COMPUTATIONAL STUDY OF (2*E*)-1-(4-chlorophenyl)-3-(4-nitrophenyl) prop-2-en-1-one BY DFT

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ABSTRACT— *Optimized geometrical structure, atomic Mulliken charges. Nonlinear optical (NLO) properties*
And thermodynamic properties of the title compound (2E)-1-(4-chlorophenyl)-3-(4-nitrophenyl) prop-2-en-1-one has been investigated by using ab initio quantum chemical computational studies dipole moment μ, the mean polarizability $α_0$, the anisotropy of polarizability $Δα$ and the mean first hyper polarizability $β0$, using the x, y, z components were calculated by B3LYP method with 6-31G(d,p), basis sets to investigate the NLO properties of the title compound.

INTRODUCTION

Chalcones are pharmacologically valuable moieties possessing 1,3diphenyl prop-2-ene-1-one (-CHCH-CO-) as a core structure in which two aromatic rings are linked by first and third carbon of α .β unsaturated carbonyl skeleton.
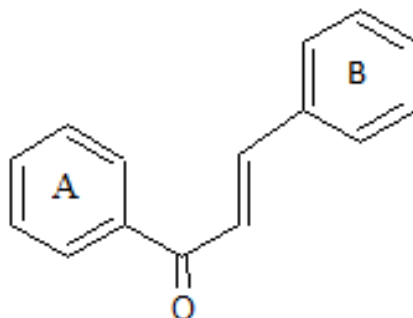
General structure of chalcones (1,3diphenyl prop-2-ene-1-one)

Due to the extended conjugation, the complete delocalisation of p electrons on both the benzene rings makes it good from bioactivity aspect. Recently many chalcones have been reported to have antimicrobial activity due the presence of a reactive α, β unsaturated keto skeleton[1] In recent years a variety of chalcones have been

reviewed for their cytotoxic, anticancer chemoprevenive and mutagenic as well as antiviral, insecticidal and enzyme inhibitory properties[2,3]. A number of chalcones having hydroxyl, alkoxy groups in different position have been reported to possess antibacterial[4], antiulcer[5],antifungal[6],antioxidant[7], vasodilatory[8], antimitotic[9], antimalarial[10], antileshmanial[11]

Chalcones are important intermediates in the synthesis of many pharmaceuticals [12-14]. In addition substituted chalcones are used as better nonlinear optical materials [15-24]. In modern years, chalcones have been used in the field of material science as optical limiting [25], electrochemical sensing [26] and Langmuir film [27]. Appreciation of these findings motivated us to carry out computational study of chalcones.

MATERIALS AND METHODS

Theoretical Calculation: The entire calculation was performed at DFT levels on a personal laptop using Gaussian(R) 09 program [28] program package, invoking gradient geometry optimization [28,29]. In the present study, the DFT/B3LYP/6-31G

(d,p) basis set level was used to calculate the optimized parameters and vibrational wave numbers of the title molecule. The vibrational frequency assignments were made with a high degree of accuracy.

RESULTS AND DISCUSSION

GEOMETRICAL ANALYSIS:

The optimised molecular structure of the mentioned compound (2*E*)-1-(4-chlorophenyl)-3-(4-nitrophenyl) prop-2-en-1-one is shown in Figure 1. The geometrical parameters of the mentioned compound are calculated using B3LYP with 6-31G (d,p) level of theory. In this study title molecule consist of two phenyl and a prop-2-en-1-one moieties. The optimized bond lengths, bond angles and dihedral angles of the compound studied are listed in Table 1 is in accordance with atom numbering scheme as shown in Fig. 1.
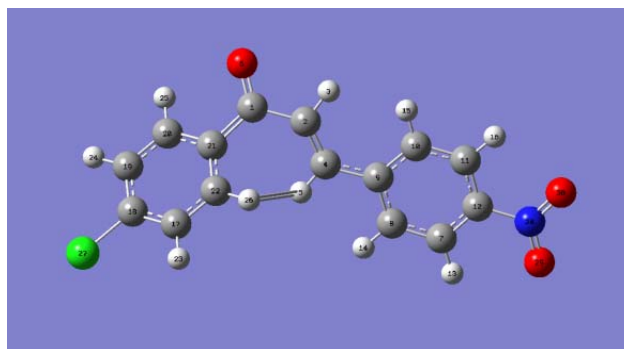

