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#### Key indicators

Single-crystal X-ray study

$T = 168$  K

Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å

$R$  factor = 0.039

$wR$  factor = 0.100

Data-to-parameter ratio = 12.9

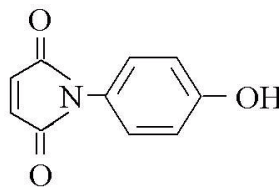
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## *N*-(4-Hydroxyphenyl)maleimide

In the title compound,  $\text{C}_{10}\text{H}_7\text{NO}_3$ , the maleimide ring is rotated by  $52.75(5)^\circ$  with respect to the phenyl ring. There is a weak  $\text{O}-\text{H}\cdots\text{O}$  intermolecular hydrogen bond between the hydroxyl group and one of the maleimide O atoms, with an  $\text{O}\cdots\text{O}$  distance of  $2.820(2)$  Å.

#### Comment

The title compound, (I), is an important building block in the formation of novel polymer materials (Park & Jang, 1992; Caulfield & Solomon, 1999). As shown in Fig. 1, the dihedral angle between the phenyl ring and the maleimide ring is  $52.75(5)^\circ$ . The rotation of the maleimide ring with respect to the phenyl ring can be attributed to the steric repulsion from adjacent carbonyl moieties. An example of a similar structure without carbonyls, 1-phenyl-3-carbethoxy-4-hydroxypyrrolone, does not show this rotation of the five-membered ring relative to the phenyl group (Paulus & Rivo, 1988). The torsion angles  $\text{C}2-\text{C}1-\text{N}1-\text{C}10$  and  $\text{C}6-\text{C}1-\text{N}1-\text{C}7$  are  $51.07(14)^\circ$  and  $54.67(14)^\circ$ , respectively. The reason for two different torsion angles is that the maleimide ring is tilted slightly away from the central axis of the molecule defined by the atoms O1, C4, C1, and N1. A packing diagram (Fig. 2) indicates that molecules stack along the  $a$  axis with identical orientation, aligning the phenyl and maleimide rings.



(I)

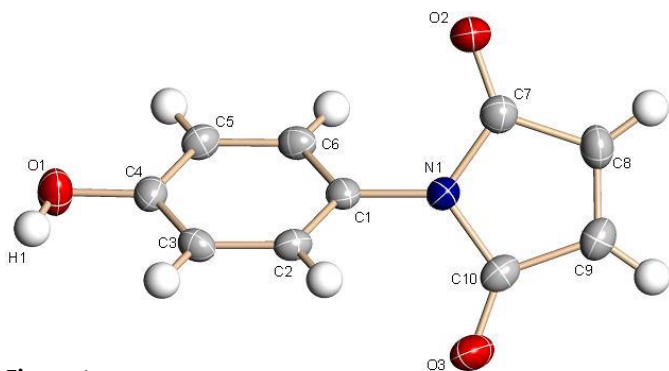
The elongation of the  $\text{N}1-\text{C}1$  bond relative to the other  $\text{N}-\text{C}$  bonds is consistent with single-bond nature of N attached to a phenyl ring (Table 1). The bond angles show a distorted trigonal planar coordination for N1. The  $\text{C}7-\text{N}1-\text{C}10$  bond angle of  $109.22(14)^\circ$  is consistent with a typical tetrahedral coordination. The  $\text{C}1-\text{N}1-\text{C}10$  and  $\text{C}1-\text{N}1-\text{C}7$  bond angles [ $125.55(13)$  and  $125.12(13)^\circ$ , respectively] reveal the distortion of the bonds away from a regular trigonal planar coordination.

Comparison of  $\text{C}-\text{O}$  bond lengths reveals the double-bond character of  $\text{C}7-\text{O}2$  and  $\text{C}10-\text{O}3$ , compared to the single bond  $\text{C}4-\text{O}1$ . The slightly longer  $\text{C}7-\text{O}2$  bond, relative to  $\text{C}10-\text{O}3$ , is attributed to the intermolecular hydrogen bond (Fig. 3 and Table 2), whereas the O3 atom has no hydrogen interaction (nearest H atom is H2 at  $2.570$  Å). The  $\text{O}1-$

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**Figure 1**

Molecular structure of (I). Displacement ellipsoids are shown at the 50% probability level.

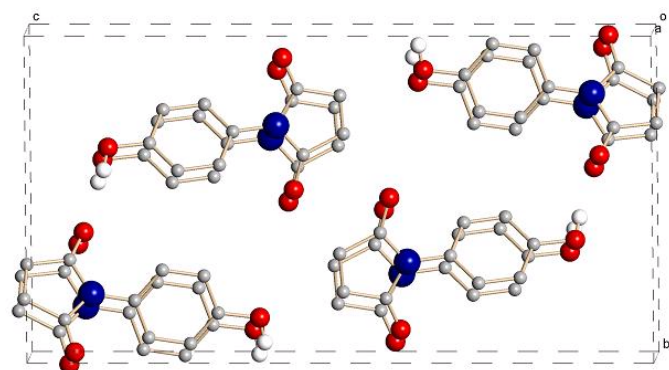
H1...O2 hydrogen bonds form a ribbon structure along the *b* axis.

