Predicted predissociation linewidths in the Schumann–Runge bands of O₂ compared with recent high resolution measurements

G. S. M. Tong and A. S-C. Cheung*  
Department of Chemistry, University of Hong Kong, Hong Kong

M. J. Jamieson  
Department of Computing Science, University of Glasgow, Glasgow, Scotland, United Kingdom

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We derive and use new parameters to quantify the semiempirical expressions of Julienne and Krauss [J. Mol. Spectrosc. 56, 270 (1975)] for the \( ^3\Pi_u, ^3\Sigma_u^+, ^3\Pi_g, \) and \(^1\Pi_u\) potentials that predissociate the rovibrational levels of the \( ^3\Sigma_u^- \) state of O₂. Using the new parameters in the model of Julienne and Krauss we evaluate fine-structure predissociation linewidths for the Schumann–Runge bands that terminate on the \( v=13,14 \) rovibrational levels of the \( ^3\Sigma_u^- \) state. We compare these linewidths and those calculated with several existing sets of parameters with the measurements of Dooley et al. [J. Chem. Phys. 109, 3856 (1998)]. We also show the deperturbing effect of the level shifts, calculated with the new parameters, on the energies of the rotationless \( v=0–17 \) vibrational levels of the \( ^3\Sigma_u^- \) state. © 2001 American Institute of Physics. [DOI: 10.1063/1.1361255]

I. INTRODUCTION

The Schumann–Runge bands of O₂ exhibit triplets that reflect the fine-structure components, \( F_1, F_2, \) and \( F_3, \) of the rovibrational levels supported by the ground electronic state, \( X^3\Sigma_g^- \), and the upper electronic state, \( B^3\Sigma_u^- \). However, the fine-structure components are not easily extracted from observed spectra because the fine-structure splittings of the \( B^3\Sigma_u^- \) and the \( X^3\Sigma_g^- \) levels and many of the predissociation linewidths are close in size.\(^1\) Cheung et al.\(^2\) obtained predissociation linewidths for vibrational levels \( v=0–12 \) of the \( B^3\Sigma_u^- \) state from photoabsorption cross section measurements of Yoshino et al.\(^3,5\) They did not distinguish between the fine-structure components and obtained averaged linewidths.

Differences in the fine-structure components were found in laser induced fluorescence experiments by Wodtke et al.\(^6\) for vibrational levels \( v=14–16 \) of the \( B^3\Sigma_u^- \) state. Few precision measurements of rotationally dependent fine-structure specific linewidths are available. Existing measurements include those obtained in laser induced fluorescence experiments by Yang et al.\(^7\) for a few high rotational states of the vibrational levels \( v=10,11 \) and by Cosby et al.\(^8\) for many rotational states of the vibrational levels \( v=0,2 \). By analyzing photoabsorption cross sections measured by Yoshino et al. at room temperature,\(^9\) Lewis et al.\(^1\) have provided more data; they inferred fine-structure specific linewidths for various rotational states of the vibrational levels \( v=1,2,5,7,9–13 \). Recently, Dooley et al.\(^10\) have made very precise width measurements by three different techniques (UV laser spectroscopy, laser induced fluorescence spectroscopy and vacuum-ultraviolet Fourier-transform spectroscopy), which agree well with each other, for many rotational levels for \( v=13,14 \).

Parameters defining the semiempirical potentials and interactions in the predissociation model of Julienne and Krauss\(^11\) have been obtained by least squares fitting techniques by Cheung et al.\(^12\) for averaged rotationally dependent linewidths for the isotopomers \( ^{16}\)O₂, \( ^{16}\)O\(^{18}\)O, and \( ^{18}\)O₂, and by Lewis et al.\(^1\) for the fine-structure linewidths found by them from the \((^{16}\)O₂) data of Yoshino et al.\(^9\) With the increasing availability of fine-structure resolved data there is a need for further exploration of the prediction of predissociation linewidths.

