

# Presentation on Ion Production and Clearing

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# Motivation and Questions to Answer

- Overarching question/goal: How can we increase the QE and thus charge lifetime of the photocathode?
- Current question: How can we reduce the number of ions reaching the photocathode and potentially damaging it, resulting in lower QE?
- Need to know:
  - ① Ion production rates between gun and VWF
  - ② Where newly formed ions go (are they trapped or do they leave the beam?)
  - ③ Distribution of ions at photocathode
- Possible solutions
  - ▶ Ion Clearing Gap (Bunch gap)
  - ▶ Clearing Electrode (Wien filter?)
  - ▶ Beam Shaking (Driving the beam at the oscillating ions' resonance frequency)

# Ion production rate

- The ion production rate for a electron beam ionizing a certain gas is given by Reiser<sup>4</sup>

$$\frac{dn}{dt} = n_b n_g \sigma_i v$$

where  $n$  is the ion density,  $n_b$  is the electron beam density,  $n_g$  is the neutral gas density,  $\sigma_i$  is the ionization cross section for a given gas species, and  $v$  is the velocity of the electrons.

# Ionization Cross Section

- The form for the ionization cross section  $\sigma_i$  for gas species  $i$  follows from Bethe's theory<sup>1</sup>. The general form used by Reiser is in the form from Slinker, Tayler and Ali's paper<sup>7</sup> shown below:

$$\begin{aligned}\sigma_i &= \frac{8a_0^2\pi I_R A_1}{m_e c^2 \beta^2} f(\beta) \left( \ln \frac{2A_2 m_e c^2 \beta^2 \gamma^2}{I_R} - \beta^2 \right) \\ &= \frac{1.872 \times 10^{-24} A_1}{\beta^2} f(\beta) \left[ \ln (7.515 \times 10^4 A_2 \beta^2 \gamma^2) - \beta^2 \right] \\ f(\beta) &= \frac{I_i}{T_e} \left( \frac{T_e}{I_i} - 1 \right) = \frac{2I_i}{m_e c^2 \beta^2} \left( \frac{m_e c^2 \beta^2}{2I_i} - 1 \right)\end{aligned}$$

Here,  $a_0$  is the Bohr radius,  $I_R = 13.6$  eV is the Rydberg energy,  $\beta = \frac{v}{c}$ ,  $\gamma = (1 - \beta^2)^{-\frac{1}{2}}$ ,  $m_e$  and  $T_e$  are the electron's mass and kinetic energy respectively,  $I_i$  is the ionization energy of gas species  $i$ ,  $f(\beta)$  is a correction function for fitting the velocity data at low energies ( $T_e \approx I_i$ ), and  $A_1 = M^2$  &  $A_2 = \frac{e^{C/M^2}}{7.515 \times 10^4}$  are empirical constants that depend on the gas species. These constants are given by Rieke and Prepejchal<sup>5</sup>.

# Ionization Cross Section vs Beam Energy

- Rewriting  $\sigma_i$  as a function of beam energy  $T_e$ , we can plot  $\sigma_i$  for various gas species that are common in the accelerator vacuum:

$$\sigma_i = \frac{1.872 \times 10^{-24} A_1}{1 - \left( \frac{m_e c^2}{m_e c^2 + T_e} \right)^2} \frac{I_i}{T_e} \left( \frac{T_e}{I_i} - 1 \right) \\ \times \left[ \ln \left( 7.515 \times 10^4 A_2 \left( 1 - \left( \frac{m_e c^2}{m_e c^2 + T_e} \right)^2 \right) \left( 1 + \frac{T_e}{m_e c^2} \right) \right) - \left( 1 - \left( \frac{m_e c^2}{m_e c^2 + T_e} \right)^2 \right) \right]$$

Gas Species	$A_1 = M^2$	$C$	$A_2$	$I_i(\text{eV})$
H <sub>2</sub>	0.695	8.115	1.5668	15.4
CH <sub>4</sub>	4.23	41.85	0.2635	12.6
N <sub>2</sub>	3.74	34.84	0.1478	15.6
CO <sub>2</sub>	5.75	55.92	0.2227	13.8

**Table:** Values for  $C$ ,  $M^2 = A_1$ , and  $A_2$  given by Rieke and Prepejchal and  $I_i$  given by NIST for some common gas species.

