Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS
ISSN 2056-9890

# Crystal structure and Hirshfeld surface analysis of (2*E*)-3-(3-chlorophenyl)-1-(3,4-dimethoxyphenyl)-prop-2-en-1-one

S. N. Sheshadri,[a] Zeliha Atioğlu,[b] Mehmet Akkurt,[c]* C. S. Chidan Kumar,[d] Ching Kheng Quah,[e] B. P. Siddaraju[f] and M. K. Veeraiah[g]

[a]Department of Chemistry, GSSS Institute of Engineering & Technology for Women, Mysuru 570 016, Karnataka, India, [b]İlke Education and Health Foundation, Cappadocia University, Cappadocia Vocational College, The Medical Imaging Techniques Program, 50420 Mustafapaşa, Ürgüp, Nevşehir, Turkey, [c]Department of Physics, Faculty of Sciences, Erciyes University, 38039 Kayseri, Turkey, [d]Department of Engineering Chemistry, Vidya Vikas Institute of Engineering & Technology, Visvesvaraya Technological University, Alanahalli, Mysuru 570 028, Karnataka, India, [e]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, [f]Department of Chemistry, Cauvery Institute of Technology, Mandya 571 402, Karnataka, India, and [g]Department of Chemistry, Sri Siddhartha Institute of Technology, Tumkur 572 105, Karnataka, India. *Correspondence e-mail: akkurt@erciyes.edu.tr

Received 25 May 2018
Accepted 6 June 2018

Edited by D.-J. Xu, Zhejiang University (Yuquan Campus), China

**Keywords:** crystal structure; 3,4-dimethoxyphenyl ring; 3-chlorophenyl ring; Hirshfeld surface analysis; hydrogen contacts; ring motif.

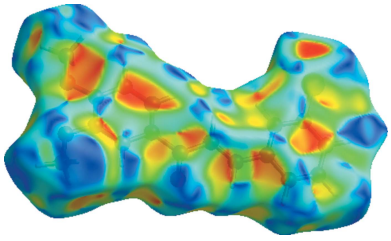
**CCDC reference**: 1847705

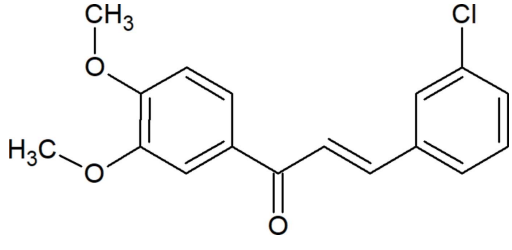
**Supporting information**: this article has supporting information at journals.iucr.org/e

In title compound, $C_{17}H_{15}ClO_3$, the dihedral angle between the benzene and chlorophenyl rings is 18.46 (7)°. In the crystal, molecules are linked by C—H···O hydrogen contacts, enclosing an $R_2^2(14)$ ring motif, and by a further C—H···O hydrogen contact, forming a two-dimensional supramolecular structure extending along the direction parallel to the *ac* plane. Hirshfeld surface analysis shows that van der Waals interactions constitute the major contribution to the intermolecular interactions, with H···H contacts accounting for 36.2% of the surface.

## 1. Chemical context

Materials exhibiting two photon absorption (TPA) have wide applications such as frequency-up lasing, multi-photon microscopy, three-dimensional fluorescence imaging, eye and sensor protection. Materials with potential non-linear optical (NLO) properties have significant applications in the field of photonics. Chalcone and its derivatives have attracted significant attention in the past few years because of their availability of high optical non-linearities resulting from the significant delocalization of π-conjugated electron clouds throughout the chalcone system, providing a large charge-transfer axis with appropriate substituents on the terminal aromatic rings. The second harmonic generation (SHG) efficiency of these compounds is due to the strong intermolecular electron–donor–acceptor interactions, which may also enhance the non-linear optical (NLO) properties. With the possibility of developing low-cost, large-area and flexible electronic devices, π-conjugated systems have been studied extensively for their optoelectronic properties (Chandra Shekhara Shetty *et al.*, 2016, 2017).





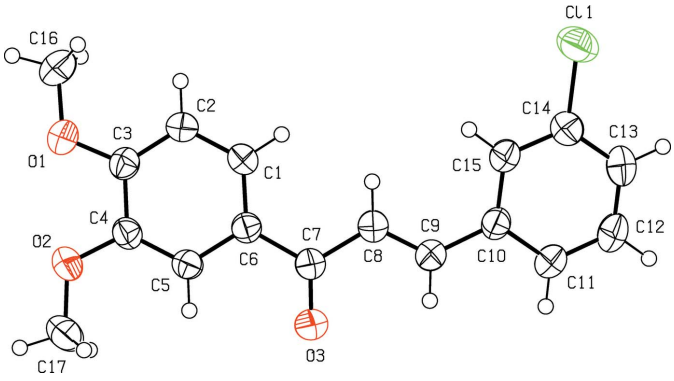



**Figure 1**
The molecular structure of the title compound, showing the atom labelling and displacement ellipsoids drawn at the 50% probability level.

