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Cyanopolyynes in the Interstellar Medium: *In Silico* Analysis of Electronic Properties and Chain Length

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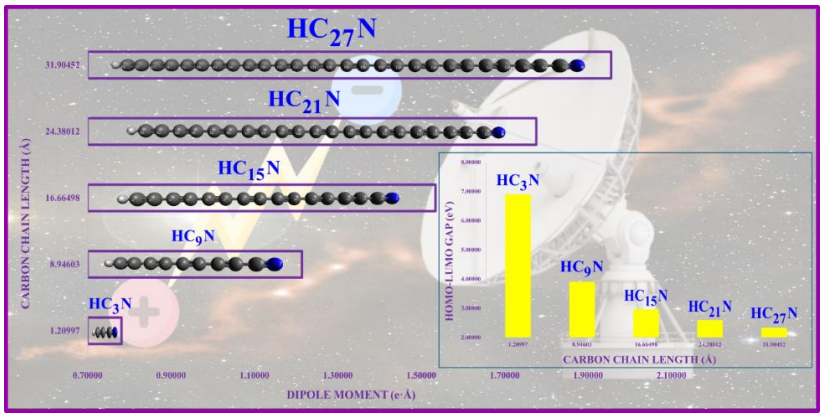
This study investigates electronic properties of linear cyanopolyynes (HCnN, with odd n from 3 to 29) by means of electron structure calculations at the DFT/B3LYP/6-311G(3df,3pd) level. Correlations between the chain length, the electric dipole moment and the HOMO-LUMO gap were analyzed. The molecular geometries were optimized and validated by vibrational calculations. The data obtained revealed that the dipole moment increases with the increase in chain length, while the gap decreases in a logarithmic way. The relationship between dipole and gap was described by by a potential model, indicating coherence between molecular structure and electronic properties. These patterns are relevant both for the detection of cyanopolyynes in the interstellar medium, by rotational spectroscopy, and for applications in molecular electronics. The statistical adjustments showed high coefficients of determination ($R^2 > 0.99$), confirming the robustness of the models used.

Graphical abstract



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1. Introduction

Astrochemistry is a fascinating field that combines knowledge from astronomy, chemistry, and physics to investigate the chemical evolution of the universe. It seeks to understand how molecules arise, transform and survive in interstellar space. Although it is a relatively young field, astrochemistry has developed rapidly, driven by technological advances, especially in radio astronomy. A significant advancement in astrochemistry occurred in 1963 with the identification of the OH radical using this technique, marking the beginning of deeper insights into molecular presence in the cosmos. Since that time, approximately 280 molecules have been detected across various space environments, particularly within the Interstellar Medium (ISM), which is renowned for its remarkable chemical diversity [1].

The ISM, which exists among the stars, consists of cosmic dust, ice, atomic and moleculares gases, as well as charged particles. Its low temperatures and densities allow for the study of the chemical characteristics of the universe [2]. Within this environment, molecular clouds contribute to the

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formation of molecules, including some that do not remain stable on Earth. For this reason, Computational Quantum Chemistry methods are commonly employed to identify and analyze these molecules more precisely [3].

Taurus Molecular Cloud 1 (TMC-1), about 450 light-years away in Taurus, is a region of the interstellar medium with temperatures near 10 K and densities between 10^4 and 10^5 particles per cm^3 — Although they appear dense compared to other areas of space, these clouds are incredibly less dense than the Earth's atmosphere, which has an average density of 10^{19} particles per cm^3 [4]. The presence of elements like carbon and nitrogen allows for the formation of complex molecules such as cyanopolyynes, which are important to both astrochemistry and technology, and provide insight into chemical processes in space and the origins of life.

Cyanopolyynes are linear chains of carbon, alternating between single and triple bonds, and terminated by a cyan group (—C≡N). In the context of astrochemistry, these molecules draw attention for their presence in molecular clouds such as TMC-1. However, they have also aroused great interest in the field of molecular electronics due to their potential as molecular wires. These carbon chains exhibit unique electronic properties, such as the potential for conducting electric current at nanometer scales, which makes them promising for applications in optoelectronic devices.

