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Research paper

A Comparative Study of Elastic Constants and Eigenvalues of Stiffness Matrices among Liquid Crystalline Compounds 4, 4'-di-3-alkyl azoxybenzene and 4,4'-di-4-alkyl azoxybenzene

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Abstract

This study investigates the elastic stiffness constants, elastic moduli and eigen values of the stiffness matrix of nematic liquid crystalline compounds 4,4'-di-3-alkyl azoxybenzene and 4,4'-di-4-alkyl azoxybenzene using two different computational processes, viz.,General Utility Lattice Program (GULP) and the ELATE Program from reported experimental data of cell parameters. The study also attempts to predict the liquid crystal structure in terms of elastic constants. Elastic constats determine the thermal stability, stiffness and degree of molecular order, which determines the range of temperature of the liquid crystalline phase. This study included the comparison of different physical parameters of the above compounds and also made an attempt to understand the reason why 4,4'-di-3-alkyl azoxybenzene exhibits the mesophase for a wider range of temperature(42°C)than smaller mesophase range of temperature(9°C)in 4,4'-di-4-alkyl azoxybenzene. The two dimensional representation of the variation of elastic moduli of the above compounds, which explore the stability of crystals are also discussed. The study revealed that the elastic stiffness constants, elastic moduli, anisotropy of elastic moduli and eigen values of the stiffness matrix of liquid crystalline compound 4,4'-di-3-alkyl azoxybenzene are more than those of 4,4'-di-4-alkyl azoxybenzene. The two dimensional variation of Young's modulus, shear modulus and Poisson's ratio in xy-plane, xz-plane and yz-plane is more in 4,4'-di-3-alkyl azoxybenzene compared tothat in 4,4'-di-4-alkyl azoxybenzene. Interestingly, the linear compressibility of compound 4,4'-di-4-alkyl azoxybenzene in xy-plane ,xz-plane and yz-plane is more compared to linear compressibility of compound 4,4'-di-3-alkyl azoxybenzene. The higher value of elastic moduli and eigenvalues of the stiffness matrix in 4,4'-di-3-alkyl azoxybenzene indicates that the intermolecular force is stronger and resists reorientation more, which may stabilize the nematic phase for a wider range of temperature(temperature range of 42°C) compared to that in 4,4'-di-4-alkyl azoxybenzene (temperature range of 9°C). Poisson's ratio of 4,4'-di-3-alkyl azoxybenzene is negative, which specifically for display devices, can contribute to improved flexibility, responsiveness and better display.

Keywords:*Liquid Crystalline Compounds; Liquid Crystal Displays; Elastic Constants; Eigenvalues;GULP;ELATE.*

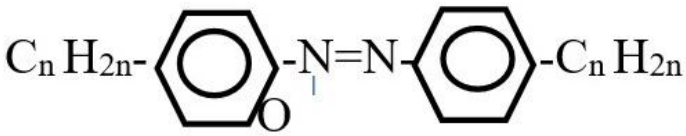
1. Introduction

The study of liquid crystalline materials is of great interest because of their wide applications, specifically in display technologies [1]. Understanding the orientation order parameters and knowing the elastic constants of liquid crystalline compounds gives the information about their stability and suitability for different applications [2, 3]. Elastic stiffness constants give information about the thermodynamic stability, stiffness, crystal resistance to deformation along a particular axis, anisotropy and molecular orientations which are important in using liquid crystalline materials for display devices [4]. Elastic stiffness constants are very important parameters in liquid crystals. They can provide information on stability, stiffness, brittleness and anisotropy of a crystal. The directional dependence of elastic constants and elastic moduli is a fundamental characteristic of most of the crystals and has significant implications in its practical applications in linear elasticity; the stiffness tensor relates stress to strain by Hooke's law. These constants are second order derivatives of the elastic energy density with respect to strain so that they encode how the crystal's internal energy changes under deformation. Elastic constants also determine mechanical properties, structural stability, anisotropy, material design, wave propagation, modeling and simulation. They are closely correlated with thermal properties and phase transformation [5].
The elastic moduli is a measure of stiffness, thermal stability, and how it responds to deformation, whereas in liquid crystals they affect the mesophase range of temperature by influencing the ordered orientation of molecules[6]. Higher elastic constants indicate the stabi-

