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ORIGINAL RESEARCH PAPER

Integrating STEAM with Astrobiology: Simulating Molecular Structures to Foster Inquiry-Based Learning in High School Science

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ABSTRACT

In this study, we have developed a framework within Pedagogical Content Knowledge (PCK) for science education, utilizing a STEM approach in combination with the Inquiry-Based Science Education (IBSE) method. The lesson plan is presented in the form of a scientific report, with a focus on investigating the potential signs of life in extraterrestrial environments. A key component of this exploration involves examining cyanide compounds, which, if present, can indicate the possibility of life in a given system. Our research methodology revolves around the simulation of DNA components—specifically, adenine, cytosine, guanine, and thymine, the fundamental building blocks of life. We simulate these DNA molecules and calculate their infrared (IR) frequency spectra. The resulting frequencies are then used to analyze astronomical data from radio telescopes, such as the Hubble Space Telescope, through astronomical spectroscopy. The simulation techniques employed in this research are grounded in Density Functional Theory (DFT), which was implemented using the Gaussian software package. This approach allows us to accurately model molecular interactions and predict the spectral signatures of life-supporting compounds in space.

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1. Introduction

The topic of extraterrestrial life has long captivated the imagination, particularly among younger generations. For high school students, this subject presents an exciting opportunity to engage in scientific inquiry through a STEM-based curriculum. By framing the study of extraterrestrial life within a STEM lesson plan, educators can not only spark student interest but also enhance their learning experience. Incorporating collaborative group activities and simulating a knowledge Enterprise model fosters motivation and promotes critical thinking. Moreover, transitioning from a traditional STEM approach to a STEAM model integrates creativity and arts into the scientific process, further enriching the educational experience【1-5】.

Pedagogical Content Knowledge (PCK) underscores the importance of instructional methods that promote learning by creating opportunities for student-teacher interaction. Thus, this course implements Inquiry-Based Science Education (IBSE) to facilitate active learning. Given the need for a structured, well-planned curriculum tailored to the resources and environment available, this manuscript presents a comprehensive report on the activities designed for this course, with clear objectives that students are expected to achieve【6-10】.

Throughout history, space has provided humankind with scientific insights through the study of electromagnetic waves. Without exploring beyond our immediate surroundings, such breakthroughs would be unattainable. For instance, past discoveries in mechanics and modern advancements in nanotechnology emerged from the study of the cosmos【11-15】. Additionally, elements like helium and unique structures such as fullerene, cumulene, and carbyne were first identified in outer space【16-20】. The question then arises: what can space teach us about biology?

Astrobiology—the study of the origin, evolution, distribution, and future of life in the universe—combines knowledge from multiple scientific disciplines, including physics, chemistry, astronomy, and biology. This field, formally established by NASA in 1998 with the creation of the Astrobiology Institute at the Ames Research Center, investigates both life on Earth and the potential for life beyond our planet【21-22】. Astrobiology's interdisciplinary nature allows it to explore a wide range of topics, from the study of planets and their moons to the conditions necessary for life in space.

Recent advancements in astrobiology have made significant contributions to our understanding of life in the universe. For example, NASA's Mars Rover missions have gathered extensive data on Mars' atmospheric properties, chemical composition, and surface conditions. Research on extremophiles—organisms that thrive in extreme conditions, such as high or low temperatures and unusual pressure environments—has revolutionized our understanding of the diversity of life【23-24】. Thermophiles, a type of extremophile, flourish in extreme environments, such as hot springs, prompting scientists to speculate that life may exist in similar conditions elsewhere in the universe【25】. This realization—that life exists in places previously thought uninhabitable—suggests the possibility of life in other regions of the cosmos. Figure 1 illustrates this concept: part (A) depicts the vibrant colors of thermophilic life found at the Grand Prism Spring, while part (B) presents electron microscope images of microfossils in Martian meteorites, which serve as preliminary evidence of possible life on Mars【26-27】.

