Journal of Interdisciplinary and Multidisciplinary Research (JIMR)
E-ISSN:1936-6264| Impact Factor: 6.886|
Vol. 16 Issue 8, August- 2021
Available online at: https://www.jimrjournal.com/
(An open access scholarly, peer-reviewed, interdisciplinary, monthly, and fully refereed journal.)

A STUDY ON MOLECULAR GEOMETRY AND BONDING THEORIES

Dr Reeta Sharma, Chemistry Department

Shyam Lal College, Shahdara, Delhi- 110032

ABSTRACT:

Through the investigation of the intricate connection that exists between bonding theories and molecular geometry, the purpose of this effort is to further our understanding of the fundamental principles that underlie chemical structures. The molecular geometry of compounds is a significant factor in determining their physical and chemical properties. This geometry also has an impact on the stability, reactivity, and overall behaviour of the compounds. In the first section of the research, the fundamental concepts of chemical bonding are investigated. These concepts include Lewis structures, molecular orbital theory, and the VSEPR (Valence Shell Electron Pair Repulsion) theory. Molecular electronic configurations may be understood and molecular structures can be predicted with the help of these theories, which give a theoretical basis. An investigation is being conducted into the manner in which orbital overlap, hybridization, and electron pair repulsion interact with one another to disclose the geometric structure of atoms inside a molecule. In addition to this, the study studies the ways in which the form of molecules influences the properties of substances. This study investigates the impact that different geometric configurations have on intermolecular forces, polarity, and dipole moments. The combination of theoretical predictions and experimental facts is what helps bonding theories become more accurate and confirmed. In addition to this, the study delves into the ways in which molecular geometry may be used in a variety of scientific domains, such as medicinal chemistry and materials research. It highlights how a comprehensive understanding of molecular geometry may be used to the fabrication of novel materials with specialised properties, enhanced catalytic processes, and the production of medications. This paper sheds light on the very important part that bonding theories and molecular geometry play in assisting with the comprehension of the complexity that are associated with chemical systems. The knowledge that was acquired from this research has practical value for a number of different fields, and it adds to the development of molecular science while also enhancing theoretical comprehension.

INTRODUCATION

The study of molecular geometry and bonding theories is based on the main objective of gaining a knowledge of chemical structures and the ways in which these shapes influence the properties and behaviours of compounds. In essence, the purpose of this research is to investigate the spatial arrangement of atoms inside molecules as well as the theoretical models that underpin the bonding patterns of these individuals. Due to the fact that it paves the way for future discoveries in a wide variety of other scientific domains, this work is more significant than just a piece of academic research. Chemical bonding, which is a key notion in molecular science, has been a subject of tremendous interest to humans ever since the birth of the field of chemistry. The Lewis model, which was developed in the early 20th century, brought about a significant shift in our understanding of chemical bonding that was brought about by the introduction of the concept of electron pair sharing. Valence electrons and the formation of electron pairs were the foundations upon which this revolutionary theory of molecule stability and covalent bonding was built. At the same time as our knowledge of atomic and molecular structures increased, it became abundantly evident that a more complex method was necessary. The emergence of the Valence Shell Electron Pair Repulsion (VSEPR) theory in the middle of the 20th century brought about a paradigm shift in the field of physics. For the purpose of reducing the amount of repulsion that occurs between electron pairs around a core atom, the notion of VSEPR postulated that these electron pairs would reject one another and adopt particular spatial arrangements. These arrangements would eventually dictate the geometry of the molecule. Through the provision of a framework for the prediction of molecule shapes, this theory contributed to the advancement of our understanding of molecular architecture.

