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COMPREHENSIVE CROSS SECTION DATABASE DEVELOPMENT FOR GENERALIZED THREE DIMENSIONAL RADIATION TRANSPORT CODES: A STATUS REPORT

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ABSTRACT

To correctly specify the composition and spectra of transmitted heavy ion radiation fields, such as those encountered in space radiation protection studies, accurate values of the total, elastic scattering, reaction cross sections, and spectral and angular distributions of all emitted particles (nucleons, light ions and heavy ions) from the nuclear interactions of propagating high-energy heavy ion (HZE) particles with target nuclei are required. For space radiation protection studies, this means that double-differential (energy and angle) isotope production cross sections must be known for all stable nuclear isotopes with mass numbers from 1 to about 60 colliding with any target nucleus at energies from tens of MeV per nucleon up to several GeV per nucleon. Currently there are several radiation transport codes that transport high-energy nucleons, light ions, heavy ions, or some combination of them. None, however, transport all of these particles in more than one dimension. In order to make a comprehensive tool for space applications that transports all of these particles, with a wide range of energies, and in three dimensions, the database described above is needed, particularly for light and heavy ions. This paper is a status report for the creation of this comprehensive cross section database.

Key Words: charged particles, heavy ions, light ions, monte carlo, cosmic rays

1. INTRODUCTION

To correctly specify the composition and spectra of transmitted heavy ion radiation fields, such as those encountered in space radiation protection studies, accurate values of the total, elastic scattering, reaction cross sections, and spectral and angular distributions of all emitted particles (nucleons, light ions and heavy ions) from the nuclear interactions of propagating high-energy heavy ion (HZE) particles with target nuclei are required. For space radiation protection studies, this means that double-differential (energy and angle) isotope production cross sections must be known for all stable nuclear isotopes with mass numbers from 1 to about 60 colliding with any target nucleus at energies from tens of MeV per nucleon up to several GeV per nucleon. Clearly, measuring all of these thousands of cross sections and distributions is virtually impossible. Hence, the databases necessary to properly describe these reactions must be obtained using nuclear models.

Currently there are several radiation transport codes that transport high-energy nucleons, light ions, heavy ions, or some combination of them. None, however, transport all of these particles in more than one dimension. In order to make a comprehensive tool for space applications that transports all of these particles, with a wide range of energies, and in three dimensions, the database described above is needed, particularly for light and heavy ions. With this database, transport codes would be able to transport nearly any radiation field that man or machine might be exposed to in space or otherwise. It would be invaluable for space radiation protection, in low earth orbit or deep space, and it could be used for terrestrial purposes as well, such as accelerator shielding or heavy charged particle radiotherapy.

2. COMPREHENSIVE CROSS SECTION DATABASE

Several algorithms necessary to transport particles using either stochastic or deterministic methods are already well known. What is lacking to create a generalized three-dimensional radiation transport code is a comprehensive cross section database of total, elastic scattering, total reaction, and double differential reaction production cross sections for virtually any colliding nuclear system.

Several cross section databases currently exist that contain part of the information needed to construct a comprehensive cross section database for transport of high-energy heavy ions in three-dimensions. In their current state these cross section databases are not designed to work together for a fully three-dimensional transport problem. The existing databases of particular interest are:

- The heavy ion total and total reaction cross section databases created by Townsend, Wilson, and Bidasaria, for incident energies above 25 MeV/nucleon [1].
- The improved total reaction cross section database, above 1 MeV/nucleon, created by Tripathi, Cucinotta, and Wilson [2].
- The nuclear fragmentation cross sections database for heavy ions created by Wilson et. al [3].
- The total and total reaction cross section database for deuteron interactions created by Townsend, Wilson, and Bidasaria, for incident energies above 25 MeV/nucleon [4].
- The nuclear fragmentation cross sections database for alpha particles created by Cucinotta, Townsend, and Wilson [5].
- The nuclear fragment momentum distribution database for heavy and light ions created by Tsao et. al [6].
- Finally, the neutron production model created by Braley et. al [7].