Fig. 1

TABLE-1-Calculated Optimized Geometrical Parameters of (2*E*)-1-(4-chlorophenyl)-3-(4-nitrophenyl) prop-2-en-1-one, at B3LYP/6-31G (d,p): bond length (Å), bond angle(º), dihedral angles(º)

S. No.	Atoms of molecule	Bond length (Å)	Angle between atoms	Bond angle (º)	Dihedral angle between atoms	Dihedral angle (º)
1	R(1,2)	1.54	A(2,1,6)	119.8865	D(6,1,2,3)	0.0
3	R(1,6)	1.2584	A(2,1,21)	119.7966	D(6,1,2,4)	180.0
3	R(1,21)	1.2731	A(6,1,21)	120.3168	D(21,1,2,3)	-179.8959
4	R(2,3)	1.07	A(1,2,3)	119.8865	D(21,1,2,4)	0.1041
5	R(2,4)	1.3552	A(1,2,4)	120.2269	D(2,1,21,20)	-179.9773
6	R(4,5)	1.07	A(3,2,4)	119.8865	D(2,1,21,22)	-0.1516
7	R(4,9)	1.4021	A(2,4,5)	120.2269	D(6,1,21,20)	0.1272
8	R(5,26)	0.5705	A(2,4,9)	117.2773	D(6,1,21,22)	179.9529
9	R(7,8)	1.3952	A(5,4,9)	122.4957	D(1,2,4,5)	0.0
10	R(7,12)	1.3948	A(4,5,26)	141.253	D(1,2,4,9)	180.0
11	R(7,13)	1.0996	A(8,7,12)	119.9985	D(3,2,4,5)	180.0
12	R(8,9)	1.3947	A(8,7,13)	119.9972	D(3,2,4,9)	0.0
13	R(8,14)	1.0997	A(12,7,13)	120.0043	D(2,4,5,26)	-0.1912
14	R(9,10)	1.3954	A(7,8,9)	120.0086	D(9,4,5,26)	179.8088
15	R(10,11)	1.3948	A(7,8,14)	119.9808	D(2,4,9,8)	180.0
16	R(10,15)	1.0997	A(9,8,14)	120.0106	D(2,4,9,10)	0.0587
17	R(11,12)	1.3951	A(4,9,8)	117.059	D(5,4,9,8)	0.0
18	R(11,16)	1.0998	A(4,9,10)	122.9468	D(5,4,9,10)	-179.9413
19	R(12,28)	1.47	A(8,9,10)	119.9942	D(4,5,26,22)	0.4751
20	R(17,18)	1.3952	A(9,10,11)	119.994	D(12,7,8,9)	0.0323
21	R(17,22)	1.3948	A(9,10,15)	119.9811	D(12,7,8,14)	179.9532
22	R(17,23)	1.0996	A(11,10,15)	120.0249	D(13,7,8,9)	-179.9729
23	R(18,19)	1.3947	A(10,11,12)	120.0047	D(13,7,8,14)	-0.052
24	R(18,27)	1.76	A(10,11,16)	120.0113	D(8,7,12,11)	0.0149
25	R(19,20)	1.3954	A(12,11,16)	119.984	D(8,7,12,28)	179.9892
26	R(19,24)	1.0997	A(7,12,11)	120.0	D(13,7,12,11)	-179.9798
27	R(20,21)	1.3948	A(7,12,28)	120.008	D(13,7,12,28)	-0.0056

