

Computational study on molecular structure, vibrational and electronic properties of a novel Schiff base: Benzyl2-(4-(bis(2-chloroethyl)benzylidene)hydrazinecarbodithioate

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Abstract

The present study reports a novel Schiff base 'Benzyl2-(4-(bis(2-chloroethyl)amino)benzylidene)hydrazinecarbodithioate' and its characterization by infra red (IR), nuclear magnetic resonance (NMR), mass spectral methods with its density functional theory (DFT) quantum chemical studies. Tautomerism in this molecule was investigated theoretically by semi-empirical methods. The molecular geometry was calculated by DFT methods using split-valence triple-zeta 6311-G(2d,2p) Pople style basis set. The vibrational frequencies were calculated by DFT method at the same basis set level. The molecular parameters such as highest occupied molecular orbital energy, lowest unoccupied molecular orbital energy, frontier molecular orbital energy gap and dipole moment were calculated by DFT methods using 6311-G(2d,2p) basis set. Molecular electrostatic surface potential and electron localization function plots were also presented. The reactive sites in the molecule studied theoretically with electronic structure in sight.

Keywords: DFT; electron localization function; HOMO-LUMO; MESP; quantum chemical calculations.

1. Introduction

The Schiff base compound under study benzy l2-(4-(bis(2-chloroethyl)amino) benzylidene hydrazinecarbodithioate (BCBHC) is a condensation product of S-benzyl ester of dithiocarbazic acid (SBDTC) and 4-(bis(2-chloroethyl) amino)benzaldehyde (BCAB) commonly known as benzaldehyde nitrogen mustard (Figure1). Nitrogen mustards and dithiocarbazic acid derivatives, both the classes are identified to possess pharmacological properties long back (Davis & Larionov, 1964; Pavan *et al.*, 2010).

The benzaldehyde nitrogen mustards and their derivatives are shown to possess anticancer properties (Modi *et al.*, 1970; Popp & Kirsch, 1961; Fu *et al.*, 2014). Chlorambucil, Predinimustine and Melapan are the medicines having phenyl nitrogen mustard moiety in them. Dithiocarbazic acid and its esters have been known for a long time and they have been compounds of interest among researchers due to their promising use as active pharmaceutical ingredient (Pavan *et al.*, 2010; Tarafder *et al.*, 2002). S-benzyl dithiocarbazate (SBDTC) has been reported to have cytotoxic effect using human breast cancer cell line MCF-7 and was found to be a potential anticancer compound (Cheah *et al.*, 2007). A combination of these two pharmacophores in a single molecule is worth to be explored as a promising future candidate in drug design. Due to the pharmacological/ medicinal activity shown by parent compounds (SBDTC and BCAB) of the title compound BCBHC, it is important to investigate and describe its geometry, electronic structure and reactivity. The main goal of the study is to theoretically investigate the structure and reactivity of BCBHC in depth and its characterization by experimental and theoretical methods. To achieve this goal, theoretical calculations were performed to optimize the geometry and to get vibrational frequencies. In the present study the title compound is investigated for molecular and electronic structure along with reactivity aspect.

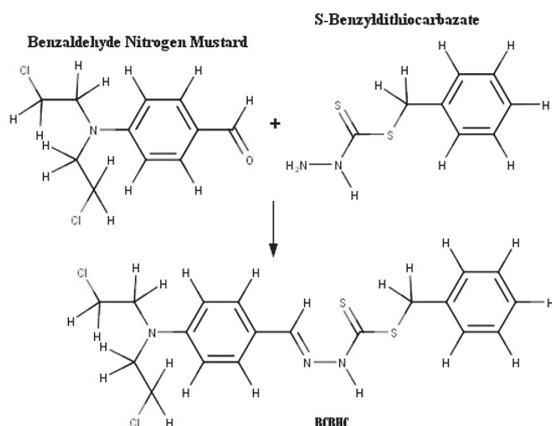


Fig. 1. 2D structural formula sketch of BCBHC

2. Experimental

2.1. Material and Instrumentation

The chemicals were purchased from Sigma-Aldrich, Merck and SRL. They were used in synthesis without any further purification. FAB-mass spectrum was recorded on a JEOL SX 102/DA 6000 mass spectrometer. The FT-IR spectrum was recorded in KBr pellets on Perkin-Elmer RXI FTIR spectrometer in the wave number region of 4000-500 cm^{-1} and ^1H NMR spectrum was recorded on a Bruker Avance DRX 200 FT-NMR spectrometer employing TMS as internal reference and CDCl_3 as a solvent.

2.2. Synthesis of BCBHC

SBDTC was prepared as described in literature (Shanmuga *et al.*, 2000). The ethanolic solutions of S-benzylthiocarbamate and benzaldehyde nitrogen mustard were mixed in 1:1 molar ratio. The mixture was made homogeneous by adding little more ethanol and then refluxed on a water bath for about 1 hour and then allowed to cool overnight. The light yellow coloured solid product obtained was filtered, washed with ethanol several times, dried in air at room temperature and finally stored under reduced pressure in a CaCl_2 desiccator (yield = 70%, MP-145°C). FAB-mass m/z : 426 (M^+ , 100%), 428 (M^{+2} , due to the presence of Cl atoms) and 303 & 305 (due to loss of $-\text{SCH}_2\text{Ph}$ group). ^1H NMR δ (ppm): 1.66 (s, 0.1H, $-\text{N}=\text{C}-\text{SH}$), 3.68-3.71 (d, 4H, $-\text{CH}_2-\text{Cl}$), 3.79-3.82 (d, 4H, $-\text{Ph}-\text{N}-\text{CH}_2-$), 4.60 (s, 2H, $-\text{S}-\text{CH}_2-\text{Ph}$), 6.68-7.65 (m, 10H, aromatic), 7.81 (s, 1H, $-\text{CH}-\text{N}=\text{}$) and 10.40 (s, 0.9H, $-\text{NH}-\text{C}=\text{S}$).