# Ionization Cross Section vs Beam Energy cont'd

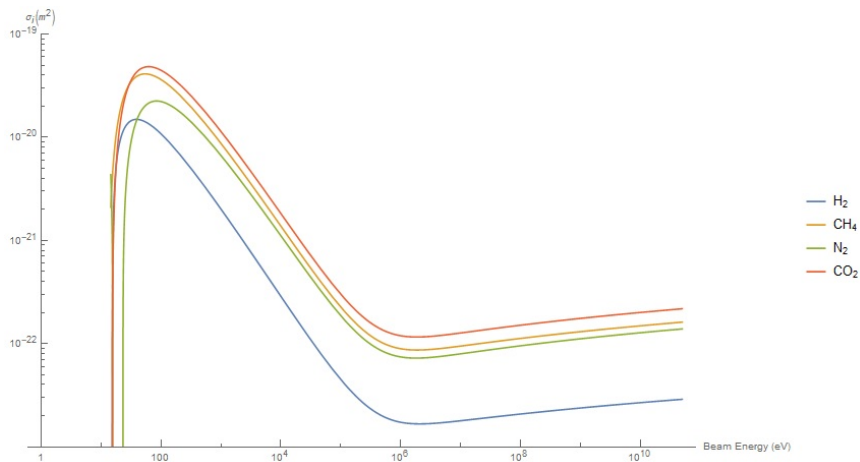
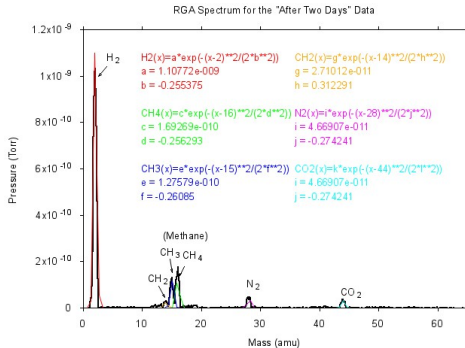


Figure: Plot of the ionization cross section  $\sigma_i$  vs. beam energy  $T_e$

# Example RGA Spectrum for Calculating Ion Production Rates

- For given values of  $n_g$ ,  $n_b$  and  $v$ , we can calculate  $\sigma_i$  and the ion production rate  $\frac{dn}{dt}$ . As an example, we can use the RGA spectrum below to get the densities of the gas species  $n_g$  in the accelerator vacuum:



**Figure:** Analysis of the RGA spectrum for the "After 2 Days" data (before correction factor)

# Gas Densities

We can assume that the residual gas behaves ideally (obeys Newton's laws, volume of gas molecules is much smaller than the gas volume, no external forces on the molecules, molecules in random motion). At standard temperature ( $T_0 = 273.15\text{K}$ ) and pressure ( $p_0 = 760\text{torr} = 1\text{atm}$ ) the density of an ideal gas in a given volume is given by Loschmidt's number:

$$n_0 = \frac{p_0}{k_B T_0} \approx 2.687 \times 10^{25} \text{m}^{-3}$$

Thus, for a given gas, its density is

$$n_g [\text{m}^{-3}] = (3.54 \times 10^{22}) p (\text{torr})$$

The partial pressures are calculated from the Gaussian fit functions (given in the RGA spectrum) using the Gaussian integral:

$$\int_{-\infty}^{\infty} e^{-a(x+b)^2} dx = \sqrt{\frac{\pi}{a}}$$
$$\int_{-\infty}^{\infty} A e^{-\frac{(x+b)^2}{2\sigma^2}} dx = A\sqrt{2\pi\sigma^2}$$



## Gas Densities cont'd

- These partial pressures then need to be corrected using correction factors that adjust the pressures of the gas species relative to nitrogen  $N_2$  (from MKS website).
- The correction factor for each parent ion is assumed to be the same for each ion in its class (as in the case of  $CH_4$ ,  $CH_3$ , and  $CH_2$ ). Assuming an extractor gauge pressure of  $2 \times 10^{-12}$  torr, we can normalize these partial pressures by a normalization factor  $\alpha$  that is equal to the sum of the corrected partial pressures divided by the extractor gauge pressure. Each partial pressure is then multiplied by  $\alpha$  so that the sum of the partial pressures is  $2 \times 10^{-12}$  torr. In this case,  $\alpha \approx 2.87 \times 10^{-3}$ .
- From the normalized partial pressures, the number densities and ion production rates can be calculated.

