iJRASET
International Journal For Research in
Applied Science and Engineering Technology

INTERNATIONAL JOURNAL FOR RESEARCH
IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY

Volume: 9 **Issue:** XI **Month of publication:** November 2021

DOI: https://doi.org/10.22214/ijraset.2021.39069

www.ijraset.com

Call: ✆08813907089 | E-mail ID: ijraset@gmail.com

International Journal for Research in Applied Science & Engineering Technology (IJRASET)
ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 7.429
Volume 9 Issue XI Nov 2021- Available at www.ijraset.com

Characterization and Theoretical study of Nonlinear Optical Properties of (2*E*)-1-(2, 4-dichlorophenyl)-3-(4-methylphenyl) prop-2-en-1-one

Virupakshi M. Bhumannavar[1], Parutagouda Shankaragouda Patil[2], Neelamma B. Gummagol[3]
[1]*Hirasugar Institute of Technology, Nidasoshi-591236, Karnataka, India*
[1, 3]*K.L.E. Institute of Technology, Opposite Airport, Gokul, Hubballi-580030, Karnataka, India*
[2]*B.L.D.E.A'S, S. B. Arts and K. C. P. Science College Vijayapur-586103, Karnataka, India*

Abstract: The structural confirmation of the title compound is done by theoretical and experimental study. Experimental techniques such as FTIR, proton NMR, UV-Visible, thermal analysis (TGA & DTA) are employed. Density functional theory is used to analyze spectroscopic data scrutinized. Second order nonlinear optical parameters are obtained. The experimental results are analyzed with theoretically obtained data from density functional theory. TD-DFT also employed for the MLDCLC at different basis set.

Keywords: DFT Study, nonlinear optical study, FTIR, ^{1}H NMR

I. INTRODUCTION

Chalcones major classes have wide range pharmacological activity importance [1]. They are found in edible plants abundantly and having many derivatives heterocyclic rings like pyrimidines, isoxazoles, pyrazolines and cynopyridines [2]. Nonlinear optical materials will have applications in lasers optical sensing, data storage etc.[3-6]. Two side of the aromatic rings of the compound consists of strong inter molecular interaction due to electron donor and electron acceptor π-conjugate system [7-9]. Due to resilient intermolecular interactions second and third order nonlinearity observed [10-16]. Also chalcone have medical applications like antimalarial, anti-fungal, anti-cancer, anti-HIV and antioxidants, anti-ulcer, anti-inflammatory, anti-mitotic etc. [17–24]. In recent DFT study were carrying out on organic, inorganic, chalcones [25–28]. The vibrational study of chalcones is done on chalcones [29-31]. Experimental study such as FTIR, ^{1}H NMR and UV–Visible–NIR was applied to determine structure characterization of chalcone [32-39]. In this research work are concentrated on investigation of molecular structure of (2*E*)-1-(2,4-dichlorophenyl)-3-(4-methylphenyl)prop-2-en-1-one (MLDCLC) compound using spectroscopic methods (FTIR, ^{1}H NMR), linear (UV–Visible). The stability of the molecule is found by thermal study. To the support of experimental results the theoretical calculations are done with B3LYP/6-311++G point of theory. Also molecular orbits, global chemical reactivity descriptors (GCRD), absorption spectra, excitation energies are done with the same theory.

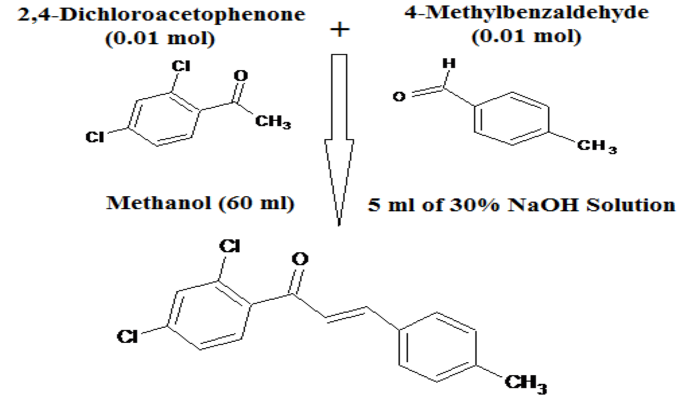
II. EXPERIMENTAL

A. Synthesis

The compound MLDCLC is synthesized with Claisen –Schmidt Condensation method. 4-Methylbenzaldehyde (0.01 mol)) with 2,4-dichloroacetophenones (0.01 mol) in methanol (60 ml) and the mixture was treated with 5 ml of 30% sodium hydroxide solution and stirred at room temperature for 2 h. The precipitate obtained was poured into ice-cold water (500 ml) and left to stand for 5 h. The resulting crude solid was filtered, dried and recrystallised by slow evaporation. The scheme of the reaction is shown in the Fig.1.

B. Computational Study

Theoretical computations for title compound are done with GAUSSIAN 09W program. Optimized geometry of MLDCLC molecule obtained at B3LYP with 6-311++G (d, p) basis set. Also DFT executed to with 6-311++G(d, p) basis set for MLDCLC molecule at different levels B3LYP, HF and CAMB3LYP. FTIR and NMR are performed with same basis set. Results are visualized in Gauss View 5 software. Obtained results of title compound were compared and discussed. Obtained results of title compound were compared and discussed. GAMESS software is run for MLDCLC molecule by writing a command.



(*E*)-1-(2,4-dichlorophenyl)-3-(4-methylphenyl)prop-2-en-1-one

Fig. 1 Scheme of reaction MLDCLC

C. Characterization

The MLDCLC compound was performed with experimental techniques ^{1}H NMR spectrum is recorded. Infra red spectrum was recorded using potassium bromide (KBr) pellet method in the range 4000-400 cm^{-1}.The ultraviolet, visible and near infrared regions spectrum for the title compound were measured in the range of 200-3000nm in DMF solution. The analysis of thermal behaviour, decaying and melting point of MLDCLC was done by TG/DTA analysis.

