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Electronic Structure and Reactivity Analysis of Bromocyclohexane, Chlorobenzene, and Iodobenzene Using Density Functional Theory

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ABSTRACT

Density functional theory study was carried out to investigate the electronic structure and vibration properties of bromocyclohexane, chlorobenzene, and iodobenzene. the calculations implemented in Gaussian 09. The results showed infrared transmittance data provided key insights into functional groups and bond vibrations. Chlorobenzene and iodobenzene exhibit maximum absorption (or minimum transmittance) at around 700 cm^{1}, corresponding to C-X (carbon-halogen) stretching vibrations, particularly C-Cl and C-I bonds. However, hexane bromosate exhibits a significant absorption at about 2900 cm^{-1}, which is associated with C-H stretching at SP3-hybridized carbon atoms (a characteristic feature of saturated aliphatic structures such as cyclohexane). In contrast, the reduced mass values provided evidence of atomic contributions to specific vibrational modes, particularly in heavy atom interactions. The reduced masses reach 6 atomic mass units (a.m.u) of Chlorobenzene and Iodobenzene, which is nearly the reduced mass between two carbon atoms, and reduced masses reach 1.3(a.m.u) for Bromocyclohexane. The positive charge value is (hydrogen - iodine - chlorine - bromine) while the negative values are for carbon. Iodine, boron, and chlorine atoms appear positively charged in Mulliken charge analysis, primarily due to differences in electronegativity and bond polarity. Together, these computational results contribute to the understanding of the molecule's electronic structure, stability, and reactive behavior, and provide information for its potential applications in pharmaceutical and materials science.

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1. INTRODUCTION

Bromocyclohexane, chlorobenzene, and iodobenzene are usually characterized with great interest in medicinal chemistry, materials science, and organic synthesis in halogenated organic compounds, because of their varied chemical reactivity and biological activities. Predicting these compounds' reactivity, interactions with biological systems, and spectroscopic characteristics requires an understanding of their electronic structure, charge distribution, and vibrational behavior. The unique electronegativity and polarity of halogen substituents (iodine, bromine, and chloride) greatly affect these compounds' electrical and spectral characteristics [1-5]. (Kausar, H. et al 2023) introduced a study of certain cancers brought on by halogen chemicals, along with their causes and consequences, to see whether there are any accessible treatments [6]. (Alla, S. K and et al 2013) This work presents a new process for creating 1,2-disubstituted benzimidazoles using m-chloroperbenzoic acid (mCPBA) as an oxidant and iodobenzene as a catalyst. These substances are significant in the field of medical chemistry [7]. (Rasul, H. H and et al 2023) It was discovered that charge transfer toward mild steel raises the capacity to donate electrons, resulting in higher inhibitory efficienc [8]. The Gaussian 09 software package's density functional theory (DFT) computations were used in this investigation, in addition to GaussView 6.0 for spectral visualization and structural modeling [9]. Infrared (IR) transmittance, which permits a better comprehension of molecular vibrations and the identification of functional groups, is one of the crucial factors that are the focus of the theoretical analysis; decreased mass, which clarifies how atoms contribute to vibrational modesMulliken charge distribution, which calculates the electron density across atoms and contributes to the explanation of polarity and reactivity in molecules; Fukui functions, which are used to locate reactive electrophilic and nucleophilic sites inside a molecule. These compounds' electrical and spectral characteristics are greatly influenced by the unique electronegativities and polarizabilities of the halogen substituents (Cl, Br, and I). This study attempts to give a thorough understanding of how various halogen atoms impact molecular geometry, charge localization, vibrational spectra, and chemical reactivity by comparing these three compounds [10]. Its aim of this work is to present a thorough understanding of the effects of various halogen atoms on gas phase chemical reactivity, vibrational spectra, charge position, and molecular geometry. It is anticipated that the findings of this investigation will aid in the development of halogenated compounds and the forecasting of their roles in chemical and biological settings. The chemical formula of Chlorobenzene is C_6H_5Cl, Iodobenzene C_6H_5I, and Bromocyclohexane (also called Cyclohexyl bromide, abbreviated CXB) is an organic compound with the chemical formula $C_6H_{11}Br$ [11]. Benzene reacts with chlorine, bromine, and iodine in the presence of a catalyst, replacing one of the hydrogen atoms on the ring with a chlorine atom, as shown in fig. (1).

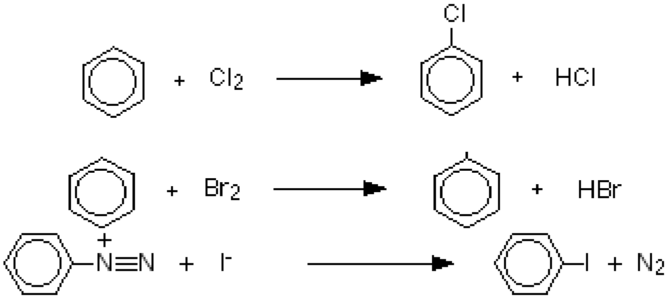


Figure 1. shows the reaction between chlorine or bromine, iodine atoms, and Benzene [12].

2. COMPUTATIONAL DETAILS

Three-dimensional forms of the compounds bromocyclohexane, chlorobenzene, and iodobenzene were drawn using the molecular imaging program Gaussian View 6.0 (Figure 2). All calculations used the Gaussian 09 software package, and density functional theory (DFT) and time-dependent density functional theory (TD- DFT) are used to perform all calculations. It is carried out using the B3LYP/6-31G(d,p) (Lee- Yang-parr) nonlocal correlation function [13-14]. Vibrational frequency calculations in density functional theory (DFT) [15-16] are very important for theoretical studies of relevant organic molecules. DFT is also a powerful and important tool for studying the relationship between the shape of a chemical compound and its electrical properties [17-18]. DFT calculations including electronic spectra, Mulliken count analysis, reduced mass and linear electro-optical properties, vibrational frequency analysis, infrared transmittance spectra, and HOMO and LUMO molecular orbital energy with different chemical reactivity parameters are presented for bromocyclohexane, iodobenzene, and chlorobenzene.

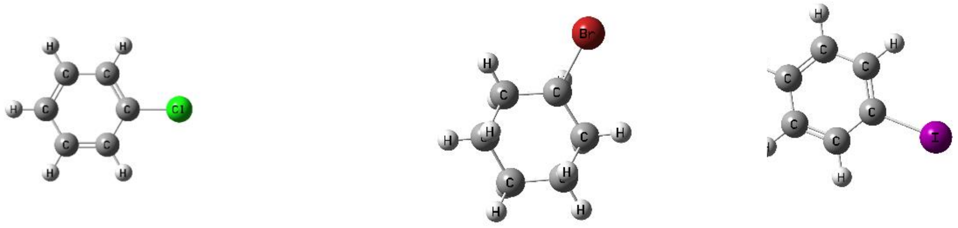


Figure 2. Shows geometry-optimisation structures of chlorobenzene, iodobenzene, and bromocyclohexane respectively.

3. RESULTS AND DISCUSSION

Theoretical quantum chemical calculations were performed to explore the relationship between specific electronic properties and the molecular structure of the studied compounds. Several important quantum descriptors, summarized in Table 1, including electronegativity (χ), electron affinity (A), ionization potential (I), and energy gap (ΔE_{Gap}) were evaluated using standard formulas. The energy gap (ΔE_{Gap}) is calculated as the difference between the energy of the lowest unoccupied molecular orbital (E_{LUMO}) and the highest occupied molecular orbital (E_{HOMO}), as shown in Equation (1), [19.20].

$$\Delta E_{gap} = E_{LUMO} - E_{HOMO} \quad (1)$$

Electron affinity (A) and ionization potential (I) are defined as the negative values of E_{LUMO} and E_{HOMO}

$$A = -E_{LUMO} \quad (2)$$

$$I = -E_{HOMO} \quad (3)$$

Electronegativity (χ), a measure of a molecule's tendency to attract electrons, is calculated as the average of I and A:

$$\chi = \frac{I+A}{2} \quad (4)$$

Additionally, to evaluate molecule stability and reactivity, the chemical hardness (η) and softness (σ) were calculated. Hardness is half of the energy gap] 21]:

$$\eta = \frac{\Delta E_{Gap}}{2} \quad (5)$$

Softness is the reciprocal of hardness:

$$\sigma = \frac{1}{\eta} \quad (6)$$

The chemical potential (μ), which represents the tendency of electrons to escape from equilibrium, is defined by:

$$\mu = -\chi^2 \quad (7)$$

Together, these parameters provide deep insight into a molecule's electronic structure, reactivity, and stability, which are crucial for understanding its potential behavior in chemical or biological environments [22].

From Table (1), it can be seen that the calculated energy gap values are 0.2069 eV, 0.241 eV, and 0.2626 eV for iodobenzene, chlorobenzene, and bromocyclohexane, respectively. This explains why iodobenzene is more stable than chlorobenzene and bromocyclohexane. The electronegativity (χ)values are 0.1221eV, 0.1329 eV, and 0.1356eV for chlorobenzene, iodobenzene, and bromocyclohexane, respectively. Chlorobenzene is more electronegative than the other two compounds. The softness values (σ) are 9.671eV^{-1}, 8.298eV^{-1}, and 7.616 eV^{-1} for iodobenzene, chlorobenzene, and bromocyclohexane, respectively. Iodobenzene has the highest value.

Table (1) Calculated chemical quantum parameters of Chlorobenzene, Iodobenzene Bromocyclohexane, respectively.

Parameters	E_{LUMO} (eV)	E_{HOMO} (eV)	ΔE_{gap} (eV)	μ (D)	η (eV)	σ (e V^{-1})	I (eV)	χ (eV)	A (eV)
Chlorobenzene	-0.01516	-0.25620	0.241	-0.0183	0.1205	8.298	0.25620	0.1356	0.01516
Iodobenzene	-0.02947	-0.23644	0.2069	-0.0176	0.1034	9.671	0.23644	0.1329	0.02947
Bromocyclohexane	0.00925	-0.25343	0.2626	-0.0149	0.1313	7.616	0.25343	0.1221	-0.0092

3.2 Mulliken charge

The distribution of atomic charges of Chlorobenzene, Iodobenzene Bromocyclohexane, respectively shown in Fig. (3). The Mulliken charges are charges based on the local electron density (charge density) [23]. The positive charge value is (hydrogen - iodine - chlorine - bromine) while the negative values are for carbon. Iodine, boron, and chlorine atoms appear positively charged in Mulliken charge analysis, primarily due to differences in electronegativity and bond polarity. Although halogens, such as chlorine and iodine, are electronegative, when bonded to higher electronegativity environments (such as oxygen, nitrogen, or conjugated systems), their ability to withdraw electron density may be relatively reduced. This can lead to partial depletion of the surrounding electron density, making them appear partially positive in atomic group analysis. Orbital Sharing and Polarization Effects: Mulliken charges depend not only on electronegativity but also on how the atomic orbitals in the molecule overlap. In many molecules, the p orbitals of the halogens participate in the bond in a way that polarizes the electron density away from them. For boron, which is inherently electron-poor (only three valence electrons), the bonding naturally causes it to lack electrons, which explains its positive charge on the Mulliken scale.

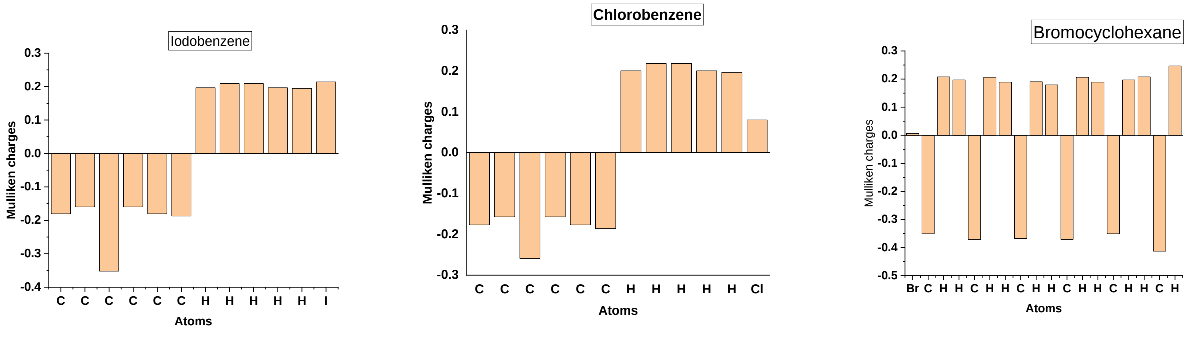
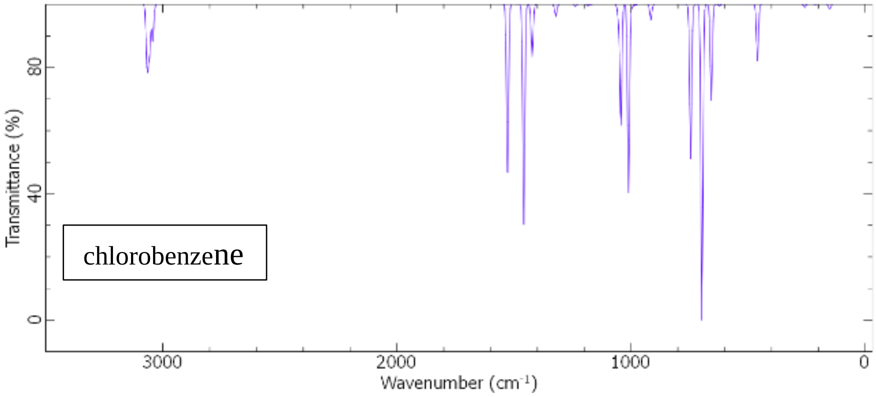
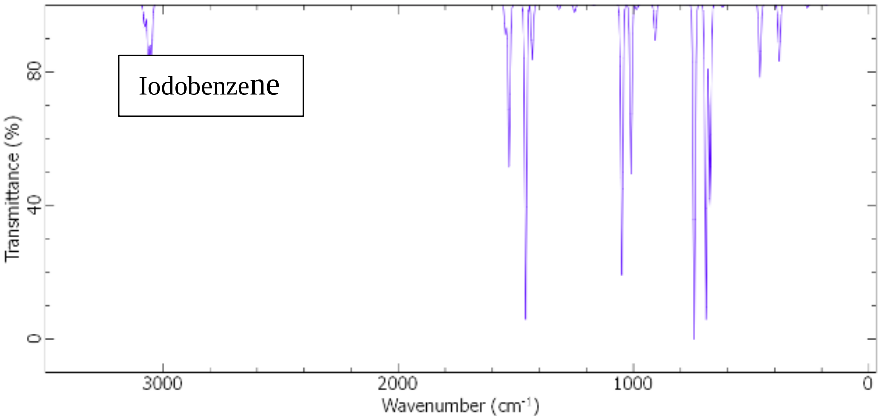


Figure 3. Shows the distribution of atomic charges of Chlorobenzene, Iodobenzene, and Bromocyclohexane, respectively.

3.3 Ultraviolet Visible Near-Infra red (UV-Vis-NIR) spectroscopy

Ultraviolet-visible-near-infrared (UV-Vis-NIR) spectroscopy is a powerful technique used to study materials' optical and electronic properties [24-25]. By measuring the amount of light transmitted (transmittance) or absorbed by a sample across a broad spectral range (from the ultraviolet to the near-infrared), scientists can gather crucial information about electronic transitions, molecular structure, and bonding within the material. Fig. (4) shows the transmittance spectra of chlorobenzene, iodobenzene, and bromocyclohexane. The spectrum is typically divided into different regions. The region from 0 to 1500 cm^{-1} is called the "fingerprint region" because it contains complex vibrations specific to each molecule, which can be used to uniquely identify the compound. Chlorobenzene and iodobenzene exhibit maximum absorption (or minimum transmittance) at around 700 cm^{-1}, which corresponds to C-X (carbon-halogen) stretching vibrations, particularly C-Cl and C-I bonds. However, hexane bromosate exhibits a significant absorption at about 2900 cm^{-1}, which is associated with C-H stretching at SP^3-hybridized carbon atoms (a characteristic feature of saturated aliphatic structures such as cyclohexane). At about 1600 cm^{-1}, the absorption is attributed to C=C double bond stretching, which is common in aromatic systems such as chlorobenzene and iodobenzene (but unexpected in hexane bromosate, which lacks aromaticity). The region at 2900 cm^{-1} corresponds to C-H stretching vibrations of sp^3-hybridized carbon atoms (saturated bonds). At about 3100 cm^{-1}, the absorptions are associated with C-H stretching at SP^2-hybridized carbon atoms, which is common in aromatic rings. Intermolecular hydrogen bonding greatly influences molecular structure and vibrational properties and often causes shifts (especially redshifts) and broadening of the infrared absorption bands. This phenomenon can change bond lengths and electron distribution, affecting the spectral signature of the material.





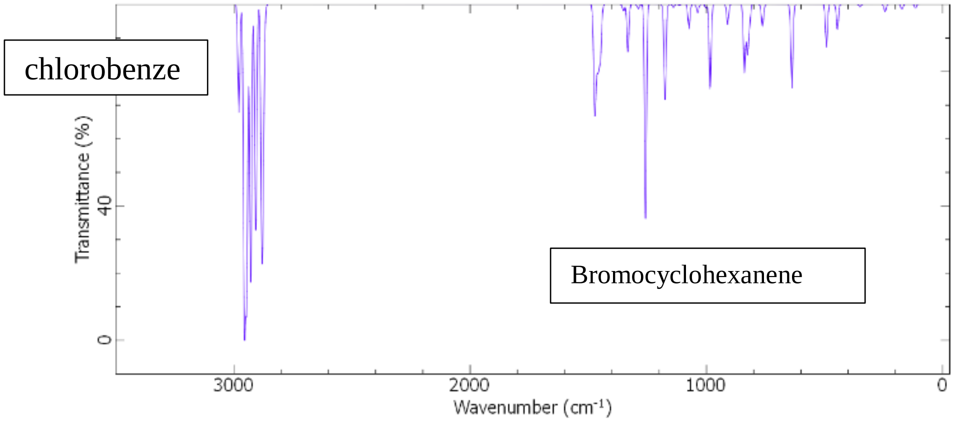


Figure 4. Shows the transmittance of Chlorobenzene, Iodobenzene, and Bromocyclohexane, respectively.

3-4 Reduced mass

Reduced mass, which is a physical quantity used when solving the two-body problem to turn it into an equivalent one-body problem that can be solved faster and easier can be seen Fig. (5). The reduced mass of two particles of masses m_1 and m_2 is given by [26]:

$$\mu = \frac{m_1 * m_2}{m_1 + m_2} \qquad (8)$$

The reduced masses reach 6 atomic mass units (a.m.u) of Chlorobenzene and Iodobenzene, which is nearly the reduced mass between two carbon atoms. This indicates that some vibrations might include one kind of atom but exclude the other. The vibrations after 1750 cm^{-1} are all hydrogen-related, since they all have the approximate reduced mass of 1 (a.m.u). But reduced masses reach 1.3(a.m.u) for Bromocyclohexane, which indicates that some vibrations might include two kinds of atoms, Bromine and Hydrogen.

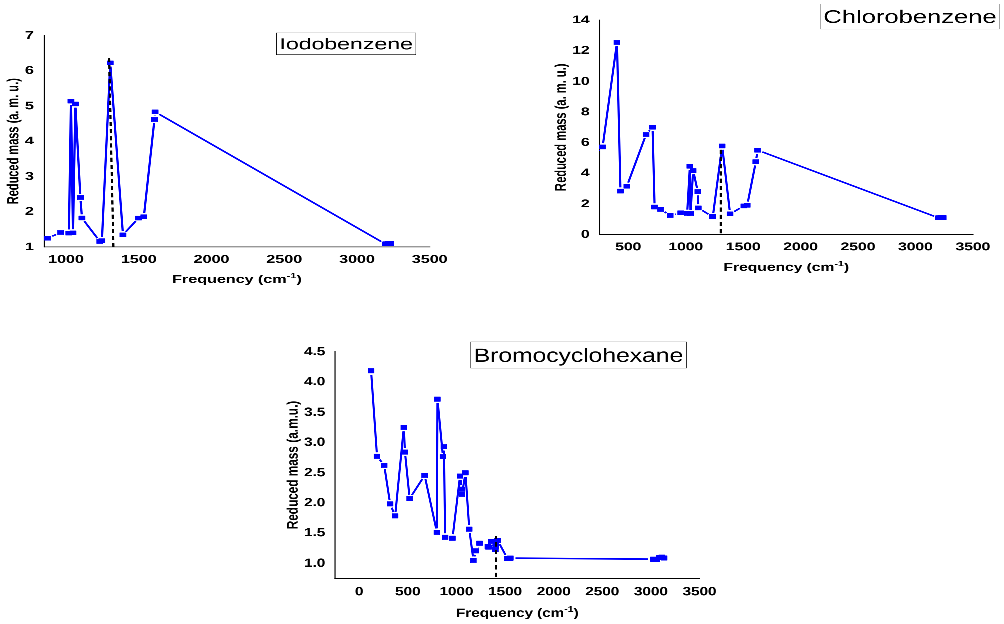


Figure 5. Shows the reduced mass of Iodobenzene, Chlorobenzene, and Bromocyclohexane, respectively.

3.5 Fukui functions

According to Mendes and Gazquez, the Fukui function f (r)

F(r) is a local reactivity descriptor that predicts a molecule's preferred location for a particular type of chemical attack—nucleophilic, electrophilic, or radical. That means consistent with the hard-soft acid-base (HSAB) principle, which states that "regions of a molecule with a large Fukui function are chemically softer," meaning they are more polar and more reactive to soft reagents. In this section, a DFT-based Fukui function analysis is applied to the neutral (N), cationic (N-1), and anionic (N+1) states of chlorobenzene, iodobenzene, and bromocyclohexane which correspond, respectively, [28, 29].

- f^+: Nucleophilic attack, calculated as ρ N+1 (r) – ρ N(r)
- f^-: Electrophilic attack, calculated as ρ N(r) - ρ N-1 (r)
- f^0: Radical attack, calculated as $\frac{1}{2}$ (ρ N+1 (r) –ρ N-1 (r))

(r) is the electron density at point r, and N is the number of electrons in a neutral molecule. These density variations give a spatial map of the molecule's chemical softness or hardness, regions with large f. f values are softer and more chemically reactive [30-31]. In this section, a DFT-based Fukui function analysis is applied to the neutral (N), cationic (N-1) and anionic (N+1) states of chlorobenzene, iodobenzene, and bromocyclohexane. These correspond, respectively, Table (2) which indicates that F^0 has a value of (0.898342, 0.717604, and 0.47005), and the values of F^- are as follows: (0.501691, 0.616665, 0.159259). Finally, the F^+ values are (0.396651, 0.479212, and 0.310791). in bromocyclohexane, iodobenzene, and chlorobenzene, respectively. A higher F^0 value indicates a greater change in electron density when an electron is added or removed, indicating greater chemical flexibility and reactivity at the free radical sites. These values indicate that iodobenzene is significantly more reactive with electrophilic compounds than the other two compounds. This high F^-value reflects greater electron density in key atomic sites when the molecule loses an electron (i.e., in the N-1 state), making it a more favorable site for electrophilic attack. These results F^+ indicate that iodobenzene is the most reactive with nucleophilic species, likely due to its ability to withdraw electrons and polarize the iodine atom, which stabilizes the added electron density. Chlorobenzene is the least reactive with nucleophilic species, consistent with chlorine's high electronegativity and low polarizability, which makes it less adaptable to the nucleophilic electron density.

Table 2. Calculated electronic energy of Chlorobenzene, Iodobenzene and Bromocyclohexane, respectively.

Number of Atoms	Atoms	F^+	F^-	F^o
Iodobenzene				
1	C	0.024729	0.008432	0.346977
2	C	0.031012	0.028168	0.297412
3	C	-0.01801	-0.09919	0.717604
4	C	0.031047	0.028179	0.297328
5	C	0.024675	0.00843	0.347057
6	C	0.047483	0.021657	0.342832
7	H	0.07892	0.083193	-0.38508
8	H	0.0657	0.073668	-0.40225
9	H	0.065684	0.073594	-0.4023
10	H	0.078905	0.083214	-0.38501
11	H	0.090645	0.073986	-0.40064
12	I	0.479212	0.616665	-0.37392
Chlorobenzene				
1	C	0.02533	0.065201	0.090531
2	C	0.039833	0.065743	0.105576
3	C	0.004934	-0.02065	-0.01571
4	C	0.039935	0.069053	0.108988
5	C	0.025194	0.062309	0.087503

6	C	0.066457	-0.01014	0.056315
7	H	0.097369	0.128916	0.226285
8	H	0.090733	0.120248	0.210981
9	H	0.090739	0.121212	0.211951
10	H	0.097331	0.128044	0.225375
11	H	0.111354	0.110805	0.222159
12	Cl	0.310791	0.159259	0.47005
Bromocyclohexane				
		0.396651	0.501691	0.898342
		0.092189	-0.16646	-0.07428
		-0.00215	0.1346	0.132451
		0.018763	0.158719	0.177482
		0.113604	-0.1493	-0.0357
		-0.02001	0.100756	0.080743
		0.011447	0.132897	0.144344
		0.112776	-0.1581	-0.04533
		0.000197	0.131457	0.131654
		-0.02511	0.096708	0.071598
		0.113604	-0.1493	-0.0357
		-0.02001	0.100756	0.080743
		0.011447	0.132897	0.144344
		0.092189	-0.16646	-0.07428
		0.018763	0.158719	0.177482
		-0.00215	0.1346	0.132451
		0.057696	-0.166	-0.1083
		0.030108	0.171819	0.201927

4. CONCLUSIONS

A comprehensive density functional theory (DFT) analysis of chlorobenzene, iodobenzene, and bromocyclohexane provides detailed insights into their structural and electronic properties. Transmittance spectra revealed distinct absorption bands corresponding to specific vibrational modes, with marked differences between compounds based on halogen substitution. Reduced-mass calculations support these vibrational differences, suggesting differences in bond rigidity and atomic mass effects. Fukui function analysis identified the most reactive sites to electrophilic, nucleophilic, and radical attacks, showing that iodobenzene exhibits higher nucleophilic reactivity (F^+), while bromocyclohexane exhibits a more balanced radical susceptibility (F^0). The Mulliken charge distribution also confirmed the variation in electron density affected by each halogen, with iodine exhibiting higher polarization and charge transfer. Ultraviolet-visible-near-infrared (UV-Vis-NIR) spectroscopy has provided a deeper understanding of electronic transitions, confirming conjugation effects in chlorobenzene and iodobenzene, and highlighting the low-energy transitions associated with larger halogens. The obtained result was presented to enhance our understanding of how molecular structure and halogen type influence the electronic behavior and chemical reactivity of these compounds, providing valuable data for use in materials science, pharmaceuticals, and organic synthesis.

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