With the introduction of the basic quantum chemistry idea known as molecular orbital theory, the development of bonding theories was advanced to a greater degree. The purpose of this theory is to investigate the behaviour of electrons in molecules by taking into consideration the way in which atomic orbitals overlap to produce molecular orbitals. In order to provide an explanation for how atomic orbitals may mix to generate new hybrid orbitals with different features, the concept of hybridization was devised. The molecular orbital theory provided a more sophisticated understanding of the electronic structure and bonding in molecules, in addition to providing a supplement to earlier bonding theories. In light of this history, the objective of our present inquiry is to make a coherent theory of molecular geometry by combining the many bonding hypotheses that have been proposed. The intricate dance that takes place between a molecule's atoms and electrons is what gives rise to its three-dimensional structure. This dance, in turn, is responsible for regulating the molecule's reactivity and other properties. This study draws on the rich tradition of scientific research in an attempt to bridge the gap between theoretical models and real molecular structures, as well as to reconcile theoretical predictions with experimental findings. Specifically, the goal of this collaboration is to narrow the gap between the two.

This research may be used in a number of different ways to the actual world. For instance, in the field of medicinal chemistry, it is necessary to have a comprehensive understanding of the molecular geometry of drug molecules in order to create compounds that possess the optimum pharmacological properties. When it comes to the study of materials, the modification of the arrangement of molecules is an essential step in the process of producing materials that possess certain characteristics. The link between theory and practice demonstrates the importance of molecular geometry in terms of stretching the frontiers of technology and finding solutions to challenges that are now being faced. The investigation of molecular geometry and bonding theories leads us on a journey that begins with the early phases of the creation of chemical bonding models and ends with the present state of things. The process of deciphering the spatial arrangements of atoms and electrons in molecules not only contributes to the advancement of our theoretical knowledge but also opens the door to prospects for innovative applications in a wide range of scientific domains. This study, which stands at the intersection of innovation and tradition, pushes the boundaries of what is known and paves the way for further developments in the field of molecular research.

Comprehending Molecular Geometry and Bonding Theories is Crucial:

It is necessary to have a comprehensive grasp of bonding theories and molecular geometry in order to successfully determine the fundamental concepts that govern the behaviour of matter at the molecular level. This understanding is essential for research and applications in a wide variety of scientific domains, including medicine, biology, chemistry, and materials science, among others.

- Predicting Chemical Behaviour: A predictive framework for predicting the behaviour of molecules is provided by bonding theories and molecular geometry. Scientists can forecast the physical and chemical characteristics of compounds by understanding the spatial arrangement of atoms and the kind of bonds, which helps in the development of novel materials and medications.

- Rational Drug Design: In medicinal chemistry, creating effective medications requires a thorough grasp of molecular geometry. The three-dimensional configuration of atoms has a significant impact on how medicinal molecules interact with biological targets, which may minimise adverse effects and increase treatment effectiveness.

- Materials engineering: To achieve certain functionality, materials' molecular geometry must be tailored. The design of materials with desirable features, such electrical conductivity, mechanical strength, and optical qualities, is guided by insights into bonding theories in the field of materials science.

- Environmental Consequences: Determining how chemical compounds will affect the environment requires an understanding of molecular geometry. It helps with the prediction of the persistence and reactivity of contaminants, which makes it easier to build pollution control and environmental remediation techniques.

- Technological Developments: Molecular geometry is essential to the creation of new technologies. Understanding bonding theories helps progress technology in a variety of domains, from building effective catalysts for industrial processes to optimising electronic gadgets.

OBJECTIVES OF THE STUDY:

1. To study on Comprehending Molecular Geometry and Bonding Theories is Crucial:
2. To study on Advancement and Developments in Bonding Theories and Molecular Geometry of molecular structures by using the repulsion that exists between electron pairs

An Overview of Previous Developments in Bonding Theories and Molecular Geometry The ground-breaking work that Gilbert Lewis did in the early 20th century is the foundation of our present understanding of molecular geometry and bonding concepts. Lewis' electron pair sharing model was crucial in laying the groundwork for a better understanding of the bonding and stability of molecules. A significant advancement was the subsequent development of the VSEPR theory, which is ascribed to Ronald Gillespie and Ronald Nyholm in the middle of the 20th century. This theory was a significant breakthrough. A spatial perspective was provided by the VSEPR technique, which described molecular structures by using the repulsion that exists between electron pairs. In order to better understand the geometry of different chemical species, it was necessary to have a three-dimensional understanding of the universe rather than a two-dimensional one.