2.3. Computational details

All the calculations were carried out on an Intel Core i7 quad-core 2.4 GHz FUJITSU make workstation having 16 GB RAM and 7200 RPM HDD. Semi-empirical calculations were performed using MOPAC 2012 (Stewart, 2012) and the DFT calculations were performed using ORCA computational chemistry package version 3.0.3 (Neese, 2012) in parallel processing at eight cores on Debian 8.0 LINUX operating system. Avogadro molecule editor and visualizer application version 1.0.3 (Hanwell *et al.*, 2012) was used for drawing the molecule

and for its initial optimization by molecular mechanics method. Input files were written with the help of Gabedit graphical user interface version 2.4.8. First, the molecule was drawn using Avogadro and it was optimized using MMFF94 molecular force field (Halgren, 1996) and the conjugate gradient algorithm at $10\text{e}-7$ convergence. The MM optimized output geometry was optimized further by DFT method at 6311-G(2d,2p) basis set level (Dill, 1975; McLean & Chandler, 1980; Francl *et al.*, 1982; Blaudeau *et al.*, 1997; Krishnan *et al.*, 1980). The DFT/6-311G(2d,2p) optimized geometry was further used as initial geometry for frequencies calculations and other studies of BCBHC. The vibrational frequencies were calculated by DFT method at the same 6311-G(2d,2p) basis set level. B3LYP (20 % HF exchange) functional was used for all the DFT calculations. Gabedit was also used for post-quantum chemical calculation result parsing, properties calculation, visualization and interpretation of the results. The theoretical assignment of the calculated wave numbers was done with vibrational animation utility of Jmol Java molecular viewer and Gabedit.

3. Results and discussion

3.1. Tautomerism

The Schiff bases derived from S-alkyl/aryl dithiocarbamate have a thione group ($\text{C}=\text{S}$) and a proton adjacent to it. The thione group ($\text{C}=\text{S}$) is relatively unstable in monomeric form and it tends to form a more stable C-S single bond by enethiolization, if there is at least one hydrogen atom available adjacent to the thione ($\text{C}=\text{S}$) bond (Mayer, 1967). Exploring relative stabilities of tautomeric forms are important for the molecular structural point of view. The IR spectrum of BCBHC does not show $\nu(\text{S}-\text{H})$ at ca. 2570 cm^{-1} and $\nu(\text{N}-\text{H})$ mode is found present at ca. 3421 and 2900 cm^{-1} . This indicates that thione form predominates in the solid state. However, ^1H -NMR spectrum of BCBHC in CDCl_3 supports that the thione and the thiol tautomeric forms exist in equilibrium in the solutions due to the presence of ^1H -NMR peaks for both the protons $-\text{N}=\text{C}-\text{SH}$ ($\delta = 1.66$) and $-\text{NH}-\text{C}=\text{S}$ ($\delta = 10.41$). The observed fractions of the protons of $-\text{N}=\text{C}-\text{SH}$ and $-\text{NH}-\text{C}=\text{S}$ were found ca. 0.1 and 0.9 respectively.

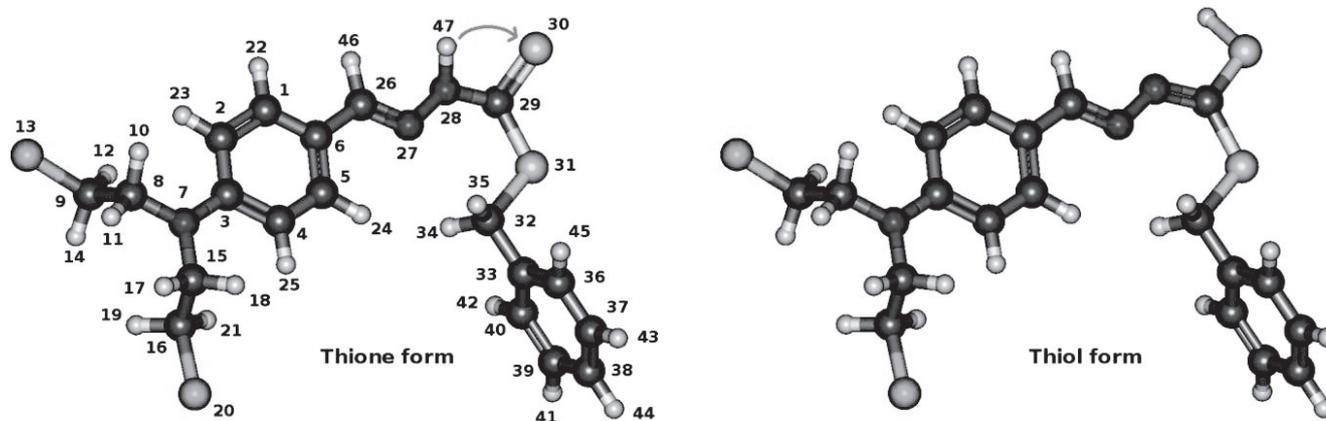


Fig. 2. Structure and atom numbering of BCBHC tautomers

To investigate thione-thiol tautomerism theoretically, the thermal properties of the thione and thiol tautomeric forms of BCBHC were computed by semi-empirical methods. The results of calculation are given in Table

1. All the semi-empirical methods except RM1 method calculated the higher heat of formation for thione form relative to thiol form in gaseous state, which predicts higher thermodynamic stability for thiol form.

