

## Molar Enthalpy Formula for the Specialized Pöschl-Teller Oscillator

\*<sup>1</sup>Ibrahim, Y., <sup>2</sup>Notani, P. P., <sup>3</sup>Ojar, J. U., <sup>4</sup>Tanko, P. U., <sup>3</sup>Mshelia, A. A., <sup>5</sup>Eyube, E. S.

<sup>1</sup>Department Science Laboratory Technology, Gombe State Polytechnic, Bajoga, Nigeria.

<sup>2</sup>Department of Pure and Applied Sciences, Taraba State Polytechnic, Suntai, Jalingo, Nigeria.

<sup>3</sup>Department of Basic Science, Adamawa State College of Agriculture, Ganye, Nigeria.

<sup>4</sup>Department of Physics Education, Federal College of education (Technical) Gombe, Gombe State, Nigeria.

<sup>5</sup>Department of Physics, Faculty of Physical Sciences, Modibbo Adama University, Yola, Nigeria.

\*Corresponding author's email: [yusufibrahim220@gmail.com](mailto:yusufibrahim220@gmail.com); Phone: +2348080850058

### ABSTRACT

In this study, an existing equation for the canonical partition function of the specialized Pöschl-Teller oscillator (SPTO) was used to develop analytical formula for the prediction of molar enthalpy of diatomic substances. The equation was used to analyze the thermodynamic property of the ground state BBr, ICl, P<sub>2</sub>, and PCI molecules. The average absolute deviation ( $\sigma_{ave}$ ) of predicted data from the observed data of the molecules was employed as accuracy indicator. The  $\sigma_{ave}$  obtained are 1.0945%, 0.5312%, 0.8178% and 0.6793% for the BBr, ICl, P<sub>2</sub>, and PCI molecules, respectively. The results predicted with the present formulation for molar enthalpy is in good agreement with the data reported in the National Institute of Standards and Technology (NIST) database. The data generated in this study could be useful in the areas of Solid-State Physics, Chemical Physics, Chemical Engineering, and Atomic and Molecular Physics.

### Keywords:

Canonical partition function,  
Diatomic molecules,  
Pöschl-Teller oscillator,  
Molar enthalpy.

### INTRODUCTION

Thermodynamics is an important subject with immense applications in the physical and biological sciences. For instance, studies associated with gelatinization of enthalpy has been used to investigate phytochemical properties of Tartary buckwheat starch, and to provide information for the application of starch in food and non-food industries (Zhang et al., 2020). Zhang and collaborators (2020) have also utilized results of measurement of thermal properties of substance to effectively produce biodiesel fuel.

The solution of wave equations in the presence of a confining potential have in the last few decades attracted much attention from the research community. The main reason is the fact that key information regarding the quantum mechanical system being analyzed is encased in the wave function describing the system. The solution of Schrödinger equation with different potential energy models have been instrumental in the understanding physical properties of a system including structural and electrical properties (Bhattacharjee and Chattopadhyaya, 2017; Rojas-Briseño, 2017).

The partition function is the master-key to obtaining useful thermodynamic equations. The vibrational partition function depends on potential energy function

describing the system, which in turn also depends on the energy levels (Gordillo-Vázquez and Kunc, 1998). Analytical model equations obtained using the vibrational partition function include entropy, enthalpy, Helmholtz free energy and mean thermal energy (Ikot et al., 2020).

Obtaining the thermochemical properties of a gaseous system is quite a challenging task, in this case, the canonical partition function is required. The canonical partition function incorporates contributions from the vibrational, rotational and translational motion of a gaseous molecule. Quite a number of diatomic molecule oscillators have been used to develop analytical (statistical-mechanical) models for the prediction of molar entropy and enthalpy of substances (Tang and Jia, 2017; Jiang et al., 2019). Equations for the prediction of molar Gibbs free energy and constant pressure (isobaric) heat capacity have been reported elsewhere (Eyube, 2022a).

