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Study of the Nuclear Magnetic Resonance and Physical Properties of Iodine

Huda M. Jawad , Faten S. Mater , Asmara S.J.M. Al-Ragehey , Sara S. Hamood

Department of physics, College of science, Mustansiriyah University, Baghdad, Iraq.

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Abstract: Iodine has long 70 years played an essential role in thyroid health, in addition to its uses in medicine. This element is used in medical applications because of its antiseptic properties. It is considered an antiseptic for healing and sterilizing wounds, and it has been proven that this element is invaluable in this field. To study the electronic characteristics, including the energy gap, HOMO-LUMO, nuclear magnetic resonance, force constant, in addition to the spectral characteristics like infrared and Raman, as a function of the frequency of iodine, UV-visible, and NMR. The methodology uses DFT and TD-DFT for all electron levels. The results display The NMR for Iodine showed a positive potential in the center of the ring due to the number of electrons being insufficient to protect for the nuclear charge The highest peak is in the high-frequency area (380 cm^{-1}) Iodine uptake analysis is used to evaluate thyroid function, diagnose benign and malignant tumors, or follow the course and progress of treatment.

Keywords: Iodine, nuclear magnetic resonance, Transmittance spectrum.

Corresponding author: (Email: drhuda293gmail.com).

Introduction

Iodine is considered an essential element in human nutrition because it is an essential element in the chemical structure of thyroid hormones (1). This element is important throughout life, but especially during pregnancy, breastfeeding and childhood. Iodine deficiency can lead to brain damage, mental retardation, neuromuscular defects, and goiter (2). Most iodine in the blood is in the form of iodide and is either absorbed by the thyroid gland and converted into thyroid hormone or excreted in the urine. Approximately 90% of the taken iodine is excreted in the urine (3 -6). “Colored violet” is a meaning of the Greek word iodides, and the name iodine is derived from it. This type of solid is considered to have a dull luster and a gray color. A violet gas emerges when heated under normal air pressure. Courtois was the discover of iodine in 1811, and brine and seaweed were a commercial source for extracting iodine (7). Iodine is also used in many medical procedures. Iodine-containing bleaching agents are used to disinfect wounds and surgical operations. Iodine is also used in X-ray images to improve diagnosis and monitor the development of diseases, and thyroid gland and vascular diseases are treated using radioactive isotopes of iodine through medical tracking (8-9). Relying on this importance, individuals should ensure that their daily iodine needs are met by eating iodine-rich foods such as marine fish and iodine-fortified foods (10-13). This research aims to study the electronic and spectroscopic properties of iodine based on the DFT method.

Theory

To study the vibrational and structural properties, we relied on the geometric optimization method and used the computer program Gaussian 09 and an associated auxiliary program Gaussian view (6.0). The theoretical estimates that predict the properties and nanostructure of iodine were predicted. DFT and (TD- DFT) were included as a term in the equation for the hybrid function B3LYP (Becke 3-parameter, Lee-Yang-Parr), which were applied with 6-31G (d,p) where the scaling factor was 0.967 and 0.960 to correct for vibration frequencies (14-15). The iodine geometry resulting from the use of self-consistent field calculations of density functional theory is illustrated in Figure (1).

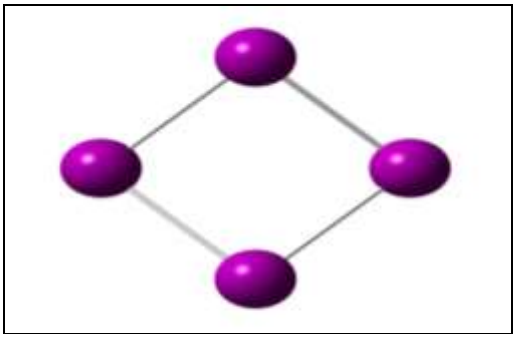

Figure (1): Geometrically optimized of Iodine.

Computational details

Spectroscopy properties

Transmission and Raman spectroscopy

Figures (2) and (3) show the transmittance and Raman spectrum of iodine as a function of frequency. The highest peak is in the high-frequency area (380 cm^{-1}). These peaks occur as a result of the interaction of iodine molecules with certain wavelengths. Iodine uptake analysis is used to evaluate thyroid function, diagnose benign and malignant tumors, or follow the course and progress of treatment (16). The interaction of matter with light leads to a change in the vibrational modes, which is accompanied by a corresponding change in the Raman spectrum, the area where the infrared ray is effective Raman inactive and vice versa. The Raman spectrum display in the area (180 cm^{-1}).

