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Research Article

**Structural Parameters, Electronic, Spectroscopic and Nonlinear Optical Theoretical Research of 1-(*m*-Chlorophenyl)piperazine (mCPP) Molecule**

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**Abstract:** In this study, the experimentally obtained IR spectrum of the meta-Chlorophenylpiperazine (C<sub>10</sub>H<sub>13</sub>ClN<sub>2</sub>) molecule, which is used in the testing phase of antimigran drugs in the literature, was obtained theoretically and the structural properties obtained for ortho and para derivatives of the title molecule were compared. moreover, the optimized molecular structure, conformational analysis, Nonlinear optics properties, HOMO-LUMO and Chemical reactivity descriptors that is the ionization potential, The electron affinity the chemical hardness, softness and the electronegativity, Molecular electrostatic potential, Natural Bonding Orbital and Raman spectrum were calculated using density functional theory method with B3LYP functional with 6-311++G (d, p) basis set in ground state. The results introduce that molecular modelling are valuable for obtainment insight into molecular structure and electronic properties of the mCPP molecule

**Keywords:** meta-Chlorophenylpiperazine, DFT, NLO, NBO, MEP, IR, Raman, HOMO-LUMO

## 1. Introduction

Piperazines have been one of the chemical groups with pharmaceutical features. Because Piperazines and their derivatives are presented in many marketed drugs for example antipsychotic, antidepressant and antitumor activity against colon, prostate, breast and lung tumors [1] These and their derivatives are now one of the cornerstones of the pharmaceutical industry. Chlorophenylpiperazine is one of piperazine components. According to the location of Cl atom in the phenyl ring of this component, three isomers can be generated as ortho-, meta- and para-chlorophenylpiperazine. Spectroscopic and quantum chemical calculations of various piperazine based components were performed and reported in literature [2, 3]. Theoretical calculation for chlorophenylpiperazine derivatives were carried

out by running density functional theory (DFT). In these studies, spectral measurements, molecular electrostatic potential (MEP), Highest Occupied Molecular Orbitals (HOMO), Lowest Unoccupied Molecular Orbitals (LUMO) and natural bond orbital (NBO) analysis for ortho-chlorophenylpiperazines were calculated [4] and spectral measurements and HOMO-LUMO energy values for para-chlorophenylpiperazine were reported recently [5] using DFT method with B3LYP functional, with 6-311++G (d, p) basis set and 6-311++G(d, 2d) basis set.

Meta-chlorophenylpiperazine (mCPP) isomer of piperazines derivatives is a psycho-active drug. This drug causes headaches in humans and is used in the testing phase of antimigran drugs [6]. Because of anorectic effects of MCPP, the treatment of obesity has been helped the

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development of selective 5-HT<sub>2C</sub> receptor agonists [7, 8]. In contrast to ortho and para chlorophenylpiperazine, the mCPP isomer has yet been studied neither theoretically nor experimentally. A number of studies made, only, were performed to investigate this molecular isomer, such as The Synthesis Of 4-(3-chlorophenyl)-1-(3chloropropyl) piperazin-1-ium chloride and two salts of a piperazine derivative 4(C<sub>17</sub>H<sub>20</sub>CIN<sub>2</sub>)+2(C<sub>4</sub>H<sub>5</sub>O<sub>4</sub>)-(C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>)-2 H<sub>2</sub>O and 2(C<sub>17</sub>H<sub>20</sub>CIN<sub>2</sub>)+C<sub>6</sub>Cl<sub>2</sub>O<sub>4</sub>-3(H<sub>2</sub>O) [9, 10]. The difference between meta- and para-chlorophenylpiperazine isomers was investigated using spectrophotometric spectroscopy [11]. The IR absorption spectroscopy was studied by Inoue et al. is in HCl of the mCPP molecule [12]. In this study, structural properties of the mCPP molecule have been investigated theoretically using the basic properties of the calculation technique known as density functional theory.

