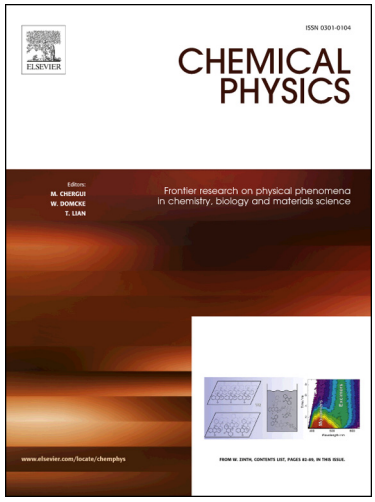


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# Effect of electric field on thermodynamic properties of confined molecules

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A detailed study of electric field effect on the thermodynamic properties namely: partition function, free energy, internal energy, entropy and specific heat of a spatially confined diatomic molecule has been presented. The molecule undertaken for study is LiH, as this molecule under confinement has recently received a lot of attention. The confinement is spherical hard wall potential. The rotational spectra for ground vibrational level and matrix elements of the form $\langle\psi_i(r)|\frac{r-r_e}{r_e}|\psi_j(r)\rangle$ have been evaluated using accurate finite difference method. Orientation and alignment of confined LiH in the presence of an applied static electric field has also been investigated.

**Keywords:** Confined molecule. Rotational spectra. Thermal properties. Orientation. Alignment.

Declarations of interest: none

## 1 Introduction

There have been many studies available in literature where the effect of environment on atomic and molecular systems has been modeled as confining potential [1]. Atoms under confinements have been subject of many works in recent times [2–4]. The supramolecular complex $H_2@C_{60}$ represents a model of quantum rotor in a nearly spherical box [5]. The experimental observation that a molecule confined in $C_{60}$ fullerene has some very interesting physical and chemical properties [6] led to the surge in the study of spatially confined molecules [7–10]. These studies have resulted in great advances in many areas of interdisciplinary interest such as nano technology, chemical synthesis methods, etc. There have been many experimental methods where diatomic molecules can be encapsulated inside fullerene cages. For example, $X_n@C_{60}$or $XY@C_{60}$ (where $X \equiv H$ and $Y \equiv O$) are now readily available. Larger molecules also have been successfully encapsulated ($CO, NH_3, CH_4$ etc.) [11, 12]. As reported by Ge. et. al. [12], the experimental technique such as NMR, IR, and inelastic neutron scattering are employed to study the vibrational and rovibrational spectra of molecules confined in fullerene cages. Synthesis of artificial atoms and molecules and even study of matter under high pressure is

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