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28	R(20,25)	1.0997	A(11,12,28)	119.992	D(7,8,9,4)	180.0
29	R(21,22)	1.3951	A(18,17,22)	119.9985	D(7,8,9,10)	-0.0568
30	R(22,26)	1.0996	A(18,17,23)	119.9972	D(14,8,9,4)	0.0791
31	R(28,29)	1.1993	A(22,17,23)	120.0043	D(14,8,9,10)	-179.9777
32	R(28,30)	1.1993	A(17,18,19)	120.0086	D(4,9,10,11)	179.9738
33			A(17,18,27)	119.9808	D(4,9,10,15)	-0.0568
34			A(19,18,27)	120.0106	D(8,9,10,11)	0.0341
35			A(18,19,20)	119.9942	D(8,9,10,15)	-179.9964
36			A(18,19,24)	120.0128	D(9,10,11,12)	0.0131
37			A(20,19,24)	119.993	D(9,10,11,16)	-179.9995
38			A(19,20,21)	119.994	D(15,10,11,12)	-179.9563
39			A(19,20,25)	119.9811	D(15,10,11,16)	0.0311
40			A(21,20,25)	120.0249	D(10,11,12,7)	-0.0376
41			A(1,21,20)	119.7934	D(10,11,12,28)	179.9881
42			A(1,21,22)	120.2017	D(16,11,12,7)	179.975
43			A(20,21,22)	120.0047	D(16,11,12,28)	0.0007
44			A(17,22,21)	120.0	D(7,12,28,29)	90.0102
45			A(17,22,26)	120.008	D(7,12,28,30)	-89.9898
46			A(21,22,26)	119.992	D(11,12,28,29)	-90.0155
47			A(5,26,22)	158.3021	D(11,12,28,30)	89.9845
48			A(12,28,29)	118.3934	D(22,17,18,19)	0.0323
49			A(12,28,30)	118.3927	D(22,17,18,27)	179.9532
50			A(29,28,30)	123.2139	D(23,17,18,19)	-179.9729
51					D(23,17,18,27)	-0.052
52					D(18,17,22,21)	0.0149
53					D(18,17,22,26)	179.9892
54					D(23,17,22,21)	-179.9798
55					D(23,17,22,26)	-0.0056
56					D(17,18,19,20)	-0.0568
57					D(17,18,19,24)	179.9619
58					D(27,18,19,20)	-179.9777
59					D(27,18,19,24)	0.041
60					D(18,19,20,21)	0.0341
61					D(18,19,20,25)	-179.9964
62					D(24,19,20,21)	-179.9846
63					D(24,19,20,25)	-0.0151
64					D(19,20,21,1)	179.8392
65					D(19,20,21,22)	0.0131
66					D(25,20,21,1)	-0.1303
67					D(25,20,21,22)	-179.9563
68					D(1,21,22,17)	-179.8629
69					D(1,21,22,26)	0.1628
70					D(20,21,22,17)	-0.0376
71					D(20,21,22,26)	179.9881
72					D(17,22,26,5)	179.6259
73					D(21,22,26,5)	-0.3998

Vibrational Assignments:

The title molecule undergoes 84 fundamental modes of vibrations. Vibrational spectral assignments have been carried on the recorded FT-IR and FT- Raman spectra based on the theoretically predicated wave number by B3LYP/6-31G (d, p) basis set and are presented in figs. 2, 3 and table 2.

C-H Vibrations: The aromatic structure shows the presence of C–H stretching vibrations in the region 3181-3214 cm−1 [34, 35], which is the characteristic region for the identification of the C–H stretching vibrations. In this region, the bands are not affected appreciably by the nature of the substituents. In this study, the C-H stretching bands observed at 3059 cm-1 in infrared spectrum and 3059 cm-1 in Raman spectrum and their corresponding harmonic value lies at 3046 cm-1 (mode no: 75-78) with the help of TED assignments ≥ 90%.

