



Resolution Infrared and UV-Vis spectrum of Naphthalene and Anthracene Compounds

Hakima Salman Jabr^{1*}, Hanan Dakhil Idan Alsaedi², Ibtesam Omran Radi³

¹Babylon university, College of Science, Physics Department, Babylon, Iraq

* Corresponding Author Email: sci.hakeima.salman@uobabylon.edu.iq - ORCID: 0009-0000-9218-9102

²Babylon university, College of Science, Physics Department, Babylon, Iraq

Email: sci884.hanan.dakial@uobabylon.edu.iq - ORCID: 0009-0000-9218-9202

³Babylon university, College of Science, Physics Department, Babylon, Iraq

Email: sci.ibtsam.omran@uobabylon.edu.iq - ORCID: 0009-0000-9218-9402

Article Info:

DOI: 10.22399/ijcesn.3232

Received : 30 April 2025

Accepted : 26 June 2025

Keywords

Infrared spectrum
Naphthalene impurities
Anthracene Structures

Abstract:

Molecular physics is studying a monocyclic aromatic hydrocarbon molecule that contains two substances: naphthalene and anthracene. The research work involved “ground state calculations at the B3LYP/6-31G level” to look into the best mix of chemicals and their spectral features for (C₁₀H₈) and (C₁₄H₁₀). Theoretical calculations of infrared spectroscopy and visible and ultraviolet spectrum calculations were performed for both compounds. The two compounds were studied in the pure state and then various impurities (aluminum, copper, silicon, nickel and nitrogen) were added and it was found that there are clear differences between the studied spectra. It has been observed that the theoretical spectra correspond well to the experimental spectra.

1. Introduction

Any gas, liquid, or solid whose molecules contain carbon and are covalently bonded-that is, their bonds have direction-is an organic compound. This opens the doors to new structures, like rings and long chains of carbon [1]. There are more than one way to classify organic substances. There is a huge difference between synthetic and natural compounds. There are two general types of organic compounds: aromatic and aliphatic. Aliphatic compounds are those that do not contain aromatic systems [2,3], like an aromatic ring system. Normally, this term is used for those substances that contain a benzene ring. Chemicals that do not contain any living component are inorganic [4]. These chemicals are formed by the geological system and do not contain any carbon or hydrogen atoms. Organic science classifies all carbon-containing molecules as organic compounds in general and by convention. Therefore, compounds that lack carbon are what inorganic chemistry focuses on. In this research study, infrared and

Raman spectra of naphthalene and anthracene shall be analyzed. Naphthene forms the key constituent of the synthesis of dyes, resins, and mothballs. It is also used in coal tar and wood preservatives. It is used as an insecticide, medicine, and other pesticide and pharmaceutical intermediates. Its chemical formula is C₁₀H₈. It carries a mothball-like smell, is insoluble in water, and exists in solid or powdered white forms [6]. It is applied in the process for phthalic anhydride manufacturing. Acute effects of human exposure to naphthalene through inhalation, ingestion, or contact of the skin include haemolytic anemia, liver damage, and brain damage. The basic tricyclic aromatic hydrocarbon is anthracene, paranthracene, or green oil, which constitutes a solid polycyclic aromatic hydrocarbon with three benzene rings produced from coal tar. This area does not absorb saturated compounds because the energy needed for exciting the electrons is much higher than that of ultraviolet rays; therefore, electronic excitation takes place when the beam is in the field of visible or ultraviolet rays. There are three types of electrons in organic molecules, one of which is

bonded to a saturated bond, such as the hydrogen-carbon bond, or in saturated compounds with carbon-carbon, called a bond. Another type of bonding links the electrons to an unsaturated molecule. In petrol and other similar compounds, and bonds are also common. The third type of electrons are those which are not involved in atomic bonding. [7].

2. Theoretical Parts

The wave function Ψ is not physically observable, but its square $[\Psi]^2$ can be interpreted as the probability density, which yields a probability when multiplied by the volume of a region. Acceptable wave function for a system has to be orthogonal and normalized [7]:

$$\int \Psi_i \Psi_j dx_N = \langle \Psi_i | \Psi_j \rangle = \delta_{ij} \quad (1)$$

an expectation value of the Hamiltonian operator of energy is [7]:

$$E = \langle \hat{H} \rangle = \frac{\int \Psi^* \hat{H} \Psi dt}{\int \Psi^* \Psi dt} \quad (2)$$

The wave function Ψ describes a many particle systems.

