

Synthesis, Spectral analysis and Computational Studies of Novel S-benzyl-β-N-(5-bromo-2-hydroxy-3methoxyphenylmethylene)dithiocarbazate Schiff base

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Abstract

Schiff bases or azomethenes are most valuable group of biomolecules, there novel synthesized dithiocabazate derivatives have been found to reveal both remarkable biological activities and other variety of valuable applications. A hard-soft nitrogen-sulphur containing Novel Schiff base derived from 5-bromo,2-hydroxy-3-methoxy benzaldehyde and S-benzyl dithiocarbazate was prepared by condensation method from their equivalent molar amounts. The structure of prepared compounds was investigated by UV-Vis, FT-IR, ¹H-NMR and the thermal stability of the Schiff base was obtained upto 800 ⁰c in inert nitrogen atmosphere. Theoretical calculations geometry optimization, UV-Vis, FT-IR, ¹H-NMR & MESP were performed by DFT method at DFT/B3LYP basis set for comparable conformity with experimental results, simultaneously theoretical investigations like Mulliken atomic charges & dipole moment has been accomplished by two different theoretical methods i,e Semi-empirical AM1, PM3, PM6, and DFT/B3LYP Quantum chemical methods for the crosscheck of the results obtained from required quantum chemicals methods.

Key Word: Schiff base, DFT, MESP, Dithiocarbazate, DFT/B3LYP.

Introduction

Synthesis and investigation of metal-complexes from certain types of N-S containing Schiff base ligands. They have been prepared by dithiocarbazic acid (NH2NHCSSH) and its derivatives ie. S-methyl/benzyl [1] which acts as donor atoms [2]. They have been synthesized, investigated and used to prepare new coordination and organometallic Compounds over past few decades.[3] N–S containing ligands and their transition metal complexes are subject of current research interest is the emerging area of research in inorganic, bioinorganic and pharmaceutical chemistry [4-5].Dithiocarbazic acid and their Schiff bases are potential multidentate ligands containing four donor atoms that derived from reaction of Dithiocarbazates with carbonyls whose properties can be modified by inserting different organic substituent's inducing different stereo-chemistry and specific condition[6-8]. Computer simulation to assist to the solution of interesting chemical problems. It has become a useful tool to design and investigate of new materials that are difficult to search or too expensive to purchase. it can give a useful information and deep understanding of the properties of molecules into chemistry by, semi-empirical method (AM1, PM3 & PM6) and Density functional theory. Computational chemistry theory and computer programs are generally based on the quantum mechanisms that provides the physical properties of atoms and subatomic particles. Density functional

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theory has been a popular method since 1970s that is available in molecules, particular atoms and the condensedmater of computational chemistry. In which selected molecules for analyzing the theoretical studies are firstly constructed in mol files as a molecular model by Gauss View 5.08, then all constructed molecular structures are optimized by minimizing electron-electron repulsion by Gaussian 9.0 using D01 version (Gaussian 09, Revision A02, Inc., Wallingford, CT, 2016, USA) [9] at B3LYP that described in 1988 as correlation energy formula which expressed as function of electron density [10] polarization type Gaussian basis set /6-311++G (d, p) which developed by optimizing exponents for heavy atoms and hydrogen respectively and self- consistent molecular orbital methods/LanL2DZ [11].The Mulliken (Electronic population analysis) [12] Frontier molecular orbitals (FMOs) are used for analysis of chemical reactivity for selected compounds to demonstrating the number of active sites that also played an important role in study of kinetic stability as well as determination of Dipole moment.[13] DFT based electronic structure calculations have been predicted by fast computational methods.[14]

2.Reaction and Mechanism

S-benzyldithiocarbazate was synthesized in the following sequence of the reactions. Potassium salt of dithiocarbazic acid in fig. (1), benzylation of potassium salt of dithiocarbazic acid by benzyl chloride. fig. (2) Synthesis of Schiff Base by Condensation of carbonyl compound 5-bromo-2-hydroxy-3-meyhoxy benzaldehyde with S-benzyl dithiocabazate. Fig. (3)