III.RESULTS AND DISCUSSIONS

A. Structure Charecterzation

The The optimization of geometry 2CBC compound carry out using DFT at B3LYP/6-311+G(d, p) level. Structure of molecule is given away in Fig. 2. From Molecule geometry bond angles, bond length and dihedral angles are obtained. The results obtained from theory and experimental XRD data are shown in Table 1. Patil et al. [40] report the XRD data of MLDCLC. The bond lengths of Cl1-C4 is 1.76 Å (DFT) and 1.74 Å (XRD), Cl2-C7 is 1.75 Å (DFT) and 1.74 Å (XRD), C13-O3 is 1.22 Å (DFT) and 1.22 Å (XRD), C14-C16 is 1.35 Å (DFT) and 1.34 Å (XRD), C19-C21 is 1.39 Å (DFT) and 1.39 Å (XRD), C23-C24 is 1.40 Å (DFT) and 1.40 Å (XRD). The bond angles of Cl1-C4-C5 is 116.52° (DFT) and 116.84° (XRD), Cl1-C4-C12 is 121.63° (DFT) and 120.92° (XRD), C21-C23-C28 is 121.50° (DFT) and 120.81° (XRD), C4-C5-H6 is 120.35° (DFT) and 120.90° (XRD), Cl2-C7-C5 is 119.06 ° (DFT) and 119.16 ° (XRD), Cl2-C7-C8 is 119.70 ° (DFT) and 118.90 ° (XRD). The torsional angles of Cl1-C4-C5-C7 is -177.12° (DFT) and -175.10° (XRD), Cl1-C4-C12-C10 is 175.24° (DFT) and 173.46° (XRD), Cl2-C7-C8-C10 is -179.84° (DFT) and -179.13° (XRD), C14-C16-C18-C19 is -179.26° (DFT) and -177.21° (XRD), C16-C18-C19-C21 is 179.89° (DFT) and 179.21° (XRD). The bond length, bond angles and torsional angles obtained from DFT and XRD results are having good agreement.

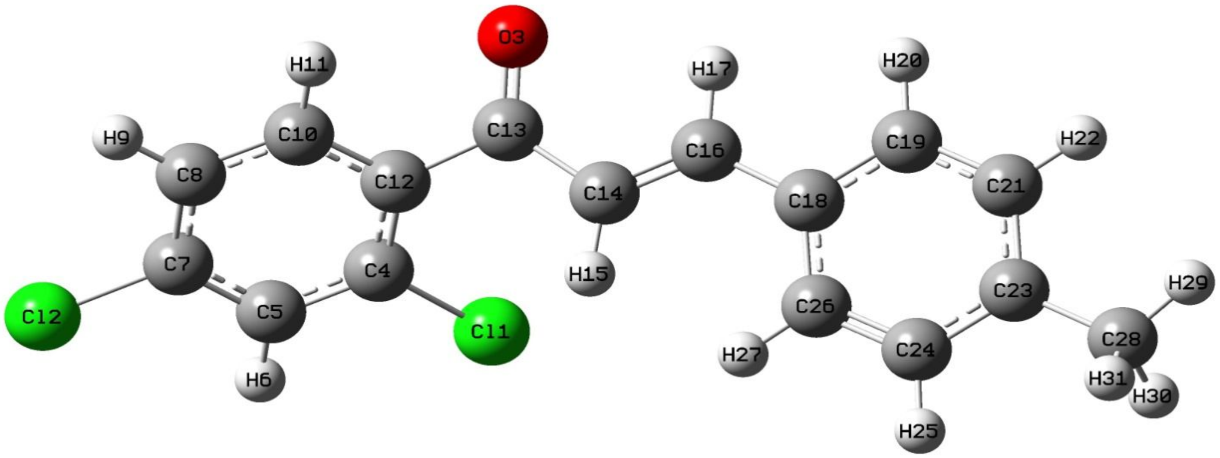


Fig.2 Optimized structure of MLDCLC

Table 1
Experimental (XRD data) and theoretical (DFT) determined bond length (Å), bond angles, and torsion angles (°) of MLDCLC molecule.

Bond length	DFT	XRD	Bond angle	DFT	XRD	Torsion angle	DFT	XRD
Cl1-C4	1.76	1.74	Cl1-C4-C5	116.52	116.84	Cl1-C4-C5-C7	-177.12	-175.10
Cl2-C7	1.75	1.74	Cl1-C4-C12	121.63	120.92	Cl1-C4-C12-C10	175.24	173.46
O3-C13	1.22	1.22	C21-C23-C28	121.50	120.81	Cl2-C7-C8-C10	-179.84	-179.13
C14-C16	1.35	1.34	C4-C5-H6	120.35	120.90	C14-C16-C18-C19	-179.26	-177.21
C19-C21	1.39	1.39	Cl2-C7-C5	119.06	119.16	C16-C18-C19-C21	179.89	179.21
C23-C24	1.40	1.40	Cl2-C7-C8	119.70	118.90	C26-C18-C19-H20	179.94	179.20
C23-C28	1.51	1.51	O3-C13-C12	118.48	118.41	C23-C24-C26-H27	179.87	180.00

B. Vibrational Spectroscopy Study

The MLDCLC compound has 31 atoms and contains 87 normal modes of vibration. MLDCLC compound functional groups are compared with experimentaly recorded FTIR spectra and theorotically obtained B3LYP/6-311++G(d, p) level. The compound has vibrational bands asssignments in the region 4000 - 400 cm^{-1}. The spectra of stretching vibrations of C-H are observed in the region 2950 - 3150 cm^{-1}. The spectra of compound are shown in Fig.3 their band assignments are shown in Table 2. Arromatic C─H stretching vibrational modes are 3059.49 (Expt) and 3196, 3180, 3156, 3108, 3076 cm^{-1} (DFT). The strong unique absorption peak of carbonyl group region in between 1750-1620 cm^{-1}. Strong peak of C = O group vibration is observed at 1780.63, 1657.24 cm^{-1} (experimental), and 1716, 1628 (theoretical) and for the molecule of MLDCLC. The theoretical and experimental C = C stretching found in the vicinity of 1600-1550 cm^{-1}. The theoretical and experimental C = C stretching found be 1589.97 cm^{-1} and 1596, 1540 cm^{-1} respectively. The MLDCLC molecule has modes of vibrations lie in the range of 1550–600 cm^{-1} for experimental spectra and calculated spectra. The stretching vibration of C–CH$_3$ of MLDCLC is obtained at 1410.42 (expt) and 1404 cm-1 (DFT). The stretching vibration of C–Cl of a molecule is observed at 747.36, 728.63, 673.84, and 577.74 cm^{-1} (expt), 740 and 692 cm^{-1} (DFT). The C-H bending of aromatic ring is found in the range of 840 cm^{-1} – 710 cm^{-1}. The C-C bending of aromatic ring is found in the range of 1600 cm^{-1} – 1450 cm^{-1}. The details of the functional vibrational frequencies are assigned. In presumption, the results of FTIR vibrations calculated and theoretical functional groups frequencies are good agreement with each other. Hence, Vibrational spectroscopic study authenticates Functional groups and their molecular structure of MLDCLC.

