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A computational study to compare some plastic polymers with potassium bromide using density functional theory and UV-Visible spectroscopy

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Abstract
This study presents the value of computer simulation in a comparative analysis of some of the most common polymers (polyamide, polyethylene, and polycarbonate) used in the plastics industry. The introduction of density functional theory (DFT) has greatly facilitated the application of computational science to these materials, in addition to the calculation of UV-visible spectra. The objective of this study was to ascertain the potential of these calculations to elucidate and compare polymers when mixed with a potassium bromide promoter. The most favorable result was observed for polyethylene, where the highest internal energy was 3812.125698 Hartree and the lowest polar moment was 8.417560 Debye. This resulted in a reduction of the total charge between the potassium bromide complex and polyethylene. Additionally, the highest UV absorbance was 800.00 nm, thus making it the safest of the remaining polymers. This provides assurance that when used as a carrier for any baked goods where potassium bromide has been used as a strengthening agent, it is the optimal choice.

Keywords: Polyamide, Polyethylene and Polycarbonate, Potassium bromide, DFT, UV-visible.

INTRODUCTION

The history of plastic production can be traced back to the mid-19th century. However, the modern era of plastics manufacturing did not begin until the early 20th century, with the development of Bakelite, the first fully synthetic plastic. Subsequently, significant developments in polymer chemistry have resulted in the creation of an extensive range of plastics, which have had a transformative impact on sectors such as packaging, transportation, construction, and healthcare (Carwile et al., 2011).

A multitude of plastic polymers are utilized in food packaging. The plastic polymers employed in food packaging can be categorized according to their chemical composition and properties. The most prevalent polymer employed is polyamide (PA) in figure 1, which is a polymer comprising imide groups and is categorized as a high-performance plastic. Polyamides possess exceptional heat resistance, rendering them suitable for a multitude of applications in contexts where durable organic materials are required, including high-temperature fuel cells, displays, and various military applications.(Braun et al., 2013), Furthermore, polyamide resin is employed as an insulating layer in the fabrication of integrated circuits and microelectromechanical system chips. Polyamide films demonstrate optimal mechanical elongation and rigidity, which is beneficial for grip between polyamide layers or between a polyamide film and a stored metal layer. (Krakuer, 2006) The minimal interaction between the gold foil and the polyamide film, coupled with the high temperature stability of the polyamide film, results in a robust framework that provides reliable protection when subjected to diverse forms of natural stress. Furthermore, polyamide is employed as a substrate for mobile phone radio wires (Ono & Erhard, 2011).

