



A COMPARATIVE STUDY OF POTENTIAL ENERGY CURVES OF CARBON MONOXIDE MOLECULE

C.T. Londhe

Department of Physics, Mahatma Gandhi Mahavidyalaya, Ahmedpur – 413515, India.

e-mail: londhect@gmail.com

Abstract:

The potential energy curves for the electronic ground state carbon monoxide molecule are constructed by the RKR method using latest molecular constants. The Generalized potential energy function and improved five-parameter exponential-type potential energy function compare each other and have good agreement with RKR curves for carbon monoxide molecules. The percentage deviations from RKR curves are drawn at the same abscissa scale. These curve shows that both potential energy curve deviation is less than 2 to 3 % error to dissociation limit.

Keywords: Potential energy curve, CO molecule, GPEF, exponential-type potential

1. INTRODUCTION

The study of experimental potential energy curves for atomic interactions is fundamental importance in chemical physics, astrophysics, gas kinetics and aerodynamics. A potential energy curve is a graphical representation of the change in potential energy of the molecule as a function of the distortion of the bond of the molecule from its equilibrium distance [1]. In the calculations of Franck Condon factors, dissociation energies and thermodynamic quantities etc, the studies of potential energy curves are necessary. The empirical potential energy functions like Morse [2], Rydberg [3] Varshni [4], Lippincott [5] and Hulbert-Hirschfelder [6] are usually applied and the potential energy curves are drawn. For all these calculations the Rydberg Klien Rees-Vanderslice RKR [7-11] curves are essential. Naturally to compute the turning points of various vibrational levels the accurate spectroscopic constants are required. The empirical potential functions also require these molecular constants.

The carbon monoxide molecule is, except molecular hydrogen, the most abundant molecule in the universe. It can be found in comet tails, interstellar space, planets, solar and stellar atmospheres. A number of carbon monoxide isotopologues have been identified in the solar spectrum [12,13] and in the spectra of different cosmic objects [14–17]. Carbon monoxide is a greenhouse gas, having contributions to the carbon cycle and global warming. In the present study the potential energy curves for the ground electronic states are constructed for the diatomic CO

molecule. The constants of ground state of carbon monoxide are taken from R. Farrenq, G. Guelachvili, A. J. Sauval, N. Grevesse, and C. B. Farmer [14] and reported in table 1.

Table 1: Molecular constants of the ground state of carbon monoxide molecule

μ	6.85620871	B_e	1.931280985
ω_e	2169.81267	α_e	-0.01750439229
$\omega_e x_e$	-13.28787634	D_e	90543
$\omega_e y_e$	0.01041106647	r_e	1.128323

Note: All constants are in cm^{-1} except r_e , which is in Å and μ , is in amu

2. THE POTENTIAL ENERGY FUNCTIONS

The method of drawing potential energy curves based on the spectroscopic constant like ω_e , $\omega_e x_e$, B_e , α_e , r_e etc was developed by Rydberg, Klien and Rees [7-9]. Further it was modified by Vanderslice [10,11]. A brief account of RKR calculation is also given by Castano et al [18].

2.1. Generalized potential energy function:

Surkus [19-29] has suggested a potential function which is known as GPEF. This function has the form

$$U_{GPEF}^{(r)} = g_0 w^2 \left(1 + \sum_{i=1}^N g_i - w_i \right) \text{--- (1)}$$

$$\text{Where } w = w(R | P, n) = \left[\frac{r^p - r_e^p}{r^p - nr_e^p} \right] \text{-----(2)}$$

Where $p \neq 0, n \neq -1$

And $s(p) = 1$ if $p > 0, s(p) = -1$ if $p < 0$

$W(R|-1,0)$ yields Dunham potential function

$W(R|1,0)$ yields SPF potential function

$W(R|P,0)$ yields Thakkar potential function

$W(R|1,1)$ yields Ogilvie-Tipping potential function

Thus all four potentials namely Dunham, Simon Parr Finlan (SPF), Thakkar and Ogilvie –Tipping are included in generalized potential energy function. The different parameters used in generalized potential energy function are calculated using turbo basic programme and shown in table 2.

2.3 IMPROVED FIVE-PARAMETER EXPONENTIAL- TYPE POTENTIAL ENERGY FUNCTION:

Recently Ke-Xue Fu , Meng Wang and Chun-Sheng Jia suggested a improved five parameter exponential type potential energy function [30] for diatomic molecule. The dissociation energy and equilibrium bond length as explicit parameters are used to establish an improved five-parameter exponential-type potential energy function for diatomic molecules. The five-parameter exponential-type potential energy model can be represented as.

$$U(r) = D_e \left(1 - \frac{e^{\alpha r_r + q}}{e^{\alpha r + q}} \right)^2 \text{-----(3)}$$

Using molecular constants the parameter α can be calculate by following expression,

$$\alpha = \pi c \omega_e \sqrt{\frac{2\mu}{D_e}} + \frac{1}{r_e} W(\pi c \omega_e r_e q \sqrt{\frac{2\mu}{D_e}} e^{-\pi c \omega_e r_e q \sqrt{\frac{2\mu}{D_e}}}) \text{-----(4)}$$

Where W represents the Lambert W function, which satisfies $z = W(z) e^{W(z)}$

The values given by Ke-Xue Fu et al. are used in this calculation [30] are shown in table 2 and drawn potential energy curve for carbon monoxide molecule.