The Pöschl-Teller potential is the main focus of the present work, the potential is known to have useful applications in chemical physics, nuclear physics, plasmas, and solid state physics. To be used as a diatomic molecule oscillator, Varshni (1957) employed conditions to be satisfied by a diatomic molecule potential to model the specialized Pöschl-Teller

oscillator (SPTO) using the equilibrium dissociation energy ( $D_e$ ), equilibrium bond length ( $r_e$ ) and equilibrium harmonic vibrational frequency ( $\omega_e$ ) as explicit parameters of the oscillator

Lately, the SPTO was used to study rotation-vibration energies of carbon monoxide within the framework of Klein-Gordon equation (Tang and Jia, 2017). In a very recent contribution, canonical partition function developed for the SPTO was used to construct statistical-mechanical models for the prediction of molar entropy and Gibbs free energy of diatomic substances, the equations obtained were used to predict the thermodynamic properties of the ground state  $F_2$ ,  $I_2$ , HI

and KH molecules (Eyube, 2022b). The explicit equations for the prediction of molar entropy and Gibbs free energy were obtained for the SPTO. However, analytical formula for the prediction of molar enthalpy have not been reported in the literature. To this end, this paper is aimed at obtaining Molar Enthalpy Formula for the Specialized Pöschl-Teller Oscillator by way of employing canonical partition function of the SPTO to construct explicit formula for the prediction of molar enthalpy of diatomic substances and use the expression to generate numerical data for some selected diatomic molecules.

## MATERIALS AND METHODS

By employing the SPTO to describe the internal vibration of a diatomic molecule, the potential energy function is given as (Varshni, 1957)

$$U(r) = D_e \left\{ 1 + \frac{\sinh^4(\alpha r_e)}{\sinh^2(\alpha r)} - \frac{\cosh^4(\alpha r_e)}{\cosh^2(\alpha r)} \right\} \quad (1)$$

where  $r$  is the internuclear separation,  $\mu$  and  $c$  are the reduced mass of the diatomic molecule and speed of light, respectively. The potential screening parameter  $\alpha$  is given as (Varshni, 1957).

$$\alpha = \pi c \omega_e (\mu/2D_e)^{1/2} \quad (2)$$

Using the equation for pure vibrational energy levels of the SPTO, the canonical partition function was obtained as (Eyube, 2020b)

$$Q(T) = Q_{\text{vib}} Q_{\text{rot}} Q_{\text{tra}} \quad (3)$$

where  $T$  is the temperature of the gas molecules,  $Q_{\text{vib}}$ ,  $Q_{\text{rot}}$ ,  $Q_{\text{tra}}$  denote the vibrational, rotational and translational components of the total partition function. By assuming a rigid-rotor approximation and using modified Poisson summation formula, the vibrational partition function was deduced as (Eyube, 2020b)

$$Q_{\text{vib}} = \frac{1}{2} \left\{ -\exp\left(\frac{2\alpha^2 \hbar^2}{\mu k_B T}\right) + \exp\left(\frac{2\alpha^2 \hbar^2 v_{\text{max}}^2}{\mu k_B T}\right) + \frac{1}{\alpha \hbar} \sqrt{\frac{\pi \mu k_B T}{2}} \left[ \text{Erfi}\left(\alpha \hbar \sqrt{\frac{2}{\mu k_B T}}\right) + \text{Erfi}\left(\alpha \hbar v_{\text{max}} \sqrt{\frac{2}{\mu k_B T}}\right) \right] \right\} \exp\left(-\frac{D_e}{k_B T}\right) \quad (4)$$

here,  $k_B$  is the Boltzmann constant,  $\hbar = h/2\pi$ ,  $h$  denotes Planck constant,  $\text{Erfi}(x)$  is the imaginary error function of parameter  $x$ . The upper bound vibrational quantum number is represented by (Eyube, 2020b)

$$v_{\text{max}} \sqrt{\frac{\mu \cosh(\alpha r_e)}{2\alpha^2 \hbar^2} + \frac{1}{16}} - \sqrt{\frac{\mu \sinh(\alpha r_e)}{2\alpha^2 \hbar^2} + \frac{1}{16}} - \frac{1}{2} \quad (5)$$