lized liquid crystalline phase [7]. A higher young's modulus of liquid crystals indicate molecules are stiffer and resist reorientation more, leading to slower switching speed. Hence liquid crystals of lower Young's modulus are preferred for faster switching devices. Bulk modulus is related to compressibility and mechanical properties that influence the liquid crystals' behavior in LCD applications [8], [9]. The value of bulk modulus directly impacts the display's electro-optical performance including response time, contract and viewing angle stability [10]. Shear modulus indicate how molecules of liquid crystals align and respond to electric fields [11]. Proper molecular alignment under shear influences the optical properties crucial to LCD performance, including the modulation of light passing through the display. Low shear modulus allow liquid crystals to realign easily under the applied voltage and gain the stability. Poisson's ratio in a crystal is significant as it describes the anisotropic elastic deformation, revealing how the crystal deforms in one direction when stressed in another direction and also it is key indicator of mechanical performance. Two and three dimensional variation of elastic moduli represents the stability of crystals, more the spatial variation of elastic moduli more will be the stability of crystal. Negative Poisson's ratio in liquid crystals indicate that they are an auxetic material; it means they get thicker when stretched and thinner when compressed[12]. A positive Poisson's ratio in liquid crystal implies that the material became thin when stretched and became thick when compressed. The negative Poisson's ratio, specifically for display devices can contribute to improved flexibility, responsiveness and better display. For liquid crystalline materials, negative Poisson's ratio indicates better optical transmissions, flicker reduction, enhanced photo stability and potentially faster response time [13]. The spatial variations of elastic moduli of liquid crystalline compounds explore the stability of crystal. The variation of elastic moduli and anisotropy is crucial for their use in display technological applications. More variations in elastic moduli are an indication of more stability of the crystal. The elastic anisotropy is the key reason for other anisotropic properties of liquid crystals, such as their electric and magnetic properties[14], [15].Liquid crystals exhibit anisotropic behavior in their physical and mechanical properties due to its unique symmetry and its dependence on the ratio vertical axis to horizontal axis. Due to high elastic moduli, high birefringence and high negative dispersions crystals have their applications in circular photonic crystal fibers and sensors in the field of communications [16]. Larger eigenvalues of liquid crystal indicate that liquid crystal resist deformation strongly in specific deformation modes and hence is stable. Small eigen values mean the structure is flexible, and a zero eigen value reveals the instability of the molecule [17]. Eigen values of elastic stiffness matrix are related to the velocity of elastic waves such as p-waves and s-waves. A larger eigen value corresponds to higher sound velocity for a wave with corresponding polarization and direction of propagation.

2. Materials and Methods

An alkyl azoxybenzene has the general formula R-N=N^+(O)-R', with one or both of the aryl groups of azoxybenzene are replaced by alkyl groups. The simplified general formula for an alkyl azoxybenzene is $C_{12+2n}H_{10+4n}N_2O$ and structural formula is



An alkyl azoxybenzene derivative with n=3 corresponds to liquid crystalline compound 4,4'-di-3-alkyl azoxybenzene and n=4 corresponds to liquid crystalline compound 4,4'-di-4-alkyl azoxybenzene, which are taken as sample for the investigation. The difference between these two compounds is the position of the alkyl group on the phenyl rings. In 4,4'-di-3-alkyl azoxybenzene, alkyl groups are attached at the meta position relative to the azoxy group whereas in 4,4'-di-4-alkyl azoxybenzenealkyl groups are attached at the para position relative to the azoxy group. The molecule of 4,4'-di-3-alkyl azoxybenzene can be represented by ($CH_3CH_2CH_2$)-C_6H_4-N=N^+(O^-)-C_6H_4-($CH_2CH_2CH_3$) [18], [19]and it shows a nematic phase from 18°C to 60°CThe nematic phase exists for a wide temperature range of 42° C [20,21]. The molecule of 4,4'-di-4-alkyl azoxybenzene can be represented by($CH_3CH_2CH_2CH_2$)-O-C_6H_4-N=N^+(O^-)-C_6H_4-O-($CH_2CH_2CH_2CH_3$) and it shows a nematic phase from 18°C to 27°C[22].The nematic phase exists only for a temperature range of 9°C.
The reported crystal structure data of 4,4'-di-3-alkyl azoxybenzeneand4,4'-di-4-alkyl azoxybenzene have been used in the present study. With the crystal structure data as an input file with slight modification in the format using Buckingham potential to General Utility Lattice Program (GULP)[23-25],we have computed elastic stiffness constants. In case of GULP, the input file must be generated by adjusting the Buckingham potential.The standard Buckingham potential form $U_{ij}(r)=A_{ij}e^{(-r/\rho ij)}-\frac{Cij}{r^6}$.$A_{ij}$is repulsive amplitude; Cijis dispersion coefficient and ρij is range parameter. These three are the only physical parameters of the basic Buckingham form in GULP.A Buckingham potential in GULP is defined with a buck line in the potential section of the .gin file, giving atom types, the three Buckingham parameters, the distance range, and (optionally) fitting flagsLATE [26] is open-source software, an online tool for analysis of elastic tensors. The input file for ELATE is 6× 6 matrix of elastic stiffness constants. It is used for computation of elastic constants and Eigen values of the elastic stiffness matrix. The 2D representation of the variation of elastic moduli which explores the stability of crystal, is also obtained from ELATE.