Two electronic properties, the dipole moment and the HOMO-LUMO gap, are fundamental to understand the electronic behavior of cyanopolyynes. The dipole moment indicates the degree of polarity of the molecule and influences its interaction with electric fields, which is relevant for its detection by rotational spectroscopy [5] and its application in electronic devices [3]. The HOMO-LUMO gap, which represents the energy difference between the highest occupied orbital (HOMO) and the lowest unoccupied orbital (LUMO) [6], is directly related to the electron transport capacity of the molecule [3]. Smaller GAPs generally mean greater ease of conducting electrons, which is desirable in electronic devices.

In this context, the relationship among cyanopolyyne chain length, dipole moment, and the HOMO-LUMO gap offers insights relevant to astrochemistry as well as applications in advanced technologies. These molecules may influence fields such as molecular electronics, which studies electronic devices at the nanometer scale where electrons pass through molecular structures, and optoelectronics, which integrates optical and electronic properties in various devices. This work seeks to explore these relationships, contributing both to the understanding of chemical processes in space and to the practical application of these molecules in cutting-edge technological systems.

The molecules analysed in this study belong to the group of cyanopolyynes, whose general formula is HCnN (with n = 3, 5, 7...). These molecules have been identified in regions of the EOM as TMC-1, Sgr B2, and Heiles 2 [7, 8]. Cyanopolyynes are of great importance both in astrochemistry (because they contribute to the formation of more complex molecules) [7] and in molecular electronics (because of their unique electronic properties, such as the potential for conducting electric current) [3]. Structurally, cyanopolyynes have a linear sequence composed of multiple acetylene units (—C≡C—), characterized by triple bonds alternating with single bonds between carbon atoms. At one end, there is a hydrogen atom (H), and at the other, a cyan group (—C≡N).

The largest molecule of this type identified in space so far is $HC_{11}N$ (cyanopentaacetylene), initially detected in the molecular cloud TMC-1 [9]. On the other hand, the smallest member of the series, HC_3N (cyanoacetylene), was discovered in 1971 by Turner in the direction of Sgr B2 [10]. In addition, both HC_3N and HC_5N (cyanodiacetylene) have been found in the atmosphere of Titan, Saturn's largest moon, rich in hydrogen, nitrogen, and carbon [11-13]. Titan's atmosphere, composed mostly of 98% N_2 and 1.8% CH_4, is exposed to solar ultraviolet radiation and energetic particles from Saturn's magnetosphere. These chemical interactions result in the formation of several species, including HC_3N and HC_5N [12].

The first five cyanopolyynes in the series — HC_3N (cyanoacetylene), HC_5N (cyanodiacetylene), HC_7N (cyanotriacetylene), HC_9N (cyanotetraacetylene) and $HC_{11}N$ (cyanopentaacetylene) — have already been detected in interstellar molecular clouds, such as TMC-1 [14]. In addition, these molecules have also been observed in circumstellar envelopes, such as that of the carbon-rich star IRC+10216, and the protoplanetary nebula CRL 2688 [15].

Studies using computational quantum chemistry methods have been instrumental in understanding the properties of cyanopolyynes in the EOM and in aiding in their detection [16]. For example, the molecules HC_9N and $HC_{11}N$ have been identified based on models that extrapolated their rotational constants [17]. In more detailed investigations, HC_9N was analyzed with the Coupled Pair Theory method, at the CCSD(T)/cc-pVTZ level [18]. The equilibrium geometries and dipole moments obtained in this study helped to determine the radial column densities of cyanopolyynes in the TMC-1 region [9]. Another study evaluated the dipole moments of small cyanopolyynes using both the Møller-Plesset Second-Order Perturbation Theory (PM2) and the Density Functional Theory (DFT), with the BP86 functional and the 6-31G* base. Comparing the results, the researchers found that the MP2 method produced dipole moment values that were more accurate than the DFT/BP86/6-31G* level [19]. In addition, other studies have focused on the electronic structure of different cyanopolyynes, employing DFT and CCSD(T) calculations to deepen the understanding about these molecules [20-22].