On the other hand, if the interactions between gas molecules are ignored, the rotational and translational partition functions are given by (Jia et al., 2018)

$$Q_{\text{rot}}(T) = \frac{T}{\sigma \Theta_{\text{rot}}} \left\{ 1 + \frac{1}{3} \frac{\Theta_{\text{rot}}}{T} + \frac{1}{15} \left(\frac{\Theta_{\text{rot}}}{T}\right)^2 + \frac{4}{315} \left(\frac{\Theta_{\text{rot}}}{T}\right)^3 \right\} \quad (6)$$

$$Q_{\text{tra}} = \left(\frac{2\pi m k_B T}{h^2}\right)^{3/2} V \quad (7)$$

where  $pV = nRT$ ,  $m$  and  $V$  are the mass and volume of gas enclosed, respectively.  $p$  is the gas pressure,  $R = N_A k_B$  denotes universal or molar gas constant,  $N_A$  being the Avogadro number and  $\Theta_{\text{rot}} = h^2/(8\pi^2 \mu r_e^2 k_B)$  is the rotational characteristic temperature of the gas. The parameter  $\sigma$  takes the value 1 if the gas consists of heteronuclear molecules, and 2 if the gas molecules are homonuclear. The molar enthalpy  $H$  (in  $\text{J mol}^{-1}$ ) can be evaluated from the formula (Jia et al., 2018)

$$H(T) = RT^2 \left(\frac{\partial}{\partial T} \ln Q\right)_V + RTV \left(\frac{\partial}{\partial V} \ln Q\right)_T \quad (8)$$

Substituting equation (3) into (8) and inserting expressions (4), (6), and (7) into the resulting equation leads to

$$H(T) = RT \left(\frac{\gamma}{Q_{\text{vib}}} + \frac{5}{2}\right) + \frac{RT}{\sigma Q_{\text{rot}}} \left\{ \frac{T}{\Theta_{\text{rot}}} - \frac{1}{15} \frac{\Theta_{\text{rot}}}{T} - \frac{8}{315} \left(\frac{\Theta_{\text{rot}}}{T}\right)^2 \right\} \quad (9)$$

where for compactness, the following notation has been used.

$$\begin{aligned}
TQ'_{\text{vib}} = & -\frac{1}{2} \left( \frac{2\alpha^2 \hbar^2 v_{\text{max}}^2}{\mu k_B T} - \frac{D_e}{k_B T} + v_{\text{max}} \right) \exp \left( \frac{2\alpha^2 \hbar^2 v_{\text{max}}^2}{\mu k_B T} - \frac{D_e}{k_B T} \right) \\
& + \frac{1}{2} \left( \frac{2\alpha^2 \hbar^2}{\mu k_B T} - \frac{D_e}{k_B T} - 1 \right) \exp \left( \frac{2\alpha^2 \hbar^2}{\mu k_B T} - \frac{D_e}{k_B T} \right) \\
& + \frac{1}{2} \left( \frac{D_e}{k_B T} + \frac{1}{2} \right) \frac{\sqrt{\pi}}{\varepsilon} \exp \left( -\frac{D_e}{k_B T} \right) \left\{ \text{Erfi} \left( \alpha \hbar v_{\text{max}} \sqrt{\frac{2}{\mu k_B T}} \right) + \text{Erfi} \left( \alpha \hbar \sqrt{\frac{2}{\mu k_B T}} \right) \right\}
\end{aligned} \tag{10}$$

prime which appears in equation (10) stands for derivative with respect to temperature. The reduced molar enthalpy is the form in which experimental data on molar enthalpy are presented, such as the data reported in the National Institute of Standards and Technology (NIST) database. Based on this reason, the analytical reduced molar enthalpy,  $H_{\text{red}}$  is defined by:

$$H_{\text{red}} = H - H_{298.15} \tag{11}$$

where  $H_{298.15}$  is the molar enthalpy value computed at  $T = 298.15$  K, and  $p = 0.1$  MPa.

## RESULTS AND DISCUSSION

The experimental values of the relevant molecular constants; consisting of  $D_e$ ,  $r_e$ , and  $\omega_e$  of the ground state BBr from (Hunt et. al. 1998), ICl (Coxon and Wicramaaratchi, 1980),  $P_2$  (Bu, 1995), and PCI (Zhang et. al., 2016) molecules are presented on Table 1. The last-three columns of Table 1 were obtained from computations using equations (2), (5) and (9). Table 1 provides the necessary data to analytically compute reduced molar enthalpy of the selected diatomic molecules. Using equation (11), the data on  $H_{\text{red}}$  were generated at  $p = 0.1$ , MPa and  $T$  ranging from 300- 6000 K, the results are shown in Table 2. Experimental (observed) data for reduced molar enthalpy of the

diatomic molecules are also listed in Table 2 under the heading  $H_{\text{NIST}}$  (NIST, 1997). The results show that in the low temperature range, data predicted by the reduced molar enthalpy are less than the observed data. However, in the moderate to high temperature region, the predicted results exceed the experimental data. It is noteworthy to highlight that, in the course of derivation of the canonical partition function, the lowest order approximation was imposed on the canonical partition function. The lowest order approximation excludes quantum correction terms from the canonical partition function, by extension, these terms could be associated with the discrepancies in the predicted and observed molar enthalpy data.

