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# Estimation of Molecular Radius, $M_r$ and Bayer's Non-Linearity Parameter, B/A in PBnA Series.

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## ABSTRACT

Thermal expansion coefficient, α estimated from density, ρ is utilized for the computation of thermodynamic parameters in case of phenylbenzylidene alkylanilines with alkyl chain varying from 4 to 10, 12, 14, 16 and 18. The thermodynamic parameters like, Beyer's nonlinearity parameter, B/A, is estimated. The molecular radius, $M_r$ is also computed from density for these compounds for which the data is available in literature. The results are discussed how these parameters vary with the temperature in a particular phase, in a liquid crystal molecule and in a homologous series. The molecular radius and Beyer's nonlinearity parameter estimated using different expressions and their nature is discussed. The results are compared with the available data in literature of other compounds.

## INTRODUCTION

It successfully finds one, it reports the found region. If it fails, the "signal graph matching" group will take over the The nonlinearity parameter *B/A* defined as the ratio of the quadratic term to that of the linear term in the equation of state, expressed as a Taylor series expansion, is an important parameter in non linear acoustics [1]. It has been used to represent the nonlinear effects such as wave form distortion, formation of higher harmonics and acoustic attenuation when a sound wave propagates through a medium. Researchers found that the acoustic nonlinearity parameter *B/A* was not only the parameter describing the degree of nonlinearity, but also the parameter which may provide some structural and state information of media.

Sehgal [2] has reported a set of relations involving the non linearity parameter, B/A for the determination of the molecular properties such as internal pressure, cohesive energy, effective Van der Walls constant, distance of closest approach of molecules, diffusion coefficient and rotational correlation time of pure liquids such as water, alcohols and fluorocarbons. Moreover, the nonlinearity parameter (*B/A*) has the potential importance in biological applications which provide information on the state of the tissues.

There have been many measurements of *B/A* in liquids from sound velocity by many workers utilizing different potentials [3]. These studies have shown that the value of B/A varies from 5 to 12. In some cases the extreme values of 2 and 13 are also reported [3]. Further, it is stated that this parameter can also be estimated from the thermal expansion coefficient, α obtained from the density data and from the sound velocity results, utilizing the expressions of Sharma [4], Hartmann et al [5] and Ballou [6]. The

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data on B/A in liquid crystals is meager and the present work provides an opportunity for the study of its variation in a liquid crystal with temperature in different phases as well as at the phase transformation. Further, systematically its variation with the alkyl and alkoxy chain numbers in a homologous series is studied. In the present manuscript, the non-linearity parameter (*B/A*) is estimated in the case of *p-n*-phenylbenzylidene-p-alkylanilines with alkyl chain number, n = 4 to 10, 12, 14,1 6 and18.

## Theory

There are a number of reports in literature describing in detail the theoretical and empirical approach for the estimation of *B/A* from α and u respectively. However, for ready reference, the manuscript presents the relevant expressions that are used in the present study. The non-linearity parameter, *B/A* is given as [7]

$$B/A = 2u\rho[du/d\rho]_T \qquad (1)$$

General formalism for *B/A* in terms of the acoustical parameters (Kand K') for liquids and polymers has been made using Moelwyn-Hughes parameter (*C1*), isobaric acoustic parameter (*K*) and the isothermal acoustic parameter (*K"*) [8] obtained from the thermal expansion coefficient, α, and from the sound velocity, u respectively. The expressions for B/A from density are given as [7]

$$B/A = 2K+2\gamma K" \qquad (2)$$
$$B/A = C_1 - 1 \qquad (3)$$

The molecular radius ($M_r$) for the LC molecule can be obtained from density and the expression is given below [9].

$$M_r = \frac{1}{2}3\sqrt{\frac{M\sqrt{2}}{\rho N}} \qquad (4)$$

where M is the molecular weight.