3. Results and Discussion

A comparison of elastic stiffness constants of two compounds is shown in Table 1.It indicates all the six elastic stiffness constants of compound 1 are higher than those of compound 2. This shows the compound 1 is thermodynamically and mechanically more stable and more anisotropic compared to compound 2.However, all the elastic stiffness constants of both the compounds are greater than zero, indicating both the compounds are mechanically and thermodynamically stable.

Table 1: Computed Elastic Stiffness Constants

Elastic stiffness constants	1	2
C_{11}	0.17	0.031
C_{22}	0.032	0.050
C_{33}	0.072	0.036
C_{44}	0.025	0.011
C_{55}	0.081	0.007
C_{66}	0.077	0.022

1-4,4'-di-3-alkyl azoxybenzene;2-4,4'-di-4-alkyl azoxybenzene ;C_{ij} in GPa.

A comparison of elastic moduli of two compounds is given inTable2. It shows the elastic moduli viz., Young's modulus, Bulk modulusand Shear modulus of compound 1 are greater than that of compound 2 in all the three averaging schemes, viz., Voigt, Reuss, and Hill. This shows compound 1 is more stable and more anisotropic compared to the compound 2.A higher value of Young's modulus in compound 1 indicate molecules are stiffer and resist orientation more than that in compound 2. The higher value of the bulk modulus of compound 1 indicates there is stronger intermolecular force which can stabilize the nematic phase for a wider range of temperature(temperature range of 42°C)compared to the nematic phase for a small range of temperature in compound 2 (temperature range of 9°C).A higher value of shear modulus of compound 1 show that molecules in it will not easily realign under the applied voltage when compared to the same phenomenon in compound 2.

Table 2: Computed Elastic Constants

Averagingscheme	Young's modulusinGPa.		Bulk modulusinGPa.		Shear modulusinGPa.	
	1	2	1	2	1	2
Voigt	0.1028	0.0337	0.0304	0.0130	0.0548	0.0158
Reuss	0.0686	0.0288	0.0196	0.0124	0.0374	0.0129
Hill	0.0857	0.0313	0.0250	0.0127	0.0461	0.0143

1- 4,4'-di-3-alkyl azoxybenzene 2-4,4'-di-4-alkyl azoxybenzene

Table 3: Computed Poisson's Ratio

Averaging scheme	Poisson's ratio12
Voigt	-0.06290.067
Reuss	-0.08400.014
Hill	-0.04610.090

1- 4,4'-di-3-alkyl azoxybenzene 2-4,4'-di-4-alkyl azoxybenzene.

Table 3 showsthe Poisson's ratio of compound1 is negative whereas that of compound 2 is positive in all three averaging schemes, viz., Voigt, Reuss, and Hill. Negative Poisson's ratio in liquid crystal indicates that it is an auxetic material. Specifically for display devices the negative Poisson's ratio can contribute to improved flexibility, responsiveness and better display. Hence compound 1 is more suitable for display devices. Therefore, compound 1 has better optical transmissions and increased photo stability compared to compound 2. Poisson's ratio of compound 2 is in the range of 0.015 to 0.090, which shows compound 2 has littletendency for lateral contraction compared to the tendency for lateral contractionof compound 1.

