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Electro-Optical Uv Spectra Analysis of Imipramine By Using First Principal

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Abstract

In ongoing paper geometry optimization of Imipramine has been done by using combination of DFT/B3LYP method and 6-311G (d,p) basis set without any symmetry constrain. The electronic properties of title molecule are calculated by HOMO LUMO MESP plot. The HOMO LUMO plot gives nature and value of chemical reactivity of title molecule. The various optical parameters are calculated by using same level theory. The UV spectra of title molecule are calculated by using time dependent theory with same level theory.

Keywords : DFT, HOMO, LUMO, MESP, UV spectra

Introduction

Last few decades after discovering fast high-performance computational facilities quantum chemical methods are important tools to determine structure stability and other properties of molecules. The quantum chemical methods are important to know about knowledge about transition states. Imipramine is tricyclic antidepressant which affects brain. This affect makes people unbalanced which cause depression. The title molecule is used as important drug for treatment of symptoms of depression [1].

Objective of the Study

Some electronics properties of Imipramine molecules are calculated by HOMO,LUMO,MESP plots.Various optical parameters like Polarisability and Hyperpolarizability are also calculated.

Review of Literature

The most common name of Imipramine is known as Melipramine, G-22355. The title molecule shows important applications as synthons of numerous natural and semi-synthetic pharmacological agents like β-lactams [2]. The pharmacological title molecule has used as anti HIV agent [3], antimutagenic [4], anticancer [5], anti- inflammatory [6], analgesic [7], antibiotic [8] activity. In present communications geometry of title molecule is fully optimized by using combination of DFT/B3LYP method and 6-311G(d,p) basis set. The UV spectra of title molecule are obtained by using TDDFT method by using same level theory which gave important aspect about optical electron. The chemical property of title molecule is calculated with help of frontier molecular orbitals. The title molecule shows antisymmetric aromatic structure so behaves as good NLO agents.The self-organized dynamic geometry of the liquid crystal (LC) equipments has immense probability for useful molecular systems [9]. From last few decades after growing fast computational technique the liquid crystalline characteristics simulation, modeling has been done by using quantum chemical properties. The HOMO,LUMO,MESP dipole moment mean polarizability anisotropic polarizability as well as hyperpolarizability molecular reactivity, charge transfer, interactions, parameters are used to determine its electro-optical properties of any arrangements.[10-12] The NLO active utensils having significant in file photosensitive switching units [13-14] and in nonlinear optics [15]. In ongoing research[16-21] we have fully optimized structure of the molecule namely, imipramine using DFT method and basis set B3LYP/6-311G (d,p). The UV spectra of title molecule are calculated by TDDFT method by using same level theory. The optical parameters like mean polarizability anisotropic polarizability MR, hyperpolarizability. In our best knowledge no such type study ever else reported .This study provides valuable information to researcher for further work on title molecule.

Computational Details

The geometry of title molecule fully optimized with Gaussian 09 suite [22]of program by using combination DFT/B3LYP[23-24] method and 6-311G (d,p) basis set without any symmetry constrain. The HOMO LUMO, MESP contour is plotted with help of Gauss View 5.0 program package.[25] The UV spectra of title molecule are studied by using time dependent theory by using same level theory. The NLO property of title molecule is calculated by using same level theory.

Results and Discussion

The geometry of title molecule (fig-1) by using combination of DFT/B3LYP method and 6-311G(d,p) basis Set.The optimized geometry is unsymmetrical so C1 symmetry having energy -2321a.u. the animated gauss view shows that title molecule

having contains three three rings fused together with a side chain of dimethylamino group. The calculated bond angle bond lengths of title molecule are listed in table-1.

Electronic properties and UV spectra

The highest occupied molecular orbital HOMO and lowest unoccupied molecular orbital LUMO are frontier molecular orbitals plays important role to determine chemical reactivity of molecule. The HOMO LUMO energy gap is indirectly varies as chemical reactivity.[26] A lower energy gap means more polarization and vice versa. The higher gap means lower chemical reactivity and vice versa. The calculated energy gap of title molecule shows that molecule is less chemically reactive. The HOMO and LUMO of title molecule is lying at -0.2154 a.u. and -0.0765 a.u. respectively. The HOMO LUMO plot of title molecule is shown in fig-2. The both HOMO LUMO are distributed over whole molecule except dimethylamino group. The HOMO LUMO of title molecule are p orbitals however nodes in HOMOs and LUMOs are located almost symmetrically.