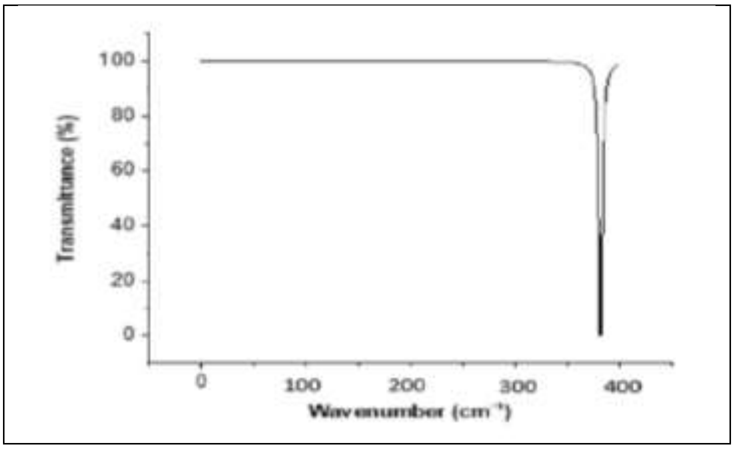

Figure (2): Transmittance spectrum of Iodine.

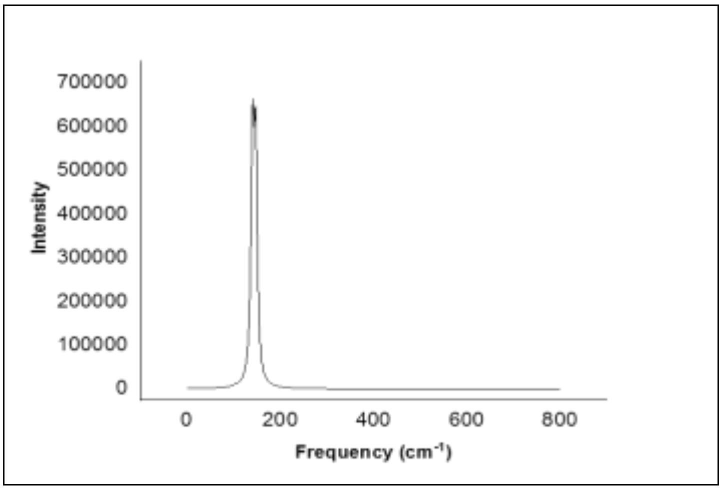

Figure (3): Raman spectrum of Iodine.

UV – Visible spectrum

Since the absorption of ultraviolet or visible radiation by a molecule leads to a transition among the electronic energy levels of the molecule, it is also often called electronic spectroscopy (17). (Figure 4) between (ε) epsilon, a constant called malar absorptivity, and excitation energy (18). It has a longer wavelength (650 nm), which means high absorbency, these are located in the visible region. The normal method for obtaining such data is to excite the iodine molecule with monochromatic radiation wherever the iodine-tracer medicine pile is in the organ or area to be examined (19).

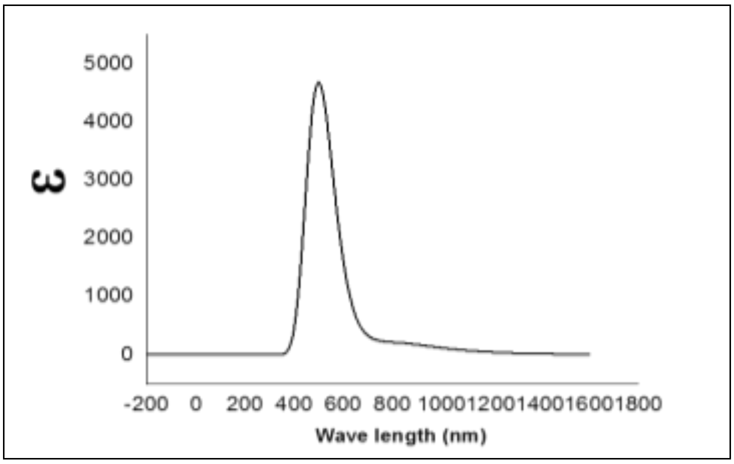

Figure (4): UV–visible spectrum for Iodine.

