

# Lennard – Jones Coefficient $C_3$ and Long – Range Retarded Potential for H,Alkali Atoms - Perfectly Conducting Surface Interaction

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## Abstract

The present work includes the theoretical study of the Lennard – Jones coefficient  $C_3$  for single valence electron atomic systems (H and Alkali atoms, in ground and first excited energy S-state) which are interacting with a perfectly conducting surface (i.e.  $\epsilon \longrightarrow \infty$ ). Our calculations depend upon the dynamic dipole polarizability formula  $\alpha_2(\hbar\omega)$ , which is given directly in terms of an effective transition frequencies  $\omega_i$  and effective oscillator strengths  $f_i$ . We calculated the retardation coefficient  $f_3(R)$  for these interactions to knowledge the retardation effect at a large separation distances  $R$ . Finally, we study the behavior of the long – range attractive potential  $V_{AtM}(R)$  for the interacting systems over a wide range of separation distances  $R$ . Our results are compared with those reported by other researchers concerning this study in the ground state interactions.

**Key Words:** Long – Range Potential, van der Waals Forces, Retardation Coefficient, Alkali Atoms, Lennard – Jones Coefficient

## Introduction

The long – range interaction potential of an atom and a surface characterizes the physics of many actual systems, and is important in many areas of physics [1]. The van der Waals interaction is a well-known example of dispersion forces. These forces are of quantum origin, and they become detectable at a small separation distance between atoms, molecule, and macroscopic bodies [2]. The van der Waals force between an atom and a cavity wall has previously been investigated, its interaction potential was found in form of  $V(R)=-C_3/R^3$  in the non relativistic approximation ( $R$  is the separation between atom and surface). The coefficient  $C_3$  was calculated and measured for different atoms and surfaces, both metallic and dielectric. The van der Waals interaction attracts a considerable interest in connection with experiments on quantum reflection of ultra cold atoms on different surfaces. With the increase of the separation distance up to hundred nanometers and even several micrometers, the relativistic and thermal effects become sufficient, changing the dependence of the van der Waals force

on separation. At moderate separations of up to 1 micrometer for atoms described by a static atomic polarizability near a wall made of ideal metal at zero temperature, the interaction potential was found by Casimir and Polder in the form  $V_4(R)=-C_4/R^4$  [3].

Both the van der Waals and Casimir – Polder interaction are of much importance in connection with the experiments on Bose-Einstein condensation of ultra cold atoms confined in a magnetic trap near a surface [2]. They may influence the stability of a condensate and the effective size of the trap. Conversely, the Bose – Einstein condensates can be used as a sensor of the van der Waals and Casimir – Polder forces. The presence of these forces leads to a shift of the oscillator frequency of the trapped condensate [3]. Note that in applications to ultra cold atoms, not their temperature, but the temperature of the wall is the characteristic parameter of the fluctuating electromagnetic field giving rise to the van der Waals interaction [2].

The interaction between a ground state atom and a dielectric or conducting surface preformed on different levels ,from a simple model of dipole – dipole interaction of the atom and its mirror image , to the full QED (Quantum Electrodynamics) relativistic quantum treatment. The full QED treated leads to the famous long – distance  $R^{-4}$  law.

Interesting in particular are the long – range casimir. Interactions that were recently observed in cavity QED experiments. When the atom – surface distance is not small compared to the wavelength of the dominant atomic transitions , the  $R^{-3}$  law associated with the instantaneous electrostatic interaction is no longer valid [4] .

**Mathematical Treatment and Calculations**

The interaction potential between an atom and a perfectly conducting surface is [5] :

$$V_{AtM}(R) = - C_3 R^{-3} \quad \text{at } R \leq 100 \text{ \AA} \dots(1)$$

where  $R$  is the separation distance between an atom and the surface ,  $C_3$  is the Lennard – Jones coefficient , and the subscript *AtM* denotes to the atom – metal surface interaction. We interested in evaluating the Lennard – Jones coefficient  $C_3$  for separation distance large sufficiently, that the exchange energy of the overlap between the atomic and the surface wave functions is not important . For a perfectly conducting surface , the coefficient  $C_3$  can be written as [6] :

