International Journal of

Chemical Separation Technology

ISSN: 2456-6691
Volume 10, Issue 2, 2024
DOI (Journal): 10.37628/IJCST

https://chemical.journalspub.info/index.php?journal=JCCST

Review IJCST

A Novel Approach to the Investigation of Molecular Polarization Using MATLAB Application

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Abstract

*Molecular polarization involves the separation of electric charge in a molecule due to the result of an induced external field leading to a dipole having a positive charge on one side and the negative charge at the other end. This helps us to know the characteristics of molecules and how they react with others. It is also helpful to know their physical and chemical properties. Molecular polarization also includes its intermolecular forces, dielectric behavior and chemical reaction. It also talks about the difference in electronegativity of the combining atom, its molecular geometry binding patterns and shows how the external field affect it. The percentage static polarization for each element in m^3 were determined as per the MATLAB program of alpha_Cl2 = 4.48e-30, % chlorine (Cl2) alpha_Be = 2.78e-30, % beryllium (Be) alpha_Ca = 4.2e-30, % calcium (Ca) alpha_Mg = 4.1e-30, % magnesium (Mg) and alpha_Br2 = 5.25e-30, % bromine (Br2). Also percentage calculation of frequency-dependent polarization using the given formula P_m_Cl$_2$ = P_s_Cl$_2$ ./ (1 + 1i * omega * tau), P_m_Be = P_s_Be ./ (1 + 1i * omega * tau), P_m_Ca = P_s_Ca ./ (1 + 1i * omega * tau), P_m_Mg = P_s_Mg ./ (1 + 1i * omega * tau) and P_m_Br$_2$ = P_s_Br$_2$ ./ (1 + 1i * omega * tau) was applied in the simulation of the process network of each element polarization.*

Keywords: Novel, approach, investigation, molecular, polarization, MATLAB application

INTRODUCTION

Polarization can be seen as a process of separating different charges making one end concentrated with a particular charge and the other the other charge. There are different mechanisms of polarization which are electronic polarization, ionic polarization, bipolar politization and space charge. Molecular polarization is one of the basic concepts in chemistry and physics which explain the separation of electric charges in a molecule. This can be seen as the uneven distribution of charges in a molecule. This separation leads to a dipole moment which can be seen as a measure of molecular polarity. When molecular polarization is studied in different molecules like water, methane and its chlorination. The dipole of the negatively and positively charged electron has a distance and magnitude of the partial charges of each of the atom bond in the molecule which can be calculated. Like for water having the hydrogen atom separated at a distance and having a given momentum form the oxygen atom. A molecule's structure appears to accept or have distinct settings

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Received Date: 17 October 2024
Accepted Date: 31 October 2024
Published Date: 18, December 2024

Citation: C. P. Ukpaka, Victor Chukwuemeka Ukpaka, Abraham Peter Ukpaka. A Novel Approach to the Investigation of Molecular Polarization Using MATLAB Application. International Journal of Chemical Separation Technology. 2024; 10(2): 1–18p.

when polarization occurs in comparison to the molecule's usual state. It facilitates comprehension of a molecule's features and attributes, including dieletric and hydrogen bonding qualities. The application of molecular polarization can be extremely beneficial in a variety of fields, including biology, medicine, engineering, materials science, and materials science. Thus, gaining additional knowledge about it facilitates and expedites life [1, 2].

OBJECTIVES OF MOLECULAR POLARIZATION

Advancing Materials Science

Molecular polarization is essential for understanding the properties of materials and designing new materials with specific applications.

Understanding Molecular Structure

The arrangement of atoms and electrons within a molecule can be seen thanks to molecular polarization.

Examining Intermolecular Forces

Molecular polarization facilitates comprehension of intermolecular forces including hydrogen bonding and van der Waals interactions.

Predicting Molecular Characteristics

Solubility, melting, and boiling temperatures are among the attributes that can be predicted using molecular polarization.

Designing Materials

To create materials with characteristics, including ferroelectrics and dielectrics, molecular polarization is essential.

Creating Novel Medications

To better understand how molecules interact with biological systems, drug designers incorporate molecular polarization in their designs.

Knowing Chemical Reactivity

Molecular polarization clarifies how molecules interact with one another.

Calculating Dipole Moments

Dipole moments are crucial for comprehending molecular characteristics and may be computed thanks to molecular polarization.

LIMITATIONS OF MOLECULAR POLARIZATION

Assumes a Hard Molecular Structure

For flexible or dynamic molecules, the assumption made by molecular polarization – a fixed molecular structure – may not be correct.

Neglects Electron Correlation

Because molecular polarization ignores electron correlation, calculations of molecular characteristics may be inaccurate.

Limited to Tiny Molecules

Larger molecules would need more involved procedures when using molecular polarization, which is normally used to smaller molecules.

Assumption of Linear Response

In the case of strong fields or nonlinear systems, the assumption of a linear response to external fields made by molecular polarization may not hold true.

Requires High-Level Quantum Computations

High-level quantum computations, which can be computationally demanding, are necessary for accurate molecular polarization calculations.

Characteristics of Molecular Polarization

These are some of the characteristics of molecular polarization.

Electronic Polarizability

The ability of a molecule to modify its electron cloud in reaction to an external electric field is known as electronic polarizability. The molecule is able to interact with the electric field because of this deformation, which creates a transient dipole moment. Studying molecular characteristics like dielectric constants and refractive indices requires an understanding of electronic polarizability.