Table 1. Thermal properties of BCBHC at 298 K

Method	Thione form				Thiol form			
	HOF	Enthalpy	Heat Capacity	Entropy	HOF	Enthalpy	Heat Capacity	Entropy
MNDO	85.606	15811.2611	91.9150	173.5985	69.196	15937.5506	92.9076	174.6291
AM1	91.932	16611.5854	94.7936	188.6789	86.041	15760.9118	93.5646	171.1818
PM3	109.204	17167.0827	98.8989	190.2707	91.819	16249.8938	97.2065	173.5327
RM1	78.909	17398.1466	99.0239	196.5823	92.351	16244.4690	96.0047	178.8054
PM6	79.222	16259.3643	96.5293	176.7297	73.468	16433.8633	98.1358	175.0414
PM7	77.421	16301.9838	96.0496	175.2376	67.913	16333.1987	96.5750	175.1948

HOF: heat of formation in kcal/mol; enthalpy in kcal/mol; heat capacity in cal/mol; entropy in cal/K/mol

We further investigated the water solvent simulation energetics of BCBHC by semi-empirical methods employing Conductor-like Screening Model (COSMO) as implemented in MOPAC and the results obtained are given in Table 2. The MNDO, AM1 and PM3 calculations predict thiol tautomeric form thermodynamically more favourable, whereas RM1 and PM6 methods predict thione tautomeric form thermodynamically more favourable. AM1 and PM7

method calculations predict the existence of both the tautomers in solutions owing to a little HOF difference between them. The calculated dipole moment values are found relatively higher for thione form, which predicts its higher proportion in polar solvents and it is consistent with NMR observations. The higher theoretical dipole moment values for thione form also confirm its dominance in the solid state as indicated by the IR spectroscopic study.

Table 2. Calculated heat of formation of BCBHC using the COSMO solvent simulation model for water as solvent (dielectric constant 78.39)

Tautomeric form		MNDO	AM1	PM3	RM1	PM6	PM7
Thione	HOF	74.678	75.905	89.962	58.445	48.089	48.500
	μ	5.277	10.263	13.291	12.369	13.157	15.640
Thiol	HOF	60.840	74.957	81.909	67.816	54.995	49.319
	μ	1.489	3.918	4.473	4.664	5.551	6.704
HOF difference		13.838	0.948	8.053	-9.371	-6.906	-0.819

HOF: heat of formation in kcal/mol; μ : dipole moment in Debye

3.2. Optimized Structure

The optimized structural parameters for thione form of BCBHC were calculated by DFT method. The number

labelling of atoms in the title compound is shown in Figure 2. The selected bond lengths and bond angles for BCBHC calculated by ORCA are given in Table 3.

Table 3. Selected bond length values and bond angle values for the thione form of BCBHC obtained by DFT/6-311G(2d,2p) method calculations

Sr.	Bond	Calculated bond length value(A)	Bond angle	Calculated bond angle value(°)
1	C1-C2	1.38360	C1-C2-C3	121.001
2	C2-C3	1.40904	C2-C3-C4	116.952
3	C3-C4	1.41387	C3-C4-C5	121.383
4	C4-C5	1.37930	C4-C5-C6	121.529
5	C5-C6	1.40179	C5-C6-C1	117.214
6	C6-C1	1.39809	C2-C3-N7	121.609
7	C3-N7	1.39071	C4-C3-N7	121.439
8	N7-C8	1.45606	C3-N7-C8	120.861
9	C8-C9	1.52922	N7-C8-C9	112.648
10	C9-Cl13	1.81564	C8-C9-Cl13	110.243
11	N7-C15	1.45649	C3-N7-C15	121.065
12	C15-C16	1.52945	N7-C15-C16	112.648
13	C16-Cl20	1.81575	C15-C16-Cl20	110.218
14	C6-C26	1.45241	C1-C6-C26	119.646
15	C26-N27	1.28410	C5-C6-C26	123.139
16	N27-N28	1.36017	C6-C26-N27	123.179
17	N28-C29	1.35577	C26-N27-N28	115.981
18	C29-S30	1.66672	N27-N28-N29	126.053
19	C29-S31	1.75847	N28-C29-S30	119.649
20	S31-C32	1.86776	N28-C29-S31	123.587
21	C32-C33	1.50297	S30-C29-S31	116.758
22	C33-C36	1.39709	C29-S31-C32	110.821
23	C36-C37	1.38872	S31-C32-C33	107.148
24	C37-C38	1.39156	C32-C33-C36	120.761
25	C38-C39	1.39030	C33-C36-C37	120.659
26	C39-C40	1.39029	C36-C37-C38	120.123
27	C40-C33	1.39612	C37-C38-C39	119.716
28			C38-C39-C40	120.067
29			C39-C40-C33	120.694
30			C40-C33-C32	120.500

3.3. Vibration frequencies

The experimental and the calculated unscaled IR fundamental vibration frequencies for BCBHC by DFT method are given in Table 4. The calculated frequencies are reported unscaled, as no scaling factor is available for

frequency calculation by DFT/6311-G(2d,2p) method. The probable assignments are also given in this table according to reported indications(Coates, 2006; Rao *et al.*, 1964; Gunasekaran *et al.*, 2008). The theoretically

predicted IR spectrum obtained from DFT method does not show any imaginary frequency implying that the optimized geometry is true ground state. Theoretical IR spectra calculated by DFT is shown in Figure 3.