2.1. Total and Total Reaction Cross Sections

First, the total cross section is calculated using Townsend and collaborators' optical potential model for total cross sections and total reaction cross sections based on quantum scattering theory [1], but it is corrected by Tripathi and collaborator's parameterization of total reaction cross sections [2]. This correction is made because Townsend and collaborator's model under predicts the total and total reaction cross section as compared to the sparse experimental data sets, especially at energies less than 50 MeV/nucleon. The total reaction cross section is calculated using only Tripathi and collaborator's parameterization of total reaction cross sections.

With this information a transport code can determine where the next interaction for a particle will occur and whether that interaction is a fragmentation/spallation event or not.

Townsend, Wilson, and Bidasaria's optical potential model for total cross sections and total reaction cross sections based on quantum scattering theory are [1]:

$$\sigma_{tot}^{optical} = 4\pi \int_0^\infty \{1 - e^{[-\operatorname{Im} \chi(\bar{b})]} \cos[\operatorname{Re} \chi(\bar{b})]\} b db \tag{1}$$

$$\sigma_{R}^{optical} = 2\pi \int_0^\infty \{1 - e^{[-2\operatorname{Im} \chi(\bar{b})]}\} b db \,. \tag{2}$$

The improved semiempirical total reaction cross section developed by Tripathi, Cucinotta, and Wilson is [2]:

$$\sigma_R^{Tripathi} = \pi * r_0^2 \left(A_P^{1/3} + A_T^{1/3} + \delta_E\right)^2 \left(1 - R_c \frac{B}{E_{cm}}\right) X_m \,. \tag{3}$$

The total cross section is not calculated directly from the optical model developed by Townsend and collaborators. Rather the ratio of the total cross section to total reaction cross section using the optical model is calculated using data that is given in the referenced paper:

$$R = \frac{\sigma_{tot}^{optical}}{\sigma_R^{optical}} \,. \tag{4}$$

No significant errors are expected for ratios obtained by interpolating between the target mass numbers or projectile mass numbers. The agreement of the total and total reaction cross sections as compared with experiment at high energies (2 GeV/nucleon) is within about 3 percent [1]. For low energies (25 MeV/nucleon) the agreement is on the order of 20 percent [1]. The ratio of the total cross section to total reaction cross section will be used because the error for the ratio is smaller than the error for the total cross section alone. Then to actually calculate the total cross section, the total reaction cross section from Tripathi and collaborator's parameterization is multiplied by the ratio of the optical model total cross section to total reaction cross section:

$$\sigma_{tot} = R * \sigma_R^{Tripathi} \,. \tag{5}$$

Tripathi and collaborator's parameterization of total reaction cross sections is a better model with smaller error than the total reaction cross section model developed by Townsend and collaborators. Most importantly, Tripathi and collaborator's model has better agreement with experiment than Townsend and collaborator's total reaction cross section model for all energies. The total reaction cross section calculated from Tripathi and collaborator's parameterization is reported as the total reaction cross section.

2.2. Elastic Scattering Cross Section

The elastic scattering cross section is calculated by subtracting the total reaction cross section from the total cross section:

$$\sigma_{elastic} = \sigma_{tot} - \sigma_R^{Tripathi} \tag{6}$$

In the event that an elastic scattering interaction occurs particle kinematics will be used to determine the new energy and direction of travel of the projectile and target [8]. This simply involves applying conservation of energy and momentum before and after the collision. However, since the energies of interest translate into speeds close to the speed of light the conservation of energy and momentum must be done in a relativistic manner.

2.3. Double Differential Fragmentation/Spallation Production Cross Sections

The next step is to determine which particles result from a fragmentation/spallation event, and what their energies and direction of travel are after the interaction occurs. *Unfortunately, there are no theoretical models currently available that are capable of accurately predicting double differential cross sections for the production of all secondaries from nuclear collisions at all of the energies of interest within a reasonable period of time (hours to days).* Neither are there sufficient experimental measurements of these double differential cross sections to use in database development for space radiation shielding and transport studies. Instead, results from NUCFRG2 [3], Cucinotta and collaborators' alpha breakup model [5], Townsend and collaborators' deuteron scattering model [4], and Braley and collaborators' neutron production model [7] will be used to calculate total yields of isotopes. Then Tsao and collaborators' [6] and Braley and collaborators' [7] models of fragment momentum distributions will be used to calculate the energy and direction of travel of the fragments produced.