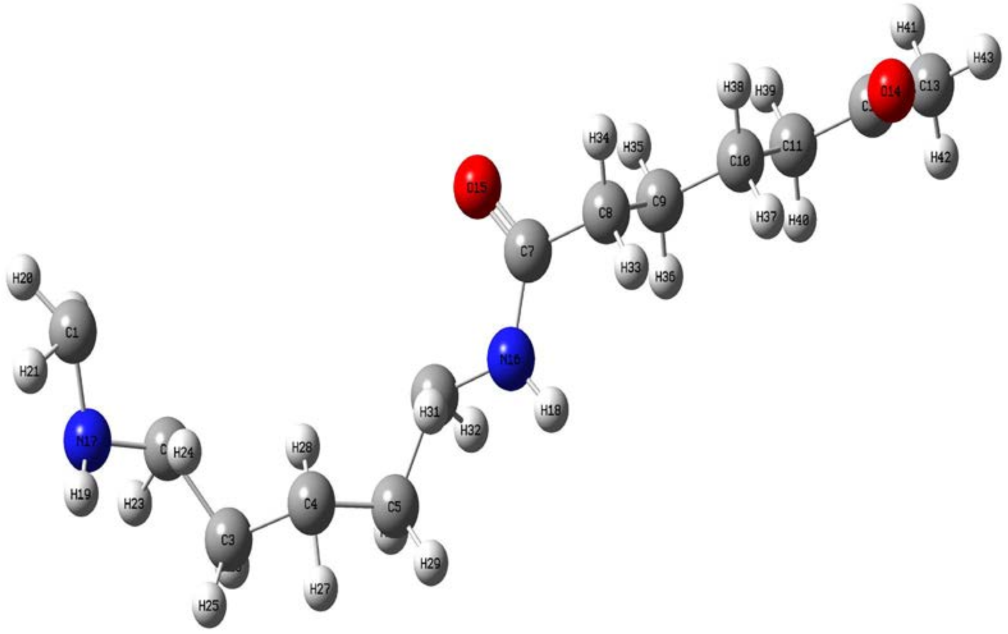

Figure: (1). The spatial structure of the polyamide composite

Polyethylene is a material that is widely employed in the packaging of foodstuffs due to its low cost, versatility, and ability to protect against moisture and synthetic chemicals Figure 2. The most commonly utilized forms of polyethylene in packaging applications are high-thickness polyethylene (HDPE) and low-thickness polyethylene (LDPE). They are the most widely manufactured plastic. HDPE is a polymer that is employed primarily for packaging purposes, including plastic sacks, plastic films, geofilms, and containers such as bottles. (Whiteley et al., 2000) Beginning in 2017, the production of polyethylene tars reached 100 million tons per year, accounting for 34% of the global plastics market.(Geyer et al., 2017), Plastics Europe.

Archived from the original on 4 February 2018] The polyethylene family encompasses a number of known types, the synthetic recipe of which is $(C_2H_4)_n$. Polyethylene is typically a blend of undifferentiated polymers of ethylene, exhibiting a range of advantageous properties. It can be classified as either low-density or high-density or alternatively, as one of the numerous transitional varieties.(Yao et al., 2022) Additionally, the material's properties can be modified through cross-linking or copolymerization. All structures are non-toxic and possess compound adaptability, which contributes to polyethylene's prominence as a flexible plastic. Furthermore, polyethylene's chemical versatility renders it resistant to degradation and corrosion when improperly discarded. As a hydrocarbon, polyethylene is characterized by a lack of impurities and coloring agents and is combustible. (Sepe, 2024).

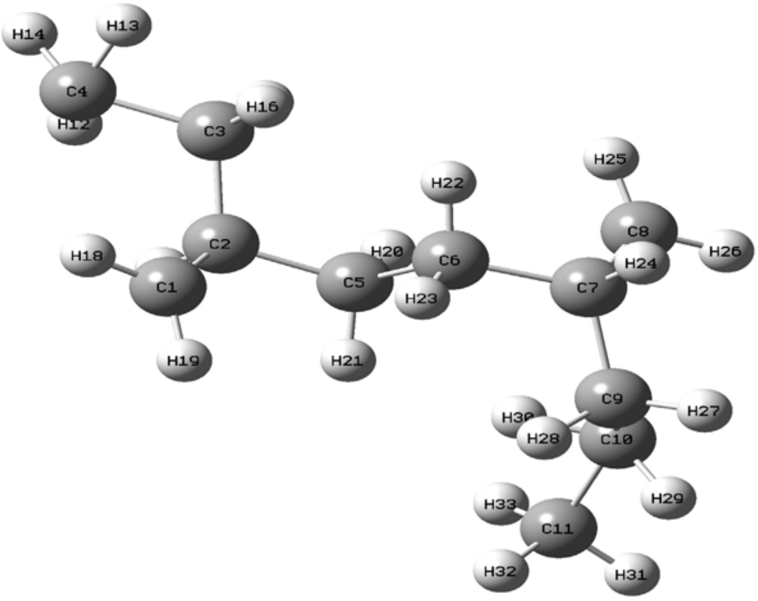

Figure:(2). The spatial structure of the polyethylene composite

Polycarbonate (PC) is a thermoplastic polymer comprising carbonate groups within its intrinsic structure Figure 3. The polycarbonates employed in the construction of various products are distinguished by their strength and versatility, with specific grades additionally exhibiting optical transparency. The aforementioned materials can be readily manipulated through processes such as shaping and thermoforming. As a consequence of these characteristics, polycarbonate is employed in a multitude of applications. Polycarbonate does not possess a unique serial number identification code (RIC).(Lexan sheet technical manual, 2015), The extensive deployment of polycarbonate in electronic applications contributes to the overall security profile of these devices. It functions as an efficacious electrical insulator, exhibiting both high-voltage and heat resistance properties. Consequently, it is utilized in the mechanical assembly of power organizations and broadcast communication equipment. It can be utilized as an electrical insulator in high-strength capacitors. (Serini, 2000).

