



Original Research Article

Investigation of Thermodynamic Properties and Hardness by DFT Calculations of S_2X_2 isomers (X: F, Cl, Br)

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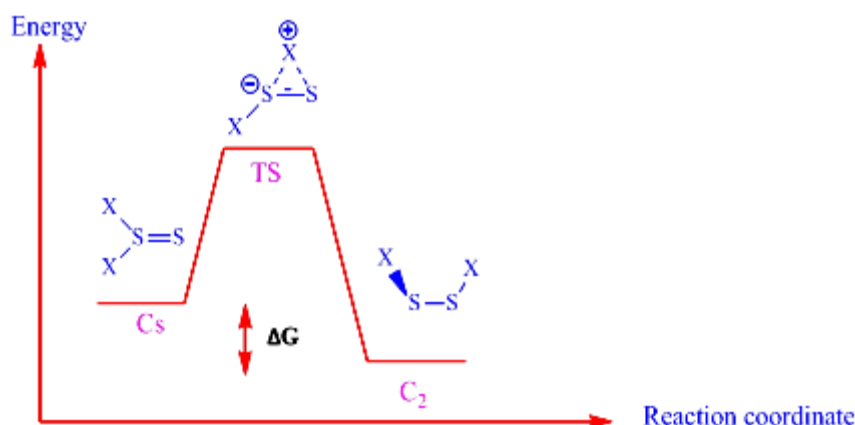
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ABSTRACT

Studying S_2X_2 compounds is of great importance due to their biochemical, atmospheric chemistry properties and protein structure, and because of the importance of this combination, it has received attention in the review. The compounds of disulfide S_2X_2 [X: F (1), Cl (2), Br (3)] and their isomers were studied with long-range-corrected functional (LC- ω PBE, LC-BLYP) with basis set Aug/pVmZ (m: 3). The analysis performed for the two forms of product (C_2) and reactant (C_S) showed that conformation C_2 is a more stable thermodynamic parameter due to greater HOMO-LUMO gap and chemical hardness higher. The difference between Gibbs free energy (ΔG) and enthalpy (ΔH), and corrected electronic energy (ΔE_0) for compounds 1 to 3 was increasing. The global hardness (η) and electronegativity (χ), ionization energy (I), electron affinity energy (A), and electrophilicity index (ω) were investigated in these compounds. There was a direct relationship between the difference in global hardness and Gibbs free energy.

GRAPHICAL ABSTRACT



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Introduction

Disulfides $XSSX$ and their isomers SSX_2 (X: H, CH_3 , F, Cl, Br) have been investigated for their importance in atmospheric chemistry as well as biochemistry. Particularly, sulfur-sulfur bond in the cysteine residue plays a significant role in biological systems as the major stabilizer of the protein's third structure [1]. Many S_2X_2 systems have been found to have two disulfide isomers ($XSSX$) with C_2 symmetry and a thiosulfoxide isomers (SSX_2) with CS symmetry. These two isomers have been separated and verifiable [2]. Based on Greenwood and Earnshaw, sulfur and fluorine have produced seven various binary compounds with a wide range of physical and chemical features involving S_2F_{10} and SF_6 [3].

Ball (2003) investigated the heat of formation and vibrational frequency of $FSSF$, SSF_2 with the theory of G2 and G3 and a complete basis set [4]. Disulfide difluoride was known for almost 170 years, but in 1963 the presence of two isomers of S_2F_2 compound by microwave and IR spectroscopy was proven [5].

Cao *et al.* [6] recently surveyed $SSF_2 \rightarrow FSSF$ isomerization reaction at 23 °C and 50 °C. HeI photo-electron spectroscopic technique (PES) was utilized to identify the kinetic parameters, the mechanism of many chemical reactions, and the isomerization reaction.

In 2007, the $SSXY \rightarrow XSSY$ (X or Y = F, Cl, Br, I) isomerization reaction applying $B_3LYP/6-311++G(2DF)$ and $MP2/6-311++G(2DF)$ and $B3LYP/6-311++G(2DF)$ was studied regarding electron density distribution theory [7].

Most experimental studies on the IR and Raman spectra of bromine species show that the molecule is transformed into a skew structure belonging to C_2 point group [8]. Applying CCSD (T) with a basic set of structural and vibrational spectrum correlations, the relative stability and heat of formation and the isomerization barrier $S=SBr_2$ and $BrSSBr$ have been surveyed [9]. Many intermolecular rearrangements resulting from the reorganization and redistribution of electron density among the atoms of a molecule are generally significant in reactivity and selectivity [10].

In 2013, the compounds of X_2Y_2 structure with two isomers $XYXY$ and X_2YY (X: Li, Na, F, Br, Cl, I) and (Y: O, S, Se, Te) applying (Density Functional Theory) DFT were studied by ZORA-BP86/QZ4P computational method [11].

Cattaraj *et al.*, surveyed the impacts of solvents as well as intermolecular rearrangements based on DFT research. They investigated the relative energy and chemical potential of electron and the chemical hardness and polarization for $F_2S_2 \rightarrow FSSF$ and $Trans-N_2H_2 \rightarrow Cis-N_2H_2$ rearrangements in the gaseous and soluble phases, respectively [12].

X_2Y_2 systems with C_2 conformation were more stable than other forms due to the anomeric impact on noncyclic and heterocyclic systems involving heteroatoms [13]. Due to the anomeric impact in $Y-X-X-Y$ systems (X: O, Y: O, N, halogen) with C_2 conformation, X-X bond length is shorter and X-Y bond length is longer [14]. The conversion reaction $XSSY \rightarrow SSXY$ (X or Y: F, Cl, Br, I) was studied by $B_3LYP/6-311++G(2df)$ and $MP2/6-311++G(2df)$ computational approach in 2007. In this reaction, there are two pathways for the transfer of atoms X and Y [15].

Due to the importance of the effect of substitution, many studies have been done in this field [16-18]. In this study, the stability of C_2 and Cs conformation of S_2X_2 compounds with X: F, Cl, Br substitution was investigated. Thermodynamic parameters ΔG , ΔH and ΔE_0 and structural parameters, hardness, softness, electronegativity parameters and electrophilic index were calculated by $LC-\omega PBE/Aug-cc-pVTZ$ and $LC-BLYP/Aug-cc-pVTZ$ methods.

Result and Dissection

Computational details

Gaussian 09W package and gaussview 5.0 [19] was utilized to compute examine the Perdew-Burke-Ernzerhof ($LC-\omega PBE$) and Becke-Lee-Yang-Parr ($LC-BLYP$) [20-22]. $Aug-cc-pVnZ$ (n: 3) are basis sets for the C_2 and CS conformations of compounds 1 to 3. The whole of electronic and zero-point energies ($E_0 = E_{el} + ZPE$), electronic and thermal enthalpies ($H = E + RT$), electronic and thermal free energy ($G = H - TS$) were explored as thermodynamic parameters. The differences within the thermodynamic information of ΔG , ΔH ,

and ΔE_0 were computed in product state C_2 and reactant states C_s for compounds 1 to 3. The structural parameters of the compound 1-3 were for the reactant C_s and product C_2 audit. The highest orbital molecular occupied (HOMO), the lowest unoccupied molecular orbital (LUMO) and gap HOMO and LUMO were recognized by

computational strategy LC-BLYP/Aug-cc-pVTZ and LC- ω PBE/Aug-cc-pVTZ. The HOMO-LUMO gap decides the degree of hardness. Figure 1 indicates the intermolecular rearengment process of the reactant (C_s) \rightarrow transition state (TS) \rightarrow product(C_2).

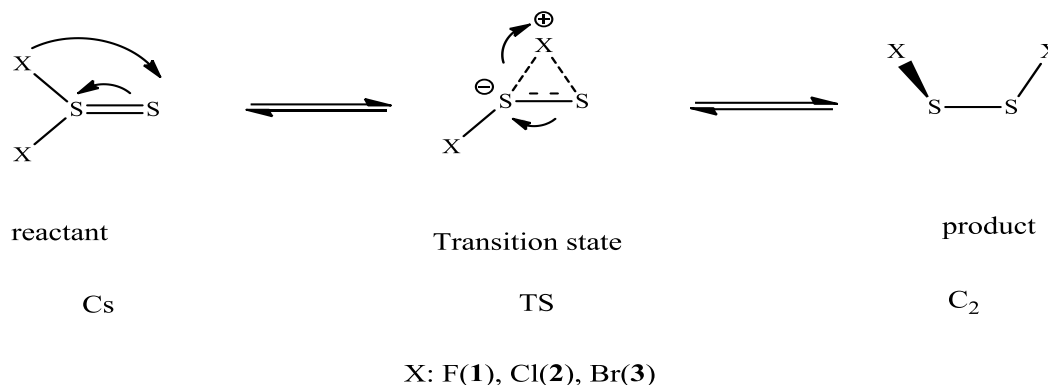


Figure 1: Symmetry variations through conformational change X: F (1), Cl (2), Br (3)

Figure 2 indicates Gibbs free energy difference between reactant $S=SX_2$ and product $XSSX$ for compounds 1- 3.

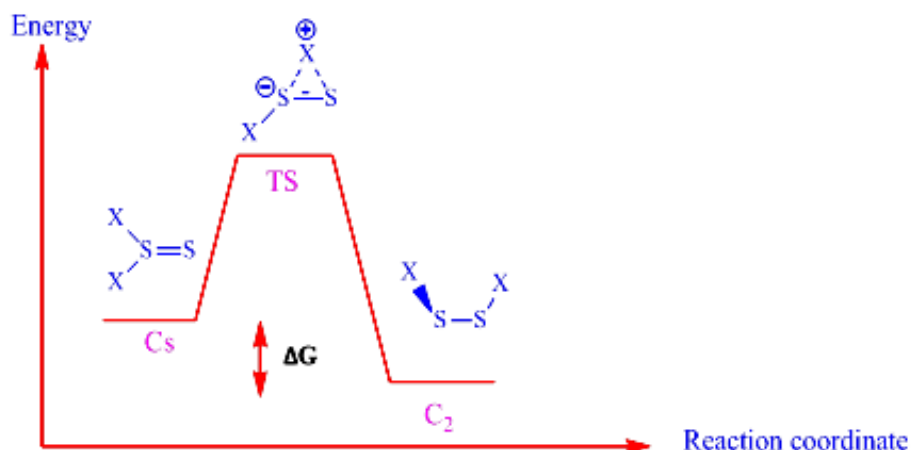


Figure 2: Diagram of Gibbs free energy changes in the conversion process $S=SX_2 \rightarrow XSSX$ [X: F (1), Cl (2), Br (3)]

Structural parameters

Structural features of bond length (r), bond angle (θ), and dihedral angle (φ) for compounds 1-3 with C_2 and C_s conformation applying LC- ω PBE/Aug-cc-pVTZ and LC-BLYP/Aug-cc-pVTZ computational approaches are indicated in Table 1. Comparing bond lengths and angles experimental and computed in C_2 and C_s conformations for compounds 1 to 3 are performed in Table 1.

Conformational properties

The difference between the enthalpy and the free energy Gibbs and the corrected electronic energy between conformations C_2 and C_s for compounds 1-3 by LC- ω PBE/Aug-cc-pVTZ and LC-BLYP/Aug-cc-pVTZ computational approaches are mentioned in Table 2. In this research, we apply enthalpy difference and Gibbs free energy and corrected electronic energy to conformation C_s and C_2 $\Delta[H(C_2) - H(C_s)]$, $\Delta[G(C_2) - G(C_s)]$ and $\Delta[E_0(C_2) - E_0(C_s)]$ is calculated according to Table 2. ΔG , ΔH , ΔE_0 increasing from compound 1 to 3.

Table 1: Computed structural parameters bond lengths (A0), bond and dihedral angles (0) of conformation (C₂) and (CS) of compounds 1 to 3

Compounds	LC- ω PBE		LC-BLYP		exp[15]	
	C ₂	C _S	C ₂	C _S	C ₂	C _S
F₂S₂	r ₁ =1.897	r ₁ =1.852	r ₁ =1.849	r ₁ =1.852	r ₁ =1.890	r ₁ =1.8744
	r ₂ =1.631	r ₂ =1.609	r ₂ =1.598	r ₂ =1.609	r ₂ =1.635	r ₂ =1.6391
	a=107.03	a ₁ =107.76	a=107.66	a ₁ =107.76	a=108.3	a ₁ =108.0
	d=87.6	a ₂ =91.95	d=91.62	a ₂ =91.95	d=87.7	a ₂ =98.0
Cl₂S₂	r ₁ =1.958	r ₁ =1.875	r ₁ =1.961	r ₁ =1.874	r ₁ =1.931	r ₁ =1.8901
	r ₂ =2.031	r ₂ =2.065	r ₂ =2.033	r ₂ =2.065	r ₂ =2.057	r ₂ =2.1599
	a=106.48	a ₁ =109.2	a=106.05	a ₁ =109.2	a=108.2	a ₁ =109.9
	d=85.8	a ₂ =96.48	d=85.27	a ₂ =96.33	d=84.8	a ₂ =106.1
Br₂S₂	r ₁ =1.97	r ₁ =1.882	r ₁ =1.971	r ₁ =1.882	r ₁ =1.98	r ₁ =1.8945
	r ₂ =2.183	r ₂ =2.233	r ₂ =2.184	r ₂ =2.232	r ₂ =2.24	r ₂ =2.3510
	a=106.49	a ₁ =109.6	a=106.22	a ₁ =109.62	a=105.0	a ₁ =110.6
	d=85.27	a ₂ =97.37	d=84.95	a ₂ =97.45	d=84.0	a ₂ =108.4

Table 2: ΔH , ΔG , ΔE_0 parameters (kcal/mol-1) in 298k and 1 atm for isomers (C₂) and (CS) structures of compounds 1 to 3

Compounds	LC- ω PBE			LC-BLYP		
	ΔE_0	ΔH	ΔG	ΔE_0	ΔH	ΔG
F₂S₂	1.88	2.51	2.51	2.74	2.52	2.62
Cl₂S₂	19.45	18.2	18.82	19.57	19.47	19.48
Br₂S₂	20.81	20.77	20.72	21.64	21.59	21.56

Global hardness and electronegativity

The highest orbital molecular occupied (HOMO) and lowest unoccupied molecular orbital (LUMO) for Compounds 1-3 with C₂ and CS conformation by LC- ω PBE/Aug-cc-pVTZ and LC-BLYP/Aug-cc-pVTZ computational approaches are indicated in Tables 3 and 4, respectively. HOMO-LUMO gap is measured by the hardness the chemical compounds. The difference in HOMO- LUMO gap of compounds 1 to 3 in the product (C₂) was 0.4321, 0.3836, 0.3588 (a. u) and product (CS) was 0.3966, 0.3443, 0.3135 (a. u) by the LC- ω PBE method, respectively. Also, the difference in HOMO- LUMO gap of compounds 1 to 3 in the product (C₂) was 0.4434, 0.3921, 0.3664 (a. u) and reactant (CS) was 0.4064, 0.3509, 0.3185 (a. u) by the LC-BLYP method, respectively. The higher the chemical hardness of compounds, the lower the chemical activity and the greater the stability [23]. The hardness difference from the compounds 1 to 3 was increasing. The relation between the hardness and the electron affinity

energy of (A) and the ionization energy (I) of a molecule is mentioned in Equation 1.

$$\eta = I - A / 2 \quad 1$$

Based on Principle Koopmans, theorem [24] the hardness of chemical compounds is explained by Equation 2.

$$\eta = 0.5(\epsilon_{\text{LUMO}} - \epsilon_{\text{HOMO}}) \quad 2$$

Based on the findings provided from the approaches LC- ω PBE/Aug-cc-pVTZ and LC-BLYP/Aug-cc-pVTZ for compounds 1-3 with C₂ and Cs conformations, the hardness of compounds with C₂ conformation is higher than CS.

The relationship between electronegativity (χ) and electron affinity energy (A) and ionization energy (I) is given according to eq 3. Tables 3 and 4 indicate the global electronegativity for compounds 1 to 3 reactant (CS) and product (C₂) conformation by LC/ ω PBE and LC/BLYP method.

$$\chi = I + A / 2 \quad 3$$

The softness (S) of chemical compounds is provided based on the relation $S = 1/2\eta$.

Regarding Tables 3 and 4, the conformation CS in compounds 1-3 is softer than that of C₂. Based on the principle maximum hardness, the hardest compounds of a molecule are the most stable form [25]. Based on the results obtained by LC-BLYP/Aug-cc-pVTZ and LC- ω PBE/Aug-cc-pVTZ computational methods, the difference in hardness among the conformations of C₂ and CS for compounds 1-3 $\Delta [\eta (C_2) - \eta (CS)]$ increased from 1 to 3 compounds which corresponds to an increase in ΔG , ΔH , ΔE_0 . The difference in hardness of compounds 1 to 3 in the reactant (CS) and product (C₂) with the LC- ω PBE method

was 0.01776, 0.01961, 0.02268 (a.u.), respectively, and for LC-BLYP approach, it was 0.02035, 0.02060, 0.0239 (a.u.), respectively. The hardness difference from the 1 to 3 compounds was increasing.

Index electrophilicity (ω) is the ability of an electrophile to provide electrical charge and system resistance to the exchange of electron charge with the environment [26]. Eq 4 indicates the hardness and electronegativity relationship with index electrophilicity.

$$\omega = \chi^2 / 2\eta \quad 4$$

Table 3: LC- ω PBE/Aug-cc-pVTZ computed energies of HOMO (ϵ_{HOMO}), LUMO (ϵ_{LUMO}), global hardness (η), softness (S), electronegativity (χ) and electrophilicity (ω) in (a. u.) parameters for the (C₂) and (CS) of compounds 1-3

	E _{HOMO}	E _{LUMO}	IP	EA	χ	μ	η	S	ω
F₂S₂									
C ₂	-0.41193	0.02022	0.41193	-0.02022	0.19585	-0.1958	0.2160	2.3148	0.0887
C _S	-0.39818	-0.00156	0.39818	0.00156	0.19987	-0.1998	0.1983	2.5214	0.1006
Cl₂S₂									
C ₂	-0.38521	-0.00161	0.38521	0.00161	0.19341	-0.1934	0.1918	2.6068	0.0974
C _S	-0.37562	-0.03124	0.37562	0.03124	0.20343	-0.2034	0.1721	2.9035	0.1202
Br₂S₂									
C ₂	-0.37364	-0.01475	0.37364	0.01475	0.19419	-0.1941	0.1794	2.7870	0.1050
C _S	-0.36588	-0.05235	0.36588	0.05235	0.20911	-0.2091	0.1567	3.1908	0.3195

Table 4: LC-BLYP/Aug-cc-pVTZ computed energies of HOMO (ϵ_{HOMO}), LUMO (ϵ_{LUMO}), global hardness (η), softness (S), electronegativity (χ) and electrophilicity (ω) in (a. u.) parameters for the (C₂) and (CS) of compounds 1-3

	E _{HOMO}	E _{LUMO}	IP	EA	χ	μ	η	S	ω
F₂S₂									
C ₂	-0.42043	0.02305	0.42043	-0.02305	0.19869	-0.19869	0.2217	2.2552	0.0889
C _S	-0.40461	0.00183	0.40461	-0.00183	0.20139	-0.20139	0.2013	2.4606	0.0997
Cl₂S₂									
C ₂	-0.39215	-0.00005	0.39215	0.00005	0.1961	-0.1961	0.1960	2.5510	0.0980
C _S	-0.38072	-0.02981	0.38072	0.02981	0.2052	-0.2052	0.1754	2.8506	0.1200
Br₂S₂									
C ₂	-0.38008	-0.01364	0.38008	0.01364	0.19686	-0.19686	0.1832	2.7292	0.1057
C _S	-0.37047	-0.05189	0.37047	0.05189	0.21118	-0.21118	0.1592	3.1407	0.1399

The process of increasing the difference hardness was be described by increasing ΔG , ΔE_0 , ΔH of compounds 1 to 3. There is a linear relationship between ΔG and $\Delta \eta$ for compounds 1 to 3 by LC-

ω PBE/Aug-cc-pVTZ and LC-BLYP/Aug-cc-pVTZ (Fig3). An increase in $\Delta \eta$ of compounds 1 to 3 corresponds to an increase in ΔG .

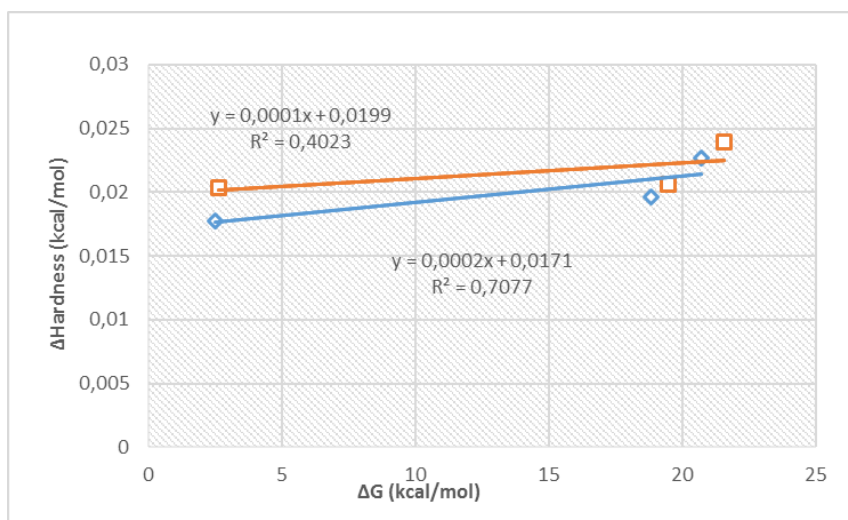


Figure 3: Relation of ΔG vs. Δ Hardness with the LC- ω PBE/aug-cc-pVTZ (\square) and LC-BLYP/aug-cc-pVTZ (\diamond)

Conclusion

In this research, for compounds 1 to 3 for two conformations C_2 and CS by LC-BLYP, LC- ω PBE with basis set Aug-pVTZ, the bond length and the bond angle and the dihedral angle were computed. ΔE_0 , ΔH , ΔG are increasing from compounds 1 to 3. The difference in hardness $\Delta[\eta(C_2)-\eta(CS)]$ of compounds 1 to 3 is increasing. There is a direct relationship between the difference in hardness and Gibbs free energy difference for compounds 1 to 3 with the LC- ω PBE/aug-cc-pVTZ and LC-BLYP/aug-cc-pVTZ approach, which shows C_2 conformation stability. Research has shown the chemical hardness of C_2 and CS conformations revealed that C_2 conformations are more stable.

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Authors' contributions

All authors contributed toward data analysis, drafting and revising the paper and agreed to be responsible for all the aspects of this work.

Conflict of Interest

We have no conflicts of interest to disclose.

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