DFT method calculated the vibrational frequencies

higher than the experimental values. The difference in the experimental values and the calculated values of the IR frequencies is due to anharmonic intermolecular interactions, approximation treatment of electron correlation effects and use of the limited basis sets.

Table 4. Selected vibration frequencies for the thione form of BCBHC experimentally obtained and the calculated vibration frequencies by DFT/6311-G (2d,2p) method

Experimental vibration frequencies		Calculated vibration frequencies		
Freq.	Assign.	Freq.	Trans. Str.	Assign.
520.7	N-H oop β	637.20	40.587	N-H oop
644.2	S-C v	651.43	22.940	C29-S31 v
713.6	ring C-H oop β	713.85	39.773	ring C-H w A2u
779.2	C-Cl v	724.76	63.446	C-Cl v
813.9	C-Cl v	735.92	73.387	C-Cl v
		834.70	36.067	ring C-H w A2u
929.6				
1022.2	C=S v	1026.96	179.855	C=S v
1091.6	C=S v	1121.35	127.775	N-N v
1176.5	sec. C-N v	1145.41	50.502	C15-N7-C8 v _a
		1204.56	206.854	ring CH β E1u
		1240.92	36.104	ring CH β E2g
		1283.87	40.720	-CH ₂ w
1253.6	tert. C-N v	1310.53	704.612	-CH ₂ r, C26-H46 β , C28-N29 v
1338.5	Ar C-N v	1323.27	161.876	-CH ₂ r, , C26-H46 β , C28-N29 v
1396.4	C-N v	1350.06	100.984	-CH ₂ r, ring C-C-C v
1423.4	C=S v	1388.03	197.792	C15-H18, C8-H10 oop β
1454.2	-CH ₂ sci.			
1508.2	ring C-C v			
1558.4	N-H β	1525.91	488.295	N-H β
1604.7	C=N v	1639.21	300.620	ring C-C v E2g
1651.0	ring	1656.83	133.380	C=N v
1685.7	ring			
1716.5	ring			
1747.4	ring			
2310.6				
2858.3	H-C-H v _s			
		3179.47	30.504	ring C-H v E1u
3421.5	N-H v			

Freq.: frequency, Assign.: assignment, Trans. Str. (transitional strength) in KM/mol, ring: aromatic ring, v: stretching, r: rocking, w: wagging, β : bending, a: asymmetric, s: symmetric, oop: out of the plane.

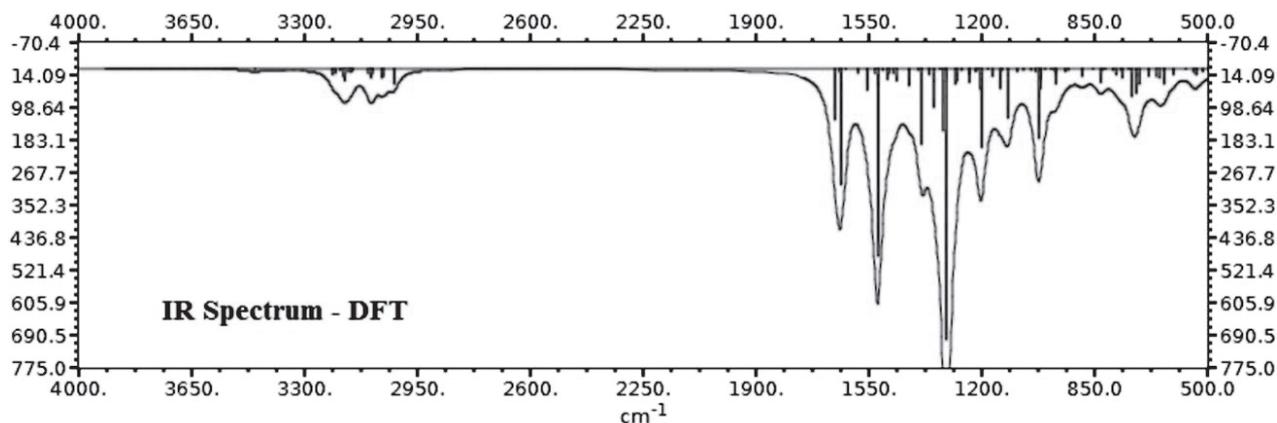


Fig. 3. Theoretical Infra-Red spectrum of BCBHC calculated by DFT/6311-G(2d,2p) method