## 2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. The title compound is constructed from two aromatic rings (chlorophenyl and terminal methoxyphenyl rings), which are linked by a C═C—C(═O)—C enone bridge. Compared to the nearly coplanar arrangement of rings in the title compound, the molecule is twisted substantially [C5—C6—C7—O3 = 3.5 (2) ° and O3—C7—C8—C9 = 10.5 (2) °] about the enone bridge, which may arise from steric repulsion with the *ortho*-O2 atom. Hence, the dihedral angle between the 3,4-methoxyphenyl and chlorophenyl rings increases to 18.46 (7)°. The C atoms of the methoxy groups are close to the plane of their attached ring: deviations of C16 and C17 are 0.252 (2) and 0.038 (2) Å, respectively. The bond lengths and angles are comparable with those in the similar compounds (*E*)-3-(3,4-dimethoxyphenyl)-1-(1-hydroxynaphthalen-2yl)prop-2-en-1-one (Ezhilarasi *et al.*, 2015), (*E*)-1-(3-bromophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one (Escobar *et al.*, 2012) and (*E*)-3-(2-bromophenyl)-1-(3,4-dimethoxyphenyl)prop-2-en-1-one (Li *et al.*, 2012).

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C11—H11*A*···O3$^{i}$ | 0.93 | 2.54 | 3.417 (2) | 157 |
| C15—H15*A*···O2$^{ii}$ | 0.93 | 2.54 | 3.4378 (18) | 163 |

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

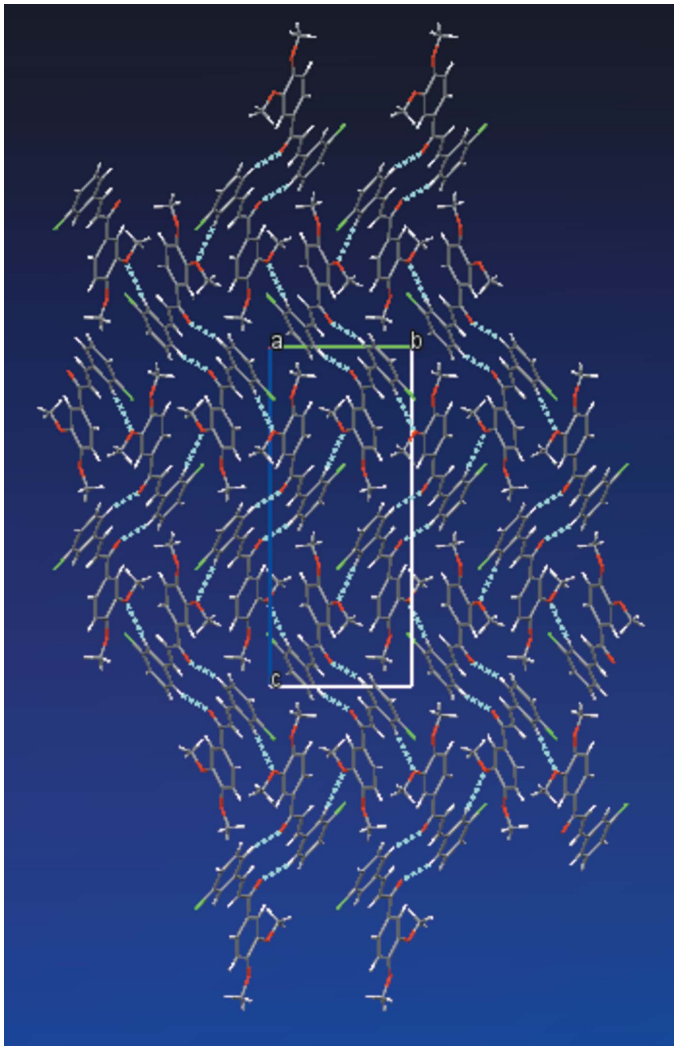



**Figure 2**
A view along the *a* axis of the crystal packing of the title compound. Intermolecular interactions are shown as dashed lines.

## 3. Supramolecular features and Hirshfeld surface analysis

In the crystal, molecules are linked by C—H···O hydrogen contacts (Table 1, Fig. 2), enclosing an $R_2^2(14)$ ring motif, and by a further C—H···O hydrogen contact, forming a three-dimensional structure extending in the *a*- and *c*-axis directions.

