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## Key indicators

Single-crystal X-ray study  
 $T = 273$  K  
Mean  $\sigma(C-C) = 0.002$  Å  
 $R$  factor = 0.053  
 $wR$  factor = 0.158  
Data-to-parameter ratio = 18.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

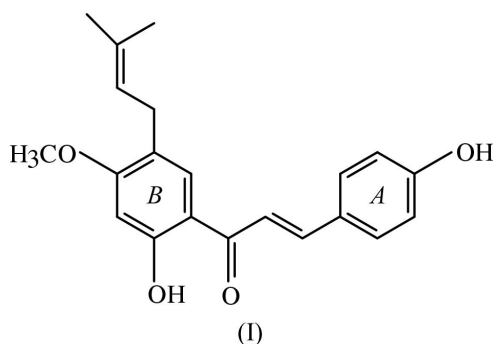
## A polymorph of bavachalcone

The title compound, 1-[2-hydroxy-4-methoxy-5-(3-methylbut-2-enyl)phenyl]-3-(4-hydroxyphenyl)prop-2-en-1-one (also known as bavachalcone),  $C_{21}H_{22}O_4$ , is a polymorphic form of a previously reported structure [Bhalla *et al.* (1968). *Tetrahedron Lett.* **20**, 2401–2406]. The molecules in both polymorphs exhibit nearly identical conformations. In each polymorph, strong intra- and intermolecular hydrogen-bonded chains, involving the hydroxyl groups, are formed. A weak  $C-H \cdots O$  interaction is seen in the present structure, but was not observed in the previously reported polymorph.

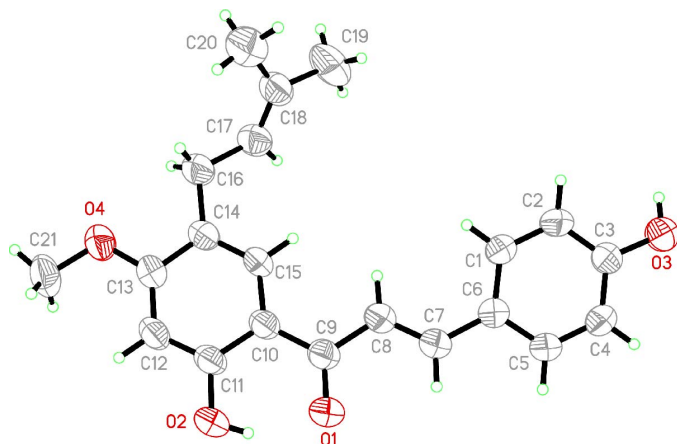
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## Comment

Despite being a structurally simple group of compounds, chalcones have displayed an impressive array of pharmacological activities (Dimmock *et al.*, 1999). Chalcones are open-chain flavonoids in which the two aromatic rings are joined by a three-carbon chain, *viz.* an  $\alpha,\beta$ -unsaturated carbonyl system. These bright-orange compounds are found in many plant parts, but most conspicuously in flowers.