3. COMPUTATIONAL PROCEDURE:

The data of turning points i.e. r_{\min} and r_{\max} values obtained from RKR curves of these molecules are substituted in equations 1, 2 and 4 respectively for extended Rydberg The Generalized potential energy function and improved five-parameter exponential-type potential energy functions along with the corresponding parameters shown in Table 2.

Table 2 : Parameters of Generalized and Improved Five-Parameter Exponential- Type Potential function for the ground state of carbon monoxide molecule

Generalized potential energy function			
p	1	g₄	-1.08667
n	1	g₅	1.30679
g₀	2437805.3	g₆	-7.06051
g₁	-3.394354	g₇	-0.10999
g₂	4.84317	C_k	35000
g₃	-2.4512	r_e(A⁰)	1.128323
Improved Five-Parameter Exponential-Type Potential Energy function			
q	-0.55	α (A⁰)⁻¹	2.19189

The potential energies obtained plotted against r values yield a potential energy curve for that potential for that particular molecule. For comparison purposes all the potential energy curves of each molecule are drawn on same scale along with their respective RKR curve. The error curves i.e. the % deviation from RKR energies which are calculated by formula $[(U_{\text{RKR}} - U_{\text{potential}}) / D_e] \times 100$.

4. RESULTS AND DISCUSSION:

The RKR curves are plotted for the ground states of carbon monoxide molecule to the extent of 75 % of their dissociation energies. The potential energy curves drawn using Generalized potential energy function and improved five-parameter exponential-type potential energy functions are shown in Figure 1 and below these curves the % deviations from RKR curves are drawn as shown in Figure 2. The average deviation of RKR reported by Londhe et al.[31]. From the graph it is clear that both the potentials show good performance over a wider range. In case of the Generalized potential curves almost overlap the RKR curves of the ground state of carbon monoxide molecule to high v values and show 2 % error to dissociation limit. On the other hand the improved five-parameter exponential-type potentials deviate from RKR with higher v values and show 3 % error to the dissociation limit.

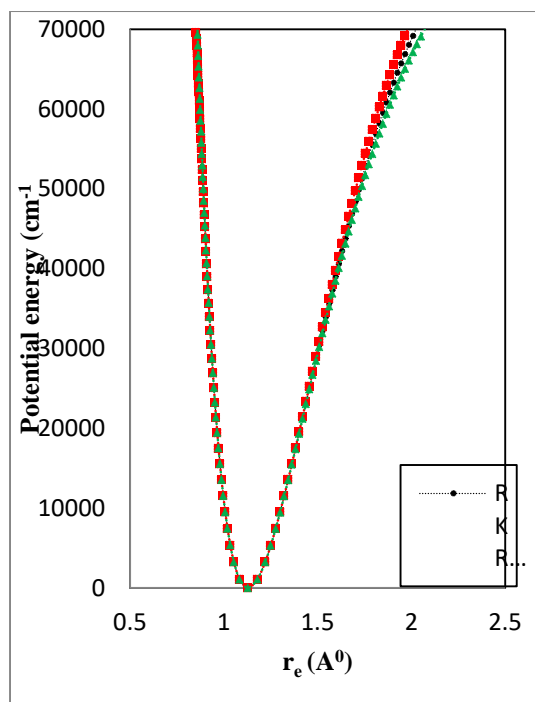


Figure 1: RKR, Generalized and Improved Five-Parameter Exponential-Type potential energy curves for the ground state of carbon monoxide molecule

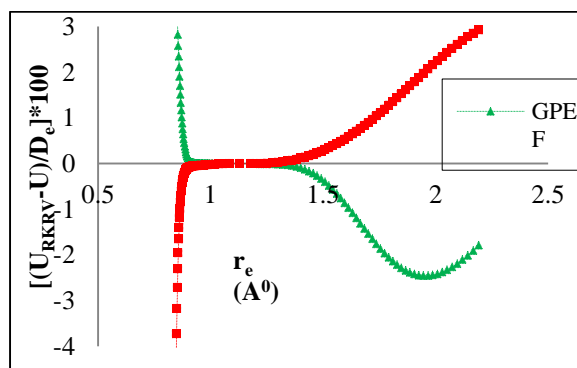


Figure 2: % Deviation of Generalized and Improved Five-Parameter Exponential-Type potential energy curves for the ground state carbon monoxide molecule

5. CONCLUSION

The Generalized potential energy function and improved five-parameter exponential-type potential energy functions almost overlap the RKR curves of the ground state of carbon monoxide molecule to high v values and shows very little deviation from RKR potential.

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