. **C=O vibrations:** A carbonyl group is an organic functional group composed of a carbon atom double-bonded to an oxygen atom. In cyclic ketones, the characteristic IR absorption frequencies of C=O group have been studied [36, 37]. The loan pair of electrons on oxygen also determines the nature of the carbonyl group. Normally carbonyl group vibrations occur in the region 1730-1654cm−1 [38]. In our present study, the carbonyl stretching vibration is observed as a medium band in FT-IR at 1710 cm−1 and in the Raman counterpart it is observed at 1650 cm−1 as a weak band. The corresponding harmonic value lies at 1636cm-1 with pure mode of vibrations (TED=86%). The C=O in plane bending vibrations are observed at 524 cm-1 (m) in infrared spectrum and 523 cm-1 (W) in Raman spectrum. The calculated value appeared at 527 cm-1 (mode no.22,23).

CH2 vibrations: The atoms in a CH2 group, commonly found in organic compounds, can vibrate in six different ways: symmetric and asymmetric stretching, scissoring, rocking, wagging and twisting. In aromatic organic compound, the C–H stretching vibrations are usually observed below 3000 cm−1 [39, 40]. These assignments are also supported by the literature Padmaja et al., [41] in addition to TED output.

C-C Vibrations: Socrates [42] mentioned that the presence of conjugate substituent such as C=C causes heavy doublet formation around the region 1625-1575 cm-1. The very strong band is appeared at 1598 cm-1 in infrared spectrum and 1597 cm-1, 1211 cm-1, 70 cm-1 in Raman spectrum due to α, β unsaturated C=C stretching vibrations in the carbonyl position [43]. In the present study, the C=C stretching vibration observed at1581 cm-1 in IR/1597 cm-1 in FT–Raman spectrum and its corresponding harmonic values lies at 1541 cm-1 (mode nos: 62) with the help of TED assignments ≥ 23%. The good agreement allows us to perform the assignments of IR and Raman bands in the whole studied spectral regions.
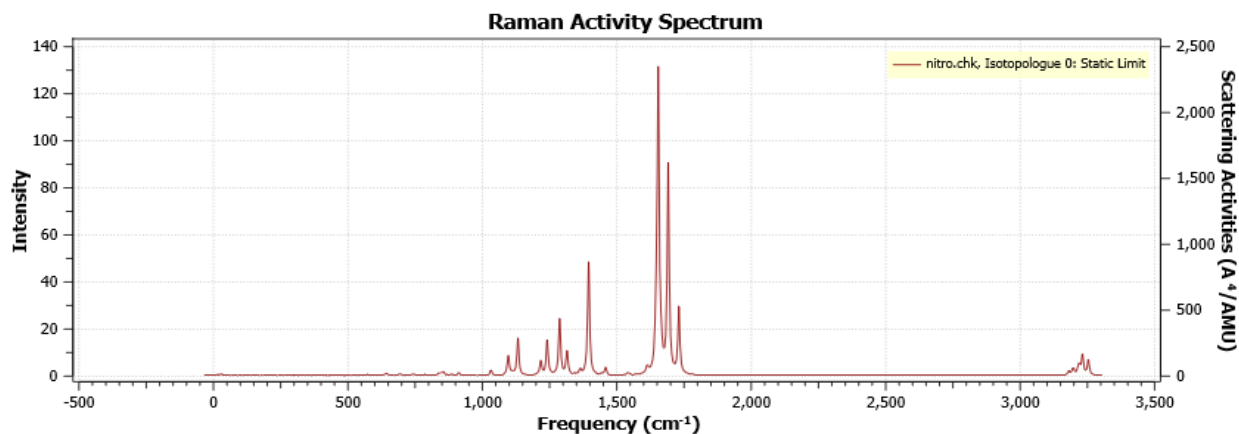
Raman Activity Spectrum
X-Axis: Frequency (cm-1)
Y-Axis: Intensity
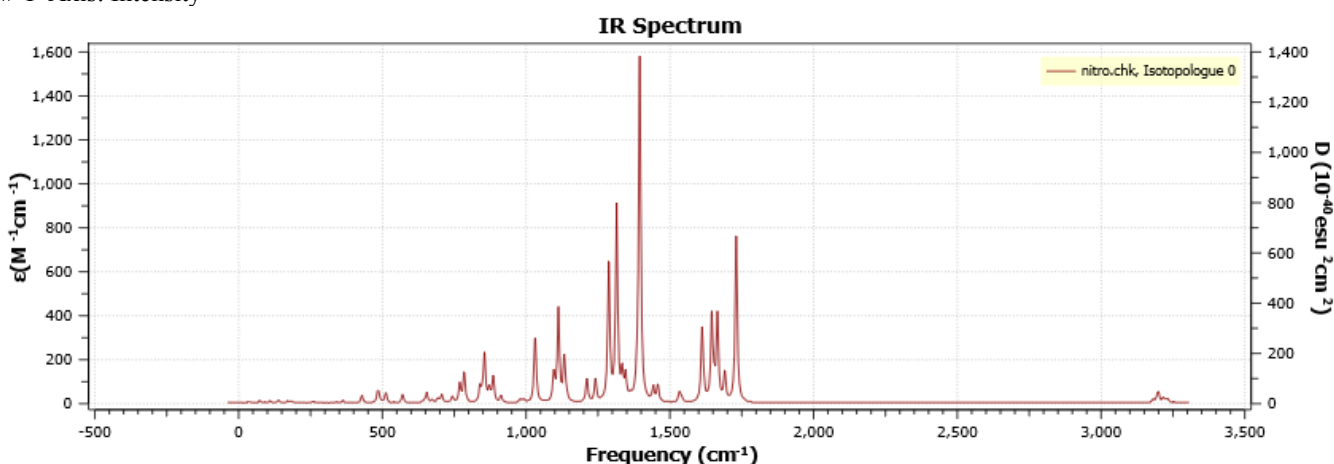
IR Spectrum
X-Axis: Frequency (cm-1)
Y-Axis: ε (M-1 cm-1)