The molecular electrostatic potential is important device to appreciate the location for the electrophilic and nucleophilic hit in a molecule. The MESP concurrently present molecular shape, size and electrostatic potential value. The MESP drawing is especially helpful in the examination of the molecular geometry with its physicochemical property relationships [27-34]. The strength of electrostatic potential inMESP is presented by various colours e.g. most red colour represents electronegative regions ,blue colour shows electropositive region Green colour stand for neutral potential region. The MESP shown in Figure 3. The surface map demonstrate obviously one negative potential regions by N ofdimethylamino group.

Time dependent density functional theory (TD–DFT) method is significant instrument for studying the nature of the transitions of UV–Vis spectrum (Fig-4) of the title compound .The calculated high oscillatory strength of electronic transitions are of are listed in Table-3 .

TD–DFT calculations display sharp peak at 175nm 174nm which originate mainly due to H-2→L+3(14%),H→L(33%),**H-1→L+1(13%)**andH-2→L+2(15%),H-1→L+3(17%), H→L+3(33%)transitions respectively.

NLO properties

Electric moments such as dipole moment, polarizability and first order hyperpolarizability have been calculated at DFT-B3LYP/6-311++G(d,p) level for the prediction of non linear optical behavior of the title molecule under examine.The optical parameter e.g dipole moment μ, mean polarizability<α> and first static hyperpolarizability β are calculated by using same level theory. The [35], the total dipole moment and the mean polarizability in a Cartesian frame is defined by

$\mu = (\mu_x^2 + \mu_y^2 + \mu_z^2)^{1/2}$

$<\alpha> = 1/3 [\alpha_{xx} + \alpha_{yy} + \alpha_{zz}]$

The total intrinsic hyperpolarizability β_{TOTAL} [36] is defined as

$\beta_{TOTAL} = [\beta_x^2 + \beta_y^2 + \beta_z^2]^{1/2}$; where $\beta_x = \beta_{xxx} + \beta_{xyy} + \beta_{xzz}$, $\beta_y = \beta_{yyy} + \beta_{yzz} + \beta_{yxx}$, $\beta_z = \beta_{zzz} + \beta_{zxx} + \beta_{zyy}$.

$\Delta\alpha = [\ ]^{1/2}$

The molar refractive index are calculated by [37-39]

MR= [ ]( )= 1.33απN

Non linear optics explain the performance of light in nonlinear media Nonlinear optical (NLO) belongings happen from the exchanges of electromagnetic fields in different media to give way new fields adjust in wavenumber. The mean polarizability and hyperpolarizability are extremely valuable standard for calculating the non linear optical actions of title molecule. All calculated optical parameter like mean polarizability, anisotropic polarizability, order parameters, molar refractivity, hyperpolarizability are listed in table- . The calculated hyperpolarizability of title molecule is11.8767×10^{-30}esu which is nearly 61 times of β_{total} of urea (0.1947×10^{-30}e.s.u).The title molecule is good NLO agent in future.

Conclusion

In this paper geometry optimization NLO property of title molecule has been done by combination of DFT/B3LYP method and 6-311G (d,p) basis set. The calculated hyperpolarizability of title molecule is nearly 61 times greater than hyperpolarizability of urea. The moment of π electron is responsible for polarization in title molecule which causes its high polarizability. The calculated HOMO-LUMO gap indicates that title molecule is less chemically reactive. The MESP plot shows that N n dimethyl amine group is most electronegative site of title molecule. The UV spectra show that prominent peak occurs at 175 nm.

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Table 1. Selected bond lengths (angstroms), bond angles (degrees) calculated at the B3LYP/6-311G (d, p) level, IMPRA MINE