Fig.(3)

3. Experimental

3.1 Materials

Hydrazine hydrate (NH2NH2.H2O) 80%, molecular weight 50.06 g/mole, weight per ml volume is 1.02 g. Potassium hydroxide (KOH) in solid pellets that molecular weight 56.11 gram per mole, Carbon di sulphide (CS2) 99%, molar mass; 76.139 g/mole, density; weight per ml volume is 1.26g, and absolute ethanol 99.9%. Benzyl chloride (C₇H₇Cl) 99%, molar mass; 126.58 g/mole, its density is similar to water and 5-Bromo 2-hydroxy-3-methoxy benzaldehyde. The solvents were purified, distilled and dried by standard procedures of conventional methods. Commercial reagents which have used in overall synthesis and condensation reactions were applied without any supplementary purification.

Synthesis of Schiff base ligand

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Synthesis of ligand molecules involves two steps:

3.2.1 Synthesis of S-benzyl dithiocarbazate.

Potassium hydroxide (11.4g, 0.2 mole) in solid pellets was completely dissolved in 70 ml alcohol-water mixture which was prepared at a time as 9:1 alcohol-water mixture and cooled this solution on ice bath for five minutes. To the cooled solution hydrazine hydrate 80% (10.01g) which was in liquid state, added slowly in the KOH solution with constant stirring. A solution of carbon disulphide 99% (15.2g, 0.2 mole), molar mass; 76.139 g/ mole, density 1.26g /ml was then added drop wise from dropping funnel with constant stirring over a period of one hour. The temperature of the mixture was kept below 5°C. After one hour two layers were formed. The light yellow oily (lower) layer was then separated using a separating funnel and dissolved in previously cooled 40% ethanol (60 ml). The mixture was kept in again on ice bath and benzyl chloride (25.3g ,0.2 mole) (C7H7Cl) 99%, molar mass; 126.58 g / mole (density 1.0 g/ml) was added slowly with vigorous mechanical stirring. After this, the mixture was stirred for further 15 min. The white product which formed was filtered off, washed with cold water and then dried in open atmosphere. The crude product was recrystallized by absolute ethanol and dried in vacuum desiccator over anhydrous CaCl2. Yield, 52% and melting point 124°C were recorded

3.2.2 Synthesis of Schiff base from S-benzyl dithiocarbazate.

S-benzyldithiocarbazate (1.220 g; 0.01 mol) was dissolved in absolute ethanol (12ml) and heating with constant stirring and added with the alcoholic solution of 5-bromo-2-hydroxy-3-methoxy benzaldehyde (4.11 g; 0.01 mol) in the same solvent (12 ml) in 1:1 molar ratio. The resultant solution becomes colored. The mixture was heated on a water bath under reflux for 23 minutes. When crystals started appearing. Then refluxing was stopped and the reaction mixture was allowed to stand overnight at room temperature. Whereupon the colored crystals that had formed were filtered off and purified by recrystallisation from ethanol and dried in vacuum over anhydrous CaCl2 in a desiccator. Colour; Yellow, Yield; 49%, m.p. 198 0C. Anal. Found; C, 45.73%; H, 3.12%; N, 5.93%; S, 14.83%; O, 7.18%. Br, 18.75%; Calc. for C16H15N2S2O2Br (Mol. wt. 411): C, 46.71%; H, 3.65%; N, 6.82%; S, 15.57%; O, 7.78%; Br, 19.46%;

4. Physical Measurements

The electronic spectra of Schiff base were measured by means of a Double Beam UV–VIS spectrophotometer of Labtronics Model LT-2203 between λ max 200 and 800 nm using 10-5 M solution in DMSO were used as reference solvent. IR spectra (4000–400 cm-1) were recorded as KBr pellet using a FTIR-105627 Perkin-Elmer spectrometer. Themo gravimetric analysis (TGA) of samples were measured weight changes as the function of temperature using TGA-50 SHIMADZU-00652 instrument under nitrogen atmosphere at constant heating rate of 100C/min., Melting points were determined on a LABTRONICS model LT-110 Digital Automatic Melting Point Apparatus in an open capillary and the elemental analysis were performed by EURO EA Elemental analyzer.