**Table 1: Model parameters of the diatomic molecules analyzed in the present study.**

Diatomic molecule	Molecular state	Molecular constant			$\alpha$ ( $\text{\AA}^{-1}$ )	$v_{\text{max}}$	$H_{298.15}$ ( $\text{kJ mol}^{-1}$ )
		$D_e$ ( $\text{cm}^{-1}$ )	$r_e$ ( $\text{\AA}$ )	$\omega_e$ ( $\text{cm}^{-1}$ )			
BBr	X $^1\Sigma^+$	32711	1.887	685.1892	0.7118	95	13.704
ICl	X $^1\Sigma^+$	17557.6	2.32091	384.27	0.9296	91	12.335
$P_2$	X $^1\Sigma^+$	40247.06	1.8934	672.20	0.8029	119	13.639
PCI	X $^1\Sigma^+$	24374.07	2.049	533.38	0.8458	91	13.016

**Table 2: Reduced Molar Enthalpy (in  $\text{kJ mol}^{-1}$ ) as a Function of Temperature (in K) of the Diatomic Molecules Investigated in this Work.**

BBr (X $^1\Sigma^+$ )			ICl (X $^1\Sigma^+$ )			$P_2$ (X $^1\Sigma^+$ )			PCI (X $^1\Sigma^+$ )		
$T$	$H_{\text{red}}$	$H_{\text{NIST}}$	$T$	$H_{\text{red}}$	$H_{\text{NIST}}$	$T$	$H_{\text{red}}$	$H_{\text{NIST}}$	$T$	$H_{\text{red}}$	$H_{\text{NIST}}$
300	0.061	0.063	300	0.066	0.066	300	0.059	0.063	300	0.064	0.064
350	1.724	1.786	350	1.857	1.854	350	1.685	1.788	350	1.818	1.817
400	3.426	3.526	400	3.669	3.657	400	3.351	3.529	400	3.599	3.586
450	5.159	5.281	450	5.496	5.470	450	5.051	5.285	450	5.400	5.369
500	6.917	7.048	500	7.334	7.293	500	6.778	7.054	500	7.216	7.162
600	10.487	10.613	600	11.033	10.961	600	10.293	10.621	600	10.881	10.777
700	14.110	14.212	700	14.756	14.652	700	13.870	14.221	700	14.577	14.420
800	17.770	17.837	800	18.494	18.361	800	17.489	17.845	800	18.294	18.085
...	...	...	...	...	...	...	...	...	...	...	...
2700	89.598	88.701	2700	90.881	90.772	2600	84.797	84.812	2700	90.432	89.571
2800	93.439	92.488	2800	94.743	94.686	2700	88.586	88.581	2800	94.279	93.401
2900	97.285	96.279	2900	98.608	98.611	2800	92.377	92.353	2900	98.130	97.238
3000	101.136	100.074	3000	102.479	102.547	2900	96.171	96.128	3000	101.986	101.082
3100	104.991	103.874	3100	106.354	106.494	3000	99.969	99.906	3100	105.845	104.933

3200	108.850	107.679	3200	110.234	110.451	3100	103.769	103.688	3200	109.709	108.793
3300	112.714	111.488	3300	114.118	114.417	3200	107.572	107.473	3300	113.577	112.660
3400	116.582	115.302	3400	118.007	118.392	3300	111.378	111.262	3400	117.450	116.535
...	...	...	...	...	...	...	...	...	...	...	...
5300	190.874	188.802	5300	192.754	194.235	5300	188.030	187.788	5300	191.801	191.594
5400	194.825	192.730	5400	196.733	198.177	5400	191.888	191.658	5400	195.755	195.598
5500	198.780	196.663	5500	200.717	202.108	5500	195.748	195.533	5500	199.713	199.604
5600	202.739	200.603	5600	204.705	206.029	5600	199.611	199.412	5600	203.675	203.612
5700	206.702	204.549	5700	208.698	209.939	5700	203.476	203.297	5700	207.641	207.620
5800	210.669	208.500	5800	212.694	213.837	5800	207.343	207.186	5800	211.610	211.629
5900	214.641	212.456	5900	216.696	217.723	5900	211.212	211.080	5900	215.584	215.638
6000	218.616	216.417	6000	220.702	221.598	6000	215.084	214.979	6000	219.562	219.645

