# A cocrystal of 1-(4-chlorophenyl)-3-(3,4,5-trimethoxyphenyl)prop-2-en-1-one and 3-(3-chloro-4,5-dimethoxyphenyl)-1-(4-chlorophenyl)prop-2-en-1-one (0.95:0.05)

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Key indicators

Single-crystal X-ray study
$T = 100$ K
Mean σ(C–C) = 0.001 Å
Disorder in main residue
R factor = 0.043
wR factor = 0.117
Data-to-parameter ratio = 34.9

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

In the title cocrystal, 1-(4-chlorophenyl)-3-(3,4,5-trimethoxyphenyl)prop-2-en-1-one–3-(3-chloro-4,5-dimethoxyphenyl)-1-(4-chlorophenyl)prop-2-en-1-one (19/1), $0.95C_{18}H_{17}ClO_4 \cdot 0.05C_{17}H_{14}Cl_2O_3$, the crystal packing is stabilized by weak intermolecular C—H$\cdots$O and π–π interactions.

Comment

Chalcone derivatives are receiving increasing interest from several disciplines because of their photochemical properties (Matsushima & Kageyama, 1985; Toda *et al.*, 1998), their structural features, and their second- and third-order nonlinear optical properties (Fichou *et al.*, 1988; Kitaoka *et al.*, 1990; Uchida *et al.*, 1998; Goto *et al.*, 1991; Patil *et al.*, 2006*a*,*b*; Zhang *et al.*, 1990; Zhao *et al.*, 2000). In order to obtain detailed information on the molecular conformation of the trimethoxy-substituted chalcone (I) in the solid state, its X-ray crystal structure was determined. Refinement revealed a cocrystal with (I) as the major component (95%) but with a minor component in which the methoxy substituent at C12 has been replaced by a Cl atom (II) (Fig. 1). The compounds crystallize in a centrosymmetric space group and therefore have no second-order nonlinear optical properties.

(I)

(II)
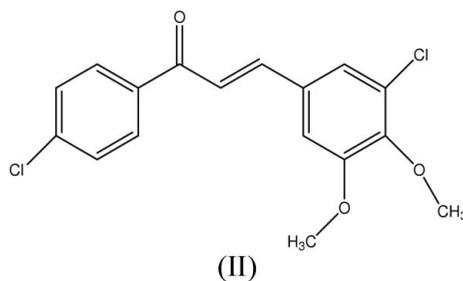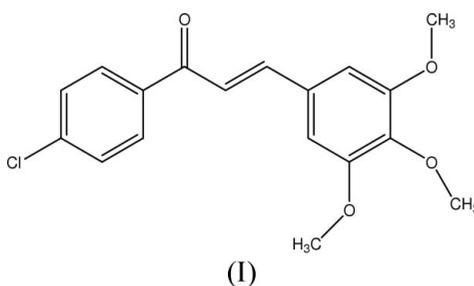
Bond lengths and angles show normal values (Allen *et al.*, 1987) and are comparable to those reported in related structures (Ng *et al.*, 2006*a*,*b*; Patil *et al.*, 2006*a*,*b*). The enone group and the two benzene rings of the chalcone are each planar, with a maximum deviation of 0.047 (1) Å from O1/C7–C9,
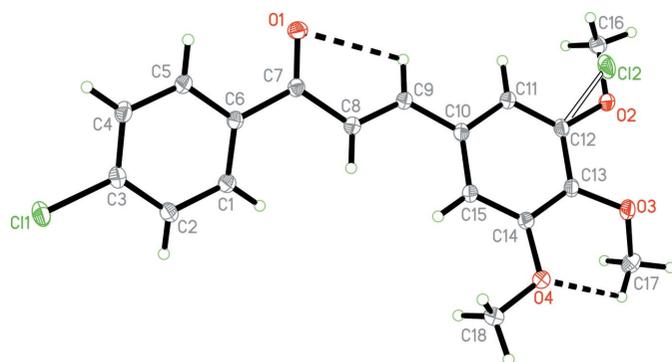
Figure 1
The structure of the title compound, showing 50% probability displacement ellipsoids and the atomic numbering. The dashed lines indicate hydrogen bonds. The hollow bond is to the Cl atom of the minor cocrystal component.
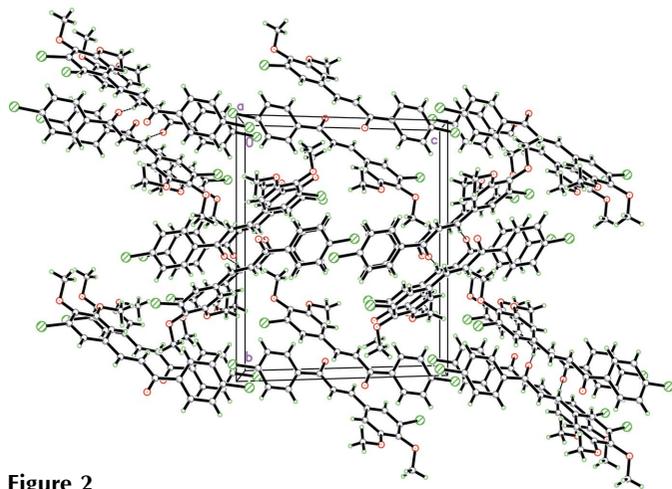
Figure 2
The crystal packing of (I), viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

