

PATHFINDER: A Tool for Calculating Pathways for Fusion-Activated Materials

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ABSTRACT

The DT fusion reaction will produce 14.1 MeV neutrons. These high-energy neutrons will interact with the surrounding material producing radioactive isotopes. Inventory codes are used to calculate the change in material composition and radiation fields produced from these irradiated materials. An isotope in the neutron environment can transmute to produce other isotopes and these next-generation isotopes can undergo nuclear reaction or radioactive decay producing a complex tree-like structure with branches, cross-linking, and loops. One of the most important results of such codes is the pathways to produce radioisotopes. Inventory codes often lack the ability to calculate these pathways. A new tool, PATHFINDER, has been developed, which probes the nuclear data and reads the reaction cross-section and decay data into a coefficient matrix. For a given initial isotope the tool can then create an activation tree. It can also be used to calculate the reverse tree describing all the parents from which the isotope can be created. Such a tool can be helpful in conjunction with the inventory codes to identify the source of a radioactive isotope or the different isotopes that can be created from a nuclide when kept in a neutron environment.

1 INTRODUCTION

The current design of fusion reactors focuses on the Deuterium-Tritium (DT) fusion reaction. This reaction will produce 14.1 MeV neutrons and as these high energy neutrons travel through the reactor vessel they will interact with the surrounding materials and initiate further reactions. These neutron-induced reactions can produce radioactive isotopes, which may further decay to produce new isotopes. The production and decay chains of isotopes forms a tree-like structure with multiple branches, cross-linking and loops. Some of the radioactive isotopes produced in the material could be responsible for long-term radioactivity, waste generation, gamma dose rates and decay heat. It thus becomes important to know the pathway through which these

isotopes could be formed, potentially to aid design engineering of materials to optimise radiological response. For example, these pathways could help identify the parent isotopes responsible for the creation of the hazardous isotopes and inform on the mitigation techniques that could be applied to minimise the production of such isotopes.

The process of changing the concentration of an isotope in a material under neutron irradiation, including its initial creation, is given by the inventory equation 1. Further details of the equation can be found in article [5].

$$\frac{dN_i}{dt} = -(\lambda_{ii} + \sigma_{ii}\phi)N_i + \sum_{j \neq i} (\lambda_{ij} + \sigma_{ij}\phi)N_j \quad (1)$$

The first term in the equation is the loss term for the isotope i , where λ_{ii} is the total decay coefficient and σ_{ii}^g is the total cross-section of isotope i for incident integrated neutron flux ϕ . The second, summation term is the gain term, which is the production of isotope i from all different isotopes j . λ_{ij} is the decay of isotope j producing i and σ_{ij} is the collapsed cross-section of producing isotope i from reactions on isotope j for incident integrated neutron flux ϕ . The collapsed cross-section is the total cross-section per unit flux under a particular neutron spectrum and obtained by multiplying the energy dependent cross section by the neutron spectrum and normalising, viz:

$$\sigma_{ij} = \frac{\sum_k \bar{\sigma}_{ij}(E_k)\phi(E_k)}{\sum_k \phi(E_k)}, \quad (2)$$

where $\bar{\sigma}_{ij}(E_k)$ is the cross-section at energy group k and $\phi(E_k)$ is the flux in energy group k .

The time evolution rate for all the isotopes in the material is given by the set of coupled first-order linear differential equations eq. bat. Inventory codes like FISPACT-II [1] calculate the final inventory of a material for a given neutron energy spectrum, initial material composition and irradiation time. Since λ_{ij} and σ_{ij} are independent of N_j , the matrix of coefficients can be defined, with terms defined as:

$$\Lambda_{ij} = \lambda_{ij} + \sigma_{ij}\Phi \quad (3)$$

The matrix Λ contains all the connections between each parent i and daughter j isotope via any decay process or neutron-induced reaction, and can be interpreted in terms of a directed graph.

In this paper, a tool called PATHFINDER is presented. It creates this coefficient matrix by reading the nuclear data library and creates the directed graphs for any isotope requested. The method and inputs required by PATHFINDER are given in section 2 and the possible kinds of outputs of the tool are discussed in the section 3.