$$\alpha_2(\pm w) = \frac{2}{3} \left[ \sum_n \sum_m C_n(\pm w) C_m(\pm w) \left\{ n B(n+m-1) + \left(\frac{n}{2}(n-1)-1\right) A(n+m-6) \pm w A(n+m) \right\} - 2 \sum_n C_n(\pm w) A(n+1) \right] \dots\dots\dots(3)$$

where  $n, m$  denote to the number of the variational constants  $C_n(\pm w)$  and  $C_m(\pm w)$  respectively . $A( \dots )$  ,  $B(\dots)$  represent the integral values for the radial wave functions corresponding to the atomic S-state for single valence electron atoms. The above formula is derived by using the double method (perturbation - variation).The mathematical details are given in Ref.[7] for the radial wave functions evaluation and the dynamic multipoles polarizabilities formula derivation . We computed the effective transition frequencies  $w_i$  by using numerical method depend directly upon the Grammar rule , where its applied to the expression of the dynamic dipole polarizability  $\alpha_2(iw)$  ,i.e. eq.(4) , and got matrix equation given in terms of the variational constants  $C_n(\pm w)$  and  $C_m(\pm w)$  . Then ,consequently , we used the computer programming to solve the problem. The effective

where  $\alpha_2(iw)$  is the dynamic dipole polarizability at imaginary frequencies. Therefore , in order to fulfil first requirement to find the Lennard – Jones coefficient  $C_3$  from equation (2) , we need to determine the dynamic dipole polarizability at imaginary frequencies formula for interacting systems ,but from the generalized formula of the dynamic multipole polarizability [7], we take the special case (where the pole degree  $L=1$ ), to get :

transition frequencies  $w_i$  are calculated when the polarization reach to sufficiently large value ( $\alpha_2(iw)$  approach to infinity).

The values of the dynamic dipole polarizability at imaginary frequencies can be obtained analytically at frequency  $w$  as a set of  $N$  of the effective transition frequency  $w_i$  and effective oscillator strengths  $f_i$  [8] :

$$\alpha_2(w) = \sum_{i=1}^N \frac{f_i}{w_i^2 - w^2} \dots(4)$$

where  $N=10$  in this study .

The effective oscillator strengths are evaluated numerically by using above equation ,where its represent the residues at the singularities points of the dynamic dipole polarizability at imaginary

frequencies , (the computational details are given in Ref. [11]).

In this study , the essential aim concerning to the Lennard – Jones coefficient  $C_3$  , therefore, by substituting equation (4) in equation (2) ,we get :

$$C_3 = \frac{1}{8} \sum_{i=1}^N \frac{f_i}{w_i} \quad \dots(5)$$

At the large separation distances between atoms and surface  $R$  relatively ,the van der Waals potential will be decreased ,this reduction in the attractive energy between the interacting bodies due

$$f_3(R) = \frac{1}{4\pi C_3} \int_0^\infty \alpha_2(iw) \exp(-2\alpha_{FS} wR) Q(\alpha_{FS} wR) dw \quad \dots\dots\dots(7)$$

where  $Q(x)=2x^2 + 2x + 1$  .  $x= \alpha_{FS} wR$  ,  $\alpha_{FS}$  is the fine structure constant ( $\alpha_{FS} = 1/137.0359895$ ) .

$$f_3(R) = \frac{R \alpha_{FS}}{2\pi C_3} \sum_{i=1}^N f_i \int_0^\infty e^{-x} \frac{[(1/2)x^2 + x + 1]}{x_i^2 - x^2} dx \quad \dots\dots\dots(8)$$

Therefore , the retardation coefficient  $f_3(R)$  depends upon the effective transition frequency  $w_i$  and the effective oscillator strengths  $f_i$  (where

to the retardation effects,which arise from the limited velocity to transfer the electromagnetic signal between them .

