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QUANTUM CHEMICAL COMPUTATIONS ON 2-[2-ETHYLAMINOTHIAZOL-5-OYL]-N-METHYL-6-CHLOROBENZIMIDAZOLE

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ABSTRACT

Quantum chemical parameters molecular geometry, vibrational frequencies and bonding features were calculated for the molecule 2-[2-ethylaminothiazol-5-oyl]-N-methyl-6-chlorobenzimidazole. The computed geometrical parameters are in close agreement with the experimental data. Charge transfer taking place within the molecule can be carried out using FMO analysis. Besides HOMO-LUMO and Mulliken atomic charges have been computed using DFT calculations.

KEYWORDS

Vibrational Frequency, DFT, Bond length, Bond angle, Gaussian and Molecular geometry.

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INTRODUCTON

Heterocyclic compounds have played a major role in pharmaceutical chemistry due to their biological activities. The syntheses of various heterocyclic compounds are known for their anti-infective, anti-bacterial and antifungal activities[1]. The compounds containing thiazole ring have shown useful biological properties and have been developed as fungicides, herbicides or plant growth regulators[2]. Various synthetic methods have been reported so far, such as refluxing in an organic solvent, the solvent free solid-phase reaction, ultra-sonication and microwave radiation[3]. Several substituted benzimidazole have been identified as potent authelmintic drugs[4]. Here we reported the complete

description of the molecular geometry and molecular vibrational assignment of 2-[2-ethylaminothiazole-5-oyl]-N-methyl-6-chlorobenzimidazole. The optimized geometry of the vibrational frequencies was calculated at DFT/B3LYP level of theory using the 6-31G basis set[5].

EXPERIMENTAL METHODS

AR grade solvents and reagents are used. All the chemicals were purchased from Sigma-Aldrich, Merck Specialities Pvt. Ltd. and Himedia Laboratories Pvt. Ltd. The compound 2-[2-ethylaminothiazol-5-oyl]-N-methyl-6-chlorobenzimidazole was prepared by the following method. A solution of 1-ethyl-3-(N,N-dimethylimidoyl) thiourea (1mmol) in DMF (2ml) was added to a solution of 2-(2-bromoacetyl)-N-methyl-6-chlorobenzimidazole (0.254g, 1mmol) which was prepared from 2-(1-hydroxyethyl)-6-chlorobenzimidazole in DMF (2ml). The reaction mixture was stirred well and triethylamine (0.15ml, 1mmol) was added. The reaction mixture was heated at 80-85^{o}C for 5 minutes. After cooling the mixture was poured into cold water and stirred constantly. The yellow precipitate thus obtained was filtered, washed with water and dried. The crude product was crystallized from ethanol-water (2:1) to give yellow crystalline solid.

RESULTS AND DISCUSSION

Optimized Geometry

The optimized geometry of 2-[2-ethylaminothiazol-5-oyl]-N-methyl-6-chlorobenzimidazole was obtained by DFT/6-31G/B3LYP level. The molecular structure along with the numbering of atoms is shown in figure.

Mulliken Analysis

The atomic charge in a molecule is fundamental to chemistry. For instance atomic charge has been used to describe the process of electro-negativity equalization and charge transfer in chemical reactions[6].

HOMO-LUMO energy gap

The HOMO-LUMO energy gap of a molecule will play an important role in determining its bioactive properties. The total energy, HOMO-LUMO energy, energy gap and dipole moment have influence on the stability of a molecule. The HOMO energy characterizes the electron donating ability and LUMO energy characterizes the electron accepting ability and the gap between HOMO and LUMO characterizes the chemical stability of the molecule. Moreover lowering the HOMO-LUMO energy gap explains the eventual charges transfer interactions taking place within the molecular.

Table No.1: Bond length data (*Å*) of 2-[2-ethylaminothiazol-5-oyl]-N-methyl-6-chlorobenzimidazole

S.No	Atoms	Bond Length
1	C2-C1	1.422
2	C3-C2	1.4026
3	C4-C3	1.3869
4	C5-C4	1.4103
5	C6-C5	1.3907
6	C7-C1	2.1746
7	H8-C3	1.0821
8	H9-C5	1.0825
9	H10-C6	1.0834
10	N11-C7	1.3360
11	C12-C2	2.5371
12	H13-C12	1.0909
13	H14-C12	1.0898
14	H15-C12	1.0903
15	N16-C2	1.3890
16	C17-C7	1.4778
17	O18-C17	1.2659
18	C19-C17	1.4408
19	C20-C19	1.3794
20	S21-C19	1.8380
21	H22-C20	1.0798
22	C23-S21	1.8333
23	N24-C23	1.3284
24	N25-C23	1.3488
25	H26-N25	1.0084
26	C27-N25	1.4750
27	H28-C27	1.0951
28	H29-C27	1.0929
29	C30-C27	1.5340
30	H31-C30	1.0961
31	H32-C30	1.0938
32	H33-C30	1.0958
33	Cl34-C4	1.8291

Table No.2: Bond angle data (*Å*) of 2-[2-ethylaminothiazol-5-oyl]-N-methyl-6-chlorobenzimidazole