Table 4: Variations of Elastic Moduli and Anisotropy

	Young's modulus inGPa. $q_{min}q_{max}$Anisotropy	Linear compressibilityin TPa^{-1} $\beta_{min}\beta_{max}$Anisotropy	Shear modulusinGPa. $n_{min}n_{max}$Anisotropy	Poisson's ratio $\sigma_{min}\sigma_{max}$Anisotropy
1	0.0320.175.312	5882.4312505.312	0.02210.08103.656	-0.60200∞
2	0.01970.052.539	20000322581.612	0.00700.02092.990	-0.09160.408∞

1 - 4,4'-di-3-alkyl azoxybenzene 2 -4,4'-di-4-alkyl azoxybenzene.

Table 4shows the variation of anisotropy in Young's modulus, shear modulus and Poisson's ratio. Anisotropy in elastic moduliviz., young's modulus, linear compressibility and shear modulus is significantly high in compound1 compared to those in compound 2.The variation of elastic moduli and anisotropy is crucial for the display of technological applications. More variations in elastic moduli in compound 1 clearly shows that it more thermodynamically stable and resist more reorientation compared to compound 2. Anisotropy is the enabling principle for liquid crystal display. High elastic anisotropy shown by compound 1 is a desirable property for using it inliquid crystal displays as it allows more precise control over the director's response to an electric field. Indication of infinite anisotropy in Poisson's ratio in both the compounds is a consequence of the materials' ordered, non-uniform structure and the unique ways in which its molecular alignment can reconfigure under stress, making the mechanical properties highly direction-dependent and unbounded by the limits of isotropic materials.

The two-dimensional variation of young's modulus, linear compressibility, Shear modulus and Poisson's ratio of two compounds are shown in figure 1(a),1(b) ; 2(a),2(b) ; 3(a),3(b)and 4(a),4(b)respectively.

The two-dimensional variation of young's modulus for both the compounds are shown in fig 1(a) and 1(b)