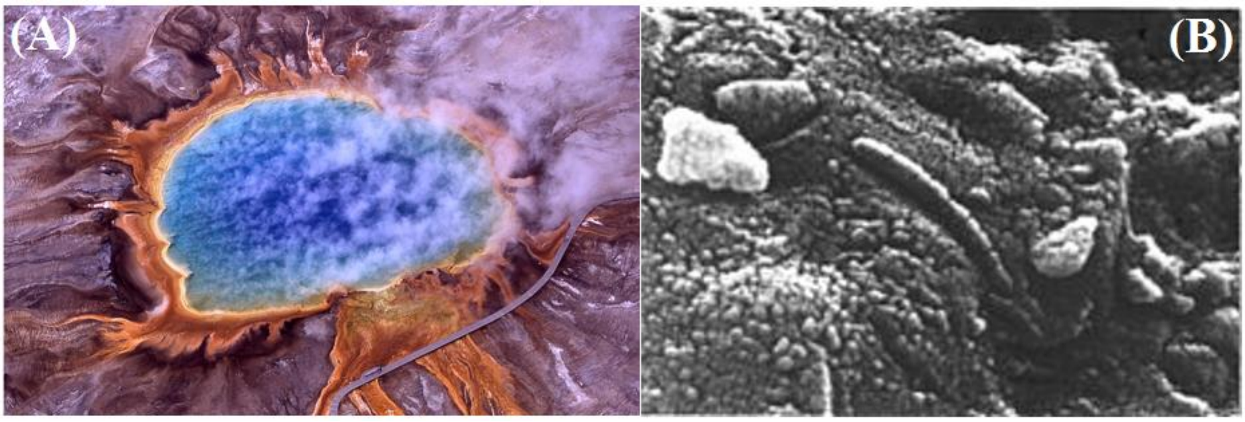

Figure 1: Above you can see with two images, part (A) of the Grand Prism Spring, which is one of the places where thermophiles are found, bright colors represent thermophilic life; and part (B) shows the Electron image of microfossils of bacteria in Martian meteorites [The above image is reconstructed from references 26 and 27].

The convergence of astronomy and biology has led to the remarkable realization that certain microbes could potentially survive in Martian environments. Despite this possibility, no definitive evidence of living organisms has yet been discovered on Mars. This poses a critical question: if we do not receive biological information from space via a meteorite, should we passively wait for the next opportunity? In response, scientists have turned to a more proactive and precise method: astronomical spectroscopy.

In April 2015, a groundbreaking discovery was made in the field of cosmology. For the first time, scientists identified complex cyanide compounds—essential precursors to life as we know it—beyond our solar system. This discovery, part of the astrophysics program at the Harvard-Smithsonian Center for Astrophysics, revealed the presence of cyanide compounds orbiting a star located 450 light-years from Earth. These compounds, specifically hydrogen cyanide (HCN), methyl cyanide (CH_3CN), and cyanoacetylene (HC_3N), were found in concentrations and formations similar to those observed in comets that existed in the early solar system【28-30】. While simpler cyanide compounds had been detected in other regions of space prior to this, this marked the first time such complex molecules were observed at this level outside the solar system【31-33】.

Methods

This manuscript presents a report on training conducted using the Inquiry-Based Science Education (IBSE) method【34】. The strategies employed are designed to promote STEM education among high school students, with an emphasis on transitioning from STEM to a STEAM model. To achieve this, students are grouped into competitive teams, simulating Knowledge Enterprise research companies【35】. This approach, inspired by the concept of the "Magic School Bus," has been adapted to meet the needs of high school students, emphasizing experiential learning in science【36】.

Throughout the course, students participate in a scientific project where they act as engineering teams, tasked with applying laboratory skills and mathematical calculations. The teams compete to develop solutions to the project's first stage, with the most successful team being the one that presents the most viable solution. This process fosters the development of critical skills, including problem-solving, critical analysis, teamwork, communication, digital literacy, independent thinking, creativity, and initiative【37】.

To integrate the use of computers, internet resources, and scientific and mathematical concepts, the project focuses on atomic molecular simulations. Specifically, this study employs Density Functional Theory (DFT) calculations to determine the optimal molecular structures and vibrational frequencies of the simulated molecules【38】. The B3LYP functional, combined with the 6-31+G(d,p) basis set, was utilized to perform these calculations【39-40】. The computational work was carried out using the Gaussian software package【41】, while the vibrational spectra were generated using GaussSum software【42】. Additionally, GaussView was employed to facilitate the graphical representation of both input and output data【43】.

