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# **GRAPHICAL ABSTRACT**



# Synthesis, crystal structure, experimental and theoretical investigations of 3-(4-ethoxy-3-methoxyphenyl)-1-phenylprop-2-en-1-one

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#### Abstract

A chalcone derivative namely, (*E*)-3-(4-ethoxy-3-methoxyphenyl)-1-phenylprop-2-en-1-one (**1v**) has been synthesized and characterized on the basis of its spectral data. The solid state self-assembly studies of **1v** were carried out through single crystal X-ray technique to see the major non-covalent interactions responsible for molecular alignment in the solid state. Furthermore, the optimized molecular geometry, vibrational frequencies, <sup>1</sup>H and <sup>13</sup>C NMR chemical shift (in gas and in chloroform solvent) values and the molecular electrostatic potential (MEP) surface parameters of **1v** were calculated using DFT/B3LYP/HF/M06 method with 6-311++G(d,p) basis set in ground state. All the theoretical calculations for **1v** were found in good agreement with experimental data.

Keywords: Alkoxychalcone, Crystal Structure, FT-IR, NMR spectroscopy, DFT calculations.

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#### Introduction

Chalcones (benzylideneacetophenones) belong to one of the largest classes of plant metabolites and are precursors of flavonoids and isoflavonoids that play major role in the plant defense mechanism to protect from microorganisms, insects and animals [1-8]. Synthetically, chalcones can easily be obtained by the Claisen-Schmidt condensation reaction between substituted acetophenones and benzaldehydes. The possibility of having different substituents on the two aromatic rings and their ability to act as Michael acceptors make this class of compounds highly attractive drug scaffolds. Hence, a large variety of their derivatives have been synthesized in recent years with interesting and diverse pharmacological activities such as anti-fungal, anti-bacterial, anti-cancer, anti-inflammatory, anti-plasmodial, immunosuppressive, anti-oxidant, anti-leishmanial, analgesic and anti-pyretic activities etc [9-16]. Other than their applications in medicinal chemistry, they have also been reported to show nonlinear optical and luminescent properties [17-20].

With the advent of various computational methods in recent years, the theoretical investigations for solving structure and chemical reactivity related problems are getting increased attention from computational chemistry community [21-29]. These methods are presently emerging as an efficient tool for predicting molecular structures, harmonic force fields, vibrational wavenumbers, IR intensities and Raman activities etc. of biologically important molecules, and may serve as an alternative tool to various spectral techniques, that are needed for structure elucidation, in near future. Therefore, a lot of energy and money may be saved by using these methods.

In this context and as continuation of our recent research interests in organic synthesis, self-assembly and theoretical spectral investigations of small organic molecules [30-44], herein, we report the synthesis, solid state self-assembly, optimized molecular geometry, vibrational IR analysis, Nuclear Magnetic Resonance (NMR) analysis and molecular electrostatic potential (MEP) calculated at the B3LYP/6-311++G(d,p) level of (*E*)-3-(4-ethoxy-3-methoxyphenyl)-1-phenylprop-2-en-1-one (**1v**), focusing on the comparison of calculated and the experimental results.

#### Experimental

#### General

All reagents and solvents were used as purchased from the supplier or recrystallized/redistilled as required. Thin layer chromatography (TLC) was performed using aluminium sheets coated with silica gel 60 F254 (Merck). The melting point of chalcone derivative (**1v**) was determined in open capillary tubes by using Gallenkamp apparatus (MP-D) and was uncorrected. The FT-IR was recorded on NICOLET 6700 FT-IR Spectrometer (4000-400 cm<sup>-1</sup>) using ATR (attenuated total reflectance) method. The <sup>1</sup>H and <sup>13</sup>C-Nuclear Magnetic Resonance (NMR) spectra of **1v** were determined on Bruker spectrometer at 300MHz and 75MHz in CDCl<sub>3</sub>, respectively, using residual solvent signals as a reference.

#### Synthesis of a chalcone derivative (1v) [45]

In a 100 mL two neck-round bottom flask equipped with reflux condenser containing DMF (10 mL) was added 4-hydroxy-3-methoxybenzaldehyde (2g, 0.01 mole) and anhydrous K<sub>2</sub>CO<sub>3</sub> (2.07g, 0.015 mole) and heated the reaction mixture at 60-65 °C for 30 minutes before the dropwise addition of bromoethane (0.01 mole). After addition of bromoethane, the whole reaction mixture was heated under N<sub>2</sub> at 80 °C for 4-5 hours. After the completion of the reaction, monitored by TLC, the reaction mixture was poured into separating funnel containing ethylacetate and washed several times with water. The organic layer was then dried over anhydrous MgSO<sub>4</sub>, evaporated by using rotary evaporator to get 4-ethoxy-3methoxybenzaldehyde intermediate, which was used in the next step without further purification. The 4-Alkoxy-3-methoxybenzaldehyde intermediate (0.01 mole, 1g) was dissolved in ethanol (10 mL) in a 100 mL round bottom flask and 37% ice cooled NaOH solution (10 mL) was then added into it. After stirring the reaction mixture for 30 minutes at 0°C, the acetophenone (0.01 mole) was added dropwise and stirred for another 4-6 hours. The precipitates thus appeared were poured into the crushed ice, filtered and washed thoroughly with water. The obtained solid was finally recrystallized from ethanol to get pure 1v.