TABLE-2: Calculated Frequencies of the Title Compound

Mode	Frequency	IR	Raman	DepolarP	Depolar-U
84	3254.09	0.9830	88.8013	0.2314	0.3758
83	3253.24	0.8151	89.9755	0.2630	0.4164
82	3232.43	2.6034	199.9637	0.1656	0.2842
81	3229.44	3.7264	53.8200	0.1463	0.2553
80	3219.69	0.1231	70.4773	0.7018	0.8247
79	3217.97	4.9895	37.9317	0.3567	0.5259
78	3214.52	3.2406	35.6160	0.6307	0.7735
77	3199.18	11.8986	45.2256	0.3883	0.5593
76	3195.45	6.4139	49.7655	0.4522	0.6228
75	3181.03	5.5249	47.2297	0.2840	0.4424
74	1730.88	220.5206	523.0595	0.2002	0.3335
73	1691.23	38.3325	1621.6432	0.3284	0.4944
72	1665.44	114.2756	149.5379	0.3385	0.5058
71	1654.02	16.0913	2285.7018	0.3656	0.5354
.70	1645.98	112.5548	317.6660	0.3893	0.5604
69	1617.33	14.3204	15.7399	0.1762	0.2996
68	1612.07	93.6907	48.4348	0.3664	0.5363
67	1541.53	6.5270	19.3744	0.3006	0.4623
66	1533.28	14.7569	4.3262	0.3963	0.5676
65	1458.21	22.8178	60.6480	0.3701	0.5403
64	1442.32	18.9691	12.1852	0.2336	0.3788
63	1395.27	453.1904	824.5477	0.2975	0.4586
62	1386.70	20.4268	17.9401	0.6002	0.7501
61	1363.44	5.3813	40.7814	0.2483	0.3978
60	1345.94	33.1902	5.2929	0.3106	0.4740
59	1334.21	27.5704	1.5865	0.5616	0.7192
58	1333.86	8.1894	3.1547	0.2378	0.3842
57	1314.87	257.1547	173.7814	0.4511	0.6217
56	1287.49	181.6148	404.8403	0.2176	0.3574
55	1241.29	30.6219	251.0776	0.3682	0.5382
54	1217.21	0.5336	101.1334	0.2477	0.3971
53	1211.46	31.6886	5.6222	0.6684	0.8012
52	1141.21	3.4868	1.0789	0.5713	0.7271
51	1139.63	7.2761	1.9787	0.4964	0.6634
50	1132.38	57.8680	258.5256	0.2614	0.4145
49	1112.41	123.0439	17.1537	0.2386	0.3853
48	1096.36	37.3446	137.6969	0.1769	0.3007
47	1033.37	23.1678	6.2293	0.2137	0.3521
46	1032.06	9.3618	32.0716	0.3203	0.4852
45	1030.62	62.2342	1.5834	0.4517	0.6223
44	991.77	4.0979	5.4436	0.6102	0.7579
43	984.58	1.7258	2.0087	0.4137	0.5853
42	982.49	0.2466	0.9226	0.4980	0.6649
41	978.05	4.2749	1.6836	0.6931	0.8188
40	912.77	9.9279	20.7163	0.4835	0.6518
39	885.53	35.2012	9.7171	0.1748	0.2976
38	871.43	18.3186	5.8777	0.1860	0.3137
37	855.13	63.1618	22.6451	0.2576	0.4096
36	849.53	1.4082	6.2722	0.4324	0.6037
35	847.94	7.7498	5.9062	0.5076	0.6734
34	839.50	19.8294	16.7163	0.3533	0.5222
33	784.49	40.5597	7.5313	0.5141	0.6791
32	769.18	25.4833	6.1349	0.3459	0.5141
31	743.50	8.8102	11.7490	0.2107	0.3481
30	706.33	11.2858	1.8561	0.2583	0.4106
29	692.36	6.0494	12.8411	0.1091	0.1968