Results

As highlighted in the introduction, essential molecules for the formation of life, including hydrogen cyanide (HCN), methyl cyanide (CH_3CN), and cyanoacetylene (HC_3N), have been identified in space. Figure 2 illustrates the ball-and-stick models of these molecular structures alongside their chemical formulas.

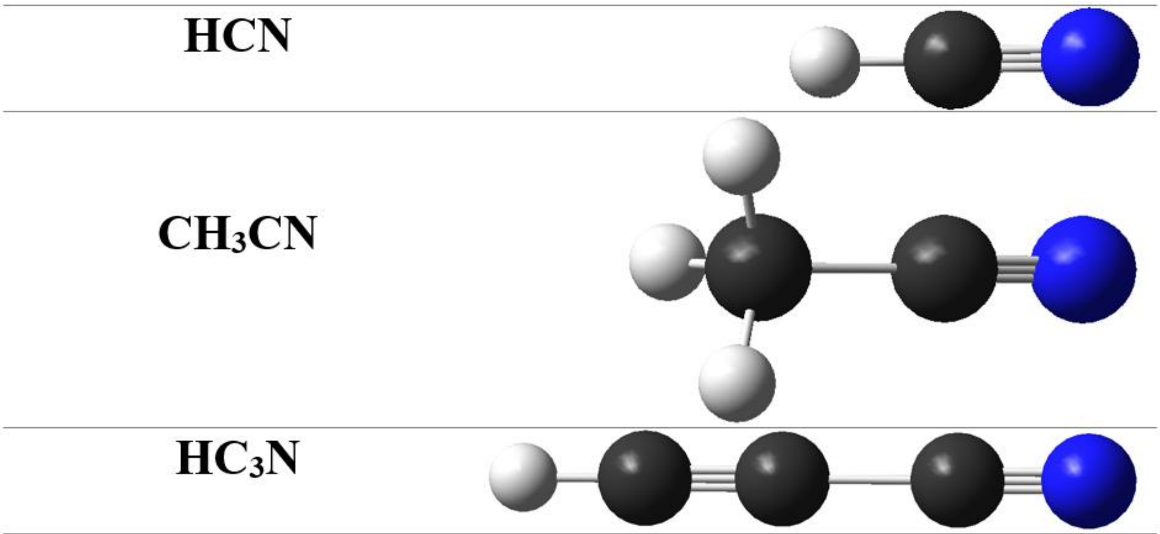

Figure 2: Hydrogen cyanide, methyl cyanide, and cyanoacetylene with their respective chemical formulas—key molecules in the formation of life.

The infrared (IR) spectra of these cyanide molecules were calculated, as shown in Figure 3, which presents the absorption spectra for these compounds.

The vibrations of these cyanide compounds generate both infrared and radio electromagnetic waves. Figure 4 depicts how hydrogen cyanide acts as a molecular transmitter, emitting electromagnetic waves that propagate in a specific direction.

In advancing our research into extraterrestrial life, particularly in the quest to determine whether human-like beings exist on other planets, astronomical spectroscopy must focus on detecting waves emitted by complex biological molecules such as DNA【45】. Figure 5 showcases two structural forms of DNA (A-DNA and B-DNA) from a cross-sectional perspective. Despite the various forms of DNA and other essential biomolecules, such as RNA, they share several common structural features【47】. Our research methodology involved simulating the components of DNA, specifically its nucleotides. The simulated DNA components include adenine, cytosine, guanine, and thymine【48-49】. We subsequently calculated their IR spectra, which are presented in Figure 6 along with the structural and chemical formulas of the DNA components.

The frequency patterns observed in Figure 6 can guide space probes in the exploration of more complex life-supporting systems. Notably, in addition to carbon and nitrogen—crucial elements for cyanobacteria—these structures also incorporate oxygen. The presence of oxygen is significant, as it plays a vital role in the formation of amino acids, proteins, and ultimately, chromosomes.