Dipole Moment

The difference between the positive and negative charges in a molecule is measured by its dipole moment. It's a key idea in the understanding of molecular polarization. Dipole moments can be created by external fields, or they can be permanent because of unequal electron sharing. They are essential for chemical reactivity, molecular characteristics, and intermolecular forces.

Polarizability Tensors

The ability to polarize Tensors are mathematical expressions that show how polarized a molecule is in various orientations. They are crucial for comprehending optical and dielectric properties because they explain how the molecule reacts to electric fields. Tensors are essential for materials science and engineering applications because they aid in the prediction of molecular behavior in a variety of domains.

Hyperpolarizability

A molecule is said to be hyperpolarizable if it can twist its electron cloud in reaction to high-frequency electric fields. This characteristic is essential to comprehending nonlinear optical phenomena like sum-frequency generation and second-harmonic generation. To create materials with distinctive optical properties, hyperpolarizability is necessary.

Molecular Orientation

Molecular orientation refers to the alignment of molecules in response to external fields, influencing polarization. This alignment can be induced by electric or magnetic fields, temperature gradients, or surface interactions. Understanding molecular orientation is vital for studying liquid crystals, ferroelectric materials, and biological systems.

Intermolecular Forces

The relationships between molecules that are altered by polarization are termed as intermolecular forces. Among these forces are Dipole-dipole forces (between permanent dipoles): – Van der Waals forces – forces between constant and induced dipoles that are caused by dipoles – London dispersion forces (between transient dipoles) – hydrogen bonding: the bonding of molecules containing hydrogen atoms to atoms that are electronegative – interactions between ions that have different charges. For the aim of looking up material qualities like melting and boiling point as well as solubility, an understanding of intermolecular forces is necessary.

Ferroelectricity

Certain materials possess an attribute known as ferroelectricity called spontaneous polarization, which allows them to hold an electric dipole moment continually despite an external field. Due to their unique properties, ferroelectric materials can be used in the following applications: – memory components, such as ferroelectric RAM – sensors, such as those for pressure harvesting and conserving energy typically, ferroelectric materials are solids with crystalline structure and certain symmetry characteristics.

Molecular Simulation

Molecule simulation is the study of molecule polarization and how it affects material characteristics through computational approaches. Methods consist of: – simulations of molecular dynamics (MD): – simulate the motion and interactions of molecules – offer details on thermodynamics and molecular dynamics – Monte Carlo simulations (MC): – use statistical techniques to model the behavior of molecules – give details about phase behavior and molecular thermodynamics: – computes quantum chemistry: - model the electrical structure and characteristics of molecules: – give details about spectroscopy and molecular reactivity. Molecular simulations aid in the understanding of intricate molecular dynamics and the creation of novel materials with targeted characteristics, such as dipole moment: A measurement of the total polarity of the molecule, denoted by the symbol μ (mu). Polarity: The degree to which a molecule’s charges are separated, ranging from extremely polar to nonpolar (no charge separation). Electronegativity: An atom’s capacity to draw electrons, which affects how charges are distributed inside molecules. Molecular shape: Charge distribution and polarization are influenced by the arrangement of atoms within a molecule. Polarizability: A molecule’s capacity to change the shape of its electron cloud in reaction to an outside electric field. Hydrogen bonding: The formation of hydrogen bonds by polar molecules affects their chemical and physical characteristics. Understanding the behavior and features of molecules in a variety of scientific domains, such as chemistry, physics, and biology, requires an understanding of these traits. Through the structure depicted, these features can be obtained or observed [3–5].

Applications of Molecular Polarization

Dielectric materials: Capacitors and other electrical devices are made of materials with high molecular polarization. Biological systems: Protein-ligand interactions and membrane transport are two examples of biological systems in which molecular polarization is essential. Chemical reactions: The reactivity of molecules and the result of chemical reactions are both influenced by molecular polarization. Materials science: The creation of materials with features, like ferroelectric materials, depends on molecular polarization.

MATERIALS/METHOD

The research explored the effects of molecular polarization by using a diverse set of molecules, including polar substances like water and methanol, to examine their properties and behavior. In this we considered methane and it’s chlorinations.

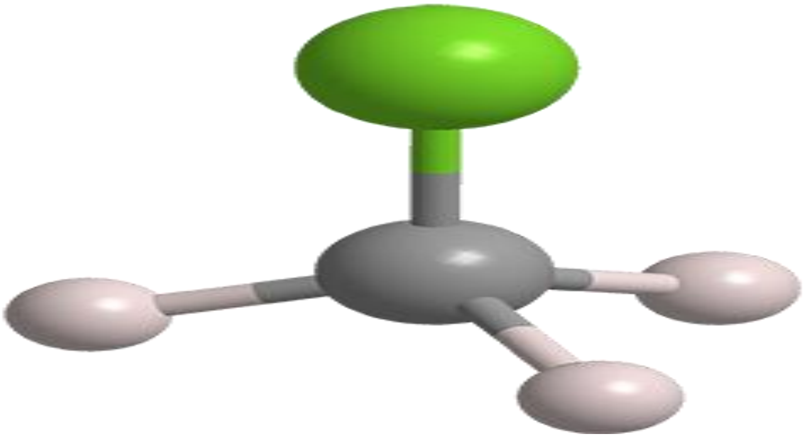
Consideration of Methane (CH_4) and Its Chlorinations (CH_3Cl, CH_2Cl_2, $CHCl_3$, CCl_4)

CH_4

Methane has a molecule that is tetrahedral in shape and it's symmetrical with some hydrogen atom bonded uniformly around the carbon (c) atom. For the fact that the carbon (c) and hydrogen atoms are evenly shared the methane is nonpolar due to the symmetrical nature of the atom in the molecule. Methane can be polarized by an induced electrical field, when the happens the electron are displaced, creating a dipole moment that is temporary, pushing the electron towards one end of the molecule thereby creating a partial negative charge and creating a partial positive charge on the protons left behind at the other end. When polarization is induced into methane it is relatively weak due to methane's relatively low polarizability and it is symmetrical shape.