## 2. Details Of Computation Procedure

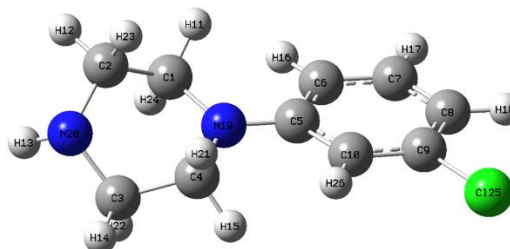
Conformation analysis of mCPP molecule was investigated by running SPARTAN 08 package program [13]. It has been carried out using Merck Molecular Force Field (MMFF) in molecular mechanic method. This analysis is defined in a detailed manner in another study [14]. The optimized structure of mCPP molecule was calculated using GAUSSIAN-09 package program [15] with density functional theory [16] with Becke three parameter Lee–Yang–Parr exchange correlation functional (B3LYP) [17] and 6-311++G(d,p) basis set [18]. The natural bonding analysis (NBO), Nonlinear optical (NLO) properties, HOMO-LUMO, Chemical reactivity descriptors, molecular electrostatic potential (MEP), IR and Raman spectrum were calculated at the same levels.

## 3. Results and discussion

### 3.1. Molecular conformation and geometrical structure analysis

The conformation analysis of mCPP molecule was determined using Spartan 08 package program with MMFF in molecular mechanic method. As a result of this analysis, a conformer was obtained. The energy value for this structure has been found as 1598.2741 kJ/mol. And then, the molecule structure optimization approached was calculated

using B3LYP/6-311++G (d, p) basis set and the most stable structure of the molecule was obtained and was shown in figure 1. Geometric parameters of title molecule have been presented in Table.1



**Figure 1.** Optimized structure of mCPP molecule Using B3LYP/6-311++G (d, p) basis set.

Bond lengths of N19-C1, N19-C4, C2-N20, N20-C3, C3-C4, N19-C5, C5-C6, C6-C7 and N20-H13 for oCPP molecule in literature have been calculated as 1.46 Å, 1.48 Å, 1.46 Å, 1.46 Å, 1.52 Å, 1.41 Å, 1.41 Å, 1.39 Å and 1.01 Å, respectively [4, 19]. These bond lengths in our study were calculated to be 1.462 Å, 1.462 Å, 1.469 Å, 1.469 Å, 1.526 Å, 1.382 Å, 1.413 Å, 1.388 Å and 1.011 Å, respectively. Bond angles of C2-C1-N19, N20-C2-C1, H13-N20-C2, N20-C3-C4, H21-C4-N19, C10-C5-C6 and C5-C6-C7 were determined to be 109.679°, 113.833°, 110.719°, 110.833°, 111.774°, 117.627° and 120.702°, respectively. These bond angles in literature were calculated as 109.79°, 108.99°, 110.86°, 109.21°, 110.04°, 116.47° and 121.98°, respectively, [4]. Dihedral angles of C5-C6-C7-C8 and N19-C5-C10-C9 were calculated as 0.38° and 179.59°, respectively, these dihedral angles in literature were calculated to be 0° and 177.66°, respectively, [4, 19]. We can say that oCPP and pCPP molecules are quite compatible with the geometric parameters gathered in literature.

### 3.2. Nonlinear optical (NLO) properties

Nonlinear optical (NLO) properties are very important for science and technology due to the development of the wide range of applications in electronic devices [20]. The NLO properties of a molecule can be foretell using dipole moment ( $\mu$ ), polarizability ( $\alpha$ ) and hyperpolarizability ( $\beta$ ) values. Total dipole moment ( $\mu_{tot}$ ) for a molecule is defined as in equation 1

$$\mu_{tot} = (\mu_x + \mu_y + \mu_z)^{1/2} \quad (1)$$

**Table. 1** Calculated bond length (Å), bond angle (°) and Dihedral angle (°) of mCPP using B3LYP/6-311++G (d,p) basis set.