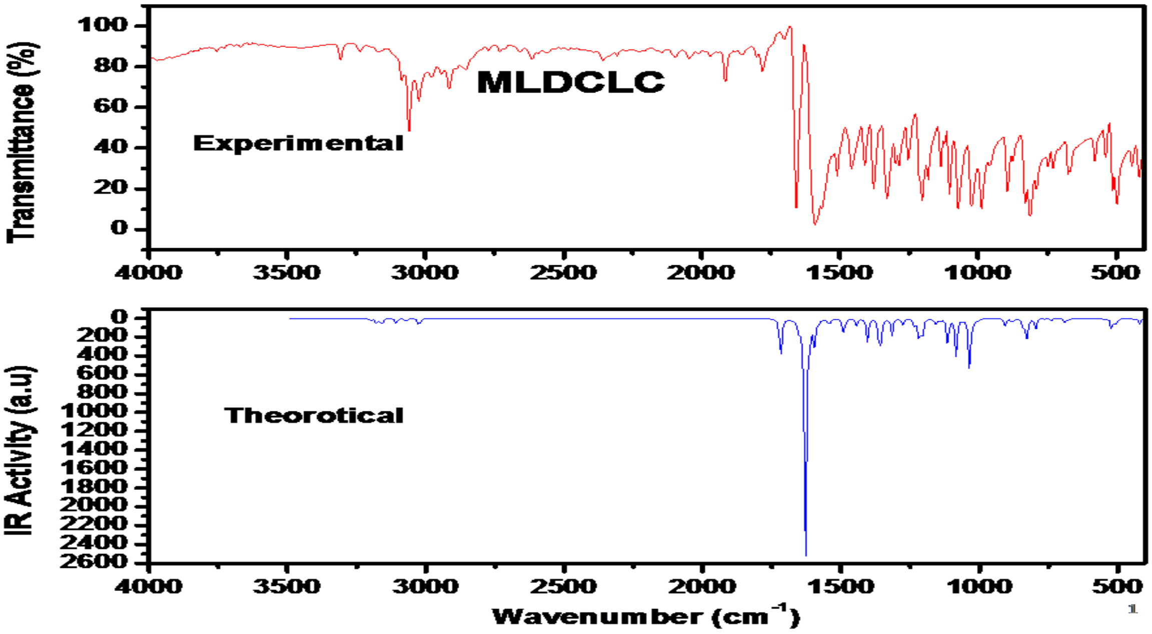


Fig. 3 Experimental FTIR spectrum

Table. 2

Experimental and theoretical FTIR vibrational assignments (wavenumber in cm^{-1}).

Experimental	Theoretical (DFT)	Assignment
3059.49	3196, 3180, 3156, 3108, 3076	ν_{Asym} (C-H stetching of CH_3 group)
3024.03	3028	ν_{Sym} (C-H Aromatic)
1780.63	1716	ν_{sym} (C=O)
1657.24	1628	ν_{sym} (C=O),
1589.97	1596, 1540	ν_{Sym} (C=C)
1509.27	1492	δ(C-C Aromatic Ring)
1457.9	1444	δ (C=C Aromatic Ring)
1410.42	1404	ν_{sym} (C-H benging of CH_3 group)
1377.44	1356	δ (C-H Aromatic)
1329.62	1316	δ (C-H Aromatic), δ (C-H)
1284.36	1276	δ (C-H CH_2 group),δ (C-H Aromatic)
1252.65	1236, 1220	δ(C-H, C-C Ring),
1202.75	1204,	δ(C-H, C-C Ring),
1135.37	1116	ν (C-C Ring), τ(HCCH Ring)
1103.08	1084, 1036	ν (C-C Ring), τ (C-H Aromatic)
1022.09	1012	γ(C-C, C-H Ring)
960.38	908	γ(C-H Ring), τ(HCCH Ring)
893.61	884	γ (C=O, Aromatic Ring),
875.52		γ (C=O γ(Ring) Wa, τ(Ring)
829.24	828	ν (C-Cl Stretching), δ(CCC Ben Ring)
811.75, 788.96	796	δ (C-C ring)
747.36,	740	ν (C-Cl Stretching)
728.63, 673.84, 577.74	692	ν (C-Cl Stretching)
538.79	524	δ (C-C, C-H Ring)
512.97, 497.47		γ(C-C, C-H Ring)
	508	t(C-C, C-H Ring)
443.27	444, 420	t(C-C, C-H Ring)

C. Proton NMR Analysis

The number of protons and molecular structure of tittle compound MLDCLC are confirmed. The combined ^1H NMR spectra of experimental and theoretical are given in Fig. 4 and their relevant chemical shifts (δ) are given in Table 3. MLDCLC molecular structure has 12 protons. The theoretical ^1H NMR spectra shows that it every proton consists of separate peaks, where as the experimental spectra shows that it consists of compound peaks because of degeneracy. The MLDCLC molecule will have chemical shifts δ=1 ppm to 8.5 ppm is observed. The chemical shifts of CH_3 group are 2.387 ppm (Expt) and 1.8497, 2.5167, 2.6195 (DFT) respectively. ^1H NMR spectral study results of experimental and theoretical values are in good correlation with their derivatives.

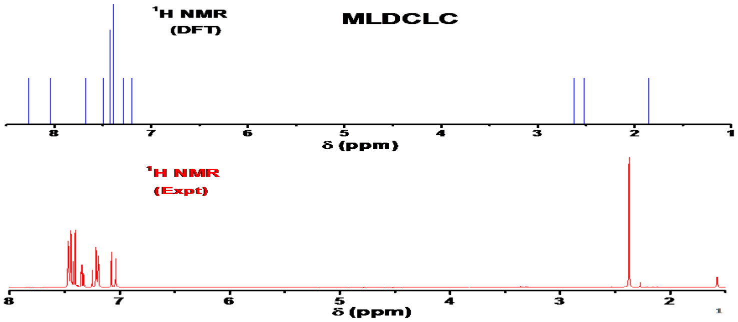


Fig. 4 Experimental and theoretical proton NMR

Table 5
The experimental and theoretical (DFT)^{1}H NMR chemical shifts (δ in ppm) of MLDCLC.

(^{1}H) type	Expt	DFT
29-H	2.387	1.8497
31-H	2.387	2.5167
30-H	2.387	2.6195
9-H	7.046, 7.086	7.2002
22-H	7.205	7.2892
25-H	7.226	7.3956
20-H	7.334, 70340, 7.355, 7.361	7.4279
6-H	7.415	7.4309
15-H	7.436	7.4969
11-H	7.455	7.6766
27-H	7.478	8.0463
17-H	7.481	8.2669

D. Thermal Analysis

The Fig.5 shows Thermo gravimetric (TG) and differential thermal (DT) analysis. A weight of 14.145 mg compound MLDCLC initially used for investigation. Thermo gravimetric (TG) curve sketch confirms that the weight loss is 1 % for a temperature 30-230 ^{0}C, due to humidity and unpredictable solvent. The major weight loss is 98.667 % at 318.63 ^{0}C because of decomposition of MLDCLC. In TGA show that final residual mass is about 1.333 % heating up to 400 ^{0}C. There is an endothermic peak observed in DTA trace at 96.03 ^{0}C which is assigned to melting point of MLDCLC molecule. The molecule is reactive up to the melting point.