The main things that determine how accurate the results are are the type of calculation used and the base set that was picked [8,9]. The Slater type orbitals (χ^{STO}) have the form [10,11]:

$$\chi^{STO} = N r^{n-1} e^{-\xi r} Y_{lm}(\theta, \varphi) \quad (3)$$

In this expression, n is one of the basic quantum numbers, and “ $3/4$ is a constant related to the effective charge” of the nucleus. The angular part of the wave function is given by the spherical harmonic $Y_{lm}(\theta, \varphi)$. It is right that Slater type functions behave in a way that stops when they get close to the nuclei where $r = 0$. One can write Gaussian type orbitals, χ^{GTO} , in terms of Cartesian coordinates as [9,11]:

$$\chi^{GTO} = N x^{lx} y^{ly} z^{lz} e^{-\xi r^2} \quad (4)$$

where: The nature of the orbitals is defined by the sum of lx , ly , and lz with a normalisation factor N . When the orbital exponent is ξ that reflects either a compact large ξ or a scattered small ξ then r^2 dependence in the exponential is an issue in GTOs as against the Slater-type orbitals STOs [12,13].

3. Results and Discussion

Oscillations include two kinds of bands, the main and non-major oscillation bands [14]. As for the

main, it is accompanied by many changes in the dipole cycles and is graded according to their high density, such as expansion, deformation, vibration, and others. Unlike non-main, excess and hot tones are low intensity [15]. Vibration analysis is only possible when the first derivative of energy relative to the displacement of atoms is zero. The frequency of photons in monogamous light changes when interacting, with the sample [16]. This effect is related to the polarization of the molecule, and is seen for molecules with net “dipole moment” and therefore do not produce a pure “rotational spectrum”. This phenomenon gives an explanation about the “inertia and therefore the structure of the molecule”. The excitation of electrons determines the absorption of visible rays and ultraviolet rays, of atoms and molecules, from low to high energy levels. Because it is measured quantitatively, it absorbs only light with energy that helps in moving from one level to another [17]. This study examines the effect of impurities on the spectral properties of naphthalene and anthracene synthesis. A mixing function (B3LYP) was employed using Gaussian View 5.0, and the output was generated from Gaussian 09 with the (6-31G) basis set. Data related to anthracene in both pure and doped forms are presented in Figure 1. The intake level has sharply increased, and the intensity of absorption varies depending on the atoms added. We also observe a sharp change in absorption peaks due to the addition of different atoms—specifically, aluminum, nitrogen, nickel, silicon, and copper atoms instead of hydrogen atoms in the ring. Notably, there is a difference in frequency values between the pure ring and the doped rings. This difference causes variations in the bending and stretching vibrations of the additive molecules compared to those of benzene. Infrared (IR) spectra and visible and ultraviolet (UV) radiation of both naphthalene and anthracene provide important information about their molecular structures, functional groups, and electron transitions. Anthracene's infrared spectrum shows distinct bands due to vibrations of C-H and C-C bonds in both the pure and doped rings. The peaks observed in the range of (2100–2300) cm^{-1} are attributed to the stretching of C-Al bonds and other added atoms. The stretching of C-H bonds appears in the region (3000–3100) cm^{-1} . Characteristic bands of bending vibrations are typically found below (1000) cm^{-1} . The stretching of the aromatic ring (C-C) occurs in the region (1300–1600) cm^{-1} , with strong bonds corresponding to around 1300 cm^{-1} and 1600 cm^{-1} . These bands are often symmetrical and typical for aromatic compounds with double bonds. The visible and ultraviolet spectrum exhibits more intense absorption areas and wavelengths. We observe maximum absorption of visible and

