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Synthesis, Crystal Growth and Characterization of (*E*)-3-(4(dimethylamino)phenyl)-1-phenylprop-2-en-1-one: An Organic Crystal

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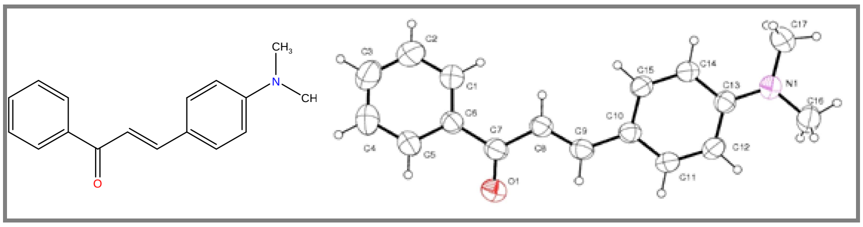
ABSTRACT

Chalcone based materials are widely used in many industrial applications. Chalcone based single crystals, (E)-3-(4-(dimethylamino)phenyl)-1-phenylprop-2-en-1-one(Crystal) were synthesized and grown as single crystals by slow evaporation solution growth technique in ethanol. The structures of the grown crystals were solved and refined by single crystal XRD and this demonstrates that crystal (E)-3-(4-(dimethylamino)phenyl)-1-phenylprop-2-en-1-one, $C_{17}H_{17}NO$*, was synthesized and characterized by infrared, NMR, HR-MS spectral studies. The compound crystallizes in monoclinic space group C2/c with unit cell parameters a=13.1956(11) Å, b=11.8396(9) Å, c=9.5664(6) Å, Z=4, and V=1408.55(18) Å*^{3}*. The crystal packing is mainly stabilized by C-H.... π interaction. There are no significant intermolecular interactions beyond van der Waals forces observed in the solid state equal to structure of the compound.*

Graphical Abstract



The structure aspects of the newly synthesized (*E*)-3-(4-(dimethylamino)phenyl)-1-phenylprop-2-en-1-one(Crystal).

Keywords: Characterization, X-ray diffraction, Chalcones, Molecular structure.

INTRODUCTION

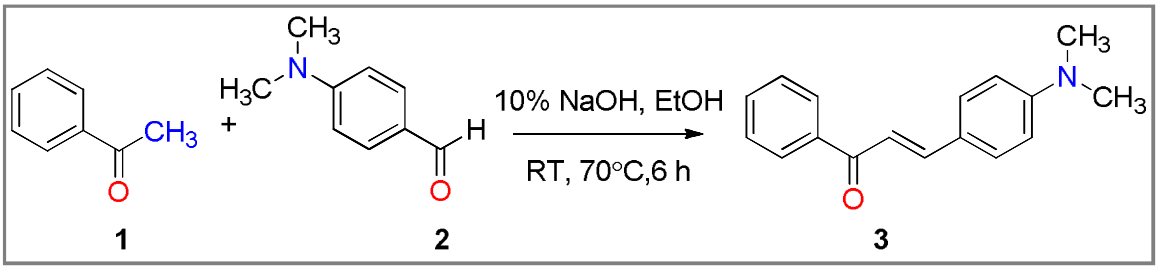
Single-crystal X-ray diffraction (XRD) method is a prevailing means for elucidating molecular structures. Single crystals larger than 20 µm are required for internal measurements [1]. The reputation of organic compounds enlarged by the existence of carbonyl group conjugating with another functional group particularly double bond C=C like α–β unsaturated carbonyl compounds [2], Chalcones assembled materials production an important role in upcoming research pitches [3]. Chalcone (Ar–CH=CH–CO–Ar) are noticeable goals for medicinal activity, significant tools for marketed drugs [4-7].Chalcones and their derivatives have been remarkable biological activity in the treatment of many diseases including such as cytotoxic [8], anticancer [9], antifungal [10], antimicrobial, antiinflammatory, [11, 12] and the chemo protective and mutagenic possessions of a sum of chalcones have been studied [13]. Some of the chalcone derivatives take a vital role innumerous field such as crystallography [14]. Fluorescence of chalcone crystals can be tuned by crystal engineering. And the strategy of tuning molecular co-planarity and J-aggregates formation through polymorphism may provide useful information into organic light-emitting materials [15]. Organic crystals play an important role in many compounds also find use in material science especially in the area of nonlinear optics [16] Chalcones are a class of cross conjugated NLO chromophores that is reported to exhibit good SHG efficiency, transparency and are easily crystallizable [17].