Electronic properties

HOMO- LUMO

Molecular electron transport properties are determined by a final interpretation of intramolecular charge transfer across the HOMO - LUMO energy gap. The high frontier orbital gap is the reason behind the weak chemical reactivity of the molecule and its high kinetic stability, and it is energetically unfavorable to add an electron to the high-lying LUMO to remove electrons from the low-lying HOMO. It is known that compounds with a high energy gap are more stable and, hence, chemically harder than those with a small energy gap (20). HOMO and LUMO is shown in figure(5). The energy gap can be calculated from the equation below.

Energy Gap = HOMO – LUMO … (1)

= ((- 0.29514 a. u.) - (- 0.12788 a.u.)) = (4.5513 eV).

Iodine is a chemical element with atomic number 53 and symbol I. As the sixty-first most plentiful element, it is the heaviest of the stable halogens. Iodine is the most densely packed essential mineral ingredient and is necessary for the thyroid to produce its hormones.

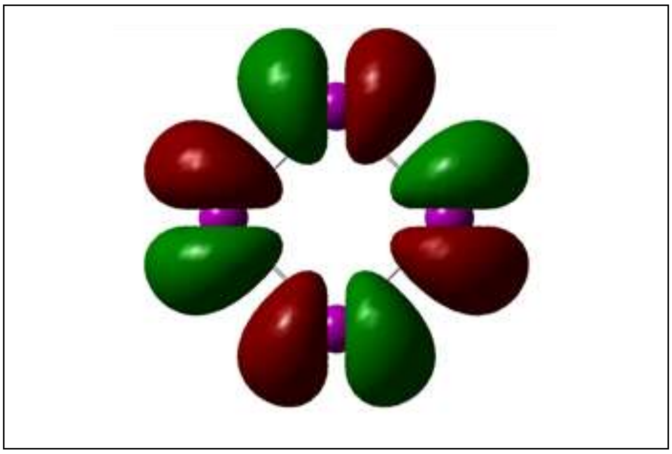

Figure (5): HOMO and LUMO of Iodine.

The chemical structure of iodine was designed through molecular modeling and molecule optimization to maintain the most stable conformation possible (Figure 6). There are different ways to understand electromagnetic contributions. Negative potentials appear in red, as shown by the Molecular Electrostatic Potential map (MESP), while positive potentials appear in blue, which expresses the derivatives of activity (21). In this figure, the positive potential appears in the center, and this explains the repulsion of the proton through the atomic nuclei in places where the density of electrons is low, so the nuclear charge is not completely protected. The green color that appears in this figure indicates that the potential is neutral in this region. The electrostatic potential of the molecule is considered a good way to determine which reactants are negatively or positively charged, and this clarifies the evaluation of molecular interactions. Therefore, MESP is considered one of the easy ways to understand the relationship between molecular structure and biological activity (22).

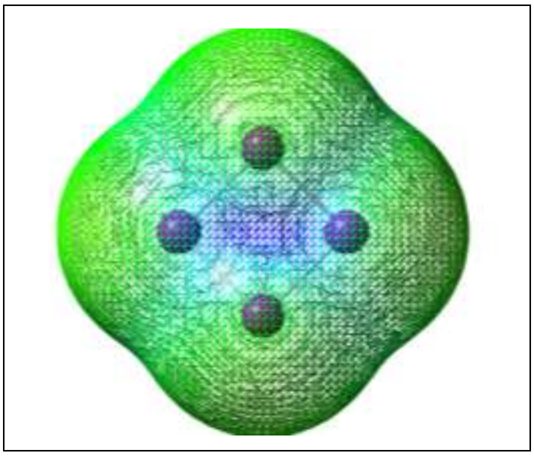

Figure (6): Molecular electrostatic potential surfaces (MESP) for Iodine.

Characterizing synthesized materials using nuclear magnetic resonance is a method routinely used by chemists and biochemists because nuclear magnetic resonance (NMR) spectroscopy has great potential in various fields of molecular and biological studies (23). The nucleus makes an electromagnetic signal with a distinct frequency when it is inside a strong magnetic field and when it is perturbed by a weak, oscillating magnetic field this procedure occurs near resonance this is a physical observation called Nuclear magnetic resonance (NMR). When atomic nuclei have magnetic properties, nuclear magnetic resonance results (24). (Figure 7) NMR for Iodine, since the ring consists of four iodine atoms that have the same number of electrons that are shielded around the protons it showed a positive potential in the center of the ring due to the number of electrons being insufficient to protect for the nuclear charge. NMR degeneracy tolerance (0.05) and peak half–width at half height (0.5) ppm.