4.1. Optical Spectra analysis

The prepared Schiff base obtained by thermal heating of the alcoholic solution of 5-bromo-2-hydroxy-3-methoxy benzaldehyde with S-methyl dithiocarbazate precursor which shown in Fig:4.



4.2 FT-IR Spectral analysis

FT-IR spectra (4000–400 cm-1) of Schiff base were obtained from FTIR-105627 PerkinElmer spectrophotometer, alkali halide KBr pellet using as transparent sheet in infrared region which present in table:1 shown FT-IR in Fig:5

S.NO.	FT-IR Bands (cm-1)	Assignments
1.	<mark>3</mark> 115	O–H stretching vibrations
2.	2935	N–H stretching vibrations
3.	2895	C–H stretching vibration
4.	1614	C=N stretching vibrations.
5.	1567	N–N stretching vibrations
6.	1468	C–N stretching vibrations
7.	1307	C=S stretching vibrations
8.	1246	N-C-S stretching vibrations
9.	1024	C-S-C stretching vibrations
10.	953	C–Br stretching vibration

Table: 1 FT-IR	Spectral	bands of	of Schiff	base



4.3. Thermo gravimetric analysis

Measurement of thermal gravimetric analysis (TGA) of Schiff base was observed from an analytical technique, performed by TGA-50 SHIMADZU-00652 instrument and the fraction of component is monitored by mass loss that occurs due to constant heating of the sample at rate of 100C/min under nitrogen atmosphere shown in Fig: 6



Fig: 6 TGA Curve of Schiff base

5. Computational Studies

Semi-empirical techniques are based on the formalism of Hartree-Fock which make many approximations from empirical data for treating large molecules. These methods exist for the calculations are much faster than the results of their ab-initio counterpart..these methods can be classified into several groups such as AM1, PM3. PM6 and PDDG. Where These Methods was required much less CPU Time as well as less accuracy can be expected than DFT calculations. and their results can be expected as similar to the DFT results. It is a modified generalization through the addition of repulsive Gaussian functions

© 2023 IJNRD | Volume 8, Issue 1 January 2023 | ISSN: 2456-4184 | IJNRD.ORG 5.1. Geometry Optimization by B3LYP/ 6-311G ++ (d, p) Methods.

Geometry optimizations are done by starting with an input structure that is believed to resemble the desired stationary point and submitting this plausible structure to a computer algorithm that systematically changes the geometry until it has found a stationary point. Dithiocarbazate Schiff base have been optimized in ground state by RB3LYP (Becke-3-Lee-Yang-Parr) /6-311++G (d, p) and /LanL2DZ basis sets. The average geometrical parameters such as bond lengths, bond angles and dihedral angles have been presented in Table 2. It is obvious that if dihedral angles associated with 4-adajacently bonded atoms are around equal to 00 or 1800, it concludes that associated atoms lie nearly in similar plane, thus no. of planes in the compound can be predicted.

5.1.1. Optimized Molecular Structure of Schiff base calculated by B3LYP/ 6-311G ++ (d, p) Methods.

A Complete geometrical optimization and optimized molecular structure of Schiff base (Stoichiometry C16H15N2S2O2Br, mol. wt. 411.33). 38 atoms, 208 electrons, has been calculated by DFT / B3LYP / 6-311G++ (d,p) (5D, 7F) method within the symmetry of C1 point group, SCF done E (RB3LYP) = -4249.44564817, A.U. after 15 Cycles, Deg. of freedom 108, 653 basis functions, 1049 primitive Gaussians, 678 Cartesian basic functions, 104 alpha electrons, 104 beta electrons. Dipole moment 1.7008 Debye, Nuclear repulsion Energy = 2440.0790020780 Hartree. Job CPU Time 13 minutes, 37 seconds. shown in Fig.7.