The expression of the interaction potential for an atom and a perfectly conducting surface including the effect of the retardation is given by[9]:

$$V_{AtM}(R) = - \frac{C_3 f_3(R)}{R^3} \quad \dots(6)$$

where  $f_3(R)$  represents the retardation coefficient , and gives the following [10] :

But from equation (4) , we get :

$N=10$ ). The final equation (8) was integrated and solved numerically by using which is called “ Gauss –Laguerre method” ,where ,its act and represent by special tables ,given in Ref. [11] .

**Results and Conclusions**

In this study , we have performed accurate calculations of the Lennard – Jones coefficient  $C_3$  which describe the van der Waals potential  $V_{AtM}(R)$  for a single valence electron atomic systems interacting with a perfectly conducting surface

(dielectric constant  $\epsilon \longrightarrow \infty$  ). The table below shows the values of the  $C_3$  coefficient in the ground and first excited energy S-state for H and alkali atoms.

**Table(1):The Values of the  $C_3$  Coefficient for Ground and First Excited S-State (in a.u.)**

		H	Li	Na	K	Rb	Cs
<b><math>C_3</math></b>	<b>Ground State</b>	0.24954	1.45351	1.62181	2.32223	2.54804	2.98896
	<b>Previous works (Ground State)</b>	0.25[1,6]	1.518[6,9]	1.89[6,10]	2.97[6,12]	3.53[6,12]	4.5[6,12]
	<b>Excited S-State</b>	3.48642	9.7528	10.49867	13.30646	14.20880	15.81840

Our results for ground state are compared with other researchers, they were used other methods in their calculations , and the values denote that there is a similarity in the results for H , Li and Na atoms with Refs. [1,6,9,10] respectively , but, the difference increased for K , Rb and Cs atoms , (i.e. with increasing of the atomic number  $Z$  for these atoms). The essential reason of increasing the difference in the results is due to the effect of Frozen Core Approximation (FCA) ; which is used to calculate the wave functions for the atoms under studying , and ,this will affect the evaluation of the dynamic dipole polarizabilities  $\alpha_2(i\omega)$  , effective transition frequencies  $\omega_i$  and effective oscillator strengths  $f_i$  respectively. Therefore, the discrepancy appeared clearly in heavy alkali atoms (K,Rb and Cs) . This coefficient is proportional directly upon the principle  $n$  and orbital  $l$  quantum numbers, in addition to the atomic number  $Z$  for H and alkali atoms, where, the  $C_3$  coefficient increased by increasing these numbers. Our results for the first excited S-state are

so greater than the ground state values , but, have the same characteristics as mentioned above for the corresponding ground state interactions.

We investigated the effect of the retardation under various separation distances  $R$  , through the numerical solution of the retardation coefficient relation by using Gauss – Laguerre method. The retardation curves start with a unity at very small separation distances  $R$  , where, this effect is neglected ,then, the retardation coefficient curve will be damped continuously with increasing of  $R$  , to reach to a saturation level at  $R > 200000$  (a.u.) for the ground and excited states . The van der Waals potential  $V_{AM}(R)$  decreases gradually with increasing of the retardation effect. Fig. (1) and Fig.(2) show the behavior of the  $f_3(R)$  coefficient for H and Na atoms in ground and first excited S-states .Other alkali atoms have the same behavior ,which is good comparable with the figures plotted in Ref.[9].