The fragmentation of nuclei in this discussion is divided into two parts, first the fragmentation of nuclei with mass number (A) greater than 4 and second the fragmentation of nuclei with mass numbers 2, 3, and 4. These two divisions have been labeled heavy ions and light ions, respectively. The fragmentation of the heavy ions is handled by NUCFRG2 [3] and various other models handle light ion fragmentation.

2.3.1. Heavy ions (A > 4)

NUCFRG2 [3] is a semiempirical nuclear fragmentation model that predicts nuclear fragmentation cross sections for colliding systems with a projectile mass number greater than 4. The processes modeled are abrasion or knockout, the process of nuclei actually breaking apart due to a direct collision, and ablation or spallation, which involves the decay of highly excited nuclear states by heavy particle emission. In this model a projectile nucleus, moving at relativistic speeds, collides with a stationary target nucleus. The parts of the two nuclear volumes that overlap are sheared away, due to the collision, in the abrasion part of this process. The remaining piece of the projectile that continues on in the original direction of travel, at the same velocity as before the collision, is left in a highly excited state. This highly excited piece of the projectile rids itself of this excess energy by emission of gamma rays and/or nuclear particles; this process is the ablation portion of the collision [9].

The number of nucleons removed through abrasion and ablation is a function of the impact parameter, b [3]:

$$\Delta N = \Delta_{abr}(b) + \Delta_{abl}(b) \tag{7}$$

where the number of nucleons removed through abrasion is [3]:

$$\Delta_{abr} = FA_p\left[1 - e^{\frac{-C_T}{\lambda}}\right] \tag{8}$$

and the number of nucleons removed through ablation is [3]:

$$\Delta_{abl} = \frac{E_s + E_x}{10} + \Delta_{spc} \tag{9}$$

Finally, the fragmentation cross section for each specific fragment isotope released due to abrasion and ablation is [3]:

$$\sigma(A_F, Z_F) = F_1 e^{-R\sqrt{\left|Z_F - SA_F + TA_F^2\right|^3}}\sigma(\Delta N) \tag{10}$$

$$\sigma(\Delta N) = \pi b_2^2 - \pi b_1^2 . \tag{11}$$

NUCFRG2 accurately accounts for the yields of all light ion and heavy ion fragments produced by a nucleus-nucleus collision, with mass numbers greater than 4. Given a nucleus-nucleus pair and beam energy, NUCFRG2 will calculate the cross sections for each possible fragment/spallation product to be produced. However, in its current state the cross sections that NUCFRG2 outputs are actually the probability of that fragment/spallation product being produced times the average multiplicity. This is adequate for deterministic codes, but for a monte carlo algorithm this probability and multiplicity need to be separated. In reality this is only a problem for the light ion products because the average multiplicity of the heavy ion products is 1. Therefore, the light ion production cross sections from NUCFRG2 will be the only cross sections corrected.

The correction of NUCFRG2 will involve Braley and collaborators' neutron production cross section, σ_n^{Braley} [7]. Braley and collaborators' model is an abrasion-ablation-coalescence model, which makes predictions of neutron spectra produced in high-energy nucleon-nucleus and nucleon-nucleon interactions. The abrasion-ablation part of this model is similar to that in NUCFRG2, but the effect of coalescence in reducing free neutron emission by composite particle formation is included [7]. The average probability for having N neutrons and Z protons that coalesce is [7]:

$$\langle P(N, Z)\rangle = \frac{(\overline{m}_Z P_Z)^Z (\overline{m}_N P_N)^N}{Z!\, N!}. \tag{12}$$

Therefore, the invariant double differential neutron production cross section is [7]:

$$\sigma_n^{Braley} = \left(\frac{Z_t + Z_p}{N_t + N_p}\right)^Z \frac{A}{Z!\, N!} \left(\frac{4\pi P_0^3}{3\sigma_0 m}\right)^{A-1} (\sigma_I(n))^A, \tag{13}$$

where the coalescence radius, P_0, is taken to be 90 MeV/c.