Theories of Molecular Bonding:

A complete understanding of molecular geometry requires a synthesis of basic bonding ideas. This is a prerequisite for the field. Due to the fact that Lewis structures are founded on valence electrons and the sharing of electron pairs, they provide a fundamental foundation for the prediction of basic covalent bonding. The VSEPR theory, which places a focus on the function that electron repulsion plays in accounting for molecular geometries, contributes to the expansion of this understanding of the subject. In quantum chemistry, the molecular orbital theory is a key idea that defines the behaviour of electrons in terms of molecular orbitals. These molecular orbitals are produced when atomic orbitals overlap. This offers a perspective from the field of quantum mechanics. The concept of hybridization, which stems from the theory of molecular orbitals, significantly contributes to the expansion of our understanding of the shapes of molecules and the electrical configurations of molecules.

Prior Studies and Developments:

Our grasp of bonding theories and molecular geometry has been enhanced and expanded thanks to the substantial number of research that have been conducted, as shown by the review of the relevant literature. Theoretical predictions have been validated and refined by the use of experimental techniques like as X-ray crystallography and advanced spectroscopy. These approaches have provided crucial insights into the three-dimensional structures of molecules. Scientists are now able to model complex chemical systems and make more accurate predictions about the properties of such systems because to the utilisation of computational approaches such as ab initio and density functional theory.

Recognised Omissions or Debates in the Text:

In spite of the fact that there has been a great deal of progress, there are still certain instances of dispute and gaps in the existing literature. Ongoing discussion is taking place on the ability of various bonding theories to accurately predict the behaviour of certain types of compounds or under certain conditions. In addition, there are challenges involved in combining experimental data with theoretical models, which is especially challenging when dealing with molecular systems that are highly reactive or complicated. Moreover, the research of uncommon bonding in unique molecules is one example of a new area of inquiry that brings to light knowledge gaps that need to be addressed.

By tracking the historical evolution of molecular geometry and bonding theories and emphasising the concepts, methodological advancements, and lasting concerns that serve as the foundation for the aims and hypotheses of this research, the literature review establishes the platform for our present examination. This is accomplished by following the historical development of these different theories.

METHODOLOGY

An explanation of the experimental procedures:

In this particular investigation, the experimental approach takes use of cutting-edge techniques in order to uncover the three-dimensional structures of molecules. Utilising X-ray crystallography, which is an essential instrument in the field of structural chemistry, one may precisely determine the arrangement of atoms in crystalline materials. This technique involves irradiating a crystal with X-rays, which results in the formation of diffraction patterns. These patterns are then analysed in order to reconstruct the electron density map of the molecule. By decoding these maps, it is possible to accurately establish the spatial coordinates of atoms, which may yield vital insights on the geometry of molecules. This may be accomplished via the process of decoding..

Information about Computational Techniques:

In order to fully understand this subject, computational methods are very necessary, particularly when paired with experimental techniques. Modelling the electronic structure of molecules is accomplished via the use of density functional theory (DFT) and ab initio approaches in quantum chemistry. These computational tools offer us with a theoretical foundation for our inquiry by allowing us to make predictions about the geometries of molecules, their energy levels, and other electronic characteristics. Simulations of molecular dynamics are used in order to explore the dynamic behaviour of molecules over certain periods of time. The ideas of classical or quantum mechanics are used in these simulations in order to provide insight on the flexibility, stability, and structural changes that occur in molecules.

Selection Criteria for Compounds or Molecules for Analysis:

In order to ensure that the study is both relevant and diverse, a set of criteria that has been explicitly specified is used to direct the selection of molecules or compounds that will be investigated. In addition to inorganic and organic compounds, the molecules that have been chosen for examination come from a wide range of chemical classes. These classes include substances that are known to have biological significance because of their chemical properties. In addition, the criteria take into consideration the complexity of molecular structures, which may range from simple diatomic molecules to more intricate organic compounds and coordination complexes. In order to provide a comprehensive image, molecules that possess a variety of bond types (covalent, ionic, and metallic) and molecular geometries are included inside the structure. Particular attention is paid to the study of molecules that have non-standard bonding patterns or electrical configurations that are not typical..

