2. Nuclear Energetics

Nuclear Units - Atomic Mass Unit and the Electron Volt

Most units used in nuclear science are based on the International System of Units or SI units (from the French "Système International d'Unités") [1]. The base SI units are the metre (length), kilogram (mass), second (time), ampere (electric current), kelvin (temperature), candela (luminous intensity), and the mole (quantity of substance). In nuclear science, in addition to SI, two units are commonly used for mass and energy i.e. the atomic mass unit and the electron volt.

Mass – The Atomic Mass Unit

Masses of atomic nuclei are generally less than 10^{-21} g. For this reason, it is more convenient to express the masses in so-called *atomic mass units* [2]. The atomic mass unit (abbreviated as amu or u) is defined such that the mass of a ¹²C atom is exactly 12 u. Hence,

 $1 u = 1.6605387 \times 10^{-27} kg$.

Energy – The Electron Volt

Energies released in chemical reactions are of the order of 10^{-19} J. For such reactions, it is more convenient to use the energy unit *electron volt*, eV. By definition, the electron volt is the kinetic energy gained by an electron after acceleration through a potential difference ΔV of one volt. This kinetic energy increase of $e\Delta V = (1.60217646 \times 10^{-19} \text{ C}) \cdot (1 \text{ V}) = 1.60217646 \times 10^{-19} \text{ J}$. Hence

 $1 \,\mathrm{eV} = 1.60217646 \times 10^{-19} \,\mathrm{J}$.

The energy equivalent of the atomic mass unit is

 $E = mc^2 = 931.494013$ MeV.

Nuclear and Atomic Masses

Tables of masses always give *atomic* rather than *nuclear* masses. This implies that the masses given include the extra-nuclear electrons. Atomic masses are more convenient than nuclear masses since it is always atomic masses or differences between atomic

masses that are measured experimentally. This distinction is reflected in the notation used in this book: rest mass of an *atom* is denoted by $M\binom{A}{Z}X$ whereas the rest mass of the *nucleus* is denoted by $m\binom{A}{Z}X$.

Notation on Masses

- rest mass of an *atom* is denoted by $M(^{A}_{7}X)$
- rest mass of the *nucleus* is denoted by $m(^{A}_{Z}X)$

According to the above notation, the electron, neutron, and proton masses are $m \begin{pmatrix} 0 \\ -1 \end{pmatrix} e$, $m \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $m \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ respectively. For convenience, however, the notation here is simplified to m_e , m_n , m_p . Since combining Z electrons with the nucleus forms a neutral atom, the atomic and nuclear masses are related by

$$M\begin{pmatrix} A\\ Z \end{pmatrix} = m\begin{pmatrix} A\\ Z \end{pmatrix} + Zm_{e} - \frac{BE_{Ze}}{c^{2}}$$

where BE_{Ze} is the energy released upon binding with the nucleus. The mass change corresponding to the electron binding energy in the above relation (BE_{Ze}/c^2) for hydrogen is approximately 10^{-8} u) is negligible compared to the mass of the atom (hydrogen mass is about 1 u) and also the electron (about 5.5×10^{-4} u), such that, to a good approximation [3]

$$M\begin{pmatrix} A\\ Z X\end{pmatrix} \cong m\begin{pmatrix} A\\ Z X\end{pmatrix} + Zm_{\rm e}.$$

Atomic and Molecular Weights

The atomic weight \mathscr{A} of an atom is the ratio of the atom's mass to 1/12th of the mass of an atom of 12 C in its ground state [3, 4]. The molecular weight of a molecule is the ratio of the molecular mass of one molecule to 1/12th of the mass of one atom of 12 C. Both the atomic and molecular weights are dimensionless. It follows that the mass of an atom measured in atomic mass units is numerically equal to the atomic weight of that atom. The atomic mass (in u) and hence the atomic weight of a nuclide is almost equal to the atomic mass number A (= Z + N) such that $\mathscr{A} \cong A$.