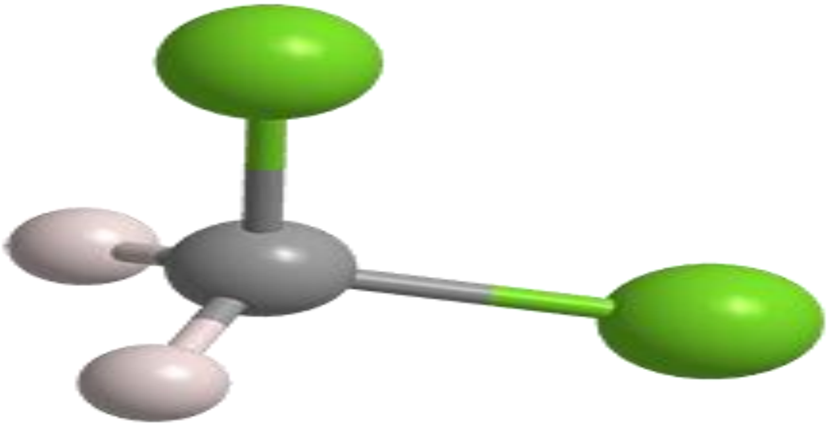
CH_3Cl

Chloromethane is identified as a polar molecule which shows difference in electronegativity in terms of carbon (C) and chlorine (Cl) atom. The C–Cl bond's polarity generates a lasting electric dipole moment, contributing to chloromethane's overall polar nature. In addition to its permanent dipole moment, CH_3Cl can also exhibit induced polarization when exposed to an electric field. This is like methane, but the effect is more pronounced in CH_3Cl due to its existing permanent dipole moment.



CH_2Cl_2

Dichloromethane as well as methylene chloride is identified as a polar molecule which shows difference in electronegativity of carbon (C) and chlorine (Cl) atom as well as the symmetrical arrangement of Cl atoms, showing the net dipole moment. When CH_2Cl_2 is acted upon by an external electric field, the electric field induces a temporary polarization in the molecule, in addition to its existing permanent dipole moment also the permanent dipole moment of CH_2Cl_2 aligns with the external electric field, resulting in a net increase in the molecule's dipole moment.



$CHCl_3$

$CHCl_3$ also known as chloroform, is a polar molecule because of the difference in electronegativity between carbon (C) and chlorine (Cl) and the symmetrical arrangement of Cl atoms, resulting in a net dipole moment. The electric field can lead to the alignment of the molecules in a particular direction, resulting in total polarization. It also induced temporary dipole moments in the molecule, in addition to its already existing permanent dipole moment. Now the molecule becomes polarized.

CCl_4

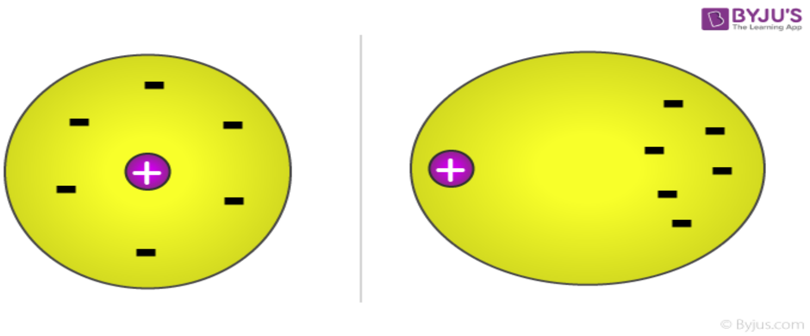
Due to a certain action, CCl_4 is a non-polar molecule. atoms of chlorine arranged symmetrically around carbon atoms. Additionally, there is a net dipole moment because all the atoms that are bound to the carbon are chlorine and have identical electronegativity. It also exhibits transient, weak polarization in response to external electric fields, no dieletric relaxation, no dipole moment alignment due to its non-polar nature, and electrical susceptibility. CCl_4's non-polar nature means that an external electric field has relatively little effect on its properties.