Bond length (Å)		Bond angle (°)		Dihedral angle (°)	
C1-C2	1,5319	H15-C4-N19	109,0626	H14-C3-C4-H15	58,7628
C1-H11	1,0936	H15-C4-H21	107,408	H14-C3-C4-N19	178,0373
C1-N19	1,4622	N19-C4-H21	111,7742	H14-C3-C4-H21	-58,1786
C1-H24	1,1012	C6-C5-C10	117,6277	N20-C3-C4-H15	179,065
C2-H12	1,0926	C6-C5-N19	121,3977	N20-C3-C4-N19	-61,6605
C2-N20	1,4695	C10-C5-N19	120,9746	N20-C3-C4-H21	62,1236
C2-H23	1,0962	C5-C6-C7	120,7022	H22-C3-C4-H15	-57,3623
C3-C4	1,5267	C5-C6-H16	120,3036	H22-C3-C4-N19	61,9122
C3-H14	1,0945	C7-C6-H16	118,9758	H22-C3-C4-H21	-174,3038
C3-N20	1,4699	C6-C7-C8	121,7605	C4-C3-N20-C2	31,6879
C3-H22	1,1007	C6-C7-H17	119,0166	C4-C3-N20-H13	156,7837
C4-H15	1,0922	C8-C7-H17	119,2182	H14-C3-N20-C2	151,5989
C4-N19	1,4626	C7-C8CC9	117,2282	H14-C3-N20-H13	-83,3053
C4-H21	1,1003	C7-C8-H18	121,7785	H22-C3-N20-C2	-89,1957
C5-C6	1,4134	C9-C8-H18	120,9932	H22-C3-N20-H13	35,9001
C5-C10	1,4129	C8-C9-C10	122,7307	C3-C4-N19-C1	29,8568
C5-N19	1,3822	C8-C9-Cl25	119,0031	C3-C4-N19-C5	-152,5717
C6-C7	1,3889	C10-C9-Cl25	118,2617	H15-C4-N19-C1	148,5596
C6-H16	1,0813	C5-C10-C9	119,9479	H15-C4-N19-C5	-33,8689
C7-C8	1,3941	C5-C10-H26	121,1556	H21-C4-N19-C1	-92,8281
C7-H17	1,0846	C9-C10-H26	118,8725	H21-C4-N19-C5	84,7434
C8-C9	1,3894	C1-N19-C4	116,9332	C10-C5-C6-C7	-0,0239
C8-H18	1,0812	C1-N19-C5	121,4382	C10-C5-C6-H16	178,3963
C9-C10	1,3873	C4-N19-C5	121,5828	N19-C5-C6-C7	179,9495
C9-Cl25	1,7654	C2-N20-C3	113,8574	N19-C5-C6-H16	-1,6302
C10-H26	1,0798	C2-N20-H13	110,7192	C6-C5-C10-C9	-0,435
H13-N20	1,0117	C3-N20-H13	110,2029	C6-C5-C10-H26	177,7661
				N19-C5-C10-C9	179,5914
				N19-C5-C10-H26	-2,2074
				C6-C5-N19-C1	-15,1606
				C6-C5-N19-C4	167,3771
				C10-C5-N19-C1	164,812
				C10-C5-N19-C4	-12,6503
				C5-C6-C7-C8	0,3899
				C5-C6-C7-H17	179,5943
				H16-C6-C7-C8	-178,0511
				H16-C6-C7-H17	1,1533
				C6-C7-C8-C9	-0,2797
				C6-C7-C8-H18	179,5919
				H17-C7-C8-C9	-179,4825
				H17-C7-C8-H18	0,3891
				C7-C8-C9-C10	-0,1982
				C7-C8-C9-Cl25	-179,4074
				H18-C8-C9-C10	179,9291
				H18-C8-C9-Cl25	0,7199
				C8-C9-C10-C5	0,5612
				C8-C9-C10-H26	-177,6809
				Cl25-C9-C10-C5	179,776
				Cl25-C9-C10-H26	1,5339
Bond angle (°)		Dihedral angle (°)			
C2-C1-H11	108,6518	H11-C1-C2-H12	61,4785		
C2-C1-N19	109,6793	H11-C1-C2-N20	-176,1956		
C2-C1-H24	110,346	H11-C1-C2-H23	-54,4605		
H11-C1-N19	109,1854	N19-C1-C2-H12	-179,2415		
H11-C1-H24	107,3081	N19-C1-C2-N20	-56,9157		
N19-C1-H24	111,5916	N19-C1-C2-H23	64,8195		
C1-C2-H12	109,4379	H24-C1-C2-H12	-55,9127		
C1-C2-N20	113,8337	H24-C1-C2-N20	66,4132		
C1-C2-H23	108,253	H24-C1-C2-H23	-171,8517		
H12-C2-N20	109,0734	C2-C1-N19-C4	26,1325		
H12-C2-H23	106,7081	C2-C1-N19-C5	-151,4427		
N20-C2-H23	109,2908	H11-C1-N19-C4	145,0841		
C4-C3-H14	108,7489	H11-C1-N19-C5	-32,4911		
C4-C3-N20	110,8331	H24-C1-N19-C4	-96,46		
C4-C3-H22	107,8879	H24-C1-N19-C5	85,9647		
H14-C3-N20	109,4046	C1-C2-N20-C3	25,9064		
H14-C3-H22	107,3427	C1-C2-N20-C13	-98,9138		
N20-C3-H22	112,4958	H12-C2-N20-C3	148,4327		
C3-C4-H15	108,121	H12-C2-N20-H13	23,6124		
C3-C4-N19	110,4728	H23-C2-N20-C3	-95,2519		
C3-C4-H21	109,8811	H23-C2-N20-H13	139,9278		