RESULT

For this particular circumstance, the utilisation of resonance calls for a weighted average of these additional traditional methods. It is generally agreed that the right-handed structure is not a provider, the centre game plan is seen to be of moderate support, and the double-handed structure is considered to be the principal beneficiary. The electron-deficient carbon atom that is present in the middle partner, which is a charge-pull out partner, removes the inclination of the electron-providers, also known as nucleophiles, to form bonds at this site. To be clear, hybridization is not a free lunch; rather, it is a last resort that needs some energy.

This is something that should be taken into consideration. Consequently, hybridization is only possible to the extent that bond designs provide a considerable amount of energy compensation throughout the process. To continue along this line, the orbitals of an atom have a preference for hybridising more centrally the more linkages it forms. This is the last choice. The ideal situation would be for hybridization to take place between the inner or centre atoms, which are responsible for the highest amount of bonds. The terminal atoms are the ones that are least likely to result in hybridization, and they also form the fewest bonds. Throughout the course of this book, we investigate the hybridization of the inside atoms and come to the realisation that every terminal atom, which only connects to a single other atom, is not hybridised. The hybridization of carbon is particularly significant since it often forms four bonds in molecules and has the ability to hybridise reliably when it is necessary to do so.

Take note of the accord that exists between the Lewis model and the valence bond speciation. Within each of the two models, the core carbon atom is responsible for the formation of two single bonds and one double bond. Valence bond speculation, on the other hand, contributes to a rise in the value of our bonds. According to the valence bond theory, the two-fold bond that exists between carbon and oxygen is composed of two distinct types of bonds, namely a s and a p. However, in the Lewis model, the two bonds that are contained within the two-fold bond give the impression of being messy. In the process of valence bond speciation, the Lewis model frequently combines a doubling bond with a s and a pi bond.

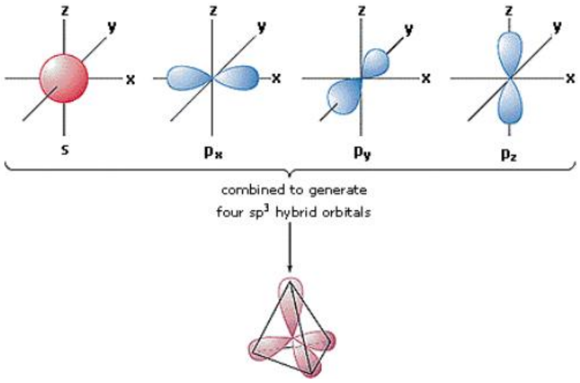

Figure 5. combined to produce four hybrid orbitals of sp3

Due to the fact that pi bonds are often weaker than s bonds, an orbital motion that goes beyond that and is side-to-side would make less sense overall from the beginning to the end. As a consequence of this, the Pbond is often simpler to dissolve than the S bond in a relationship that consists of two people. The Lewis model does not give us with a greater knowledge of the twofold bond probability than the valence bond speciation does, despite the fact that it is quite definite.

Table 1. Using the C2v symmetry operations on the water molecule's oxygen 2px, 2py, and 2pz atomic orbitals

C2v	E	C2	σv (xz)	σ′v (yz)
A1	1	1	1	1
A2	1	1	-1	-1
B1	1	-1	1	-1
B2	1	-1	-1	1
2px	1	-1	1	-1
2py	1	-1	-1	1
2pz	1	1	1	1

within the context of the identical symmetry operation, the matrix representation of this action may be understood as

$$\begin{array}{ccc} & sH1 & sH2 \\ sH1 & 1 & 0 \\ sH2 & 0 & 1 \end{array} \xrightarrow{\hat{E}} \begin{array}{ccc} & sH1 & sH2 \\ sH1 & 1 & 0 \\ sH2 & 0 & 1 \end{array}$$