Parameter	Calculated	Parameter	Calculated	
C1-C2	1.524		C2-C1-C3	117.9
C1-C3 1.535			C2-C1-H22	108.1
C1-H22 1.097			C3-C1-H22	108.0
C1-H23 1.096			H22-C1-H23	105.8
C2-C4 1.415			C1-C2-C4	126.3
C2-C5 1.401			C1-C2-C5	115.6
C3-C10	1.503		C1-C3-C10	111.9
C3-H24	1.094		C10-C3-H24	109.8
C3-H25	1.095		H24-C3-H25	107.4
C4-N6	1.426		C2-C4-N6	122.6
C4-C7	1.408		N6-C4-C7	118.9
C5-C14	1.389		C2-C5-C14	123.0
C5-H26	1.086		C2-C5-H26	117.9
N6-C8	1.431		C4-N6-C8	118.2
N6-C9	1.467		C8-N6-C9	117.3
C7-C13	1.389		C4-C7-H27	119.4
C7-H27	1.082		N6-C8-C10	118.6
C8-C10	1.403		C10-C8-C11	119.8
C8-C11	1.399		N6-C9-C17	112.7
C9-C17	1.533		N6-C9-H28	112.6
C9-H28	1.102		C17-C9-H28	109.6
C9-H29	1.092		C3-C10-C8	118.5
C10-C12	1.396		C8-C11-C16	120.5
C11-C16	1.393	C8-C11-H30	119.9	
C11-H30	1.084	C10-C12-H31	119.1	
C12-C15	1.393	C15-C12-H31	119.8	
C12-H31	1.086	C5-C14-H33	120.4	
C13-C14	1.391	C12-C15-H34	120.1	
C13-H32	1.085	C11-C16-C15	120.0	
C14-H33	1.084	C9-C17-C18	110.9	
C15-C16	1.393	C9-C17-H36	110.9	
C15-H34	1.084	C18-C17-H36	108.7	
C16-H35	1.084	H36-C17-H37	107.3	
C17-C18	1.532	C17-C18-N19	113.8	
C17-H36	1.093	C17-C18-H38	108.7	
C18-N19	1.463	N19-C18-H38	107.0	
C18-H38	1.095	C18-N19-C20	111.2	
C18-H39	1.109	C18-N19-C21	112.9	
N19-C20	1.457	N19-C20-H40	109.9	
N19-C21	1.458	H40-C20-H42	108.1	
C20-H40	1.093	N19-C21-H43	110.7	
C20-H42	1.107	H44-C21-H45	108.0	
C21-H43	1.091			

Table-2
The calculated electronic transitions: *E* (eV), oscillatory strength (*f*), *λ*max(nm) using TD–DFT/B3LYP/6–311G(d,p)

S. N.	Electronic transitions	E (eV)	Oscillatory strength (*f*)	Calculated(λ max)	% contribution	Assignment
1	H-2→L+3 H→L **H-1→L+1**	7.07	0.101	175	14% 33% 13%	$n_p \rightarrow n^*_p$
2	H-2→L+2 H-1→L+3 H→L+3	7.13	0.060	174	15% 17% 33%	$n_p \rightarrow \pi^*$

3	H-3→L+1 H-1→L H-1→L+2	7.25	0.007	171	38% 21% 15%	$n_p \rightarrow \sigma^*$

Table-3
Polarizability and Hyperpolarizability of title molecule

S.NO.	PARAMETER	POLARIZABILITY
1.	α_{XX}	126.1245
2.	α_{YY}	126.2536
3.	α_{ZZ}	124.5006
4.	α_{XY}	3.7274
5.	α_{XZ}	2.2809
6.	α_{YZ}	-0.4862
α_{total}		125.6262

S.NO.	Parameter	Hyper Polarizability
1.	β_{XXX}	246.6415
2.	β_{YYY}	152.8932
3.	β_{ZZZ}	71.445
4.	β_{XYY}	17.7618
5.	β_{XXY}	5.977
6.	β_{XXZ}	-15.3954
7.	β_{XZZ}	-3.4028
8.	β_{YZZ}	1.4464
9.	β_{YYZ}	-1.6516
10.	β_{XYZ}	1.4176
β_{total}		11.8767×10^{-30} esu
$\alpha_{anisotropic}$		81.6543
MR		46.993
$\Delta\alpha$		0.1291

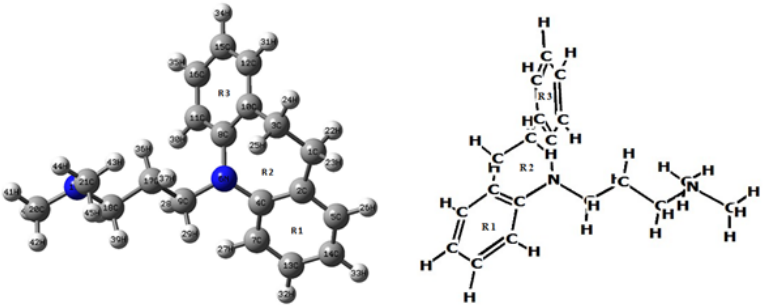

Figure 1. Molecular structure of IMIPRAMINE optimized at B3LYP/6-311G (d, p) level.