Cheung et al.\(^12\) determined the parameters by fitting data for vibrational levels \( v=0–12 \). In this investigation we have modified the parameters by including, in the fitted data, the fine-structure data of Cosby et al.\(^8\) for vibrational levels \( v=0,2 \) and of Lewis et al.\(^1\) for vibrational levels \( v=1,2,9–12 \); we used neither the data of Yang et al.\(^7\) nor the data of Lewis et al. for vibrational levels \( v=5,7 \) because they contain comparatively little rotational information. We made the new fit to the same range of rotational levels used by Cheung et al.\(^12\) (\( v=0–12 \)). Then we used the new data of Dooley et al.\(^10\) as a sensitive test of our choice of parameters by comparing the predicted linewidths with these measurements. Finally, we calculated the level shifts and studied their deperturbing effect on the rotationless \( v=0–17 \) vibrational energies.

II. THE CALCULATIONS

A. Widths

We calculated the widths according to the model of Julienne and Krauss\(^11\) as did Lewis et al.\(^1\) The method is as follows.

The equation
\[
-\frac{\hbar^2}{2\mu} \frac{d^2}{dR^2} + V_p(R) + \frac{\hbar^2}{2\mu R^2} J(J+1) - E \chi_{\xi J}(R) = 0
\]
is solved where \( \mu \) is the reduced mass of the molecule, \( R \) is the nuclear separation and \( R^{-1} \chi_{ij}(R) \) is the normalized radial wave function for the bound rovibrational state \((v,J)\) with energy \( E \) supported by the \( B^3\Sigma_u^- \) potential \( V_B(R) \) and, for each predissociated electronic state, the equation

\[
\left[ -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + V_C(R) + \frac{\hbar^2}{2\mu R^2} J(J+1) - E \right] \chi_{ij}(R) = 0
\]

(2)
is solved where \( R^{-1} \chi_{ij}(R) \) is the radial continuum wave function with wave number \( k = (1/\hbar) \sqrt{2\mu[E + V_B(\infty) - V_C(\infty)]} \) (asymptotic) in the predissociating potential \( V_C(R) \), normalized so that its amplitude is \( 1/(2\pi k) \) at infinite separation. Numerical methods are necessary to solve Eqs. (1) and (2). With these solutions the matrix elements

\[
\xi = \int_0^\infty dr \, \chi_{ij}(R) V_{so}(R) \chi_{kl}(R)
\]

(3)
are evaluated where \( V_{so}(R) \) is the spin-orbit interaction between the \( B^3\Sigma_u^- \) bound state and the predissociated state. The fine-structure widths are determined from the formulas given for these energies by Miller and Townes \(14,15\) parameters, \( a \) and \( b \) are given by

\[
a = a(v,J) = \sqrt{\frac{F_3(v,J) - F_2(v,J)}{F_3(v,J) - F_1(v,J)}},
\]

(4)

\[
b = b(v,J) = \sqrt{\frac{F_3(v,J) - F_2(v,J)}{F_3(v,J) - F_1(v,J)}}.
\]

(5)
where \( F_1(v,J) \), \( F_2(v,J) \), and \( F_3(v,J) \) are the energies of the three fine-structure components for level \((v,J)\). The expressions given for these energies by Miller and Townes\(14,15\) imply that

\[
a(v,J) = \sqrt{\frac{1 + \frac{\lambda}{2} - \left( \frac{B - \gamma}{2} \right)}{2 \sqrt{\left[ \frac{\lambda}{2} - \left( \frac{B - \gamma}{2} \right) \right]^2 + 4J(J+1) \left( \frac{B - \gamma}{2} \right)^2}}}
\]

(6)
and

\[
b(v,J) = \sqrt{\frac{1 - \frac{\lambda}{2} - \left( \frac{B - \gamma}{2} \right)}{2 \sqrt{\left[ \frac{\lambda}{2} - \left( \frac{B - \gamma}{2} \right) \right]^2 + 4J(J+1) \left( \frac{B - \gamma}{2} \right)^2}}}
\]

(7)
where \( B \) denotes the rotational constant and \( \lambda \) and \( \gamma \) denote other constants for vibrational level \( v \). In our calculations we used the values of \( B, \lambda, \gamma \), and \( \eta \) that were fitted to experimental data by Cheung et al.\(16\).