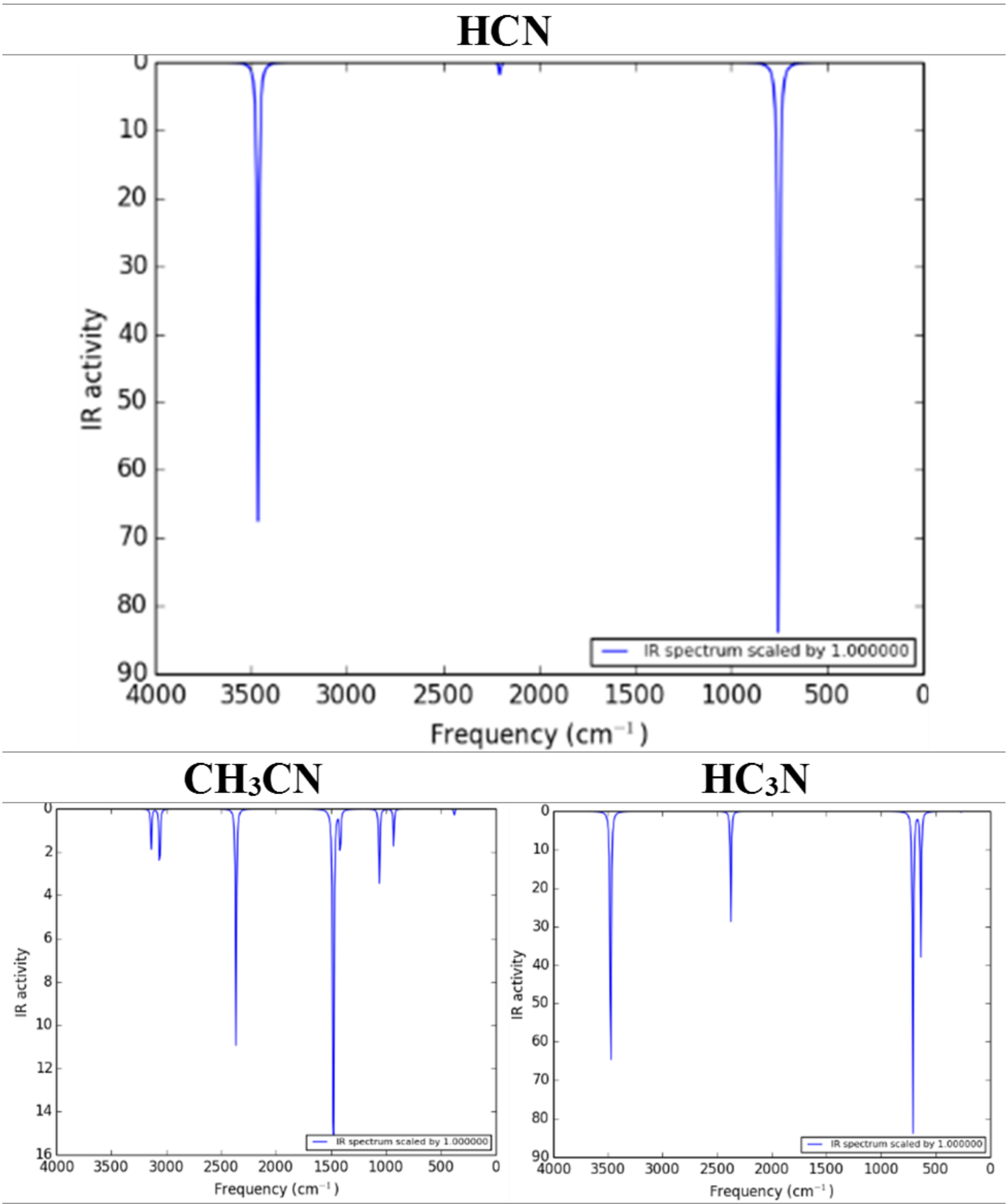

Figure 3: Infrared absorption spectra for hydrogen cyanide (HCN), methyl cyanide (CH_3CN), and cyanoacetylene (HC_3N)—essential molecules for the formation of life.