2. Material and Methods

In this study, linear molecules of the cyanopolyynes family were analyzed, with the general formula HCnN, in which n to 3, 5, 7.... Fig. 1 shows the representative molecular structures used in the simulations.

The molecular geometries were optimized through the Density Functional Theory (DFT) [23, 24], using the hybrid functional B3LYP and the base set 6-311G(3df,3pd), as implemented in the ORCA 5.0.1 program [25]. The functional B3LYP was chosen for its balanced performance between computational accuracy and cost, and is widely used for π-conjugate systems and long molecular chains [26-28]. Although there are more modern functionals, such as M06-2X or ωB97XD, the choice of B3LYP is justified by its robustness and wide acceptance in the literature for the type of system under study [21, 29-31].

The base 6-311G(3df,3pd) was chosen because it provides an adequate description of the valence and polarization functions for linear molecules, such as cyanopolyynes, ensuring a good balance between accuracy and computational cost [32-34]. Comparative tests performed by QI and collaborators indicate that the inclusion of fuzzy functions, present in the base 6-311++G(3df,3pd), results in small variations in the dipole moment (~1 to 2%) and

negligible impact on the HOMO–LUMO gap (< 0.05 eV) for typical neutral systems of the HCnN series [21]. Methodological reviews, such as Jensen's, also argue that the need for fuzzy functions depends on the property studied, recommending their use especially for tail-sensitive properties of the electron density [35]. Thus, the exclusion of diffuse functions is justified for the scope of this work, in which trends and correlations are prioritized throughout the series, without compromising the quality of the electronic and structural results.

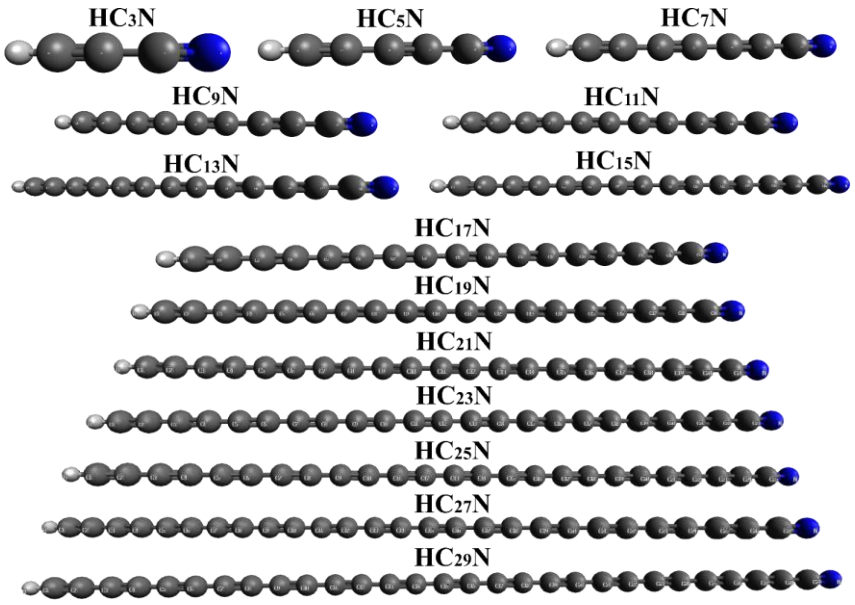

Fig. 1. Representative molecular structures of linear cyanopolyynes HCnN (n = 3 a 29), level optimized DFT/B3LYP/6-311G(3df,3pd).

The geometries have been optimized without restrictions, allowing all degrees of freedom, using the standard ORCA convergence criteria. Subsequently, vibrational frequency calculations were performed in the harmonic approximation to ensure that the structures obtained corresponded to local minima on the potential energy surface. The absence of imaginary frequencies confirmed the stability of the geometries, validating the physical interpretation of the results obtained.