This procedure yields widths for a given value of the total angular momentum quantum number \( J \). The experimental data are reported in terms of the quantum number \( N \) of the angular momentum of the end over end rotation. For electronic \( \Sigma \) states these angular momenta differ only by the spin angular momentum of the pair of unmatched electrons and \( N \) is related to \( J \) for each fine-structure component as indicated in Table I. The fine-structure specific widths are clearly seen to differ.

B. Shifts

In the current and previous work\(17\) we used the Green’s function method described by Du et al.\(18\) to obtain the shifts at the band heads where \( J=0 \), Lewis et al.\(1\) found the shifts differently. For each predissociating electronic state and a range of energies \( E \) they solved the coupled equations, to which Eqs. (1) and (2) are approximations for \( J=0 \),

\[
\left[ -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + V_B(R) - E \right] \chi_i(R) = V_{so}(R) \chi'_i(R)
\]

(8)
and

\[
\left[ -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + V_C(R) - E \right] \chi'_i(R) = V_{so}(R) \chi_i'(R),
\]

(9)
where \( R^{-1} \chi_i'(R) \) and \( R^{-1} \chi_i(R) \) are radial wave functions; they found the shifted energies by seeking resonances in the phase shifts of \( \chi_i'(R) \) and determined the shifts by subtracting the corresponding eigenenergies, for \( J=0 \), of Eq. (1). The Green’s function method that we used is simpler in that it requires no search of phase shifts but it does require the solution of an inhomogeneous differential equation.

C. Potentials and interactions

We used the empirical \( B^3\Sigma_u^- \) RKR potential of Friedman.\(19\) Molecules in the \( 5\Pi_u, 3\Sigma^+_u, 3\Pi_u, \) and \( 1\Pi_u \) electronic states dissociate by separating two \( \sigma(3p) \) atoms; the interaction between these molecular states and the \( B^3\Sigma_u^- \) state predissociates the bound levels of the \( B^3\Sigma_u^- \) state. For these predissociating state potentials we used the expression of Julienne and Krauss,\(11\)

\[
V(R) = V_s \exp[-(M_s/V_s)(R-R_s)],
\]

(10)
with various sets of values of the parameters \( V_s \) and \( M_s \), which are the values and slopes of each potential where it crosses the \( B^3\Sigma_u^- \) potential, and \( R_s \), which is the location of each crossing; each potential is referred to its asymptotic value at infinite atomic separation.

We used the representation of Julienne and Krauss\(11\) for the spin–orbit interaction of each predissociated state with the \( B^3\Sigma_u^- \) state:

\[
V_{so}(R) = A_s \exp[-a(R-R_s)^2]
\]

(11)
\( (a=1 \text{ bohr}^{-2}) \), where \( A_s \) is a parameter. We represented the additional Coriolis interaction by the ratio \( \rho \) defined in Sec. II A; its contribution to the widths is shown in Table I.
TABLE I. Fine-structure widths $\Gamma$ in the Julienne and Krauss model.

<table>
<thead>
<tr>
<th>State</th>
<th>$\Gamma(F_1)$</th>
<th>$\Gamma(F_2)$</th>
<th>$\Gamma(F_3)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^3\Pi_u$</td>
<td>$1 + \frac{b^2}{6}$</td>
<td>$\frac{7}{6}$</td>
<td>$1 + \frac{a^2}{6}$</td>
</tr>
<tr>
<td>$^3\Sigma_u^+$</td>
<td>$b^2$</td>
<td>$1$</td>
<td>$a^2$</td>
</tr>
<tr>
<td>$^3\Pi_u$</td>
<td>$1 + a^2 + 2[J(J + 1) - 1] \rho^2 - 4\sqrt{2} a b \rho (J + 1)$</td>
<td>$1 + 2J(J + 1) \rho^2 + 2 \sqrt{2} \rho$</td>
<td>$1 + b^2 + 2[J(J + 1) - 1] \rho^2 + 4\sqrt{2} a b \rho (J + 1)$</td>
</tr>
<tr>
<td>$^1\Pi_u$</td>
<td>$b^2$</td>
<td>$1$</td>
<td>$a^2$</td>
</tr>
</tbody>
</table>

N = J - 1

III. RESULTS AND DISCUSSION

We show the new values of the parameters and also, for comparison, the values found in other work, in Table II.