**Table 3: Average absolute deviation (%) of predicted data from experimental data of the molecules.**

$H_{\text{red}}$ model	Diatomic molecule			
	$\text{BBr} (X^1\Sigma^+)$	$\text{ICl} (X^1\Sigma^+)$	$\text{P}_2 (X^1\Sigma^+)$	$\text{PCl} (X^1\Sigma^+)$
SPTO	1.0945	0.5312	0.8178	0.6793
MHT	...	...	0.8939	...
IRM	...	...	0.9318	...
HAR	...	...	1.1938	...

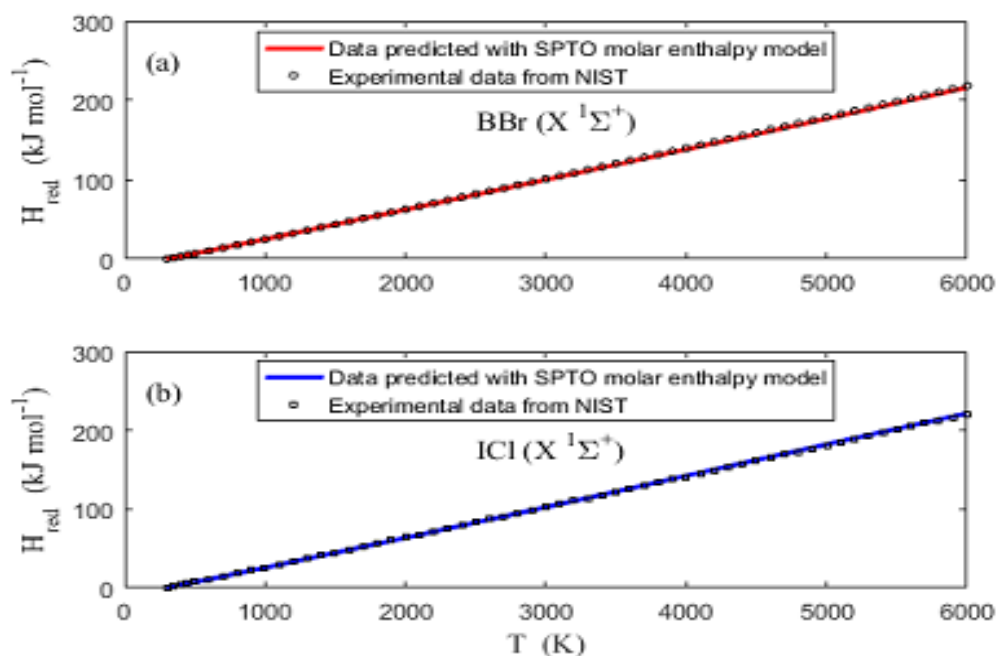


Figure 1: Fitting of the predicted molar enthalpy to observed data for the ground state: (a) BBr molecule. (b) ICl molecule.