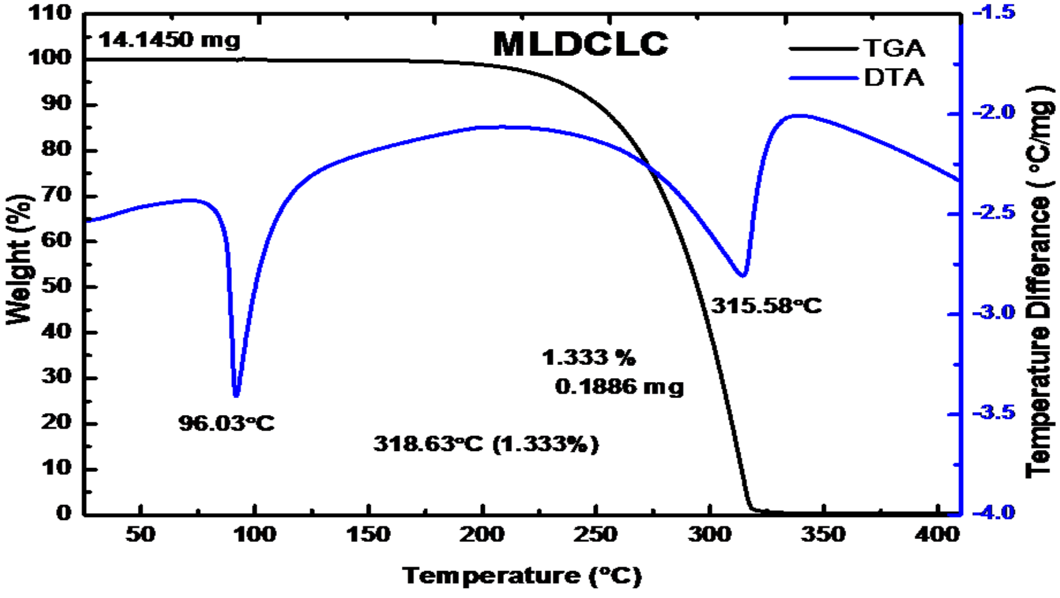


Fig. 5 Thermal study plots of MLDCLC molecule

E. Ultra Violet-Visible- Absorption Spectrum

Ultra Violet-Visible absorption spectrum was obtained for the sample MLDCLC at the range 200nm-800nm. Two peaks in absorption spectrum are observed and they corresponding to electronic transitions of π–π* and *n*–π* and their absorption peaks are 238 nm and 312 nm respectively. The maximum absorption energy of molecule will have the peak at 312 nm as shown in Fig.6. From absorption spectrum the energy gap of MLDCLC was computed using Tauc's plot [41]. Plotting graph of $(\alpha h\nu)^{1/n}$ verses photon (hν) by taking n=0.5, intersects x-axis and the value of energy gap (E_g) was found to be 3.29 eV (indirect method) and 3.38 eV (direct method) as shown in Fig. 6.

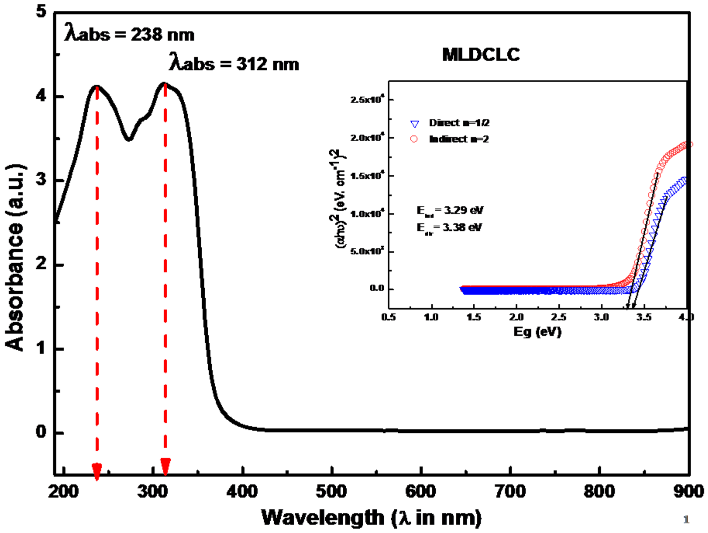


Fig.6 Experimental UV-Visible spectra of MLDCLC molecule

F. TD-DFT Linear Absorption Study

The electronic excitation, wavelength absorption and oscillator strength can be calculated for three different levels by TD-DFT method with B3LYP/6-311++G(d, p), CAM-B3LYP/6-311++G(d, p) and HF/6-311++G(d, p) basis in gas phase [42] as shown in Fig.7. The vertical absorption in UV-Vis spectrum corresponds to highest absorption peak. The theoretical absorption vales from TD-DFT Absorption spectrum at for basis set HF, CAM-B3LYP and B3LYP found to be 276.83 nm, 303.55 nm, and be 334.66 nm. The absorption wavelength, excitation energy, oscillation strength and contribution of HOMO-LUMO orbital are revealed in Table 4. Excitation energy of MLDCLC from TD-CAMB3LYP predicted 4.084 eV.

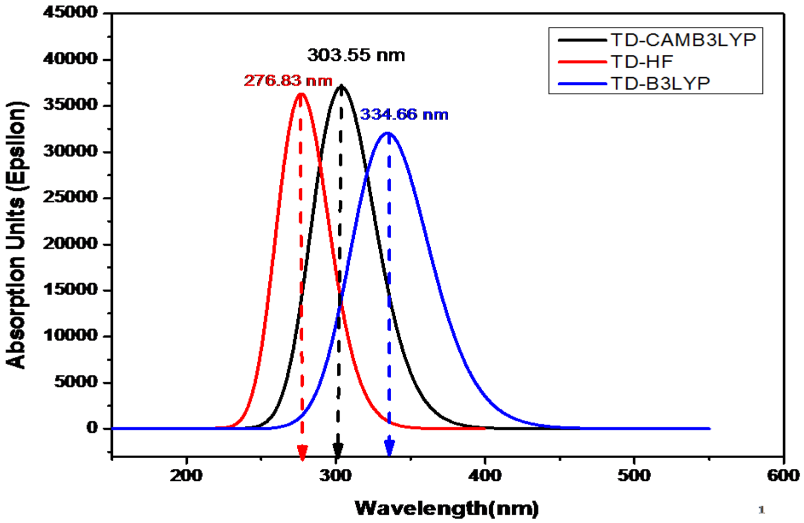


Fig.7 TD-DFT Linear absorption study plot of MLDCLC

Table 4

The excitation energy Δ*E*, oscillator strengths f_0 and major contributions of HOMO-LUMO orbitals of MLDCLC molecule at different states under TD-DFT using 6-311++G(d, p) basis set.