**1v**: Yield 94%; yellow crystals; m. p. 105-108°C;  $R_f = 0.47$  (n-hexane : ethyl acetate, 4:1), IR( $\overline{\nu}$ , cm<sup>-1</sup>): 1652 (C=O), 1574 (C=C), 1237, 1035 (Ar-O-R); <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>), 1.51 (3H, t, J = 6.9 Hz), 3.99 (3H, s), 4.17 (2H, q, J = 6.9 Hz), 6.91 (1H, d, J = 8.4 Hz), 7.18-7.28 (2H, m), 7.40 (1H, d, J = 15.6 Hz), 7.49-7.54 (3H, m), 7.78 (1H, d, J = 15.6 Hz), 8.03 (2H, d, J = 6.9 Hz);

<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) δ 14.07, 56.03, 64.03, 110.32, 112.16, 119.95, 123.21, 127.67, 128.45, 128.58, 132.58, 138.53, 145.17, 149.41, 150.86, 190.72; EIMS (*m*/*z*), 282.

#### 2.3. Crystallographic data collection and structural refinement

The single crystal X-Ray diffraction measurements for the **1v** were carried out using Bruker APEX-II CCD area-detector equipped with graphite monochromator at 296(2) K with Mo K $\alpha$  radiations ( $\lambda = 0.71073$  Å). The structure is solved by direct methods [46] full-matrix least-squares refinement on F<sup>2</sup> and 236 parameters for 4323 unique intensities (R<sub>int</sub> = 0.011). The crystal data and refinement details of **1v** are summarized in Table 1.

#### **Computational details**

In the present work, all computations were performed with the Gaussian 09 program package [47]. GaussView 5 molecular visualization program [48] was used for visual animation and also for the verification of the normal modes assignment. The molecular structure and vibrational calculations of chalcone derivative **1v** were computed by using Becke-3-Lee Yang Parr (B3LYP), HF and M06 levels of theory [49-51]. The standard 6-311++G(d,p) basis set is used for all the calculations. The VEDA4 program [52] was used to characterize the normal vibrational modes on the basis of Potential Energy Distribution (PED). The wavenumbers and their intensities obtained from the computation were used to simulate infrared spectra. For the NMR computations, the optimized molecular geometry of **1v** was first obtained at the B3LYP/6-311++G(d,p), HF/6-311++G(d,p) and M0/6-311++G(d,p) levels and then, the <sup>1</sup>H and <sup>13</sup>C NMR chemical shifts were calculated using the gauge-invariant atomic orbital (GIAO) method after the molecular geometry of **1v** was computed using DFT/ B3LYP method with 6-311++G(d,p) basis set.

#### **Results and discussion**

#### Synthesis and spectral characterization

The synthesis of chalcone 1v was initiated by the preparation of 4-ethyloxy-3methoxybenzaldehyde intermediate by reacting equimolar quantities of 4-hydroxy-3methoxybenzaldehyde with ethyl bromide in DMF solvent using K<sub>2</sub>CO<sub>3</sub> as a base at 80  $^{0}$ C. The reaction proceeded smoothly providing excellent yield. The 4-ethyloxy-3-methoxybenzaldehyde intermediate was then reacted with acetophenone under base catalyzed Claisen-Schmidt

condensation reaction conditions for 4-6 hours to get our desired chalcone derivative **1v** in 94% yields (Scheme 1). The structure of **1v** was confirmed by its physical and spectral (IR, <sup>1</sup>H and <sup>13</sup>C NMR) data and were found geometrically pure with E configuration (Jtrans =  $\sim$ 16 Hz) around double bond by <sup>1</sup>HNMR spectroscopy.

In FT-IR spectrum, the characteristic bands at 1652 and 1574 cm<sup>-1</sup> were assigned to the carbonyl group (C=O) and olefinic double bond (–CH=CH–), respectively [53-55]. Furthermore, two bands at 1237 and 1035 were indicative of the presence of alkyl-aryl ether (Ar-O-R) moiety. Similarly, the two prominent doublets, one at 7.40 ppm and the other at 7.78 ppm with coupling constants 15.6 Hz each in the <sup>1</sup>H-NMR spectrum of **1v** confirmed the presence of  $\alpha$  and  $\beta$  - hydrogen atoms of the olefinic double bond in the  $\alpha$ ,  $\beta$ -unsaturated carbonyl system. The coupling constant ( $J_{\text{trans}} = \sim 16$  Hz) also confirmed *E*-configuration and geometrical purity of **1v**. Furthermore, the methoxy (-OCH<sub>3</sub>) and methylene (ArO–CH<sub>2</sub>–) protons appeared as a singlet and a quartet at 3.99 ppm and 4.17 ppm, respectively. Likewise, the conclusions drawn from the <sup>13</sup>C NMR data also supported the formation of desired chalcone derivative **1v**.