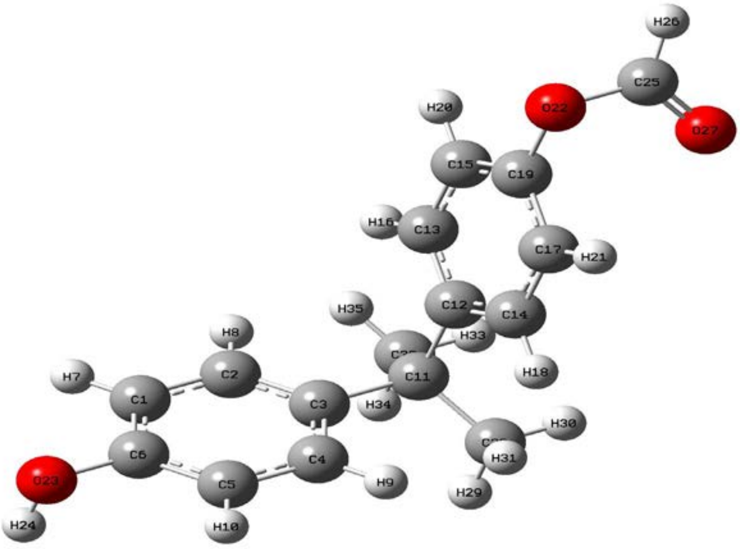

Figure: (3). The spatial structure of the polycarbonate composite

The use of plastic polymers has become ubiquitous in contemporary culture, assuming a pivotal role in numerous facets of daily life. The flexibility, durability, and cost-effectiveness of these materials have facilitated their extensive utilization across a diverse range of industries, including food and beverage packaging, medical services, electronics, and automotive manufacturing. (Kubwabo et al., 2009), Although plastic polymers offer a number of advantages, their unavoidable use has also given rise to concerns about the potential for contamination of natural materials, particularly in light of the potential risks associated with the presence of added substances and impurities. One such risk is the potential for substance migration, whereby plastic materials may transfer harmful synthetics into foodstuffs via an interaction known as migration. The rate and degree of compound movement can be influenced by a number of factors, including temperature, contact time, and the corrosiveness of the food in question. Furthermore, the movement of substances from plastic packaging to food occurs via various pathways that may be influenced by temperature.

The process of dispersion refers to the movement of particles from an area of higher concentration to an area of lower concentration. The transfer of synthetic compounds from plastic packaging to foodstuffs can occur via the process of diffusion. (González-Sálamo et al., 2018), As atoms move from areas of high fixation (e.g., plastic) to areas of low focus (e.g., food), the rate of dispersion can be significantly accelerated by elevated temperatures, thereby expediting the relocation of designed materials into food. In order to address these difficulties, a number of measures have been implemented. These include improvements to biodegradable plastics, which form the basis of reuse programs, and the implementation of administrative measures with the specific aim of monitoring plastic waste and promoting the use of financial packaging arrangements.(Rhim & Ng, 2007).

A variety of contextual analyses conducted in authentic settings have identified the potential risks associated with the relocation of synthetic compounds from plastic bundling materials utilized for food storage and organization. For example, a review published in Ecological Well-Being Perspectives found that plastic containers designed for microwave warming delivery may leach BPA and phthalates into food, potentially exposing consumers to harmful synthetic compounds. Furthermore, studies examining the transfer of synthetic compounds from plastic baby bottles and food containers have highlighted potential health concerns regarding the use of these items, particularly for infants and young children., There has been a notable increase in consumer awareness and concerns about the safety of plastic food packaging in recent years. This is driven by a combination of growing scientific evidence and media coverage that has highlighted the potential health risks associated with the use of plastics in food packaging.

These risks are attributed to the cost-effectiveness and versatility of plastics, which have become ubiquitous in food packaging. Plastic materials, which are pervasive in food packaging due to their cost-effectiveness and versatility, have been subjected to intensifying scrutiny regarding their capacity to leach potentially harmful chemicals into food, particularly under conditions of heat or acidity.(Geyer et al., 2017), An additional creative methodology entails the integration of dynamic fixings into plastic bundling materials, with the objective of extending the usability period of transient food sources and reducing food waste. For example, antimicrobial additives can be incorporated into packaging materials to inhibit microbial growth and extend the shelf life of packaged food products. Similarly, the use of oxygen scavengers and moisture scavengers can prevent oxidation and decay, thereby maintaining the quality and safety of packaged items. (Thompson et al., 2009), Nevertheless, the extensive adoption of novel packaging technologies gives rise to a number of challenges and constraints. A significant challenge is to guarantee that new packaging materials and additives comply with the relevant regulatory requirements and safety standards. It is incumbent upon regulatory agencies to subject new packaging solutions to exhaustive testing and evaluation in order to ascertain their safety with respect to food contact and environmental impact. Furthermore, the expansion of production operations for novel packaging technologies may necessitate substantial investments in equipment and infrastructure, in addition to a meticulous examination of supply chain logistics and associated costs (Ragaert et al., 2017).