It is possible to simplify this notation by taking into account the fact that the sH1 atomic orbital is represented by the first column and the first line of the matrices, and the sH2 atomic orbital is represented by the second column and the second line. In addition, the character or trace of the matrix, denoted by the symbol χ, which is responsible for representing the sum of its principal diagonal components, is also shown.

$$\hat{E}\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}=\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}; \qquad \chi(\hat{E})=\mathrm{tr}\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}=2$$

$$\hat{C}_2\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}=\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}; \qquad \chi(\hat{C}_2)=\mathrm{tr}\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}=0$$

$$\hat{\sigma}_v^{(xz)}\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}=\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}; \qquad \chi(\hat{\sigma}_v^{(xz)})=\mathrm{tr}\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}=0$$

$$\hat{\sigma}'_v{}^{(yz)}\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}=\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}; \qquad \chi(\hat{\sigma}'_v{}^{(yz)})=\mathrm{tr}\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}=2$$

These findings demonstrate that the hydrogens' 1s atomic orbitals provide a reducible representation, which can be shown to be produced by adding A1 and B2 (see Table 2).

Table 2. Utilising the C2v symmetry operations on the water molecule's hydrogen 1s atomic orbitals

C2v	E	C2	σv (xz)	σ′v (yz)	
A1	1	1	1	1	z
A2	1	1	-1	-1	
B1	1	-1	1	-1	x
B2	1	-1	-1	1	y
(Sh1,Sh2)	2	0	0	0	A1 + B2

Taking into consideration the fact that atomic orbitals of the same symmetry species cannot come together, it is possible to create the energy level diagram for the molecular orbitals of water (Figure 5). This diagram may be produced using the information presented here. Lowercase symmetry designations are used to designate atomic and molecular orbitals, respectively. It is important to keep in mind that the b1 nonbonding molecular orbital of the 2px oxygen atomic orbital is preserved. This is because the 2px atomic orbital does not have any hydrogen orbitals to couple with due to the fact that it does not possess any hydrogen orbitals.

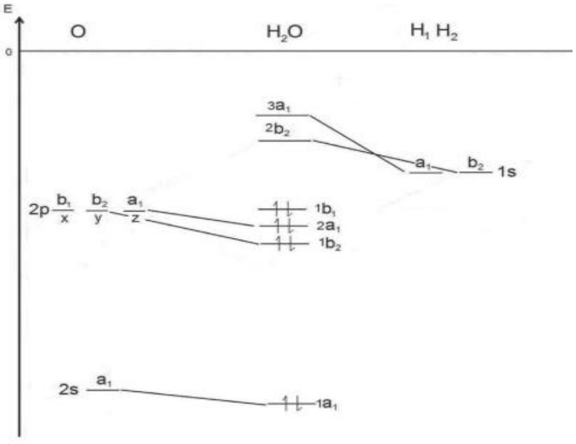

Figure 6. Water in the bent geometry: a qualitative molecular orbital energy-level diagram (C2v)

Now, let's investigate the possibility that the water molecule has a linear structure. This particular case will include a molecule belonging to the point group D∞h, as seen in Figure 1. Utilising the information that is included in the last column of the Character Table (Table 3).

Table 3. Utilising the D∞h symmetry operations on the linear water molecule's hydrogen 1s atomic orbitals

D∞h	E	2C∞ ϕ	…	∞σ	i	2S∞ ϕ	…	∞C2	
Σg +	1	1	…	1	1	1	…	1	
Σg -	1	1	…	-1	1	1	…	-1	
Πg	2	2cosϕ	…	0	2	−2cosϕ	…	0	
Δg	2	2cos2ϕ	…	0	2	2cos2ϕ	…	0	
Σu +	1	1	…	1	-1	−1	…	-1	z
Σu -	1	1	…	-1	-1	−1	…	1	
Πu	2	2cosϕ	…	0	-2	2cosϕ	…	0	(x,y)
Δu	2	2cos2ϕ	…	0	-2	−2cos2ϕ	…	0	
(sH1,sH2)	2	2		2	0	0		0	Σg + + Σu +

The ammonia molecule

It is possible to describe the most stable shape of a number of other simple molecules by utilising the same mechanism that is used to explain the water molecule. Taking a look at the NH3 molecule in its two unique geometries, which are planar (D3h) and pyramidal (C3v) (Figure 7), we can see that it has two distinct shapes. The results that are shown in Table 4 are obtained by using the same concepts of symmetry.

