

# Theoretical Investigation Of Spectroscopic And Some Electronic Properties Of (E)-4-((P-Tolylimino) Methyl)Phenyl Acrylate Schiff Base By DFT Method

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## ABSTRACT

The present study aims to theoretically investigate the spectroscopic and electronic properties of (E)-4-((P-tolylimino)methyl) phenyl acrylate Schiff base using the Density Functional Theory (DFT) method. The optimized molecular geometry and electronic properties of the Schiff base were calculated using DFT with B3LYP/6-311++G(d,p) level of theory. The calculated results revealed that the Schiff base molecule exists in the trans conformation and has a stable structure. The vibrational frequencies were calculated, and the corresponding FT-IR spectra were simulated, which showed good agreement with the experimental results. Non-linear optical (NLO) properties of the Schiff base were calculated, and it was found to possess considerable NLO activity. Finally, HOMO-LUMO molecular orbital energies and molecular electrostatic potential (MEP) analysis was performed to study the reactivity and potential sites of electrophilic and nucleophilic attacks. The results of this study provide valuable insights into the spectroscopic and electronic properties of the (E)-4-((P-tolylimino)methyl) phenyl acrylate Schiff base and could be useful in designing novel organic materials with promising optical and electronic properties.

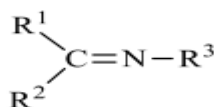
**Key words:** FT-IR, NMR, NLO, DFT, HOMO- LUMO

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## I. INTRODUCION

Since a scientist named Schiff first created them in 1864, compounds with the (-C=N-) group in their structure are referred to as "Schiff Bases" (Schiff 1869). The generic formula  $RCH=NR'$ , where R and R' in the formula signify aryl or alkyl substituents, is used to describe Schiff bases (Fig. 1).



**Figure 1.** General representation of Schiff bases. R1, R2, R3 = aryl or alkyl

Depending on the amount of donor atoms in their structure, Schiff bases can function as polydentate ligands. By giving the metal electron pairs on the nitrogen atoms they contain, they can create complexes. The stability of the cyclic complexes formed by the azomethine groups is increased by the transport of other functional groups (like hydroxyl) that contain displaceable hydrogen atoms adjacent to the azomethine groups.

The bond created by a reaction with an aldehyde is known as an azomethine or an aldimine, whereas the bond created by a reaction with a ketone is known as an imine or a ketimine. Because they are stable and simple to synthesize, schiff bases (imines) have succeeded in being among the compounds of interest. Imines' employment in numerous biological systems (Sharaby et al. 2017), chemical catalysis (Redshaw 2017), medicine and pharmacy (Roberts et al. 2017), chemical analyses, and new technologies (Dirisio et al. 2017, Upadhyay et al. 2008), among other applications, can be used to explain this interest in them.

Coordination chemicals are becoming more and more significant in both biological systems and the industry. Schiff bases are among the ligands widely used in coordination chemistry due to their structural and biological properties.

Metal complexes of Schiff bases, whose use as ligands was initially described by Pfeiffer in 1933 (Pfeiffer et al. 1933, Seçkin et al. 2003), are being researched with interest.

According to (Ashraf et al. 2011), metal-imine complexes have been extensively studied for their potential as herbicides and anticancer agents. Diabetes and AIDS are also treated with it (Golcu et al. 2005, Silva et al. 2011, Rehman et al. 2004). Additionally, Schiff bases are employed in a variety of industries, including the paint industry (Serin and Gök 1988), cation carrier, ion selective electrode production (Aydnlı 2006).

## II. MATERIAL AND METHOD

Calculations were made using Becke's three-parameter energy functional hybrid approach and Lee-Yang and Parr's B3LYP theory, which consists of the correlation functional, in the Gaussian 09W program. In the all calculations 6-311++G(d,p) base set was used. This basis set includes polarized functions added to eliminate the polarization effect, as well as diffuse functions added to model the electron density in excited, ionic molecules to be more dispersed compared to the ground state of the molecule.