Despite these challenges, continued technological advances hold the promise of enhancing the safety, sustainability, and performance of plastic packaging. By employing innovative materials, coatings, and manufacturing processes, the industry can address consumer concerns regarding chemical migration while simultaneously reducing its environmental impact and enhancing food security (Kefeni et al., 2011). Moreover, the current analytical techniques employed for the detection and quantification of migrating chemicals in food samples may lack the requisite sensitivity or specificity for some compounds, particularly those of an emerging nature or degradation products of plastic polymers. It is imperative that methodological advances be made in order to improve the accuracy, precision, and throughput of analytical techniques, thereby allowing for more comprehensive screening of a wider range of chemicals at trace levels (Groh et al., 2017).

In order to address these complex research questions, it will be essential to engage in interdisciplinary collaboration between food scientists, materials engineers, toxicologists, and analytical chemists. An interdisciplinary approach that integrates experimental studies, computational modeling, and risk assessment frameworks can facilitate a comprehensive understanding of the factors that influence chemical migration and their potential health effects (Muncke, 2009), Although significant progress has been made in understanding the effects of plastic polymers on hot food, there are still knowledge gaps and research methodologies that require further investigation. By addressing these gaps and adopting a multidisciplinary approach, researchers can advance their understanding of this complex issue and develop evidence-based strategies to mitigate potential risks to human health and food safety (Wagner & Oehlmann, 2011).

One of the most well-known additives that has significantly influenced its incorporation into polymer plastic molecules is potassium bromide. Modern salt was extensively employed as an anticonvulsant and narcotic throughout the late nineteenth and mid-twentieth centuries, with over-the-counter use becoming prevalent in the United States by 1975. The pharmacological action of this substance is attributed to the bromide ion, and sodium bromide has a similar effect. Potassium bromide Figure 4 is employed in the treatment of epilepsy in canines as a veterinary pharmaceutical.
The white crystalline powder that constitutes potassium bromide is its typical physical form under standard conditions. The problematic substance is insoluble in acetonitrile; however, water has the capacity to dissolve it. In a diluted aqueous solution, potassium bromide has been described as having a sweet flavor. However, at higher concentrations, the substance is perceived as bitter, and at even higher concentrations, it is perceived as salty. The characteristics of the potassium ion are the primary cause of these effects. The perception of sodium bromide as salty remains constant regardless of the concentration. At elevated concentrations, it has been demonstrated that potassium bromide is a significant irritant to the gastric mucosa, resulting in symptoms such as nausea and vomiting. This phenomenon is not exclusive to potassium bromide, as it is a common occurrence in soluble potassium salts (ChemIDplus, 2014).

Until 1975, bromide was present in a number of over-the-counter medications in the United States. This was due to the fact that bromide compounds, particularly sodium bromide, were outlawed from such products due to their chronic toxicity. Such products included the original formulation of Bromo-Seltzer. The long half-life of bromide in the body presented a challenge in determining the appropriate dosage without adverse effects. As a consequence of the advent of a plethora of superior sedatives with shorter durations of action, bromide was no longer employed for medical purposes in the United States at this juncture (Adams, 1907).