The current work deals with the synthesis, growth, characterization and evaluation of two new chalcone based single crystals, namely *(E)*-3-(4-(dimethylamino)phenyl)-1-phenylprop-2-en-1-one **3** (crystal). The physico chemical properties and theoretical analysis of these two materials were subjected to different characterization techniques such as TGA, single crystal XRD, solvent effect FT-IR, UV-Visible analysis, and molecular structure the properties are entirely different from each other and are discussed.

MATERIALS AND METHODS

Melting points are uncorrected. Infrared spectra were recorded on a Perkin-Elmer Paragon 1000 FT-IR spectrophotometer as potassium bromide discs unless otherwise indicated. NMR spectra were obtained on a Brucker (500 MHz) instrument in $CDCl_3$ solutions using tetramethylsilane as an internal standard. *J* Values are given in Hz. Perkin Elmer clarus 600 Mass spectrum were obtained at the Vellore Institute of Technology, Vellore, Tamilnadu, India. Column chromatography utilized Merck silica gel 60-120 mesh and hexane and ethyl acetate as eluents. All the basic chemicals were purchased from Merck and Avira chemical (India).

Synthesis of materials: Synthesis of *(E)*-3-(4-(dimethylamino)phenyl)-1-phenylprop-2-en-1-one **3.**



Scheme 1. Synthesis of *(E)*-3-(4-(dimethylamino)phenyl)-1-phenylprop-2-en-1-one 3.

First synthesized novel *(E)*-3-(4-(dimethylamino)phenyl)-1-phenylprop-2-en-1-one **3** were designed and synthesized by a standard Claisen–Schmidt condensation reaction of Dimethyl aminobenazaldehyde **2** with acetophenone**1**produced the correspond in α–β unsaturated carbonyl compounds*(E)*-3-(4-(dimethylamino)phenyl)-1-phenylprop-2-en-1-one **3** respectively scheme **1**.

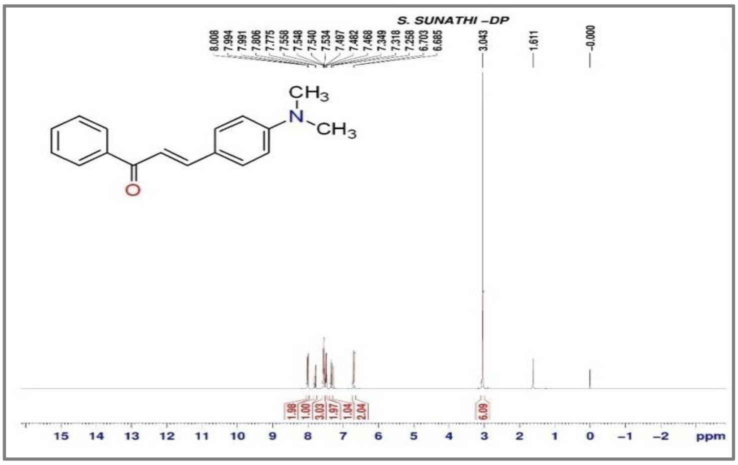


Figure 1. ^{1}H-NMR spectrum of *(E)*-3-(4-(dimethylamino)phenyl) -1-phenylprop-2-en-1-one **3.**

Chalcone derivatives were synthesized by the reaction of an equimolar amount dimethylaminobenzaldehyde and the corresponding active ketone 1was dissolved in dry ethanol in Sodium hydroxide as catalyst, refluxing in a steam bath. After six-hour thin layer chromatography displayed the highest conversion of substrates to the product. Then the reaction was monitored with TLC and checked on 30 min intervals; after complete disappearance of starting material spot, the excess ethanol was distilled out and cooled to room temperature. It was poured into ice-cold water; the precipitate was filtered and purified by recrystallization from ethanol. The yield was quite good and it melts at 135°C.