#### Solid state self-assembly

The dependence of outstanding bulk properties of solids on the molecular alignment is the main driving force for crystal engineers to understand solid state self-assembly process and to explore new functional solids. The solid state self-assembly studies of **1v** were carried out to identify the structural features that play major role in the molecular alignment in the solid state. For this purpose, good-quality single crystals of **1v** suitable for X-ray analysis were grown in ethanol solvent. The crystal data and structural refinement parameters of **1v** are summarized in Table 1.

The 3D-network of 1v is composed of various 1D-tapes (Figure 1). Each 1D-tape is formed by the connection of various antiparallel/centrosymmtric-arranged molecules of 1v through CH···O and CH··· $\pi$  interactions (Figure 1a). These tapes are also connected to the neighbouring chains by CH···O interactions to form 2D-sheets which by means of CH···O and CH··· $\pi$ interactions form 3D-network of 1v (Figure 1b).

#### Molecular geometry

The optimized molecular structure along with the numbering of atoms of 1v calculated at B3LYP/6-311++G(d,p) level of theory is given in Fig. 2. The geometrical parameters (bond lengths and bond angles) corresponding to the optimized geometries of the title compound are given in Table 2 along with the X-ray experiment data. Generally, most of the optimized bond lengths and angles are slightly different from the experimental ones. This is expected because,

one isolated molecule is considered in theoretical gas phase calculation, whereas packed molecules are considered in solid phase during the experimental measurement. However, the calculated geometric parameters are in good agreement with the experimental results. To be specific, the root mean square (RMS) errors are 0.0835 Å, 0.0780 Å and 0.0851 Å for the bond lengths calculated at HF, B3LYP and M06 respectively; while the RMS values for the bond angles are found to be 1.09°, 1.13° and 1.04° calculated at HF, B3LYP and M06 respectively.

#### Vibrational IR Spectra Analysis

The optimized structural parameters were used to compute the vibrational wavenumbers for the title compound at HF/6-311++G(d,p), B3LYP/6-311++G(d,p) and M06/6-311++G(d,p)levels of theory. Since, the calculated vibrational wavenumbers are generally larger than the observed values due to the well-known systematic errors and the neglect of anharmonicity and incomplete treatment of electron correlation and basis set truncation. The differences are accounted for by using scaling factor. However, the high frequency region for the vibrational modes contains the stretching vibrational modes related to functional groups of a molecule and the lower frequency region can include the overlapped bands of the compounds, the characteristic properties of high and low frequency regions require different scaling factors. For these reasons, the calculated vibrational wavenumbers were scaled as 0.983 for frequencies less than 1700 cm<sup>-1</sup> and 0.958 for frequencies higher than 1700 cm<sup>-1</sup> for B3LYP/6-311++G(d,p) basis set [56, 57]. Table 3 presents the calculated (scaled) vibrational wavenumbers and IR intensities along with the assignment of vibrational modes for the 1v compound. The Table also shows the observed infrared wavenumbers of 1v for comparison. The assignment of the fundamental vibrational modes is proposed on the basis of Potential Energy Distribution using VEDA 4 program and the animation option of Gauss View graphical interface of Gaussian program. A detailed description of the normal modes based on PED is given in the last column of Table 3. The (E)-3-(4-(pentyloxy)phenyl)-1-phenylprop-2-en-1-one molecule (1v) has 39 atoms and the number of fundamental vibration modes is 111 which are all IR active. The absence of imaginary wavenumbers in the calculated vibrational spectrum confirms that the optimized structure corresponds to the minimum energy on the potential energy surface.

The vibrational wavenumbers and the corresponding intensities obtained from calculations at the three levels of theory were used to simulate the IR spectra of the title compound. For simulation, pure Lorentizian band shape with a bandwidth of full width and half maximum (FWHM) of 10 cm-1 was used to plot the calculated IR and Raman spectra. The

experimental and simulated IR spectra of 1v molecule are presented in Figure 3. This figure clearly shows the spectral characteristics of the title molecule. Generally, the aromatic C-H stretching modes appears in the region  $3100 - 3000 \text{ cm}^{-1}$  [58]. In the present study, the vibrational mode at 3067 cm<sup>-1</sup> in the FTIR spectrum of 1v (Fig. 3) is attributed to aromatic C-H stretching vibrations. This mode was found to be 3230, 3267 and 3055 cm<sup>-1</sup> at B3LYP/6-311++G(d,p), HF/6-311++G(d,p) and M06/6-311++G(d,p) respectively and this show good agreement between experimental and theoretical vibrational wavenumbers.