Hirshfeld surfaces and fingerprint plots were generated for the title compound based on the crystallographic information file (CIF) using *CrystalExplorer* (McKinnon *et al.*, 2007). Hirshfeld surfaces enable the visualization of intermolecular interactions by different colors and color intensity, repre-

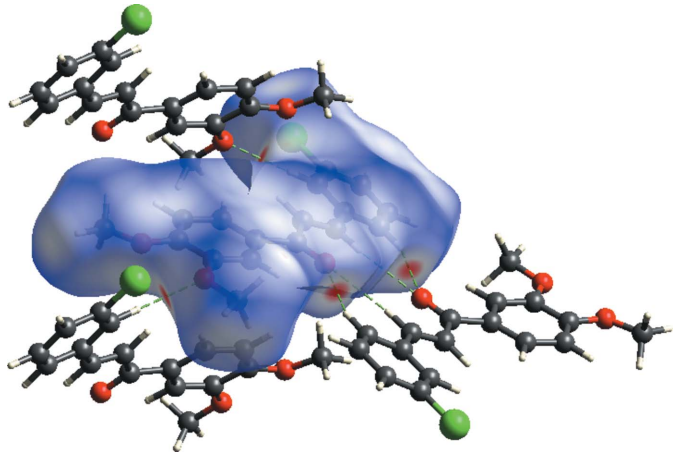


**Figure 3**
View of the three-dimensional Hirshfeld surface of the title compound mapped over $d_{norm}$.

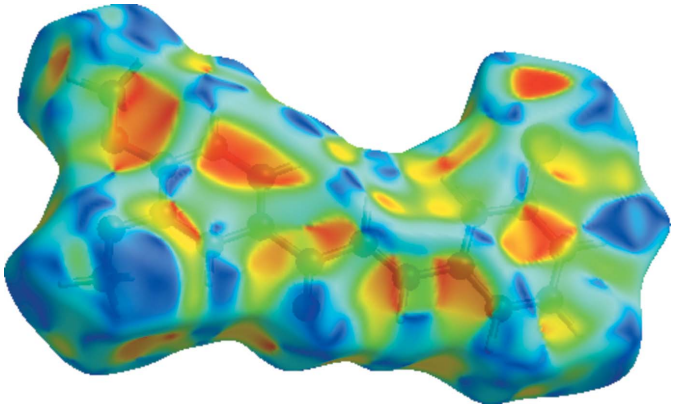


**Figure 4**
Hirshfeld surface of the title complex plotted over shape-index.

**Table 2**
Summary of short interatomic contacts (Å) in the title compound.

| Contact | Distance | Symmetry operation |
|---|---|---|
| Cl1···H17*B* | 3.05 | $-1+x, 1+y, z$ |
| Cl1···C1 | 3.4666 (15) | $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$ |
| O2···H15*A* | 2.54 | $\frac{3}{2}-x, -\frac{1}{2}+y, \frac{1}{2}-z$ |
| O1···H17*A* | 2.86 | $\frac{5}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$ |
| H17*C*···C10 | 2.88 | $1+x, y, z$ |
| H11*A*···O3 | 2.54 | $1-x, 1-y, -z$ |
| C1···Cl1 | 3.4666 (15) | $\frac{1}{2}-x, -\frac{1}{2}+y, \frac{1}{2}-z$ |
| H15*A*···O2 | 2.54 | $\frac{3}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$ |
| C10···H17*C* | 2.88 | $-1+x, y, z$ |
| C13···C13 | 3.497 (2) | $-x, 2-y, -z$ |
| H13*A*···H16*A* | 2.46 | $-\frac{3}{2}+x, \frac{3}{2}-y, -\frac{1}{2}+z$ |
| H16*A*···H13*A* | 2.46 | $\frac{3}{2}+x, \frac{3}{2}-y, \frac{1}{2}+z$ |
| H17*A*···O1 | 2.86 | $\frac{5}{2}-x, -\frac{1}{2}+y, \frac{1}{2}-z$ |
| H17*B*···Cl1 | 3.05 | $1+x, -1+y, z$ |