3D Structure of S-benzyl-β-N-[5-bromo-2-hydroxy-3-methoxyphenylmethylene] dithiocarbazate Fig.7 5.1.2:Calculated bond lengths, bond angles and dihedral angles of S-benzyl-β-N-[5-bromo-2-hydroxy-3-methoxyphenylmethylene]dithiocarbazate.

Bond-length (in Å)	Bond-Angle (in	0)	Dihedral Angle (in 0)
C(1)-C(2) 1.35	C1-C2-C3	120	C1-C2-C3-C4 00
C(1) - C(6) 1.54	C2-C1-C6	120	C6-C1-C2-C3 0.00
C(1) - Br(21) 1.893	C2-C3-C4	120	С6-С1-С2-Н24 -179
C(2) - C(3) 1.54	C2-C3-O22	120	Br21-C1-C2-C3 180
C(3) - C(4) 1.35	N8-N9-C10	109.47	Br21-C1-C2-H24 00
C(4) - C(5) 1.54	N8-N9-H27	109.47	C2-C1-C6-C5 -0.00
C(5) - C(6) 1.35	N9 <mark>-C1</mark> 0-S11	120	Br21-C1-C6-C5 179
C(5) - C(7) 1.54	N9-C10-S11	120	Br21-C1-C6-H25 0001
C(7) - N(8) 1.29	N9-C10-S12	120	C1-C2-C3-O22 -179
N(8) - N(9) 1.4	S11-C10-S12	120	C2-C3-C4-C5 00
N(9) - C(10) 1.47	C10-S12-C13	109.47	C2-C3-C4-O20 180
C(10) - S(11) 1.57	S12-C13-C14	109.47	O22-C3-C4-C5 180
S(10) - S(12) 1.78	<mark>S12-C13-H</mark> 28	109.47	С2-С3-О22-Н23 150
S(12) - C(13) 1.78	S12-C13-H29	109.47	С4-С3-О22-Н23 -30
C(13) - C(14) 1.54	H28-C13-H29	109.47	C3-C4-C5-C7 179.99
C(14) - C(15) 1.36	C13-C14-C15	120	O20-C4-C5-C6 179.99
C(15) -C(16) 1.54	C13-C14-H29	120	С3-С4-О20-Н35 150
C(16) - C(17) 1.54	C18- <mark>C19-H3</mark> 4	120	C4-C5-C6-C1 0.0001
C(18) - C(19) 1.36	C4-O <mark>20-H35</mark>	109.47	C7-N8-N9-C10 90
C(4)- O(20) 1.43	C3-O2 <mark>2-C23</mark>	109.47	N8-N9-C10-C11 -90
C(3) - O(22) 1.43	C3-O22-H23	109.47	N8-N9-C10-S12 90
O(22)- (C23) 1.43	O22-C23-H23	109.47	H27-N9-C10-S11 30
C(2)- H(24) 1.07	O22-C23-H37	109.47	H27-N9-C10-S12 -150
N(9)-H (29) 1.00	O22-C23-C38	109.47	С13-С14-С19-Н34 000
C(23)- H(37) 1.57	H36-C23-H37	109.47	C19-C14-C15-H30 -180
O(22)- H(35) 0.96	H36-C23-H37	109.47	C13-C14-C19-C18 -180

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5.2: Comparison of Dipole Moments of Schiff base calculated by and DFT/ B3LYP/ 6-311G ++ (d, p) Methods. Table 3