Total polarizability ( $\alpha_{tot}$ ) for a molecule can be evaluated by equation 2

$$\alpha_{tot} = \frac{1}{3} (\alpha_{xx} + \alpha_{yy} + \alpha_{zz})^{1/2} \quad (2)$$

The total first hyperpolarizability ( $\beta_{tot}$ ) can be calculated by equation 3

$$\beta_{tot} = (\beta_x^2 + \beta_y^2 + \beta_z^2)^{1/2} \quad (3)$$

Here  $\beta_x$ ,  $\beta_y$  and  $\beta_z$

$$\beta_x = (\beta_{xxx} + \beta_{xyy} + \beta_{xzz}) \quad (4)$$

$$\beta_y = (\beta_{yyy} + \beta_{yzz} + \beta_{yxx}) \quad (5)$$

$$\beta_z = (\beta_{zzz} + \beta_{zxx} + \beta_{zyy}) \quad (6)$$

Total first hyperpolarizability from Gaussian 09 output is given in equation 7.

$$\beta_{tot} = [(\beta_{xxx} + \beta_{xyy} + \beta_{xzz})^2 + (\beta_{yyy} + \beta_{yzz} + \beta_{yxx})^2 + (\beta_{zzz} + \beta_{zxx} + \beta_{zyy})^2]^{1/2} \quad (7)$$

Because these  $\beta$  and  $\alpha$  values of Gaussian 09 program are given in atomic units (a.u), the calculated  $\beta_{tot}$  and  $\alpha_{tot}$  values were converted into electrostatic units (esu) [1 a.u. =  $8.6393 \times 10^{-33}$  esu] and [1 a.u. =  $0.1482 \times 10^{-24}$  esu], respectively, [21, 22]. The nonlinear properties of mCPP molecule were calculated using DFT/B3LYP method with 6-311++G (d,p) basis set and was given in Table 2.

**Table.2** Calculated Dipole moment ( $\mu$ ) in Debye, polarizability ( $\alpha$ ) and hyperpolarizability ( $\beta$ ) of mCPP by B3LYP/6-311++G (d,p) method.

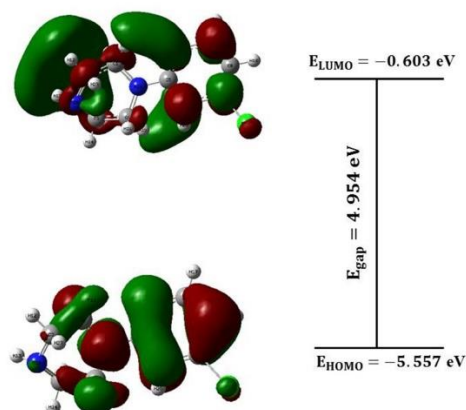
Parameters	Values
<b>Dipole moment (Debye)</b>	
$\mu_x$	-3.4994
$\mu_y$	1.5306
$\mu_z$	-0.8915
$\mu_{tot}$	3.9221
<b>Polarizability (a.u)</b>	
$\alpha_{xx}$	201.934
$\alpha_{yy}$	150.023
$\alpha_{zz}$	97.630
$\alpha_{tot}$ (a.u)	149.8623
$\alpha_{tot}$ (esu)	$22.209 \times 10^{-24}$
<b>Hyperpolarizability (a.u)</b>	
$\beta_{xxx}$	546.381
$\beta_{xxy}$	233.413
$\beta_{xyy}$	-67.300
$\beta_{yyy}$	-69.443
$\beta_{xxz}$	-159.808
$\beta_{xyz}$	158.966
$\beta_{yyz}$	-54.229
$\beta_{xzz}$	150.626
$\beta_{yzz}$	-72.531
$\beta_{zzz}$	-196.221
$\beta_{tot}$ (a.u)	757.102
$\beta_{tot}$ (esu)	$6540.83 \times 10^{-33}$