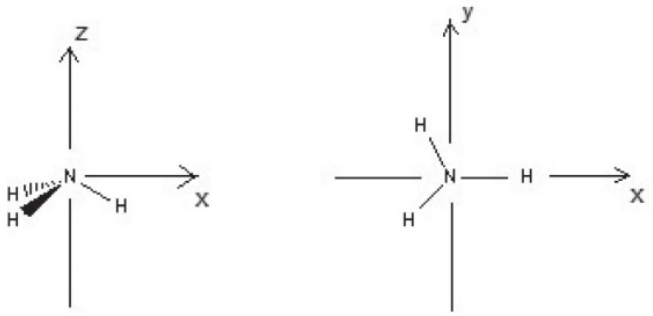

Figure 7. The ammonia molecule has two potential geometries: pyramidal (C3v) and planar (D3h).

Table 4. Using the C3v symmetry operations on the NH3 molecule's atomic orbitals

C3v	E	2C3	3σv	
A1	1	1	1	z
A2	1	1	-1	
E	2	-1	0	(x,y)
(sH1,sH2,sH3)	3	0	1	A1 + E

Taking into account these observations, we are able to draw the conclusion that the atomic orbitals of nitrogen, which are 2s and 2pz, are associated with the irreducible representation A1, whereas the orbitals of py and x are associated with the irreducible representation E. When the three hydrogen 1s orbitals are combined, a reducible representation is produced, and this representation may be broken down into A1 and E.

DISCUSSION

Analysis of the Data in Light of Bonding Theories:

Putting the findings within the context of various bonding theories is an important step in the process of analysing the data. The observed spatial arrangements of atoms for compounds that were investigated by X-ray crystallography and spectroscopy are compared with the predictions of Lewis structures, the VSEPR theory, and the molecular orbital theory. It is thoroughly evaluated whether or not each hypothesis is capable of explaining the experimental findings, as well as whether or not it has any faults. The theories are considered to be verified when they are in agreement with the outcomes of the experiments; however, when they do not, more study into the characteristics that impact the geometry of molecules is required.

Comparing Various Bonding Theories for Particular Situations:

The comparison of different bonding theories that are applied to specific molecular examples is a significant area of research that is being conducted. By meticulously comparing the predictions of each theory with the data obtained from experiments, we hope to get a better understanding of the benefits and drawbacks associated with each hypothesis. Each theory functions most effectively when applied to certain situations. There are circumstances in which the VSEPR theory or the molecular orbital theory deviates from the accurate prediction of molecular geometry that Lewis structures provide. These circumstances highlight the need of having a detailed understanding of when each theory is most applicable. The results of these comparative studies contribute to the development of existing theories and enable the appropriate application of such ideas in a variety of chemical environments.

Resolving Unexpected Results or Inconsistencies:

During the course of scientific inquiry, it is not uncommon for unexpected findings or inconsistencies to arise, which presents scientists with several options for additional investigation. Every circumstance in which the experimental results demonstrate a significant departure from the theoretical predictions is subjected to a thorough examination by our team. It is possible that this will include revisiting the presumptions that were made in the theoretical models, taking into account environmental factors that were not initially taken into consideration, or investigating the possibility of atypical bonding. Because doing so may result in the production of new hypotheses or the enhancement of present ones that give a better explanation for the events that are being observed, addressing unexpected outcomes is an essential component of scientific study. This is because doing so may lead to the development of new hypotheses.