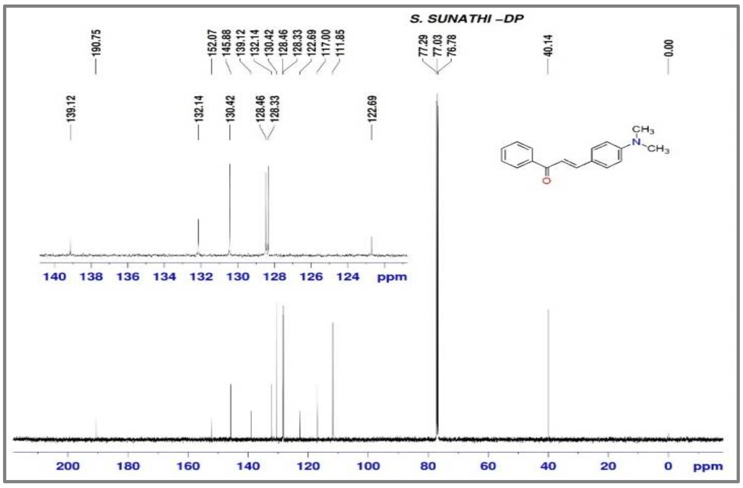


Figure 2. ^{13}C-NMR spectrum of *(E)*-3-(4-(dimethylamino)phenyl) -1-phenylprop-2-en-1-one **3.**

The purified products were characterized by EI-MS m/z (rel. int.%): FT-IR, ^{1}H NMR, ^{13}C NMR. The IR spectra of compounds **3** showed the characteristic band, aromatic C-H stretching at 3051 cm^{-1}, methyl C-H stretching 2908 cm^{-1} and carbonyl C=O stretching at 1644 cm^{-1} of chacones **3**. This is due to the conjugation of the π-electrons on the benzene moiety with those on the ethylene moiety in the enon linkage. ^{1}H NMR spectra, is a proven diagnostic tool for the positional elucidation of the proton. Assignments of the signals are based on chemical shift and intensity pattern. The ^{1}H-NMR spectrum (Figure 1) of compound **3** showed six protons of two CH_3 as a singlet at δ 3.04 ppm and α, β -unsaturated benzylic proton appear at 7.78 and 7.99 ppm for the CO,CH indicating that the ethylene moiety in the non linkage is in the trans-conformation which conform the formation of chalcones.^{13}C-NMR spectrum (Figure 2) showed a signal at δ 40.14 and 40.67 in the region of secondary carbon atom for C-H and disappearance of a signal at the olefinic carbon region confirmed the structure **3**of chalcones was recorded in $CDCl_3$ and spectral signals are in good agreement with the probable structures.

Characteristic peaks were observed in the EI mass spectra of compounds, which followed the molecular ion peak and similar fragmentation pattern, the mass spectrum of compound 3 as molecular formula $C_{17}H_{17}NO$ m/z (%): 252 (60) [M+1].

***(E)*-3-(4-(dimethylamino)phenyl)-1-phenylprop-2-en-1-one: 3 :** A mixture of Dimethylamino benzaldehyde (2) (14.9g, 0.1 mole) and butan-2-one (1) (7.2 mL, 0.1 mole) in dry ethanol (25 mL) was refluxed with added NaOH (1.0 g), monitoring the progress of reaction by TLC. The reaction was stopped at the appropriate point 6 h, the reaction mixture was worked up and subjected to column chromatography over silica gel (60-120 mesh) using 02:98% ethyl acetate in petroleum ether as eluent. The Single crystal suitable for X-ray diffraction study was grown by slow evaporation method and was dimerized during crystallization. Orange crystal, m.p. 180-181°C; 82% yield; IR (KBr, ν_{max}, cm^{-1}): 3343, 2977, 2900, 2818, 1677, 1578, 1519, 1229, 1000; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.52 (d, 1H, *J* =16 Hz, benzylic-H), 7.45 (d, 1H, phenyl-C_2) 6.58 (d, 1H, *J* = 16, benzylic-H), 6.67 (d, 2H, *J* = 9, phenyl-C_3-C_5), 2.66 (q, 2H, CH_2), 1.14 (t, 3H, CH_3) 3.08 (s, 6H, N-CH_3); ^{13}C NMR (120 MHz, $CDCl_3$): δ 201.12, 151.89, 143.09, 129.99, 122.22, 121.25, 111.88,111.01,40.12, 33.59, 8.65; GC-MS: m/z [M+1] 204 (16%).