#### Nuclear Magnetic Resonance (NMR) analysis

The <sup>1</sup>H and <sup>13</sup>C NMR spectroscopy is a very important analytical tool used by chemist for the identification and characterization of organic compounds. However, since there is no simple correlation between the measured chemical shifts and structural parameters, the interpretation of experimental NMR spectra could be awkward. The calculation of NMR chemical shifts can provide in many cases the necessary information for the correct interpretation of experimental NMR spectra. Thus, the combined use of experimental and quantum mechanical calculation of chemical shifts offers a powerful tool for the reliable interpretation and prediction of the structures of bulky molecules. In the present work, the <sup>1</sup>H and <sup>13</sup>C NMR isotropic shielding for 1v molecule were calculated with the Gauge Invariant Atomic Orbitals (GIAO) method using the optimized geometrical parameters obtained from the HF/6-311++G(d,p), B3LYP/6-311++G(d,p)and M06/6-311++G(d,p) levels of theory. The chemical shifts are reported in ppm relative to TMS isotropic chemical shifts for <sup>1</sup>H and <sup>13</sup>C calculated at the same level of theory. The experimental and calculated <sup>1</sup>H and <sup>13</sup>C NMR chemical shift values of **1v** molecule are presented in Table 4. Generally, the <sup>13</sup>C NMR chemical shifts for aromatic ring are greater than 100 ppm. As can be seen from Table 3, the <sup>13</sup>C NMR chemical shift values of aromatic carbons of 1v compound have been observed at the interval of 110 - 151 ppm. The observed and calculated chemical shift values of  $C_{11}$  and  $C_{12}$  atoms (that are connected to the oxygen atoms  $O_{10}$  and  $O_{20}$ respectively) are higher than those of other ring carbon atoms. The chemical shifts of methyl and methylene carbon atoms which are shielded by their own hydrogen atoms are observed down field. On the other hand, the <sup>13</sup>C chemical shift of carbonyl group (CO) was observed at 190.72 ppm and calculated to be at 189.59, 192.02 and 186.75 ppm at HF, BELYP and MO6 methods respectively. In general, both <sup>1</sup>H and <sup>13</sup>C NMR calculations are in reasonable agreement with the experimental values. The correlation between the observed and calculated <sup>13</sup>C (<sup>1</sup>H) chemical shift values were found to be 0.9872(0.9695), 0.9944(0.9868) and 0.9922(0.9814) for HF, B3LYP and M06 respectively.

#### Molecular electrostatic potential (MEP)

Molecular Electrostatic Potential (MEP) mapping is very important in the study of molecular interactions, prediction of relative sites for nucleophilic and electrophilic attack, molecular cluster and predication wide range of macroscopic properties [59, 60]. To predict reactive sites for nucleophilic and electrophilic attack for 1v molecule, the MEP at the B3LYP/6-311++G(d,p) optimized geometry was calculated and the result is illustrated in Figure S1 (Supporting Information). The electrostatic potentials at the surface are represented by different colors; red, blue and green represent the regions of negative, positive and zero electrostatic potentials respectively. In addition, the negative regions (red color) of MEP are related to electrophilic reactivity. As can be seen from Figure 4, the negative electrostatic potentials are mainly localized over the carbonyl oxygen atom, and is a potential site for electrophilic attack. The MEP of 1v is dominated by the green regions which correspond to electrostatic potential halfway between the red and the blue and are potential sites for intermolecular interactions.

#### Conclusions

In conclusion, we have synthesized a chalcone derivative namely, (*E*)-3-(4-ethoxy-3methoxyphenyl)-1-phenylprop-2-en-1-one (**1v**), characterized on the basis of its spectral (IR, <sup>1</sup>H & <sup>13</sup>C NMR and MS) data and its solid state self-assembly studies were carried out through single crystal X-ray technique. The CH···O and CH··· $\pi$  interactions were found to be the main supramolecular forces involved in stabilization of its self-assembly in the solid state. Furthermore, spectral and crystallographic structural data have been verified through quantum chemical computations of **1v** at HF/6-311++G(d,p), B3LYP/6-311++G(d,p) and M06/6-311++G(d,p) levels of theory. The optimized molecular geometry, vibrational frequencies, <sup>1</sup>H and <sup>13</sup>C NMR chemical shift (in gas and in chloroform solvent) values and the molecular electrostatic potential (MEP) surface parameters of **1v** showed good agreement with experimental data. Therefore, these computational methods may be considered as powerful tools not only to compliment the experimental results but also as a replacement to some expensive and tedious experimental characterizations.