28	673.36	4.5414	1.6132	0.6069	0.7554
27	654.06	13.5222	3.9820	0.3694	0.5395
26	643.86	1.9525	8.2927	0.7323	0.8454
25	641.35	0.9546	7.5330	0.7490	0.8565
24	570.81	11.9872	6.3719	0.1719	0.2933
23	538.27	1.1132	3.1579	0.7124	0.8321
22	511.56	14.0989	2.9032	0.3273	0.4932
21	488.21	8.7039	0.6963	0.3525	0.5213
20	483.42	13.4558	0.4231	0.7105	0.8308
19	428.78	9.5099	1.3953	0.4367	0.6079
18	424.76	1.1785	1.8354	0.4067	0.5782
17	418.99	0.2053	0.0631	0.6291	0.7723
16	362.10	3.5888	1.2104	0.3518	0.5205
15	342.00	2.0216	4.5597	0.5470	0.7072
14	312.56	0.3002	1.2237	0.5332	0.6956
13	298.47	0.2328	1.5871	0.5062	0.6721
12	260.83	2.8877	4.2213	0.7499	0.8571
11	237.36	0.5854	2.0507	0.7013	0.8244
10	183.60	2.8380	2.6821	0.4767	0.6456
9	170.66	3.0400	2.8891	0.7401	0.8506
8	139.49	4.4033	3.9230	0.5906	0.7426
7	108.58	3.2206	1.4550	0.7305	0.8443
6	89.17	1.2860	1.2543	0.6204	0.7657
5	74.45	3.7878	4.6121	0.7265	0.8416
4	63.72	0.0324	0.2773	0.7376	0.8490
3	35.34	1.7774	3.8676	0.7393	0.8501
2	29.02	0.5619	5.1282	0.7057	0.8275
1	18.60	0.0519	6.6094	0.7500	0.8571

Thermodynamic Properties

The standard thermodynamic functions: heat capacity (CV), entropy (S) and enthalpy (E) based on the Vibrational analysis using the B3LYP/6-31G (d,p) level to Investigate thermodynamically properties of the title compound Were calculated and listed in Table 3 the frequency calculations compute the zero point energies, thermal correction to internal energy and entropy as well as the heat capacity for a molecular system. These functions describe the thermodynamic stability of the system at the given conditions of pressure and temperature.