S.No	Atoms	Bond Angle
1	C3-C2-C1	121.8398
2	C4-C3-C2	115.7284
3	C5-C4-C3	123.9079
4	C6-C5-C4	119.7468
5	C7-C1-C6	161.10566
6	H8-C3-C2	123.2357
7	H9-C5-C4	119.4239
8	H10-C6-C5	121.3832
9	N11-C7-C1	37.8636
10	C12-C2-C1	134.2301
11	H13-C12-C2	81.6032
12	H14-C12-C2	122.1417
13	H15-C12-C2	121.2306
14	N16-C2-C1	105.9805
15	C17-C7-C1	163.244
16	O18-C17-C7	119.3048
17	C19-C17-C7	119.6929
18	C20-C19-C17	133.4163
19	S21-C19-C17	117.1759
20	H22-C20-C19	122.3639
21	C23-S21-C19	86.2143
22	N24-C23-S21	114.8140
23	N25-C23-S21	121.4699
24	H26-N25-C23	118.9097
25	C27-N25-C23	122.3229
26	H28-C27-N25	107.0141
27	H29-C27-N25	107.3026
28	C30-C27-N25	113.0454
29	H31-C30-C27	110.0964
30	H32-C30-C27	110.1577
31	H33-C30-C27	111.3201
32	Cl34-C4-C3	118.1683

Table No.3: Dihedral angle data (*Å*) of 2-[2-ethylaminothiazol-5-oyl]-N-methyl-6-chlorobenzimidazole

S.No	Atoms	Dihedral Angle
1	C4-C3-C2-C1	-0.03179
2	C5-C4-C3-C2	0.01108
3	C6-C5-C4-C3	0.01489
4	C7-C1-C6-C5	-179.8281
5	H8-C3-C2-C1	179.9635
6	H9-C5-C4-C3	-179.9960
7	H10-C6-C5-C4	179.9856
8	N11-C7-C1-C6	-0.16930
9	C12-C2-C1-N11	0.03044
10	H13-C12-C2-C1	178.9292
11	H14-C12-C2-C1	70.7575
12	H15-C12-C2-C1	-72.9909
13	N16-C2-C1-N11	0.03210
14	C17-C7-C1-N11	0.07160
15	O18-C17-C7-C1	179.8101
16	C19-C17-C7-C1	-0.2143
17	C20-C19-C17-C7	-0.09440
18	S21-C19-C17-C7	179.9197
19	H22-C20-C19-C17	0.011100
20	C23-S21-C19-C17	-179.9591
21	N24-C23-S21-C19	0.10226
22	N25-C23-S21-C19	-179.3014
23	H26-N25-C23-S21	-3.4056
24	C27-N25-C23-S21	-179.4071
25	H28-C27-N25-C23	-153.7459
26	H29-C27-N25-C23	-37.8160
27	C30-C27-N25-C23	83.8169
28	H31-C30-C27-N25	179.2315
29	H32-C30-C27-N25	-61.39222
30	H33-C30-C27-N25	59.2590
31	Cl34-C4-C3-C2	-179.99498

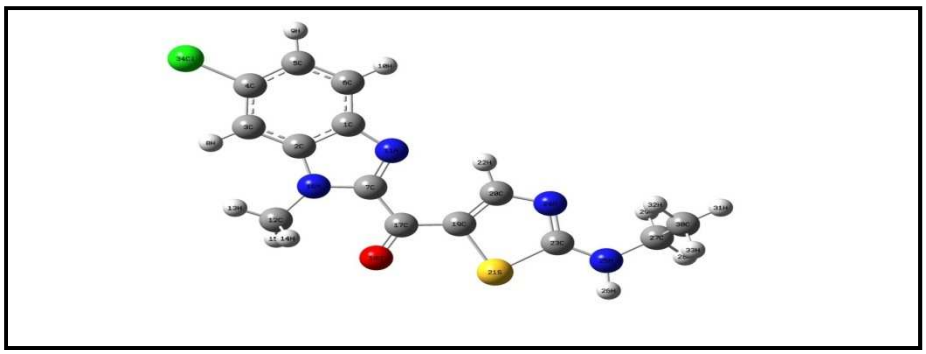
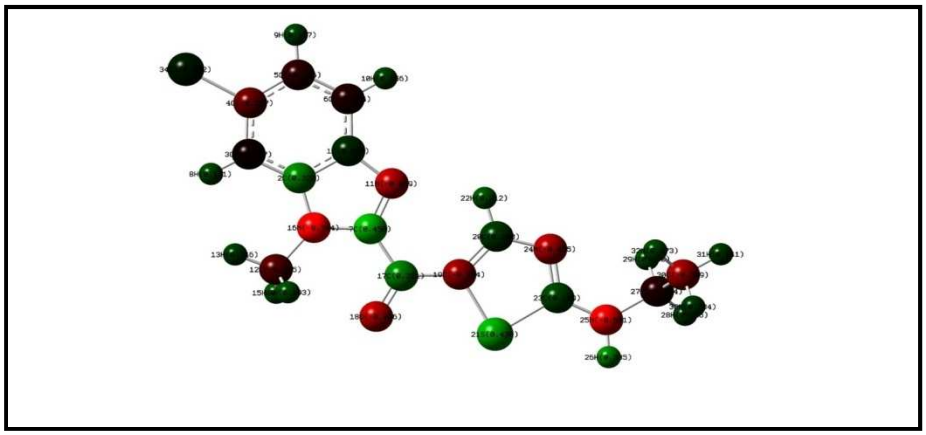


Figure No.1: Optimized structure of 2-[2-ethylaminothiazol-5-oyl]-N-methyl-6-chlorobenzimidazole



CONCLUSION

The geometry of 2-[2-ethylaminothiazol-5-oyl]-N-methyl-6-chlorobenzimidazole was optimized in different levels with DFT-B3LYP method using 6-31G. The complete molecular structural parameters of the optimized geometry of the compound have been obtained from *ab initio* and DFT calculations.

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CONFLICT OF INTEREST

We declare that we have no conflict of interest.

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