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# **Table 1.** Crystallographic data for chalcone derivative 1v

Bond	X-Ray	Calcula	ited bond le	ngth (Å)	Bond Angle *	X-Ray	Calculated bond angle (°)		
(Å)	(Å)	HF	B3LYP	M06	(°)	(°)	HF	<b>B3LYP</b>	M06
R(1-8)	1.438	1.432	1.406	1.417	A(8-1-11)	116.9	119.1	120.4	118.8
R(1-11)	1.365	1.353	1.338	1.343	A(1-8-4)	107.3	107.6	107.7	107.5
(2-12)	1.369	1.359	1.343	1.349	A(1-8-9)	110.3	109.5	109.8	109.7
$\frac{(2-32)}{(2-30)}$	1.428	1.422	1.398	1.406	A(1-8-10)	110.3	109.5	109.8	109.7
$\frac{x(3-20)}{x(4-5)}$	1.220	1.220	1.190	1.218	A(1-11-12) A(1-11-28)	115.7	125.0	124.0	115.8
$\frac{(4-5)}{2(4-6)}$	0.980	1.092	1.086	1.093	A(1-11-20) A(12-2-32)	1167	118.4	119.8	117.8
(4-7)	0.980	1.092	1.084	1.093	A(2-12-11)	115.1	115.7	115.9	115.7
R(4-8)	1.508	1.516	1.514	1.504	A(2-12-13)	124.7	125.0	124.8	125.0
(8-9)	0.989	1.097	1.087	1.100	A(2-32-33)	109.4	111.4	111.5	111.5
R(8-10)	0.990	1.097	1.087	1.100	A(2-32-34)	109.5	105.7	106.1	106.4
(11-12)	1.409	1.418	1.408	1.413	A(2-32-35)	109.4	111.4	111.5	111.6
$\frac{(11-28)}{(12,12)}$	1.385	1.396	1.380	1.390	A(3-20-18)	122.0	121.7	121.6	121.8
$\frac{(12-13)}{(12-14)}$	1.380	1.387	1.373	1.381	A(5-20-21)	120.2	109.5	109.8	109.9
(13-14)	1 403	1.082	1.073	1.085	A(5-4-0) A(5-4-7)	109.4	108.5	108.7	108.3
(15-16)	1.463	1.456	1.471	1.450	A(5-4-8)	109.5	110.7	110.6	110.6
(15-30)	1.391	1.398	1.379	1.391	A(6-4-7)	109.5	108.5	108.7	108.5
(16-17)	0.950	1.088	1.077	1.091	A(6-4-8)	109.5	109.8	109.9	110.3
(16-18)	1.335	1.348	1.329	1.342	A(7-4-8)	109.5	110.7	110.6	110.6
(18-19)	0.949	1.082	1.072	1.086	A(4-8-9)	110.3	111.0	110.6	111.1
(18-20)	1.475	1.479	1.488	1.473	A(4-8-10)	110.3	111.0	110.6	111.2
(20-21)	1.495	1.505	1.505	1.490	A(9-8-10) A(12,11,28)	108.5	108.5	108.2	110/./
(21-22) (21-36)	1 393	1.402	1 390	1.390	A(12-11-20) A(11-12-13)	120.2	119.1	119.0	119.2
(22-23)	0.950	1.083	1.073	1.085	A(11-28-29)	119.8	119.9	120.2	119.9
(22-24)	1.385	1.389	1.382	1.384	A(11-28-30)	120.3	120.9	121.0	120.8
(24-25)	0.950	1.084	1.075	1.086	A(12-13-14)	119.7	119.8	119.8	120.0
(24-26)	1.380	1.396	1.388	1.390	A(12-13-15)	120.6	121.8	121.7	121.7
(26-27)	0.950	1.084	1.076	1.086	A(14-13-15)	119.7	118.4	118.5	118.3
<u>(26-38)</u>	1.387	1.393	1.384	1.387	A(13-15-16)	118.6	118.2	118.0	118.4
(28-29)	0.950	1.081	1.072	1.084	A(13-15-30)	118.8	118.0	118.3	118.2
(30-31)	0.950	1.392	1.390	1.387	A(10-13-30) A(15-16-17)	1167	115.0	125.7	123.4
(32-33)	0.980	1.095	1.086	1.098	A(15-16-18)	126.5	128.3	127.7	128.0
(32-34)	0.980	1.089	1.080	1.090	A(15-30-28)	120.9	120.8	120.6	120.8
(32-35)	0.980	1.095	1.086	1.098	A(15-30-31)	119.6	120.4	120.8	120.3
(36-37)	0.950	1.083	1.074	1.085	A(17-16-18)	116.8	115.8	116.6	115.8
<u>(36-38)</u>	1.387	1.394	1.386	1.388	A(16-18-19)	119.0	121.0	121.5	120.9
(38-39) DM	0.950	1.084	1.075	1.080	A(10-18-20) A(10, 18, 20)	121.9	120.4	120.0	120.0
KIVI.	<i>5D</i>	0.004	0.078	0.005	A(19-18-20) A(18-20-21)	117.8	118.0	118.4	119.0
					A(20-21-22)	119.6	117.8	118.0	117.6
					A(20-21-36)	120.9	123.4	123.0	123.4
					A(22-21-36)	119.4	118.8	119.1	118.9
					A(21-22-23)	120.0	118.2	118.8	118.1
					A(21-22-24)	120.2	120.7	120.5	120.6
					A(21-36-37)	119.9	120.5	120.6	120.5
					A(23-22-24)	110.1	120.0	120.3	120.3
					A(22-24-25)	120.0	119.9	119.9	120.0
					A(22-24-26)	120.1	120.1	120.0	120.0
					A(25-24-26)	120.0	120.0	120.1	120.0
					A(24-26-27)	119.8	120.1	120.0	120.1
					A(24-26-38)	120.3	119.8	119.9	119.9
					A(27-26-38)	119.9	120.1	120.0	120.0
					A(26-38-36)	119.9	120.1	120.0	120.0
					A(20-38-39) A(20-28-30)	120.0	120.1	120.2	120.1
					A(29-20-30) A(28-30-31)	119.9	119.1	118.6	119.2
					A(33-32-34)	109.5	109.4	109.1	109.1
					A(33-32-35)	109.5	109.5	109.4	109.0
r					A(34-32-35)	109.5	109.4	109.1	109.1
					A(37-36-38)	119.9	118.9	118.9	119.0
					A(36-38-39)	120.1	119.8	119.8	119.9
					RMSI	)	1.1	1.1	1.0