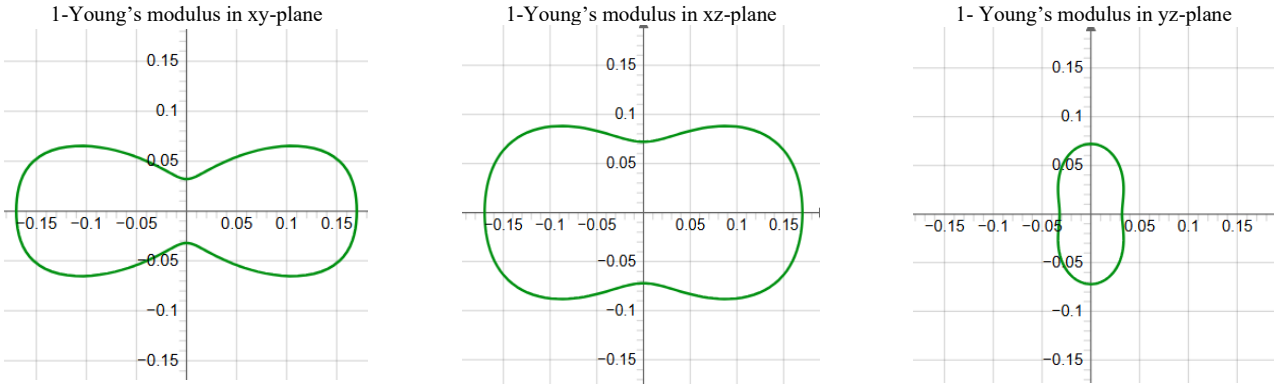


Fig. 1: A) 2D Variation of Young's Modulus in Compound 1

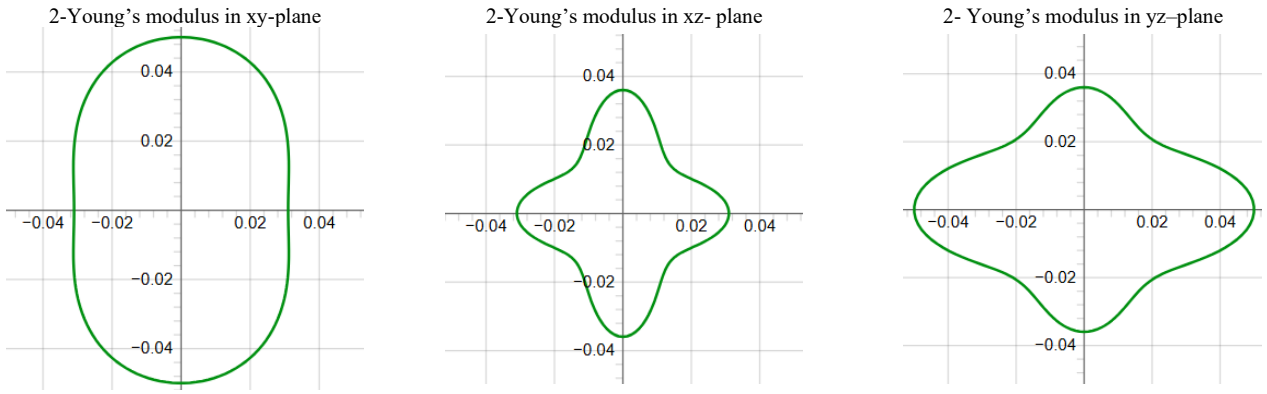


Fig. 1: B) 2D Variation of Young's Modulus in Compound 2 1- 4,4'-Di-3-Alkyl Azoxybenzene 2- 4,4'-Di-4-Alkyl Azoxybenzene.

From fig1(a) and 1(b),it is clear that the 2D variation of Young's modulus is more in compound1 in all xy-plane, xz-plane and yz-plane compared to the variation of the same in compound 2. This also shows there will be more spatial variation in Young's modulus in compound1 than that in compound 2.Hence compound 1 is more thermodynamically stable and more orderly oriented compared to compound 2.

The two-dimensional variation of linear compressibility for both the compounds are shown in fig 2(a) and 2(b)