Ligand	AM1	PM3	PM6	PDDG	DFT/ B3LYP
Ligand	2.4160	1.1463	1.4925	1.2522	1.7008

5.3.. Mulliken atomic charges

Atomic charges are widely used in quantum chemistry. The electronic charges are firstly calculated by R.S. Mulliken in 1833 in the overlap region. later on, this overlap population study was performed by computational AM1, PM3, PM6, PDDG Semi-empirical Methods and DFT/B3LYP methods which processed with 6-311++G (d, p) basis level that can be used to expressed the electronic charges distribution and these values are recorded in Table: 3

3.3.1; Comparison of Mulliken atomic charges of Schiff base calculated by AM1, PM3, PM6, PDDG Semiempirical Methods and DFT/ B3LYP/ 6-311G ++ (d, p) Methods.

Atom	AM1	PM3	PM6	PDDG	DFT/ B3LYP
C1	-0.199485	0.026004	0.041855	-0.181229	-0.138196
C2	0.096961	0.155347	-0.032931	0.062585	0.102796
C3	0.015363	-0.181873	0.213092	0.017041	0.026412
C4	0.128369	0.082749	0.206615	0.128446	0.040962
C5	-0.130775	0.122682	-0.120440	-0.160781	-0.087417
C6	0.08 <mark>5680</mark>	0.082749	0.003148	0.063949	0.078846
C7	0.051243	0.122682	<mark>0</mark> .135164	0.084061	0.087203
N8	-0.086189	-0.178474	<mark>-0</mark> .204798	-0.166707	-0.125453
N9	0.013151	0.270734	0.059890	<mark>0</mark> .234 <mark>4</mark> 46	0.126246
C10	-0.134085	-0.200201	0.288167	- <mark>0.4605</mark> 46	-0.259684
S11	-0 <mark>.191</mark> 567	-0.244276	-0.462388	-0.039771	-0.122026
S12	0.283415	0.112269	0.017535	0.392577	0.099674
C13	0.025295	0.108238	0.067302	-0.028379	0.173492
C14	-0.081967	-0.094820	0.033647	-0.069192	-0.098087
C15	0.015009	0.022414	-0.014742	0.016670	0.083073
C16	0.001893	0.000346	0.019099	0.010088	0.009632
C17	0.011288	0.012083	-0.001644	0.004082	0.018490
C18	0.005718	0.006283	0.019103	0.008297	0.009261
C19	0.039174	0.041907	-0.014747	0.012884	0.033708
O20	0.014393	0.003991	-0.098111	0.004460	-0.024819
Br21	0.063370	0.010162	-0.090531	0.054416	0.027437
O22	-0.208840	-0.183052	-0.345872	-0.138770	-0.177017
C23	0.182107	0.168132	0.281608	0.151375	0.155468

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5.4; Comparison of Job CPU Time of Schiff base calculated by AM1, PM3, PM6, PDDG Semi-empirical Methods and and DFT/ B3LYP/ 6-311G ++ (d, p) Methods, given in Table: 5

Ligand	AM1	PM3	PM6	PDDG	DFT/ B3LYP
Ligand	36 sec.	21 sec.	15 sec.	11 sec.	13 min. 37 sec.
Reze	arch Tl	nrough Ir	novati	DA	

5.5. 1H NMR of Schiff base calculated by B3LYP/ 6-311G ++ (d, p) Methods.

1H-NMR (300 MHz, CDCl3, ppm) δ: 3.85 (s, 3H, OCH3), 4.43 (s, SCH2), 8.74 (s, CH), 8.6 (s, 1H NH), 7.19 - 7.44 (m, 7H-ar), 13.78 (s, OH), shown in Fig:8



Fig.9 1H NMR spectra of Schiff base

6.Results and discussion

6.1Physico-chemical data analysis

The melting point of Schiff bases and their transition metal complexes are shown in 1980C this indicates the synthesized Schiff base compound is thermal stable. The solubility of this Schiff base was appeared in acetone on appearing the characteristic yellow color that indicates the d-d transitions from their ground states to various excited states.