Table 2: The calculated and experimental molecular geometry parameters of the 1v.

\*Atomic number are given in Figure 3.

Table 3: The experimental and calculated wavenumbers  $(cm^{-1})$  and their assignment of 1v.

Fynt	HF		B3LYP		MO6		Assignment (PFD $> 10\%$ )	
Expt.	IR <sup>a</sup>	Intensity <sup>b</sup>	IR <sup>a</sup>	Intensity <sup>b</sup>	IR <sup>a</sup>	Intensity <sup>b</sup>	Assignment ( $\Gamma ED \ge 1076$ )	
	3234	19.45	3075	12.17	3057	9.73	vCH(99)	
3067 w	3230	1.09	3067	11.52	3055	10.43	vCH(96)	
	3228	6.40	3066	1.91	3053	10.43	vCH(88)	
	3225	6.73	3065	13.49	3052	12.79	vCH(78)	
	3215	6.57	3056	2.52	3043	14.93	vCH(78)	
	3206	31.76	3051	28.71	3040	17.29	vCH(69)	
	3204	12.26	3048	4.46	3036	3.02	vCH(90)	
	3193	11.77	3039	10.68	3031	10.39	vCH(90)	
	3189	0.42	3030	0.48	3022	0.07	vCH(86)	
•	3181	0.08	3012	1.14	3006	21.49	vC=CH(83)	
2976 w	3146	42.21	3004	23.59	2999	2.17	vCH <sub>3</sub> (99)	
2973 w	3116	46.72	2984	25.14	2994	20.48	vCH <sub>3</sub> (86)	
2972 w	3101	40.12	2975	22.20	2990	17.47	vCH <sub>3</sub> (97)	
	3085	47.25	2935	34.59	2932	32.45	vCH <sub>3</sub> (100)	
	3061	29.74	2911	25.37	2909	22.91	vCH <sub>2</sub> (99)	
	3040	37.39	2909	26.95	2901	28.37	vCH <sub>3</sub> (99)	
2880 w	3028	46.30	2879	45.99	2866	46.93	υCH <sub>3</sub> (99)	
2839 w	3025	35.25	2873	36.88	2859	40.05	vCH <sub>2</sub> (100)	
1707 w	1839	236.08	1683	149.36	1728	155.04	υCO(77)	
	1735	418.40	1619	144.85	1646	318.34	vCC(73) + vC = C(10)	
1652 s	1756	11.19	1608	11.86	1622	20.46	$\upsilon C = C(66) + \delta HCC(13) + \delta CCC(11)$	
	1751	200.89	1593	280.89	1614	424.18	vCC(66)	
	1734	70.12	1585	163.97	1600	21.64	vCC(49)	
1576 sh	1730	6.50	1576	288.76	1596	142.97	$\nu$ CC(55) + $\delta$ HCC(11)	
1574 s	1659	468.16	1523	358.94	1531	553.01	δHCH(75) +τHCCO(12)	
1515 w	1621	61.18	1494	0.38	1489	3.71	δHCC(73)	
1512 s	1620	2.51	1493	81.09	1466	44.48	δHCH(77)	
	1602	32.23	1479	52.34	1454	42.51	δHCH(79)	
	1594	8.06	1475	8.16	1446	49.49	δHCH(79)	
	1590	4.62	1467	9.36	1444	10.16	δHCH(26)	
1448 w	1584	26.29	1458	7.58	1441	7.48	$vCC(15) + \delta HCC(59) + \delta CCC(10)$	
1446 s	1572	5.74	1456	27.92	1431	15.60	δHCH(92)	
1444 w	1564	16.81	1450	5.02	1427	8.45	δHCH(78)	
	1539	62.93	1419	32.94	1414	7.84	$\upsilon CC(29) + \delta HCC(46)$	
	1531	81.71	1403	71.36	1391	88.46	vCC(56)	
	1495	8.42	1378	10.19	1356	94.90	δHCH(10)	
1336 w	1446	9.54	1346	271.86	1354	215.84	$vCO(56) + \delta HCC(15)$	
1335 s	1427	485.03	1338	26.48	1330	6.93	δHCC(68)	
	1420	65.86	1323	4.51	1327	1.49	δHCC(65)	
	1410	165.96	1316	3.97	1313	34.79	$\nu CO(13) + \delta HCC(51)$	
	1405	51.68	1305	5.60	1289	82.12	$vCC(19) + \delta HCC(53)$	
	1396	1.57	1292	30.31	1278	185.04	δHCC(80)	
	1360	278.60	1283	0.76	1275	365.57	δHCC(44)	
1240 w	1318	238.11	1264	691.14	1272	248.73	$\upsilon CC(32) + \delta HCC(35)$	
1238 s	1308	56.80	1242	232.92	1250	219.14	$vCC(15) + vC-O(10) + \delta HCC(29)$	
	1297	28.14	1206	187.60	1198	129.31	$\delta$ HCC(67) + $\delta$ CCO(10)	
	1289	63.63	1196	40.64	1183	21.27	$\delta$ HCC(24) + $\tau$ HCOC(31)	
	1266	16.71	1180	45.97	1172	52.00	δHCC(12)	
	1264	4.51	1176	61.03	1165	66.74	0HCC(65)	
1142	1257	2.53	1162	4.75	1145	4.42	0HCC(20)	
1142 W	1241	265.93	1157	5.59	1142	1.03	0HCH(28)	
1140 W	1216	8.04	1149	0.95	1136	125.29	0HCH(20)	
115/8	1206	24.20	1141	242.00	1123	133.28	$\mathcal{V} \cup \mathcal{U}(25) + OHU(22)$	
	1193	10.09	1114	1.08	1117	0.89	VUU(43) + 0HUU(11)	
	1153	19.08	1088	1.90	1088	2.13	$v CO(25) + v CC(19) + \delta CCC(15)$	