First, the optimization calculation was performed to find the stable structure of the molecule. Then, the vibration frequencies of these compounds will be estimated using the same method and basis set. The  $^1\text{H-NMR}$  and  $^{13}\text{C-NMR}$  calculations of the molecule were calculated in the DMSO phase to compare with the experimental values. On the level of the DFT/B3LYP/6-311++G (d, p) theory, HOMO and LUMO molecular orbital energies, nonlinear optical characteristics (NLO), and molecular electrostatic potential (MESP)map will be examined. Upon completion of the computations, the theoretical findings will be compared to the known experimental values. All computations will be performed using the packages Gaussian 09 and Gauss View 5.

## III. RESULTS AND DISCUSSION

### 3.1 Geometrical Optimization of the (E)-4-((p-tolylimino)methyl)phenyl acrylate

The three-dimensional geometry of the molecule was drawn with the program Gauss View 5.0. Then, full geometry optimization was performed with the DFT/B3LYP/6-311+G (d, p) method and the lowest energy structure of the molecular system was found (Figure 3.1).

The bond lengths, bond angles and dihedral angles of the compound are given in Table 4.1. According to our knowledge of the literature so far, no experimental data on the structural parameters of the compound have been found. For this reason, the comparison of certain structural parameters was made according to similar molecules studied in the literature.

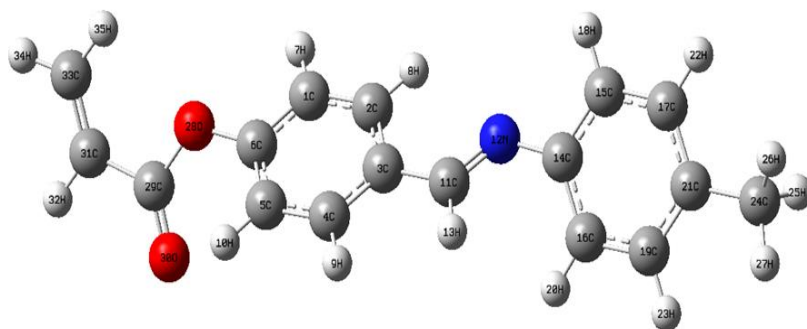


Figure 3.1 Optimized structure of the (E)-4-((p-tolylimino)methyl)phenyl acrylate

The N-C bond length was experimentally determined as 1.470Å they found 1.468Å theoretically by (Alyar *et al.* 2012). In this study, the N-C bond length was calculated as 1.405Å.

**Table 3. 1** Some molecular geometric parameters (bond lengths, bond and torsion angles) of (E)-4-((p-tolylimino)methyl)phenyl acrylate

Bond Length	B3LYP-6311++G(d,p)	Bond Angles	B3LYP-6311++G(d,p)	Torsion Angle	B3LYP-6311++G(d,p)
C1-C2	1.386	C2-C1-C6	119.6	C6-C1-C2-C3	-0.028
C1-C6	1.394	C2-C1-H7	121.2	C6-C1-C2-H8	179.939
C1-H7	1.083	C6-C1-H7	119.1	H7-C1-C2-C3	179.906
C2-C3	1.403	C1-C2-C3	120.4	H7-C1-C2-H8	-0.125
C2-H8	1.082	C1-C2-H8	120.7	C2-C1-C6-C5	0.232
C3-C4	1.401	C3-C2-H8	118.8	C2-C1-C6-O28	176.241
C3-C11	1.467	C2-C3-C4	118.7	H7-C1-C6-C5	-179.703
C4-C5	1.391	C2-C3-C11	121.7	H7-C1-C6-O28	-3.695
C4-H9	1.085	C4-C3-C11	119.4	C1-C2-C3-C4	-0.045
C5-C6	1.390	C3-C4-C5	121.3	C1-C2-C3-C11	-179.942
C5-H10	1.080	C3-C4-H9	119.5	H8-C2-C3-C4	179.985
C6-O28	1.393	C5-C4-H9	119.1	H8-C2-C3-C11	0.088
C11-N12	1.276	C4-C5-C6	118.6	C2-C3-C4-C5	-0.081
C11-H13	1.098	C4-C5-H10	120.7	C2-C3-C4-H9	-179.989
N12-C14	1.405	C6-C5-H10	120.5	C11-C3-C4-C5	179.818
C14-C15	1.402	C1-C6-C5	121.1	C11-C3-C4-H9	-0.089
C14-C16	1.402	C1-C6-O28	116.3	C2-C3-C11-N12	2.113
C15-C17	1.388	C5-C6-O28	122.3	C2-C3-C11-H13	-178.841
C15-H18	1.083	C3-C11-N12	122.8	C4-C3-C11-N12	-177.784
C16-C19	1.392	C3-C11-H13	115.5	C4-C3-C11-H13	1.262
C16-H20	1.084	N12-C11-H13	121.6	C3-C4-C5-C6	0.277
C17-C21	1.401	C11-N12-C14	120.4	C3-C4-C5-H10	179.661
C17-H22	1.085	N12-C14-C15	118.02	H9-C4-C5-C6	-179.814
C19-C21	1.397	N12-C14-C16	123.5	H9-C4-C5-H10	-0.431