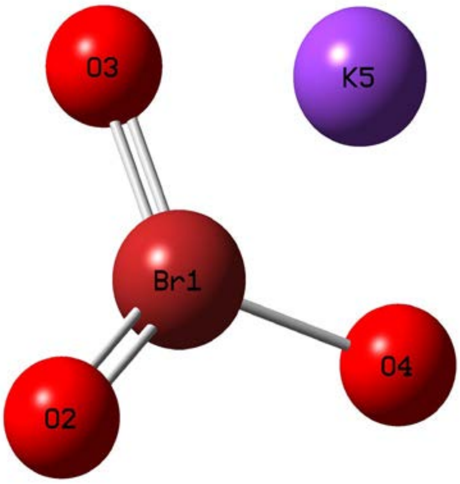

Figure: (4). The spatial structure of the potassium bromide complex

The objective of this study is to quantify the migration of chemicals from plastic polymers to heated foods, which represents a significant hazard to human health. The objective of this study is to ascertain which types of plastic are the most stable and prevent the interaction of plastic particles with potassium bromide on baked foods, and to determine their ability to withstand the surrounding conditions. This will be achieved by simulating their interaction with potassium bromide, a food improver used to improve the specifications of bread and baking.

MATERIALS & METHODS

The study of electron behavior through mathematical approximations concerns the examination of the properties of matter. Consequently, the equations of quantum mechanics were initially employed solely for single-electron systems. Over time, a plethora of mathematical techniques have been devised to approximate solutions for many electron systems through computational means (Esposito et al., 2004).

The significance of quantum computing emerged from the inability of classical physics to elucidate certain phenomena, including the blackbody effect, the photoelectric effect, the Kempton effect, and other such occurrences. (Rai-Choudhury, 1997) The geometric structures of the complexes were constructed on the foundation of the structures derived from the crystal parameters furnished by Cambridge Structural and were subsequently optimized through the utilization of the Density Functional Theory (DFT) method, employing the Gaussian 09 software package. The initial geometries of the compact complexes were constructed using HyperChem version 8.0, developed by Hypercube, Gainesville, FL, USA.

The objective of the geometry optimization process is to ascertain the position of the stable point at which the molecule is most stable. The stable point may be identified as the minimum energy configuration, which is indicative of the molecular system being most stable at low energies (Natelson et al., 2000)

The process of optimizing the input structure in order to reach the transition state structure commences with a structure that exhibits a lower energy state. The calculation of vibrational frequencies is frequently undertaken subsequent to the identification of the stable point through the process of geometry optimization (Tsuji, 2015). The DFT method is a frequently employed technique for calculating electron density in a diverse array of compounds. It is employed in the treatment of large molecules in computational chemistry, where it is particularly advantageous. A quantum chemistry approach based on the Schrödinger equation is the DFT method.(Natelson et al., 2000). B3LYP is a widely employed methodology in the field of chemical systems, primarily due to its high degree of accuracy in determining the final geometry, approximate structural formula, final energy, and bond lengths. It is also crucial to consider the internal bond lengths and angles (Tsuji, 2015).

RESULTS & DISCUSSION

The results and discussion demonstrate the significance of examining the total energy and the spectrum of absorbed ultraviolet rays, in addition to the polar moment, which encapsulates the strength of the activity of the physically interfering compounds between the polymers used with potassium bromide. As illustrated in Table 1, the lowest polar moment was observed for polyethylene, which exhibited the highest absorption and a relatively high energy level among the other polymers. Conversely, there is a marked increase in the polar moment of potassium bromide and a notable reduction in energy, which renders it highly stable. However, this increased stability may pose a risk if the permitted limit is exceeded in the bread and baking industry. Accordingly, the utilization of a specific type of plastic for polymers with a low polar moment was imperative to circumvent interference and absorption within the ultraviolet spectrum. This phenomenon was observed in the case of the polymer (polyethylene) in its individual state. However, to gain a comprehensive understanding of the interplay between the components and to ascertain the most optimal configuration, computational integration is essential. This will facilitate the identification of the lowest polar moment, which will ultimately determine the most active component and the most suitable integration strategy. This is a provisional measure.

Table 1: Energy of the polymers polyamide, polyethylene, polycarbonate and potassium bromide individually.

Structure	EN, hartree	Dipole moment, Debye	UV-Vis, nm
PA	- 769.644140	7.642117	750.00
PE	- 431.592646	1.641764	786.00
PC	- 844.570386	2.410575	265.03
KBr	-3382.703071	10.748100	760.00

As evidenced in Table 2, there is a notable discrepancy in the total internal energy values of the polymer complexes with potassium bromide. Among the polymers, polyethylene exhibits the most favorable interaction with bromide, characterized by a low polar moment and high absorption. While the energy remains relatively high for the other polymers, it has decreased significantly from its single-case value.

