This results in intramolecular O(ether)—O(carbonyl) interactive distances of 2·643 (10) (*A*) and 2·637 (10) Å (*B*) compared with 2·51 and 2·50 Å found in the previous determination of 2-CPA (Chandrasekhar & Pattabhi, 1977). The range and mean for this distance over 19 phenoxyalkanoic acids, irrespective of their conformation, is 2·605 Å [(2,4,5-trichlorophenoxy)acetic acid] to 2·775 Å [2-(4-chlorophenoxy)propionic acid]; mean 2·711 Å (Kennard *et al.*, 1981). Bond distances and angles for both molecules *A* and *B* are essentially the same and are similar to those found in the previous determination and in all other members of the series. This includes the usual distortion of the *exo*-C(1) bond angles [*A*, 125·3 (8), 115·0 (8); *B*, 125·0 (8), 114·1 (8)°]. The structure is comparable to that of (±)-2-(2-chlorophenoxy)propionic acid (Smith, Kennard & White, 1981) in that there is no evidence of orientational disorder in the carboxylic acid dimer unit, the C=O and C—O(H) distances being 1·230 (11), 1·213 (11); 1·288 (11), 1·305 (11) Å respectively, and the C—C=O and C—C—OH angles 123·6 (8), 125·5 (8); 113·0 (8), 110·1 (8)°. In 2-CPA the angle between the benzene plane and the plane of the carboxylic acid group in the same molecule is 5·6 (8) and 8·2 (8)° for *A* and *B* respectively.

Packing of molecules *A* and *B* in the triclinic cell gives a pseudo $2_1/c$ relationship (x,y,z; $x, \frac{1}{2} - y, \frac{1}{2} + z$) and results in an absence of observed reflections of the $0k0$ set for k = odd and a paucity of observed reflections of the $h0l$ set for l = odd (for l = 1, 3, 5, number of observed reflections = 11, 5, 0 respectively; maximum $|F_o| = 23{\cdot}0$ for $\bar{6}03$). The reason for this subtle deviation from perfect $P2_1/c$ space symmetry is not understood since all other examples, even of lower molecular symmetry, pack with only one molecular asymmetric unit in either triclinic or monoclinic cells.

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Structure of 1,4-Diacetyl-2,5-dimethoxybenzene

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Abstract. $C_{12}H_{14}O_4$, monoclinic, $P2_1/n$, $a = 9{\cdot}618$ (3), $b = 14{\cdot}097$ (4), $c = 4{\cdot}118$ (1) Å, $\beta = 98{\cdot}6$ (1)°, $Z = 2$, $D_m = 1{\cdot}33$, $D_x = 1{\cdot}337$ Mg m^{-3}. The structure was solved by direct methods and refined by least squares to a final $R = 0{\cdot}053$ for 785 observed reflections. The molecules are centrosymmetric and are linked by van der Waals forces only.

Introduction. It has been reported (Madeja-Kotkowska, 1974) that 2,5-diacetylhydroquinone (I) can be very easily reduced to 3,6-dihydro-2,5-diacetylhydroquinone (II). The reduction of its methoxy derivative 1,4-diacetyl-2,5-dimethoxybenzene (III) in the same experimental conditions does not give any stable dihydro derivative. Short communications about structures (I) and (II) have been published previously (Wajsman, Grabowski, Stępień & Cygler, 1978*a*,*b*). The crystal-structure investigation of (III) was undertaken to elucidate the above statement concerning chemical reactivity and compare the molecular structures of these compounds.

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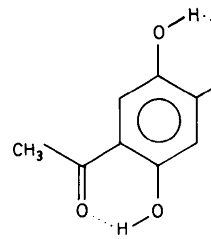
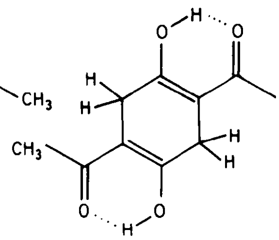
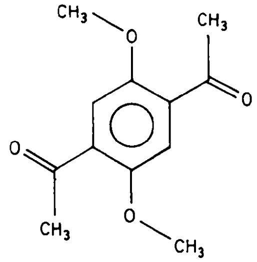