Alyar measured the C-C bond length as 1.392Å experimentally and calculated 1.402Å theoretically. In this study, the bond C-C length was calculated as 1.394Å.

The C-O bond length was found 1.364Å theoretically by (S. Alyar and Sevki 2014). In this study, the C-O bond length was calculated as 1.393Å. These results show us that our theoretical calculations are compatible with the experimental and theoretic data found in the literature for similar molecular systems.

### 3.2 Vibrational Assignment of (E)-4-((p-tolylimino)methyl)phenyl acrylate

In this section of our thesis, we formed and interpreted the assignments of the fundamental vibrational frequencies computed for the stable structure of the molecular structure (E)-4-((p-tolylimino)methyl)phenyl acrylate at minimal energy. The 35 atom molecule (E)-4-((p-tolylimino)methyl)phenyl acrylate compound exhibits 99 fundamental vibration frequencies. Theoretical and experimental vibration frequencies are given in this section (Table 3.2).

**Table 3.2** Theoretical and experimental (FT-IR) vibration frequencies of the (E)-4-((p-tolylimino)methyl)phenyl acrylate

Mode	Exp. (Silku 2014)	Calculated	Intensity	Descriptions
99		3240	4.60	$\nu_{as} (C_{33}H_2) + \nu (C_{31}H_{32})$
98		3218	3.73	$\nu (CH)_{R1}$
97		3204	3.18	$\nu (CH)_{R1}$
96		3188.35	3.03	$\nu (CH)_{R1}$
95		3187.89	3.40	$\nu (C_{31}H_{32}) + \nu (C_{33}H_{35})$
94		3187	6.53	$\nu (CH)_{R2}$
93		3179	9.46	$\nu (CH)_{R2}$
92		3167	8.28	$\nu (CH)_{R1}$
91		3156	23.28	$\nu (CH)_{R2}$
90		3155	1636	$\nu (CH)_{R2}$
89		3148	4.81	$\nu_s (C_{33}H_2) + \nu (C_{31}H_{32})$
88		3099	16.73	$\nu_{as} (C_{24}H_2) + \nu_s (C_{24}H_2)$
87	3033	3071	20.08	$\nu_s (C_{24}H_2) + \nu_{as} (C_{24}H_2)$
86		3019	47.03	$\nu_s (C_{24}H_2)$
85	2919	3005	43.36	$\nu (C_{11}H_{13})$
84	1749	1791	264.56	$\nu (C_{29} = O_{30}) + \nu (C_{31} = C_{33}) + \beta (C_{33}H_2) + \beta (C_{29}CH_{32})$