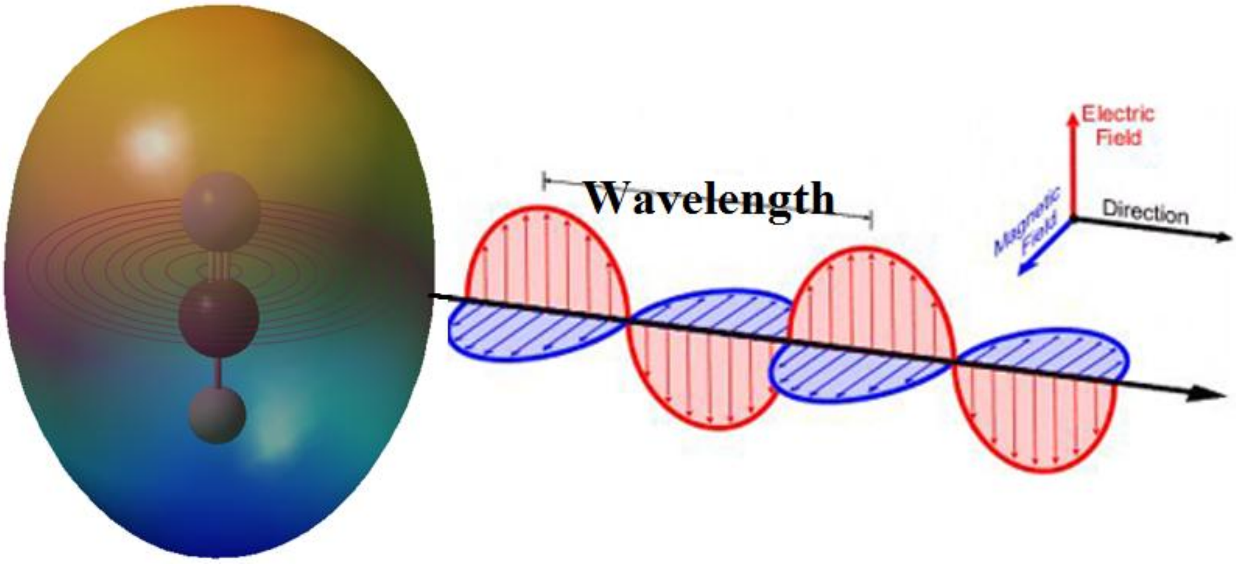

Figure 4: Formation of electromagnetic waves by hydrogen cyanide, illustrating its role as a molecular transmitter and the propagation of waves in one direction. The source of the wave section in the image is adapted from the NOAA site【44】.

