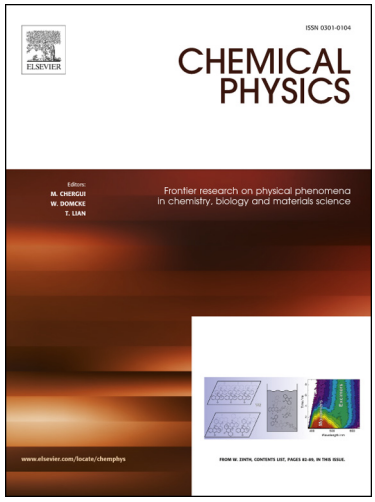

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Relativistic Spinless Energies and Thermodynamic Properties of Sodium Dimer Molecule

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Relativistic spinless rotational-vibrational energy eigenvalue relation has been obtained by solving the Klein-Gordon equation in the presence of General Molecular potential (GMP). The relativistic energy eigenvalue relation has been reduced to the non-relativistic one in the non-relativistic limit. Relativistic and non-relativistic vibrational energies have been computed for the $5\ ^1\Delta_g$ state of Na_2 molecule and compared with Rydberg-Klein-Rees (RKR) data. It has been concluded that depending on relation between scalar and vector potentials, relativistic effect can cause a slight decrease in the vibrational energies or can lead to an increase. In addition, thermodynamic properties such as vibrational mean energy U, vibrational specific heat C, vibrational free energy F and vibrational entropy S for $Na_2(5\ ^1\Delta_g)$ molecule have been examined with respect to temperature and the values of principal quantum number.

I. INTRODUCTION

In order to explain atomic and molecular structures theoretically in non-relativistic and relativistic frameworks, various potential energy functions have been suggested. It is known that the success of potential energy functions in explaining experimental data for diatomic molecules changes depending on the examined diatomic molecule. Therefore, it is necessary to determine which diatomic molecules can be best modeled by which potential energy functions. In this regard, some diatomic molecules have been examined by considering various potential energy models [1–8]. One of these diatomic molecules is also the $5\ ^1\Delta_g$ state of Na_2 molecule. The sodium dimer molecule has been examined in the non-relativistic framework by using Morse [9], improved Rosen-Morse [9, 10], improved Tietz [11] and GMP [12] models. In reference [9], Liu et al. have obtained non-relativistic rotational-vibrational energies for the $Na_2(5\ ^1\Delta_g)$ molecule by considering both the Morse and improved Rosen-Morse potentials and compare these energies with experimental RKR data. They have showed that the energies obtained by using the improved Rosen-Morse potential are in better agreement with the RKR data than those found by using Morse potential. In Reference [11], Tang et al. have handled the same problem by using the improved Tietz potential and compared their results with the experimental RKR data. It has been seen from these results that the improved Tietz potential is better than the improved Rosen-Morse potential for the $Na_2(5\ ^1\Delta_g)$ molecule. In another new study, Yanar et al. have obtained non-relativistic vibrational energies of $Na_2(5\ ^1\Delta_g)$ molecule by considering GMP and proved that GMP's special case modified Rosen-Morse potential is better than the improved Tietz and other potentials given in the literature, in explaining the experimental RKR data for $Na_2(5\ ^1\Delta_g)$ molecule (see Reference [12] and references therein).

It is significant to examine diatomic molecules in the relativistic framework as well as in the non-relativistic case to get more accurate energy level structures for molecules [13, 14]. Relativistic spinless energies of the $Na_2(5\ ^1\Delta_g)$ molecule have been found by solving the Klein-Gordon equation in the presence of improved Rosen-Morse potential [15]. However the GMP which includes the best potential model for the $Na_2(5\ ^1\Delta_g)$ molecule has not been addressed in the relativistic frame as far as we know. In this context, one of the goals of present study is to find relativistic spinless energies of the $Na_2(5\ ^1\Delta_g)$ molecule interacting with the GMP and compare them with the experimental RKR data and non-relativistic energies. The other aim is to investigate thermodynamic properties of the $Na_2(5\ ^1\Delta_g)$ molecule when it interacts with the GMP. Although thermodynamic properties of the ground electronic state of sodium dimer molecule have been studied previously by using improved Rosen-Morse potential [16], they have not been discussed for $5\ ^1\Delta_g$ state and in the framework of the GMP which includes the best model for this molecule. The GMP has been defined as [12]

$$V(r) = \frac{A - Be^{-\alpha(r-r_e)} + \widetilde{q}[C - De^{-\alpha(r-r_e)}]^2}{[1 - qe^{-\alpha(r-r_e)}]^2} \qquad (1)$$

where A, B, C, D, α and dimensionless $\widetilde{q}$ and q denote adjustable real potential parameters while r_e indicates the equilibrium bond length. The potential parameters must satisfy the condition $r \neq \frac{1}{\alpha}\ln q + r_e$ to avoid singularity.

The scheme of paper is as follows. In section II, the Klein-Gordon equation with centrifugal term has been solved for the GMP. Then the relativistic rotational-vibrational energy eigenvalue equation and eigenfunctions have been obtained. In section III, we have made a discussion on what potential parameters should be for diatomic molecules. Then, relativistic vibrational energies have been calculated for the $5\ ^1\Delta_g$ states of Na_2

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