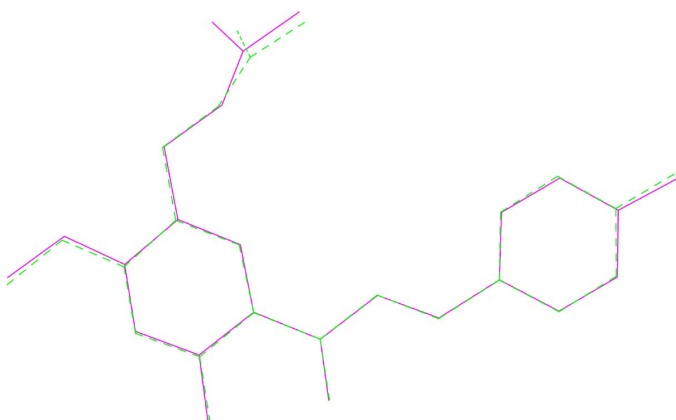


*Psoralea corylifolia* L. (Fabaceae) is distributed from India to southeast Asia. The seeds of this plant, a well known traditional Chinese medicine, are widely applied for the cure of gynaecological bleeding, vitiligo and psoriasis (Yin *et al.*, 2004). The seed oil is used externally for the treatment of leucodermy and leprosy in Indian folk medicine (Kondo *et al.*, 1990). The seed extract is also suggested to be useful as a remedy for bone fracture, osteomalacia and osteoporosis (Miura *et al.*, 1996). In the course of our search for bioactive compounds from botanical sources, the title compound, bavachalcone, (I), was isolated from the seed extract of *P. corylifolia*. However, bavachalcone was reported previously from the same plant (Bhalla *et al.*, 1968) and its crystal structure [polymorph 1,  $a = 9.631$  (5),  $b = 11.068$  (3),  $c = 17.915$  (5) Å and  $\beta = 105.27$  (3)°] was determined (Roychowdhury & Roychowdhury, 1988). Incidentally, the title compound, (I), recrystallized from isopropyl alcohol,



**Figure 1**

A view of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.



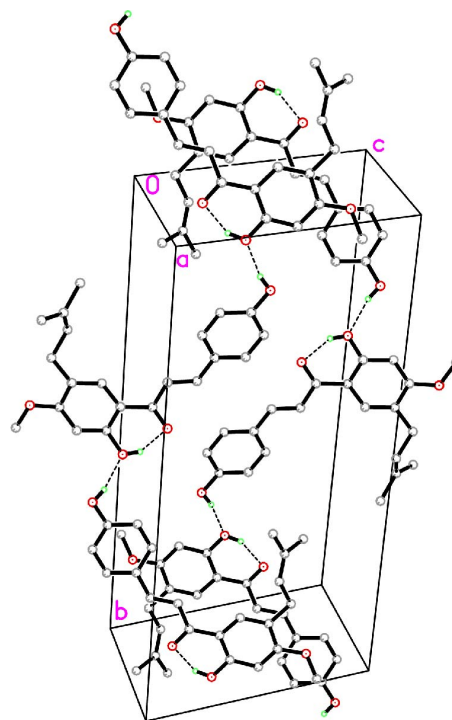
**Figure 2**

A least-squares fit of polymorph 2 (solid lines) and polymorph 1 (dashed lines).

crystallized in the same space group  $P2_1/c$ , but differed in the unit-cell dimensions (polymorph 2); its structure is reported here.

The key geometric parameters defining the chalcone structures, in the enone entity  $O=C-C=C$  (Table 1), are equal, within experimental error, to those in polymorph 1. The geometric data given hereafter in square brackets refer to polymorph 1. In both polymorphs, the enone system adopts an *s-cis* conformation, as seen from the  $C7-C8-C9=O1$  torsion angle of  $3.4(2)^\circ$  [ $0.8(1)^\circ$ ].

The molecule on the whole may not be considered as strictly planar in either polymorph. The two benzene rings on either side of the central enone system subtend a dihedral angle of  $17.8(1)^\circ$  [ $12.15(1)^\circ$ ]. From a molecular perspective, the polymorphs differ slightly in the orientation of the isoprenoid side chain attached to ring *B* (see scheme). A least-squares fit of the enone plane (r.m.s. deviation =  $0.014 \text{ \AA}$ ) of polymorphs 1 and 2 is shown in Fig. 2. The isoprenoid side chain is in an extended conformation, [ $C14-C16-C17-C18 = -132.30(19)^\circ$  [ $-124.9(1)^\circ$ ]] and forms an angle of  $60.1(1)^\circ$  [ $68.8(1)^\circ$ ] with the plane of ring *B*. There is a weak inter-



**Figure 3**

Perspective view of part of the unit cell contents of the title compound.  $O-H \cdots O$  hydrogen bonds are indicated by dashed lines. H atoms attached to C atoms have been omitted for clarity.

molecular  $C-H \cdots O$  interaction (Table 2), which is not observed in polymorph 1.

Ring *A* is twisted slightly with respect to the enone plane  $C1/C6/C7/C8$  [ $12.7(2)^\circ$  [ $12.6(1)^\circ$ ]], whereas ring *B* is coplanar [ $C8-C9-C10-C15 = 0.8(2)^\circ$  [ $-1.4(1)^\circ$ ]] with it. There is an intramolecular  $O-H \cdots O$  hydrogen bond between the hydroxyl group and the enone carbonyl O atom, a common feature observed in similar substituted chalcones.