2 METHOD TO CALCULATE THE PATHWAYS

A directed graph is set of vertices connected by directed edges. Each vertex or node in this work is an isotope and each edge corresponds to a nuclear reaction or radioactive decay between the parent and daughter isotope (vertices). Each directed graph can be represented by an adjacency matrix. The elements of the matrix indicate whether pairs of vertices are in the graph or not. This adjacency matrix can be created from the coefficient matrix described via 3. The adjacency matrix, referred in this tool as the connection matrix, contains all the possible connections between the isotopes that exists in the nuclear data libraries of decay and (neutron) reactivity.

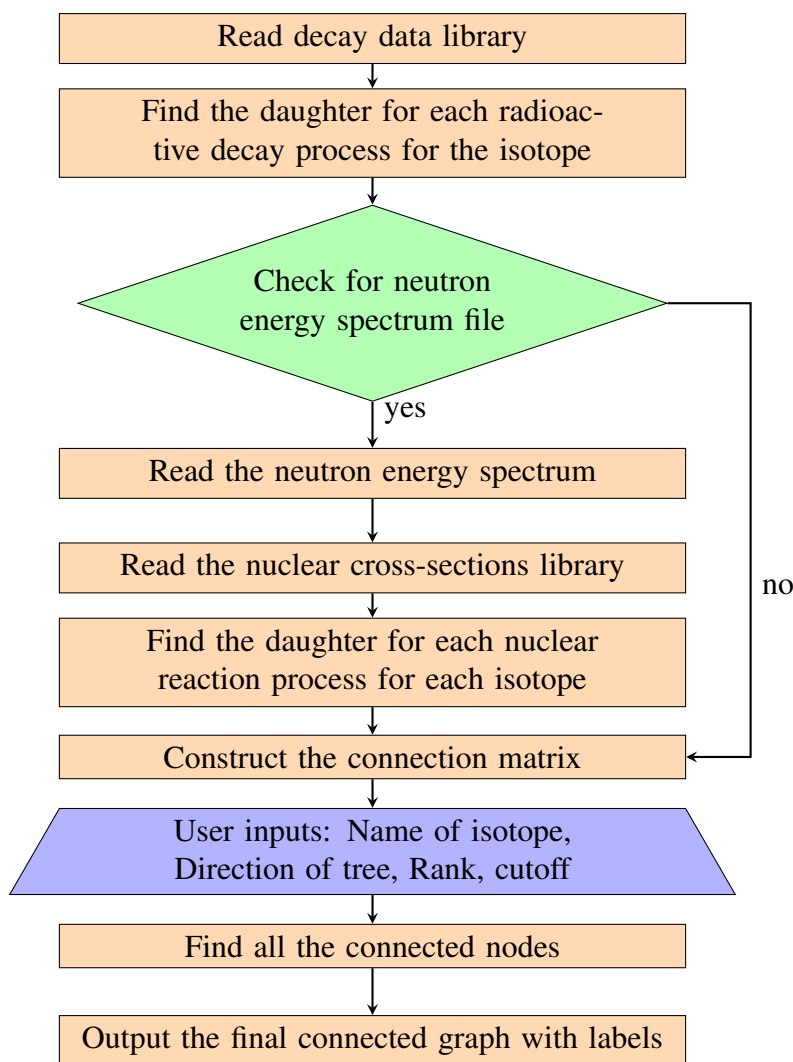


Figure 1: Overview of PATHFINDER

PATHFINDER is a python program that reads the nuclear data libraries, constructs the coefficient matrix and then generates the pathways for the requested isotope. A simplified flow chart of the code is given below:

Inputs required by PATHFINDER tool:

- The address for the nuclear data library and the neutron spectrum file. If the neutron spectrum file is missing, the tool will not read the neutron reaction cross-section library and only create directed graphs for radioactive decay.
- Name of the isotope and kind of the directed graph (forward or backward). Forward will show all the daughters of the isotope, and backward will show all the parents of the (daughter) isotope.
- In case of a directed graph with the neutron reactions included, rank is also required as input. Rank puts a limit on the connections from a parent to the daughter, for example if the rank is 1 then only paths like $A \rightarrow B$ will be shown. This is to make the visualisation more easy and as such there is no limitation in the tool to create paths or directed graphs of any rank.