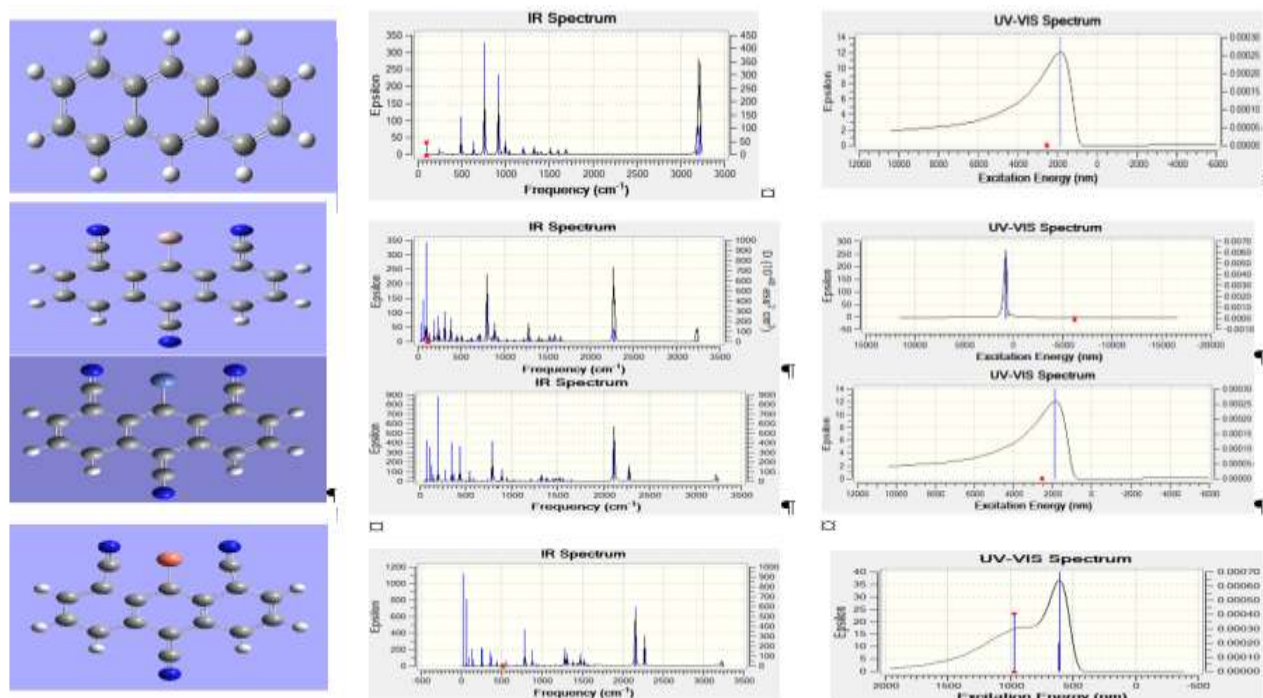


Figure 1. Geometrical Structures for Anthracene of Infrared (IR) and (UV-VIS) spectrum