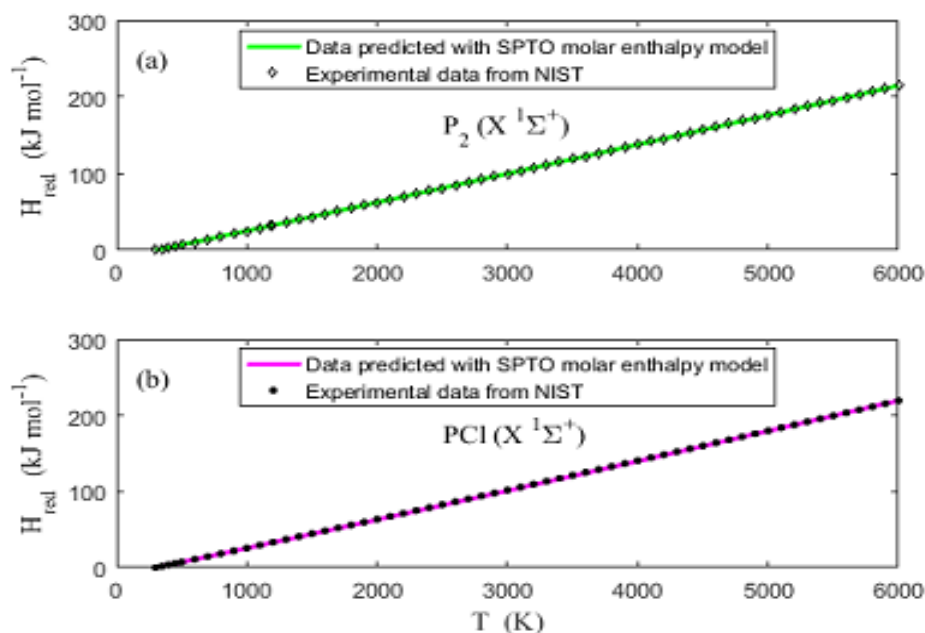


Figure 2: Fitting of the predicted molar enthalpy to observed data for the ground state: (a)  $\text{P}_2$  molecule. (b)  $\text{PCl}$  molecule.

Figures 1 and 2 are the graphical representation of the variation of reduced molar enthalpy (predicted and observed) as a function of temperature of the molecules. The plots evidently reveal that the predicted results are in good agreement with the observed data. Graphical plots only give a picture of the fitted data. Statistically, the average absolute deviation of predicted data from the experimental data can be used to authenticate the applicability of an analytical equation. The average absolute deviation is given by (Eyube, 2022c)

$$\sigma_{\text{ave}} = \frac{100}{N_p} \sum_{j=1}^{N_p} \left| \left( 1 - \frac{H_{\text{red}}}{H_{\text{NIST}}} \right)_j \right| \quad (12)$$

where  $N_p$  is the number of experimental data points, for a quite satisfactory model,  $\sigma_{\text{ave}} \leq 1\%$  of observed data. In the present calculations, taking the temperature range 300- 6000 K of the NIST data,  $N_p = 60$  for  $\text{BBr}$ ,  $\text{ICl}$  and  $\text{PCl}$  molecules, and 61 for the  $\text{P}_2$  molecule. Using equation (12) and the data given in Table 2, the average absolute deviation obtained are displayed in Table 3.

To allow comparison with existing literature results, Table 3 also includes the average absolute deviation obtained with other molar enthalpy models developed from; Modified Hyperbolic-Type (MHT) oscillator, Improved Rosen-Morse (IRM) oscillator and Harmonic (HAR) oscillator models. The tabulated results show that within an error limit of 1% of the NIST data, the proposed molar enthalpy equation is a near perfect model for the diatomic molecules. The results obtained are in good agreement with existing literature on gaseous molecules.

## CONCLUSION

By employing the SPTO to describe the internal vibration of a diatomic molecule, explicit equation for the prediction of molar enthalpy was deduced from the canonical partition function of the system. The equation was used to examine the spectroscopic data of some selected diatomic molecules which includes  $\text{BBr}$  ( $X^1\Sigma^+$ ),  $\text{ICl}$  ( $X^1\Sigma^+$ ),  $\text{P}_2$  ( $X^1\Sigma^+$ ) and  $\text{PCl}$  ( $X^1\Sigma^+$ ). In order to affirm the efficiency of the analytical model, the average absolute deviation ( $\sigma_{\text{ave}}$ ) of predicted data from experimental results of the molecules was employed as goodness-of-fit index. The  $\sigma_{\text{ave}}$  obtained are 1.0945%, 0.5312%, 0.8178% and 0.6793% of the results given by the NIST database for the ground state  $\text{BBr}$  ( $X^1\Sigma^+$ ),  $\text{ICl}$  ( $X^1\Sigma^+$ ),  $\text{P}_2$  ( $X^1\Sigma^+$ ) and  $\text{PCl}$  ( $X^1\Sigma^+$ ) molecules. The obtained data are in good agreement with available literature on gaseous molecules. The results obtained in this study could be applicable to chemical physics, atomic and molecular physics, solid-state physics and plasma physics.

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