### 3.3. HOMO-LUMO and Chemical reactivity descriptors studies

Molecular orbitals are very important for quantum chemistry. The most important molecules orbitals in a molecule are the highest occupied molecular orbital (HOMO) and the lowest unoccupied (LUMO) orbitals. Molecular interactions and chemical reactivity can be examined by interpreting

HOMO and LUMO values. Also, chemical reactivity descriptors such as the ionization potential (I), the electron affinity (A), the chemical hardness ( $\eta$ ), softness (S) and electronegativity ( $\chi$ ) can be calculated. HOMO, LUMO and HOMO-LUMO gap energy values have been shown in Figure 2 and Table 3. These values were calculated

using DFT/B3LYP method with 6-311++G (d, p) basis set.

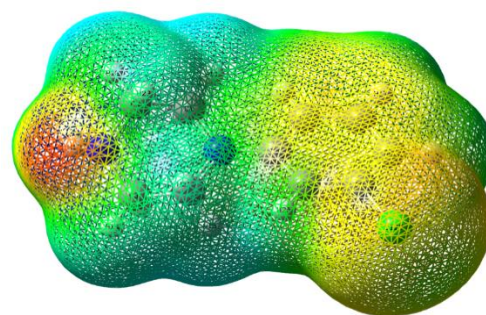


**Figure 2.** HOMO-LUMO energy gap of mCPP molecule Using B3LYP/6-311++G (d, p) basis set.

Ionization potential is the energy required to remove an electron from the molecule and it is calculated with  $I = -E_{\text{HOMO}}$  [23]. The electron affinity is the energy that increases when the molecule gains an electron and it is determined by  $A = -E_{\text{LUMO}}$  [23]. The chemical hardness and softness are calculated by  $\eta = \frac{1}{2}[E_{\text{LUMO}} - E_{\text{HOMO}}]$  and  $S = \frac{1}{2\eta}$ . The electronegativity is determined by  $\chi = -\frac{1}{2}[E_{\text{HOMO}} + E_{\text{LUMO}}]$  [24]. The obtained chemical reactivity descriptors have been given in Table 3.

### 3.4. Molecular electrostatic potential surface (MEPS) analysis

The chemical stability and reactivity of a molecule are examined with the help of molecular electrostatic potential surface (MEP). The different colors in MEP are corresponding to the different electrostatic potential. Red and yellow colors on MEP correspond to negative electrostatic potential regions while blue color corresponds to positive electrostatic potential region. The MEP surface of mCPP molecule were calculated using the DFT/B3LYP method with 6-311++G (d, p) basis set and has been shown in figure 3. The color code of this map ranges from  $-3.876 \times 10^{-2}$  and  $+3.876 \times 10^{-2}$  a.u. The positive electrostatic potential areas are on the hydrogen atoms. But the negative electrostatic potential areas are on the nitrogen and the chlorine atoms.



**Figure 3.** Molecular electrostatic potential surface of mCPP molecule Using B3LYP/6-311++G (d, p) basis set.

### 3.5. Natural Bonding Orbital (NBO) analysis

The natural bond orbital (NBO) analysis is an effective method to examine intermolecular bonding and interaction among bonds. Also, it provides an useful method to investigate charge transfer and conjugative interactions in a molecule [25]. Some electron donor orbital, acceptor orbital and the interacting stabilization energy resulting from the second-order micro disturbance theory was reported [26, 27]. The second-order Fock matrix has been calculated to evaluate the donor and acceptor from the NBO analysis of mCPP molecule [25, 28]. The interaction result is losse occupier turn the localized NBO of electrons in the Lewis structure into the empty non-Lewis structure. The stabilization energy  $E(2)$  associated with the delocalization donor (i)  $\rightarrow$  acceptor (j) can be calculated by equation 8 [29, 30].