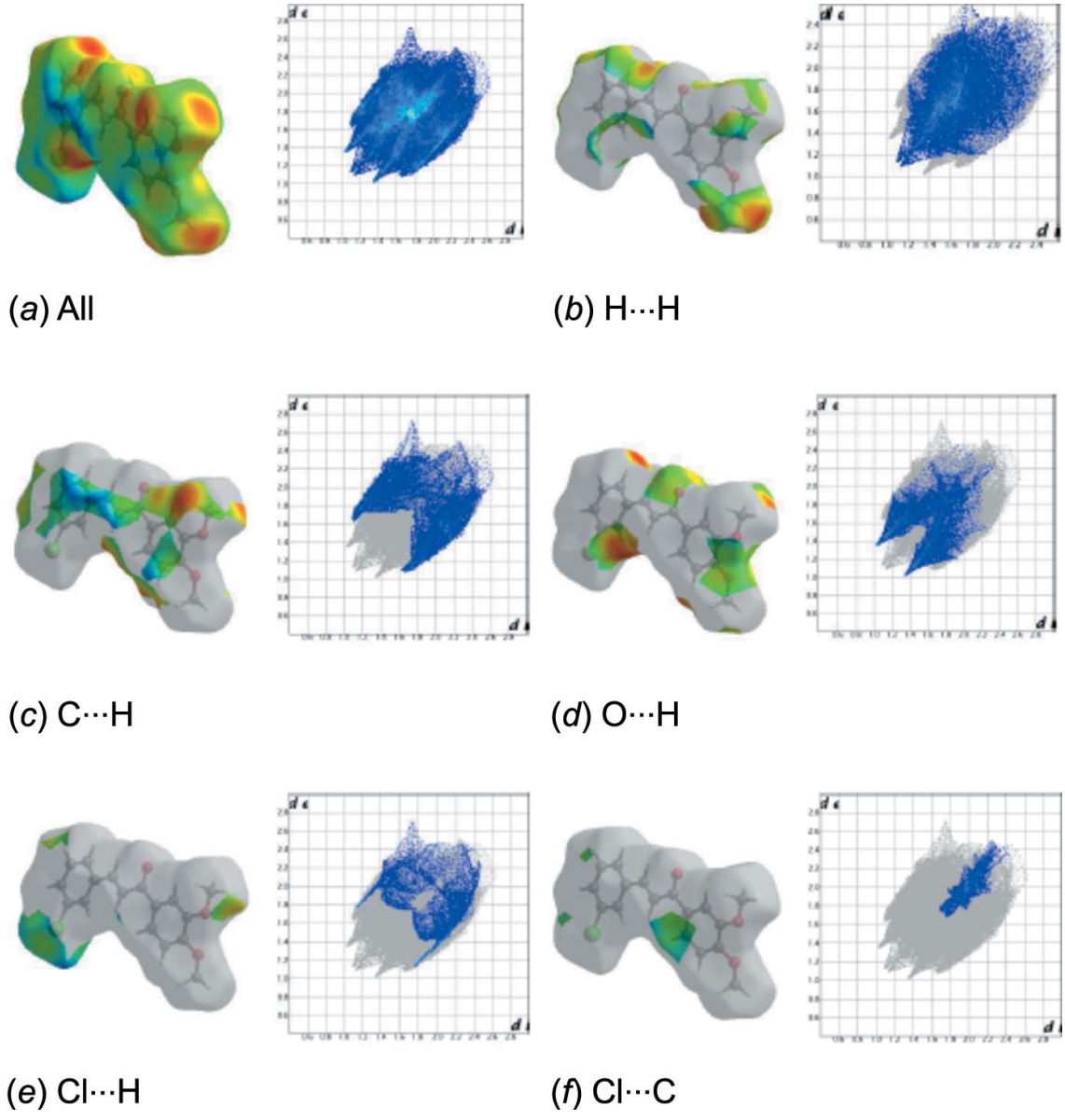



**Figure 5**
The two-dimensional fingerprint plots of the title compound, showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) C···H, (*d*) O···H, (*e*) Cl···H and (*f*) Cl···C interactions [$d_e$ and $d_i$ represent the distances from a point on the Hirshfeld surface to the nearest atoms outside (external) and inside (internal) the surface, respectively].

Table 3
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{17}H_{15}ClO_3$ |
| $M_r$ | 302.74 |
| Crystal system, space group | Monoclinic, $P2_1/n$ |
| Temperature (K) | 294 |
| $a, b, c$ (Å) | 9.0491 (4), 8.3257 (4), 20.2857 (9) |
| $\beta$ (°) | 99.484 (1) |
| $V$ (Å$^3$) | 1507.44 (12) |
| $Z$ | 4 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.26 |
| Crystal size (mm) | 0.40 × 0.24 × 0.19 |
| | |
| Data collection | |
| Diffractometer | Bruker APEXII CCD |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 39332, 5506, 3732 |
| $R_{int}$ | 0.036 |
| $(\sin \theta/\lambda)_{max}$ (Å$^{-1}$) | 0.758 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.049, 0.158, 1.01 |
| No. of reflections | 5506 |
| No. of parameters | 190 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.31, −0.43 |

Computer programs: *APEX2* and *SAINT* (Bruker, 2007), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

senting short or long contacts and indicating the relative strength of the interactions. Figs. 3 and 4 show the Hirshfeld surfaces mapped over $d_{norm}$(−0.16 to 1.25 a.u.) and shape-index (−1.0 to 1.0 a.u.).

In Fig. 3, the spots near atoms O2 and O3 result from the C15—H15*A*···O2$^{ii}$ and C11—H11*A*···O3$^{i}$ interactions significant in the molecule packing of the title compound (Table 1). Some of the short intermolecular contacts for the title compound are listed in Table 2. The Hirshfeld surfaces illustrated in Fig. 3 also reflect the involvement of different atoms in the intermolecular interactions through the appearance of blue and red regions around the participating atoms, which correspond to positive and negative electrostatic potential, respectively.

