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Calculation of the Second Virial Coefficient of The TMGa Molecule

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Abstract **–** In this work, interaction energy values were calculated using ab initio method for Trimethylgallium (TMGa) molecule. For the Trimethylgallium molecules, the minimum energy values obtained by the ab initio method have been used to calculate second virial coefficient by placing in Yukawa potential. The obtained second virial coefficient results are compared to theoretical data reported in the literature. Furthermore, the obtained results for Yukawa potential compared to with other potentials such as Lennard Jones (12-6) potential and Morse potential in the literature. For most of the varied temperatures of the investigated TMGa molecule, the second virial coefficient predicted by theoretical result computations showed reasonable agreement with theoretical second virial coefficient values.

Keywords – Second Virial Coefficient, Yukawa Potential, Interaction Energy, Ab Initio Method, TMGa

I. INTRODUCTION

Trimethylgallium (TMGa, (CH3)3Ga) was initially described in a thesis [1-3]. Following then, a variety of methods for TMGa production have been offered in studies [3-5]. Because of its broad band gap, trimethylgallium Ga (CH3)3 has lately become the most utilized primary material [4]. TMGa has been utilized in welding to create GaAs [6-9]. TMGa is employed for common organic metal compounds in addition to established GaAs [10-12]. In an aqueous solution, TMGa hydrolyzes [5].

The heat capacity of the TMGa molecule was evaluated in this research at temperatures ranging from 30(Trimethylgallium (TMGa, (CH3)3Ga) was initially described in a thesis [1-3]. Following that, a variety of approaches for TMGa production have been presented in studies [3-5]. Because of its broad band gap, trimethylgallium Ga (CH3)3 has lately become the most utilized primary material [4]. TMGa welding has been utilized to create GaAs [6-9]. TMGa is employed for common organic metal compounds in addition to established GaAs [10-12]. In an aqueous solution, TMGa hydrolyzes [5].

The heat capacity of the TMGa molecule was measured in this work across a temperature range of various K. The theoretical second virial coefficient values were compared to experimental and theoretical values given in the literature. The theoretical second virial coefficient values were derived using Mathematica Software 7.0.

Aside from second virial coefficient, the DFT technique has been utilized to determine the characteristics of the TMGa molecule's intermolecular potential. The Gaussian09 software was used to calculate the intermolecular potential parameter. The Yukawa potential parameters for TMGa have been defined using the calculated intermolecular potential parameters and the programmed fitting technique of Mathematica Software 7.0. The acquired outcomes were compared to theoretical data.

II. MATERIALS AND METHOD

As is well known, determining the intermolecular interaction parameters accurately and precisely is critical. The thermodynamic and transport characteristics of molecules may be determined by estimating the intermolecular interaction potentials based on the structure of the molecule. The energy of intermolecular contact has been defined as [6].

$$\Delta E_{\text{int}}\left(AB\right) = E_{AB} - \left(E_A + E_B\right) \qquad (1)$$

where E_A and E_B represent the energies of the monomers' optimization geometries in their respective basis sets and is the energy of the bimolecular complex AB assessed on a dimer basis [6–8].

In this study, Eq. (1) has been used to compute the intermolecular interaction potential energy for dimer TMGa molecules that is optimized utilizing the 6-31G basis sets of the DFT theory without the symmetry restriction in the gas phase. The heat capacity was computed using the second virial coefficient to show the correctness of the derived potential parameters.

The following form is used to write the second virial coefficient:

$$B_2\left(T\right) = -2\pi N_A \int_0^{\infty} \left(e^{\frac{u\left(r_{ij}\right)}{k_B T}} - 1 \right) r^2 dr \qquad (2)$$

where N_A is the Avogadro constant and $u\left(r_{ij}\right)$ is the intermolecular potential [9].