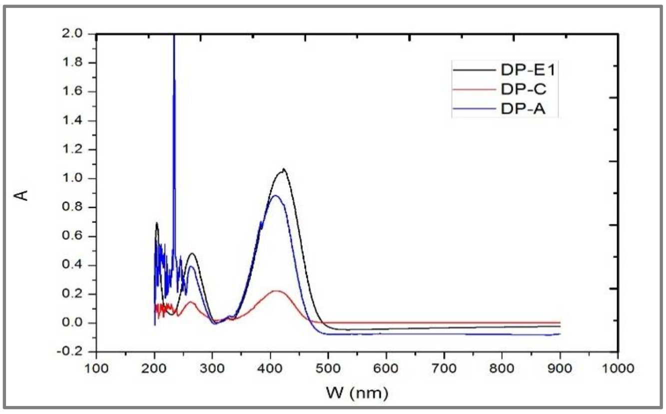


Figure 3. UV-Vis spectra Comparison of (*E*)-3-(4-(dimethylamino)phenyl)-1-phenylprop-2-en-1-one **3.**

In the solvent effect on the UV-Vis spectra of (*E*)-3-(4-(dimethylamino)phenyl)-1-phenylprop-2-en-1-one(**3**) $\pi \longrightarrow \pi^*$ transition were observed in all the solvent in the range of 265nm. In $CHCl_3$ it is observed at 262.83 nm 410nm, acetonitrile λ_{max} is slightly decreased to 262.07 nm 408 nm. While in highly polar protic solvent it has increased to 264.13 nm 463. These absorptions may be attributed to $\pi \longrightarrow \pi^*$ transition. The solvent effect in the intensity of λ_{max} of n to π^* transition is higher than that of π to π^* transition (Figure 3).

Crystal growth: The *(E)*-3-(4-(dimethylamino)phenyl)-1-phenylprop-2-en-1-onecrystals were grown by slow evaporation solution growth technique. The resulting compound 3 was crystallized using several solvents such as acetone, ethanol, ethyl acetate, methanol, chloroform, hexane, DMF, THF and ether, the ethanol was creating to be the best solvent to grow crystals as good value crystals. The (E)-3-(4 (dimethylamino)phenyl)-1-phenylprop-2-en-1-one product (5 g) was dissolved with ethanol and stirred for 1h at room temperature. the resultant homogeneous solution was filtered off in

Whatman 40 filter paper and then concentrated. The concentrated solution was kept for 1 days at room temperature for crystallization to obtain non-hygroscopic needle like crystals with the maximum size of approximate dimensions 0.100 mm x 0.220 mm x 0.250 mm (E)-3-(4-(dimethylamino) phenyl)-1-phenylprop-2-en-1-one (crystal).

Measurements: High-resolution ^{1}H-NMR spectrum of the compound was recorded on a 500 MHz AVANCE III spectrometer in $CDCl_3$ with TMS as an internal standard. The Fourier Transform Infrared (FT-IR) spectra of respective aldehyde, ketone and material was recorded between the regions of 600 to 4000 cm$^-$1 using a Bruker IFS 66V Fourier transform spectrometer, Thermo gravimetric analysis (TGA) was performed on a Mettler TA 3000 thermal analyzer under nitrogen atmosphere at a heating rate of 5°C min^{-1} with a sample weight of 3–5 mg. The optical band gap energies of crystals A and B were calculated using diffuse reflectance UV-Vis spectroscopy. The spectra were recorded between 190 and 800 nm on a Shimadzu UV-Vis spectrophotometer (model 2450) using $BaSO_4$ as the reference.