(I)



(II)



(III)

Crystals of (III) suitable for X-ray analysis were obtained by evaporation from ethanol. The space group $P2_1/n$ was determined from systematic absences observed on Weissenberg photographs. The intensities were collected on a Syntex $P2_1$ diffractometer with a graphite monochromator using Cu $K\alpha$ radiation. 935 independent reflections within the θ range 1 to 71 ° were measured by the θ–2θ scan mode. 785 of them with $I > 3\sigma(I)$ were treated as observed. The structure was solved by direct methods using *SHELX* 76 (Sheldrick, 1976). Difference syntheses gave all H atoms. The structure was refined by the full-matrix least-squares method with anisotropic temperature factors for C and O atoms and isotropic temperature factors for H atoms. The final reliability index was $R = 0{\cdot}053$. Final atomic coordinates with e.s.d.'s are given in Table 1 with atoms numbered as shown in Fig. 1.* Bond lengths and bond angles are shown in Fig. 1.

Table 1. *Final fractional coordinates* ($\times 10^4$, *for* H $\times 10^3$) *and mean isotropic temperature factors with e.s.d.'s in parentheses*

For non-H atoms $U_{\rm iso} = \frac{1}{3}(U_{11} + U_{22} + U_{33})$.

	x	y	z	$U_{\rm iso}$ (Å^2)
C(1)	1364 (2)	9927 (1)	−759 (4)	0·041 (1)
C(2)	794 (2)	9168 (1)	810 (4)	0·040 (1)
C(3)	575 (2)	739 (1)	−1523 (5)	0·042 (1)
C(21)	1524 (2)	8250 (1)	1862 (5)	0·050 (1)
C(22)	3042 (3)	8101 (2)	1727 (8)	0·066 (2)
C(11)	3333 (2)	615 (2)	−2811 (6)	0·059 (1)
O(1)	2693 (2)	9825 (1)	−1477 (4)	0·058 (1)
O(21)	853 (2)	7625 (1)	2879 (8)	0·102 (2)
H(31)	92 (2)	123 (2)	−246 (6)	0·046 (5)
H(111)	281 (3)	77 (2)	−500 (8)	0·071 (8)
H(112)	339 (2)	111 (2)	−117 (7)	0·061 (7)
H(113)	430 (3)	39 (2)	−273 (6)	0·062 (7)
H(221)	362 (4)	859 (3)	301 (11)	0·127 (14)
H(222)	324 (3)	826 (2)	−29 (9)	0·075 (8)
H(223)	326 (4)	749 (3)	273 (9)	0·081 (9)

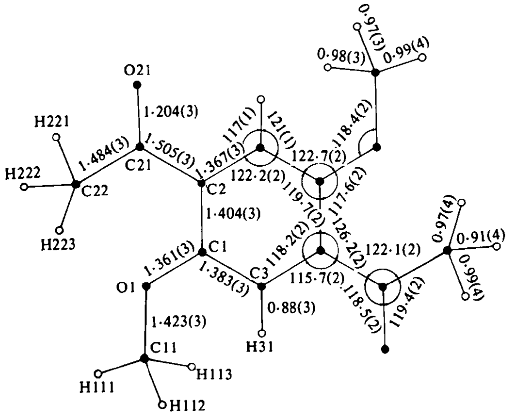


Fig. 1. Bond lengths (Å), angles (°) and atom-numbering scheme.

Discussion. The molecule of 1,4-diacetyl-2,5-dimethoxybenzene is centrosymmetric. The planarity of the molecule is disturbed by the rotation of the $-\mathrm{COCH_3}$ group about the C(2)–C(21) bond. The angle of rotation is 8·9 °.

Intramolecular hydrogen bonds are not possible and the molecule is a typical benzene derivative. In contrast, in (I) and (II) the $-\mathrm{COCH_3}$ groups are in a configuration that enables the formation of strong intramolecular hydrogen bonds. Two quasi-aromatic rings, formed thus, increase the reactivity of atoms in positions 3 and 6 in the benzene ring. The molecules of (III) are linked by van der Waals forces only.

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35987 (6 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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