$$E_2 = \Delta E_{ij} = q_i \frac{F(i,j)^2}{\epsilon_j - \epsilon_i} \quad (8)$$

The stabilization energy  $E(2)$  values in table 4 have been presented for values only 5 and greater than 5. The bonding C8-C9, N19 and C5-C10 interacts with anti-bonding C6-C7, C5-C10 and C8-C9, and stabilization energy values are 273.14, 43.12 and 25, 89 kcal/mol, respectively. Also, these values show that interaction is taken place between C8-C9 and C6-C7 antibonding of charge transfer causing stabilization of molecule

### 3.6. FT-IR and Raman measurements

The mCPP molecule has 72 normal modes of vibrations because it has 26 atoms. The experimental IR spectra of mCPP molecule have been obtained between 1500 and 1680  $\text{cm}^{-1}$  [31]. The theoretical vibrational calculations were done in the B3LYP/6-311++G (d,p) level.

**Table. 3** Calculated HOMO, LUMO, HOMO-LUMO gap and chemical reactivity descriptors of mCPP by B3LYP/6-311++G (d, p) method

Parameters	Values (eV)
HOMO	-5.557
LUMO	-0.603
HOMO-LUMO gap	4.954
I	5.557
A	0.603
η	2.477
S	0.201
χ	3.08

**Table. 4** Second Order perturbation theory analysis of Fock matrix in NBO basis for mCPP by B3LYP/6-311++G (d,p) method.

Donor (i)	ED (i)	Acceptor (j)	ED (j)	E(2) (kcal/mol)	E(j)-E(i) (a.u)	F(i,j) (a.u)
C8-C9	0,42578	C6-C7	0,34675	273,14	0,01	0,084
N19	1,73437	C5-C10	0,42782	43,12	0,27	0,1
C5-C10	1,62882	C8-C9	0,42578	25,89	0,27	0,076
C6-C7	1,72177	C5-C10	0,42782	21,77	0,28	0,072
C8-C9	1,69498	C6-C7	0,34675	21,59	0,29	0,072
C6-C7	1,72177	C8-C9	0,42578	16,2	0,27	0,062
C8-C9	1,69498	C5-C10	0,42782	15,9	0,29	0,062
C5-C10	1,62882	C6-C7	0,34675	15,58	0,28	0,06
Cl25	1,93329	C8-C9	0,42578	12,02	0,33	0,062
N19	1,73437	C4-H21	0,03072	8,21	0,63	0,068
N19	1,73437	C1-H24	0,03025	8,2	0,63	0,068
N20	1,92294	C3-H22	0,02841	6,16	0,67	0,058
C7-C8	1,96965	C9-Cl25	0,03341	5,6	0,84	0,061
N20	1,92294	C1-C2	0,02399	5,5	0,66	0,054

### 3.6. FT-IR and Raman measurements

The mCPP molecule has 72 normal modes of vibrations because it has 26 atoms. The experimental IR spectra of mCPP molecule have been obtained between 1500 and 1680 cm<sup>-1</sup> [31]. The theoretical vibrational calculations were done in the B3LYP/6-311++G (d,p) level.

The calculated FT-IR and FT-Raman frequencies for 72 modes of vibrations are presented in table 5. The DFT/B3LYP functional tends to overestimate the fundamental modes; therefore scaling factors have to be used for obtaining a very agreement with experimental results. The scaling factor used in the study is 0.9668 for B3LYP/6-311++G(d, p) [14, 32]. The calculated FT-IR and FT-Raman frequencies for 72 modes of vibrations are presented in table 5. The DFT/B3LYP functional tends to overestimate the fundamental modes; therefore scaling factors have to be used for obtaining a very agreement with experimental results. The scaling factor used in the study is 0.9668 for B3LYP/6-311++G(d, p) [14, 32].