The overall two-dimensional fingerprint plot for the title compound and those delineated into H···H, C···H/H···C, H···O/O···H, Cl···H/H···Cl and Cl···C/C···Cl contacts are illustrated in Fig. 5; the percentage contributions from the different interatomic contacts to the Hirshfeld surfaces are as follows: H···H (36.2%), C···H/H···C (24.6%), H···O/O···H (19.2%), Cl···H/H···Cl (10.5%), Cl···C/C···Cl (5.8%), C···C (3.3%), Cl···O/O···Cl (0.3%) and O···C/C···O (0.2%), as shown in the two-dimensional fingerprint plots in Fig. 4.

## 4. Synthesis and crystallization

The reagents and solvents for the synthesis were obtained from the Aldrich Chemical Co. and were used without additional purification. 1-(3,4-Dimethoxyphenyl) ethanone (0.01 mol) and 3-chlorobenzaldehyde (0.01 mol) were dissolved in 20 ml methanol. A catalytic amount of NaOH was added to the solution dropwise with vigorous stirring. The reaction mixture was stirred for about 5–6 h at room temperature. The progress of the reaction was monitored by TLC. The formed crude products were filtered, washed successively with distilled water and recrystallized from ethanol to get the title chalcone. Crystals suitable for X-ray diffraction studies were obtained from acetone solution by slow evaporation at room temperature. The melting point (371–373 K) was determined by a Stuart Scientific (UK) apparatus. The purity of the compound was confirmed by thin layer chromatography using Merck silica gel 60 F254 coated aluminum plates.

## 5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. C-bound H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C) for C—H and C—H = 0.96 Å and $U_{iso}$(H) = 1.5$U_{eq}$(C) for methyl H atoms.

## Acknowledgements

The authors extend their appreciation to the Vidya Vikas Research & Development Centre for the facilities and their encouragement.

## References

Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chandra Shekhara Shetty, T., Chidan Kumar, C. S., Gagan Patel, K. N., Chia, T. S., Dharmaprakash, S. M., Ramasami, P., Umar, Y., Chandraju, S. & Quah, C. K. (2017). *J. Mol. Struct.* **1143**, 306–317.
Chandra Shekhara Shetty, T., Raghavendra, S., Chidan Kumar, C. S. & Dharmaprakash, S. M. (2016). *Appl. Phys. B*, **122**, 205.
Escobar, C. A., Trujillo, A., Howard, J. A. K. & Fuentealba, M. (2012). *Acta Cryst.* E**68**, o887.
Ezhilarasi, K. S., Reuben Jonathan, D., Vasanthi, R., Revathi, B. K. & Usha, G. (2015). *Acta Cryst.* E**71**, o371–o372.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Li, Z., Wang, Y., Peng, K., Chen, L. & Chu, S. (2012). *Acta Cryst.* E**68**, o776.
McKinnon, J. J., Jayatilaka, D. & Spackman, M. A. (2007). *Chem. Commun.* pp. 3814–3816.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

# supporting information

*Acta Cryst.* (2018). E**74**, 935-938 [https://doi.org/10.1107/S205698901800837X]

## Crystal structure and Hirshfeld surface analysis of (2*E*)-3-(3-chlorophenyl)-1-(3,4-dimethoxyphenyl)prop-2-en-1-one

**S. N. Sheshadri, Zeliha Atioğlu, Mehmet Akkurt, C. S. Chidan Kumar, Ching Kheng Quah, B. P. Siddaraju and M. K. Veeraiah**

### Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009).

### (2*E*)-3-(3-Chlorophenyl)-1-(3,4-dimethoxyphenyl)prop-2-en-1-one

*Crystal data*

$C_{17}H_{15}ClO_3$
$M_r = 302.74$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 9.0491$ (4) Å
$b = 8.3257$ (4) Å
$c = 20.2857$ (9) Å
$\beta = 99.484$ (1)°
$V = 1507.44$ (12) Å$^3$
$Z = 4$
$F(000) = 632$
$D_x = 1.334$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8862 reflections
$\theta = 2.7$–$30.8°$
$\mu = 0.26$ mm$^{-1}$
$T = 294$ K
Block, yellow
0.40 × 0.24 × 0.19 mm

*Data collection*

Bruker APEXII CCD diffractometer
$\varphi$ and $\omega$ scans
39332 measured reflections
5506 independent reflections
3732 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 32.6°$, $\theta_{min} = 2.0°$
$h = -13 \rightarrow 13$
$k = -12 \rightarrow 12$
$l = -30 \rightarrow 30$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.158$
$S = 1.01$
5506 reflections
190 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0758P)^2 + 0.3034P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.31$ e Å$^{-3}$
$\Delta\rho_{min} = -0.43$ e Å$^{-3}$