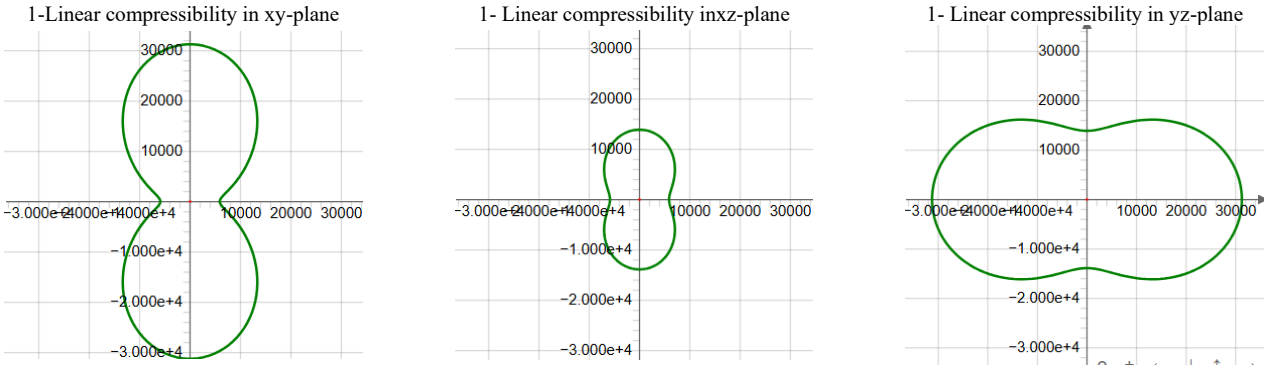


Fig. 2: A) 2D Variation of Linear Compressibility in Compound 1

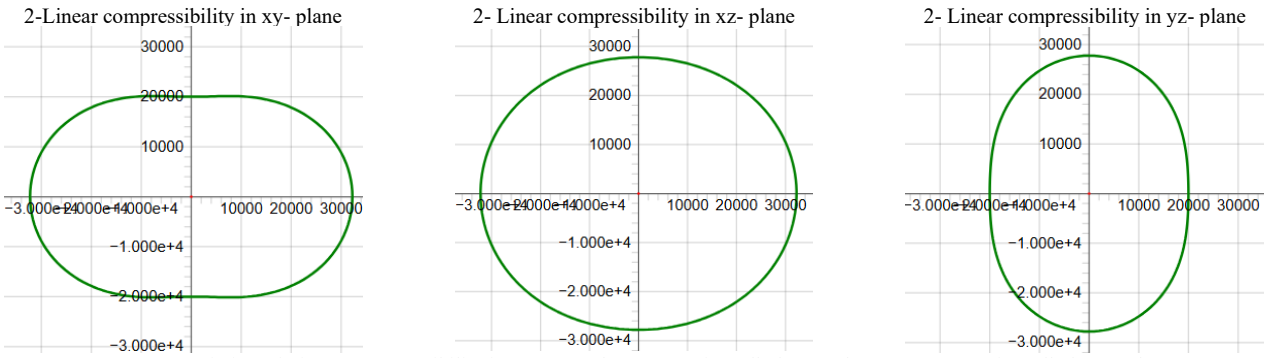


Fig. 2: A) 2D Variation of Linear Compressibility in Compound 2 1- 4,4'-Di-3-Alkyl Azoxybenzene 2- 4,4'-Di-4-Alkyl Azoxybenzene.

Interestinglyf rom fig 2(a) and 2(b),2Dvariation of linear compressibility is more in compound 2 in all xy-plane, xz-plane and yz- plane compared to that in compound 1.This also shows there will be more spatial variation in linear compressibility in compound 2 than that in compound 1.

The two-dimensional variation of Shear modulus for both the compounds are shown in fig 3(a) and 3(b)

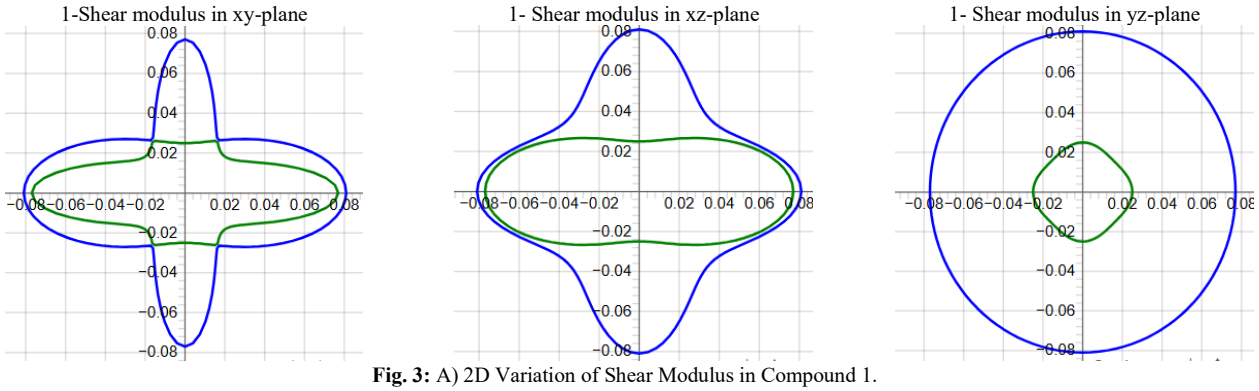


Fig. 3: A) 2D Variation of Shear Modulus in Compound 1.

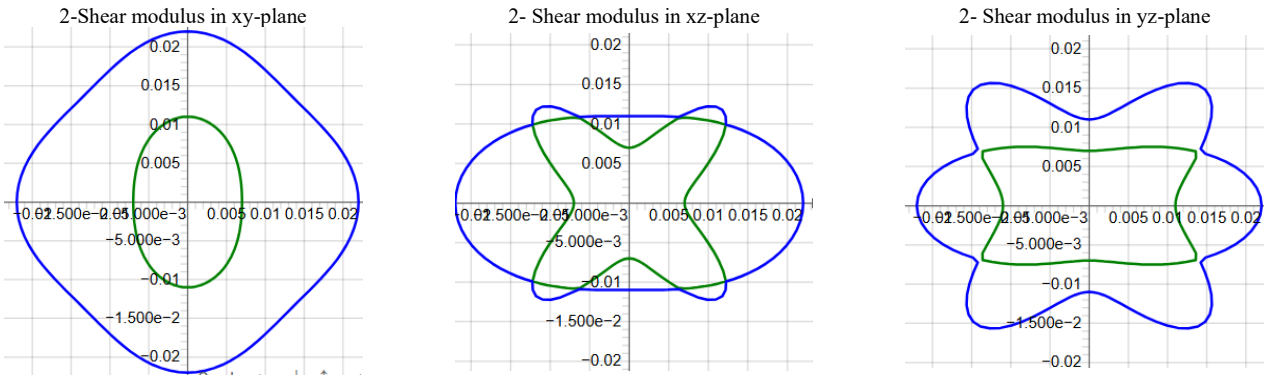


Fig. 3: B) 2D Variation of Shear Modulus in Compound 2 1- 4,4'-Di-3-Alkyl Azoxybenzene 2- 4,4'-Di-4-Alkyl Azoxybenzene.