TABLE-3

Zero-point correction	0.218333 (Hartree/Particle)
Thermal correction to Energy	0.235159
Thermal correction to Enthalpy	0.236103
Thermal correction to Gibbs Free Energy	0.170230
Sum of electronic and zero-point Energies	-1317.911607
Sum of electronic and thermal Energies	-1317.894781
Sum of electronic and thermal Enthalpies	-1317.893837
Sum of electronic and thermal Free Energies	-1317.959710

TABLE-4

	Enthalpy (E) (Thermal)	Heat Capacity (CV)	Entropy(S)
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	147.565	63.135	138.642
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	42.861
Rotational	0.889	2.981	35.201
Vibrational	145.787	57.174	60.580
Vibration 1	0.593	1.986	6.779
Vibration 2	0.593	1.984	5.896

Vibration 3	0.594	1.982	5.504
Vibration 4	0.597	1.972	4.339
Vibration 5	0.599	1.966	4.032
Vibration 6	0.602	1.957	3.678
Vibration 7	0.606	1.942	3.294
Vibration 8	0.615	1.914	2.811
Vibration 9	0.626	1.879	2.428
Vibration 10	0.631	1.862	2.291
Vibration 11	0.656	1.783	1.823
Vibration 12	0.669	1.744	1.656
Vibration 13	0.692	1.677	1.425
Vibration 14	0.701	1.650	1.349
Vibration 15	0.721	1.592	1.203
Vibration 16	0.736	1.550	1.113
Vibration 17	0.782	1.429	0.895
Vibration 18	0.787	1.416	0.876
Vibration 19	0.790	1.408	0.863
Vibration 20	0.840	1.287	0.701
Vibration 21	0.844	1.276	0.688
Vibration 22	0.867	1.224	0.630
Vibration 23	0.893	1.165	0.569
Vibration 24	0.927	1.094	0.503

Nonlinear optical effects:

NLO is the important role of current research because it provides the key functions of frequency shifting, optical logic, optical modulation, optical switching and optical memory for the technologies in areas such as telecommunications, signal processing and optical interconnection [30,31].

The total static dipole moment μ, the mean polarizability α_0, the anisotropy of polarizability $\Delta\alpha$ and the mean first hyper polarizability β0, using the x, y, z components are defined as [32]

$$\mu = (\mu^2_x + \mu^2_y + \mu^2_z)^{1/2}$$
$$\alpha_0 = \frac{(\alpha xx + \alpha yy + \alpha zz)}{3}$$

$$\Delta\alpha = \frac{1}{\sqrt{2}} [(\alpha_{xx}-\alpha_{yy})^2 + (\alpha_{yy}-\alpha_{zz})^2 + (\alpha_{zz}-\alpha_{xx})^2 + 6(\alpha^2_{xy}+\alpha^2_{yz}+\alpha^2_{xz})]^{1/2}$$

$$\beta_0 = [(\beta_{xxx}+\beta_{xyy}+\beta_{xzz})^2 + (\beta_{yyy}+\beta_{yzz}+\beta_{yxx})^2 + (\beta_{zzz}+\beta_{zxx}+\beta_{zyy})^2)]^{1/2}$$

Calculated dipole moment (μ, in Debye), mean polarizability (α_0, in a.u.), anisotropy of polarizability ($\Delta\alpha$, in a.u.) and first hyper polarizability (β, in a.u.) of (2E)-1-(4-chlorophenyl)-3-(4-nitrophenyl) prop-2-en-1-one by DFT by B3LYP/6-31G(d,p). Dipole moment (field-independent basis, Debye): is given in Table-4

Table 5: Calculated dipole moment (μ, in Debye), mean polarizability (α_0, in a.u.), anisotropy of polarizability ($\Delta\alpha$, in a.u.) and first hyper polarizability (β, in a.u.) of (2*E*)-1-(4-chlorophenyl)-3-(4-nitrophenyl) prop-2-en-1-one .