*Special details*

**Geometry**. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

**Refinement**. Refinement on $F^2$ for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses of fit S are based on $F^2$, conventional R-factors R are based on F, with F set to zero for negative $F^2$. The observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs etc. and is not relevant to the choice of reflections for refinement. R-factors based on $F^2$ are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | −0.02901 (5) | 1.02517 (6) | 0.15452 (2) | 0.0710 (2) |
| O1 | 1.07019 (12) | 0.65283 (15) | 0.35402 (5) | 0.0576 (3) |
| O2 | 1.13649 (12) | 0.52216 (16) | 0.24887 (6) | 0.0634 (4) |
| O3 | 0.67255 (12) | 0.57110 (17) | 0.07167 (5) | 0.0632 (4) |
| C1 | 0.72153 (15) | 0.73479 (17) | 0.23869 (7) | 0.0458 (4) |
| C2 | 0.82535 (15) | 0.73642 (17) | 0.29717 (7) | 0.0463 (4) |
| C3 | 0.96267 (14) | 0.66310 (15) | 0.29901 (6) | 0.0420 (3) |
| C4 | 0.99836 (14) | 0.59071 (16) | 0.24086 (6) | 0.0415 (3) |
| C5 | 0.89499 (14) | 0.59023 (15) | 0.18335 (6) | 0.0405 (3) |
| C6 | 0.75372 (13) | 0.66142 (14) | 0.18154 (6) | 0.0394 (3) |
| C7 | 0.64331 (14) | 0.64884 (17) | 0.11929 (7) | 0.0444 (4) |
| C8 | 0.49469 (15) | 0.72588 (18) | 0.11575 (7) | 0.0495 (4) |
| C9 | 0.38379 (15) | 0.69300 (18) | 0.06640 (6) | 0.0452 (4) |
| C10 | 0.22936 (14) | 0.75164 (16) | 0.05882 (6) | 0.0424 (3) |
| C11 | 0.12555 (17) | 0.69543 (19) | 0.00574 (7) | 0.0525 (4) |
| C12 | −0.02283 (18) | 0.7421 (2) | −0.00148 (8) | 0.0610 (5) |
| C13 | −0.07040 (16) | 0.8446 (2) | 0.04383 (8) | 0.0564 (5) |
| C14 | 0.03261 (16) | 0.90063 (17) | 0.09633 (7) | 0.0470 (4) |
| C15 | 0.18120 (15) | 0.85720 (16) | 0.10468 (7) | 0.0447 (3) |
| C16 | 1.0326 (2) | 0.7046 (3) | 0.41599 (8) | 0.0826 (7) |
| C17 | 1.1814 (2) | 0.4431 (2) | 0.19409 (9) | 0.0669 (6) |
| H1A | 0.62888 | 0.78375 | 0.23788 | 0.0550* |
| H2A | 0.80242 | 0.78689 | 0.33512 | 0.0560* |
| H5A | 0.91867 | 0.54216 | 0.14504 | 0.0490* |
| H8A | 0.47900 | 0.79854 | 0.14872 | 0.0590* |
| H9A | 0.40642 | 0.62539 | 0.03295 | 0.0540* |
| H11A | 0.15612 | 0.62577 | −0.02523 | 0.0630* |
| H12A | −0.09113 | 0.70376 | −0.03734 | 0.0730* |
| H13A | −0.17036 | 0.87545 | 0.03911 | 0.0680* |
| H15A | 0.24886 | 0.89746 | 0.14035 | 0.0540* |
| H16A | 1.11764 | 0.69130 | 0.45069 | 0.1240* |
| H16B | 1.00432 | 0.81587 | 0.41282 | 0.1240* |
| H16C | 0.95044 | 0.64175 | 0.42628 | 0.1240* |
| H17A | 1.28064 | 0.40096 | 0.20705 | 0.1000* |
| H17B | 1.11330 | 0.35669 | 0.17988 | 0.1000* |