Method	Electronic transitions	λ_{Ex}	ΔE (eV)	f_0	Major contributions (in %)
Experimental	-	312	3.9763	-	-
B3LYP	$S_0 \rightarrow S_1$	368.48	3.3647	0.0126	H-1→L (62)
	$S_0 \rightarrow S_2$	334.66	3.7047	0.7758	H→L (94)
	$S_0 \rightarrow S_3$	299.43	4.1406	0.0324	H-2→L (68)
CAM-B3LYP	$S_0 \rightarrow S_1$	336.98	3.6792	0.0054	H-4→L (46)
	$S_0 \rightarrow S_2$	303.55	4.0844	0.9133	H→L (94)
	$S_0 \rightarrow S_3$	259.74	4.7735	0.0038	H-2→L (59)
HF	$S_0 \rightarrow S_1$	276.83	4.4788	0.8919	H→L+1 (75)
	$S_0 \rightarrow S_2$	266.00	4.6611	0.0063	H-5→L+1 (54)
	$S_0 \rightarrow S_3$	228.83	5.4182	0.0021	H-1→L+1 (34)

G. HOMO-LUMO Study

The molecular orbit (MO) consists of unoccupied molecular orbital (LUMO) and highest occupied molecular orbital (HOMO). HOMO-LUMO energy gap of compound MLDCLC theoretically determined by B3LYP/6-311++G (d, p) is 3.98 eV are listed in Table 5. Molecular orbits are shown in Fig. 8. Transition of π→π* orbital strongly suggest that it is system of donor and acceptor. The energy gap of HOMO-LUMO is good agreement calculated is 3.98 eV and excited energy gap 3.976 eV.

Table 5

The frontier molecular orbital energies (in eV), and global chemical reactivity descriptors (in eV), chemical hardness (η), potential (μ), softness (S), electronegativity (χ), and electrophilic index (ω) of MLDCLC molecule

E_H	E_L	E_{H-1}	E_{L+1}	ΔE_{H-L}	$\Delta E_{H-1-L+1}$	η	μ	S	χ	ω	I	A
-6.57	-2.59	-7.14	-1.29	-3.98	-5.85	1.99	-4.58	0.25	4.58	5.27	-6.57	-2.59

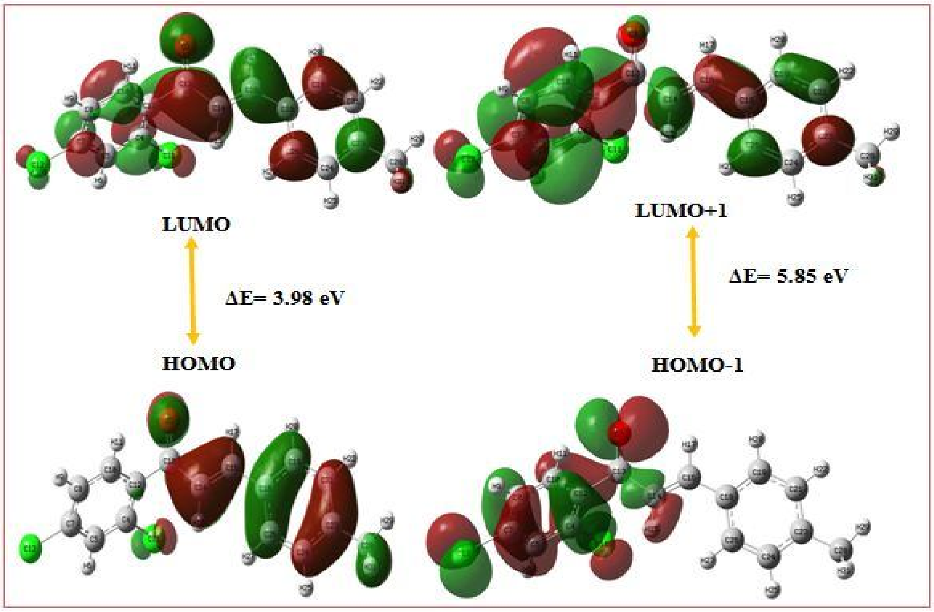


Fig. 8 HOMO-LUMO plots of MLDCLC

H. Computational NLO Studies

From its components dipole moment, mean polarizability, anisotropic polarizability, first hyperpolarizability and second hyperpolarizability were calculated [43-44]. The calculated dipole moment is presented in table 6. Static polarizability, first hyperpolarizability and second hyperpolarizability are calculated from DFT by the basis set B3LYP/6-311+G(d, p). Dynamic polarizability, first hyperpolarizability and second hyperpolarizability are calculated for different frequencies are determined by writing a command in GAMESS software. From GAMESS software dynamic mean polarizability anisotropic polarizability, first hyperpolarizability and second hyperpolarizability are determined.

Table 1
The calculated values of static dipole moment (μ) of MLDCLC in Debye

Components	
μ_x	-3.07
μ_y	-1.73
μ_z	-1.59
μ_{tot}	3.87

Table 2
The calculated values of static and dynamic polarizability (α) of MLDCLC

Components ($\times 10^{-24}$) esu	ω=0.00	ω=0.0569
α_{xx}	31.12	32.17
α_{xy}	0.21	0.28
α_{yy}	16.99	17.23
α_{xz}	-2.25	-2.25
α_{yz}	0.43	0.44
α_{zz}	7.19	7.27
α_{tot}	18.43	18.89
$\Delta\alpha$	21.21	22.07

The results of static (ω=0.0) and dynamic (ω=0.0569) mean polarizability is presented in Table 7. The results of static (ω=0.0) and dynamic (ω=0.0569) anisotropic polarizability are given in Table 7. The results of static (ω=0.0) and dynamic (ω=0.0569) first hyperpolarizability are given in Table 8. The results of static (ω=0.0) and dynamic (ω=0.0569) second hyperpolarizability are given in Table 9.