From the optimized structures, the electric dipole moments and the energies of the boundary orbitals (HOMO and LUMO) were extracted, from which the HOMO-LUMO gap was calculated as the difference between LUMO and HOMO. The length of the chain was defined as the length of the cyanopolyyne, excluding the terminal hydrogen atom and the cyan group, along the molecular axis. This choice aims to focus the analysis on the repetitive units of the conjugate carbon chain, which are the main responsible for the electron properties analyzed, such as the HOMO-LUMO gap and the dipole moment. Although the total length of the molecule (from H to the CN group) is slightly longer, the adoption of this definition does not compromise the comparison between different species, in addition to providing a more direct representation of the influence of the effective size of the carbon chain on molecular properties.

The geometric and electron variables were statistically correlated by means of nonlinear regressions, adopting polynomial, logarithmic or potential models, according to the trend observed in each case. The adjusted coefficients (a and b), their standard errors and the R^2 values were obtained by adjusting curves in Microsoft Excel. The results of these analyses are summarized in Table 2 and graphically represented in Figs. 2, 3 and 4.

3. Results and Discussion

3.1 Results

In this section, we present the results of the correlation between the linear carbon chain length, the dipole moment and the HOMO-LUMO gap of the cyanopolyynes analyzed in this study. The calculated values can be seen in Table 1, while the graphical analyses of these relationships are presented in Fig. 2, Fig. 3 and Fig. 4. The regression models applied to these data, with their respective adjusted parameters and coefficients of determination (R^2), are summarized in Table 2.

Table 1. Values of Chain Length, Dipole Moment and HOMO-LUMO gap of the Chemical Species Studied.

Molecule	Cyanopolyyne Chain Length (Å)	Dipole Moment (e·Å)	HOMO-LUMO Gap (eV)
HC_3N	1.210	0.781	6.903
HC_5N	3.794	0.942	5.371
HC_7N	6.371	1.085	4.484
HC_9N	8.946	1.214	3.907
$HC_{11}N$	11.520	1.331	3.501
$HC_{13}N$	14.093	1.438	3.200
$HC_{15}N$	16.665	1.534	2.965
$HC_{17}N$	19.235	1.622	2.786
$HC_{19}N$	21.809	1.702	2.638
$HC_{21}N$	24.380	1.776	2.590
$HC_{23}N$	26.792	1.842	2.489
$HC_{25}N$	29.348	1.901	2.404
$HC_{27}N$	31.905	1.955	2.332
$HC_{29}N$	34.461	2.004	2.270

CYANOPOLYYNE CHAIN LENGTH (Å): cyanopolyyne chain length (excluding the terminal hydrogen atom and the CN group). DIPOLE MOMENT (e· Å): dipole moment, in electron-angstrom. HOMO-LUMO gap (eV): energy difference between the HOMO and LUMO orbitals, in electronvolts.

3.1.1 Chain Length versus Dipole Moment

Table 1 and Fig. 2 shows that, as the carbon chain length of cyanopolyynes increases, there is also a growth in the dipole moment. This indicates that as more carbon atoms are added to the molecule, the distribution of electronic charge along the chain becomes more polarized. For example, while the HC_3N molecule has a dipole moment of 0.781 e·Å, the $HC_{29}N$ molecule reaches 2.004 e·Å.

The regression applied to this correlation was well described by a second-order polynomial model, with R^2 = 0.9996, indicating an almost perfect fit to the data. This quantitative result reinforces the observed trend and confirms the coherence between the increase in molecular length and the intensification of the dipole moment. The adjusted parameters are presented in Table 2.

Table 2. Parameters of the regression models applied to the variables studied, with respective standard errors and coefficients of determination (R^2).