CONCLUSION

Furthermore, the discussion extends beyond the specific molecules that are the subject of the inquiry to take into consideration the larger implications that the discoveries have for the scientific community. The findings contribute to the ongoing debate about the boundaries of existing bonding theories and the extent to which they may be applied. The insights gained from the research are expanded upon in order to provide recommendations for enhancing or expanding the theoretical frameworks that are already being used. The implications for practice are taken into consideration, including the ways in which they could influence the creation of medications, the study of materials, and catalysis procedures. For the purpose of improving our understanding of bonding theories and molecular geometry, which will serve as a foundation for our future theoretical and practical chemical research initiatives, the significance of the study is brought to light. The purpose of the discussion part is to extract major insights from the study by addressing unexpected discoveries, comparing bonding ideas, interpreting the facts, and taking into consideration bigger repercussions. Not only does this collection of data contribute to the advancement of our understanding of molecular geometry, but it also serves as a guide for future research, therefore establishing a dynamic and ever-evolving environment within the field of chemical science.

REFERENCES

[1] W. Ren, Y. Liu, X. Wu, L. Zhang, and X. Yao, Integ. Ferroelectrics 15, 271 (2017).

[2] D. A. Neumayer, R. J. Purtell, W. F. Kane, and A. Grill, Integ. Ferroelectrics 14, 85 (2020).

[3] N. Nagao, T. Takeuchi, and K. Iijima, Jpn. J. Appl. Phys. 32, 4065 (2019).

[4] J. Mendiola, M. L. Calzada, P. Ramos, M. L. Martin, and F. AgulloRueda, Thin Solid Films. 315, 195 (2020).

[5] Sonalee Chopra, Seema Sharma, T. C. Goel, and R. G. Mendiratta, Solid State Communiications 127, 299 (2020).

[6] Sonalee Chopra, A. K. Tripathi, T. C. Goel, and R. G. Mendiratta, J. Mat. Sci. Eng. B. 100, 180 (2019).

[7] C. Vijayaraghavan, T. C. Goel, and R. G. Mendiaratta, IEEE Trans. on Diel. and Electr. Insul. 6, 69 (2019).

[8] K. Iijima, R. Takayama. Y. Tomita, and I. Ueda, J. Appl. Phys. 60, 2914 (2020).

[9] E. Yamaka, H. Watanabe, H. Kimura, H. Kanaya, and H. Ohkuma, J. Vac. Sci. Technology. 6, 2921 (2018).

[10] Brady, J. E.; Russell, J. W.; Holum, J. A.; Chemistry: The Study of Matter and Its Changes, 3rd ed., John Wiley & Sons: New York, 2000.

[11] Kotz, J. C.; Treichel, P. Jr.; Chemistry and Chemical Reactivity, 9th ed., CENGAGE Learning: Stamford, 2015.

[12] Brown, T. E.; LeMay, H. E., Jr.; Bursten, B. E.; Murphy, C.; Woodward, P.; Stoltzfus, M. E.; Chemistry: The Central Science, 13th ed., Pearson Education Ltd.: Harlow, 2015.

[13] Weller, M.; Overton, T.; Rourke, J.; Armstrong, F.; Inorganic Chemistry, 6th ed., Oxford University Press: Oxford, 2014.

[14] Miessler, G. L.; Fischer, P. J.; Tarr, D. A.; Inorganic Chemistry, 5th ed., Pearson Education Ltd.: Harlow, 2013.

[15] Housecroft, C.; Sharpe, A. G.; Inorganic Chemistry, 4th ed., Pearson Education Ltd.: Harlow, 2012.

[16] Bernath, P. F.; Spectra of Atoms and Molecules, Oxford University Press: Oxford, 1995

[17] Walsh, A. D.; J. Chem. Soc. 1953, 2260.

[18] Orchin, M. M.; Jaffé, H. H.; J. Chem. Educ. 1970, 47, 372

[19] Harris, D. C.; Bertolucci, M. D.; Symmetry and Spectroscopy, Oxford University Press: Oxford, 1978.

[20] Cotton, F.A.; Chemical Applications of Group Theory, 3rd. ed., John Wiley & Sons: New York, 1990