigorous overall planarity probably being enforced by packing considerations.

The mean C–C bond length is 1·385 Å, and the mean C–O bond length 1·372 Å, which compare with the values of 1·39 and 1·36 Å respectively found in resorcinol (Robertson, 1936). The mean hydrogen bond length (2·801 Å) is however rather longer than the mean (2·70 Å) in the resorcinol structure.

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Short Communications

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The space group and unit cell of cyclohex-2-ene-1, 4-dione.

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With an interest in the conformation of cyclohex-2-ene-1,4-dione, $C_6H_6O_2$, prepared by Garbisch (1965), we started the crystal structure determination of this compound. Short needle-shaped crystals were enclosed in capillaries to prevent sublimation. From precession photographs (Mo $K\alpha$, $\lambda=0{\cdot}7107$ Å), the monoclinic cell dimensions were found to be

$$a=6{\cdot}92\pm0{\cdot}01\ \text{Å}$$
$$b=6{\cdot}82\pm0{\cdot}01$$
$$c=6{\cdot}07\pm0{\cdot}01$$
$$\beta=97^\circ 20'\pm10'$$

where a is the needle axis. From systematic extinctions ($0k0$, $k=2n+1$; $h0l$, $h+l=2n+1$) the space group was determined to be $P2_1/n$. By comparison with the molecular volumes of quinol (132 Å^3/molecule) and quinhydrone (2 × 126 Å^3/molecule), it was concluded that there are two molecules per unit cell, since this would give a molecular volume for cyclohex-2-ene-1,4-dione of 142.1 Å^3. Also, crystals sink very slowly in glycerin, which suggests that the density is slightly greater than 1·28 g.cm^{-3}, the value for glycerin. For $Z=2$, the calculated density is 1·285 g.cm^{-3}.

With two molecules per unit cell, for space group $P2_1/n$, the molecule must lie on a center of symmetry. Since no reasonable structure for cyclohex-2-ene-1,4-dione contains a center of symmetry, the structure must be disordered. Therefore, we plan no further work on this compound.

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