Table 2: Energy of complexes formed between polymers and potassium bromide.

	KBr		
	EN, hartree	Dipole moment, Debye	UV-Vis, nm
PA	- 4166.32120	23.207191	760.00
PE	-3812.125698	8.417560	800.00
PC	-4241.374936	16.330985	680.00

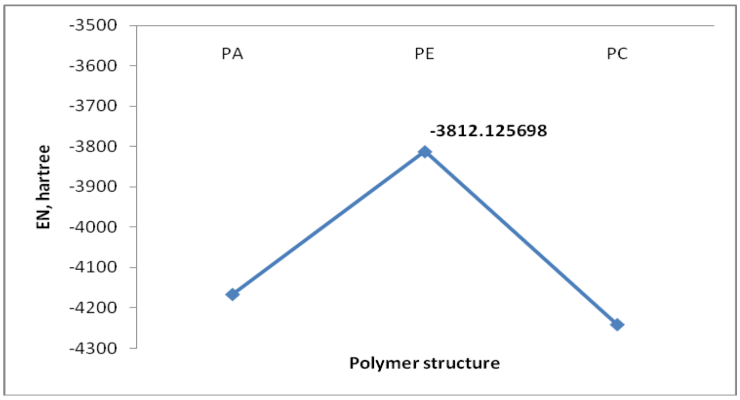

Figure: (5). Energy of complexes combined between polymers and potassium bromide

The energy of the polymer complexes combined with potassium bromide exhibits a discernible distinction in figure 5. In this regard, polyethylene displays the most notable energy profile, imparting heightened activity without undue interference over an extended duration. This distinguishes it from the other polymers, which exhibit less pronounced energy profiles.

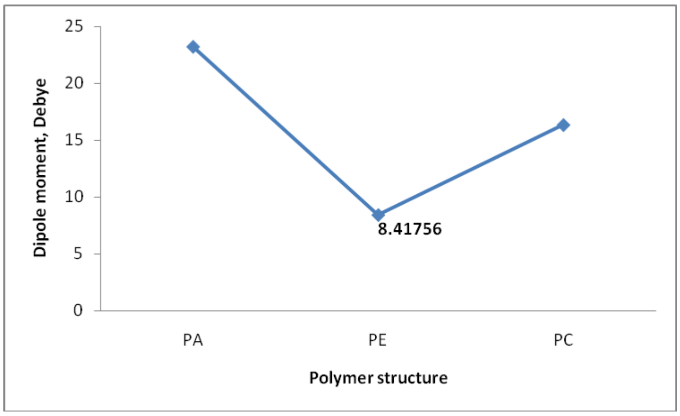

Figure: (6). Polar moment values for the complexes combined between polymers and potassium bromide

Figure 6 illustrates a reduction in the polar moment value for the polyethylene-potassium bromide mixture, which lends further support to the use of polyethylene plastic as a safe carrier. This is due to the decrease in bromide activity, which is reduced to a lower degree among the other polymers used.

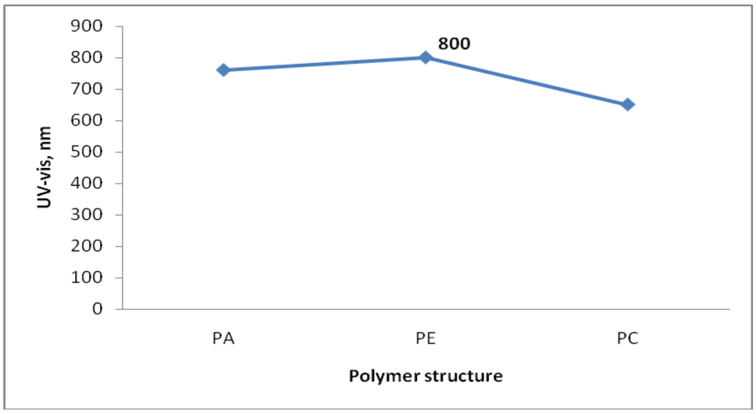

Figure: (7). UV spectrum curve of the complexes combined between polymers and potassium bromide

The UV absorption spectrum of polyethylene complex with potassium bromide, as illustrated in Figure 7, exhibits the highest absorption rate of polymers under consideration. This result corroborates the suitability of polyethylene as a safe carrier in the presence of bromide. The subsequent figures (8, 9, 10, 11, 12, and 13) illustrate the integrated complexes and simulated UV absorption spectrum of samples of polymers, namely polyamide, polyethylene, and polycarbonate with potassium bromide. It is notable that there is a discernible difference in the absorption curves.