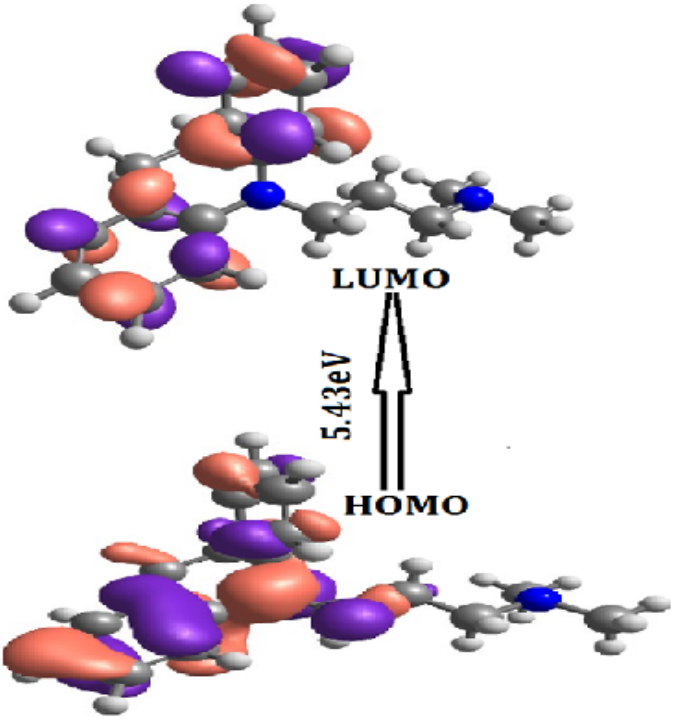

Figure 2 HOMO and LUMO surfaces of IMIPRAMINE.

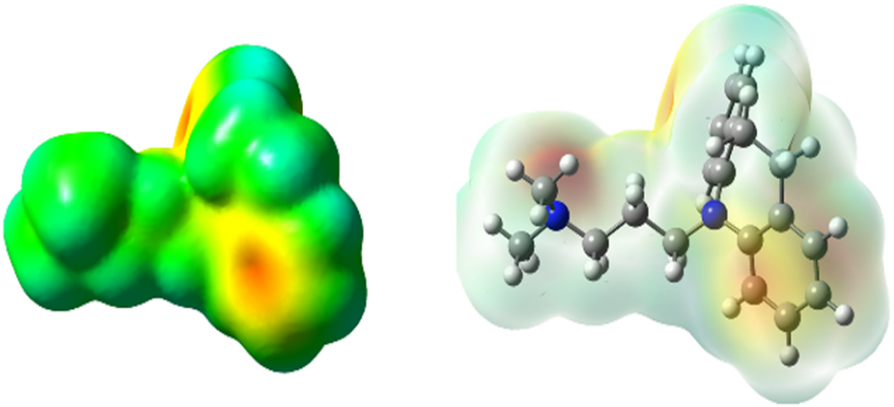

Figure 3. MESP surfaces of IMIPRAMINE

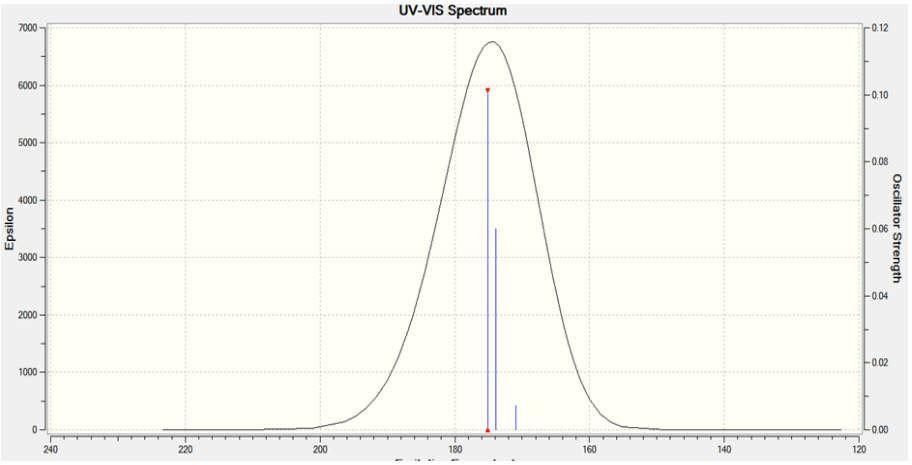

Fig-4 UV spectra of Imipramine