The tool starts by reading the ENDF format data libraries [3] and creates an object with attributes like half-life, decay channels, branching ratios, MT numbers and reaction cross-section (in the given group structure). It also reads the neutron energy spectrum and collapses the reaction cross-section. The program then calculates the daughter isotopes resulting from the decay or the nuclear reactions. Using this information two matrices are created, first is the connection matrix and second is the name matrix. If there exists a non-zero reaction cross-section or a decay from isotope j to isotope i then the connection matrix element C_{ij} is set to 1, else it is zero. A cutoff can also be put in the connection matrix to include only the reactions which have a reaction rate above a certain value. This cutoff is used to prune the connections so that only the important reactions are shown in the directed graph. The second matrix contains the name of the reaction or decay between the isotopes. It also contains the branching ratio in case of radioactive decay and the ratio of reaction cross-section from the parent to a daughter to the total cross-section of the parent. These ratios show among the various branches of the directed graph which branch is most probable. The daughters or the parents of the input isotope are then extracted from the connection matrix using the Python module Networkx [2]. All the paths connecting these sets of isotopes are then plotted using the same module.

3 RESULTS

The results obtained in this paper are using the DECAFY–2020 [4] and the TENDL–2017 [6] nuclear data libraries. Examples of various kinds of outputs that can be generated from PATHFINDER are given below.

3.1 Directed graphs for decay

PATHFINDER can create forwards and backwards directed graphs for isotopes which are connected only via radioactive decay. These graphs don't contain any loops. The forward

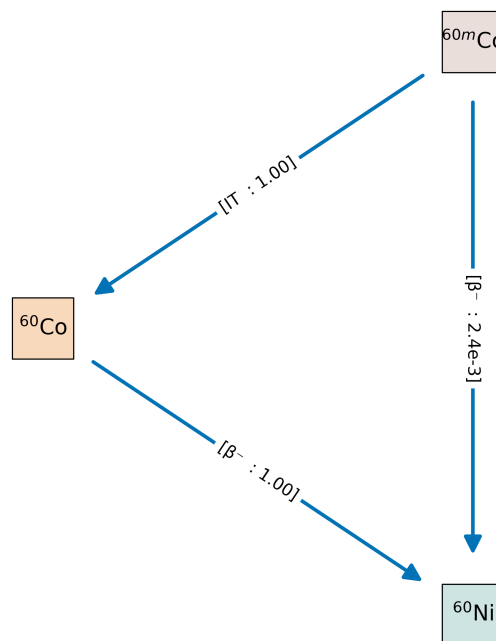


Figure 2: All the daughters of ^{60m}Co

directed graph from a radioactive isotope always terminates at a stable isotope. Thus these graphs have a natural termination condition. The figure 2 is a forwards directed graph for ^{60m}Co . The root node or the isotope for which the graph is requested is given in the mauve color box at the top. The radioactive isotopes are given an orange color box and stable isotopes are in blue. The edge connecting the isotopes gives the name of the radioactive decay and the branching ratio for that decay. A backward graph can also be generated using PATHFINDER, which contains all the parents from which a particular isotope can be created.

3.2 Directed graphs including decay and transmutation

The directed graphs that include the nuclear reaction cross-section typically contain many more connections than the decay-only directed graph.