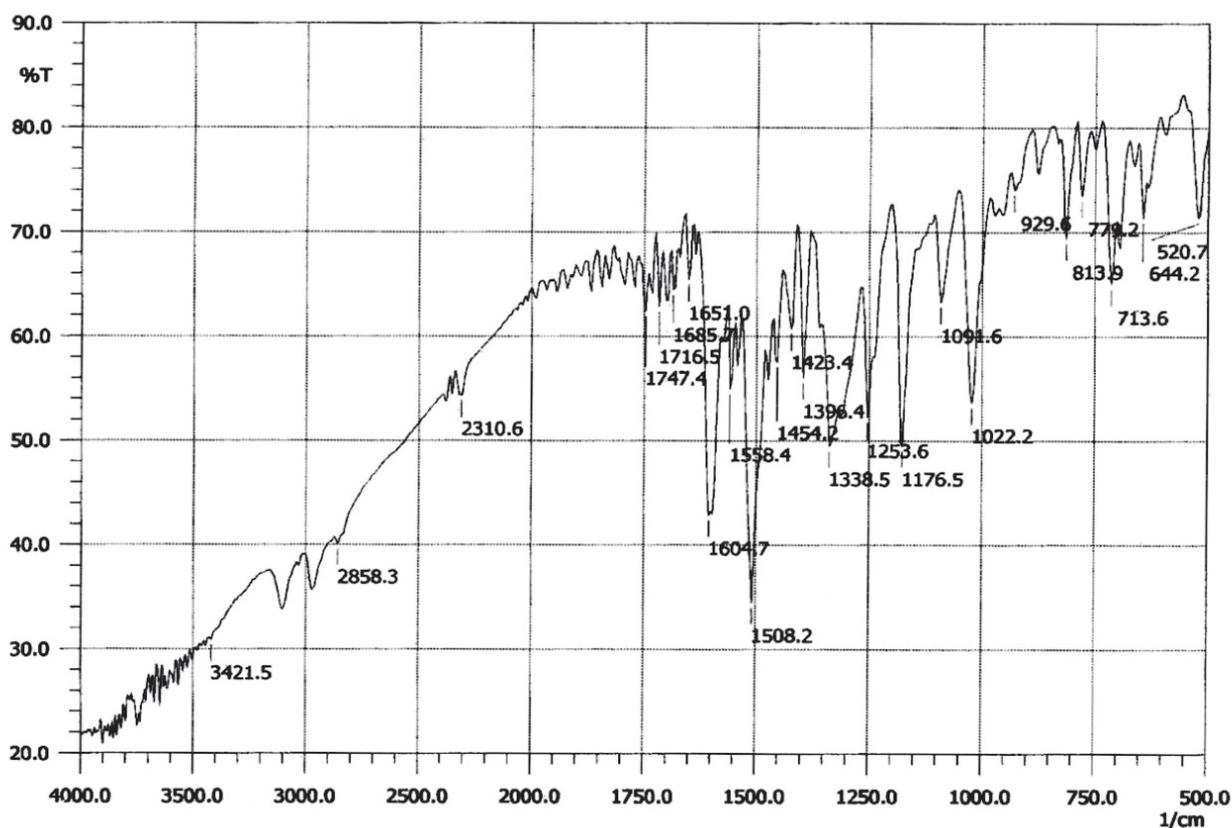


Fig. 4. Scanned copy of the observed vibrational spectrum of BCBHC

3.4. Molecular electrostatic surface potential

Molecular electrostatic surface potential (MESP) is related to electron density and it is a very useful descriptor for determining of sites for electrophilic and nucleophilic attack as well as hydrogen-bonding interactions (Okulik & Jubert, 2005; Scrocco & Tomasi, 1978). Molecular electrostatic potential (MEP), $V(r)$ may be calculated by using the following formula:

$$V(\mathbf{r}) = \sum_A \frac{Z_A}{|\mathbf{R}_A - \mathbf{r}|} - \int \frac{\rho(\mathbf{r}')}{|\mathbf{r}' - \mathbf{r}|} d\mathbf{r}'$$

Where, Z_A is the charge of nucleus A located at \mathbf{R}_A , $\rho(\mathbf{r}')$ is electronic density function of the molecule and \mathbf{r}' is integration variable.

To predict reactive sites for electrophilic and nucleophilic attack for the title molecule, MEP was calculated for DFT/6311-G(2d,2p) optimized geometry by MOLDEN using charge. The presented MEP surface, an overlaying of the electrostatic potential (the attraction or repulsion of a positive charge for a molecule) is valuable for describing the overall molecular distribution as well as for anticipating sites for electrophilic addition. The MESP 3D isosurface plot of BCBHC is shown in Figure 5. The red colour represents negatively charged areas of the

surface (i.e. those areas where accepting an electrophile is most favourable), the blue colour represents positively charged areas of the surface (i.e. those areas where accepting a nucleophile is most favourable) and the green colour represents the neutral surface area. It can be seen in Figure 5, there are possible sites in the title compound for electrophilic attack i.e. negative region, which is localized over N, S and Cl atoms. However, the most negative region is localized over N27 and N28 atoms.