From fig 3(a) and 3(b), it is clear that the variation of shear modulus is more in xy-plane, xz-plane and yz- plane in compound 1than that in compound 2. This shows that spatial variation in shear modulus is more in compound1 than the spatial variation in shear modulus of compound 2.

The two-dimensional variation of Poisson's ratio for both the compounds are shown in fig 4(a) and 4(b)

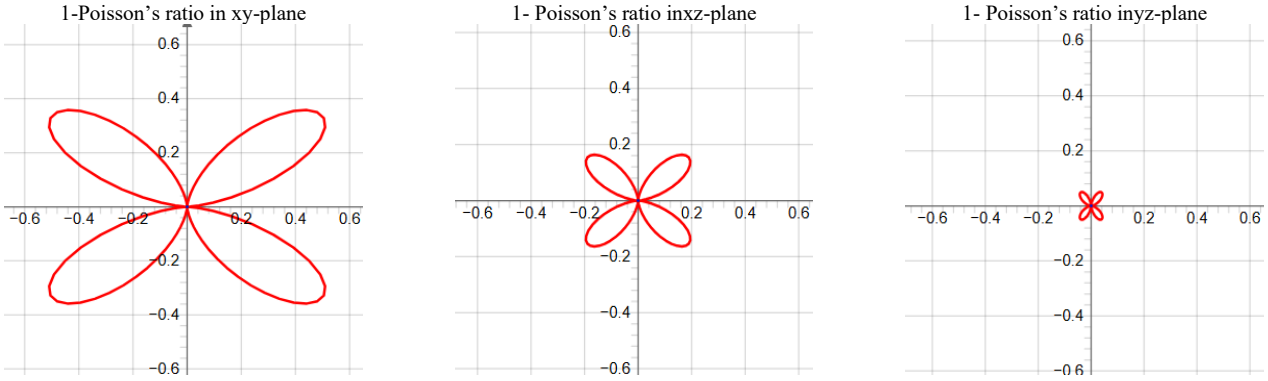


Fig. 4:A)2D Variation of Poisson's Ratio in Compound 1.

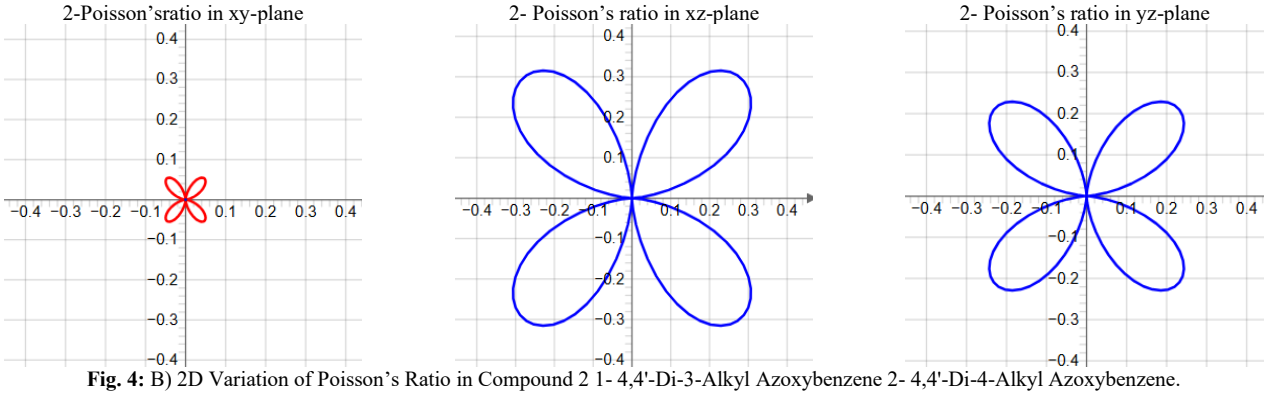


Fig. 4: B) 2D Variation of Poisson's Ratio in Compound 2 1- 4,4'-Di-3-Alkyl Azoxybenzene 2- 4,4'-Di-4-Alkyl Azoxybenzene.