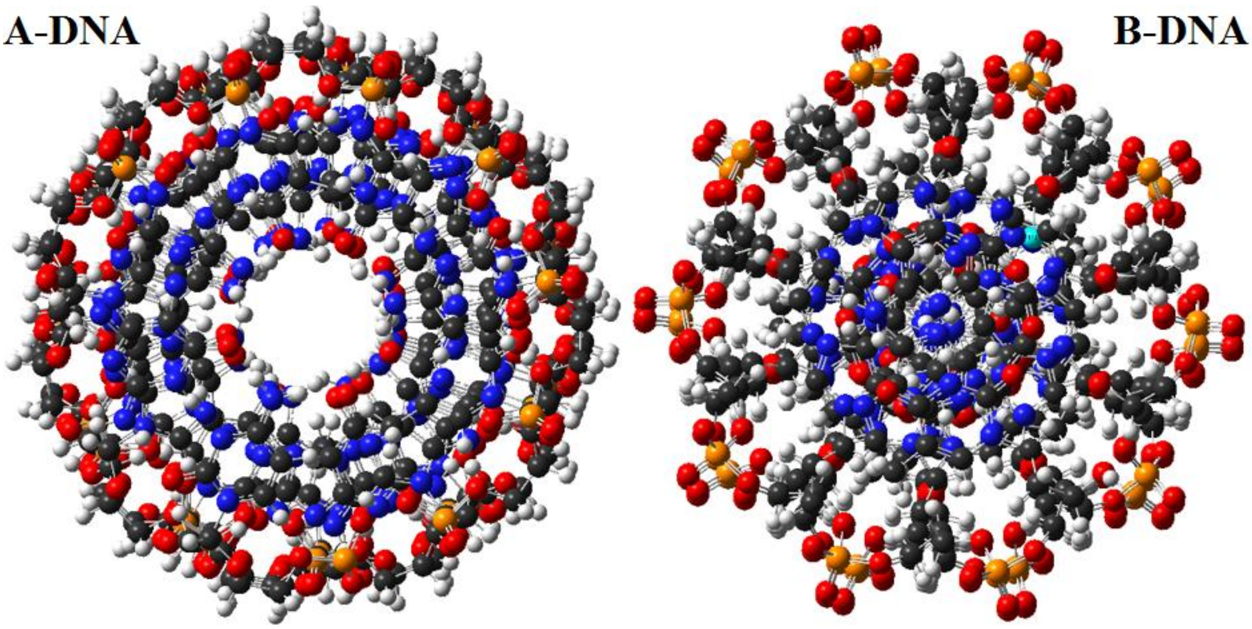

Figure 5: Diagram of the structure of a DNA molecule.

