were from *International Tables for X-ray Crystallography* (1974, Vol. IV). The *PARST* program (Nardelli, 1983) was used for molecular geometry calculations. The atomic parameters are given in Table 1.* The bond lengths, valence angles and geometrical parameters of selected intermolecular interactions are given in Table 2. A perspective view of the title compound is given in Fig. 1. The crystal packing along the *a* axis is shown in Fig. 2.

Related literature. The geometry at S(1) conforms to that found for related *p*-tolylsulfinyl derivatives (de la Camp & Hope, 1970; Hua, Badejo, McCann & Takusagawa, 1987). In the epoxidic ring the C(2)—O(1) and C(3)—O(1) bond lengths of 1.453 (8) and 1.435 (9) Å, respectively, are close to the accepted value of 1.446 (14) Å for C(sp^3)—O bonds in epoxides with any substitution (Allen, Kennard, Watson, Brammer, Orpen & Taylor, 1987). In the structure two short contacts, C—H···O and C—H···F, exist, which can be reasonably described as hydrogen bonds (Taylor & Kennard, 1982).

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54857 (7 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: GE0292]

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Structure of 4,6-Diacetylresorcinol

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Abstract. $C_{10}H_{10}O_4$, $M_r = 194.19$, monoclinic, $P2_1/c$, $a = 7.089$ (1), $b = 11.361$ (1), $c = 11.656$ (1) Å, $\beta = 100.45$ (3)°, $V = 922.92$ (1) Å^3, $Z = 4$, $D_m = 1.410$ (5), $D_x = 1.397$ Mg m^{-3}, λ(Cu $K\alpha$) = 1.5418 Å, μ(Cu $K\alpha$) = 0.89 mm^{-1}, $T = 300$ K, $F(000) = 408$, final $R = 0.057$ for 1701 observed reflections. The molecule is almost planar, with O(9) and O(12) of the acetyl groups deviating by 0.074 (1) and 0.071 (2) Å from the mean plane of the benzene ring. The bond lengths and bond angles of the benzene ring are normal. There are intramolecular hydrogen bonds between O(9) and H(14) and between O(12) and H(13); there are no intermolecular hydrogen bonds. The molecules are packed in layers parallel to the *ac* plane and are held together essentially by van der Waals interactions.

Experimental. The title compound is obtained by the reaction of acetic anhydride and resorcinol in the presence of $ZnCl_2$; crystals suitable for X-ray analysis were grown in benzene solution by slow evaporation; orange crystal 0.3 × 0.4 × 0.2 mm mounted on an Enraf–Nonius CAD-4 diffractometer, $\omega/2\theta$ scan; cell dimensions from least-squares refinement of 25 reflections in the 2θ range 0 to 55°; density measurements by flotation technique using potassium iodide

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Table 1. *Fractional coordinates* ($\times 10^4$) *and equivalent isotropic temperature factors* ($Å^2 \times 10^4$) *for non-H atoms; e.s.d.'s are given in parentheses*

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq}
C(1)	3057 (2)	6414 (1)	35 (1)	433 (5)
C(2)	2310 (2)	6121 (1)	−1113 (1)	480 (6)
C(3)	1750 (2)	4981 (1)	−1393 (1)	441 (5)
C(4)	1900 (2)	4095 (1)	−517 (1)	405 (5)
C(5)	2618 (2)	4418 (1)	629 (1)	395 (5)
C(6)	3207 (2)	5564 (1)	935 (1)	402 (5)
C(7)	4003 (2)	5890 (1)	2144 (1)	483 (5)
C(8)	4111 (4)	5019 (2)	3107 (2)	654 (7)
O(9)	4586 (2)	6904 (1)	2374 (1)	641 (5)
C(10)	1315 (2)	2881 (1)	−838 (1)	478 (5)
C(11)	1426 (3)	1949 (2)	75 (2)	594 (7)
O(12)	727 (3)	2619 (1)	−1865 (1)	720 (6)
O(13)	1067 (2)	4726 (1)	−2517 (1)	642 (5)
O(14)	3612 (2)	7534 (1)	269 (1)	611 (5)

Table 2. *Bond lengths* (Å), *bond angles* (°) *and hydrogen-bonding parameters; e.s.d.'s are in parentheses*