A. Widths

In Figs. 1–7 we compare the new calculated widths with the data to which they were fitted. The agreement is good but we note some deviations; first, the $F_1$ components are a little small for $v = 0$, $N \leq 12$ and for $v = 10$ and all $N$ shown; second, the $F_2$ components are too small for $v = 0$, $N \leq 16$ and for $v = 1$ and 10 and all $N$ shown; third, the $F_3$ component is too small for $v = 10$ and, finally, all three components fit the data of Lewis et al.\(^1\) better than that of Cosby et al.\(^8\) for $v = 2$.

In Figs. 8–13 we compare the widths predicted by the new parameters and by the others listed in Table II, with the

TABLE II. Parameters for interactions with the $B^3\Sigma_u^-$ state.

<table>
<thead>
<tr>
<th>State</th>
<th>$^3\Pi_u$</th>
<th>$^3\Sigma_u^+$</th>
<th>$^3\Pi_u$</th>
<th>$^1\Pi_u$</th>
</tr>
</thead>
<tbody>
<tr>
<td>New values</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$A_v$ (cm$^{-1}$)</td>
<td>70</td>
<td>46</td>
<td>35</td>
<td>28</td>
</tr>
<tr>
<td>$R_v$ (Å)</td>
<td>1.879</td>
<td>1.999</td>
<td>1.454</td>
<td>1.724</td>
</tr>
<tr>
<td>$M_v$ (cm$^{-1}$  Å$^{-1}$)</td>
<td>38.650</td>
<td>49.000</td>
<td>64.000</td>
<td>22.700</td>
</tr>
<tr>
<td>$\rho$</td>
<td>0.024</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Values given by Cheung et al. in Table I(a) of Ref. 12</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$A_v$ (cm$^{-1}$)</td>
<td>70</td>
<td>46</td>
<td>35</td>
<td>33</td>
</tr>
<tr>
<td>$R_v$ (Å)</td>
<td>1.879</td>
<td>1.999</td>
<td>1.429</td>
<td>1.711</td>
</tr>
<tr>
<td>$M_v$ (cm$^{-1}$  Å$^{-1}$)</td>
<td>38.600</td>
<td>49.000</td>
<td>74.000</td>
<td>25.000</td>
</tr>
<tr>
<td>$\rho$</td>
<td>0.029</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Values of Lewis et al. (Ref. 1)

| $A_v$ (cm$^{-1}$) | 69.9 | 29.7 | 30.8 | 28.3 |
| $R_v$ (Å) | 1.8787 | 2.009 | 1.454 | 1.724 |
| $M_v$ (cm$^{-1}$  Å$^{-1}$) | 41.000 | 27.600 | 55.600 | 23.000 |
| $\rho$ | 0.0189 | | | |

Ab initio values (Refs. 1 and 11)

| $A_v$ (cm$^{-1}$) | 65 | 45 | 28 | 25 |
| $R_v$ (Å) | 1.880 | 2.004 | 1.457 | 1.724 |
| $M_v$ (cm$^{-1}$  Å$^{-1}$) | 41.900 | 40.800 | 58.700 | 23.000 |
| $\rho$ | 0.018 | | | |
experimental results of Dooley et al.\textsuperscript{10} for $v = 13,14$; the tabulated measurements were obtained by vacuum-ultraviolet laser spectroscopy (VUVLS) and laser-induced fluorescence spectroscopy (LIFS). It is seen that, except for the $F_1$ and $F_3$ components with $v = 14$, the predictions from the new parameters represent the best overall fit to the experimental data although the widths of the $F_1$ and $F_3$ components with $v = 13$ predicted from the parameters of Lewis et al.\textsuperscript{1} are better for the higher values of $N$. Our calculated $F_1$ linewidths for the levels with $v = 13$ and $N < 14$ agree well with the experimental measurements; however, at $N = 14$ the calculated and experimental values begin to differ.