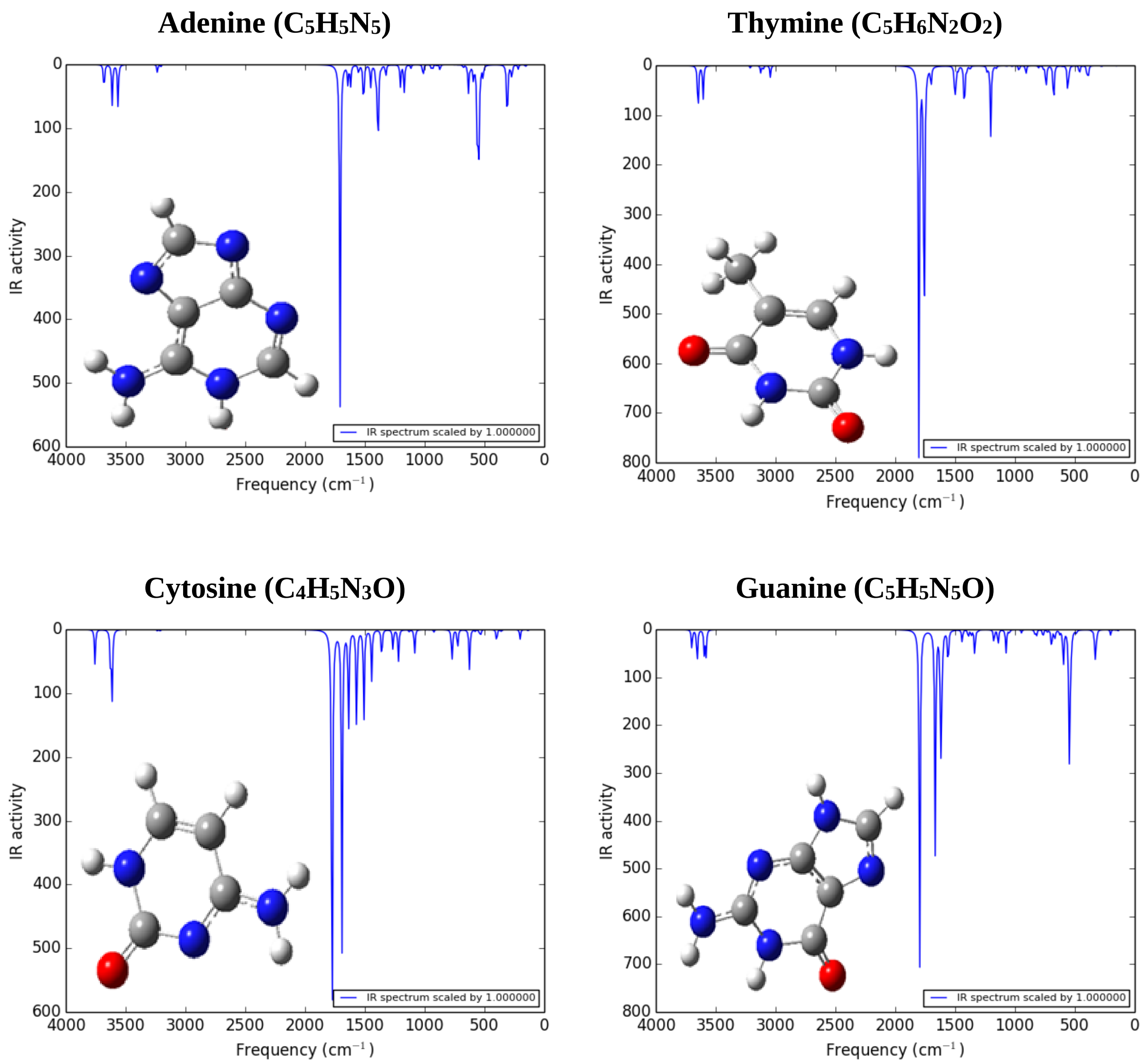

Figure 6: IR spectrum of DNA components, including their structural and chemical formulas.

Applications

Theoretical calculations indicate that the vibrations of hydrogenated silicon nanoparticles correspond to a wavelength of approximately 2000 cm^{-1}, which is equivalent to 15 megahertz. Consequently, the radio waves emitted from these nanoparticles possess a wavelength of about 50 meters, placing them within the high-frequency (HF) wave category. These radio waves occupy the atmospheric window and can serve as fundamental components for transmitters and receivers in radio telescopes, particularly in the field of astrobiology. Figure 7 presents a schematic representation of a silicon-dot coating layer utilized in astronomical radio receiver devices【50-55】.

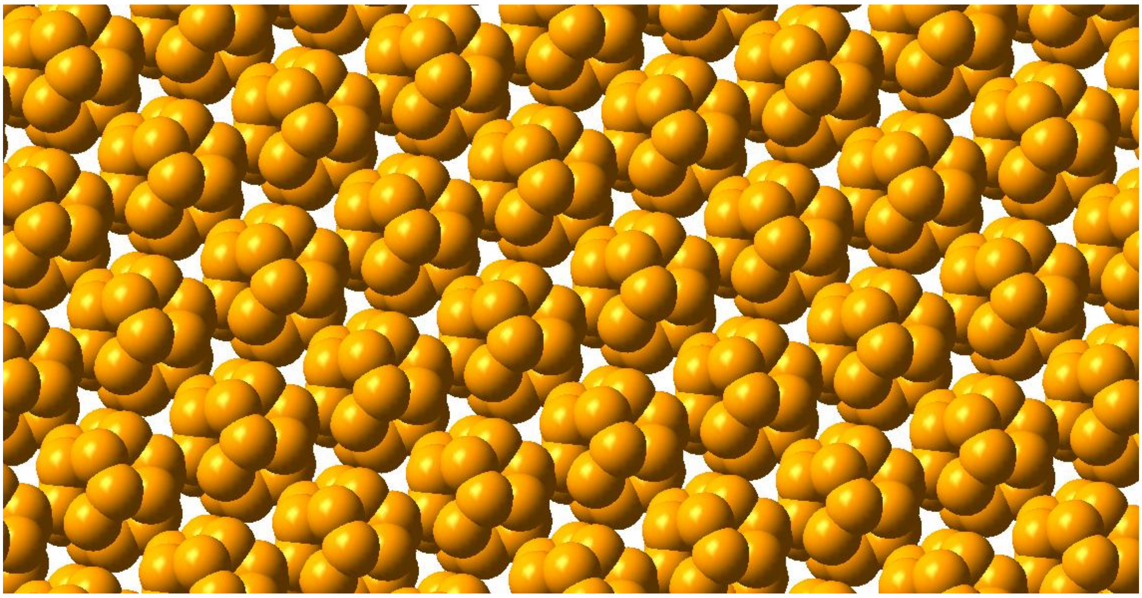

Figure 7: A schematic of the silicon-dot coating layer for an astronomical radio receiver device.