83		1687	96.16	$\nu (C_{11}=N_{12}) + \nu (CC)_{R1,2} + \beta (C_3CH_{13})$
82	1652	1680	10.22	$\nu (C_{31}=C_{33}) + \nu (C_{29}=O_{30}) + \beta (C_{33}H_2) + \beta (C_{29}CH_{32})$
81		1647	16.42	$\nu (CC)_{R1,2} + \nu (C_{11}=N_{12}) + \beta (CCH)_{R1,2}$
80		1636	57.67	$\nu (CC)_{R1,2} + \nu (C_{11}=N_{12}) + \beta (CCH)_{R1,2} + \beta (C_{11}NH)$
79		1614	47.09	$\nu (CC)_{R1} + \nu (C_{11}=N_{12}) + \beta (C_5CH_9) + \beta (C_2CH_7) + \beta (C_4CH_{10})$
78		1601	2.81	$\nu (CC)_{R2} + \beta (C_{19}CH_{20}) + \beta (C_{19}CH_{20}) + \beta (C_{17}CH_{18}) + \beta (C_{21}CH_{26}) + \beta (C_{21}CH_{27}) + \beta (C_{24}H_2)$

Table 3.1 (Continued)

77		1539	137.45	$\nu (CC)_{R1,2} + \beta (CCH)_{R1,2} + \nu (C_3C_{11}) + \nu (C_{14}N_{12}) + \nu (C_6O_{28}) + \nu (C_{21}C_{24})$
76		1531	0.95	$\nu (CC)_{R1,2} + \beta (CCH)_{R1,2} + \nu (C_3C_{11}) + \nu (C_{14}N_{12}) + \nu (C_6O_{28}) + \nu (C_{21}C_{24})$
75		1494	8.22	$\nu (CC)_{R2} + \beta (C_{24}H_2)$
74		1488	6.95	$\beta (C_{24}H_2) + \gamma (C_{24}H_{25}H_{26})$
73		1447	6.68	$\nu (CC)_{R1,2} + \nu (C_{11}=N_{12}) + \beta (CCH)_{R1,2} + \beta (C_{33}H_2)$
72		1439	28.79	$\nu (CC)_{R2} + \nu (C_{31}=C_{33}) + \beta (C_{33}H_2) + \beta (C_{24}H_2)$
71		1438	29.12	$\nu (CC)_{R1,2} + \beta (CCH)_{R2} + \beta (C_{33}H_2) + \beta (C_{24}H_2)$
70		1414	0.09	$\gamma (C_{24}H_2)$
69		1402	11.54	$\nu (CC)_{R1,2} + \nu (C_{11}=N_{12}) + \beta (CN_{12}H)$
68		1337	0.25	$\nu (CC)_{R1,2} + \beta (CCH)_{R2} + \beta (CN_{12}H) + \beta (C_6CO_{28})$
67		1333	3.71	$\nu (CC)_{R1,2} + \beta (CCH)_{R2} + \beta (C_{21}CH_{27}) + \gamma (C_{24}H_{25}H_{26})$
66		1325	7.18	$\nu (CC)_{R2} + \beta (CCH)_{R1} + \gamma (C_{24}H_{25}H_{26})$
65		1313	10.62	$\nu (C_{31}=C_{33}) + \beta (C_{31}CH_{35}) + \beta (C_{33}CH_{32})$
64		1311	3.63	$\nu (CC)_{R1,2} + \beta (C_{21}CH_{27}) + \gamma (C_{24}H_{25}H_{26}) + \beta (C_{14}CH_{18})$