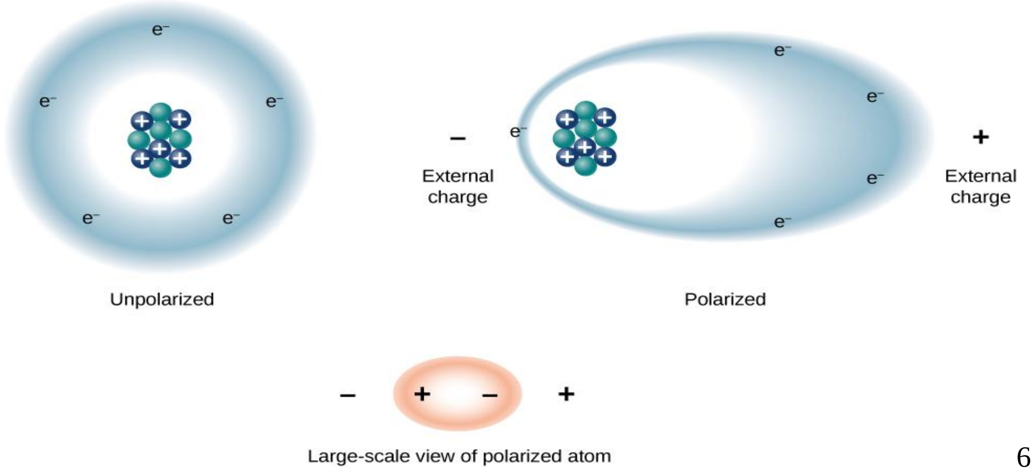
METHODS

Computational software was employed to model and optimize molecular structures, calculating their dipole moments and polarizabilities.

The molecules were subsequently synthesized using established laboratory techniques, and their optical and dielectric properties were measured using spectrophotometry and polarimetry.

Data analysis and comparison of experimental results with computational predictions were conducted to elucidate the role of molecular polarization in determining molecular behavior [6–8].





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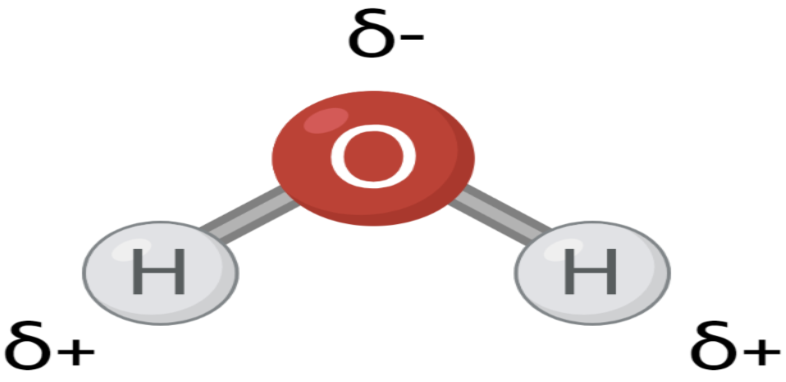

RESULTS AND DISCUSSION

- The results confirm that molecular polarization is a critical factor in determining molecular behavior, influencing both optical properties and intermolecular forces.
- The strong correlation between dipole moment and molecular polarity suggests that dipole moment can be used as a reliable indicator of molecular polarization.
- The results also underscore the value of computational modeling in understanding molecular polarization and its effects on molecular behavior as demonstrated in Table 1.

Table 1. Chlorination properties of methane.

Mathane and Its Chlorination	**Dipole Moment**	**Induced Dipole Moment**	**Polarizability**
CH_4	0	0.01	2.6
CH_3Cl	1.86	0.05	4.6
CH_2Cl_2	1.60	0.08	6.2
$CHCl_3$	1.08	0.12	8.5
CCl_4	0	0.02	1.8

Polarization in Elements (Molecule)

Chlorine

The distribution of electric charge within a chlorine molecule (Cl_2) in response to an external electric field is known as molecular polarization in chlorine. The refractive index, dielectric constant, and polarizability of the molecule are all influenced by this distribution. With both chlorine atoms sharing an equal number of electrons, chlorine molecules have a symmetrical, linear form. Molecule polarization is what causes this induced dipole moment. The ease with which an external field can distort the electron cloud can be determined by polarizability (α), which characterizes the molecular polarization of chlorine.

Polarization in Group 2 Elements

The distribution of electric charge within group 2 elements (calcium, bellerilium, magnesium molecules, etc.) that results in a transient electric dipole moment is known as “molecular polarization of that element.” This is the result of differences in electronegativity where other atoms can draw electrons to themselves because of alkali metals (group two) low electronegativity. The following variables affect group 2 molecular polarization, such as: Strength and duration of bonds, variations in electronegativity, the geometry of molecules and character ionic.

Polarization Calculations

The formula for molecular polarization P_m in terms of molecular dipole moment μ and other parameters depends on the context, but a common one is derived from the Clausius-Mossotti relation or its general form in dielectric materials.

For a gas or dilute solution, molecular polarization is given by:

$$P_m = N\alpha E \tag{1}$$

where: P_m is the molecular polarization., *N* is the number of molecules per unit volume.
α is the polarizability of a single molecule and *E* is the applied electric field.

If You're Considering Dielectric Polarization

Using the Clausius-Mossotti relation for the dielectric constant ε_r, the polarizability α is linked to the dielectric constant by:

$$\frac{\varepsilon_r - 1}{\varepsilon_r + 2} = \frac{N\alpha}{3\varepsilon_0} \tag{2}$$

where:ε_r is the relative permittivity of the material and ε_0 is the permittivity of free space.

Molecular polarization in this case is proportional to how much the medium is polarized in the presence of an external electric field.

Molecular polarization P_m is dependent on both frequency and velocity in systems involving oscillating electric fields, such as in dielectric materials under the influence of alternating fields. The behavior of polarization as a function of frequency is tied to the frequency-dependent dielectric response of the material. This leads to the concept of *dispersion* and *relaxation times* in molecular polarization.

Polarization and Frequency

The polarization P_m in response to an electric field $E(t)$ can vary with frequency due to different molecular mechanisms (electronic, atomic, and orientation polarization). The general behavior is described by *Debye relaxation* for polar molecules, where the molecular polarization P_m is frequency dependent.