# Table of Values for $n_g$ , $\sigma_i$ and $\frac{dn}{dt}$

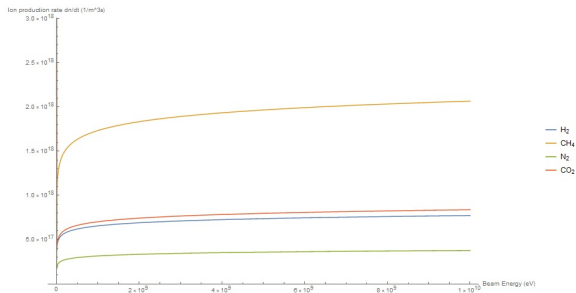
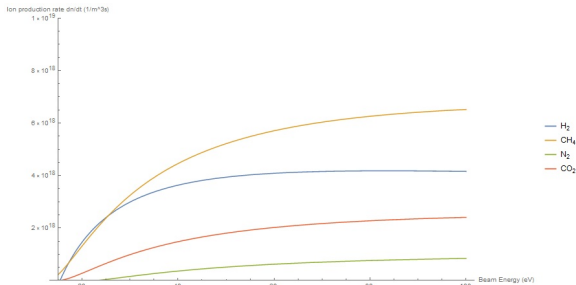
Gas species	Uncorrected Pressure (torr)	Correction factor	Corrected Pressure (torr)	Normalized Pressure (torr)
H <sub>2</sub>	$7.09085 \times 10^{-10}$	0.46	$3.26 \times 10^{-10}$	$9.28 \times 10^{-13}$
CH <sub>4</sub>	$1.08744 \times 10^{-10}$	1.40	$1.52 \times 10^{-10}$	$4.33 \times 10^{-13}$
CH <sub>3</sub>	$8.34180 \times 10^{-11}$	1.40	$1.17 \times 10^{-10}$	$3.33 \times 10^{-13}$
CH <sub>2</sub>	$2.12148 \times 10^{-11}$	1.40	$2.97 \times 10^{-11}$	$8.45 \times 10^{-14}$
N <sub>2</sub>	$3.20961 \times 10^{-11}$	1.00	$3.21 \times 10^{-11}$	$9.14 \times 10^{-14}$
CO <sub>2</sub>	$3.20961 \times 10^{-11}$	1.42	$4.56 \times 10^{-11}$	$1.30 \times 10^{-13}$

Gas species	Gas Density $n_g$ (molecules/m <sup>3</sup> )	Ionization Cross Section $\sigma_i$ (m <sup>2</sup> )	Ion Production Rate (ions/m <sup>3</sup> s)
H <sub>2</sub>	$3.29 \times 10^{10}$	$2.99 \times 10^{-23}$	$4.06 \times 10^{17}$
CH <sub>4</sub>	$1.53 \times 10^{10}$	$1.53 \times 10^{-22}$	$9.66 \times 10^{17}$
CH <sub>3</sub>	$1.18 \times 10^{10}$	$8.00 \times 10^{-23}$ *	$3.89 \times 10^{17}$
CH <sub>2</sub>	$2.99 \times 10^9$	$9.00 \times 10^{-23}$ *	$1.11 \times 10^{17}$
N <sub>2</sub>	$3.24 \times 10^9$	$1.27 \times 10^{-22}$	$1.70 \times 10^{17}$
CO <sub>2</sub>	$4.60 \times 10^9$	$2.04 \times 10^{-22}$	$3.87 \times 10^{17}$