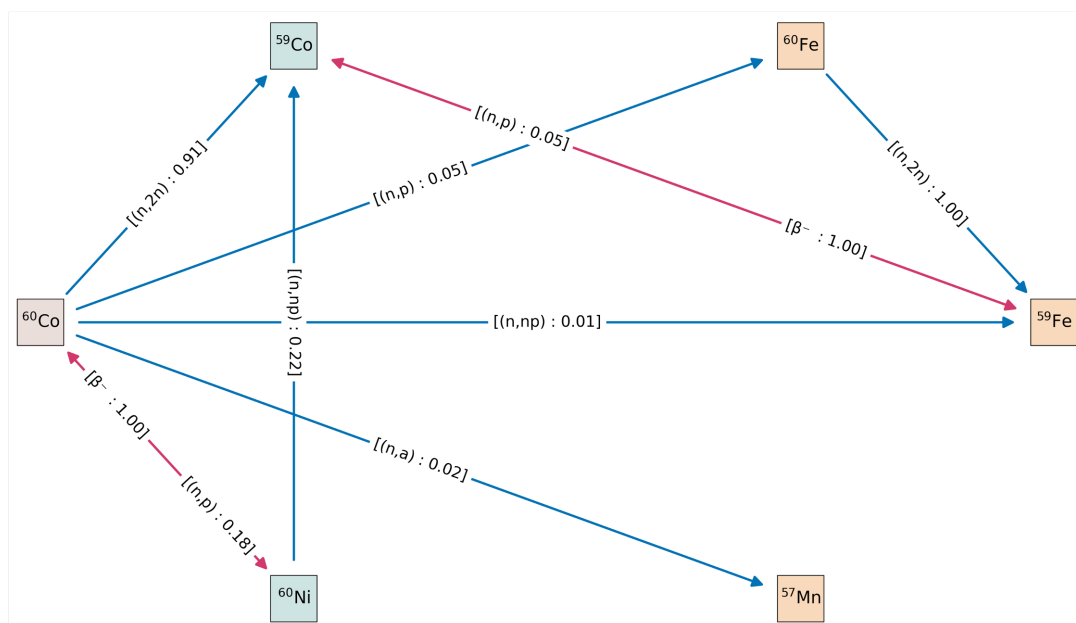


Figure 3: All the daughters of ^{60}Co with rank 1

To prune the directed graph to show only the relevant or most dominant paths, a few constraints are required. First, to create the connection matrix the collapsed cross-section is used, this is done to show only the reactions relevant for a particular neutron spectrum. Second, a cutoff is used during the creation of the connection matrix to identify and use only the dominant connections. Third, since there is no natural termination condition in case of nuclear reactions, a rank is given as an input. This rank puts a limit on the number of connections from a source/request nuclide (either as parent or daughter). The graphs shown in figures 3 and 4 were produced for 14 MeV mono-energetic neutrons with a cutoff of 1% and rank 1.

Figure 3 is a forward directed graph of ^{60}Co including the neutron induced reactions. In a combined nuclear reactions and decay graph there could exist single-step loops between two isotopes; these loops are indicated in a directed graph in pink color with double-headed arrows. In figure 3, loops can be seen between ^{60}Co and ^{60}Ni , and ^{60}Co and ^{59}Co . In case of a simple, mono-directional path (reaction), the edge labels are written in the middle of the edge. However, in case of a loop, the edge labels from a parent are written close to that parent isotope. For example, in the loop between ^{60}Co and ^{60}Ni in figure 3, the paths are $^{60}\text{Ni} - (n, p) \rightarrow ^{60}\text{Co}$ and $^{60}\text{Co} - \beta^- \rightarrow ^{60}\text{Ni}$, written as labels next to ^{60}Ni and ^{60}Co , respectively. Also, since more than one reaction can create the same daughter from a parent, the edges contain all the reactions