## RESULTS AND DISCUSSION

The *p-n*-phenylbenzylidene-*p*-alkylanilines with alkyl chain number, n=4 to 10, 12, 14, 16 and 18 are chosen to evaluate, the Beyer's nonlinearity parameter (B/A) molecular radius, ($M_r$). The experimental data required for the estimation was taken from the literature [10, 11]. The estimated values of the above parameters are presented in tables 1 and 2 respectively.

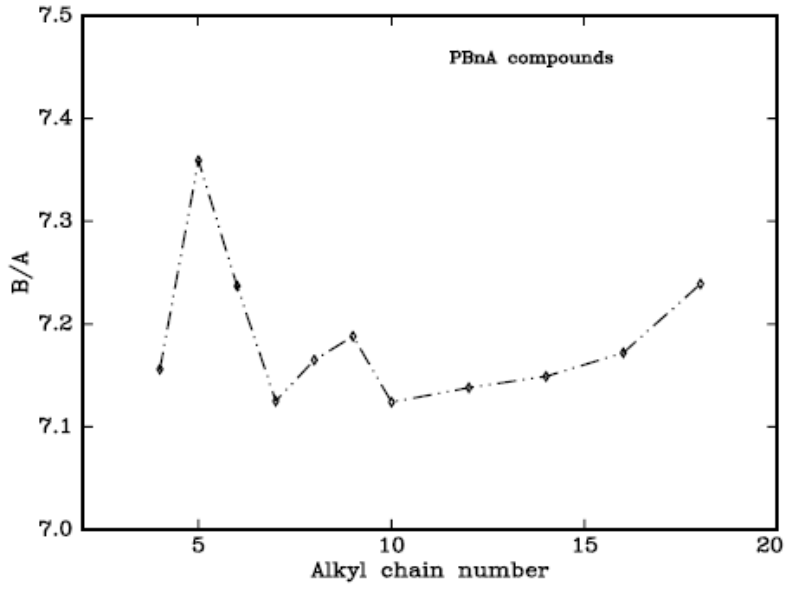


Figure 1: Variation of B/A with alkyl chain number in PBnA series.

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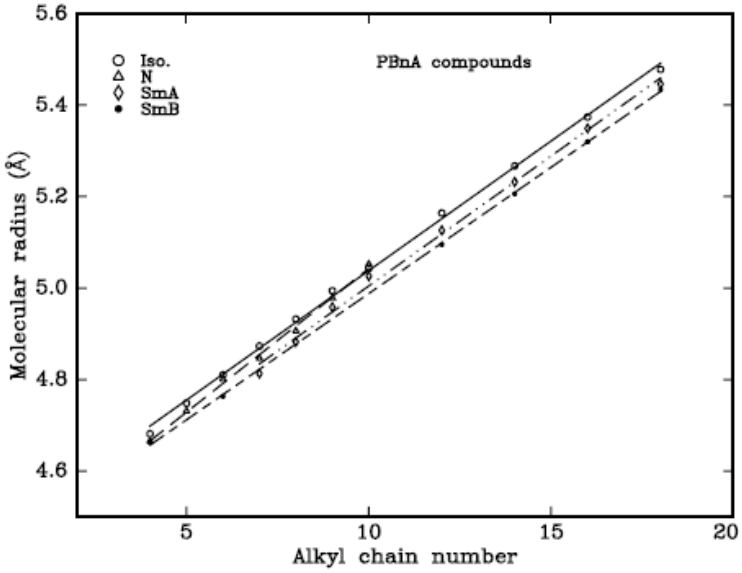


Figure 2: Variation of molecular radius ($M_r$) with alkyl chain number in different phases of PBnA series