RESULTS AND DISCUSSION

Single crystal X-ray diffraction: A clear light yellow Rectangular-like specimen of $C_{17}H_{17}NO$, approximate dimensions 0.100 mm x 0.220 mm x 0.250 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. A total of 637 frames were collected. The total exposure time was 1.77 h. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm [18]. The integration of the data using a monoclinic unit cell yielded a total of 9301 reflections to a maximum θ angle of 24.76° (0.85 Å resolution), of which 2402 were independent (average redundancy 3.872, completeness=99.8%, R_{int}=3.10%, R_{sig}=3.37%) and 1307 (54.41%) were greater than $2\sigma(F^2)$. The final cell constants of a=13.1956(11) Å, b=11.8396(9) Å, c=9.5664(6) Å, β=109.533(3)°, volume=1408.55(18) Å^3, are based upon the refinement of the XYZ-centroids of 1657 reflections above 20 σ(I) with 4.750° < 2θ <39.42°. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.903. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9820 and 0.9930 (table 1and 2).

Table 1. Summary of X-ray crystallographic crystal data for (*E*)-3-(4-(dimethylamino)phenyl)-1-phenylprop-2-en-1-one **3**

Identification code	AU_Sumathi_Dp
Chemical formula	$C_{17}H_{17}NO$
Formula weight	251.31 g/mol
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal size	0.100 x 0.220 x 0.250 mm
Crystal habit	clear light yellow Rectangular
Crystal system	Monoclinic
Space group	P 1 21/c 1
Unit cell dimensions	a = 13.1956(11) Å α = 90°
	b = 11.8396(9) Å β = 109.533(3)°
	c = 9.5664(6) Å γ = 90°
Volume	1408.55(18) Å^3
Z	4
Density (calculated)	1.185 g/cm^3
Absorption coefficient	0.073 mm^{-1}
F(000)	536

Table 2. Data collection and structure refinement for (*E*)-3-(4-(dimethylamino)phenyl)-1-phenylprop-2-en-1-one **3.**

Theta range for data collection	1.64 to 24.76°
Index ranges	-15<=h<=15, -13<=k<=13, -11<=l<=9
Reflections collected	9301
Independent reflections	2402 [R(int) = 0.0310]
Coverage of independent reflections	99.8%
Absorption correction	multi-scan
Max. and min. transmission	0.9930 and 0.9820
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)
Function minimized	$\Sigma\ w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	2402 / 0 / 175
Goodness-of-fit on F^2	1.032
Final R indices	1307 data; I>2σ(I) R1 = 0.0534, wR2 = 0.1438
	all data R1 = 0.1070, wR2 = 0.1810
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0809P)^2+0.2344P]$ where $P=(F_o^2+2F_c^2)/3$
Extinction coefficient	0.0150(30)
Largest diff. peak and hole	0.155 and -0.126 eÅ^{-3}
R.M.S. deviation from mean	0.029 eÅ^{-3}

The compound is recrystallized using acetone-chloroform in the ratio 1:1 and subjected to single crystal XRD analysis. The hydrogen atomic coordinates and isotropic atomic displacement factors and corresponding anisotropic displacement parameter. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) are calculated. The selected bond length and bond angles and torsional angles are listed in tables 3, 4, 5.

Bond Geometry: The molecular structure (*E*)-1-(4-(dimethylamino)phenyl)pent-1-en-3-one **3** shown in figure 4 (ORTEP). It comprises of chalcone derivative with *N*, *N*- Dimethylamine. The chalcone moiety bears one aromatic substituent on *N*, *N* Dimethylamine and phenyl group atom. The structural parameters, including bond distances and bond angles (Table 3) show normal geometry. The chalcone compound, (*E*)-3-(4-(dimethylamino)phenyl)-1-phenylprop-2-en-1-one, which the structure shows two aromatic rings. The central C6 C1 phenyl ring forms the dihedral angles of and with the adjacent C10 C15 aromatic rings. The molecule is bent at N1 with the C12 C13 N1 C17 torsion angle of 179.5 (3)◦. The molecule exists in *E* configuration with respect to the central prop-en-one group which is defined by the C7-C8-C9-C10 torsion angle of 176.9 (2)◦.