In this study, we calculated the specific heat capacity of the Yukawa potential numerically while accounting for the second virial coefficient. The Yukawa potential is expressed as follows:

$$u\left(r\right) = \begin{cases} \infty & r \le \sigma \\ -\varepsilon \dfrac{e^{\kappa\sigma\left(1-r/\sigma\right)}}{r/\sigma} & r \ge \sigma \end{cases} \qquad (3)$$

III. RESULTS

Table 1. The comparative reduced temperature dependence values of the second virial coefficient with Yukawa and Lennard-Jones (12-6) potentials

T*	This work	Lennard-Jones (12-6)
0.5	-15.487	-8.72021
1	-5.88407	-2.53808
5	-0.226904	0.243344
10	0.394439	0.460875
30	0.799849	0.526925
50	0.880111	0.508361
100	0.940131	0.464069
200	0.970084	0.411432
300	0.98006	0.380128
400	0.985047	0.358351

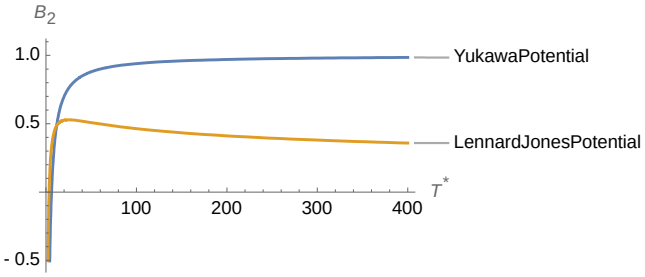

Figure 1. The reduced temperature dependence of the second virial coefficient with Yukawa and Lennard-Jones (12-6) potentials

IV. DISCUSSION

In this work, the TMGa molecule was first optimized at Gaussian 09, and then the trimethylgallium (TMGa) interaction energy was calculated using ab initio molecular orbital and density functional theory (DFT) approaches. The Yukawa potential parameters calculated for the TMGa molecule were calculated. The results are given in Table 1. The second virial coefficient of the TMGa molecule has been computed for wide temperature levels. Table 1 shows the second virial

coefficient value that is regarded as acceptable. The Yukawa potential parameter is κ=1.00229.

CONCLUSION

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

References

[1] C. A. Kraus, F. E. Toonder, *Proc. Acad. Sci.* vol. 19 pp. 292 1933.

[2] C. A. Kraus, F. E. Toonder, *Proc. Acad. Sci.* vol.19 pp. 298 1933.

[3] C. A. Kraus, F. E. Toonder, *J. Am. Chem. Soc.* vol. 55 pp.3547 1933.

[4] M. Fikri, A. Makeich, G. Rollmann, C. Schulz, P. Entel, *J. Phys. Chem. A* 1vol.12 pp. 6330–6337 2013.

[5] A. Charlres, C. A. Kraus, E. F. Toonder Chemical Laboratory, Brown University Communicated January 26, 1933.

[6] Z. Zhang, B. Huang, D. Cui, *Master Sci Eng B* vol.86 pp. 147 2001.

[7] T. Barfels, H. J. Fitting, J. Jansons, I. A. Tale, A. Veispals, A. Von Czarnowski, et al. *Appl Surf Sci* vol. 179 pp.191 2001.

[8] S. P. Watkins, T. Pinnington , J. Hu, P. Yeo, M. Kluth, N. Mason et al. J Cryst Growth vol.221 pp.166 2002.

[9] Z. J. Liu, B. Atakan, K. Kohse-Hoinghaus, J. Katharina, “” *Cryst Growth* vol. 219 pp.176 2002.

[10] H. U. Schwering, H. Olapinski, E. Jungk, J. J. Weidlein, *J Organomet Chem* vol. 76 pp. 315 1974

[11] I. L. Wilson, K. J. Dehnicke, *Organomet Chem* vol. 67 pp. 229 1974.

[12] R. N. Grimes, W. J. Rademaker, M. L. Denniston, R. F. Bryan, P. T. Greene, *J Am Chem Soc* vol. 94 pp. 1865 1972.