The frequency-dependent molecular polarization $P_m(\omega)$ is given by:

$$P_m(\omega) = \frac{P_s}{1 + j\omega\tau} \tag{2a}$$

where: $P_m(\omega)$ is the polarization at angular frequency ω, P_s is the static polarization (polarization at low frequencies or DC field), ω is the angular frequency $\omega = 2\pi f$, where *f* is the frequency, $\tau$is the relaxation time (the time it takes for polarization to relax after the removal of the field) and *j* is the imaginary unit.

As the frequency increases:

- *Low frequencies:* Polarization follows the field, and $P_m(\omega) \approx P_s$.
- *High frequencies:* Polarization can't keep up with the field, and $P_m(\omega)$ drops, leading to a decrease in polarization response (dielectric dispersion).

Molecular Polarization and Velocity

In this context, velocity refers to how fast the dipoles reorient themselves in response to the oscillating field. The *relaxation time* $\boldsymbol{\tau}$ is a key factor here, and it is related to the molecular reorientation speed (or velocity). Molecules with higher velocities (due to thermal energy, for example) will have shorter relaxation times, meaning they can reorient faster.

Molecular polarization changes with velocity through the relationship with the relaxation time τ, where:

$$\tau = \frac{\eta V}{k_B T} \tag{3}$$

where: η is the viscosity of the medium, V is the volume of the molecule, k_B is the Boltzmann constant and T is the temperature.

SUMMARY

- *Frequency dependence:* At low frequencies, polarization follows the field closely, while at high frequencies, polarization decreases due to molecular inertia.
- *Velocity dependence:* Faster molecular reorientation (lower relaxation time) allows better response at higher frequencies, and the viscosity and temperature of the medium influence this reorientation.

Calculation for Molecular Polarization

$$P_m = N\alpha E \tag{4}$$

Step 1: Calculate the Number Density *N*

We can use the *ideal gas law* to determine the number density *N*. The ideal gas law is:

$$N = \frac{P_{\text{gas}}}{k_B T} \tag{5}$$

Assumptions: $P_{\text{gas}} = 1.013 \times 10^5$ Pa is the pressure of the gas (1 atmosphere), $k_B = 1.38 \times 10^{-23}$ J/K is the Boltzmann constant and $T = 300$ K is the temperature (room temperature). Now, let's calculate *N*:

$$N = \frac{1.013 \times 10^5}{1.38 \times 10^{-23} \times 300} \approx 2.45 \times 10^{25} \text{ molecules/m}^3 \tag{6}$$

Polarizability α for Each Element

- *Chlorine (Cl):* $\alpha_{\text{Cl}_2} = 4.48 \times 10^{-30}$ m^3,
- *Beryllium (Be):* $\alpha_{\text{Be}} = 2.78 \times 10^{-30}$ m^3,
- *Calcium (Ca):* $\alpha_{\text{Ca}} = 4.2 \times 10^{-30}$ m^3**,** Mg): $\alpha_{\text{Mg}} = 4.1 \times 10^{-30}$ m^3 and
- *Bromine (Br}_2):* $\alpha_{\text{Br}_2} = 5.25 \times 10^{-30}$ m^3.

Step 2: Use the Applied Electric Field *E*

We assume the applied electric field E is 1V/m for simplicity, although this could vary based on experimental conditions.

Step 3: Calculate the Molecular Polarization *Pm*

Now we can calculate molecular polarization using the formula:

$$P_m = N\alpha E$$

Chlorine (Cl)
Polarizability α: 4.48×10^{-30} m^3 and
Number density N: 2.45×10^{25} molecules/m^3
Substituting the values:

$$P_m = 2.45 \times 10^{25} \times 4.48 \times 10^{-30} \times 1 = 1.1 \times 10^{-4}\ \mathrm{C/m^2}$$

Beryllium (Be)
Polarizability α: 2.78×10^{-30} m^3 and
Number density N: 2.45×10^{25} molecules/m^3
Substituting values:

$$P_m = 2.45 \times 10^{25} \times 2.78 \times 10^{-30} \times 1 = 6.8 \times 10^{-5}\ \mathrm{C/m^2}$$

Calcium (Ca)
Polarizability α: 2.78×10^{-30} m^3 and
Number density N: 2.45×10^{25} molecules/m^3
Substituting values:

$$P_m = 2.45 \times 10^{25} \times 4.2 \times 10^{-30} \times 1 = 1.03 \times 10^{-4}\ \mathrm{C/m^2}$$

Magnesium (Mg)
Polarizability α: 4.1×10^{-30} m^3 and
Number density N: 2.45×10^{25} molecules/m^3
Substituting values:

$$P_m = 2.45 \times 10^{25} \times 4.1 \times 10^{-30} \times 1 = 1.0 \times 10^{-4}\ \mathrm{C/m^2}$$

Bromine (Br_2)
Polarizability α: 5.25×10^{-30} m^3 and
Number density N: 2.45×10^{25} molecules/m^3
Substituting values:

$$P_m = 2.45 \times 10^{25} \times 5.25 \times 10^{-30} \times 1 = 1.29 \times 10^{-4}\ \mathrm{C/m^2}$$

Table 2. Summary of molecular polarization calculations

Element	**Polarizability α (m³)**	**Number Density N (molecules/m³)**	**Molecular Polarization P_m (C/m²)**
Chlorine (Cl)	4.48×10^{-30}	2.45×10^{25}	1.1×10^{-4}
Beryllium (Be)	2.78×10^{-30}	2.45×10^{25}	6.8×10^{-5}
Calcium (Ca)	4.2×10^{-30}	2.45×10^{25}	1.03×10^{-4}
Magnesium (Mg)	4.1×10^{-30}	2.45×10^{25}	1.0×10^{-4}
Bromine (Br_2)	5.25×10^{-30}	2.45×10^{25}	1.29×10^{-4}

This Table 2 summarizes the polarizabilities, number densities, and molecular polarization values for each element under the same conditions.