The IR spectra as a result of theoretical calculation and IR spectra obtained experimentally were compared to a region between 1500 and 1680 cm<sup>-1</sup>. The experimentally obtained IR spectra with our theoretical calculations are quite in coherence. The theoretical and experimental IR spectra are shown in Figure 4 and Figure 5. Experimental IR spectra of mCPP molecule have shown peaks in the region about 1562 and 1597 cm<sup>-1</sup>. Theoretical IR spectra of mCPP molecule were shown in the region 1538 and 1582 cm<sup>-1</sup>. The C-C stretches in this region actually give rise to two IR active peaks. In the literature, C-C ring stretching vibrations usually occur between 1600 and 740 cm<sup>-1</sup> [33, 34]. The Raman spectrum of the mCPP molecule was calculated between 0-3560 cm<sup>-1</sup> using the B3LYP/6-311++G (d, p) basis set and the theoretical Raman spectra were shown in Figure 6. In this Raman spectrum, the most intense band was observed at 2960.14 cm<sup>-1</sup>. In this region is a found vibrational frequency of the C-H stretching. The C-C stretching vibrations are occurring in the 1279,

1321, 1466, 1509 and 1590 cm<sup>-1</sup>. These values are compatible with the values given in the literature for the aromatic C–C stretching vibration [35]. The N-H stretching vibration of title molecule was calculated as band at 3559 cm<sup>-1</sup>.

**Table 5** calculated vibrational wavenumbers (cm<sup>1</sup>) of the mCPP compound by B3LYP/6-311++G (d, p) method.

Mode	Frequency	Scaled Freq	Infrared	Raman Activity
1	36.38	35.17	0.1849	1.1964
2	66.54	64.33	0.9962	1.1041
3	90.60	87.59	6.8938	0.5849
4	121.55	117.51	0.6552	1.3065
5	191.12	184.77	0.9559	0.9954
6	213.01	205.94	0.1502	1.5714
7	260.84	252.18	1.5193	3.3818
8	279.91	270.61	0.5215	1.1273
9	294.99	285.20	5.1018	1.9256
10	322.44	311.74	0.0146	3.2285
11	402.15	388.80	7.1054	5.7669
12	449.11	434.20	4.0004	0.2578
13	480.19	464.25	4.2043	0.3249
14	487.61	471.42	8.7074	1.5439
15	525.61	508.16	12.9654	2.1252
16	587.37	567.87	0.3376	0.5967
17	613.93	593.55	4.0339	0.5097
18	684.30	661.58	10.0088	8.1031
19	693.73	670.70	19.2026	1.0646
20	715.74	691.98	96.6482	1.0711
21	765.21	739.80	38.5553	1.8426
22	780.73	754.81	22.6198	1.6395
23	837.49	809.68	19.4438	0.5995
24	856.74	828.30	0.3412	1.1844
25	867.79	838.98	3.8110	3.0559
26	891.75	862.15	6.5749	4.0973
27	931.91	900.97	3.3574	2.3735
28	969.45	937.26	49.0598	8.2854
29	970.15	937.94	18.5348	5.7986
30	997.01	963.91	48.8286	55.1687
31	1042.96	1008.33	5.2774	4.4998
32	1069.03	1033.54	6.4126	10.7060
33	1087.49	1051.39	1.0167	3.2482
34	1100.60	1064.06	17.0357	17.7761
35	1112.64	1075.70	9.4586	1.8707
36	1119.15	1081.99	18.4212	4.3243
37	1167.15	1128.40	36.5438	2.2083
38	1196.39	1156.67	11.3078	1.9182
39	1198.04	1158.26	17.9496	0.7474
40	1243.49	1202.20	37.9604	5.3811
41	1259.64	1217.82	17.5032	4.6193
42	1279.42	1236.94	30.0970	6.1673
43	1309.20	1265.74	38.1150	9.0617
44	1321.55	1277.67	2.7495	12.3593
45	1336.22	1291.86	5.3860	3.1472
46	1372.36	1326.79	3.2854	2.6903
47	1386.30	1340.28	45.7518	8.0288
48	1396.55	1350.19	15.0900	3.1962
49	1408.95	1362.17	21.6294	4.3722
50	1414.11	1367.16	72.2036	4.9024
51	1466.26	1417.58	16.0575	1.9488