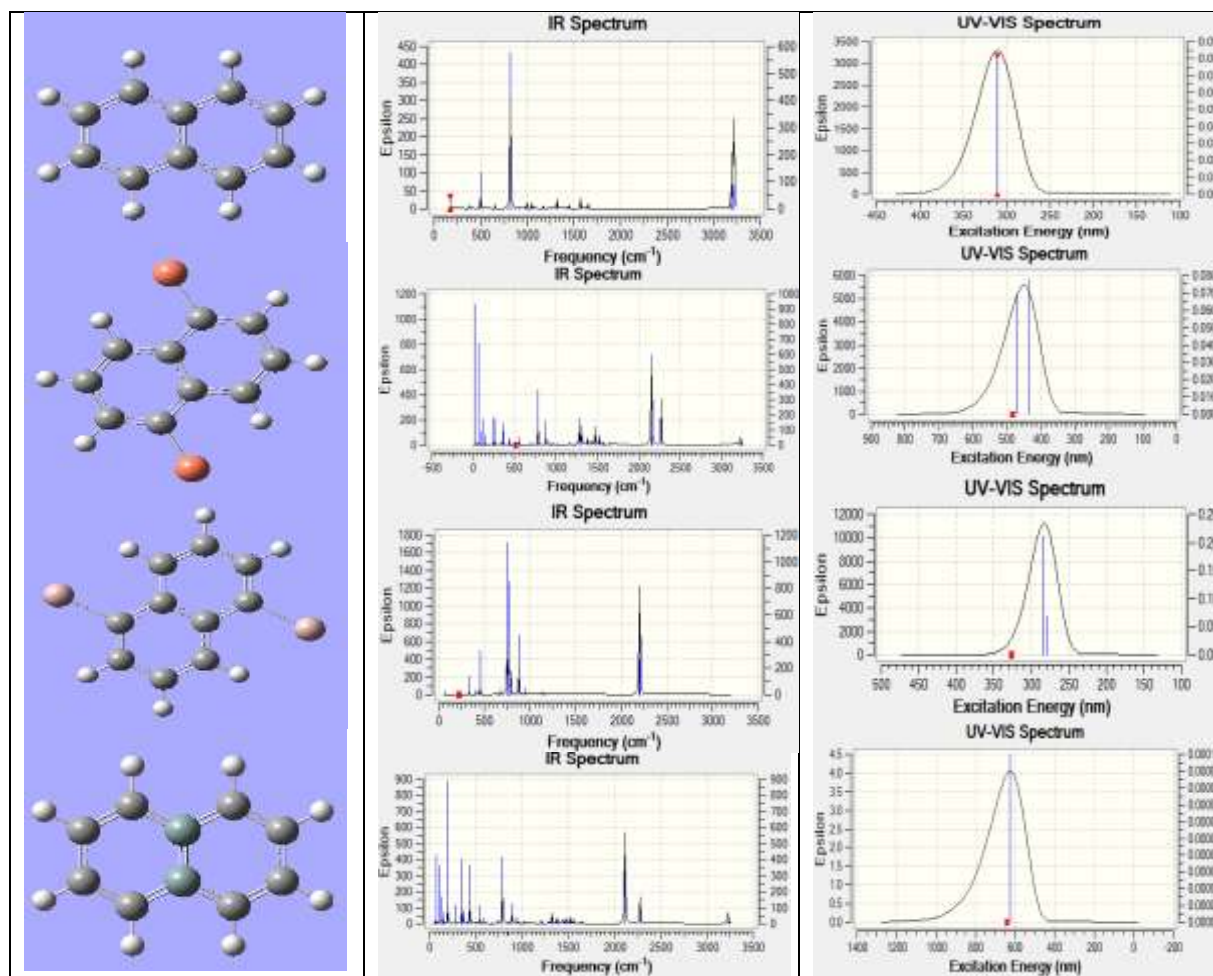


Figure 2. Geometrical Structures for Naphthalene of Infrared (IR) and (UV-VIS) spectrum.

ultraviolet rays at 550 nm, as shown in Figure 2 which presents the results for the naphthalene compound in both pure and doped states. When hydrogen atoms are replaced with copper, peaks in the range (2150–2250) cm^{-1} are due to the stretching of C-Cu bonds. Aluminum affects the vibration of C-H and C-C bonds, and in the case of replacing hydrogen with aluminum, vibrations appear at 2150 cm^{-1} . C-Al bonds appear in the range of (750–850) cm^{-1} . For silicon, C-Si bond peaks are observed in the range (2100–2250) cm^{-1} . C-C and C-H bonds typically fall within the range of 500–1000 cm^{-1} . In the ultraviolet (UV) spectrum of naphthalene, clear absorption is observed due to electronic transitions in the molecule. Since aluminum has a high ionization energy, replacing hydrogen with aluminum results in a change in the absorption spectrum in the ultraviolet region. Silicon, on the other hand, may lead to a change in the wavelength of absorbed light up to 600 nm.

4. Conclusion

Both naphthalene and anthracene exhibit distinct absorption zones in the infrared, ultraviolet, and visible spectra, reflecting their conjugated aromatic structures. Naphthalene has simpler spectra due to its smaller size, while anthracene shows new absorption zones and extended spectral features. When a hydrogen atom is replaced by the mentioned atoms, a change in the spectrum occurs in several regions where new absorption peaks appear due to different electron transitions. This contributes to a better understanding of the molecular behavior of the two compounds.

5. Recommendations

Recommendations Inferentially from the study, the following recommendations are made:

Experiments for Further Verification: Real experiments should be conducted to verify the obtained theoretical results. This will contribute to validate the veracity of the theoretical predictions and will render a complete knowledge of the spectral properties for naphthalene and anthracene type compounds. **Further Impurities:** Study other possible impurities and their influence on the spectral behavior of naphthalene and anthracene. Such substances and mixtures might be experienced for example, in an industrial or environmental setting. **Advanced Computational Methods** Use improved computational techniques and larger basis sets to improve theory calculations. That could provide a more detailed understanding of the electronic structures and vibrational modes of the compounds. **Other Research:** Investigate the

application of this work in material science, specifically in the creation of new materials with designed optical and electronic properties. The knowledge obtained herein may be valuable for developing materials for targeted applications such as sensors, photovoltaics, and optoelectronics. **Impact on Health and the Environment:** Considering the possible effects on health and the environment of naphthalene and anthracene, additional research is needed to determine the effects of these substances and any impurities on human health and the environment. This might help with regulatory guidelines and safer industrial practices. These suggestions would enable further investigation that could expand on the work reported here and might increase our insight into spectral characteristics of naphthalene and anthracene derivatives and their applications.