Table 3
The calculated values of static and dynamic first hyperpolarizability (β) of MLDCLC

Component ($\times 10^{-30}$) esu	ω=0.00	ω=0.05695
β_{xxx}	-3.85	-6.24
β_{yyy}	-0.09	-0.14
β_{zzz}	0.13	0.14
β_x	-12.88	-20.49
β_y	-8.06	-11.25
β_z	-2.44	-3.67
β-V	15.38	23.66

Table 4
The calculated values of static and dynamic second hyperpolarizability (γ) of MLDCLC

Components ($\times10^{-36}$) esu	ω=0.00	ω=0.05695
γ_{xxxx}	44.76	140.79
γ_{yyyy}	0.15	0.31
γ_{zzzz}	0.19	0.28
γ_{xxyy}	4.21	11.23
γ_{xxzz}	1.07	2.72
γ_{yyzz}	0.17	0.31
γ_{yyzz}	0.17	0.31
‹γ›	11.20	33.98

I. Global Chemical Reactivity Descriptors (GCRD)

This is the important utensils to identify the chemical stability, hardness, softness, potential, electronegativityand electrophilic index. Calculated GCRD are listed in the table 5. The value hardness must larger so that molecule will be more stable. Hardness (η) of MLDCLC compound is found to be 1.99 eV, softness (S) is 0.25 eV, Potential (μ) is -4.58 eV, Electronegativity (χ) is 4.58 eV, Electrophilic index (ω) is 5.27 eV, Ionization energy (I) is 6.57 eV and Electron affinity (A) is 2.59 eV.

J. Molecular Electrostatic Potential

The molecular electrostatic potential will give the information of shape, size and positive, negative and neutral sites of the molecule. MEP of the molecule MLDCLC is given in Fig. 9. Blue colour which will be preferred area for positive region. Red region, red colour which will indicate the preferred area of negative region and white colour represents the proton rich region[45].

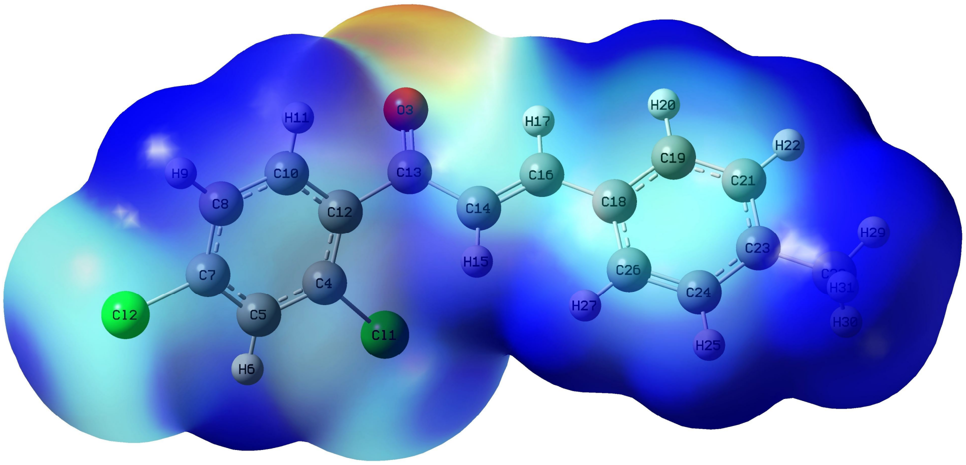


Fig. 9 Molecular electrostatic potential of MLDCLC

IV. CONCLUSIONS

The compound MLDCLC are confirmed with spectroscopic experiments results of FTIR, proton NMR and UV-Visible. The density functional theory is used to obtain optimized geometry by keeping B3LYP/6-311G++(d,p) at the basis set. Theoretical results of bond length, bond angle and torsinal angle are obtained from DFT are compared with XRD results of the crystal. The results are good agreement with each other. Also confirmation of molecular structure is done with proton NMR. Experimental and theoretical (DFT) FTIR spectrum of functional group frequency results are good agreement with each other. The MLDCLC compound is having the total dipole moment 3.87 D. The static (ω=0.0) and dynamic (ω=0.0569) mean polarizability are 18.43 x$10^{-24}$and 18.89 x 10^{-24}esu. Static (ω=0.0) and dynamic (ω=0.0569) anisotropic polarizability are 21.21 x10^{-24} esu and 22.07 x 10^{-24}esu. Static (ω=0.0) and dynamic (ω=0.0569) first hyperpolarizability are 15.38 x10^{-30} esu and 23.66 x 10^{-30} esu. Static (ω=0.0) and dynamic (ω=0.0569) second hyperpolarizability are 11.20x10^{-36} esu and 33.98x10^{-36} esu. The values of static and dynamic first hyperpolarizability are close agreement with already reported nonlinear compounds. This compound will be helpful in the field nonlinear optics applications.

V. ACKNOWLEDGMENT

I thank Dr. Basavaraj Anami Principal KLE Institute of Technology Hubballi, India for encouraging carrying out the study. I thank Dr. S.C.Kamate Principal Hirasugar Institute of Technology Nidasoshi for constant support. I thank USIC karnatak University Dharwad for providing the instrumental help.