\*Denotes values from NIST here

<https://physics.nist.gov/PhysRefData/Ionization/intro.html>

# Ion Production Rate vs Beam Energy



# Ion Production Rates at Various Beam Energies

Gas Species	IPR at 50eV ( $\text{m}^{-3} \text{s}^{-1}$ )	IPR at 100eV ( $\text{m}^{-3} \text{s}^{-1}$ )	IPR at 500eV ( $\text{m}^{-3} \text{s}^{-1}$ )	IPR at 1keV ( $\text{m}^{-3} \text{s}^{-1}$ )
H <sub>2</sub>	$3.93 \times 10^{18}$	$4.15 \times 10^{18}$	$3.03 \times 10^{18}$	$2.45 \times 10^{18}$
CH <sub>4</sub>	$5.22 \times 10^{18}$	$6.52 \times 10^{18}$	$5.81 \times 10^{18}$	$4.95 \times 10^{18}$
N <sub>2</sub>	$5.22 \times 10^{17}$	$8.43 \times 10^{17}$	$9.07 \times 10^{17}$	$7.99 \times 10^{17}$
CO <sub>2</sub>	$1.80 \times 10^{18}$	$2.41 \times 10^{18}$	$2.26 \times 10^{18}$	$1.94 \times 10^{18}$
Gas Species	IPR at 100keV ( $\text{m}^{-3} \text{s}^{-1}$ )	IPR at 130keV ( $\text{m}^{-3} \text{s}^{-1}$ )	IPR at 180keV ( $\text{m}^{-3} \text{s}^{-1}$ )	IPR at 1MeV ( $\text{m}^{-3} \text{s}^{-1}$ )
H <sub>2</sub>	$4.88 \times 10^{17}$	$4.52 \times 10^{17}$	$4.16 \times 10^{17}$	$3.46 \times 10^{17}$
CH <sub>4</sub>	$1.15 \times 10^{18}$	$1.07 \times 10^{18}$	$9.91 \times 10^{17}$	$8.46 \times 10^{17}$
N <sub>2</sub>	$2.00 \times 10^{17}$	$1.87 \times 10^{17}$	$1.73 \times 10^{17}$	$1.50 \times 10^{17}$
CO <sub>2</sub>	$4.60 \times 10^{17}$	$4.29 \times 10^{17}$	$3.97 \times 10^{17}$	$3.40 \times 10^{17}$

**Table:** Ion Production Rates (IPR) of each gas species for selected beam energies.

# Normalizing IPR to Beam Current

- We can rewrite the equation for IPR and normalize to beam current

$$\frac{dn}{dt} = n_g \sigma_i (n_b v)$$

- The quantity in parentheses can be thought of as the volume *number* density of electrons moving at velocity  $v$ . We can relate this to conventional current  $I$  via the definition of the volume *current* density  $J$  for a volume *charge* density  $\rho$ :

$$J = \rho v \equiv e n_b v = \frac{dI}{da_{\perp}}$$

where  $e$  is the elementary charge and  $a_{\perp}$  is the geometric transverse area of the electron beam.

# Normalizing IPR to Beam Current Cont'd

- We can integrate through the entire electron beam and rewrite this as:

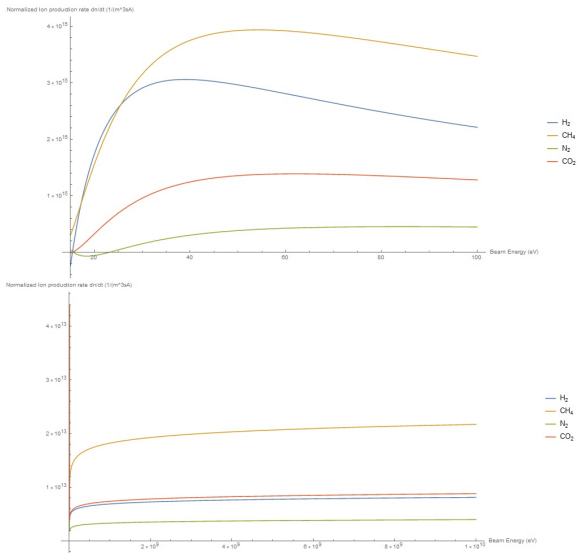
$$J = \frac{I}{a_{\perp}} = en_b v$$
$$n_b v = \frac{I}{ea_{\perp}}$$

Thus,

$$\frac{dn}{dt} = n_g \sigma_i \frac{I}{ea_{\perp}}$$
$$\frac{dn/dt}{I} = \frac{n_g \sigma_i}{ea_{\perp}}$$

- The above equation yields the number of ions produced per second per ampere per cubic meter. Note that, in most cases,  $a_{\perp}$  and  $n_g$  are *not* constant and have distance dependence.