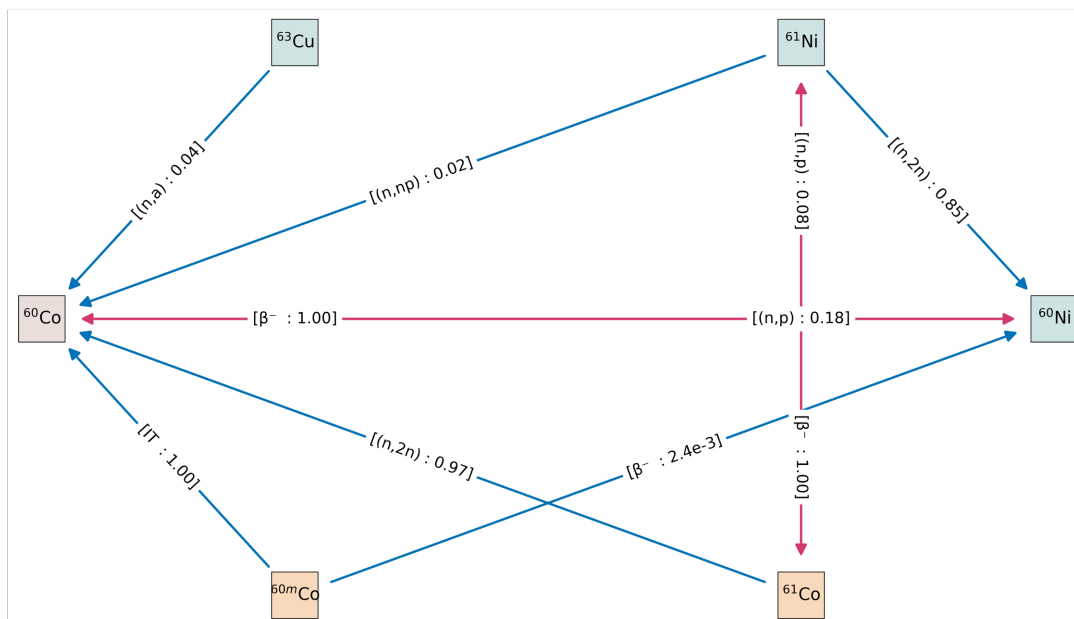


Figure 4: All the parents of ^{60}Co with rank 1

contributing to the production of the daughter with their respective probability. Figure 4 shows the backward directed graph for ^{60}Co , containing all the parents and reactions that can produce ^{60}Co .

An example of a more complex directed graph created using PATHFINDER is given in Figure 5. This forward directed graph shows all the daughters of ^{186}W with rank 2, created using the DEMO first wall neutron spectrum with cutoff of 1%.

3.3 Directed graphs between a parent and a daughter

PATHFINDER can also give the directed graphs between a given parent and daughter. These directed graphs show all the connections between the given pair. Figure 6 shows all the connection (decay and nuclear reaction) that connect ^{160}W and ^{156}Lu for 14 MeV mono-energetic neutrons and rank 2.

4 CONCLUSION AND FUTURE WORKS

PATHFINDER is a python tool that can construct forward and backward directed graphs for any isotope. It can evaluate the collapsed reaction cross-section and print the name and the probability of the nuclear reaction on the edge connecting the isotopes. It can also print the branching ratio and decay type on the edge connecting the isotopes. In conjunction with inventory simulations, the forward graph can be used to understand the creation of various hazardous isotopes in a material. Similarly, the backward graph can be used to interrogate the parents of a radioactive isotope, which may have been identified as part of an inventory solution, and hence, for example, guide the development of mitigation techniques to minimise production of hazardous isotopes. It can also be used to evaluate how different neutron spectra or nuclear data libraries can lead to production of different set of isotopes, where the former can aid understanding of different nuclear environments and differences identified in the latter can point the way towards improvements in nuclear data libraries.

PATHFINDER is in beta stage and is still under development. There are many planned

