1. Mass Excesses and Binding Energies

   The Periodic chart of Elements is a useful graphical presentation of the elements of nature. The elements are identified via the number of electrons in the neutral atom. (Z) which corresponds to the element name (e.g. Hydrogen [H] has $Z = 1$, Helium [He] has $Z = 2$ and Iron [Fe] has $Z = 26$). The atoms of an element consist of Z- electrons orbiting a nucleus with charge $+Z$. The nucleus is made of protons and neutrons. Since neutrons have no charge and protons +1 charge, there are Z-protons. A single element can have more than one isotope; when the number of protons is fixed, but the number of neutrons varies from isotope to isotope. The natural abundance of the element hydrogen is dominated by the isotope ^{1}H, with smaller quantities of heavy hydrogen (or deuterium) ^{2}H. The number in this notation is the associated mass number, it is the sum of the number of protons and neutrons. The element hydrogen has 1 proton, thus ^{1}H has 0 neutrons and ^{2}H has 1 neutron. One can see that the Periodic chart of Elements is not adequate to graphically show this richness of nuclei, thus we create what is known as a chart of nuclides, a graphical representation of nuclei. The chart is organized with the number of neutrons (N) situated on the horizontal axis and the number of protons (Z) on the vertical axis. Please visit the National Nuclear Data Center's chart of nuclides to get familiar with the chart (`http://www.nndc.bnl.gov/chart/`).

   You may recall that in atomic physics, we use carbon to define a mass scale. The so-called atomic mass unit (m_u). This provides a convenient mass scale that we can use to estimate the mass of an atom.

$$M(Z,N) \approx (Z+N)m_u \tag{1}$$

   Since the mass of the atom is dominated by the nucleus (i.e. $m_u \sim M_p \sim M_n$), a better guess of the mass is simply the sum of the constituent masses; the sum of the electron, proton and neutron masses:

$$M(Z,N) \approx ZM_H + NM_n \approx Z(M_p + M_e) + NM_n \tag{2}$$

   The masses listed in the periodic table are in fact in terms of the atomic mass unit (e.g. $A(Z,N) = M(Z,N)/m_u$). One can use the values in the periodic table to define the "excess" mass in the nuclide.

$$\Delta(Z,N) \equiv M(Z,N) - (Z+N)m_u \tag{3}$$

   One can also define a nuclear binding energy, the difference between the actual mass of an atom and the total mass of the electrons, protons and neutrons in the system (assumes atomic binding is negligible).

$$B(Z,N) \equiv ZM_H + NM_n - M(Z,N) \approx Z(M_p + M_e) + NM_n - M(Z,N) \tag{4}$$

2. Nuclear Reactions and their Q-values

   Nuclear reactions involve the rearrangement of the constituent neutrons and protons to form new nuclide(s). As in any reactive process there is an energy cost or benefit, that can enhance or inhibit particular reactions (chemists usually speak in terms of an enthalpy of reaction). We can calculate the amount of energy released or required for a reaction, by comparing the total mass (i.e. energy) of the initial and final nuclides in the reaction. We will define the Q-value to be the energy released in a reaction, such that it is a positive number for an energetically favored reaction. For simplicity we will consider binary reactions (i.e. reactions between 2 nuclides).

$$reaction: \quad = \quad A + B \rightarrow C + D \tag{5}$$

$$M_A + M_B \quad = \quad M_C + M_D + Q[A(B,C)D] \tag{6}$$

   Remembering our work from the previous problem, we can substitute the relations for mass excess or binding energy here. Since the total number of neutrons and protons is unchanged in nuclear reactions (charge and mass conservation), we know that the "bulk" mass terms (i.e. $(Z+N)m_u$ and $ZM_H + NM_n$) will cancel on both sides. We are left with an equation for the Q-value that depends on only the mass excesses or only on the binding energies.

$$\Delta_A + \Delta_B = \Delta_C + \Delta_D + Q[A(B,C)D] \tag{7}$$

$$B_A + B_B = B_C + B_D - Q[A(B,C)D] \tag{8}$$

3. Weak rate Q-value calculation

Q-values can be calculated as above for any nuclear reaction. Given charge and mass conservation, we do not need to differentiate between nuclear and atomic masses. The electron mass contribution cancels, as does the overall "bulk" mass terms. All one needs is to use whatever particular mass convention consistently; all should be nuclear or all atomic masses.