REFERENCES

[1] Yao, B. Zhang, C. Ge, S. Peng, J. Fang, J. Agric. Food Chem. 63 (2015) 1521-1531.
[2] O.S. Moustafa, R.A. Ahmad, Phosphorus, Sulfur, and Silicon and Relat. Elem. 178 (2003) 475-484.
[3] M. Shkir, S. Muhammad, S. AlFaify, A. Irfan, P.S. Patil, M. Arora, H. Algarni,Z. Jingping, RSC Adv. 5 (2015) 87320-87332.
[4] S.D. Smith, Lasers, nonlinear optics and optical computers, Nature 316 (1985) 319–324.
[5] P. Huber, High power in the near ultraviolet using efficient SHG, Opt. Commun. 15 (1975) 196–200.
[6] P. Franken, J.Ward, Optical harmonics and nonlinear phenomena, Rev. Mod. Phys. 35 (1963) 23.
[7] Y. Goto, A. Hayashi, Y. Kimura, M. Nakayama, Second harmonic generation and crystal growth of substituted thienyl chalcone, J. Cryst. Growth 108 (1991) 688–698.
[8] W.T. Harrison, H. Yathirajan, B. Sarojini, B. Narayana, H. Anilkumar, Do C—H···O and C—H···π interactions help to stabilize a non-centrosymmetric structure for racemic 2, 3-dibromo-1, 3-diphenylpropan-1-one? Acta Crystallogr. Sect. C: Cryst. Struct. Commun. 61 (2005) 728–730.
[9] T. Uchida, K. Kozawa, T. Sakai, M. Aoki, H. Yoguchi, A. Abdureyim, Y. Watanabe, Novel organic SHG materials, Mol. Cryst. Liq. Cryst. 315 (1998) 135–140.
[10] B. Gu, W. Ji, P. Patil, S. Dharmaprakash, Ultrafast optical nonlinearities and figures of merit in acceptor-substituted 3, 4, 5-trimethoxy chalcone derivatives: Structure - property relationships, J. Appl. Phys. 103 (2008) (103511-103511-103516).
[11] H. Ravindra, A.J. Kiran, S. Dharmaprakash, N.S. Rai, K. Chandrasekharan, B. Kalluraya, F. Rotermund, Growth and characterization of an efficient nonlinear optical D–π–A–π–D type chalcone single crystal, J. Cryst. Growth 310 (2008) 4169–4176.
[12] P.S.Patil,M. Bannur, D. Badigannavar, S. Dharmaprakash, Study on nonlinear optical properties of 2, 4, 5-trimethoxy-4′-bromochalcone single crystal, Opt. Laser Technol. 55 (2014) 37–41.
[13] B.K. Sarojini, B. Narayana, B.V. Ashalatha, J. Indira, K.G. Lobo, Synthesis, crystal growth and studies on non-linear optical property of new chalcones, J. Cryst. Growth 295 (2006) 54–59.
[14] E.D. D'silva, G.K. Podagatlapalli, S.V. Rao, D.N. Rao, S.M. Dharmaprakash, New, high efficiency nonlinear optical chalcone Co-crystal and structure–property relationship, Cryst. Growth Des. 11 (2011) 5362–5369.
[15] M. Cockerham, C. Frazier, S. Guha, E. Chauchard, Second-harmonic generation in derivatives and analogs of benzophenone and chalcone, Appl. Phys. B 53 (1991) 275–278.
[16] P. S. Patil, V.M. Bhumannavar, M. Bannur, H.N. Kulkarni, G. Bhagavannarayana, Second Harmonic Generation in Some Donor-acceptor Substituted Chalcone Derivatives, 2013.
[17] M. Shigeru, M. Makoto, A. Hironaka, O. Susumu, Inhibition of gastric H+, K+- ATPase by the anti-ulcer agent, sofalcone, Biochem. Pharmacol. 42 (1991) 1447–1451.R.J. Anto, K. Sukumaran, G. Kuttan, M. Rao, V. Subbaraju, R. Kuttan, Anticancer and antioxidant activity of synthetic chalcones and related compounds, Cancer Lett. 97 (1995) 33–37.
[18] S. Ducki, R. Forrest, J.A. Hadfield, A. Kendall, N.J. Lawrence, A.T. McGown, D. Rennison, Potent antimitotic and cell growth inhibitory properties of substituted chalcones, Bioorg. Med. Chem. Lett. 8 (1998) 1051–1056.
[19] F. Herencia, M.L. Ferrandiz, A. Ubeda, J. Domínguez, J.E. Charris, G.M. Lobo, M.J. Alcaraz, Synthesis and anti-inflammatory activity of chalcone derivatives, Bioorg. Med. Chem. Lett. 8 (1998) 1169–1174.
[20] M. Liu, P. Wilairat, M.-L. Go, Antimalarial alkoxylated and hydroxylated chalones: structure-activity relationship analysis, J. Med. Chem. 44 (2001) 4443–4452.
[21] S.N. López, M.V. Castelli, S.A. Zacchino, J.N. Domínguez, G. Lobo, J. Charris-Charris,J.C. Cortés, J.C. Ribas, C. Devia, A.M. Rodríguez, In vitro antifungal evaluation and structure–activity relationships of a new series of chalcone derivatives and synthetic analogues, with inhibitory properties against polymers of the fungal cell wall, Bioorg. Med. Chem. 9 (2001) (1999–2013).
[22] J.-H. Wu, X.-H. Wang, Y.-H. Yi, K.-H. Lee, Anti-AIDS agents 54. A potent anti-HIV chalcone and flavonoids from genus Desmos, Bioorg. Med. Chem. Lett. 13 (2003) 1813–1815.
[23] L. Mathiesen, K.E. Malterud, R.B. Sund, Antioxidant activity of fruit exudates and C-methylated dihydrochalcones from Myrica gale, Planta Med. 61 (1995) 515–518.
[24] X. Tao, T. Watanabe, K. Kono, T. Deguchi, M. Nakayama, S. Miyata, Synthesis and characterization of poly(aryl ether chalcone) s for second harmonic generation, Chem. Mater. 8 (1996) 1326–1332.
[25] P.S. Patil, S. Dharmaprakash, K. Ramakrishna, H.-K. Fun, R.S.S. Kumar, D.N. Rao, Second harmonic generation and crystal growth of new chalcone derivatives, J. Cryst. Growth 303 (2007) 520–524.
[26] B. Gu,W. Ji, X.-Q. Huang, P. Patil, S. Dharmaprakash, Nonlinear optical properties of 2, 4, 5-trimethoxy-4′-nitrochalcone: observation of two-photon-induced excitedstate nonlinearities, Opt. Express 17 (2009) 1126–1135.
[27] J. Chen, X.Wang, Q. Ren, P. Patil, T. Li, H. Yang, J. Zhang, G. Li, L. Zhu, Investigation of third-order nonlinear optical properties of NNDC-doped PMMA thin films by Zscan technique, Appl. Phys. A 105 (2011) 723–731.
[28] S. Guidara, H. Feki, Y. Abid, Vibrational spectral studies and non-linear optical propertiesof L-leucine L-leucinium picrate: a density functional theory approach, Spectrochim. Acta A Mol. Biomol. Spectrosc. 115 (2013) 437–444.
[29] N. Elleuch, W. Amamou, A.B. Ahmed, Y. Abid, H. Feki, Vibrational spectroscopic study, charge transfer interaction and nonlinear optical properties of Lasparaginium picrate: a density functional theoretical approach, Spectrochim. Acta A Mol. Biomol. Spectrosc. 128 (2014) 781–789.
[30] S. Elleuch, H. Feki, Y. Abid, HF,MP2 and DFT calculations and spectroscopic study of the vibrational and conformational properties of N-diethylendiamine, Spectrochim. Acta A Mol. Biomol. Spectrosc. 68 (2007) 942–947.
[31] M. Shkir, H. Abbas, on the ground and excited state of glycine–glutaric acid: a new organicmaterial, Spectrochim. Acta AMol. Biomol. Spectrosc. 125 (2014) 453–457.
[32] N. Sudharsana, S. Muthunatesan, G.J. Priya, V. Krishnakumar, R. Nagalakshmi, Experimental and theoretical studies of 2, 5-dichloroanilinium picrate, Spectrochim. Acta A Mol. Biomol. Spectrosc. 121 (2014) 53–62.
[33] A.Reshak,W. Khan, The density functional study of electronic structure, electronic charge density, linear and nonlinear optical properties of single crystal alpha-LiAlTe 2, J. Alloys Compd. 592 (2014) 92–99.

[34] M. Shkir, S. Muhammad, S. AlFaify, A. Irfan, I. Yahia, A dual approach to study the electro-optical properties of a noncentrosymmetric L-asparagine monohydrate, Spectrochim. Acta A Mol. Biomol. Spectrosc. 137 (2015) 432–441.