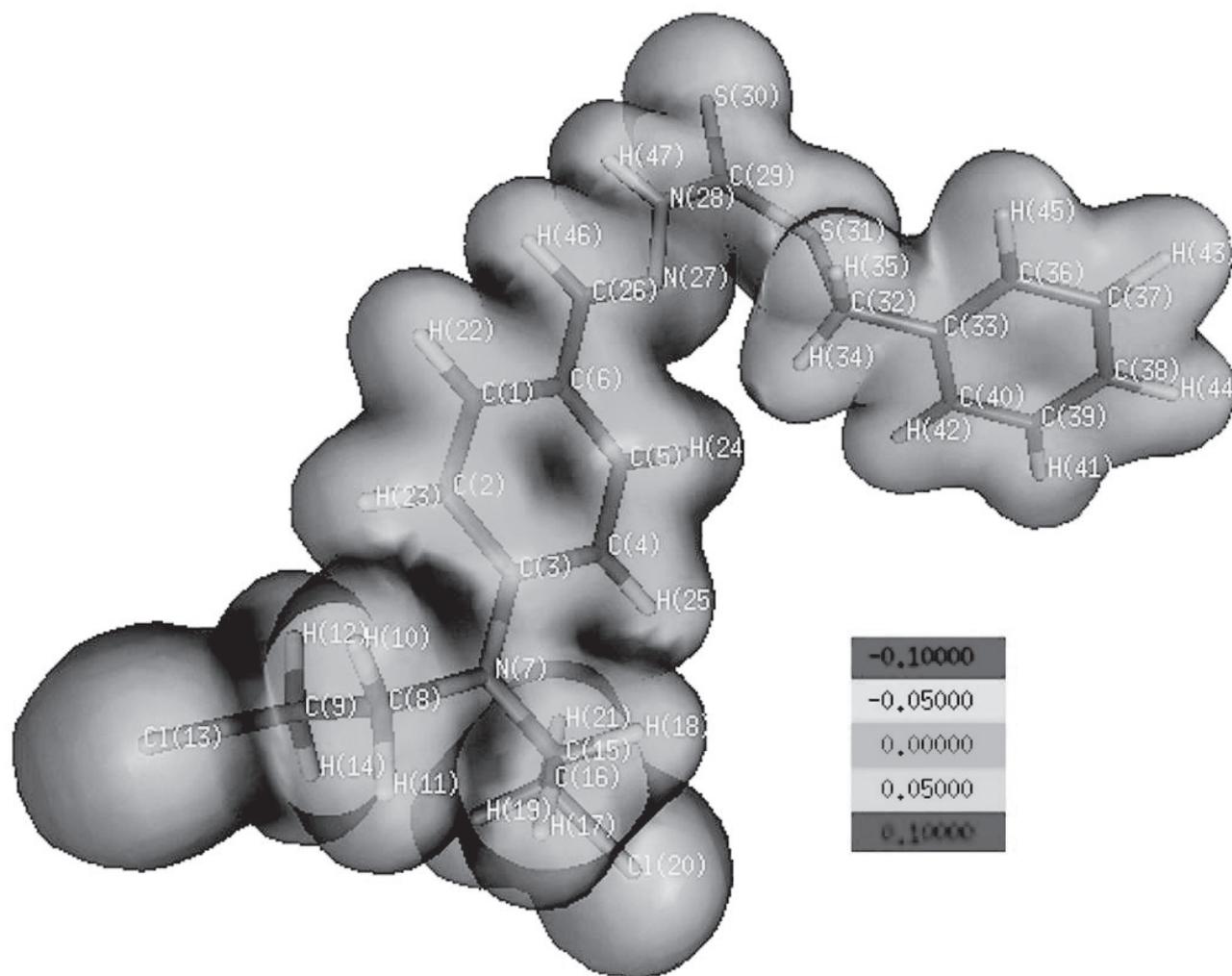


Fig. 5. MESP 3D isosurface plot of BCBHC thione form for DFT/B3LYP optimized geometry

3.5. Frontier molecular orbital analysis

The frontier molecular orbitals (HOMO and LUMO) of a chemical species are very important in defining its reactivity (Fukui *et al.*, 1952; Mendoza-Huizar & Rios-Reyes, 2011). A Higher value of HOMO shows the tendency of a molecule to donate the electrons to an appropriate acceptor molecule having low energy and empty molecular orbital. Three-dimensional plots of the

HOMO and the LUMO for BCBHC calculated by the DFT method at iso value 0.04 are shown in Figure 6. Both the HOMO and the LUMO are mainly spread from N7 to S30 through benzene ring. The blue colour illustrates the positive phase of the wave function and the red colour illustrates the negative phase of the wave function. Using HOMO and LUMO energy values for a molecule, we can

compute absolute electronegativity (χ), absolute hardness (η) and softness (s) operationally and approximately (Pearson, 1986; Pearson, 2005) as follows:

$$\chi = (I + A)/2 \quad \eta = (I - A)/2 \quad s = 1/\eta$$

where I and A are ionization potential and electron affinity. Within the limitations of Koopmans' theorem, I and A may be approximated as $(-E_{\text{HOMO}})$ and $(-E_{\text{LUMO}})$ respectively.

The HOMO and the LUMO energies, the ionization potential (I), the electron affinity (A), the electronegativity (χ), the chemical hardness and the chemical softness for the title molecule have been calculated by DFT method at 6311-G(2d,2p). The results obtained are given in Table 5. The absolute hardness (η) corresponds the gap between the HOMO and the LUMO orbital energies. The larger the HOMO-LUMO orbital energy gap, the harder the molecule. The hardness has been associated with stability of the chemical systems. A larger HOMO-LUMO gap corresponds to a less reactive molecule and a smaller gap corresponds to a more reactive molecule. In the present study, the calculated HOMO-LUMO gap of the molecule comes out as 0.13492 a.u. by DFT/6311-G(2d,2p) method which, indicates that the title structure is stable. The ionization energy (IE) can be expressed through

HOMO orbital energy as $\text{IE} = -E_{\text{HOMO}}$. The ionization potential values obtained by theoretical study also support the stability of the title molecule. The calculated Dipole moment values show that BCBHC is polar in nature.

Table 5. Calculated values of HOMO-LUMO energy, Hardness (η) and related molecular properties for the thione form of BCBHC

Energies/Properties	Computed values
$E_{\text{LUMO}+1}$ (a.u.)	-0.03420
E_{LUMO} (a.u.)	-0.07223
E_{HOMO} (a.u.)	-0.20715
$E_{\text{HOMO}-1}$ (a.u.)	-0.21570
$E_{\text{HOMO}} - E_{\text{LUMO}}$ (a.u.)	0.13492
Energy gap $\Delta E_1 = E_{\text{LUMO}+1} - E_{\text{HOMO}-1}$ (a.u.)	0.18150
Ionization potential ($I = -E_{\text{HOMO}}$) (a.u.)	0.20715
Electron affinity ($A = -E_{\text{LUMO}}$) (a.u.)	0.07223
Absolute electronegativity ($\chi = (I+A)/2$)	0.13969
Absolute hardness ($\eta = (I - A)/2$)	0.06746
Absolute softness ($s = 1/\eta$)	14.82360
Dipole moment (Debye)	6.83165