Author Statements:

- **Ethical approval:** The conducted research is not related to either human or animal use.
- **Conflict of interest:** The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper
- **Acknowledgement:** The authors declare that they have nobody or no-company to acknowledge.
- **Author contributions:** The authors declare that they have equal right on this paper.
- **Funding information:** The authors declare that there is no funding to be acknowledged.
- **Data availability statement:** The data that support the findings of this study are available on request from the corresponding author. The data are not publicly available due to privacy or ethical restrictions.

References

- [1] *Environmental Health Association of Nova Scotia*. (2013).
- [2] *CDC-Niosh pocket guide to chemical hazards-naphthalene*. (2022).
- [3] Igor A. Fedorov, Yurii N. Zhuravleva and Victor P. Bervenob. (2011). Electronic structure and chemical bond in naphthalene and anthracene *Chem. Phys*, 13, 5679–5686.
- [4] Patrick J. Lynch, Luke O'Neill, David Bradley, Hugh J. Byrne, Mary McNamara, (2007). Systematic Study of the Effects of Naphthalene and Anthracene Substitution on the Properties of PPV Derivative Conjugated Systems, *Macromolecules*, 40, 7895-7901.

- [5] Liu Satoshi Kaneko, Yuki Komoto, Shintaro Fujii, Manabu Kiguchi, (2015). Highly conductive single naphthalene and anthracene molecular junction with well-defined conductance, *Appl. Phys. Lett.* 106, 103103.
- [6] Nigam, C. Majumder and Skkulshreshtha, (2006). Teoretical study of aromaticity in inorganic tetramer Clustres, *J. Chem.*, vol. 118(6), 575-578.
- [7] H. H. Fadhal, (2019). Investigate of the Energy Gap, Ionic Charge and Infrared Spectra (IR) Of Ge Nanocrystals, *Journal of University of Babylon for Pure and Applied Sciences*, vol. 27(3) 151-160.
- [8] M.C. Shane, (2000). M.Sc. Thesis, University of Western Australia, Department of physics.
- [9] R. F. Stewart, (1970). Small Gaussian Expansions of Slater-Type Orbitals, *The Journal of Chemical Physics*, vol. 52(1), 431-438.
- [10] G. M. Merdan, (2005). Self-Consistent Field Calculation for the effect of Pressure and Temperatureonsome Properties of Greyt in Crystal, M. Sc. Thesis, University of Babylon.
- [11] K. A. Saeed, (2010). A theoretical Study of the Structural Properties and its Correlation with the Bbiological Activity of Stavudine and some Derivatives, M. Sc. Thesis, University of Kufa.
- [12] H. Dorsett, A. White, (2000). Overview of Molecular Modeling and Ab Initio Molecular Orbital Methods Suitable for Use with EnergeticMaterials, *Deference science and Technology Organization*, Australia.
- [13] Tim Holtum, Julien Bloino, Christos Pappas, Vikas Kumar,Vincenzo Barone,Sebastian Schlücker, (2021). Ultraviolet resonance Raman spectroscopy of anthracene: Experiment and theory. doi: 10.1002/jrs.6223.wiley,23.
- [14] T. R. Morrison, N. R. Boyd, (2007). Organic Chemistry, 6th Edition, New York University.
- [15] Sadasivam and R. kumaresan, (2011). Computational and Theoretical Chemistry, 963, 227-235.
- [16] Ketterer, (2011). Raman Spectroscopy of GaAs Nanowires: Doping Mechanisms and Fundamental Properties, Ph.D Thesis NO. 5211.
- [17] Gatzkeyx, S. J. Webby, K.Fobeletsz and R. A. Stradlingy, (1998). In Situ Raman Spectroscopy of the Selective Etching of Antimonides in GaSb/AlSb/InAs Heterostructures, *Semicond. Sci. Technol.* Vol. 13, 399–403.