Correlation	Model	a (± error)	b (± error)	R^2
Dipole vs Length	Polynomial	0.7247 ± 0.0066	0.0595 ± 0.00085	0.9996
GAP vs Length	Logarithmic	7.1090 ± 0.1019	−1.4210 ± 0.0370	0.9919
GAP vs Dipole	Power	4.985 ± 0.048	−1.1623 ± 0.0206	0.9964

This behavior can be explained by the greater spacing between the opposite charges within the molecule, caused by the elongation of the carbon chain. For example, considering only the cyanopolyyne chain (i.e., disregarding the terminal hydrogen and the cyan group), the HC_3N molecule has an extension of approximately 1.21 Å, while in HC_9N this value reaches about 8.95 Å. This structural elongation contributes to increased charge separation along the molecule, resulting in progressively larger dipole moments with increasing chain length. This structural elongation directly contributes to the increase of the dipole vector. This characteristic is important because molecules with larger dipole moments interact more intensely with electric fields, which facilitates their detection in rotational spectroscopy and enhances their use in electronic devices.

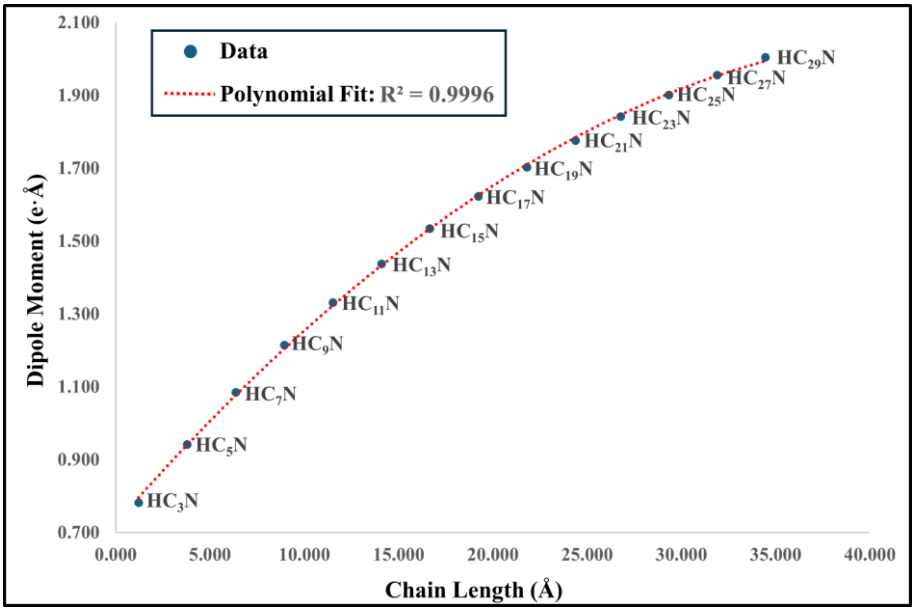

Fig. 2. Correlation between the dipole moment and the cyanopolyyne chain length (excluding the terminal hydrogen atom and the CN group).

3.1.2 Chain Length versus HOMO-LUMO Gap

The HOMO-LUMO gap, which represents the energy difference between the highest occupied orbital (HOMO) and the lowest unoccupied orbital (LUMO), decreases significantly as the length of the carbon chain increases. This trend is clearly observed in Table 1 and illustrated in Fig. 3. For example, the HC_3N molecule has a gap of 6.903 eV, while the $HC_{29}N$ molecule has only 2.270 eV.

The regression applied to this relationship was better adjusted by a logarithmic model, with a coefficient of determination R^2 = 0.9919, which indicates a strong correlation between the length of the chain and the reduction of the gap. This type of decay is typical of long π-conjugate systems, in which the amplification of electron delocalization reduces the energy required to promote an electron from HOMO to LUMO.

Physically, this is because, with the increase in the number of carbon atoms in the chain, the molecular orbitals become more spaced and distributed throughout the molecule, reducing the energy difference between the occupied and unoccupied levels. This characteristic is essential for applications in molecular electronics, as it indicates that larger molecules can behave as semiconductors with a lower electronic barrier, favoring charge transport.

3.1.3 Dipole Moment versus HOMO-LUMO Gap

The relationship between the electric dipole moment and the HOMO-LUMO gap of the cyanopolyynes reveals an inverse behavior: the higher the dipole moment, the smaller the electron gap tends to be. This trend can be observed in the data in Table 1 and is graphically evidenced in Fig. 4.