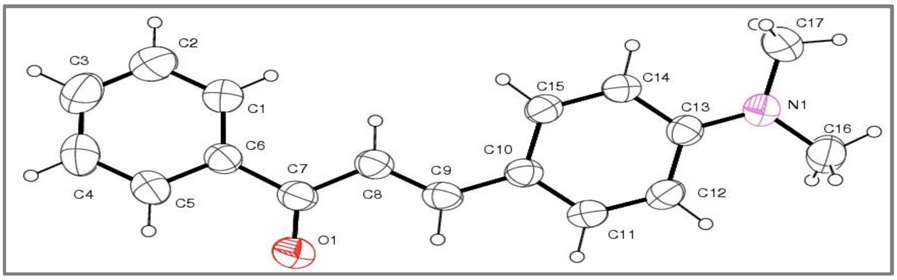


Figure 4. ORTEP view of the molecule (*E*)-1-(4-(dimethylamino)phenyl)pent-1-en-3-one **3**

The crystal structure is mainly stabilized by C5—H5…*π* *i*nteractions (Symmetry code: *x*, −*y*, *z*−1/2) involving the centroid of the C10—C12 benzene (*Cg*3) ring connecting the molecules into head-to-tail fashion propagating along *c*-axis direction (Figure 4). No significant intermolecular hydrogen bonds were found for the investigated structure. The crystal packing is consolidated by van der Waals contacts. The bond length and bond angles agree with the literature values [19].

Table 3. Bond lengths (Å) for (*E*)-3-(4-(dimethylamino)phenyl)-1-phenylprop-2-en-1-one **3**

C1-C2	1.367(5)	C1-C6	1.369(4)
C1-H1	0.93	C2-C3	1.367(5)
C2-H2	0.93	C3-C4	1.342(5)
C3-H3	0.93	C4-C5	1.368(5)
C4-H4	0.93	C5-C6	1.368(4)
C5-H5	0.93	C6-C7	1.480(4)
C7-O1	1.223(3)	C7-C8	1.462(3)
C8-C9	1.330(3)	C8-H8	0.93
C9-C10	1.444(3)	C9-H9	0.93
C10-C11	1.386(3)	C10-C15	1.398(3)
C11-C12	1.367(4)	C11-H11	0.93
C12-C13	1.400(4)	C12-H12	0.93
C13-N1	1.363(3)	C13-C14	1.402(3)
C14-C15	1.367(3)	C14-H14	0.93
C15-H15	0.93	C16-N1	1.450(3)
C16-H16A	0.96	C16-H16B	0.96
C16-H16C	0.96	C17-N1	1.437(4)
C17-H17A	0.96	C17-H17B	0.96
C17-H17C	0.96		

Table 4. Bond angles (°) for(*E*)-3-(4-(dimethylamino)phenyl)-1-phenylprop-2-en-1-one**3**.

C2-C1-C6	121.2(3)	C12-C11-C10	123.1(2)	C2-C1-H1	119.4	C12-C11-H11	118.4
C6-C1-H1	119.4	C10-C11-H11	118.4	C1-C2-C3	119.7(4)	C11-C12-C13	120.9(3)
C1-C2-H2	120.1	C11-C12-H12	119.5	C3-C2-H2	120.1	C13-C12-H12	119.5
C4-C3-C2	119.7(4)	N1-C13-C12	121.8(2)	C4-C3-H3	120.1	N1-C13-C14	121.8(2)
C2-C3-H3	120.1	C12-C13-C14	116.4(2)	C3-C4-C5	120.5(4)	C15-C14-C13	121.6(2)
C3-C4-H4	119.8	C15-C14-H14	119.2	C5-C4-H4	119.8	C13-C14-H14	119.2
C4-C5-C6	121.1(3)	C14-C15-C10	122.1(2)	C4-C5-H5	119.5	C14-C15-H15	119.0
C6-C5-H5	119.5	C10-C15-H15	119.0	C5-C6-C1	117.7(3)	N1-C16-H16A	109.5
C5-C6-C7	119.4(3)	N1-C16-H16B	109.5	C1-C6-C7	122.9(3)	H16A-C16-H16B	109.5
O1-C7-C8	121.1(3)	N1-C16-H16C	109.5	O1-C7-C6	119.0(2)	H16A-C16-H16C	109.5
C8-C7-C6	119.9(3)	H16B-C16-H16C	109.5	C9-C8-C7	121.7(3)	N1-C17-H17A	109.5
C9-C8-H8	119.2	N1-C17-H17B	109.5	C7-C8-H8	119.2	H17A-C17-H17B	109.5
C8-C9-C10	129.3(2)	N1-C17-H17C	109.5	C8-C9-H9	115.3	H17A-C17-H17C	109.5
C10-C9-H9	115.3	H17B-C17-H17C	109.5	C11-C10-C15	115.7(2)	C13-N1-C17	122.0(2)
C11-C10-C9	120.4(2)	C13-N1-C16	120.8(2)	C15-C10-C9	123.8(2)	C17-N1-C16	117.1(2)