C(1)—C(2)	1.387 (2)	C(5)—C(6)	1.394 (2)
C(1)—C(6)	1.416 (2)	C(6)—C(7)	1.467 (2)
C(1)—O(14)	1.345 (2)	C(7)—C(8)	1.487 (3)
C(2)—C(3)	1.376 (2)	C(7)—O(9)	1.238 (2)
C(3)—C(4)	1.425 (2)	C(10)—C(11)	1.493 (2)
C(3)—O(13)	1.343 (2)	C(10)—O(12)	1.230 (2)
C(4)—C(5)	1.389 (2)		
C(4)—C(10)	1.469 (2)		

C(6)—C(1)—C(2)	121.1 (1)	C(7)—C(6)—C(5)	121.8 (1)
O(14)—C(1)—C(2)	118.0 (1)	C(8)—C(7)—C(6)	121.0 (2)
O(14)—C(1)—C(6)	120.9 (1)	O(9)—C(7)—C(6)	119.8 (2)
C(3)—C(2)—C(1)	119.9 (1)	O(9)—C(7)—C(8)	119.1 (2)
C(4)—C(3)—C(2)	120.9 (1)	O(13)—C(3)—C(2)	118.2 (2)
O(13)—C(3)—C(4)	120.9 (2)	C(11)—C(10)—C(4)	120.5 (1)
C(5)—C(4)—C(3)	118.0 (1)	O(12)—C(10)—C(4)	120.3 (2)
C(10)—C(4)—C(3)	120.0 (1)	O(12)—C(10)—C(11)	119.2 (2)
C(10)—C(4)—C(5)	122.0 (1)	C(6)—C(5)—C(4)	122.3 (1)
C(5)—C(6)—C(1)	117.9 (1)	C(7)—C(6)—C(1)	120.3 (1)

X—H···Y	X—H (Å)	H···Y (Å)	X···Y (Å)	X—H···Y (°)
O(14)—H(14)···O(9)	1.055 (29)	1.534 (30)	2.528	155 (3)
O(13)—H(13)···O(12)	0.959 (34)	1.644 (33)	2.536	153 (3)

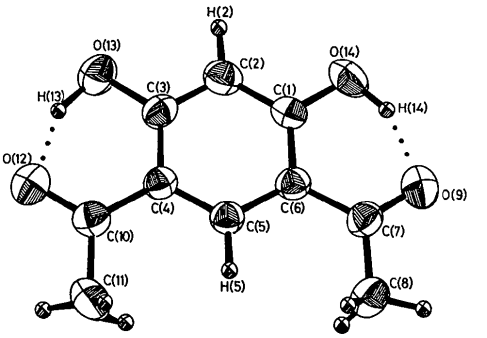

Fig. 1. A perspective view of the molecule with 50% probability thermal ellipsoids.

solution; intensity data collected using Cu $K\alpha$ radiation to a maximum $\theta = 75°$; three standard reflections ($12\bar{1}$, $\bar{1}02$, $2\bar{1}2$) monitored after every 50 reflections; h, -8 to 8, k, 0 to 14, l, 0 to 13; total of 3850 reflections of which 1853 were unique ($R_{int} = 0.019$); 1701 reflections with $I \geq 3\sigma(I)$ were considered observed; data corrected for Lorentz–polarization effects. The structure was solved using *MULTAN*84 (Main, Germain & Woolfson, 1984) and *DIRDIF* (Beurskens, Bosman, Doesberg, Van den Hark, Prick, Noordik, Beurskens, Gould & Parthasarathy, 1984); all the H atoms were located from difference Fourier maps; full-matrix least-squares refinement with anisotropic thermal parameters for non-H atoms and isotropic thermal parameters for H atoms using *SHELX*76 (Sheldrick, 1976); 167 parameters refined and 10 reflections per parameter; final $R = 0.0570$ and $wR = 0.0781$, $w = [\sigma^2(F) + gF^2]^{-1}$, $g = 0.0011$, σ's based on counting statistics; the refinement terminated when shift/e.s.d.'s for non-H atoms was less than 0.1; the minimum and maximum residual electron densities in the final difference Fourier map were -0.10 and 0.11 e $Å^{-3}$, respectively. The final positional parameters of the non-H atoms with U_{eq} are given in Table 1.* The *ORTEP* (Johnson, 1965) plot of the molecule with 50% probability ellipsoids is shown in Fig. 1; the bond lengths, bond angles and hydrogen-bonding parameters are given in Table 2.

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