| Dipole Moment μ in Debye		Polarizability α in a.u.		Hyper polarizability β in a.u.	
μ_X	-2.0936	α_{XX}	-150.2854	β_{XXX}	-238.6193
μ_Y	-1.4740	α_{YY}	-122.7101	β_{YYY}	-58.5140
μ_Z	0.0010	α_{ZZ}	-125.7387	β_{ZZZ}	-0.0130
Tot μ	2.5605	α_{XY}	8.0679	β_{XYY}	58.4810
		α_{XZ}	-0.0027	β_{XXY}	76.9751
		α_{YZ}	0.0103	β_{XXZ}	0.0067
				β_{XZZ}	-10.5104
				β_{YZZ}	1.6611
				β_{YYZ}	0.0153
		α_0	-132.9114	β_{XYZ}	0.0010
		$\Delta\alpha$	263.6921	β_0	191.7077

Mulliken Atomic charges:

In the uses of quantum mechanical calculation to molecular system, the calculation of effective Mulliken atomic charge plays an important role of the system [33]. The charges are calculated by DFT/ B3LYP/6-31G (d, p) level of theory which is tabulated in table 7 and displayed in fig 7. The Mulliken charge is directly related to the dipole moment, molecular polarization, electronic structure, vibrational properties of the molecule, and quantifies how the electronic structure changes under atomic displacement; it is therefore related directly to the chemical bonds present in the molecule. The maximum negative charge belongs to 6 'O' atom -0.518996) high positive charge belongs 28 "N"atom (0.366169).

Table 6: the muliken Atomic Charges of chalcone

1 C	0.302051	11 C	-0.146747	21 C	0.144474
2 C	-0.249664	12 C	0.270869	22 C	-0.072970
3 H	0.157326	13 H	0.164181	23 H	0.153057
4 C	-0.070287	14 H	0.145649	24 H	0.164720
5 H	0.122513	15 H	0.165722	25 H	0.187008
6 O	-0.518996	16 H	0.167504	26 H	0.155180
7 C	-0.135818	17 C	-0.201279	27 Cl	0.000464
8 C	-0.203355	18 C	-0.041025	28 N	0.366169
9 C	0.152596	19 C	-0.150747	29 O	-0.371298
10 C	-0.160395	20 C	-0.125585	30 O	-0.371316

HOMO - LUMO Energy: The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) plots of the title compound is shown in fig 5.The HOMO is orbital that acts as an electron donor and the LUMO is the orbital that acts as an electron acceptor. The energy value of HOMO is -0.25826ev and LUMO= -0.11214 ev .The energy difference is -0.14612 ev which illustrates the stability of chalcone.
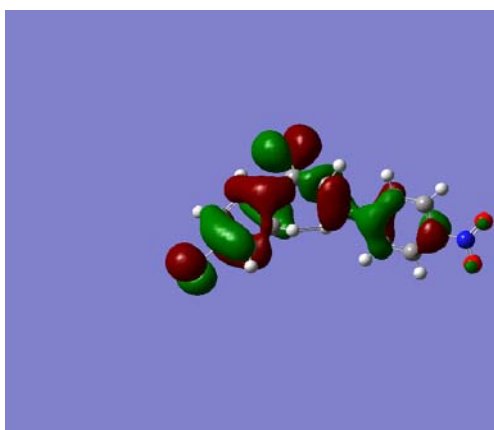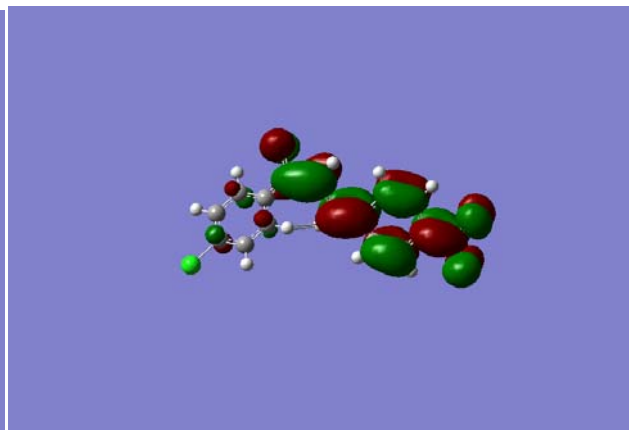
HOMO= -0.25826ev   **LUMO= -0.11214 ev**

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