| | | | | |
|---|---|---|---|---|
| H17C | 1.18073 | 0.51778 | 0.15799 | 0.1000* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0650 (3) | 0.0704 (3) | 0.0809 (3) | 0.0083 (2) | 0.0216 (2) | −0.0176 (2) |
| O1 | 0.0518 (6) | 0.0735 (7) | 0.0440 (5) | 0.0124 (5) | −0.0028 (4) | −0.0031 (5) |
| O2 | 0.0487 (6) | 0.0881 (8) | 0.0518 (6) | 0.0278 (5) | 0.0039 (4) | −0.0044 (5) |
| O3 | 0.0479 (6) | 0.0898 (8) | 0.0505 (6) | 0.0088 (5) | 0.0038 (4) | −0.0226 (6) |
| C1 | 0.0400 (6) | 0.0500 (7) | 0.0472 (7) | 0.0080 (5) | 0.0064 (5) | −0.0052 (5) |
| C2 | 0.0462 (7) | 0.0506 (7) | 0.0420 (6) | 0.0063 (5) | 0.0074 (5) | −0.0069 (5) |
| C3 | 0.0425 (6) | 0.0424 (6) | 0.0398 (6) | 0.0012 (5) | 0.0028 (5) | 0.0021 (5) |
| C4 | 0.0382 (6) | 0.0423 (6) | 0.0441 (6) | 0.0057 (5) | 0.0073 (5) | 0.0033 (5) |
| C5 | 0.0404 (6) | 0.0425 (6) | 0.0396 (6) | 0.0032 (5) | 0.0093 (5) | −0.0010 (5) |
| C6 | 0.0382 (6) | 0.0393 (5) | 0.0403 (6) | 0.0007 (4) | 0.0057 (4) | −0.0005 (4) |
| C7 | 0.0384 (6) | 0.0510 (7) | 0.0434 (6) | 0.0014 (5) | 0.0055 (5) | −0.0046 (5) |
| C8 | 0.0426 (6) | 0.0562 (8) | 0.0476 (7) | 0.0070 (6) | 0.0014 (5) | −0.0090 (6) |
| C9 | 0.0424 (6) | 0.0539 (7) | 0.0388 (6) | 0.0028 (5) | 0.0050 (5) | −0.0017 (5) |
| C10 | 0.0401 (6) | 0.0469 (6) | 0.0384 (6) | −0.0001 (5) | 0.0011 (5) | 0.0006 (5) |
| C11 | 0.0493 (7) | 0.0603 (8) | 0.0449 (7) | 0.0006 (6) | −0.0014 (6) | −0.0093 (6) |
| C12 | 0.0468 (8) | 0.0733 (10) | 0.0568 (8) | −0.0030 (7) | −0.0092 (6) | −0.0092 (7) |
| C13 | 0.0379 (6) | 0.0642 (9) | 0.0643 (9) | 0.0002 (6) | −0.0002 (6) | 0.0022 (7) |
| C14 | 0.0452 (7) | 0.0445 (6) | 0.0519 (7) | −0.0005 (5) | 0.0094 (5) | 0.0004 (5) |
| C15 | 0.0419 (6) | 0.0476 (6) | 0.0427 (6) | −0.0022 (5) | 0.0016 (5) | −0.0030 (5) |
| C16 | 0.0814 (12) | 0.1149 (17) | 0.0452 (8) | 0.0267 (12) | −0.0080 (8) | −0.0161 (10) |
| C17 | 0.0583 (9) | 0.0781 (11) | 0.0673 (10) | 0.0238 (8) | 0.0189 (8) | −0.0001 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C14 | 1.7310 (15) | C12—C13 | 1.374 (2) |
| O1—C3 | 1.3570 (16) | C13—C14 | 1.376 (2) |
| O1—C16 | 1.422 (2) | C14—C15 | 1.376 (2) |
| O2—C4 | 1.3593 (17) | C1—H1A | 0.9300 |
| O2—C17 | 1.408 (2) | C2—H2A | 0.9300 |
| O3—C7 | 1.2273 (18) | C5—H5A | 0.9300 |
| C1—C2 | 1.387 (2) | C8—H8A | 0.9300 |
| C1—C6 | 1.3832 (18) | C9—H9A | 0.9300 |
| C2—C3 | 1.3794 (19) | C11—H11A | 0.9300 |
| C3—C4 | 1.4088 (17) | C12—H12A | 0.9300 |
| C4—C5 | 1.3698 (17) | C13—H13A | 0.9300 |
| C5—C6 | 1.4041 (17) | C15—H15A | 0.9300 |
| C6—C7 | 1.4792 (18) | C16—H16A | 0.9600 |
| C7—C8 | 1.4810 (19) | C16—H16B | 0.9600 |
| C8—C9 | 1.3241 (19) | C16—H16C | 0.9600 |
| C9—C10 | 1.4643 (19) | C17—H17A | 0.9600 |
| C10—C11 | 1.3884 (19) | C17—H17B | 0.9600 |
| C10—C15 | 1.4005 (19) | C17—H17C | 0.9600 |
| C11—C12 | 1.382 (2) | | |