1039 s	1151	0.13	1044	60.06	1079	20.77	vC-C(32) + vC-O(10)
1036 s	1133	77.72	1037	44.17	1059	72.22	vC-C(28) + vC-O(11)
1034 s	1108	42.93	1036	97.91	1035	12.73	τHCCC(63)
	1105	54.46	1018	223.74	1019	178.14	$\tau$ HCCC(70) + $\tau$ CCCC(11)
	1100	4.67	1007	26.59	997	24.05	$\tau$ HCCC(79) + $\tau$ CCCC(15)
	1089	4.58	999	1.88	991	12.17	δCCC(74)
	1083	182.75	992	0.11	989	2.42	vCC(72)
971 vs	1063	5.84	975	0.76	975	0.62	δCCC(55)
	1039	4.76	948	1.60	953	5.54	τHCCC(83)
	1029	3.55	931	1.52	928	2.54	τHCCC(80)
	1014	4.01	918	21.36	925	12.72	$vCC(36) + \tau HCCC(19)$
	988	12.49	911	1.11	904	1.54	$vCC(17) + \delta CCC(10)$
	977	0.27	875	1.15	869	3.43	тНССС(78)
	953	33.16	865	1.74	866	2.80	τHCCC(97)
851 vs	935	0.53	849	23.11	844	25.15	τHCCC(68)
	929	5.33	844	2.29	843	1.30	$\delta COC(10) + \tau HCCC(39)$
	905	27.94	825	0.94	815	2.95	τHCCC(40)
801s	877	5.28	798	14.35	792	7.89	τHCOC(68)
777 vs	858	36.34	784	25.72	791	9.97	$\tau$ HCCC(53) + $\tau$ CCCC(24)
775 s	846	16.75	783	27.56	778	41.97	$\upsilon CO(36) + \delta CCO(12) + \delta CCC(15)$
	813	2.95	739	8.43	741	9.81	$\tau CCCC(13) + \tau OCCC(66)$
	787	6.27	738	3.39	735	4.07	$vCC(16) + \delta CCC(27)$
712 vs	770	68.43	698	52.50	696	46.52	$\tau$ HCCC(25) + $\tau$ CCCC(47)
	742	10.51	686	5.53	683	9.28	$\tau CCCC(11) + \tau OCCC(43)$
655 vs	711	22.16	665	18.63	660	19.48	δCCC(31)
	662	1.01	621	1.29	611	1.79	δCCC(81)
	654	9.35	606	4.83	607	5.61	δCCO(64)
	643	6.19	594	10.65	588	8.82	τCCCC(42)
565 s	612	75.90	573	78.01	569	65.88	δCCC(39)
	557	6.29	522	6.05	521	6.64	δCCO(18)
	543	2.24	503	2.86	501	2.60	-
	511	1.78	467	1.51	466	0.93	τCCCC(59)
	472	6.09	438	5.46	435	5.36	$\delta CCO(10) + \tau CCCC(26)$
	444	0.35	408	1.89	410	1.05	$\tau \text{HCCC}(17) + \tau \text{CCCC}(77)$
	432	0.06	404	0.00	400	0.17	$\delta COC(34) + \tau CCCC(11)$
	412	2.25	375	1.82	376	1.89	$\tau OCCC(68) + \tau CCCC(10)$
	373	2.62	351	2.38	360	2.89	$\delta CCO(12) + \delta COC(38)$
	364	3.10	341	3.83	344	3.22	δCCO(60)
	324	5.77	305	6.30	311	6.55	$\tau HCOC(44) + \tau CCCC(29)$
	309	0.34	285	0.14	285	0.56	δCOC(46)
	270	0.38	246	0.27	250	0.48	τHCCO(28)
	257	0.74	241	0.87	245	0.31	$\tau$ HCOC(12) + $\tau$ CCCC(19)
	246	0.19	225	0.16	218	0.16	τHCCO(92)
	205	0.92	189	0.92	192	0.96	$\delta CCO(11) + \tau CCCC(27)$
	193	0.18	181	0.05	183	0.08	$vCC(28) + \delta CCC(22)$
	181	0.21	166	0.19	168	0.17	$\tau CCCC(34) + \tau CCOC(11)$
	142	2.97	133	3.27	137	3.02	$\delta CCO(41) + \tau CCCC(16)$
	126	0.80	117	0.75	122	0.65	$\delta CCO(54) + \tau CCCC(11)$
	108	0.10	107	0.10	106	0.24	$\tau$ HCCO(10) + $\tau$ COCC(58)