Silicon nanoparticles offer two primary advantages. First, their IR vibrational spectrum closely resembles that of biological molecules, allowing for effective adaptation to the desired spectral domain through functionalization. Figure 8 illustrates the vibrational spectrum of an ideal silicon-dot type, demonstrating its proximity to biological molecular vibrations【56-57】.

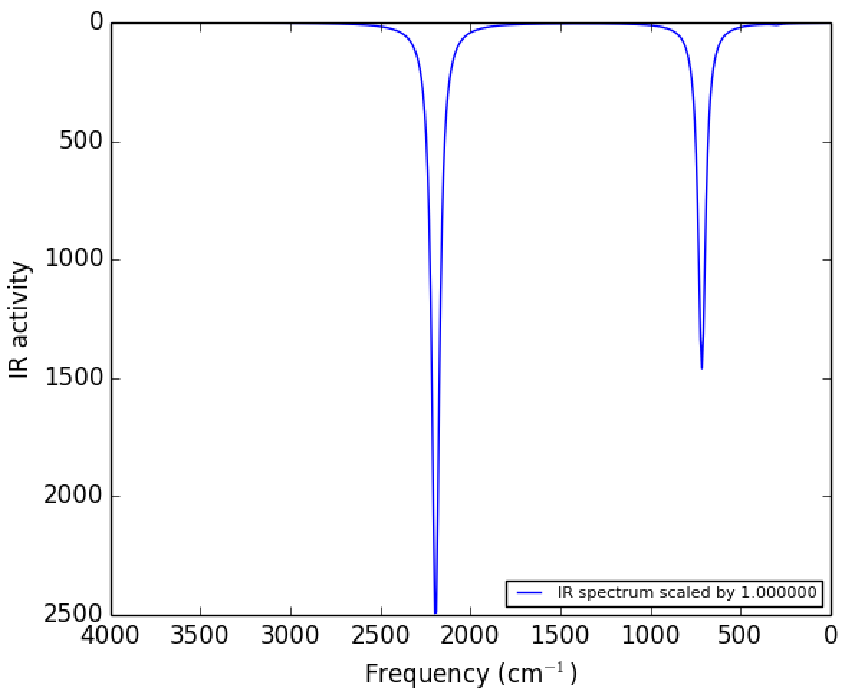

Figure 8: The vibrational spectrum of an ideal silicon-dot type, illustrating its similarity to the vibrations of biological molecules.

Additionally, unlike other nanoparticles that operate under the principle of the particle-in-a-box model or quantum confinement effects, silicon nanoparticles exhibit a gentler slope. This characteristic allows for less precision in production, making their manufacturing process more cost-effective【58-63】.

Within the Earth's atmosphere, particularly in the upper mesosphere and at altitudes reaching approximately 1000 kilometers, there exists a high density of electric charge. High-energy solar radiation entering these upper atmospheric layers breaks molecular bonds, resulting in the release of free electrons and leaving the remaining atoms ionized; this region is referred to as the ionosphere. The intensity of ionization varies with altitude, creating layers of differing electron and ion densities.

The electric charge density within the ionosphere forms a conductive layer that reflects radio waves from distant parts of the universe, functioning similarly to a metallic sheet. As a result, radio telescopes, such as the Hubble Space Telescope, are strategically positioned outside the ionosphere to avoid signal distortion【64-67】. If these telescopes can successfully detect spectra associated with chemical structures containing nitrogen and oxygen, it would parallel the breakthroughs nanoscience has brought to our understanding on Earth【68-70】. This spectroscopic astronomy may ultimately provide compelling evidence for the existence of extraterrestrial life【71-73】.

Conclusion

In summary, this course demonstrates how high school students can engage with key scientific concepts through a STEM approach combined with the Inquiry-Based Science Education (IBSE) method. The following topics can be effectively taught:

- Physics: Topics include the electromagnetic spectrum, transmitting antennas, types of radio and infrared telescopes, the ionosphere and plasma, the interaction of electromagnetic waves with the atmosphere, and astronomical spectroscopy.
- Chemistry: Discussions can encompass functional groups, organic structures, molecular vibrations, computational chemistry, and nanostructures.
- Biology: Key concepts include the formation of life, biological molecules, and the structure of DNA.

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