It is noteworthy that structure-activity studies on the antileishmanial activity of chalcones by Nielsen *et al.* (1998) emphasized that it is important that ring *B* is *para*-substituted with oxygenated and non-bulky substituents for desirable activity. Recently, Liu *et al.* (2003) reported that antileishmanial activity is associated with 4'-hydroxy-substituted *B* rings and hetero/polyaromatic *A* rings, while chalcones with good antimalarial activity have alkoxyated *B* rings and electron-deficient *A* rings. It appears that different physicochemical and structural requirements exist for chalcones towards these activities.

In the crystal packing, glide-related molecules are linked by an intermolecular hydrogen bond between the two hydroxyl groups, forming chains along the *b* axis (Fig. 3). As observed in polymorph 1, hydroxyl group O2 plays a dual role as donor and acceptor in the hydrogen-bonding network.

## Experimental

The shade-dried seeds of the plant were powdered and extracted with petroleum ether in a Soxhlet apparatus for 24 h. The solvent was evaporated under reduced pressure in a rotary flash evaporator,

yielding a residue. The residue was absorbed on silica gel and subjected to column chromatography over silica gel (60–120 mesh), and eluted with a gradient of ethyl acetate in petroleum ether to yield fractions monitored by thin-layer chromatography. Later, one of the major fractions was rechromatographed using silica gel to obtain the compound in a pure form. The spectroscopic data of this compound are identical to those of bavachalcone (Bhalla *et al.*, 1968). An orange crystalline powder recrystallized from isopropyl alcohol gave block-shaped crystals suitable for X-ray studies.

Crystal data

$C_{21}H_{22}O_4$	$D_x = 1.214 \text{ Mg m}^{-3}$
$M_r = 338.39$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 5568 reflections
$a = 7.5025 (5) \text{ \AA}$	$\theta = 2.6\text{--}27.0^\circ$
$b = 22.5080 (15) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$c = 11.1960 (7) \text{ \AA}$	$T = 273 (2) \text{ K}$
$\beta = 101.639 (1)^\circ$	Block, orange
$V = 1851.8 (2) \text{ \AA}^3$	$0.30 \times 0.18 \times 0.11 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	3210 reflections with $I > 2\sigma(I)$
$\omega$ scans	$R_{\text{int}} = 0.020$
Absorption correction: none	$\theta_{\text{max}} = 28.0^\circ$
15 814 measured reflections	$h = -9 \rightarrow 9$
4328 independent reflections	$k = -28 \rightarrow 29$
	$l = -14 \rightarrow 14$

Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0863P)^2 + 0.191P]$
$R[F^2 > 2\sigma(F^2)] = 0.053$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.158$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.04$	$\Delta\rho_{\text{max}} = 0.26 \text{ e \AA}^{-3}$
4328 reflections	$\Delta\rho_{\text{min}} = -0.15 \text{ e \AA}^{-3}$
231 parameters	
H-atom parameters constrained	

Table 1

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

O1—C9	1.2506 (16)	C14—C16	1.5053 (19)
O3—C3	1.3568 (17)	C17—C18	1.312 (2)
O4—C13	1.3521 (17)		
C5—C6—C7	119.61 (12)	C17—C16—C14	114.80 (14)
C11—C10—C9	119.63 (12)	C18—C17—C16	128.19 (18)
C15—C14—C16	122.71 (12)		

Table 2

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2—H2A $\cdots$ O1	0.82	1.75	2.488 (2)	148
O3—H3 $\cdots$ O2 <sup>i</sup>	0.82	1.94	2.743 (2)	166
C17—H17 $\cdots$ O2 <sup>ii</sup>	0.93	2.70	3.470 (2)	140

Symmetry codes: (i)  $2 - x, y - \frac{1}{2}, \frac{1}{2} - z$ ; (ii)  $1 - x, 1 - y, -z$ .

H atoms were included in calculated positions ( $C-H = 0.93\text{--}0.98 \text{ \AA}$ ) using a riding model, with  $U_{\text{iso}}(H)$  values set at 1.2 (O and CH H atoms) and 1.5 ( $\text{CH}_3$ ) times the  $U_{\text{eq}}$  values of the parent atoms. The methyl and hydroxyl groups were allowed to rotate but not to tip.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL/PC (Sheldrick, 1990); software used to prepare material for publication: SHELXL97 and PARST (Nardelli, 1995).

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