# Normalized IPR vs. Beam Energy



# Where do newly formed ions go?

- According to Reiser<sup>4</sup>, if the ions have the *same* charge as the beam particles (i.e. if the ions are negatively charged), then they are expelled to the walls by the beam's space charge in the absence of magnetic fields. If the ions have *opposite* charge to the beam particles, they are trapped in the beam and contribute to neutralization
- In order to consider the degree of ionization and neutralization, we have to consider several different cases and ask:
  - ▶ How does  $v_e$  compare with  $v_g$ ?
  - ▶ How likely is ionization to occur? Qualitative ion production rate?
  - ▶ Are the collisions elastic or inelastic?
  - ▶ Under what conditions does recombination occur?



# When does $v_e = v_g$ ?

- First, we need to calculate  $v_g$ , the average speed of a gas molecule. From the equipartition theorem,

$$K_{avg} = \frac{3}{2}kT$$

Thus,

$$\begin{aligned}\frac{1}{2}mv_g^2 &= \frac{3}{2}kT \\ v_g &= \sqrt{\frac{3kT}{m}}\end{aligned}$$

where  $k$  is the Boltzmann constant,  $T$  is the gas temperature and  $m$  is the mass of the gas molecule.

## When does $v_e = v_g$ ? cont'd

Below are values for velocity for various gas molecules in the accelerator vacuum

Gas Molecule	Mass of one molecule (kg)	Velocity at 298.15K (m/s)
H <sub>2</sub>	$3.348 \times 10^{-27}$	1921
N <sub>2</sub>	$4.652 \times 10^{-26}$	515.2
CO <sub>2</sub>	$7.308 \times 10^{-26}$	411.1
CH <sub>4</sub>	$2.664 \times 10^{-26}$	680.9

# When does $v_e = v_g$ ? cont'd

- Average gas speed:

$$v_{g,avg} = \frac{1921 + 515.2 + 411.1 + 680.9}{4} \frac{\text{m}}{\text{s}} = 882.05 \frac{\text{m}}{\text{s}} \approx 900 \frac{\text{m}}{\text{s}}$$

- Speed of electron at 200keV is  $0.695c$  or  $2.084 \times 10^8 \frac{\text{m}}{\text{s}}$  ...6 orders of magnitude higher!
- For a potential difference of 200kV through 10cm (cathode-anode gap),

$$E = \frac{V}{d} = 2 \times 10^6 \text{N C}^{-1} \text{ (Electric Field)}$$

$$F_e = eE = 3.204 \times 10^{-13} \text{N (Electric Force)}$$

$$v_f^2 = v_0^2 + 2a\Delta x \text{ (from Kinematics)}$$

## When does $v_e = v_g$ ? cont'd

- Assuming the electrons start from rest,  $v_0 = 0$ . When the electrons reach a speed of  $900 \frac{\text{m}}{\text{s}}$ , they have travelled

$$\begin{aligned}\Delta x &= \frac{v_f^2}{2a} \\ &= \frac{mv_f^2}{2F_e} \\ &= \frac{(9.11 \times 10^{-31} \text{kg}) (900 \frac{\text{m}}{\text{s}})^2}{2 (3.204 \times 10^{-13} \text{N})} \\ &= 1.151 \text{pm!!!!}\end{aligned}$$

- From Carter and Colligon<sup>2</sup>, the maximum energy transfer (i.e. for a head-on collision) from a 200keV electron to a hydrogen molecule is:

$$\begin{aligned}T_{\text{max}} &= \frac{4M_e M_{H_2}}{(M_e + M_{H_2})^2} T_e \\ &= \frac{4 (9.11 \times 10^{-31} \text{kg}) (3.348 \times 10^{-27} \text{kg})}{(9.11 \times 10^{-31} \text{kg} + 3.348 \times 10^{-27} \text{kg})^2} (200 \text{keV}) \\ &= 0.2175 \text{keV} \approx 0.001 T_e\end{aligned}$$

- Thus, we can assume that, throughout the accelerator,  $v_e \gg v_g$

# Do we have to worry about electron-ion recombination?

- The recombination cross section is given by Derbenev<sup>3</sup>:

$$\sigma_{rec} = \frac{16\pi z^2 e^6}{3\sqrt{3}m^2 v^2 c^3 \hbar} \ln \frac{2I}{mv^2} \text{ for } mv^2 \ll 2I$$
$$I = \frac{z^2 e^4 m}{2\hbar^2}$$

We see that, since  $v$  is very large and  $\frac{1}{2}mv^2 = T_e \gg I$ , recombination is highly unlikely. Thus, newly formed ions remain ions.