Calculation for Polarization and Frequency

for $P_m(\omega) = \frac{P_s}{1+j\omega\tau}$ for chlorine, beryllium, calcium, magnesium, and bromine at a given frequency.

Given:

- P_s is the static (low frequency) polarization for each element (in C/m^2).
- $\omega = 2\pi f$ is the angular frequency (with f in Hz).
- τ is the relaxation time (assumed 1×10^{-9} s for simplicity).
- j is the imaginary unit.

Let's use an example frequency of $f = 1 \times 10^6$ Hz 106 Hz (1 MHz) to demonstrate the calculation step-by-step.

Static Polarization Values:

Chlorine (Cl_2): $P_s = 1.1 \times 10^{-4}$ C/m^2,
Beryllium (Be): $P_s = 6.8 \times 10^{-5}$ C/m^2,
Calcium (Ca): $P_s = 1.03 \times 10^{-4}$ C/m^2,
Magnesium (Mg): $P_s = 1.0 \times 10^{-4}$ C/m^2 and
Bromine (Br_2): $P_s = 1.29 \times 10^{-4}$ C/m^2

Angular Frequency: $f = 1 \times 10^6$ Hz:

$$\omega = 2\pi f = 2\pi \times 10^6 \text{ Hz} = 6.283 \times 10^6 \text{ rad/s}$$

Relaxation Time:

Assumed $\tau = 1 \times 10^{-9}$ s.

For each element, we'll calculate $P_m(\omega) = \frac{P_s}{1+j\omega\tau}$, which involves both real and imaginary parts.

I. Chlorine (Cl_2):

$$P_m(\omega) = \frac{1.1 \times 10^{-4}}{1 + j(6.283 \times 10^6)(1 \times 10^{-9})}$$

Simplifying:

$$1 + j\omega\tau = 1 + j(6.283 \times 10^6 \times 1 \times 10^{-9}) = 1 + j(6.283 \times 10^{-3})$$

Thus:

$$P_m(\omega) = \frac{1.1 \times 10^{-4}}{1 + j(6.283 \times 10^{-3})}$$

The denominator is a complex number, so we use the complex division formula:

$$\frac{a}{b+jc}=\frac{a(b-jc)}{b^2+c^2}$$

Here $a = 1.1 \times 10^{-4}$, $b = 1$, and $c = 6.283 \times 10^{-3}$:

$$P_m(\omega)=\frac{1.1\times 10^{-4}(1-j(6.283\times 10^{-3}))}{1^2+(6.283\times 10^{-3})^2}$$

$$P_m(\omega)=\frac{1.1\times 10^{-4}(1-j(6.283\times 10^{-3}))}{1+3.947\times 10^{-5}}$$

$$P_m(\omega)=\frac{1.1\times 10^{-4}(1-j(6.283\times 10^{-3}))}{1.00003947}$$

Thus:

$P_m(\omega) \approx 1.1 \times 10^{-4}(1 - j(6.283 \times 10^{-3}))$(for small denominator)

The real and imaginary parts are:

Real Part:$P_m(\omega)_{\text{real}} \approx 1.1 \times 10^{-4}$

Imaginary Part:$P_m(\omega)_{\text{imag}} \approx -6.911 \times 10^{-7}$

II. Beryllium (Be):

$$P_m(\omega)=\frac{6.8\times 10^{-5}}{1+j(6.283\times 10^{6})(1\times 10^{-9})}$$

Simplifying similarly as before:

$$1+j\omega\tau = 1+j(6.283\times 10^{-3})$$

$$P_m(\omega)=\frac{6.8\times 10^{-5}(1-j(6.283\times 10^{-3}))}{1+3.947\times 10^{-5}}$$

$$P_m(\omega)\approx 6.8\times 10^{-5}(1-j(6.283\times 10^{-3}))$$

Thus:

$$P_m(\omega)_{\text{real}} \approx 6.8\times 10^{-5}$$

$$P_m(\omega)\approx 1.03\times 10^{-4}(1-j(6.283\times 10^{-3}))$$

III. Calcium (Ca):

$$P_m(\omega) = \frac{1.03 \times 10^{-4}}{1 + j(6.283 \times 10^{6})(1 \times 10^{-9})}$$

$$P_m(\omega) \approx 1.03 \times 10^{-4}(1 - j(6.283 \times 10^{-3}))$$

Thus:

$$P_m(\omega)_{\text{real}} \approx 1.03 \times 10^{-4}$$

$$P_m(\omega)_{\text{imag}} \approx -6.47 \times 10^{-7}$$

IV. Magnesium (Mg):

$$P_m(\omega) = \frac{1.0 \times 10^{-4}}{1 + j(6.283 \times 10^{6})(1 \times 10^{-9})}$$

$$P_m(\omega) \approx 1.0 \times 10^{-4}(1 - j(6.283 \times 10^{-3}))$$

Thus:

$$P_m(\omega)_{\text{real}} \approx 1.0 \times 10^{-4}$$

$$P_m(\omega)_{\text{imag}} \approx -6.283 \times 10^{-7}$$

V. Bromine (Br_2):

$$P_m(\omega) = \frac{1.29 \times 10^{-4}}{1 + j(6.283 \times 10^{6})(1 \times 10^{-9})}$$

$$P_m(\omega) \approx 1.29 \times 10^{-4}(1 - j(6.283 \times 10^{-3}))$$

Thus:

$$P_m(\omega)_{\text{real}} \approx 1.29 \times 10^{-4}$$

$$P_m(\omega)_{\text{imag}} \approx -8.11 \times 10^{-7}$$

Table 3. Summary of results (at f = 1 MHz).