From fig 4(a) and 4(b), it is clear that the 2D variation of Poisson's ratio in compound 1is more in xy-plane, xz-plane and yz-plane than the corresponding variations in compound 2.These shows there will be more spatial variation in Poisson's ratio in compound1 than that in compound 2.

Table 4 shows eigen values of the stiffness matrix.

Table 4: Eigenvalues of Stiffness Matrix

	λ_1 in GPa	λ_2 in GPa	λ_3 in GPa	λ_4 in GPa	λ_5 in GPa	λ_6 in GPa
1	0.125	0.032	0.072	0.077	0.081	0.17
2	0.007	0.011	0.022	0.031	0.036	0.05

1- 4,4'-di-3-alkyl azoxybenzene2-4,4'-di-4-alkyl azoxybenzene.

From table 4, it is clear that all the eigen values are positive for both the compounds 1 and 2. This indicates both the liquid crystalline compounds are stable against corresponding deformation modes. However, the magnitude of each eigen value corresponds to the stiffness of the compound against a specific deformation mode (eigenvector). Compound 1 is, therefore more stable for different specific deformation modes compared to compound 2. A crystal is mechanically stable if and only if all eigen values of its elastic matrix are positive.Sinceall the eigenvalues are positive for both the compounds, both are stable. Further, higher eigen values of compound 1 may be one of the reasons for the exhibition of a nematic crystalline phase for a wide temperature range of 42°C.

4. Conclusions

The elastic stiffness constants, elastic moduli and eigenvalues of the stiffness matrix of the liquid crystalline compounds 4,4'-di-3-alkyl azoxybenzene and 4,4'-di-4-alkyl azoxybenzene are computed and compared using GULP and ELATE. The elastic stiffness constants C_{11}, C_{33}, C_{44}, C_{55},and C_{66} are high for 4,4'-di-3-alkyl azoxybenzene compared to that of 4,4'-di-4-alkyl azoxybenzene, indicating 4,4'-di-3-alkyl azoxybenzene is more thermodynamically stable. Interestingly, the elastic stiffness constant C_{22} is high for 4,4'-di-4-alkyl azoxybenzene. However, all the elastic stiffness constants of both the compounds are greater than zero indicating that both are mechanically stable. Further, elastic moduli viz., young's modulus, bulk modulus and shear modulus are high for 4,4'-di-4-alkyl azoxybenzene which shows the crystal is stable and also it may be the reason for long-range stability in the nematic mesophase. More anisotropy is observed in elastic moduli for 4,4'-di-3-alkyl azoxybenzene compared to anisotropy in elastic moduli of 4,4'-di-4-alkyl azoxybenzene. High elastic anisotropy shown by 4'-di-3-alkyl azoxybenzene is a desirable property for creating liquid crystal displays, as it allows more precise control over the director's response to an electric field. Two-dimensional variations in young's modulus, shear modulus and Poisson's ratio are more for4,4'-di-3-alkyl azoxybenzene. Interestingly, the two-dimensional variations in linear compressibility is more the inin 4,4'-di-4-alkyl azoxybenzene. The negative Poisson's ratio is observed in 4,4'-di-3-alkyl azoxybenzene, which specifically for display devices, it can contribute to improved flexibility, responsiveness and better display. Hence 4,4'-di-3-alkyl azoxybenzene is more suitable for display devices. Higher eigen values and higher bulk modulus of 4,4'-di-3-alkyl azoxybenzene may be one of the reasons for the existence stabilized nematic crystalline phase for the wide temperature range of 42°C.

Suggestion for Future Work

1) The study can be extended to derivatives of alkoxy-azoxybenzene liquid crystalline homologous series.
2) The study can be extended to derivatives of azobenzene and azoxybenzene liquid crystalline compound and comparing the physical parameters with experimental results.
3) Computation of elastic stiffness constants and elastic moduli of inorganic crystals and its comparison with experimental results, there by analyzing their applications can be carried out.
4) Electro-optical response simulations with respect to their elastic anisotropy can be studied.

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Competing Interests

The authors declare no competing interests.

Response Letter

1) The grammatical errors have been rectified.
2) Units and symbols have been standardized.
3) More information about Buckingham potential has been incorporated.
4) Figures are captioned bellow.
5) Minor inconsistencies in conclusion part have been rectified.
6) All citation of the references has been formatted properly to PAA format.
7) Suggestion for future work has been mentioned.

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