# Space Charge: Can the ion ever leave the beam?

- Imagine a positive ion surrounded by many electrons in a circular beam. The ion feels a net Coulomb force *towards* the center of beam. Since the electron beam is travelling, the electrons can be thought of a parallel currents (which is a good approximation, since  $v_e \gg v_g$ ) in which case the ion feels a net magnetic force *away* from the center of the beam. This effect is known as the space charge effect<sup>6</sup>.
- The Lorentz force on the ion is

$$\vec{F} = q \left( \vec{E} + \vec{v} \times \vec{B} \right)$$

- Assuming the ion is travelling parallel to the beam, the electric field is purely radial due to symmetry:

$$E_r = \frac{I}{2\pi\epsilon_0\beta c} \frac{r}{R^2}$$

where  $R$  is the radius of the electron beam and  $r$  is the radial distance of the ion from the center of the beam.

# Space Charge cont'd

- The magnetic field is purely azimuthal, also due to symmetry:

$$B_{\phi} = \frac{I}{2\pi\epsilon_0 c^2} \frac{r}{R^2}$$

- The force on the ion, which is purely radial, is thus:

$$F_r = -\frac{el}{2\pi\epsilon_0\beta c} \frac{1}{\gamma^2} \frac{r}{R^2}$$

Due to the  $1/\gamma^2$  factor, this effect is only applicable at non-relativistic beam energies. The negative sign indicates that  $F_r$  is a restoring force and the ion will undergo oscillations about the center of the beam.

# Can the ion leave the beam?

- Let's look at the extreme case: Assume that the ion is travelling radially away from the beam at  $v_g = 900 \frac{\text{m}}{\text{s}}$ . For  $I = 1\text{mA}$ ,  $\beta c = 0.695$  (200keV),  $r = R = 1\text{mm}$ , and  $\gamma = 1.39$ . Let's calculate how far the ion goes before stopping:

$$a = \frac{F_r}{m}$$
$$v_f^2 = v_0^2 + 2a\Delta x$$

In this case,  $v_f = 0$  and  $v_0 = v_g$ . Solving for  $\Delta x$ :

$$\begin{aligned}\Delta x &= \frac{-v_g^2}{2a} \\ &= \frac{-v_g^2 m}{2F_r} \\ &= \left( \frac{1}{4\pi\epsilon_0} \right)^{-1} \frac{v_g^2 m \beta c \gamma^2}{4eI} \frac{R^2}{r}\end{aligned}$$



## Can the ion leave the beam? cont'd

- For a hydrogen ion,  $\text{H}_2^+$ ,  $m = 3.346 \times 10^{-27} \text{kg}$ , so

$$\Delta x = \frac{1}{9 \times 10^9 \frac{\text{N m}^2}{\text{C}^2}} \frac{\left(900 \frac{\text{m}}{\text{s}}\right)^2 (3.346 \times 10^{-27} \text{kg}) (0.695c) (1.39)^2}{4 (1.6 \times 10^{-19} \text{C}) (10^{-3} \text{A})} (10^{-3} \text{m})$$
$$= 0.1892 \text{mm}$$

- For the heaviest ion,  $\text{CO}_2^+$ ,  $m \approx 7.308 \times 10^{-26} \text{kg}$ ,  $\Delta x = 4.131 \text{mm}$
- We see that no ion, once made, can escape the beam. All ions stay very close to the electron beam, if not inside it.

# Distribution of Ions at Photocathode

- Gas molecules lose electrons when ionized by electrons, thus all newly formed ions are positively charged (not sure how gas molecules can *gain* electrons from the electron beam), thus they are trapped in the electron beam.
- When electrons are accelerated forward, positively charged ions are accelerated backward. Since they are trapped by the beam, it stands to reason the ions would remain within the electron beam shape at the photocathode (beam shape determines distribution).
- We can use GPT to confirm these hypotheses. A more rigorous approach may be to use an approximate solution to the Boltzmann/Landau kinetic equation that would show exactly what the distribution of the ions are as a result of ionization (i.e. collisions).

# References

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