<sup>a</sup> Scaled vibrational IR wavenumbers (cm<sup>-1</sup>); 0.983 scaling factor for the vibrational wavenumbers below 1800 cm<sup>-1</sup> and 0.958 for the vibrational wavenumbers above 1800 cm<sup>-1</sup>. <sup>b</sup> Calculated infrared intensities in km mol<sup>-1</sup>.

Nucleus	Experiment Chemical Shifts	Calculate 6-311+	d Chemical S +G(d,p) GIA	hifts TMS O (ppm)	Nucleus	Experiment Chemical Shifts in	Calculated Chemical Shifts TMS 6-311++G(d,p) GIAO (ppm)			
	in CHCl3-d	HF	B3LYP	M06		CHCl <sub>3</sub> -d		B3LYP	M06	
C4	14.70	17.48	16.82	15.67	H5	1.51	1.76	1.48	1.19	
C8	64.41	57.65	68.68	61.28	H6	1.51	1.30	1.03	0.82	
C11	150.86	156.05	159.34	156.78	H7	1.51	1.79	1.50	1.15	
C12	149.41	153.40	157.36	154.95	H9	4.17	4.02	3.69	3.39	
C13	110.32	120.20	119.86	118.08	H10	4.17	4.01	3.69	3.38	
C15	127.67	131.56	134.12	132.50	H14	7.18-7.28	7.01	6.73	6.90	
C16	145.17	156.41	151.17	151.57	H19	7.40	8.15	7.81	8.23	
C18	119.5	119.26	118.76	118.23	H17	7.78	7.77	7.40	7.38	
C20	190.72	189.59	192.02	186.75	H23	8.03	8.60	8.34	8.21	
C21	138.53	144.73	146.99	143.89	H25	7.49-7.54	7.61	7.37	7.60	
C22	128.45	139.70	136.61	135.71	H27	7.49-7.54	7.77	7.51	7.64	
C24	128.58	134.38	135.26	134.27	H29	6.91	6.90	6.63	6.45	
C26	132.58	140.32	138.15	138.33	H31	7.18-7.28	7.89	7.51	7.62	
C28	112.16	114.92	114.95	114.75	H33	3.99	3.69	3.40	3.38	
C30	123.21	125.00	123.22	121.99	H34	3.99	4.14	3.92	4.04	
C32	56.03	49.69	56.76	55.60	H35	3.99	3.73	3.43	3.57	
C36	128.45	136.53	133.81	133.38	H37	8.03	8.27	7.87	7.76	
C38	128.58	132.61	133.44	133.32	H39	7.49-7.54	7.66	7.50	7.49	
RMSD		6.34	5.79	4.83			1.36	0.38	0.53	
			3							
	K									

			1	12					
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1 a 0 10 + 1	The calculated	and experimental	II and		chennear	SIIIIUS	(ppm)		



Figure 1: Solid state self-assembly of **1v**: a) 1D-supramolecular tapes; b) 3D-network



Figure 2: Optimized structure and atom numbering for (E)-(4-Ethoxy-3-methoxyphyl)-1phenylprop-2-en-1-one (**1**v)



Figure 3. IR spectra (a) experimental and simulated at (b) B3LYP/6-311++G(d,p), (c) HF/6-311++G(d,p) and (d) M06/6-311++G(d,p) of 1v.



Scheme 1. Synthesis of new chalcone derivative 1v

## **Research Highlights:**

- Chalcones are attractive organic molecules with diverse applications.
- Synthesis of (*E*)-3-(4-ethoxy-3-methoxyphenyl)-1-phenylprop-2-en-1-one.
- Spectral characterization and theoretical calculations.
- B3LYP/6-311++G(d,p), HF/6-311++G(d,p) and M06/6-311++G(d,p).

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