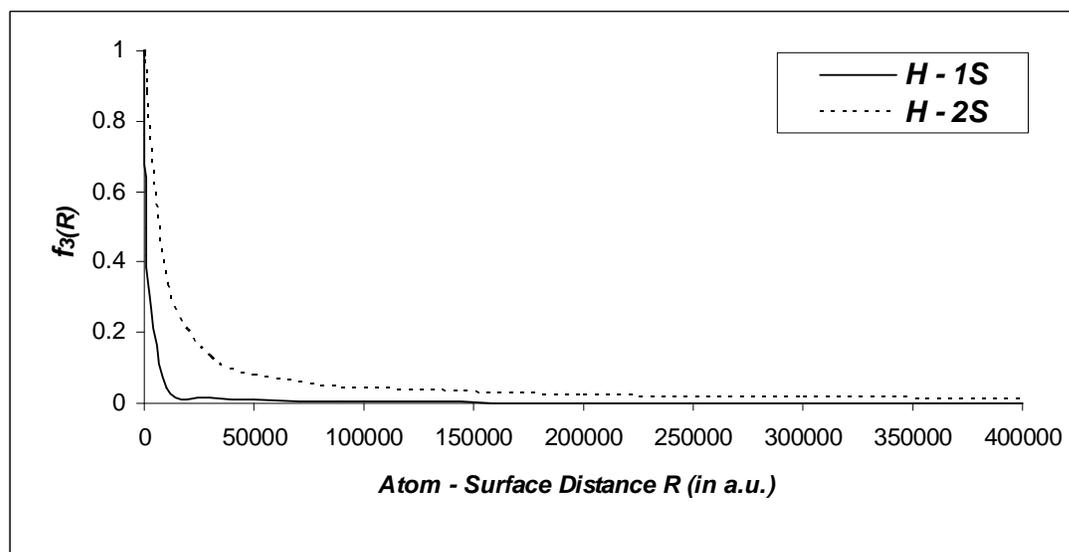


Fig. (1) Retardation Coefficient Curves for H-Atom in Ground & Excited State

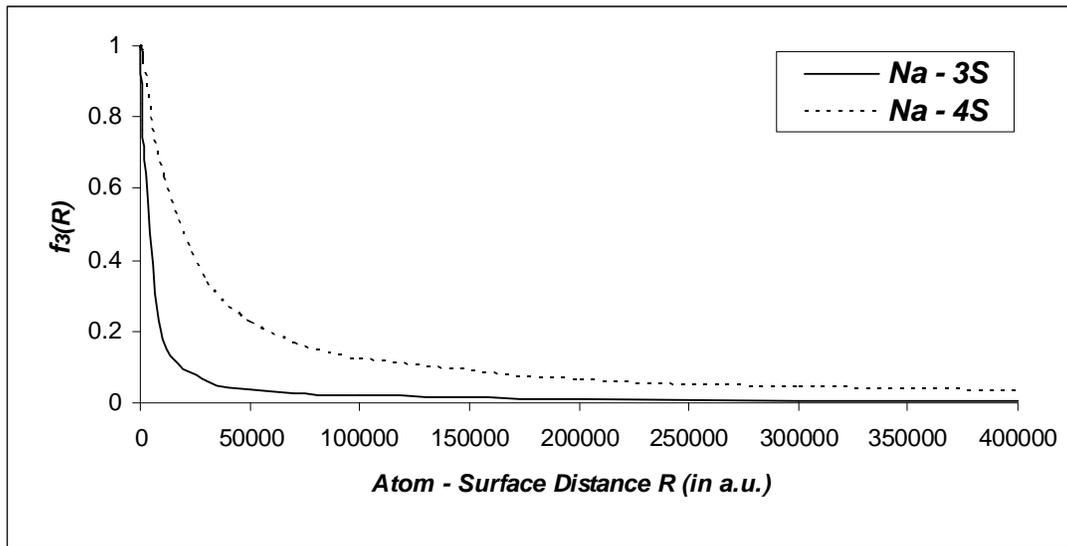


Fig. (2) Retardation Coefficient Curves for Na-Atom in Ground & Excited State

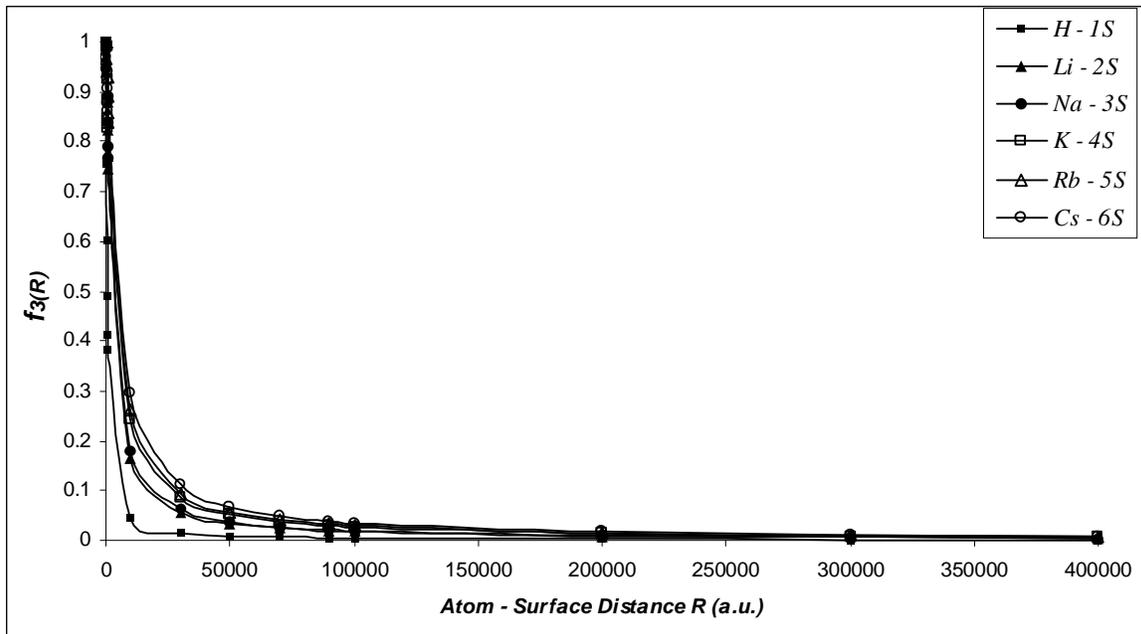
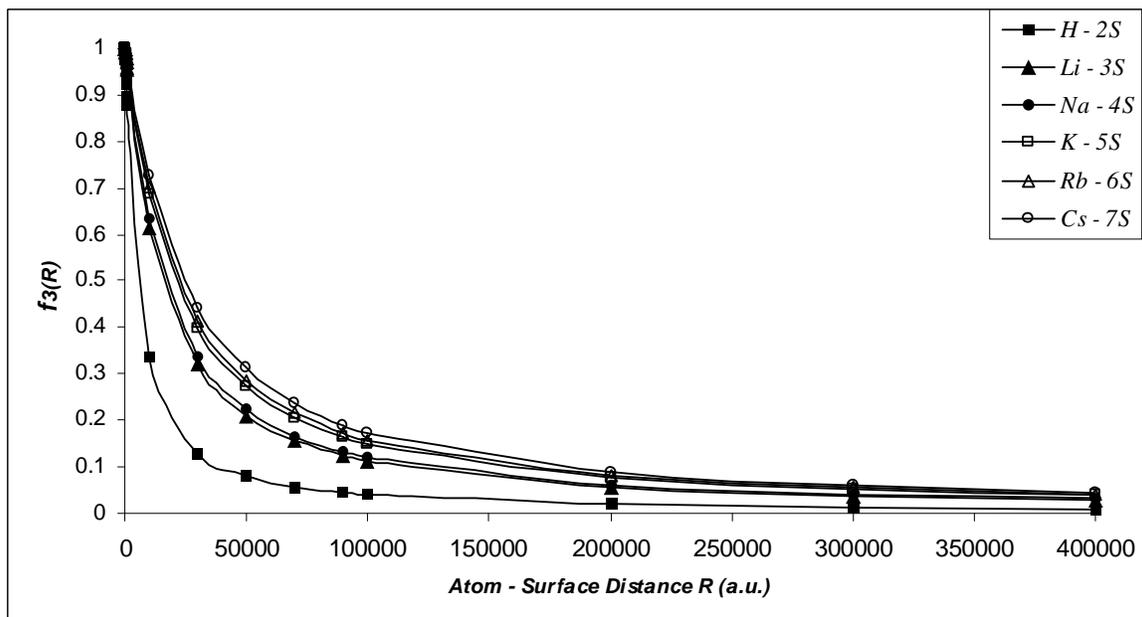


Fig. (3) Retardation Coefficients Curves for H & Alkali Atom in Ground State



**Fig. (4) Retardation Coefficients Curves for H & Alkali Atom in First Excited S-State**

Fig.(3) and Fig.(4) show the behavior of the retardation coefficient curves for all the interacting systems in each ground and first excited S-states respectively. From above figures, our conclusions are as follows: the attractive long-range potential (van der Waals)  $V_{AIM}(R)$  at a certain separation distance  $R$ , increases for the excited state interactions with a surface under the effect of the retardation, this is correct for all atoms, it appears clearly for the H atom and becomes weaker for alkali atoms (Li to Cs gradually).