Element	**Real Part ($P_m(\omega)_{\text{real}}$**	**Imaginary Part ($P_m(\omega)_{\text{imag}}$**
Chlorine	1.1×10^{-4} C/m^2	-6.911×10^{-7} C/m^2
Beryllium	6.8×10^{-5} C/m^2	-4.27×10^{-7} C/m^2
Calcium	1.03×10^{-4} C/m^2	-6.47×10^{-7} C/m^2
Magnesium	1.0×10^{-4} C/m^2	-6.283×10^{-7} C/m^2
Bromine	1.29×10^{-4} C/m^2	-8.11×10^{-7} C/m^2

These results show the real and imaginary parts of the molecular polarization for each element at 1 MHz. (Table 3).

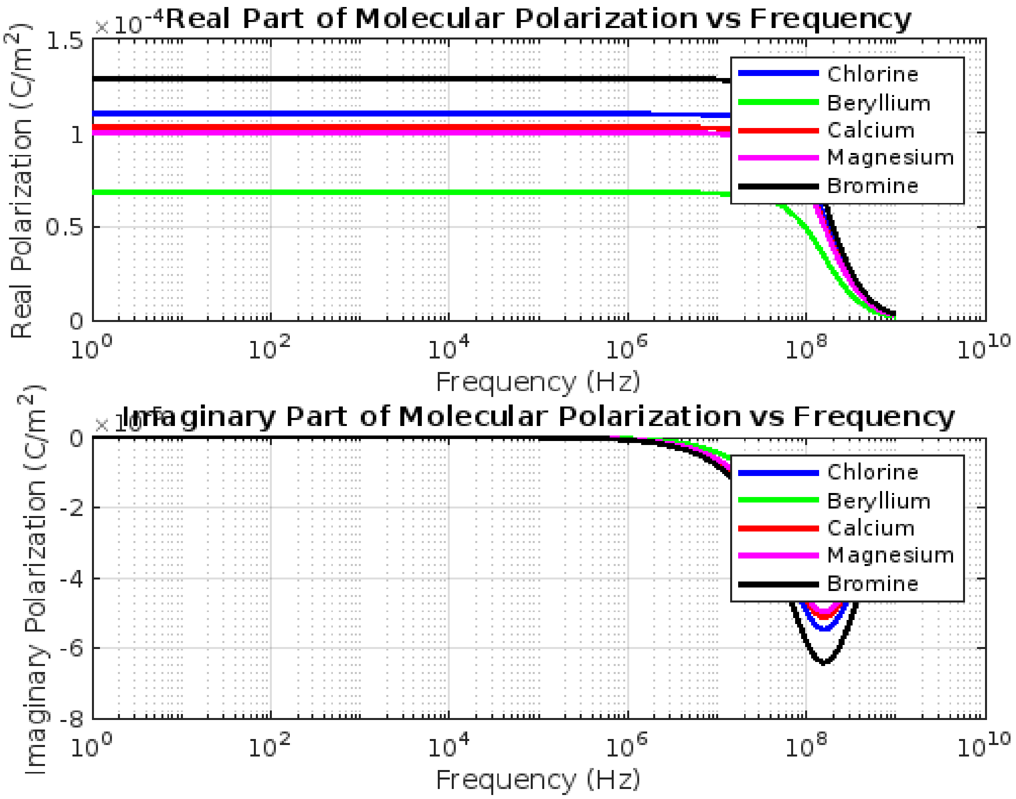

Figure 1. Integrity of polarization versus frequency

Explanations of the integrity of the polarization upon the effect of frequency were outlined as stated below: Figure 1.

1. *Frequency range:* The code computes the polarization for frequencies between 1 Hz and 1 GHz using a logarithmic scale.
2. *Static polarizations (P_S):* The static polarization values for chlorine, beryllium, calcium, magnesium, and bromine are provided.
3. *Debye model:* The molecular polarization is calculated using

$$P_m(\omega) = \frac{P_s}{1 + j\omega\tau}$$

4. *Plotting:*
   - The *real part* of the molecular polarization is plotted in the first subplot.
   - The *imaginary part* of the molecular polarization is plotted in the second subplot.
5. *Logarithmic frequency scale:* The frequency is plotted on a logarithmic scale to capture the behavior over a wide frequency range.

Graph Description

- The *real part* of polarization decreases with increasing frequency, reflecting the inability of the dipoles to align quickly with the electric field.

- The *imaginary part* exhibits a peak, representing energy dissipation (loss) near the relaxation frequency ($\omega\tau \approx 1$) [9–10].