6.2. Electronic spectra analysis

S-benzyl dithiocabazate Schiff base possesses excellent optical properties. Absorption curve first increases from 300 nm to 315 nm which shows the characteristics absorption at 315 nm this peak indicates the λ max of the analyzed Schiff base compounds, then absorption curve gradually decreases to 460 nm and becomes constant towards higher wavelength up to 500 nm.

6.3. Vibrational studies of Schiff base.

Schiff bases synthesized from S- benzyl dithiocarbazate are capable to existing as the thioketo (C=S) form that observed at 1307 cm-1 in FT-IR spectra [15]. and S-H stretching vibration which have not seen at about 2615-2705 cm-1 that indicates the existence of only the thione tautomer in the solid state [16]. the broad band range of IR spectra assigned to v(N-H) at 2935 cm-1 that exhibit the thioketo form of the presently investigated synthesized novel Schiff bases. The broadness of this band is occurred due to possibly hydrogen bonding between hydrogen of aldimine group and sulphur of thione group. The strong band stretching of azomethine (C=N) in Schiff base spectrum appeared at 1614 cm-1 which shown in table 1 of FT-IR spectra of the Schiff base. [17]. The N-N

© 2023 IJNRD | Volume 8, Issue 1 January 2023 | ISSN: 2456-4184 | IJNRD.ORG stretching vibration of Schiff base ligands is assigned at 1567 cm-1. The v(N-C-S) and v(C-S-C) are found in the free ligand at the region of 1246 cm-1 and 1024 cm-1 respectively. the stretching vibration of v(C-Br) of synthesized Schiff base are observed at 953cm-1

6.4. Thermogravimetric analysis

TGA curve of the ligand against temperature from zero to 8000C, that exhibit 68.40% random weight loses. The first estimated weight loss of 40 % is attributed at 195 0C to C1H3S molecule as a gas in the second and third stages of the compound exhibits weight loss of 15 % and 3.4 % decomposition as gases at 240 and 710 ^oC finally residue (ash).

6.5. Geometry Optimization;

Bond length of C=S of dithiocabazate Schiff base is calculated as 1.57 which resembles the 1.64 A of thioketo group.

7. Conclusion

This synthesized novel S-benzyl dithiocarbazate Schiff base has been prepared from precursor SBDTC, by condensation reaction between precursor and carbonyl compounds viz, 5-bromo-2-hydroxy-3-methoxy benzaldehyde in 1:1 molar ratio. They have exhibit different denticity that refers to the donor groups of the ligands to the central metal ion and different basicity that will play a key role in the formation of complexes which will influence the stability and development the properties of the complexes in the coordination chemistry. This synthesized S-substituted Schiff bases was successfully characterized by the physiochemical properties, usual elemental and spectroscopic techniques are presented in this proposed work and found in yellow-coloured solid compounds which are readily soluble in acetone which representing as nonpolymeric structure. Characterization with, UV-Visible, FT-IR and TGA spectroscopic techniques, as well as theoretically Computational semi-empirical AM1,PM3,PM6 and PDDG methods suggests the synthesized species of Schiff base have formed different stoichiometries, The electronic spectra in uv-vis region 200-800 nm of Schiff base provide a number of evidences that the Schiff base are formed for coordination used, the synthesized Schiff base compound is thermal stable and soluble in non-polar solvents which exists in the thicketo (C=S) free state. Theoretical calculations are also supporting that the optimized molecular structure of Schiff base is stable by parameterization of all bond lengths and bond angles.

8. Future perspectives of this work

The aim to attempt new bidentate S-benzyl dithiocarbazate Schiff base ligands and also developed and their utilization as theoretical computational studies were the main purpose of present work. Detail description regarding the synthesis, spectral, thermal characterization and Theoretical studies that predict the chemical properties and various applications in coordination chemistry and to study the potential active site for chelation in transition metal ions with new dithiocarbazate Schiff bases.

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