Table 1: Variation of nonlinearity parameter (B/A) in PBnA series in different phases

| | Phase | B/A = 2(K+K") | B/A = ($C_1$-1) |
|---|---|---|---|
| PB4A | Iso | 7.156 | 6.324 |
| | N | 7.136 | 6.167 |
| | B | 7.126 | 5.881 |
| PB5A | Iso | 7.359 | 7.372 |
| | N | 7.164 | 6.384 |
| PB6A | Iso | 7.237 | 6.796 |
| | N | 7.168 | 6.409 |
| | B | 7.209 | 5.661 |
| PB7A | Iso | 7.125 | 6.034 |
| | N | 7.142 | 5.769 |
| | A | 7.752 | 7.760 |
| PB8A | Iso | 7.165 | 5.711 |
| | N | 7.633 | 5.802 |
| | A | 7.799 | 5.927 |
| PB9A | Iso | 7.188 | 6.540 |
| | N | 7.144 | 5.762 |
| | A | 7.239 | 5.646 |
| PB10A | Iso | 7.124 | 5.992 |
| | N | 7.126 | 5.867 |
| | A | 7.161 | 5.719 |
| PB12A | Iso | 7.138 | 5.787 |
| | A | 7.140 | 5.776 |
| | B | 7.140 | 5.778 |
| PB14A | Iso | 7.149 | 6.284 |
| | A | 7.129 | 5.840 |
| | B | 7.153 | 5.736 |
| PB16A | Iso | 7.172 | 6.439 |
| | A | 7.223 | 5.652 |
| | B | 7.267 | 5.640 |
| PB18A | Iso | 7.239 | 6.813 |
| | A | 7.185 | 6.520 |
| | B | 7.176 | 6.467 |

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Table 2: Variation of molecular radius ($M_r$) in PBnA series in different phases.

| Compound | Phase<br>Phase P | Temp. (°C) | Mol. Rad(Å) |
|---|---|---|---|
| **PB4A** | Iso | 135 | 4.681 |
| | N | 125 | 4.665 |
| | B | 120 | 4.662 |
| **PB5A** | Iso | 145 | 4.748 |
| | N | 135 | 4.731 |
| **PB6A** | Iso | 135 | 4.810 |
| | N | 130 | 4.801 |
| | B | 125 | 4.763 |
| **PB7A** | Iso | 140 | 4.873 |
| | N | 130 | 4.846 |
| | A | 126 | 4.813 |
| **PB8A** | Iso | 135 | 4.932 |
| | N | 129 | 4.906 |
| | A | 126 | 4.882 |
| **PB9A** | Iso | 137 | 4.994 |
| | N | 131 | 4.978 |
| | A | 127 | 4.958 |
| **PB10A** | Iso | 133 | 5.052 |
| | N | 126 | 5.026 |
| | A | 119 | 4.990 |
| **PB12A** | Iso | 129 | 5.164 |
| | A | 121 | 5.126 |
| | B | 114 | 5.095 |
| **PB14A** | Iso | 123 | 5.267 |
| | A | 115 | 5.232 |
| | B | 110 | 5.206 |
| **PB16A** | Iso | 120 | 5.374 |
| | A | 113 | 5.349 |
| | B | 106 | 5.320 |
| **PB18A** | Iso | 116.7 | 5.478 |
| | A | 107 | 5.446 |
| | B | 102.5 | 5.434 |

The Nonlinearity parameter (*B/A*) calculated using eq. (2) and eq. (3) are presented in Table 1. The *B/A* value almost remains constant in a particular phase except at the vicinity of the phase transition where it shows a peak and the peak magnitude depends on α. The magnitude of *B/A* is slightly smaller in LC phases compared to that in isotropic phase,

The values of B/A estimated from eq. 3 are slightly lower to those obtained from eq.2. The results in table 1 reveal that the values obtained in isotropic phase are slightly higher compared to those obtained in liquid crystalline phases. Further, it is found that there is no regualr variation B/A with the n value and at the same it cannot be conclude conclusively about odd-even effect.

The molecular radius ($M_r$) is calculated using the eq. (4) and their values in different liquid crystalline phases in all the compounds is depicted in table 2. The variation of molecular radius with temperature follows as that of molar volume in all the cases. It exhibits jumps at the phase transition temperature and it is found that the molecular radius, $M_r$ increases with the increase of alkyl chain number. From the results it is found that the core radius is 4.49 Å and the increment for methylene unit is 0.056 Å. In the case of alkoxy benzoic acids [12] it is found that these values are 3.58 Å and 0.084 Å respectively.

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