(a) As an example, let us consider the first reaction in the pp-chain which powers the Sun, $p + p \rightarrow d + e^+ + \nu_e$. This reaction fuses 2 protons (p) into a deuteron (d, nucleus of Deuterium atom, or heavy Hydrogen ^{2}H), a positron (e^+ or β^+) and electron neutrino (ν_e). Substituting nuclear masses from the Particle Data Group (`http://pdg.lbl.gov/`), we find:

$$\begin{aligned} p + p &\rightarrow d + e^+ + \nu_e \\ 2M_p &= M_d + M_e + Q \\ Q &= 2M_p - M_d - M_e \\ Q &= 2(938.272) - 1875.613 - 0.511 \\ Q &= 0.42\text{MeV} \end{aligned} \tag{9}$$

Existing in a plasma, where free electrons roam, a decay emitting a positron will annihilate quite rapidly, dumping an extra $2M_e$'s worth of energy into the plasma per reaction ($e^- + e^+ \rightarrow 2\gamma$). Thus, adding to energy release from the original reaction:

$$\begin{aligned} Q_{eff} &= Q + 2M_e \\ Q_{eff} &= 0.42 + 2(0.511) \\ Q_{eff} &= 1.44 \text{ MeV} \end{aligned} \tag{10}$$

We can repeat this exercise using atomic masses instead, assuming $M_{atm} \approx M_{nuc} + ZM_e$:

$$\begin{aligned} p + p &\rightarrow d + e^+ + \nu_e \\ 2(M_H - M_e) &= (M_D - M_e) + M_e + Q \\ Q &= 2M_H - M_D - 2M_e \\ Q &= 2\Delta_H - \Delta_D - 2M_e \quad \text{substituting mass excess formula} \\ Q &= 2(7.289) - 13.138 - 2(0.511) \\ Q &= 0.42 \text{ MeV} \end{aligned} \tag{11}$$

Adding the annihilation energy, we find:

$$\begin{aligned} Q_{eff} &= Q + 2M_e \\ Q_{eff} &= 2M_H - M_D - 2M_e + 2M_e \\ Q_{eff} &= 2M_H - M_D \\ Q_{eff} &= 1.44 \text{ MeV} \end{aligned} \tag{12}$$

Note that the annihilation energy cancels the electron mass corrections, leaving only the atomic masses (or mass excesses) relevant. This is true of all β^+ decays.

(b) For a second example, let us consider a "sister" reaction to the first, $p + p + e^- \rightarrow d + \nu_e$. Otherwise known as an electron capture reaction, in this case the *pep* reaction. We find using nuclear masses:

$$\begin{aligned} p + p + e^- &\rightarrow d + \nu_e \\ 2M_p + M_e &= M_d + Q \\ Q &= 2M_p - M_d + M_e \\ Q &= 1.44 \text{ MeV} \end{aligned} \tag{13}$$

Repeating with atomic masses, assuming $M_{atm} \approx M_{nuc} + ZM_e$:

$$\begin{aligned} p + p + e^- &\rightarrow d + \nu_e \\ 2(M_H - M_e) + M_e &= (M_D - M_e) + Q \\ Q &= 2M_H - M_D \\ Q &= 1.44 \text{ MeV} \end{aligned} \tag{14}$$

Note that the electron mass drops out of the equation using atomic masses again. The electron capture reaction transmutes the same nuclides as the positron decay reaction. As long as we are in a astrophysical situation for which the positrons annihilate, the Q-values for electron capture and positron decay are identical for all nuclides.

(c) For our last example, let us consider the group of reactions in the pp-chain making ^{4}He, $4p \to {}^4\text{He} + 2e^+ + 2\nu_e$. We find:

$$\begin{aligned}
4p &\to {}^4\text{He} + 2e^+ + 2\nu_e \\
4M_p &= M_\alpha + 2M_e + Q \\
Q &= 4M_p - M_\alpha - 2M_e \\
Q &= 4(938.272) - 3727.379 - 2(0.511) \\
Q &= 3753.088 - 3727.379 - 1.022 \\
Q &= 24.687 \text{ MeV} \qquad (15)
\end{aligned}$$

Taking into account the annihilation of positrons, $2M_e$ for every positron; yielding a total of $4M_e$ for this reaction, we find:

$$\begin{aligned}
Q_{eff} &= Q + 2(2M_e) = Q + 4M_e \qquad (16) \\
Q_{eff} &= 24.687 + 4(0.511) \\
Q_{eff} &= 26.731 \text{ MeV}
\end{aligned}$$

Now we repeat using atomic masses, assuming $M_{atm} \approx M_{nuc} + ZM_e$:

$$\begin{aligned}
4p &\to {}^4\text{He} + 2e^+ + 2\nu_e \\
4(M_H - M_e) &= (M_{4He} - 2M_e) + 2M_e + Q \\
Q &= 4M_H - M_{4He} - 4M_e \\
Q &= 4\Delta_H - \Delta_{4He} - 4M_e \\
Q &= 4(7.289) - 2.425 - 4(0.511) \\
Q &= 24.687 \text{ MeV} \qquad (17)
\end{aligned}$$

Adding the annihilation energy:

$$\begin{aligned}
Q_{eff} &= Q + 4M_e \qquad (18) \\
Q_{eff} &= 4\Delta_H - \Delta_{4He} - 4M_e + 4M_e \\
Q_{eff} &= 4\Delta_H - \Delta_{4He} \\
Q_{eff} &= 26.731 \text{ MeV}
\end{aligned}$$

Again, note that the annihilation energy cancels the electron mass corrections, leaving only the atomic masses (or mass excesses) relevant.