Finally, Fig.(5) and Fig.(6), represent the values of the  $R^3V_{AIM}(R)$  potential for H and alkali atoms in ground and first excited S-state interacting with a perfectly conducting surface. The  $V_{AIM}(R)$  is an attractive potential, and the curve starts at the value of the Lennard-Jones coefficient  $C_3$ , then, increases to reach the zero value at sufficiently large separation distances ( $R \rightarrow \infty$ ). The curves of the Lennard-Jones potential have the same

behavior for all interacting systems in ground and first excited energy S-state. Our presented curves of the  $R^3V_{AIM}(R)$  potential are similar extremely to those given in Refs.[1,5,8,9] for ground state interactions. In our work, we conclude that in the case of the interacting between atoms and perfectly conducting surface, the Frozen Core Approximation is suitable for H and light alkali atoms (Li and Na), where, the discrepancy can be traced back to the contribution that only includes the valence electron ( $N_e=1$ ), thereby, the interference between the electronic clouds in each of atoms and perfectly conducting surface appears clearly in atoms of a large ionic core (K, Rb and Cs), therefore, it leads to inaccurate  $C_3$  coefficient for these atoms relatively. Thus, the present results may be useful in analyzing the interactions of atoms with metallic surfaces for spectroscopy or atom interferometry experiments.