63		1268	5.48	$\nu (CC)_{R1,2} + \nu (C_3C_{11}) + \nu (C_{14}N_{12}) + \beta (C_2CH_7) + \beta (C_3CH_{13}) + \beta (C_3NH_{13})$
62		1251	335.53	$\nu (CC)_{R1} + \nu (C_6O_{28}) + \nu (C_{29}O_{28}) + \nu (C_{29}C_{31}) + \beta (C_{29}CH_{32}) + \beta (C_{31}CH_{35}) + \beta (C_{33}H_2) + \beta (C_6CO_{28})$
61		1230	26.67	$\nu (CC)_{R2} + \nu (C_{21}C_{24}) + \gamma (C_{24}H_2)$
60		1220	651.34	$\nu (CC)_{R1,2} + \nu (C_6O_{28}) + \nu (C_{29}O_{28}) + \nu (C_{14}N_{12}) + \beta (CCH)_{R1} + \beta (C_{29}CH_{32}) + \beta (C_{33}H_2)$
59	1202	1214	24.11	$\nu (CC)_{R1,2} + \nu (C_6O_{28}) + \nu (C_{21}C_{24}) + \nu (C_{14}N_{12}) + \nu (C_3C_{11}) + \beta (C_5CH_9) + \beta (C_2CH_7)$
58		1191	1.31	$\nu (CC)_{R2} + \nu (C_{14}N_{12}) + \beta (CCH)_{R2}$
57		1181	217.77	$\nu (CC)_{R1} + \nu (C_6O_{28}) + \beta (CCH)_{R1}$
56		1136	8.29	$\nu (CC)_{R2} + \beta (C_{19}CH_{20}) + \gamma (C_{24}H_{25}H_{26})$
55		1126	12.74	$\nu (CC)_{R1} + \beta (C_4CH_{10})$
54		1059	12.11	$\beta (C_{21}CH_{25}) + \beta (C_{21}CH_{26}) + \gamma (C_{24}H_{26}H_{27})$
53		1033	211.97	$\nu (CC)_{R1} + \nu (C_{29}O_{28}) + \beta (C_{33}H_2) + \beta (C_{33}CH)$
52		1031	11.89	$\nu (CC)_{R2} + \beta (CCH)_{R2} + \gamma (C_{24}H_2)$
51		1029	42.85	$\nu (CC)_{R1} + \beta (CCH)_{R1} + \beta (C_{33}H_2) + \beta (CCC)_{R1} + \beta (CCH)_{R1}$
50		1027	18.43	$\tau (C_{33}H=CH_2)$
49		1009	3.29	$\beta (C_{21}CH_{27}) + \gamma (C_{21}H_2)$
48		1007	36.48	$\gamma (C_{33}H_2)$
47		1001	5.53	$\beta (C_{21}CH_{27}) + \gamma (C_{21}H_2) + \gamma (CH=N_{12}) + \tau (CCCH)_R$
46		990	0.72	$\tau (CCCC)R + \tau (CCCH)R$
45		977	0.42	$\tau (CCCC)R + \tau (CCCH)R$
44		962	1.35	$\tau (CCCC)R + \tau (CCCH)R$
43		954	2.12	$\tau (CCCC)R + \tau (CCCH)R$
42		912	32.24	$\beta (C_{33}H_2) + \nu_s (C_{31}CO_{28}) + \tau (CCCC)R + \tau (CCCH)R$
41		899	34.49	$\nu (CC)_{R1,2} + \beta (C_3CH_{13}) + \beta (C_{11}NH)$
40		867	25.13	$\beta (C_{33}H_2) + \tau (CCCC)R + \tau (CCCH)R$
39		852	16.71	$\nu (CC)_{R1,2} + \tau (CCCC)R + \tau (CCCH)R$