Table 5 continue

52	1488.48	1439.07	8.7473	2.8987
53	1498.77	1449.01	65.7179	10.6920
54	1509.40	1459.29	114.2521	6.3965
55	1514.72	1464.43	23.1759	2.4309
56	1521.57	1471.05	54.1150	4.8841
57	1526.56	1475.88	15.7500	9.1408
58	1590.98	1538.16	75.8847	5.7226
59	1637.23	1582.87	296.6146	82.0706
60	2949.76	2851.82	55.7566	63.7183
61	2960.14	2861.86	48.9679	322.9880
62	2973.36	2874.65	78.9915	43.8006
63	3011.74	2911.75	42.7893	78.5399
64	3042.14	2941.14	48.2542	147.1256
65	3053.44	2952.06	28.0384	81.1001
66	3069.49	2967.58	26.7370	40.2936
67	3076.31	2974.17	33.8770	182.9935
68	3169.75	3064.52	12.1396	101.3182
69	3204.02	3097.65	8.7541	60.7152
70	3211.70	3105.07	1.7425	147.4444
71	3222.57	3115.59	1.8246	49.0397
72	3559.19	3441.03	2.1724	128.5324

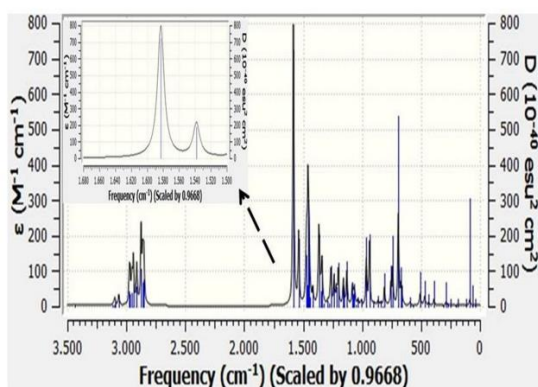


Figure 3. FT-IR spectra of mCPP molecule Using B3LYP/6-311++G (d, p) basis set.

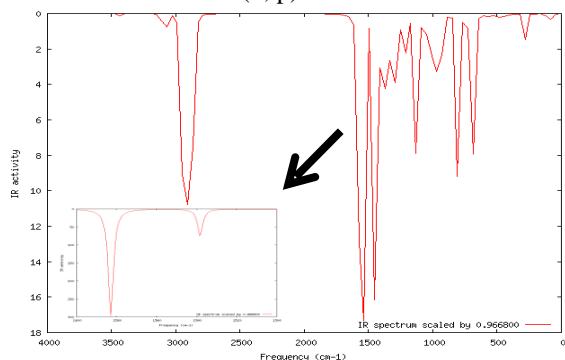


Figure 4. IR spectra of mCPP molecule Using B3LYP/6-311++G (d, p) basis set.

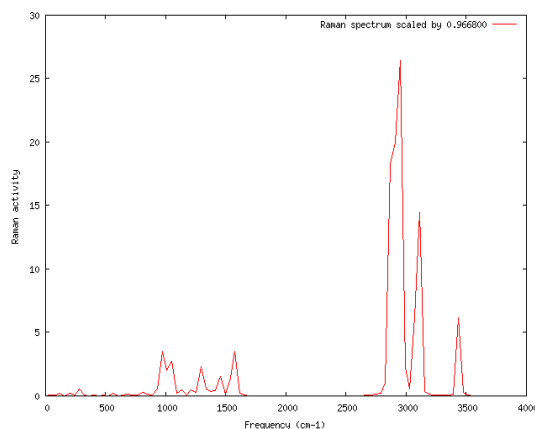


Figure 5. Raman spectra of mCPP molecule Using B3LYP/6-311++G (d, p) basis set.

#### 4. Conclusion

In this study, the structural and electronic as well as optical properties of the mCPP molecule, which is a psychoactive drug of the phenylpiperazine class, have been calculated using B3LYP/6-311++G (d, p) basis set. Theoretically obtained IR spectrum is in good agreement with experimental results. Also, the title molecule has been characterized by the conformational stabilities, optimized molecular structure, nonlinear optics properties HOMO-LUMO analysis, chemical reactivity descriptors, the natural bond orbital and the molecular electrostatic potential using Gaussian 09 program. The results introduce that molecular modelling is valuable for obtainment insight into molecular structure and electronic properties of the mCPP molecule.



The theoretical results obtained for mCPP molecule can be used to understand the activity. Since neither experimental nor theoretical enough published data about the mCPP molecule have been reported in literature, we think that our study will be a pioneering study for both experimental and theoretical studies and we think that this paper presents some good data for the pharmaceutical industry.

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