The first step in the correction of the NUCFRG2 light ion production cross sections will be to modify Braley and collaborators' model so that it also calculates proton production cross sections, σ_p^{Braley}. Then the production cross section for protons (σ_p), neutrons (σ_n), deuterons (σ_d), and tritons (σ_t) will be calculated using Braley and collaborators' cross sections and the same production cross sections from NUCFRG2 ($\sigma_p^{NUCFRG2}$, $\sigma_n^{NUCFRG2}$, $\sigma_d^{NUCFRG2}$, $\sigma_t^{NUCFRG2}$):

$$\sigma_p = \sigma_p^{Braley} \qquad \sigma_n = \sigma_n^{Braley}$$

$$\frac{\sigma_d}{\sigma_p + \sigma_d + \sigma_t} = \frac{\sigma_d^{NUCFRG2}}{\sigma_p^{NUCFRG2} + \sigma_d^{NUCFRG2} + \sigma_t^{NUCFRG2}} = d \tag{14}$$

$$\frac{\sigma_t}{\sigma_p + \sigma_d + \sigma_t} = \frac{\sigma_t^{NUCFRG2}}{\sigma_p^{NUCFRG2} + \sigma_d^{NUCFRG2} + \sigma_t^{NUCFRG2}} = t.$$

Equation 14 forms a system of linear equations that can be solved for σ_d and σ_t:

$$(1 - d)\sigma_d - d\sigma_t = d\sigma_p \qquad -t\sigma_d + (1 - t)\sigma_t = t\sigma_p$$

$$\sigma_t = \frac{t}{1 - t - d}\sigma_p \qquad \sigma_d = \frac{dt + d(1 - t - d)}{(1 - d)(1 - t - d)}\sigma_p. \tag{15}$$

Next, using Tripathi and collaborators' total reaction cross section, $\sigma_R^{Tripathi}$, the production cross section for isotopes with z equal 2 ($\sigma_{z=2}$) will be calculated. First the sum of all NUCFRG2 production cross sections for isotopes with z > 2 ($\sigma_{z>2}^{NUCFRG2}$) is calculated:

$$\sigma_{z>2}^{NUCFRG2} = \sum_{z=3}^{z_p} \sigma_z^{NUCFRG2}$$

$$\sigma_{z=2} = \sigma_R^{Tripathi} - \sigma_{z>2}^{NUCFRG2} - \sigma_p - \sigma_n - \sigma_d - \sigma_t, \qquad (16)$$

where z_p is the charge number of the projectile. With the production cross section for isotopes with z equal 2 ($\sigma_{z=2}$) the production cross section for alphas (σ_α) and helium-3 (σ_{He-3}) can be calculated using NUCFRG2's alpha and helium-3 production cross sections ($\sigma_\alpha^{NUCFRG2}$ and $\sigma_{He-3}^{NUCFRG2}$):

$$\sigma_\alpha = \frac{\sigma_\alpha^{NUCFRG2}}{\sigma_\alpha^{NUCFRG2} + \sigma_{He-3}^{NUCFRG2}} \sigma_{z=2} \qquad (17)$$

$$\sigma_{He-3} = \frac{\sigma_{He-3}^{NUCFRG2}}{\sigma_\alpha^{NUCFRG2} + \sigma_{He-3}^{NUCFRG2}} \sigma_{z=2}. \qquad (18)$$

With the above corrections for NUCFRG2's light ion production cross sections, NUCFRG2's heavy ion production cross sections, and Braley and collaborators' nucleon production cross sections the cross sections for producing nucleons, light ions, and heavy ions resulting from nucleus-nucleus collisions, with mass number greater than 4, is complete.

2.3.2. Light ions (2 ≤ A ≤ 4)

The deuteron scattering cross section model created by Townsend, Wilson, and Bidasaria [4] uses the same physics as their total and total reaction cross section model [1]. It is an optical potential model based on quantum scattering theory. However, it is now applied to deuterons colliding with different nuclei. This model provides the total cross section and total reaction cross section for deuterons interacting with different nuclei starting at 25 MeV/nucleon up to 22.5 GeV/nucleon.

The simplest projectile to determine fragmentation/spallation products of is the deuteron. Using Townsend and collaborators' deuteron scattering model [4] the total deuteron-nucleon cross section and the total deuteron-nucleon reaction cross section is calculated. When the deuteron breaks up there is only possible fragmentation channel. Therefore, the total reaction cross section of the deuteron interaction is equal to the fragmentation cross section for this single channel:

$$\sigma_{pn} = \sigma_R^{Tripathi} \qquad (19)$$

If the interaction is elastic then the process described previously about elastic scattering will determine the outcome of the reaction. If the interaction is inelastic then the reaction will produce a proton and a neutron.