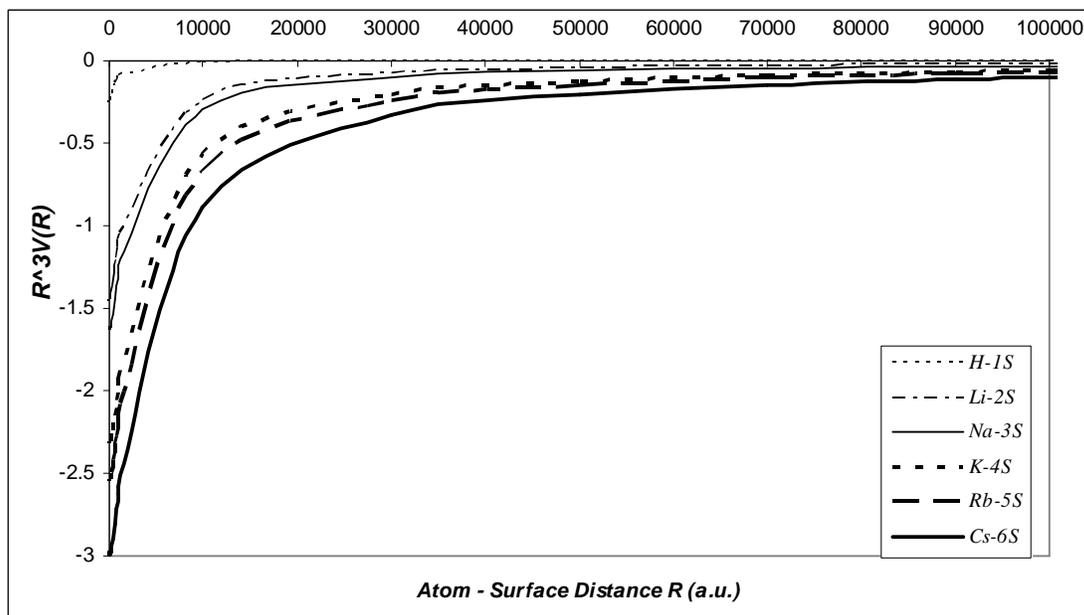


Fig.(5) Values of  $R^3 V_{AtM}(R)$  for H & Alkali Atoms in Ground S-State

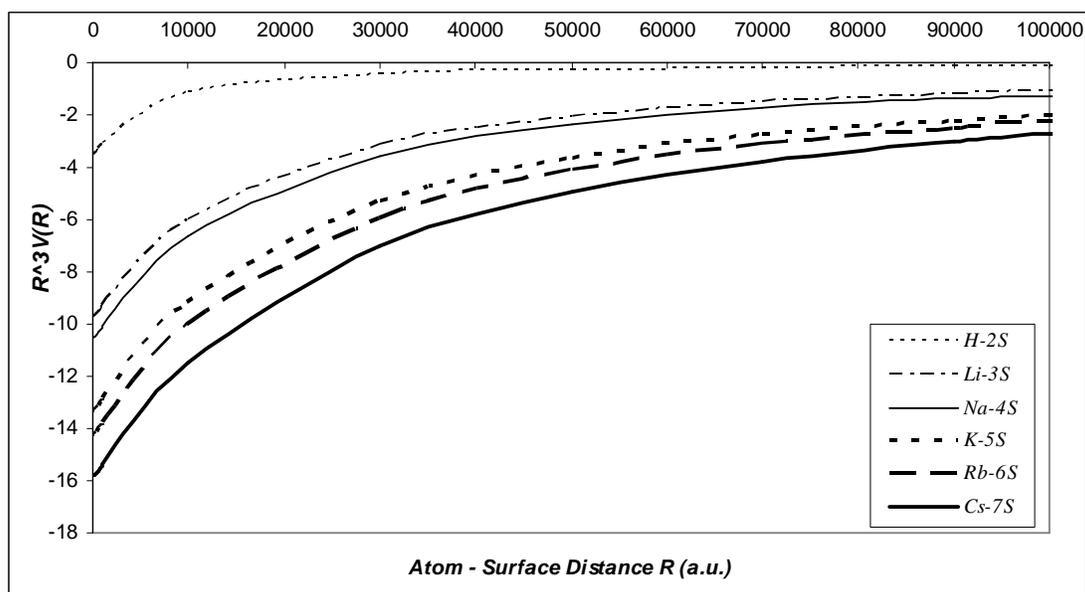


Fig.(6) Values of  $R^3 V_{AtM}(R)$  for H & Alkali Atoms in First Excited S-State

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## معامل لينارد - جونز $C_3$ وجهد الارتداد الطويل المدى لتفاعل ذرة الهيدروجين و الذرات القلوية مع سطح جيد التوصيليه

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### الخلاصة

تضمن هذا البحث دراسة نظريه لمعامل لينارد - جونز  $C_3$  للانظمة الذريه ذات الكترولون التكافؤ المنفرد ( ذرة الهيدروجين والذرات القلويه ) والمتفاعله مع سطح جيد التوصيليه ( $\epsilon \rightarrow \infty$ ) ، وذلك للحاله الارضييه والمثاره الاولى من النوع-S . ان حساباتنا لهذا المعامل يعتمد بصوره اساسيه على صيغه استقطابيه ثنائي القطب الديناميكيه  $\alpha_2(i\omega)$  ، والتي بدورها تعطى بدلالة ترددات الانتقال المؤثره  $w_i$  وشدات التذبذب المؤثره  $f_i$  ، وقد حسبنا الترددات المؤثره والشدات المؤثره لهذا الغرض. كذلك تم حساب معامل الارتداد  $f_3(R)$  لدراسة تأثير الاعاقه الذي يظهر عند المسافات الفاصله الكبيره نسبياً . اخيرا ، تضمن هذا البحث دراسه تصرف جهد التجاذب الطويل المدى (جهد فان در فالز)  $V_{AIM}(R)$  للانظمة المتفاعله مع السطح الجيد التوصيليه ولمديات واسعه من المسافه الفاصله بينهما  $R$  . بينت نتائج الدراسه ضمن تفاعلات الحاله الارضييه بأنها مقاربه لدراسات سابقه .

**الكلمات المفتاحيه:** الجهد الطويل المدى ، قوى فاندر فالز ، معامل الارتداد ، الذرات القلويه ، معامل لينارد - جونز