CONCLUSIONS

Through the examination of the relationships between dipole moment and refractive index, we were able to determine the effects of molecular polarization on molecular properties, which has important implications for material design and innovation with potential applications in a variety of fields. Additionally, future research can explore the effects of molecular polarization on molecular interactions and biological functions, further solidifying its importance in understanding molecular behavior.

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MATLAB CODE TO CALCULATE THE MOLECULAR POLARIZATION

```
% MATLAB code to calculate molecular polarization.
% Constants.
T = 300; % Temperature in Kelvin.
P_gas = 1.013e5; % Atmospheric pressure in Pa.
k_B = 1.38e-23; % Boltzmann constant in J/K.
E = 1; % Electric field in V/m.

% Number density (ideal gas law approximation for gases).
N = P_gas / (k_B * T); % Number density in molecules/m^3.

% Polarizabilities for each element in m^3.
alpha_Cl2 = 4.48e-30; % Chlorine (Cl2).
```

```
alpha_Be = 2.78e-30;  % Beryllium (Be).
alpha_Ca = 4.2e-30;  % Calcium (Ca).
alpha_Mg = 4.1e-30;  % Magnesium (Mg).
alpha_Br2 = 5.25e-30; % Bromine (Br2).

% Calculating molecular polarization for each element
P_m_Cl2 = N * alpha_Cl2 * E;
P_m_Be = N * alpha_Be * E;
P_m_Ca = N * alpha_Ca * E;
P_m_Mg = N * alpha_Mg * E;
P_m_Br2 = N * alpha_Br2 * E;

% Displaying the results
Fprintf ('Molecular Polarization Results (C/m^2):\n');
Fprintf ('Chlorine (Cl2): %.2e C/m^2\n', P_m_Cl2);
Fprintf ('Beryllium (Be): %.2e C/m^2\n', P_m_Be);
Fprintf ('Calcium (Ca): %.2e C/m^2\n', P_m_Ca);
Fprintf ('Magnesium (Mg): %.2e C/m^2\n', P_m_Mg);
Fprintf ('Bromine (Br2): %.2e C/m^2\n', P_m_Br2);
```

OUTPUT RESULT:

```
Molecular Polarization Results (C/m^2):
Chlorine (Cl2): 1.10e-04 C/m^2
Beryllium (Be): 6.80e-05 C/m^2
Calcium (Ca): 1.03e-04 C/m^2
Magnesium (Mg): 1.00e-04 C/m^2
Bromine (Br2): 1.28e-04 C/m^2
```

MATLAB CODE TO PLOT POLARIZATION VS. FREQUENCY:

```
% MATLAB code to calculate and plot molecular polarization for multiple elements

% Define parameters
tau = 1e-9;  % Relaxation time in seconds
f_min = 1;   % Minimum frequency in Hz
f_max = 1e9; % Maximum frequency in Hz
frequencies = logspace(log10(f_min), log10(f_max), 100); % Frequency range (logarithmic scale)

% Calculate angular frequencies
omega = 2 * pi * frequencies;

% Static polarization values for each element (from previous calculations)
P_s_Cl2 = 1.1e-4;  % Chlorine
P_s_Be = 6.8e-5;   % Beryllium
P_s_Ca = 1.03e-4;  % Calcium
P_s_Mg = 1.0e-4;   % Magnesium
P_s_Br2 = 1.29e-4; % Bromine
```

```
% Calculate frequency-dependent polarization using the given formula
P_m_Cl₂ = P_s_Cl₂ ./ (1 + 1i * omega * tau);
P_m_Be = P_s_Be ./ (1 + 1i * omega * tau);
P_m_Ca = P_s_Ca ./ (1 + 1i * omega * tau);
P_m_Mg = P_s_Mg ./ (1 + 1i * omega * tau);
P_m_Br₂ = P_s_Br₂ ./ (1 + 1i * omega * tau);

% Plot the real part of molecular polarization for all elements
figure;
subplot (2,1,1);
semilogx (frequencies, real (P_m_Cl2), 'b', 'LineWidth', 2); hold on;
semilogx (frequencies, rea l(P_m_Be), 'g', 'LineWidth', 2);
semilogx (frequencies, real (P_m_Ca), 'r', 'LineWidth', 2);
semilogx (frequencies, real (P_m_Mg), 'm', 'LineWidth', 2);
semilogx (frequencies, real (P_m_Br2), 'k', 'LineWidth', 2);
xlabel ('Frequency (Hz)');
ylabel ('Real Polarization (C/m^2)');
title ('Real Part of Molecular Polarization vs Frequency');
legend ('Chlorine', 'Beryllium', 'Calcium', 'Magnesium', 'Bromine');
grid on;

% Plot the imaginary part of molecular polarization for all elements
Subplot (2,1,2);
Semilogx (frequencies, imag(P_m_Cl2), 'b', 'LineWidth', 2); hold on;
Semilogx (frequencies, imag(P_m_Be), 'g', 'LineWidth', 2);
Semilogx (frequencies, imag(P_m_Ca), 'r', 'LineWidth', 2);
Semilogx (frequencies, imag(P_m_Mg), 'm', 'LineWidth', 2);
Semilogx (frequencies, imag(P_m_Br2), 'k', 'LineWidth', 2);
Xlabel ('Frequency (Hz)');
Ylabel ('Imaginary Polarization (C/m^2)');
Title ('Imaginary Part of Molecular Polarization vs Frequency');
Legend ('Chlorine', 'Beryllium', 'Calcium', 'Magnesium', 'Bromine');
grid on;
```