Viriális: A Web-based Program that Calculates the Second Virial Coefficient

Alberto Seleto de Souza(IC)*[1], Patrícia Regina Pereira Barreto(PQ) [2].

albertoseleto@usp.br; prpbarreto@gmail.com

[1]*Departamento de Engenharia de Materiais, Escola de Engenharia de Lorena da USP - Área II - Lorena – SP,*
[2]*Laboratório Associado de Plasma, Instituto Nacional de Pesquisas Espaciais, CP515, São José dos Campos – SP – Brasil.*

Keywords: *Monte Carlo Integration, Potential Energy Surface, Second Virial Coefficient, Interactive web based program, non linear regression.*

Introduction

A web-based program called *Viriális* has been developed in order to calculate the classical second virial coefficient *B(T)*[1], alongside with its quantum corrections, for a molecular system of A_2-B_2 type as a rigid rotor. The intermolecular interaction energy $V(R, \theta_a, \theta_b, \varphi)$ is defined as:

$$V(R,\theta_a\theta_b,\varphi) = 4\pi \sum_{L_a,L_b,L} V^{L_a,L_b,L}(R) Y^{L0}_{L_aL_b}(\theta_a\theta_b,\varphi)$$

Where R is the distance between the centers of mass, θ_a and θ_b are the angles between the molecule axis and the center of mass coordinates, and φ is the dihedral angle between A_2 and B_2. $Y^{L0}_{L_aL_b}$ represents the bipolar spherical harmonics, and $V^{L_a,L_b,L}$ are the moments, that can be write in terms of the leading configuration (LCs) and can be described as Pirani potential[2] or the fifth degree Rydberg potential[3].
The goal of this work is to obtain the value of the second virial coefficient through a computational numeric method hosted in the web, so other research can avail from it.

Methods

Using ab initio points from electronic structure calculation made in *Molpro, Gaussian, and SAPT*, it was possible to create a code in *Python* that fits these points to the fitting function of choice, and calculates *B* for various temperatures(*T*) using Monte Carlo integration through the *VEGAS* library[4]. The final outputs are a downloadable information table, and plots of *B x T*, *V x R*, and $V^{L_a,L_b,L}$ *x R*. Several different systems were used to test the code, but only the results for H_2F_2 will be shown here.

Results

The software can be accessed through https://virialis.streamlit.app/. Figure 1 represents the Home Page of *Virialis*. From there, the user can read the instructions on how to use it, and proceed to page “Regression”, where he can input his ab initio points’ files and choose the desired fitting function. Once the fitting is done, the energy information is displayed in a plot (figure 2), and the generated information can be used as input for the page “Polyatomic Molecules A_2B_2”. There, a few options ought to be specified, such as the number of temperatures, and the atoms that are being used. *Viriális* uses the equation of state[5] as a reference data.

Figure 1: Virialis Home Page.

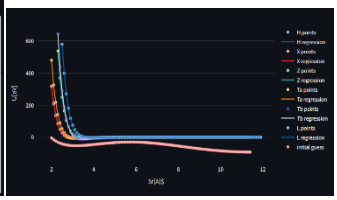
Figure 2: Graph of *V x R* of H_2F_2, for the six LCs.

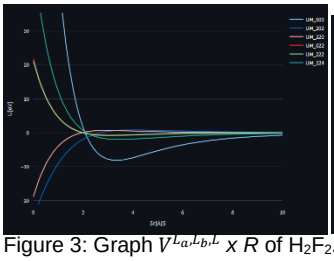
Figure 3: Graph $V^{L_a,L_b,L}$ *x R* of H_2F_2.

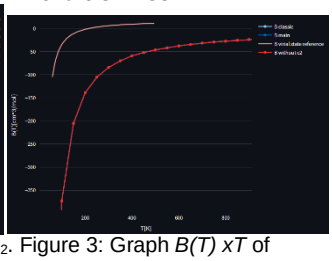
Figure 3: Graph *B(T) xT* of H_2F_2.

Conclusions

As shown in the previous figures, *Viriális* is a working and functioning code that returns valuable information about *B(T)* of A_2-B_2 type systems. However, its precision is imperfect, and corrections are still underway. Apart from A_2-B_2, it also works for A-B molecules, and we wish to expand it to a wider range of molecules, including the most general case AB-CD.

References

[1] BARRETO, P.; CRUZ, A.; EUCLIDES, H.; ALBERNAZ, A.; CORREA, E. J. Mol. Mod., v. 26, p. 277, 09 2020. 3, 5
[2] CORREA, E.; ALBERNAZ, A.; BARRETO, P.; AQUILANTI, V. Chem. Phys. Lett., v. 779, p. 138845, 06 2021. 5, 6
[3] CORREA, E.; ALBERNAZ, A.; BARRETO, P.; AQUILANTI, V.. Chem. Phys. Lett., v. 779, p. 138845, 06 2021. 5, 6
[4] LEPAGE, G. P. J. of Comp. Phys., v. 27, n. 2, p. 192–203, 1978.
[5] MENG, L.; DUAN, Y.-Y.; WANG, X.-D.. Fluid Phase Equilibria, v. 260, n. 2, p. 354–358, 2007.

Acknowledgements

I thank CNPq for funding my undergraduate research for the past three years.