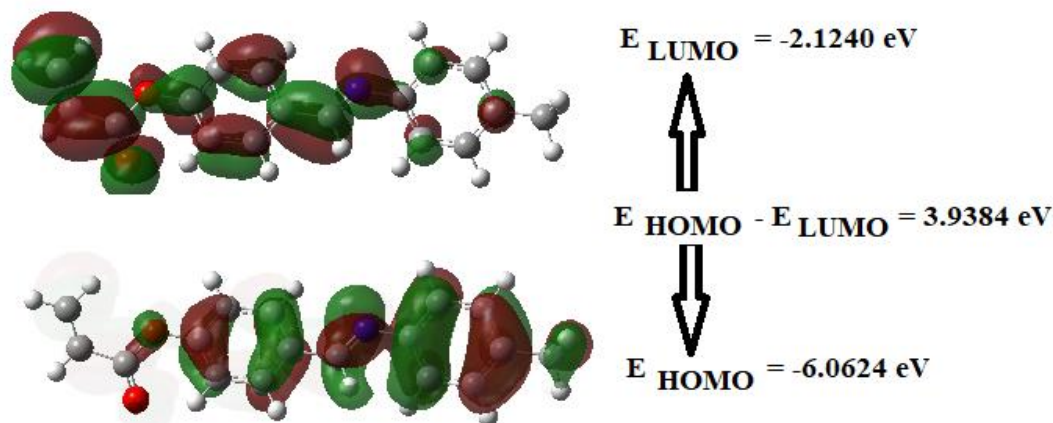
38		842	7.79	$\tau$ (CCCC)R + $\tau$ (CCCH)R
37		835	4.97	$\tau$ (CCCC)R + $\tau$ (CCCH)R
36		828	1.44	$\tau$ (CCCC)R + $\tau$ (CCCH)R
35		823	45.46	$\gamma$ (C33H2) + $\tau$ (CCCH)R
34		806	2.07	$\beta$ (C29O2) + $\gamma$ (C33H2) + $\tau$ (CCCH)R
33		771	1.83	$\nu$ (C21C24) + $\beta$ (C33H2) + $\beta$ (CCC)R2
32		735	3.94	$\tau$ (CCCC)R + $\tau$ (CCCH)R
31		721	3.74	$\gamma$ (C24H2) + $\tau$ (CCCC)R + $\tau$ (CCCH)R
30		665	15.01	$\beta$ (C33H2) + $\beta$ (CCC)R1
29		657	0.12	$\beta$ (CC)R2 + $\beta$ (C33H2)
28		646	0.27	$\beta$ (CC)R1 + $\beta$ (C33H2)
27		568	14	$\beta$ (C31CO) + $\tau$ (CCCC)R + $\tau$ (CCCH)R
26		548	21.80	$\tau$ (CCCC)R + $\tau$ (CCCH)R + $\tau$ (CCCN) + $\tau$ (CNCC)
25		535	2.15	$\nu$ (CC)R2 + $\beta$ (C33H2) + $\beta$ (C33CC)
24		533	5.07	$\tau$ (CCCC)R + $\tau$ (CCCH)R + $\tau$ (CCCN) + $\tau$ (CNCC)
23		504	2.38	$\gamma$ (C33H2) + $\tau$ (C33H=CH2) + $\tau$ (C31H=CO)
22		486	5.58	$\beta$ (C11=CN) + $\tau$ (CCCC)R + $\tau$ (CCCH)R

When the IR spectrum of the compound numbered (Figure 3.2) is examined, the peak belonging to the carbonyl group ( $>C=O$ ) is seen at  $1749\text{ cm}^{-1}$ , were calculated at  $1791\text{ cm}^{-1}$  theoretically. As a result of acryloylation, it was determined that the broad peak of the OH group, seen at  $3291 - 2388\text{ cm}^{-1}$ , disappeared. The aliphatic C-H stretch at  $2919\text{ cm}^{-1}$  and  $2850\text{ cm}^{-1}$  theoretically were calculated at  $3005\text{ cm}^{-1}$ .

The aromatic and aliphatic  $-C=C-$  stretch peaks at  $1652\text{ cm}^{-1}$ , theoretically were calculated at  $1680\text{ cm}^{-1}$ . While the peaks of  $-C(O)-O$  stretching are detected at  $1202\text{ cm}^{-1}$ ,  $1164\text{ cm}^{-1}$  and  $1138\text{ cm}^{-1}$ , theoretically were calculated at  $1214\text{ cm}^{-1}$ . The aromatic  $-C-H$  peak belonging to the  $-CH_3$  group is observed at  $3033\text{ cm}^{-1}$  (Erdik 2008), were calculated at  $3071\text{ cm}^{-1}$  theoretically.