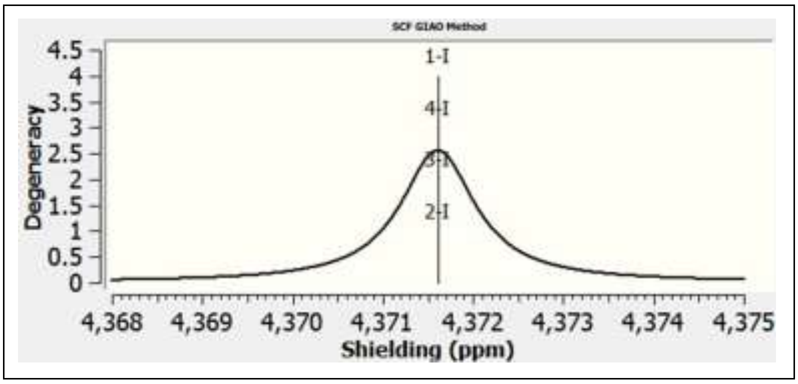

Figure (7): Nuclear magnetic resonance (NMR) for Iodine.

Force Constant

Elastic waves have three different modes of vibration: two are orthogonal modes of transverse vibration and one is longitudinal. Elastic waves are used in various fields and applications. For example, elastic X-rays are used to image internal tissues in medicine, and elastic sound waves are used in embryo screening and ultrasound imaging, in addition to their use in sonar, engineering, materials, manufacturing, and other fields. Vibration. The reduced mass is calculated by summing the equivalent mass of each particle involved in the vibration and reducing it. Considering four iodine atoms bonded together, the reduced mass will be one equivalent mass expressing the effective mass of the molecular system during vibration. The inverted mass is used in calculations of energy and atomic and molecular frequencies. The force and mass constants are used in many scientific and technical applications, such as the study of molecular vibrations, spectrum analysis, and the design of electronic devices and composite materials (25). This equation below displays the relationship between the frequencies at the boundary Brillion zone (26).

$$\upsilon = \frac{1}{2\pi}\sqrt{\frac{K}{\mu}} \quad \ldots\ldots$$

Force constant is shown figure (8). Force constant increasing with increasing frequency because there is a proportionality between the square root of the force constant and the vibrational frequen (27). Force constant is being maximum vibrations at around (763 cm-1) to the Symmetric mode. As a result, it shows that the nanoscale and molecular limits are red-shifted. The iodine atoms' vibrational modes.

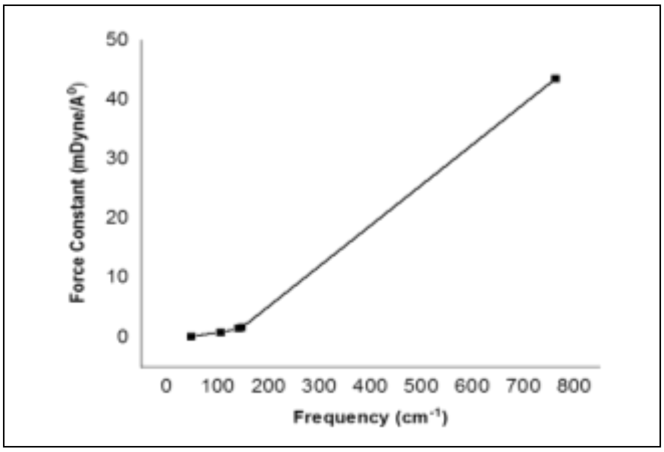

Figure (8): Force constants of Iodine.

Conclusion

The absorption of ultraviolet or visible radiation Maximum light absorption in the range (650cm^{-1}) is in the visible region The normal method for obtaining such data is to excite the iodine molecule with monochromatic radiation wherever the iodine-tracer medicine pile is in the organ or area to be examined. The NMR for Iodine showed a positive potential in the center of the ring due to the number of electrons being insufficient to protect for the nuclear charge. the energy gap is (4.5513 eV) and the Force constant is being maximum vibrations at around (763 cm^{-1}) to the Symmetric mode. As a result, it shows that the nanoscale and molecular limits are red-shifted for iodine atoms' vibrational modes. High absorbency helped iodine be absorbed by thyroid cells and be a treatment for hyperthyroidism.

Acknowledgment

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