| | | | |
|---|---|---|---|
| C3—O1—C16 | 117.66 (12) | C6—C1—H1A | 120.00 |
| C4—O2—C17 | 118.77 (12) | C1—C2—H2A | 120.00 |
| C2—C1—C6 | 120.98 (13) | C3—C2—H2A | 120.00 |
| C1—C2—C3 | 119.94 (13) | C4—C5—H5A | 120.00 |
| O1—C3—C2 | 124.80 (12) | C6—C5—H5A | 120.00 |
| O1—C3—C4 | 115.43 (11) | C7—C8—H8A | 119.00 |
| C2—C3—C4 | 119.77 (12) | C9—C8—H8A | 119.00 |
| O2—C4—C3 | 114.38 (11) | C8—C9—H9A | 116.00 |
| O2—C4—C5 | 125.88 (12) | C10—C9—H9A | 117.00 |
| C3—C4—C5 | 119.72 (12) | C10—C11—H11A | 120.00 |
| C4—C5—C6 | 120.80 (11) | C12—C11—H11A | 120.00 |
| C1—C6—C5 | 118.76 (11) | C11—C12—H12A | 120.00 |
| C1—C6—C7 | 122.74 (11) | C13—C12—H12A | 120.00 |
| C5—C6—C7 | 118.45 (11) | C12—C13—H13A | 121.00 |
| O3—C7—C6 | 120.42 (12) | C14—C13—H13A | 121.00 |
| O3—C7—C8 | 120.14 (13) | C10—C15—H15A | 120.00 |
| C6—C7—C8 | 119.40 (12) | C14—C15—H15A | 120.00 |
| C7—C8—C9 | 121.08 (13) | O1—C16—H16A | 109.00 |
| C8—C9—C10 | 127.00 (13) | O1—C16—H16B | 109.00 |
| C9—C10—C11 | 118.76 (12) | O1—C16—H16C | 109.00 |
| C9—C10—C15 | 122.38 (12) | H16A—C16—H16B | 109.00 |
| C11—C10—C15 | 118.81 (12) | H16A—C16—H16C | 109.00 |
| C10—C11—C12 | 120.58 (14) | H16B—C16—H16C | 109.00 |
| C11—C12—C13 | 120.63 (15) | O2—C17—H17A | 109.00 |
| C12—C13—C14 | 118.77 (14) | O2—C17—H17B | 109.00 |
| Cl1—C14—C13 | 118.53 (11) | O2—C17—H17C | 109.00 |
| Cl1—C14—C15 | 119.45 (11) | H17A—C17—H17B | 109.00 |
| C13—C14—C15 | 122.00 (13) | H17A—C17—H17C | 110.00 |
| C10—C15—C14 | 119.21 (13) | H17B—C17—H17C | 109.00 |
| C2—C1—H1A | 120.00 | | |

| | | | |
|---|---|---|---|
| C16—O1—C3—C2 | 7.7 (2) | C1—C6—C7—C8 | 3.84 (19) |
| C16—O1—C3—C4 | −171.77 (15) | C5—C6—C7—O3 | 3.5 (2) |
| C17—O2—C4—C3 | 178.44 (13) | C5—C6—C7—C8 | −178.75 (12) |
| C17—O2—C4—C5 | 0.3 (2) | O3—C7—C8—C9 | 10.5 (2) |
| C6—C1—C2—C3 | −0.5 (2) | C6—C7—C8—C9 | −167.28 (13) |
| C2—C1—C6—C5 | −1.0 (2) | C7—C8—C9—C10 | 175.76 (13) |
| C2—C1—C6—C7 | 176.44 (13) | C8—C9—C10—C11 | −175.75 (15) |
| C1—C2—C3—O1 | −177.65 (13) | C8—C9—C10—C15 | 1.6 (2) |
| C1—C2—C3—C4 | 1.8 (2) | C9—C10—C11—C12 | 177.04 (14) |
| O1—C3—C4—O2 | −0.40 (17) | C15—C10—C11—C12 | −0.4 (2) |
| O1—C3—C4—C5 | 177.86 (12) | C9—C10—C15—C14 | −176.57 (13) |
| C2—C3—C4—O2 | −179.87 (12) | C11—C10—C15—C14 | 0.8 (2) |
| C2—C3—C4—C5 | −1.60 (19) | C10—C11—C12—C13 | −0.2 (2) |
| O2—C4—C5—C6 | 178.20 (13) | C11—C12—C13—C14 | 0.4 (2) |
| C3—C4—C5—C6 | 0.2 (2) | C12—C13—C14—Cl1 | −178.21 (12) |
| C4—C5—C6—C1 | 1.13 (19) | C12—C13—C14—C15 | 0.0 (2) |

| | | | |
|---|---|---|---|
| C4—C5—C6—C7 | −176.39 (12) | Cl1—C14—C15—C10 | 177.64 (10) |
| C1—C6—C7—O3 | −173.88 (14) | C13—C14—C15—C10 | −0.6 (2) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C9—H9*A*···O3 | 0.93 | 2.45 | 2.7888 (18) | 102 |
| C11—H11*A*···O3$^{i}$ | 0.93 | 2.54 | 3.417 (2) | 157 |
| C15—H15*A*···O2$^{ii}$ | 0.93 | 2.54 | 3.4378 (18) | 163 |

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) −*x*+3/2, *y*+1/2, −*z*+1/2.