## Experimental

The title compound, (I), was prepared in two steps. In the first step, 1 mole of maleic anhydride was reacted with 1 mole of 4-aminophenol in excess acetone. The product, *cis*-4-[(4-hydroxyphenyl)amino]-4-oxo-2-butenoic acid, was obtained in nearly quantitative yield as an insoluble yellow precipitate which was isolated by filtration and washed with excess acetone. 4-Hydroxyphenyl maleimide was then obtained in the second step by cyclodehydration. One mole of *cis*-4-[(4-hydroxyphenyl)amino]-4-oxo-2-butenoic acid, 0.26 mole of sulfuric acid, and 0.2 mole of phosphorus pentoxide were dissolved in excess dimethylformamide and reacted at 343 K for a minimum of 4 h. The solution was poured over ice to obtain crude product, (I), as a solid orange precipitate. The precipitate was isolated by filtration and washed with excess water and dried. The crystals of (I) were grown from an isopropyl alcohol solution; yield *ca* 60%. The melting point of the crystals is 455–457 K.

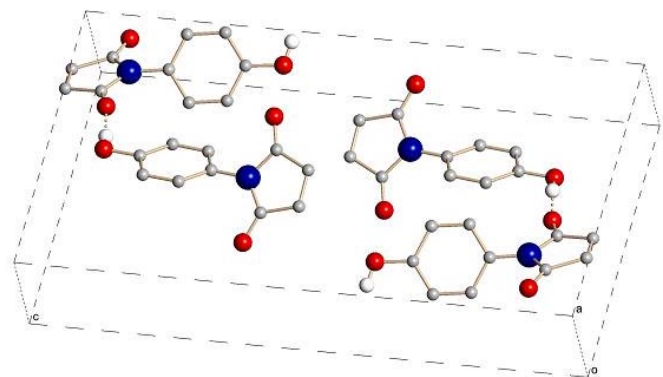
### Crystal data

$C_{10}H_7NO_3$	$D_x = 1.489 \text{ Mg m}^{-3}$
$M_r = 189.17$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 753 reflections
$a = 3.864 (1) \text{ \AA}$	$\theta = 2.0\text{--}23.3^\circ$
$b = 10.691 (3) \text{ \AA}$	$\mu = 0.11 \text{ mm}^{-1}$
$c = 20.461 (5) \text{ \AA}$	$T = 168 (2) \text{ K}$
$\beta = 93.036 (5)^\circ$	Needle, orange
$V = 844.0 (4) \text{ \AA}^3$	$0.18 \times 0.08 \times 0.08 \text{ mm}$
$Z = 4$	



**Figure 2**

Packing diagram for (I), viewed down the *a* axis.



**Figure 3**

Packing diagram showing the intermolecular hydrogen bond. Several molecules in the packing diagram were removed for clarity.

### Data collection

Bruker AXS CCD diffractometer	1252 reflections with $I > 2\sigma(I)$
$\omega$ and $\varphi$ scans	$R_{\text{int}} = 0.035$
Absorption correction: multi-scan (SADABS; Sheldrick, 1999)	$\theta_{\text{max}} = 26.2^\circ$
$T_{\text{min}} = 0.94, T_{\text{max}} = 0.99$	$h = -4 \rightarrow 3$
4735 measured reflections	$k = -13 \rightarrow 13$
1685 independent reflections	$l = -20 \rightarrow 25$

### Refinement

Refinement on $F^2$	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.039$	$w = 1/[\sigma^2(F_o^2) + (0.0506P)^2]$
$wR(F^2) = 0.100$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{\text{max}} = 0.002$
1685 reflections	$\Delta\rho_{\text{max}} = 0.17 \text{ e \AA}^{-3}$
131 parameters	$\Delta\rho_{\text{min}} = -0.20 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

N1—C7	1.390 (2)	O3—C10	1.208 (2)
N1—C10	1.408 (2)	C7—C8	1.483 (2)
N1—C1	1.434 (2)	C8—C9	1.318 (2)
O1—C4	1.371 (2)	C9—C10	1.486 (2)
O2—C7	1.215 (2)		
C7—N1—C10	109.22 (14)	N1—C7—C8	106.66 (14)
C7—N1—C1	125.12 (13)	O3—C10—N1	124.72 (16)
C10—N1—C1	125.55 (13)	O3—C10—C9	128.99 (15)
O2—C7—N1	125.29 (16)	N1—C10—C9	106.29 (14)
O2—C7—C8	128.05 (16)		

**Table 2**

Hydrogen-bonding geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
O1—H1...O2 <sup>i</sup>	0.87 (2)	1.95 (2)	2.820 (2)	175.17 (15)

Symmetry code: (i)  $\frac{5}{2} - x, \frac{1}{2} + y, \frac{3}{2} - z$ .

H-atom positions were idealized, with H atoms riding on the atoms to which they were attached. These idealized H atoms had their isotropic displacement parameters fixed at 1.2 or 1.5 times the  $U_{\text{eq}}$  of the C atoms to which they were bonded. The H1 hydrogen was the exception, in that it was located from a difference Fourier map; its

atomic positional parameters and isotropic displacement parameter were refined.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT-Plus* (Bruker, 2001); program(s) used to solve structure: *SHELXTL* (Bruker, 1998); program(s) used to refine structure: *XSHELL* (Bruker, 2000); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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