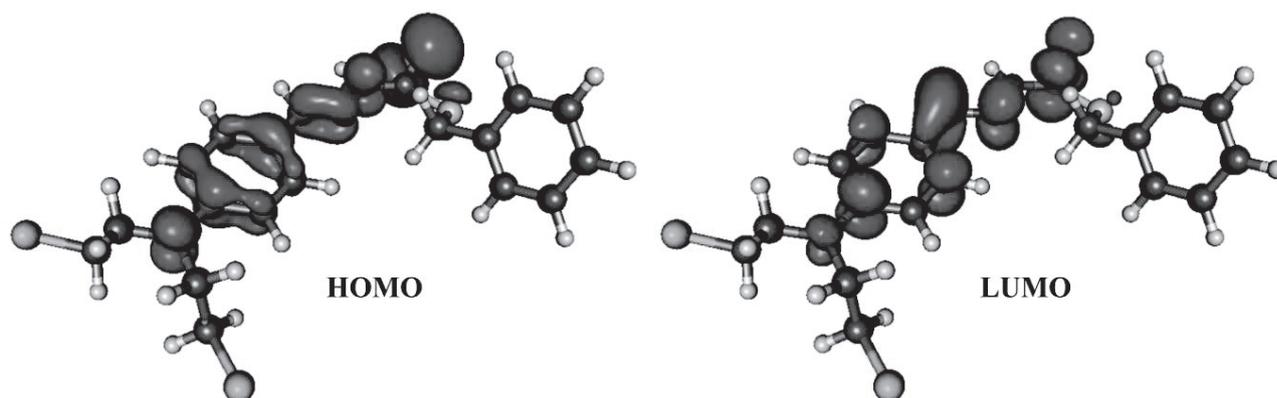


Fig. 6. HOMO-LUMO 3D isosurface plots by DFT/6311-G(2d,2p) method for BCBHC thione form

3.6. Population analysis

Population analysis gives an idea of the charge distribution in a molecule. Despite the method and basis set dependency, the Mulliken atomic charges have an important role in the application of quantum chemical calculations to molecular systems, because they may be used to interpret the atomic charge, dipole moment, molecular polarizability, electronic structure and other properties

of molecular systems. The histogram for the calculated partial charge by the natural population analysis of BCBHC obtained by Mulliken population analysis by DFT/6311-G(2d,2p) method is shown in Figure 7. Most negative value predicted by both the methods stands for N7 atom followed by N27 and S30 atoms, whereas most positive values predicted by both the methods stands for C4 atom followed by C26 and C29 atoms.

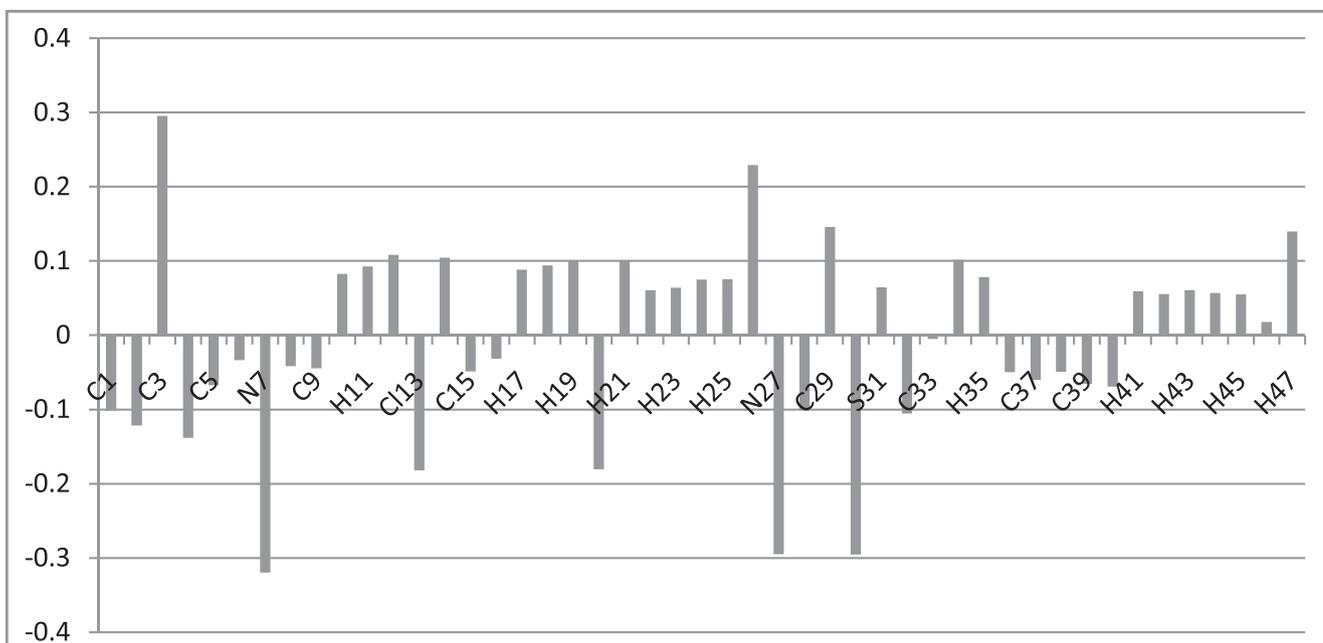


Fig. 7. Histogram of partial charges calculated by DFT/6311-G(2d,2p) method

3.7. Electron localization function plot

Becke and Edgecombe propounded the electron localization function (ELF) as a simple measure of localization of electron in atomic and molecular systems (Becke & Edgecombe, 1990). They defined ELF as follows:

$$ELF(r) = \frac{1}{1+\chi_{\sigma}^2(r)} \quad 0 \leq ELF \leq 1, \text{ where}$$

$$\chi_{\sigma}^2(r) = D_{\sigma} / D_{\sigma}^0$$

where D_{σ} is the difference of kinetic energy density of the non-interacting system and von Weizsäcker kinetic energy density, D_{σ}^0 is the value of D_{σ} term for

homogeneous electron gas. Savin further generalized the ELF approach to a variety of chemical systems (Savin *et al.*, 1997). The ELF isosurfaces plots explain the bonding type in a chemical species. The ELF 3D isosurface (Savin *et al.*, 1996) calculated by Gabedit for DFT/6311-G(2d,2p) calculation output is shown in Figure 8. Non-bonding ring attractor domains are visible on C113, C120 and S30. The non-bonding attractors on N atoms are visible as merged with nearby bonding attractors. The disynaptic basins $V(C,C)$ for aromatic rings show an intermediate shape as shown by a typical C-C single bond and C=C double bond. The $V(C,H)$ disynaptic basins show their typical shape. A single bean shaped $V(C,S)$ disynaptic basin arisen for C29=S30 bond.

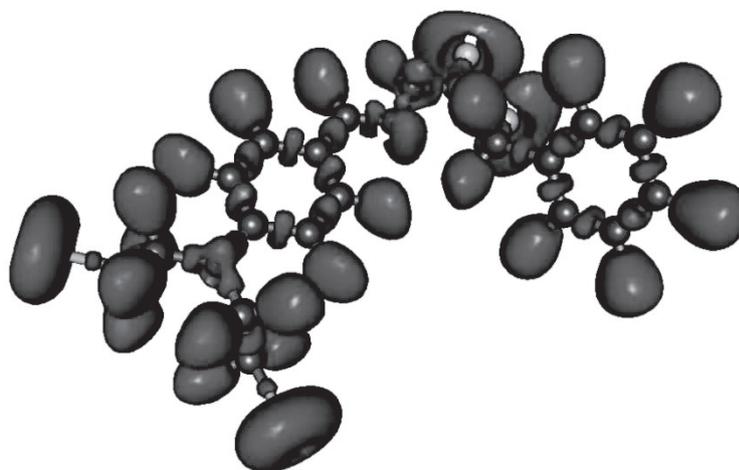


Fig. 8. ELF of BCBHC thione form at level 0.8

4. Conclusion

A novel Schiff base, Benzyl2-(4-(bis(2-chloroethyl)amino)benzylidene)hydrazinecarbodithioate was synthesized and characterized. ¹H-NMR and IR spectral studies indicate that the thione tautomeric form predominates in solid state, while thiol tautomeric forms exist in solution, and is thermodynamically more stable. Theoretical findings conclude the same. MEP surface analysis indicates N27-N28 atom pair as possible site for electrophilic attack. $E_{\text{HOMO}}-E_{\text{LUMO}}$ gap values predict it a reactive species. The ELF isosurface plots show typical localization domains for BCBHC.

5. Acknowledgments

Rajeev Singh and Bhoop Singh gratefully acknowledge the financial support for this work by the Madhya Pradesh Council of Science and Technology (MPCST), Bhopal by means of Research Grant No. 1076/CST/R&D/2012.

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- Submitted** : 18/03/2016
Revised : 15/11/2016
Accepted : 16/11/2016

دراسة حسابية على التركيب الجزيئي والخصائص الالكترونية والاهتزازية لقاعدة شيف Schiff base جديدة: بنزيل 2-4-(مكرر (2-كلورو إيثيل) أمينو) بنزيليدين) هيدرازين كاربوديثيوات (Benzyl2-(4-(bis(2-chloroethyl)amino)benzylidene) hydrazinecarbodithioate)

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خلاصة

تشير هذه الدراسة إلى قاعدة شيف Schiff base جديدة «بنزيل 2-4-(مكرر (2-كلورو إيثيل) أمينو) بنزيليدين) هيدرازين كاربوديثيوات» (Benzyl2-(4-(bis(2-chloroethyl)amino)benzylidene) hydrazinecarbodithioate) وخصائصها بواسطة الأشعة تحت الحمراء (IR)، الرنين المغناطيسي النووي (NMR)، وطرائق قياس الطيف الكتلي mass spectral methods مع الدراسات الكيميائية الكمية لنظرية الدالة الوظيفية لكثافتها (DFT). تمت دراسة الصنوانية tautomerism في هذا الجزيء نظرياً بطرق شبه تجريبية. تم حساب الهندسة الجزيئية من خلال طرق نظرية الدالة الوظيفية للكثافة (DFT) باستخدام مجموعة أساس التكافؤ المقسم ثلاثي-زيتا (6-311G(2d,2p) من نمط بوبل Pople. تم حساب الترددات الاهتزازية بواسطة طريقة نظرية الدالة الوظيفية للكثافة على نفس مستوى مجموعة الأساس. تم حساب المعلمات الجزيئية مثل أعلى طاقة مدار جزيئي مشغول، وأدنى طاقة مدار جزيئي غير مشغول، وفجوة طاقة المدار الجزيئي الحدودية والعزم القطبي بواسطة طرق نظرية الدالة الوظيفية للكثافة DFT باستخدام مجموعة أساس المقسم ثلاثي-زيتا (6-311G(2d,2p). وكذلك تم عرض جهد السطح الكهروستاتيكي الجزيئي والخرائط الديناميكية لتوطن الإلكترون. وتمت دراسة المواقع التفاعلية في الجزيء نظرياً مع وضع التركيب الإلكتروني في الاعتبار.