### 3.3 HOMO-LUMO Analyze

The majority of the time boundary orbitals are utilized to describe how molecules behave with one another. In this instance, the boundary orbitals are the occupied molecular orbital with the greatest energy (HOMO) and the empty molecular orbital with the lowest energy (LUMO). Most chemical reactions occur when a molecule acquires or loses an electron. Hence HOMO and LUMO have a direct impact on the behavior of the molecule. The energy of the lowest energy empty molecular orbital (LUMO), where the electron will be placed, decreases with the ease with which an electron may be taken. Since electrons will be released from the molecular orbital with the maximum energy (HOMO), the more energy this orbital contains, the more probable it is to release electrons. Figures 3.2 presents HOMO-LUMO graphs of the (E)-4-((p-tolylimino)methyl)phenyl acrylate. HOMO and LUMO energies of the compounds were calculated using the 6-311++G (d, p) basis set of the B3LYP technique. In accordance with the computation, the energy band gap between the ground state and the first excited level of (E)-4-((p-tolylimino)methyl)phenyl acrylate is around  $3.94\text{ eV}$ .



**Figure 3.2** Energy levels and the 3D plots of the HOMO and LUMO of the (E)-4-((p-tolylimino)methyl)phenyl acrylate compound at the B3LYP/6-311++G(d,p) level

### 3.4 Nonlinear Optical (NLO) Properties

Nonlinear optics, which investigates how intense light fields interact with materials, is a recent field within physics with numerous potential applications in both basic science and technology (R.W. Boyd 2002). Analyzing nonlinear optical (NLO) effects are analyzed by considering the response of the dielectric material at the atomic level to the electric fields of an intense light beam.

static polarizability ( $\alpha_0$ ), initial static hyperpolarizability ( $\beta_{tot}$ ) of structures, and The dipole moment ( $\mu$ ) are all intimately connected to their nonlinear optical (NLO) activity. by The Gaussian 5.0 output, polarizabilities and hyperpolarizabilities have been translated from atomic to electrostatic units.

Urea is viewed as a general reference due to its unique characteristics in the study of nonlinear optical properties. The NLO characteristics of the molecules under consideration are assessed by comparing them to urea. Urea values acquired from DFT/B3LYP/6-311G calculations (d),  $\mu = 1.3732$  Debye,  $\alpha = 3.8312 \text{ \AA}^3$  and  $\beta = 0.37289 \times 10^{-30} \text{ cm}^5/\text{esu}$  (Meganathan *et al.* 2012).

Table 3.4 displays the examined The computed electric dipole moment, polarizability, and first-order hyperpolarizability properties of the investigated substance.

**Table 3.3** The electric dipole moment  $\mu$  (D), the mean polarizability  $\langle\alpha\rangle$  and the first hyperpolarizability ( $\beta_{tot}$ ) of (E)-4-((p-tolylimino)methyl)phenyl acrylate by DFT/B3LYP/6-311++G(d,p) level of theory

Parameter	4-((p-tolylimino)methyl)phenyl acrylate	Parameter	4-((p-tolylimino)methyl)phenyl acrylate
$\mu_x$	-0.3285	$\beta_{xxx}$	-1347.83
$\mu_y$	0.3296	$\beta_{xyx}$	-232.97
$\mu_z$	0.5267	$\beta_{xyy}$	37.37
$\mu_{tot}$	0.7028	$\beta_{yyy}$	19.40
$\alpha_{xx}$	419.41	$\beta_{xxz}$	95.49
$\alpha_{xy}$	-5.37	$\beta_{xyz}$	16.04
$\alpha_{yy}$	198.40	$\beta_{yyz}$	29.65
$\alpha_{xz}$	-5.65	$\beta_{xzz}$	-3.04
$\alpha_{yz}$	0.88	$\beta_{yzz}$	10.19
$\alpha_{zz}$	129.90	$\beta_{zzz}$	42.62
$\langle\alpha\rangle$ (a.u)	249.23	$\beta_{tot}$ (a.u)	1339.69
$\langle\alpha\rangle$ (esu)	$36.93 \times 10^{-24} \text{ esu}$	$\beta_{tot}$ (esu)	$11573.98 \times 10^{-33} \text{ esu}$