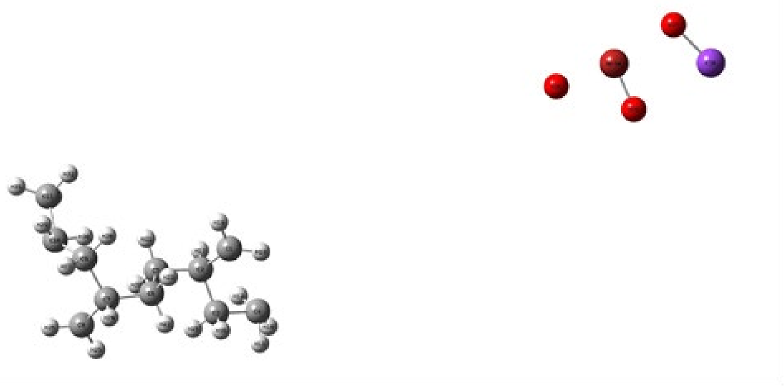

Figure 8: (9). Polyamide integrated with potassium bromide

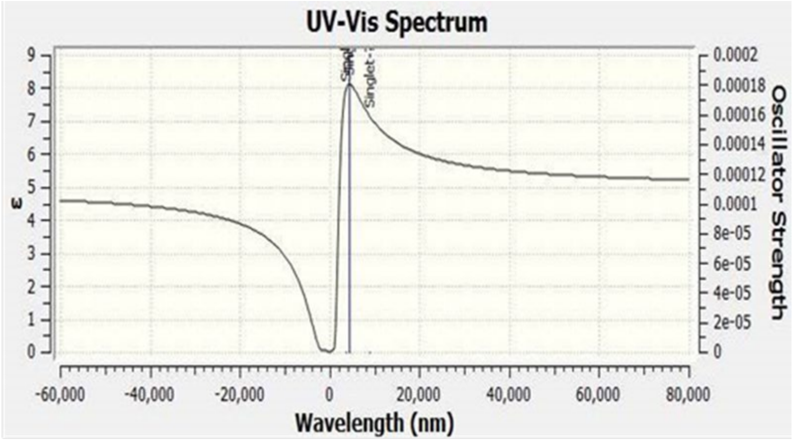

Figure : (9). UV spectrum curve of polyamide complex with potassium bromide

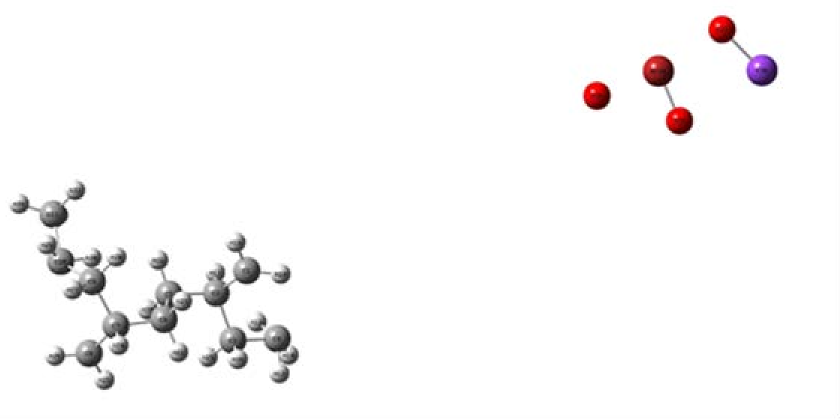

Figure: (10). Polyethylene combined with potassium bromide

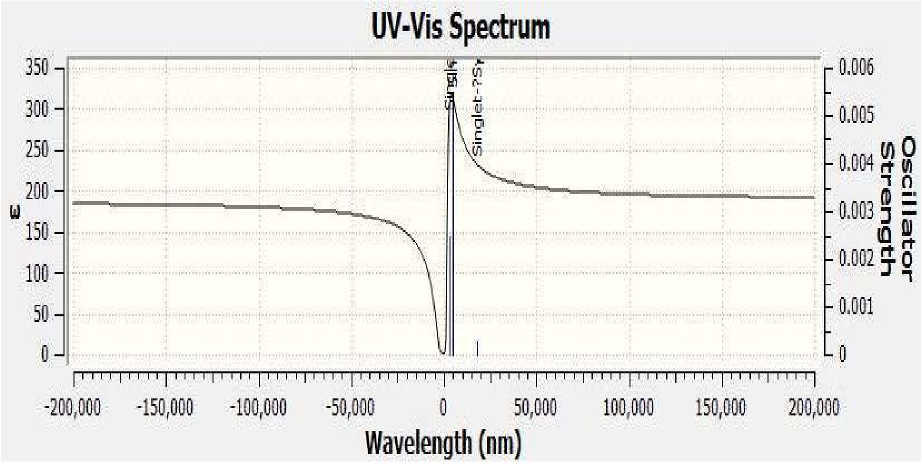

Figure: (11). UV spectrum curve of polyethylene complex with potassium bromide

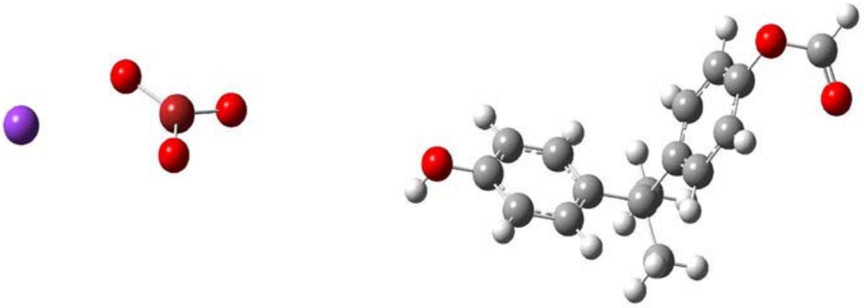

Figure: (12). Polycarbonate combined with potassium bromide

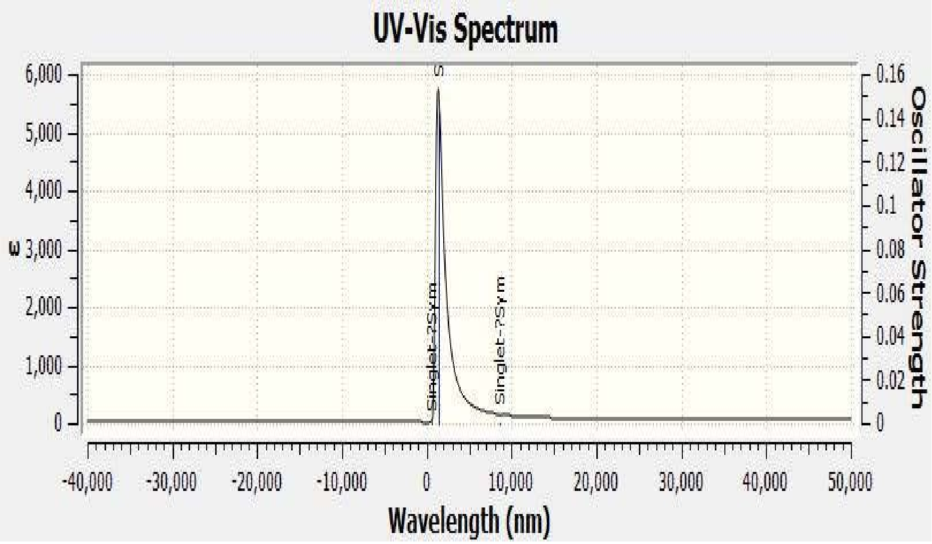

Figure: (13). UV spectrum curve of polycarbonate complex with potassium bromide

CONCLUSION

The findings of this study indicate that there are significant differences in the energy of the integrated complexes, polar moment, and UV absorption spectrum of the polymers under examination. It is evident that polyethylene is the optimal choice, as it exhibits the greatest degree of non-interference, providing a high degree of assurance when employed as a carrier for baked foods in which potassium bromide was utilized as an improving material.

RECOMMENDATIONS

It is imperative that this line of research be continued, and that the quality of plastic be enhanced. This can be achieved through collaboration between researchers in this field and stakeholders in the baked food industry. By doing so, we can guarantee the safety of baked foods and ensure that packaging meets the scientific specifications set forth in this study and other studies in this field.

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