Compound **3** crystallizes in clear light yellow Rectangular in a Monoclinic type structure and exhibits crystallographic disorder between the *N*, *N*-Dimethyl amino positions. When measuring the bond lengths of C16-N1 and C17-N1 distances of 1.450(3) Å and 1.437(4) Å, respectively, are observed.

The final anisotropic full-matrix least-squares refinement on F^2 with 140 variables converged at R1= 4.44%, for the observed data and wR2 = 12.68% for all data. The goodness-of-fit was 1.042. The largest peak in the final difference electron density synthesis was 0.191 e^-/Å^3 and the largest hole was -0.119 e^-/Å^3 with an RMS deviation of 0.029 e^-/Å^3. On the basis of the final model, the calculated density was 1.154 g/cm^3 and F (000), 440 e^-. The molecular structure **(3)** shown in Figure **2** (ORTEP) [**20**]. It comprises of chalcone derivative with *N*, *N*- Dimethylamine. The chalcone moiety bears one aromatic substituent on *N*, *N*- Dimethylamine and Ethyl group atom. The structural parameters including bond distances and bond angles were (Table **3** and 4) show normal geometry.

Table 5. Torsion angles (°) for(*E*)-3-(4-(dimethylamino)phenyl)-1-phenylprop-2-en-1-one **3**.

C6-C1-C2-C3	2.0(7)	C1-C2-C3-C4	-3.0(7)
C2-C3-C4-C5	1.9(8)	C3-C4-C5-C6	0.3(7)
C4-C5-C6-C1	-1.3(5)	C4-C5-C6-C7	-179.1(4)
C2-C1-C6-C5	0.1(5)	C2-C1-C6-C7	177.9(3)
C5-C6-C7-O1	18.9(4)	C1-C6-C7-O1	-158.8(3)
C5-C6-C7-C8	-161.8(3)	C1-C6-C7-C8	20.5(4)
O1-C7-C8-C9	1.0(4)	C6-C7-C8-C9	-178.3(2)
C7-C8-C9-C10	176.9(2)	C8-C9-C10-C11	-176.7(3)
C8-C9-C10-C15	0.9(4)	C15-C10-C11-C12	-2.0(4)
C9-C10-C11-C12	175.8(2)	C10-C11-C12-C13	0.1(4)
C11-C12-C13-N1	-176.8(2)	C11-C12-C13-C14	2.3(4)
N1-C13-C14-C15	176.2(2)	C12-C13-C14-C15	-3.0(4)
C13-C14-C15-C10	1.1(4)	C11-C10-C15-C14	1.4(4)
C9-C10-C15-C14	-176.4(2)	C12-C13-N1-C17	-179.5(3)
C14-C13-N1-C17	1.3(4)	C12-C13-N1-C16	-2.8(4)
C14-C13-N1-C16	178.1(2)		

APPLICATION

Chalcones are pharmacologically active compounds, chemically known as derivatives of (E)-3-(4(Dimethylamino)phenyl)-1-phenylprof-2-en-1-one. They have found applications are antimicrobial, anti-tubercular agents. On the foundation of the results obtained from single XRD studies the novel chalcone.

CONCLUSION

A novel (*E*)-3-(4-(dimethylamino)phenyl)-1-phenylprop-2-en-1-one (chalcone) is synthesized and crystals of this compound were successfully grown by the solution growth technique. The functional groups present in the synthesized compound were identified using FT-IR and NMR spectra. Single crystal XRD studies confirm the conformation of the investigated compound. There exists ample scope for synthesis and crystal growth studies on other chalcone possessing which might show better biological activities or optical properties.

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