[35] Kumar, V. Deval, P. Tandon, A. Gupta, E.D. D'silva, Experimental and theoretical (FT-IR, FT-Raman, UV–vis, NMR) spectroscopic analysis and first order hyperpolarizability studies of non-linear optical material:(2E)-3-[4-(methylsulfanyl) phenyl]-1-(4-nitrophenyl) prop-2-en-1-one using density functional theory, Spectrochim. Acta A Mol. Biomol. Spectrosc. 130 (2014) 41–53.

[36] M. Shkir, H. Abbas, S. Kumar, G. Bhagavannarayana, S. AlFaify, Experimental and theoretical studies on bis (glycine) lithium nitrate (BGLiN): a physico-chemical approach,J. Phys. Chem. Solids 75 (2014) 959–965.

[37] M. Shkir, S. AlFaify, H. Abbas, G. Bhagavannarayana, A physico-chemical approach to study the experimental and theoretical properties of l-ornithine monohydrochloride: an organic nonlinear optical material, Mater. Chem. Phys. 155 (2015) 36–46.

[38] M. Shkir, S. Muhammad, S. AlFaify, Experimental and density functional theory (DFT): a dual approach to study the various important properties of monohydrated L-proline cadmium chloride for nonlinear optical applications, Spectrochim. Acta A Mol. Biomol. Spectrosc. 143 (2015) 128–135.

[39] Hoong-Kun Fun, P. S. Patil, S. M. Dharmaprakash and Suchad Chantrapromma Acta Crystallographica Section E (2008). E**64**, o936

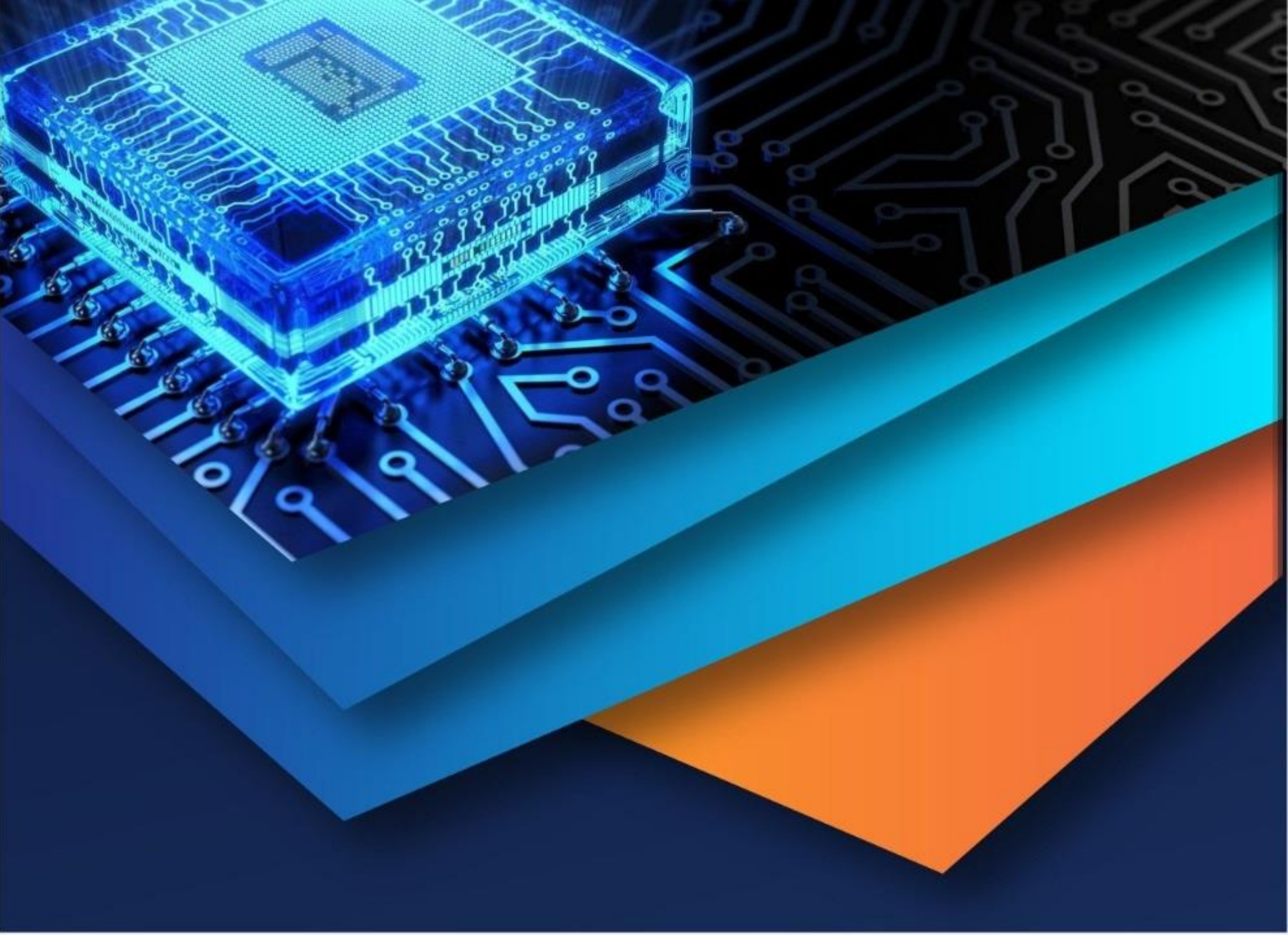
[40] J. Tauc, The Optical Properties of Solids, Academic Press, New York, 1966.

[41] C.S. Nair Lakshmi, S. Balachandran, Dhas D.Arul, Anuf A. Ronaldo, Joe I. Hubert. "DFT Analysis on Spectral and NLO properties of (2E)-3-[4-(dimethylamino) phenyl]-1-(naphthalen-2-yl) prop-2-en-1-one; a D-π-A Chalcone Derivative and its Docking studies as a potent Hepatoprotective agent", Chemical Data Collections, 2019

[42] H.A. Kurtz, J.J.P. Stewart, K.M. Dieter, Calculation of the nonlinear optical properties of molecules, J. Comput. Chem. 11 (1990) 82–87.

[43] G. Maroulis, Hyperpolarizability of H2O, J. Chem. Phys. 94 (1991) 1182–1190.

[44] Shivaraj R. Maidur, Parutagouda Shankaragouda Patil, S. Venugopal Rao, Mohd Shkir, S.M. Dharmaprakash, Experimental and computational studies on second-and third-order nonlinear optical properties of a novel D-π-A type chalcone derivative: 3-(4-methoxyphenyl)-1-(4-nitrophenyl)prop-2-en-1-one,Optics & Laser Technology,Volume 97,2017,Pages 219-228.



INTERNATIONAL JOURNAL FOR RESEARCH

IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY