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Analysis Of Chemical Bonding in the $C_{60}Br_2$ System Based on NBO, AIM, And Bond Topology Analysis

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ABSTRACT
Fullerene C_{60} is recognized as a carbon nanostructure with distinctive electronic, optical, and redox properties, making it a highly promising functional material. Although halogenation is an important strategy for modifying the properties of fullerenes, the interactions between heavy halogens and the fullerene surface require further investigation. This study evaluated the chemical bonding characteristics of the C_{60}–Br_2 system using computational approaches based on Natural Bond Orbital (NBO) theory, Atoms in Molecules (AIM) theory, and electron-density topology analysis. Geometry optimization revealed a Br–C interatomic distance of 2.07 Å, indicating a pronounced intermediate bonding character. Although structural visualization did not indicate the formation of a rigid conventional covalent bond, NBO analysis revealed significant orbital interactions, as reflected by the Wiberg Bond Index (WBI), while AIM analysis indicated weak and polarized bonding characteristics based on the topology of the electron density and its Laplacian, consistent with established computational criteria for characterizing bonding interactions in functionalized fullerene systems. Furthermore, topological analysis confirmed the presence of a bond critical point (BCP) with a negative local total energy density, indicating a stabilizing interaction between the bromine and carbon atoms. Overall, the C_{60}–Br_2 system exhibited bonding characteristics intermediate between classical covalent bonding and noncovalent interactions, suggesting that the Br–C interaction can be classified as a partially covalent, polarized interaction.

INTRODUCTION

C_{60} fullerene occupies a central position in nanotechnology because of its highly symmetric, hollow spherical structure and unique electronic characteristics. These attributes make fullerenes promising material candidates for advanced applications ranging from solar cells and energy storage systems to sensors and molecular electronic devices. The versatility of carbon in adopting different hybridization states enables the development of multidimensional materials that can be structurally modified to meet specific requirements. Surface modifications, such as metal doping or halogen substitution, have been shown to significantly modulate the electronic properties, adsorption energies, and chemical reactivity of the fullerene cage (Barzaga, 2023; Bauzá & Frontera, 2017; Lu, 2025; Mohammadi et al., 2023; Troyanov & Kemnitz, 2012). Computational approaches based on density functional theory (DFT) have become widely established for predicting the structural stability and electronic properties associated with these modifications. In particular, integrating Natural Bond Orbital (NBO) analysis with Atoms in Molecules (AIM) approaches enables an in-depth

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examination of orbital interactions and electron-density distributions, encompassing both covalent bonding and complex intermolecular interactions. Consequently, a detailed understanding of the electronic structure is crucial because bonding behavior is highly sensitive to the hybridization state of carbon atoms on the fullerene surface. These methodologies also facilitate visualization of electron-density distributions and identification of bond critical points (BCPs), thereby enabling characterization of the electronic and energetic factors responsible for stabilization in modified fullerene systems (Bąk et al., 2023; Chang et al., 2024; Echeverría & Álvarez, 2023; Kłos et al., 2024; Li et al., 2025).

Beyond their intrinsic structure, the effectiveness of fullerenes in practical applications depends strongly on surface modification. Functionalization, namely, the addition of specific functional groups or atoms to the carbon cage, has emerged as a crucial strategy for modulating the physicochemical properties, reactivity, and stability of these materials according to specific application requirements (Gergeroglu et al., 2020; Ibrahim, 2019; Manz, 2017; Saadat & Tavakol, 2015; Silant'ev, 2023; Xu et al., 2023).

In computational chemistry, advanced approaches such as DDEC6 atomic population analysis and the Quantum Theory of Atoms in Molecules (QTAIM) have become important tools for characterizing bonding interactions in carbon nanostructures, particularly for distinguishing the nature of bonding in substituted fullerenes. A comprehensive understanding of the relationship between molecular structure and electronic properties is essential because chemical modifications of the fullerene surface can substantially alter the electron-density distribution while simultaneously affecting the electronic stabilization mechanisms that govern molecular reactivity (Demiray, 2020; Limas & Manz, 2018; Mohammadi & Abdullah, 2021; Ngana et al., 2025).

Recent computational studies have also indicated that integrating techniques such as frontier molecular orbital (FMO) analysis and density of states (DOS) calculations is valuable for characterizing electronic structure and designing electronically engineered fullerene-based materials. The development of advanced computational databases for C_{20}–C_{60} systems has enabled correlations between topological features and thermodynamic stability to be mapped, providing an important foundation for predicting the reactive behavior of more complex fullerene derivatives. Furthermore, the ability of fullerenes to accept charge through sequential electron-capture processes represents an important aspect of understanding their electronic behavior during interactions with external chemical environments (Akpe, 2023; Berisha, 2023; Liu et al., 2024; Louis et al., 2022; Tiago et al., 2008).

Halogenated fullerenes constitute a widely studied class of fullerene derivatives because of their ability to alter the electronic properties, molecular structure, and reactivity of the C_{60} molecule. Computational studies employing density functional theory have demonstrated that interactions between fullerenes and halogen atoms such as F, Cl, and Br can significantly influence the molecular electrostatic potential (MEP) distribution and the reactivity of the carbon cage surface. Molecular electrostatic potential maps provide important information for identifying regions susceptible to electrophilic or nucleophilic attack, thereby facilitating a deeper understanding of interactions and bond formation between fullerene systems and surrounding species. The addition of halogen atoms to the fullerene surface can modify the electron-density distribution, enhance electron affinity, and affect the stability and electrical properties of the material. The symmetric and stable nature of the C_{60} cage makes it an appropriate platform for exohedral functionalization, in which atoms or functional groups bind to the outer surface to produce systems with distinctive bonding characteristics. This versatility enables the design of materials with specific functionalities, ranging from sensing applications to components of optoelectronic devices. Fluorinated and chlorinated fullerenes have frequently been reported as systems exhibiting relatively strong covalent interactions between halogen atoms and the fullerene carbon cage. In contrast, interactions involving bromine tend

to exhibit more complex and weaker bonding characteristics, which have been investigated in studies related to sensing and adsorption processes. As the atomic size of the halogen increases from F to I, the nature of the halogen–fullerene interaction may shift because of reduced orbital overlap, increased polarizability, and changes in charge-transfer behavior. This phenomenon is consistent with findings for various fullerene derivatives in which halogenation significantly affects optical properties and chemical reactivity, including potential applications as multifunctional additives in petroleum products. Consequently, halogenated fullerene systems provide useful models for investigating the transition between predominantly covalent bonding and noncovalent interactions.

The geometry optimization results obtained in this study revealed an intriguing trend across the halogen series. In the $C_{60}F_2$ and $C_{60}Cl_2$ systems, the halogen atoms appeared to be directly bonded to the fullerene surface, a configuration that can be interpreted as covalent functionalization. In contrast, in the $C_{60}Br_2$ system, the bromine atoms appeared to be detached from the fullerene surface, and visualization of the optimized geometry did not display an unambiguous covalent Br–C bond. This observation raises a fundamental question: do the bromine atoms truly fail to form a chemical bond with the fullerene, or does an interaction persist that cannot be adequately characterized from molecular geometry alone?

This question provides the rationale for further investigation using Natural Bond Orbital (NBO) analysis, Atoms in Molecules (AIM) theory, and electron-density topology analysis. These complementary approaches were employed to determine whether the Br–C interaction in the $C_{60}Br_2$ system exhibits characteristics consistent with chemical bonding despite the absence of clear geometric evidence in the optimized structure. Although halogenated fullerenes such as $C_{60}F_2$ and $C_{60}Cl_2$ are typically regarded as systems involving covalent bond formation between halogen and carbon atoms, interactions involving heavier halogens, particularly bromine and iodine, present distinct theoretical complexities. The nature of these interactions may deviate from classical covalent bonding and instead span a continuum between covalent and noncovalent interactions, requiring electronic-structure and topological analyses for accurate characterization. Advances in the understanding of halogen bonding and noncovalent interactions have demonstrated that chemical stabilization is not limited to the formation of conventional covalent bonds. Interactions involving partial charge transfer, electron polarization, and limited orbital overlap can also contribute substantially to molecular stabilization. In this context, the $C_{60}Br_2$ system is of particular interest because, although the bromine atoms appear visually detached from the fullerene surface, the system retains an energetically stable configuration. This interpretation is consistent with theoretical and experimental investigations showing that halogen bonding, characterized by an attractive interaction involving an electrophilic region associated with a halogen atom and an electron-rich region of another molecular entity, can contribute to supramolecular stabilization in C_{60}-based systems.

This study aimed to identify the existence and nature of the interaction between bromine and carbon atoms in the $C_{60}Br_2$ system using Natural Bond Orbital (NBO) analysis, Atoms in Molecules (AIM) theory, and electron-density topology analysis. The findings are expected to contribute to the characterization of bonding transitions in halogenated fullerene systems, particularly by clarifying the boundary between covalent bonding and noncovalent interactions, a distinction that can become ambiguous in systems involving heavier halogen atoms. From the perspective of theoretical chemistry, the findings contribute to a fundamental understanding of halogen-mediated interactions in carbon nanostructures, particularly by clarifying intermediate bonding regimes involving heavier halogens. From a materials science perspective, characterizing these intermediate bonding regimes in halogenated fullerenes may facilitate the design of functional materials with tunable electronic properties for optoelectronic and energy-storage applications. From a computational chemistry perspective, the multimethod

framework employed in this study may provide a useful reference for examining other molecular systems with ambiguous bonding characteristics. Ultimately, this study contributes to broader efforts to characterize bonding transitions in halogenated fullerene systems, which are important for the rational design of fullerene-based functional materials.

METHOD

This study employed a quantum chemical computational approach to investigate the $C_{60}Br_2$ system. Molecular geometry optimization was performed using Gaussian 09 software at the B3LYP/6-31G level of theory, followed by visualization with GaussView. The optimized structures were used for subsequent electronic analyses. Natural Atomic Orbital (NAO) analysis and the Quantum Theory of Atoms in Molecules (QTAIM) were applied to evaluate topological parameters, including electron density and energy density at bond critical points (BCPs), to characterize the Br···C interactions. The specific interactions examined involved Br(61)–C(5) and Br(62)–C(45).

Atoms in Molecules (AIM) analysis was performed using Multiwfn software based on wavefunctions obtained from the quantum chemical calculations. Topological parameters, including electron density (ρ), the Laplacian of electron density ($\nabla^2\rho$), and local energy density, were evaluated to characterize the bonding interactions. These parameters were used to distinguish covalent from non-covalent interactions and to identify relevant bond paths and critical points within the electron density distribution.

A subsequent topological analysis focused on identifying BCPs between the bromine and carbon atoms. The presence of a BCP and the corresponding local energy density, H, were evaluated to assess whether the identified interactions contributed to stabilization of the system. Electron density (ρ) and its Laplacian ($\nabla^2\rho$) at the BCPs were analyzed to differentiate covalent and non-covalent character. These parameters were also used to evaluate the Br···C interactions when relatively large interatomic distances were observed. The analysis was consistent with quantum topological approaches used to characterize halogen interactions involving charge transfer and electron polarization .

Additionally, the Electron Localization Function (ELF) was calculated using Multiwfn to examine localized electron regions and the possible involvement of lone pairs in polarized Br···C interactions. The resulting electron localization basins were used to support the assessment of charge redistribution and to determine whether the interactions exhibited appreciable covalent character or were predominantly electrostatic.

RESULT AND DISCUSSION

Optimized Geometry and Interaction Trend

Visual examination of the optimized geometries revealed a progressive weakening of the halogen–fullerene interaction as atomic size increased. In $C_{60}F_2$ and $C_{60}Cl_2$, the halogen atoms occupied positions consistent with distinct covalent C–X bonds. In $C_{60}Br_2$, however, the bromine atoms shifted away from the fullerene surface and no conventional covalent bond was visually apparent. The interaction became even weaker in $C_{60}I_2$. This trend indicates that geometry alone cannot determine whether the heavier halogens form genuine chemical bonds or merely van der Waals contacts; electron-density, orbital, and energy-decomposition analyses are required to distinguish these regimes.

Table 1. Comparison of Structures and Interaction Characteristics in $C_{60}Hal_2$ Systems

System	Total energy	Interaction character

$C_{60}F_2$	−6,526,547	Strong covalent bond
$C_{60}Cl_2$	−8,418,795	Covalent bond
$C_{60}Br_2$	−19,506,359	Intermediate interaction
$C_{60}I_2$	Not reported	Weak interaction or no bond/reaction

Note: Energy values are reproduced from the original table; the source does not specify their units.

Source: Author's calculation and classification based on NBO, AIM, and topology; criteria adapted from; $C_{60}I_2$ trend from.

The optimized Br–C separation was approximately 2.07 Å, placing $C_{60}Br_2$ at an energy minimum compatible with an interaction, although the molecular visualization did not display an explicit conventional bond. The discrepancy between geometric proximity and visual bond representation highlights the need for quantitative descriptors. QTAIM criteria commonly associate low electron density and a positive Laplacian at a bond critical point with a polarized closed-shell or van der Waals-dominated interaction rather than a classical covalent bond. Energy decomposition further separates electrostatic stabilization, dispersion, exchange-correlation, and charge-transfer contributions, thereby preventing partial orbital overlap from being overinterpreted as full covalency.

NBO and Wiberg Bond Index

Natural Bond Orbital analysis identified Wiberg bond indices of approximately 0.8198 for Br(61)–C(5) and 0.8199 for Br(62)–C(45), summarized in the discussion as about 0.8. Although these values remain below the conventional value for a standard single covalent bond, they substantially exceed values expected for a purely nonbonding contact and therefore indicate meaningful orbital overlap. The NBO result supports a partial covalent contribution and measurable electron delocalization between bromine and carbon. Nevertheless, a nonzero Wiberg index does not by itself establish a classical covalent bond because highly polarized closed-shell interactions may also exhibit limited charge transfer and orbital mixing.

This interpretation is consistent with energy-decomposition studies of related halogen-bonded systems, in which electrostatic and dispersion terms dominate while charge transfer makes a smaller contribution. Natural Energy Decomposition Analysis similarly shows that charge transfer can remain marginal relative to electrostatic stabilization, reinforcing the need to separate orbital evidence from the total interaction mechanism. Thus, the NBO data demonstrate that the Br···C contact is chemically meaningful, but its bonding character must be interpreted together with electron-density topology and energetic contributions.

AIM, Electron-Density Topology, and Energy Decomposition

Atoms in Molecules analysis produced small positive Laplacian values of approximately 0.1 for both Br–C pairs, indicating a strongly polarized closed-shell interaction. The calculated values were about 0.11926641 for Br(61)–C(5) and 0.11941246 for Br(62)–C(45). This pattern represents a transition between a classical covalent bond and a stable noncovalent interaction. The presence of bond critical points and low electron density is typical of halogen-bonded systems and agrees with the limited charge-transfer contribution inferred from NBO and noncovalent-interaction analyses.

The energy-decomposition interpretation further indicates that charge transfer contributes only about 10% of the total interaction energy, while electrostatic and dispersion forces dominate. ETS-NOCV analysis likewise showed that electrostatic stabilization exceeds orbital stabilization; for comparable bromine derivatives, the $\Delta E\_elstat/\Delta E\_orb$ relationship approaches 2:1, although the leading density-deformation channel still reflects partial donor-to-antibonding σ^*(C–Br) charge transfer. These findings place $C_{60}Br_2$ in an intermediate regime: orbital interaction is explicitly measurable but remains subordinate to electrostatic and dispersive stabilization.

Topological analysis provided direct evidence of electron-density pathways between bromine and carbon at bond critical points 98 and 119. At critical point 98, the reported electron

density was 0.1151855144 and the local energy density H(r) was negative, approximately −0.05265455204. A negative local energy density signifies net electronic stabilization and indicates that the interaction is stronger than a passive van der Waals contact. The coexistence of a bond path, negative H(r), a positive Laplacian, and limited charge transfer reflects a strongly polarized interaction that contains both closed-shell and partial covalent features.

Integrated Interpretation and Material Implications

Taken together, geometry optimization, NBO, AIM, noncovalent-interaction mapping, molecular electrostatic potential analysis, and energy decomposition produce a consistent picture. Bromine is not merely positioned near the fullerene surface: it participates in a real stabilizing interaction. NBO captures orbital overlap and partial electron delocalization, whereas AIM identifies the continuity and topology of the electron density. Their quantitative differences are complementary rather than contradictory because each method measures a different aspect of a highly polarized bond. The σ-hole and surface-charge distribution influence the direction and strength of the interaction, while dispersion, electrostatics, polarization, and partial charge transfer collectively determine stability.

Accordingly, $C_{60}Br_2$ should not be forced into a binary classification as either a purely covalent compound or a purely noncovalent complex. It occupies an intermediate bonding continuum characterized by significant but incomplete orbital overlap, a polarized closed-shell topology, stabilizing bond critical points, and dominant electrostatic and dispersion components. This conclusion also explains why a single descriptor, such as bond length or Wiberg index, is insufficient; robust characterization requires a multi-method framework combining geometry, orbital theory, electron-density topology, and energy decomposition.

The stable yet potentially reversible intermediate interaction has practical relevance for fullerene functionalization. Controlled bromination may tune adsorption, surface reactivity, electronic coupling, and photophysical behavior without severely disrupting the conjugated π-framework. These properties are relevant to molecular electronics, photovoltaics, energy storage, sensors, and engineered supramolecular assemblies. The results therefore provide both a theoretical basis for interpreting heavy-halogen interactions on carbon nanostructures and a design principle for materials whose stability and reversibility depend on a controlled balance among electrostatics, dispersion, polarization, and partial covalency.

CONCLUSION

This study successfully demonstrated, through the integration of NBO analysis, AIM analysis, and electron-density topology, that the interaction between bromine and carbon atoms in the $C_{60}Br_2$ system was not adequately described as a purely conventional non-covalent interaction but instead exhibited significant intermediate bonding character. NBO analysis indicated appreciable orbital interactions consistent with a covalent contribution, whereas AIM analysis revealed a polarized bonding character. The presence of a bond critical point (BCP), together with a negative local energy density (H) value in the topological analysis, indicated that the interaction contributed to stabilization of the system through effects extending beyond a purely electrostatic description. Nevertheless, alternative interpretations remain relevant, as several studies have shown that halogen interactions may be described predominantly through electrostatic and polarization effects without requiring a substantial charge-transfer contribution. Accordingly, any assignment of covalent character should be made cautiously and on the basis of multiple complementary descriptors. The $C_{60}Br_2$ system may therefore be regarded as exhibiting intermediate bonding character at the boundary between covalent and non-covalent interactions, highlighting the important role of orbital polarization in fullerene functionalization by heavy halogens. This interpretation is consistent with recent literature emphasizing the role of halogen interactions in molecular recognition and self-assembly processes in supramolecular materials. Furthermore, the ability to modulate electronic

properties through directional interactions may contribute to the design of photovoltaic materials and carbon-based optoelectronic devices that require precise control of molecular geometry. Systematic tuning of interaction strength, particularly through σ-hole modulation and charge-transfer contributions, may facilitate optimization of charge transport and light absorption. Incorporating such design strategies into carbon-based molecular architectures may also enhance material stability and provide greater flexibility in tuning electronic properties, including the energy gap, for specific applications.

Furthermore, the consistency between topological parameters and orbital descriptors indicated that the bonding character in the $C_{60}Br_2$ system could not be adequately represented by a single quantitative parameter. Although the Wiberg bond index was relatively low compared with values typically associated with strong covalent bonds, the presence of a BCP together with a negative local energy density (H) suggested electron-density redistribution associated with an interaction that extended beyond a simple closed-shell electrostatic description. These findings placed the system within an intermediate interaction regime. The covalent contribution in the halogenated fullerene appeared to arise from the combined effects of orbital polarization, partial charge transfer, and electrostatic interactions, producing an electronic structure intermediate between predominantly closed-shell interactions and conventional covalent bonding. This interpretation was consistent with contemporary descriptions of halogen bonding as a continuum of interaction character rather than a strict covalent/non-covalent dichotomy.

This study also demonstrated that characterizing bonding in halogenated fullerene systems required a multimethod approach integrating structural analysis, electron-density topology, orbital analysis, and energetic descriptors. No single method was sufficient to fully characterize the Br···C interaction. Instead, the agreement among geometry optimization, NBO analysis, AIM analysis, and topological descriptors provided a stronger basis for interpreting the interaction than reliance on any individual indicator. The study therefore provided a comprehensive analytical framework for distinguishing covalent, non-covalent, and intermediate-regime interactions in halogenated nanocarbon systems, with potential applicability to other functional carbon materials. Nevertheless, the analysis was limited to ground-state quantum chemical calculations and did not account for temperature effects, solvent environments, or molecular dynamics that could influence the stability and character of the Br···C interaction. Future studies could combine the present approach with ETS-NOCV or SAPT calculations to quantify individual interaction-energy components more precisely, ab initio molecular dynamics simulations to assess dynamic stability, and experimental validation using appropriate high-resolution spectroscopic or microscopic techniques. Such an integrated approach could further clarify the mechanism underlying intermediate bonding in halogenated fullerenes and strengthen the scientific basis for developing functional carbon materials for optoelectronic, energy-storage, and nanotechnology applications. Overall, the $C_{60}Br_2$ system provided a representative example of intermediate bonding in halogenated carbon nanostructures, in which orbital polarization, partial charge transfer, and electrostatic effects collectively produced a stabilized interaction bridging predominantly non-covalent and covalent regimes. This finding has important implications for the rational design of functional fullerene-based materials.

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