Cucinotta, Townsend, and Wilson have developed a parameterization of helium-3, triton, and deuteron production due to alpha particle fragmentation on hydrogen [5]. The cross section for helium-3 production is [5]:

$$\sigma_{He-3}^{Cucinotta} = 42.5\left[\frac{2}{1 + e^{(T_{th}-T)/6.8}} - 1\right]\left(1 - \frac{0.51}{1 + 6.7e^{-T/34}}\right)^3 * \left[1 + 0.36\sqrt{\frac{T}{520}}\right]\left(e^{(780-T)/2300}\right), \tag{20}$$

where T_{th} is the threshold energy for the possible fragmentation events, which are listed below in Table I, and T is the kinetic energy of the projectile in units of MeV per nucleon. The cross section for triton production is [5]:

$$\sigma_{t}^{Cucinotta} = 15.5\left[\frac{2}{1 + e^{(T_{th}-T)/7}} - 1\right]\left(1 - \frac{0.45}{1 + 7e^{-T/55}}\right)^3 * \left[1 + 1.8\sqrt{\frac{T}{550}}\right]\left(e^{(750-T)/4500}\right). \tag{21}$$

Lastly, the cross section for deuteron production is [5]:

$$\sigma_{d}^{Cucinotta} = 17\left[\frac{2}{1 + e^{(T_{th}-T)/12}} - 1\right]\left(1 + \frac{\frac{0.21T}{145} - 0.21}{1 + e^{(145-T)/6}}\right)^3\left(e^{-T/3000}\right). \tag{22}$$

Table I list the threshold energies for each of the possible alpha fragmentation channels [5].

Table I: Threshold Energies for Alpha-Hydrogen Fragmentation Channels

Fragmentation Channel	Threshold, MeV
proton + triton	24.77
neutron + helium-3	25.72
deuteron + deuteron	29.81
deuteron + proton + neutron	32.59
proton + proton + neutron + neutron	35.37

For alpha breakup the products of the reaction will actually be determined by choosing the entire reaction channel of the alpha breakup. The 5 possible fragmentation channels for alpha breakup are listed above in Table I. The production cross section for each alpha fragmentation channel is:

$$\sigma_{pt} = \sigma_t^{Cucinotta} \qquad \sigma_{nHe-3} = \sigma_{He-3}^{Cucinotta}$$

$$\sigma_{dd} = \sigma_d^{Cucinotta}\left(T_{th} = 29.81\right) \qquad \sigma_{dpn} = \sigma_d^{Cucinotta}\left(T_{th} = 32.59\right) \tag{23}$$

$$\sigma_{ppnn} = \sigma_R^{Tripathi} - \sigma_{pt} - \sigma_{nHe-3} - \sigma_{dd} - \sigma_{dpn}.$$

One issue with Cucinotta and collaborator's alpha breakup model is that it applies to alpha-hydrogen reactions. Therefore it will need to be generalized to alpha-nucleus reactions. This will be done using a scaling algorithm the best of which was developed by Tsao et. al. [10].

This then leaves to determine the products of triton-nucleus and helium-3-nucleus interactions. No models have been found specifically for each of these breakup processes, however, a backdoor way of getting the necessary fragmentation cross sections is being investigated. This method would use Braley and collaborators' modified model, which will calculate neutron [7] and proton production cross sections for nucleus-nucleus interactions. This is feasible because triton and helium-3 breakup each only have 2 fragmentation channels. For helium-3 breakup the fragmentation channels are 2 protons and a neutron or a deuteron and a proton. For triton breakup the fragmentation channels are 2 neutrons and a proton or a deuteron and a neutron. Therefore, the production cross sections for each helium-3 fragmentation channel would be:

$$\sigma_{ppn} = \sigma_n^{Braley} \qquad \sigma_{dp} = \sigma_p^{Braley} \tag{24}$$

and the production cross sections for each triton fragmentation channel is:

$$\sigma_{dn} = \sigma_n^{Braley} \qquad \sigma_{nnp} = \sigma_p^{Braley}. \tag{25}$$

Please note that this method is still being investigated.