0.013 (1) Å from C1–C6, and 0.017 (1) Å from C10–C15 for atoms C8, C6 and C14, respectively.

The short H1A···H8A (2.21 Å) contact causes the C1—C6—C7 [123.28 (7)°] and C6—C7—C8 [118.37 (7)°] bond angles to deviate significantly from 120°. Similarly, the short H8A···H15A (2.17 Å) contact produces a slight widening of the C9—C10—C15 angle to [121.83 (7)°]. These result in the molecules being twisted about the C6—C7 bond for both (I) and (II). The least-squares plane through the enone group makes dihedral angles of 16.94 (3) and 13.61 (3)° with the C1–C6 and C10–C15 benzene rings, respectively. The dihedral angles between the two benzene rings is 30.28 (3)°.

The methoxy groups at C12 and C14 are almost coplanar with the attached rings, with torsion angles C16—O2—C12—C11 = −4.1 (1)° and C18—O4—C14—C15 = 3.0 (1)°, while the methoxy group at C13 is twisted away from the attached ring, with a torsion angle C17—O3—C13—C14 = 56.4 (1)°.

In the crystal structure, atom O1 is involved in both intra- and intermolecular hydrogen bonds (Table 1). The intra-molecular C17—H17C···O4 and C9—H9A···O1 interactions generate $S(5)$ and $S(6)$ ring motifs, respectively (Bernstein *et al.*,1995). The crystal packing is further stabilized by weak intermolecular π–π interactions, involving the C1–C6 ring at

(x, y, z) and the C10–C15 ring at (1 − x, −y, 1 − z); the centroid–centroid distance is 3.8771 (5) Å.

Experimental

Crystal data

$0.95C_{18}H_{17}ClO_4 \cdot 0.05C_{17}H_{14}Cl_2O_3$	$Z = 4$
$M_r = 332.99$	$D_x = 1.403$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 7.5517$ (1) Å	$\mu = 0.27$ mm^{-1}
$b = 15.9894$ (2) Å	$T = 100.0$ (1) K
$c = 13.6914$ (2) Å	Block, yellow
$\beta = 107.491$ (1)°	$0.48 \times 0.29 \times 0.20$ mm
$V = 1576.76$ (4) Å^3	

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer	54905 measured reflections
ω scans	8205 independent reflections
Absorption correction: multi-scan ($SADABS$; Bruker, 2005)	6659 reflections with $I > 2\sigma(I)$
$T_{min} = 0.829$, $T_{max} = 0.949$	$R_{int} = 0.048$
	$\theta_{max} = 37.5°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0593P)^2 + 0.3778P]$
$R[F^2 > 2\sigma(F^2)] = 0.043$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.118$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.03$	$\Delta\rho_{max} = 0.60$ e Å^{-3}
8205 reflections	$\Delta\rho_{min} = -0.29$ e Å^{-3}
235 parameters	
Only H-atom coordinates refined	

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9A···O1	0.93	2.51	2.829 (1)	100
C17—H17C···O4	0.96	2.34	2.866 (1)	114
C9—H9A···O1^i	0.93	2.51	3.414 (1)	166
C18—H18C···O1^{ii}	0.96	2.59	3.526 (1)	164

Symmetry codes: (i) $-x$, $-y$, $-z + 1$; (ii) $-x + 1$, $-y$, $-z + 1$.

H atoms were placed in calculated positions, with C—H distances in the range 0.93–0.96 Å, and refined as riding. The U_{iso} values were freely refined. The ratio of (I) and (II) in the cocrystal was obtained by refinement as 0.954 (3):0.046 (3).

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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