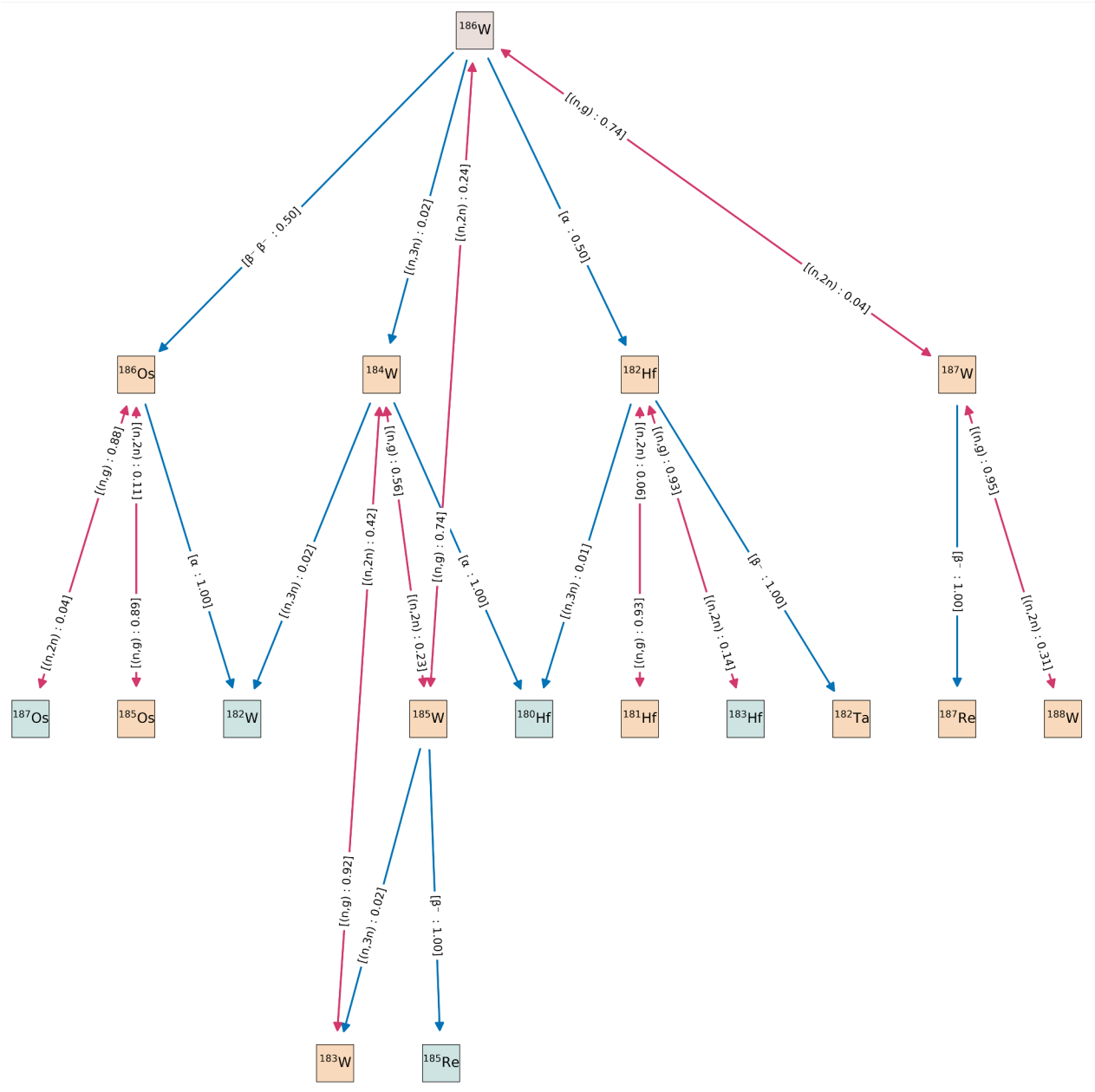


Figure 5: All daughters of ^{186}W with rank 2

future works for the tool. First is to make an interactive output. The next planned work is to include a compare function, where the users can input multiple neutron cross-section libraries in the same run and examine the differences in the resulting graphs that are calculated. Another future development is to create connection matrix for different incident projectiles like protons, photons etc.

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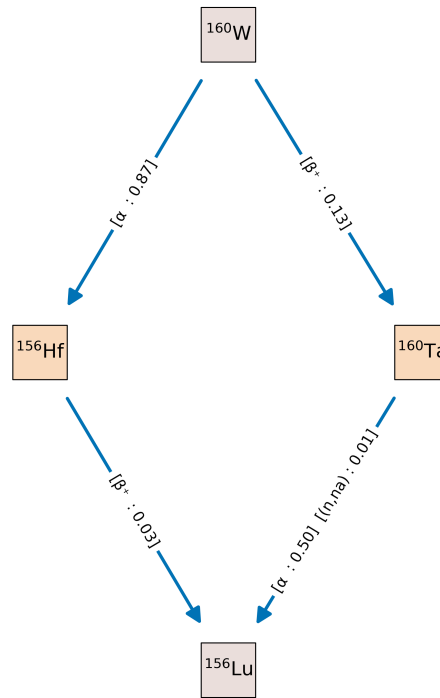


Figure 6: All paths between ^{160}W and ^{156}Lu

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