2.3.3. Nuclear fragmentation momentum distributions

Once the proper fragmentation/spallation product yields have been predicted for a nucleus-nucleus collision, the energy and direction of travel of those products must be determined. The fragment transverse momentum distributions are well described by a phenomenological parameterization due to Tripathi and Townsend [11]. Further work was done by Tsao et. al. to produce a computer code that calculates these momentum distributions in both the longitudinal and transverse directions [6]. Their model assumes that the momentum distributions of fragmentation/spallation products in the projectile rest frame are Gaussian distributed, as is suggested by experimental data. The variance of this Gaussian distribution has a parabolic dependence on the fragment mass [6]. The average kinetic energy loss per nucleon parallel to the original direction of travel of the projectile in the projectile frame, which can easily be related to the momentum loss, for projectile fragments with mass, A_f, less than A is [6]:

$$\langle dKE \rangle_{\parallel} = E_A - E_{\Delta A} - M_f . \quad (26)$$

The average kinetic energy loss per nucleon perpendicular to the original direction of travel of the projectile in the projectile frame, which can easily be related to the momentum loss, for projectile fragments with mass, A_f, less than A is [6]:

$$\langle dKE \rangle_{\perp} = \sqrt{2} * \left| \langle dKE \rangle_{\parallel} \right| . \quad (27)$$

The variance of the kinetic energy distribution, σ^2_{dKE}, is [6]:

$$\sigma^2_{dKE} = \frac{9T^2_{eff}\Delta A}{A_P}\left[\sqrt{\frac{2\langle dKE \rangle}{3T_{eff}}} + 1\right]^2 , \quad (28)$$

where the variance is for the parallel momentum distribution when $\langle dKE \rangle$ is the mean of the parallel distribution and for the perpendicular momentum distribution when $\langle dKE \rangle$ is the mean of the perpendicular distribution.

This computer code, given a nucleus-nucleus pair, energy, and fragment/spallation product of interest, reports the parallel and perpendicular momentum distribution components of the fragment/spallation product in the projectile frame of reference [6]. A small modification to the code needs to be made so that the momentum distribution components are reported in the LAB frame of reference, which will be done via a Lorentz transformation. This code will be used as the source of momentum distribution for all fragmentation/spallation products excluding nucleons. With this information the parallel and perpendicular momentum distributions of each individual fragment/spallation product can be defined as Gaussian distributions, and then sampled in order to select an energy and direction of travel for each fragment/spallation product. Of course momentum and kinetic energy before and after the collision will be conserved.

The neutron production model developed by Braley et. al. reports double differential neutron production cross sections [7]. The modified version of the neutron production model that will provide proton production cross sections will also report double differential neutron and proton production cross sections. Therefore, it is not necessary to use Tsao and collaborators' model to determine the energy and direction of travel for nucleons produced in the fragmentation/spallation reactions.

3. SUMMARY OF DATABASE STATUS

To date (October 2002) the total, total reaction, and elastic cross sections of this database are complete. The heavy ion production cross sections for nucleus-nucleus interactions, with mass number greater than 4, are also complete. The double differential neutron production cross sections for nucleus-nucleus interactions is complete as well. Light ion production cross sections for nucleus-nucleus interactions, with mass number greater than 4, are not complete because they are dependent on double differential proton production cross sections for nucleus-nucleus interactions. The double differential neutron production cross section model still needs to be modified in order to create a double differential proton production cross section model. Production cross sections for deuteron-nucleus and alpha-nucleus interactions are complete. Production cross sections for triton-nucleus and helium-3-nucleus interactions are not complete. Currently a model for triton-nucleus and helium-3-nucleus production cross sections using the double differential neutron and proton production cross section model is being investigated. All that remains to complete the model of fragment momentum distributions for light ion and heavy ion fragments is the Lorentz transformation from the projectile rest frame to the LAB frame.

Once the modifications and coupling of all these databases is complete a comprehensive cross section database for generalized three dimensional radiation transport codes will exist. In order to test the cross section database and to create a truly generalized three-dimensional radiation transport code, this database will be added to the monte carlo radiation transport code, HETC [12]. This generalized three-dimensional radiation transport code, HETC/HEDS [13], will be very useful in the fields of space radiation protection, accelerator shielding, and heavy charged particle radiotherapy.

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