$\alpha$ : 1a. u =  $0.1482 \times 10^{-24} \text{ esu}$ ,  $\beta$ : 1a. u =  $8.6393 \times 10^{-33} \text{ esu}$

The ( $\mu$ ) dipole moment was determined 0.7028 and mean polarizability ( $\alpha_{tot}$ ) was determined to be  $36.93 \times 10^{-24} \text{ esu}$ . the compound's first order hyperpolarizability ( $\beta_{tot}$ ) was determined to be  $11573.98 \times 10^{-33} \text{ esu}$  which is nearly 31 times larger than that of urea. Based on the results, We reach our conclusion that the topic of this chemical and its derivatives represent a promising field for further research into nonlinear optical properties.

### 3.5 Molecular Electrostatic Potential (MEP)

The MEP determines whether a proton positioned at any point surrounding the molecule will find the region of the molecule to be attractive or repulsive (Al-Ahmary *et al.* 2018). The electronic density of a molecule is the focus of MEP mapping. According to (Yeşilkaynak *et al.* 2010), this is a great descriptor for comprehending hydrogen bond interactions and pinpointing hydrogen bond positions in electrophilic and nucleophilic processes. As shown in Fig. 3.3, the MEP surfaces were examined using the DFT method (B3LYP) and basis set (6-311++G\*\*) for geometry optimization. The MEP surface's color scheme is as follows: red indicates an electron-rich, partially negative charge; blue indicates an electron-deficient, partially positive charge; light blue indicates a region that is slightly electron-deficient; yellow indicates a region that is slightly electron-rich; and green indicates neutral (zero potential). (Poltzer and Murray 2002)



**Figure 3.3** MEP's map of 4-((p-tolylimino)methyl)phenyl acrylate compound

#### IV. CONCLUSIONS

In the study, (E)-4-((p-tolylimino)methyl)phenyl acrylate molecule, First of all, the stable structure with minimum energy of the studied molecule was obtained by DFT method by performing geometry optimization calculation at B3LYP/6-311++G(d,p) level. Since the molecule studied in the literature has no experimental structural parameters, the theoretically calculated bond lengths and bond angles of the compound were compared with the experimental values of similar molecules in the literature. The N-C, C-C and C-O bond lengths were calculated as 1.405, 1.394 and 1.393 Å. It was seen that the calculated results and the experimental values in the literature were compatible with each other. In the FT-IR analysis results obtained with the 6-311++G(d,p) basis set we used with the DFT/B3LYP method, it is seen that the value of 3071 cm<sup>-1</sup> calculated for the –C-H stretching vibration almost coincide with the value of similar molecule groups (Erdik 2008). In addition, the absence of virtual vibration frequency values (negative number) indicates that the molecule is optimized with correct calculation methods and has a stable structure. The HOMO and LUMO energies of the (E)-4-((p-tolylimino)methyl)phenyl acrylate molecule were calculated by the DFT method at the B3LYP/6-311++G(d,p) level. The obtained HOMO and LUMO energy difference was found to be 3.94 eV. The nonlinear optical properties and molecular potential energy surface map of the studied compound were calculated using the same method and basis set. As a result of calculation, the compound was found to have a hyperpolarizability of 11573.98\*10<sup>-33</sup>esu. This value indicates that the hyperpolarizability of the compound is approximately 31 times larger than that of urea. Therefore, it can be said that the compound exhibits nonlinear optical properties. On the molecular potential energy surface, the red regions indicate electron-rich regions, and the gray and blue regions indicate electron-poor regions. In this thesis, all calculations were performed with Gaussian 09 and Gauss View 5.0 package program.

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