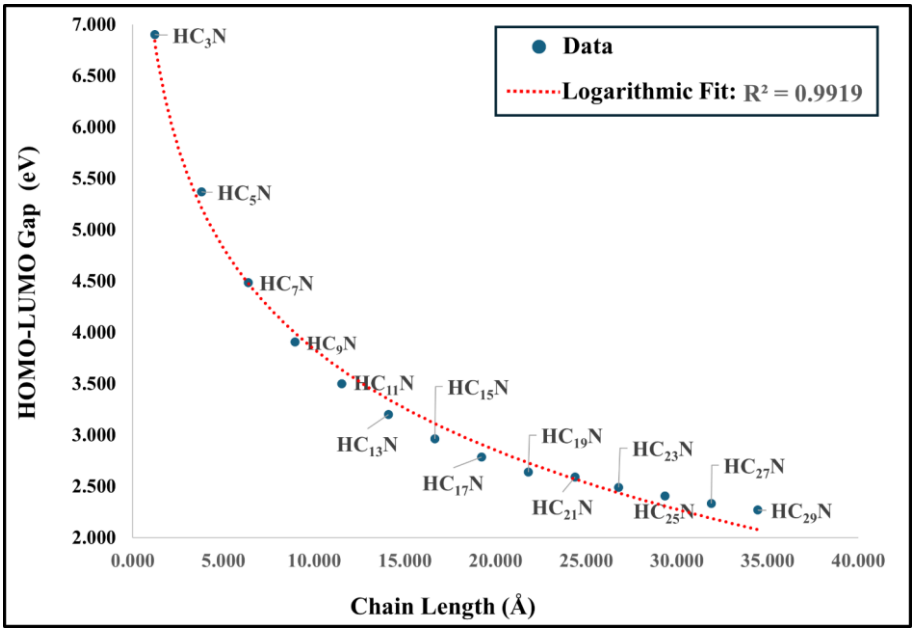

Fig. 3. Correlation between the HOMO-LUMO gap and the cyanopolyyne chain length (excluding the terminal hydrogen atom and the CN group).

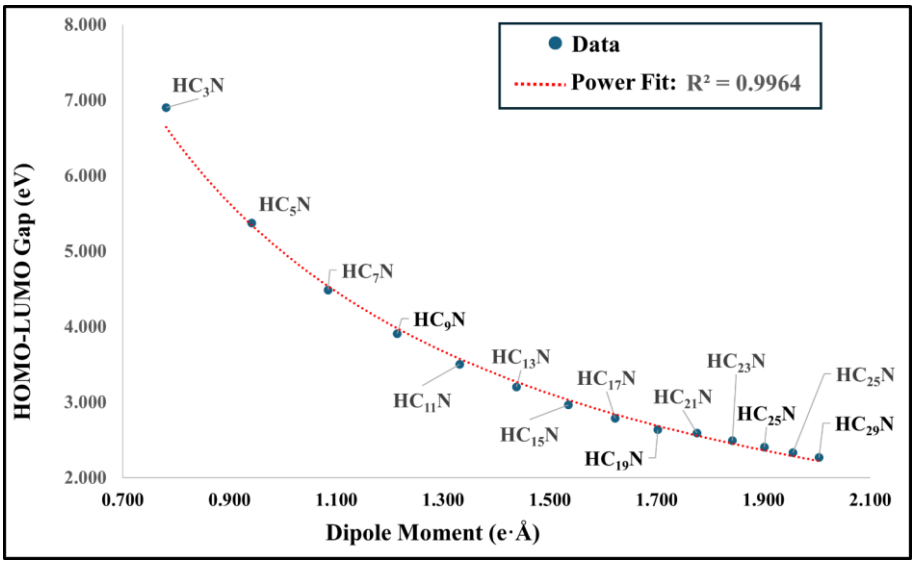

Fig. 4. Correlation between the dipole moment and the HOMO-LUMO gap of cyanopolyynes.