The fits to experiment of the $F_1$ linewidths with $v = 14$ obtained with the \textit{ab initio}\textsuperscript{1,11} and the Lewis parameters are good for the values of $N$ shown, the better fit being that obtained from the Lewis values; although the $N$ dependence of these linewidths obtained from the new parameters is qualitatively correct in having the expected ‘‘S’’ shape, the fit to experiment is not satisfactory. Previous calculations\textsuperscript{1,12,17} and the present work suggest that there is considerable sensitivity to the fitted data. To allow these discrepancies in the $F_1$ linewidths to be investigated properly any uncertainties in the calculated values that reflect uncertainties in the fitted data must be eliminated. New measurements of the $v = 0–12$ fine-structure data, made with precision comparable to that achieved by Dooley et al.,\textsuperscript{10} are needed in such a study. The fits of the $F_2$ linewidths with $v = 14$ obtained with the new parameters and with the \textit{ab initio} parameters are also only satisfactory but the fit obtained from the Lewis parameters is good. In all cases the parameters of Cheung et al.\textsuperscript{12} yield widths which are too large and, except for the $F_1$ and $F_3$ components with $v = 14$, the \textit{ab initio} parameters yield widths which are too small.

Cheung et al.\textsuperscript{12} calculated the value of $p$ as 0.029 within the hypothesis of pure precession; they used the value of $\xi$ obtained by Chiu et al.\textsuperscript{17} in their analysis, for $J = 0$, of measurements on the isotopomers $^{16}$O$_2$, $^{16}$O$^{18}$O, and $^{18}$O$_2$. We would obtain the same value for $p$ if we assumed pure precession because the new parameters for the $^{1}$I$_u$ potential are the same as those used by Cheung et al.\textsuperscript{12} and Chiu et al.\textsuperscript{17} the new value of 0.024 differs from the value above, reflecting the departure from pure precession. Lewis et al.\textsuperscript{1} ob-

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**FIG. 1.** Linewidths for $v = 0$. Calculated: this work $F_1$ full line, $F_2$ dashed line, $F_3$ dotted line. Experiment: Cosby et al. (Ref. 8) $F_1 \Diamond$, $F_2 \times$, $F_3 \ast$.

**FIG. 2.** Linewidths for $v = 1$. Calculated: this work $F_1$ full line, $F_2$ dashed line, $F_3$ dotted line. Experiment: Lewis et al. (Ref. 1) $F_1 \triangle$, $F_2 \circ$, $F_3 \ast$.

**FIG. 3.** Linewidths for $v = 2$. Calculated: this work $F_1$ full line, $F_2$ dashed line, $F_3$ dotted line. Experiment: Cosby et al. (Ref. 8) $F_1 \Diamond$, $F_2 \times$, $F_3 \ast$, Lewis et al. (Ref. 1) $F_1 \Delta$, $F_2 \triangledown$, $F_3 \Box$.

**FIG. 4.** Linewidths for $v = 9$. Calculated: this work $F_1$ full line, $F_2$ dashed line, $F_3$ dotted line. Experiment: Lewis et al. (Ref. 1) $F_1 \Diamond$, $F_2 \times$, $F_3 \ast$. 

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FIG. 5. Linewidths for $v=10$. Calculated: this work $F_1$ full line, $F_2$ dashed line, $F_3$ dotted line. Experiment: Lewis et al. (Ref. 1) $F_1 \bigcirc$, $F_2 \times$, $F_3 \ast$.

FIG. 6. Linewidths for $v=11$. Calculated: this work $F_1$ full line, $F_2$ dashed line, $F_3$ dotted line. Experiment: Lewis et al. (Ref. 1) $F_1 \bigcirc$, $F_2 \times$, $F_3 \ast$.

FIG. 7. Linewidths for $v=12$. Calculated: this work $F_1$ full line, $F_2$ dashed line, $F_3$ dotted line. Experiment: Lewis et al. (Ref. 1) $F_1 \bigcirc$, $F_2 \times$, $F_3 \ast$.

FIG. 8. $F_1$ linewidths for $v=13$. Calculated: this work full line, Lewis et al.\textsuperscript{1} dashed line, \textit{ab initio} Lewis et al. (Ref. 1) and Julienne and Krauss (Ref. 11) dotted line, Cheung et al. (Ref. 12) dotted/dashed line. Experiment: Dooley et al. (Ref. 10) VUVLS \times, LIFS \ast.

