Calculation of Second Virial Coefficient of DNA

Bahtiyar Akber Mamedov[1], Elif Somuncu[2], Ebru Karatas[3]

[1]*Department of Physics, Faculty of Arts and Sciences, Gaziosmanpaşa University, Tokat, Turkey 60100*
[2]*Department of Medical Services and Techniques, Usak Ulubey Vocational School, Usak University, Usak, Turkey,64000*
[3]*Department of Medical Imaging Techniques, Avrasya Vocational School of Health Services, Avrasya University, Trabzon Turkey 61000*

Email:karatasebru08@gmail.com

Abstract – In this work, a new calculate method has been presented to calculate second virial coefficient with structure factor. The second virial coefficient for DNA have been defined using the calculated structure factor and the programmed fitting technique of Mathematica Software 7.0. The obtained results have been compared with theoretical data and shown in good agreement with literature.

Keywords – Equation of State, Virial Coefficient, DNA, Structure Factor, Concentration

I. INTRODUCTION

In recent years, the second virial coefficient has been considerable interest in the structure factor and protein crystal growth [1-3]. Many authors have been offered theoretical and experimental method for calculation second virial coefficient of DNA and protein [1-5]. Deszczynski et al. has been investigated second virial coefficient as predictors of protein crystal growth [1]. Suzette et al. have been presented structure factor and second virial coefficient of DNA [5]. Despite many developments, the evaluation of the second virial coefficients of DNA is still one of the main problems in biophysical chemistry [1-4].

In this work, aims to calculate the second virial coefficient of DNA with structure factor and compare the obtained results with the theoretical data available in the literature. By using the structure factor and concentration data have determined using the Mathematica Software 7.0. programming fitting method. The obtained results are in good agreement with the theoretical data.

II. MATERIALS AND METHOD

The structure factor depend on second virial coefficient can be written following form [5]:

$$\frac{P(Q=0)}{I(Q=0)} = \frac{1}{S(c,Q=0)} = 1 + 2\,MA_2 c$$

where c is concentration of DNA, M is molecular weight of DNA and A_2 is second virial coefficient. The second virial coefficient cab be calculated by fitting method. Second virial coefficient is defined as [5]:

$$A_2 = \frac{N_A}{2\,M^2} \int 1 - Exp[\frac{u(r)}{k_B\,T}]dr$$

III. RESULTS

Table 1. The comparative the second virial coefficient of DNA

DNA	This work	Ref. [6]
Dumbbell DNA	1.36261E-04	1.4E-04
Semi-Dumbbell DNA	2.11249E-04	-2.2E-04
Double-Strand DNA	5.87194E-04	-5.9E-04

IV. DISCUSSION

A new method for calculation of the second virial coefficient with DNA has been presented. The suggested method can be used to calculate some thermodynamic properties of DNA considering intermolecular interaction energy. We constructed programs for calculation of second virial coefficient using fitting method Mathematica 7.0 international mathematical software. To show the accurate of the fitting method, calculation results have been given in Tables 1. In Tables 1, the obtained results are comparison with other method available literature [6] and the second virial coefficient are in good agreement with Ref. [6].

CONCLUSION

In this work, a new method for calculation of the second virial coefficient with DNA has been offered. The presented method can be used to calculate many thermodynamic properties of DNA with virial coefficient.

References

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