The most appropriate fit to describe this correlation was a potential model, with a coefficient of determination R^2 = 0.9964, indicating a strong functional dependence between the variables. The nonlinear behavior suggests that the effect of polarization on gap reduction intensifies in molecules with longer dipole moments.

Physically, this pattern can be interpreted as a result of the greater ability of the more polar molecules to rearrange their electron density. This reduces the energy barrier between the HOMO and LUMO orbitals, facilitating electronic transitions. This relationship is particularly relevant for the design of semiconductor molecular materials or chemical sensors, in which polarity can be manipulated to adjust electronic performance.

3.2 Discussion

The results obtained reinforce the role of cyanopolyynes as molecules with significant potential both in fundamental research and in technological applications. In particular, longer species, such as $HC_{29}N$, have desirable electronic characteristics for molecular semiconductor materials, combining high dipole moments and reduced HOMO-LUMO gaps.

In the context of astrochemistry, the increase in the dipole moment with the length of the chain is highly relevant, as it favors the detection of these molecules by rotational spectroscopy (one of the main techniques for identifying compounds in dense molecular clouds, such as TMC-1). The increasing polarity facilitates interaction with microwave radiation, which contributes to the success of astronomical observation of these species.

From the perspective of molecular electronics, the systematic reduction of the HOMO-LUMO gap with the increase of the carbon chain is in line with the typical behavior of extended π-conjugate systems. This property indicates that the larger cyanopolyynes can act as organic nanowires with

adjustable conductivity, an important feature for molecular-scale devices.

In addition, the observed patterns point to opportunities for structural modulation: variations in the terminal groups or in the introduction of substituents along the chain can alter in a controlled manner both the polarity and the electronic behavior, expanding the range of functionalities of these compounds in specific applications. Finally, although the results obtained by electronic structure methods provide a reliable overview of the behavior of these molecules, their experimental validation is an essential step. Techniques such as UV-Vis spectroscopy, photoelectron spectroscopy, or electron transport experiments will be able to confirm and expand the understanding of the performance of cyanopolyynes in real environments, whether in interstellar space or in functional devices.

4. Conclusions

In this study, we investigated the electronic properties of a series of linear cyanopolyynes (HCnN) by means of electron structure calculations at the DFT/B3LYP/6-311G(3df,3pd) level. The analyses showed that the electric dipole moment increases with the increase in the length of the chain, while the HOMO-LUMO gap shows a logarithmic downward trend. These statistically robust correlations were described by regression models with high coefficients of determination (R^2 > 0.99), evidencing the direct relationship between the molecular structure and the electronic properties of the compounds studied. The strong polarization of the larger molecules favors their detectability in rotational spectroscopy, which is particularly relevant for astrochemistry. Simultaneously, the reduction of the HOMO-LUMO gap suggests that these systems can exhibit significant electronic conductivity, positioning cyanopolyynes as promising candidates for applications in molecular electronic devices and sensors. The results obtained offer a solid basis for understanding the role of these molecules both in the ISM and in emerging technological contexts.

Based on the findings of this work, some directions are proposed for the deepening of the investigation on cyanopolyynes. The experimental validation of theoretical data through techniques such as UV-Vis spectroscopy, photoelectron spectroscopy, and electron transport experiments is essential to confirm the applicability of the proposed models. The use of more modern and specific functionals to describe systems with electronic relocation, such as CAM-B3LYP, ωB97X-D or M06-2X, may offer even more accurate estimates. In addition, studying the effect of different substituents on the ends of the chains, as well as simulating external environments such as solvents or surfaces, can reveal ways to modulate the electronic properties of these molecules. Finally, the application of dynamic approaches, such as electronic transport simulations based on Landauer's theory, may expand the understanding of the behavior of cyanopolyynes in real operational contexts, allowing the advancement in the development of functional molecular devices.

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Author Contributions

Gilberto Anders Ferreira: Conceptualization, Methodology, Investigation, Formal analysis, Software, Data curation, Visualization, Writing – original draft. Eloi Alves da Silva Filho: Supervision, Validation, Writing – review and editing.

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