FIG. 9. $F_2$ linewidths for $v=13$. Calculated: this work full line, Lewis et al. (Ref. 1) dashed line, \textit{ab initio} Lewis et al. (Ref. 1) and Julienne and Krauss\textsuperscript{11} dotted line, Cheung et al. (Ref. 12) dotted/dashed line. Experiment: Dooley et al. (Ref. 10) VUVLS \times, LIFS \ast.

FIG. 10. $F_3$ linewidths for $v=13$. Calculated: this work full line, Lewis et al. (Ref. 1) dashed line, \textit{ab initio} Lewis et al. (Ref. 1) and Julienne and Krauss\textsuperscript{11} dotted line, Cheung et al. (Ref. 12) dotted/dashed line. Experiment: Dooley et al. (Ref. 10) VUVLS \times, LIFS \ast.
We solved the quadratic equation \( \Delta^2 F_2(v) = F_2(v+1,0) - 2F_2(v,0) + F_2(v-1,0) \) (14) for the \( F_2 \) vibrational level \( v \) with \( J=0 \) (and therefore \( N=0 \)). We calculated the shifts that are induced by the predissociating interactions for \( v=0-17 \). The level shift contribution to the second vibrational difference is given by

\[
\Delta^2 S(v) = S(v+1) - 2S(v) + S(v-1),
\]

where \( S(v) \) is the shift in the \( F_2 \) energy of the vibrational level with vibrational quantum number \( v \) with \( J=0 \). The unperturbed second difference

\[
\Delta^2 F_0(v) = \Delta^2 F_2(v) - \Delta^2 S(v)
\]

is expected to show smoother dependence on \( v \) than does the second difference in Eq. (14).11,13 The second differences are negative because the spacing of the levels in the \( B \, 3\Sigma_u^- \) potential decreases as \( v \) increases and the contributions from the level shifts in Eq. (15) are small; we show the second differences in Fig. 14 with the signs reversed. Figure 14 demonstrates the smoothing effect of the shifts, calculated with the new parameters, on the energies given by Cheung et al.;16 the differences are centered on vibrational levels \( v=1-16 \).

**IV. CONCLUSION**

In conclusion we have obtained a new set of parameters to describe the potentials and interactions responsible for...
predisassociating the levels supported by the $B \ ^3\Sigma_u^-$ potential. The agreement between measured widths and the widths obtained when our parameters are used in the model of Julienne and Krauss\textsuperscript{11} is good for the $F_1$, $F_2$, and $F_3$ fine-structure levels of the $v=13$ vibrational state and for the $F_2$ fine-structure level of the $v=14$ vibrational state, but is not satisfactory for the $F_1$ and $F_3$ fine-structure levels of the $v=14$ vibrational state. The new parameters yield an approximately smooth dependence of the deperturbed second order rotationless energy on vibrational quantum number. Agreement with experiment is better in some cases when predicted with the parameters of Lewis et al.\textsuperscript{1} and better in some cases when predicted with our new values; either set provides a plausible account of the predissociation of the rovibrational levels of the $B \ ^3\Sigma_u^-$ state. The branching ratio for the products $O(\ ^3\Pi)+O(\ ^3\Pi)$ and $O(\ ^3\Pi)+O(\ ^1\Delta)$ has been measured by Lin et al.\textsuperscript{21} but its value does not lead to a sensitive distinction between the sets of parameters; for example the calculations of Balakrishnan et al.\textsuperscript{22} show good agreement with experiment when either of the sets of parameters given by Cheung et al. in Tables I(a) and I(b) of Ref. 12 is used. The new parameters and those of Lewis et al.\textsuperscript{1} depend largely on linewidths that were obtained from photoabsorption cross sections. As the determination of these fine-structure linewidths is probably close to the limit of information that can be extracted from the photoabsorption measurements, experimental data for $v=0–12$ of as high quality as that of Dooley et al.\textsuperscript{10} would be very valuable in a further search for a better set of parameters.

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