Most naturally occurring elements consists of two or more isotopes. The isotopic abundance a_i is defined as the relative number of atoms of a particular isotope in a mixture of the isotopes of a chemical element, expressed as a fraction of all the atoms of the element. The *elemental atomic weight* \mathscr{A} is the weighted average of the atomic weights \mathscr{A}_i of the naturally occurring isotopes of the elements, weighted by the isotopic abundance a_i of each isotope i.e.

$$\mathscr{A} = \sum_{i} \frac{a_i}{100} \mathscr{A}_i \,.$$

Atomic Weight of Magnesium

Naturally occurring magnesium consists of three stable isotopes $-{}^{24}Mg$, ${}^{25}Mg$, ${}^{26}Mg$ – with isotopic abundances 78.99, 10, and 11.01 atom-percent respectively. The atomic weights are 23.985041700 (${}^{24}Mg$), 24.98583692 (${}^{25}Mg$), and 25.982592929 (${}^{26}Mg$).

The atomic weight of magnesium \mathscr{A}_{Mg} is then:

$$\mathcal{A}_{Mg} = \frac{a_{24}\mathcal{A}_{24} + a_{25}\mathcal{A}_{25} + a_{26}\mathcal{A}_{26}}{100}$$

= (0.7899 × 23.985042) + (0.1 × 24.985837) + (0.1101 × 25.982593)
= 24.3050

Avogadro's Number

A mole of a substance is defined to contain as many "elementary particles" as there are atoms in 12 g of ¹²C and is equal to 6.0221415×10^{23} (2002 CODATA recommended value). This number is known as Avogadro's number N_a . The mass in grams of a substance that equals the dimensionless atomic or molecular weight is called the gram atomic weight or the gram molecular weight. Hence one gram atomic weight of a substance represents one mole and contains N_a atoms or molecules.

Basic Relation between Mass and Number of Atoms

Consider a substance of mass \mathcal{M} (in grams). This mass corresponds to \mathcal{M}/\mathcal{A} moles and therefore contains $(\mathcal{M}/\mathcal{A}) \cdot N_a$ atoms. Hence the basic relation between the *number of atoms* and the *mass of a substance* is given by:

$$N = \frac{\mathscr{M}}{\mathscr{A}} \cdot N_{\mathrm{a}} \, .$$

Calculations usually involve an initial mass or an activity of a parent nuclide. The first step is then to convert this mass to a number of atoms, N, before the solutions to the decay equations is evaluated, for example.

The activity, A, is defined by A = kN where k is the decay constant $\ln 2/\tau(s)$. Given an activity, the number of atoms is given by

$$N = \frac{A}{k} = A \cdot \frac{\tau(s)}{\ln 2}$$

where τ (s) is the half-life in seconds. The relationship between the mass and the activity is given by

$$A \cdot \frac{\tau(\mathbf{s})}{\ln 2} = \frac{\mathscr{M}}{\mathscr{A}} \cdot N_{\mathbf{a}}$$

from which it follows

$$A = \frac{\ln 2}{\tau(s)} \cdot \frac{\mathscr{M}}{\mathscr{A}} \cdot N_{a}$$

or
$$\mathscr{M} = A \cdot \left[\frac{\mathscr{A}}{N_{a}}\right] \cdot \frac{\tau(s)}{\ln 2}$$

Mass of an Atom and Atomic Number Density

With Avogadro's number, the mass of an individual atom can be evaluated. One mole of a substance, with mass of \mathscr{A} grams, contains N_a atoms. Hence, the mass of an individual atom is

$$M = \frac{\mathscr{A}}{N_{\rm a}} \cong \frac{A}{N_{\rm a}}$$

where the atomic weight has been approximated by the atomic mass number. That this approximation is good can be seen for the case of 208 Pb:

Approximate relation $M \cong A/N_a$

$$M(^{208}\text{Pb}) \cong \frac{208 \text{ g}}{6.022142 \times 10^{23}} = 3.4539 \times 10^{-22} \text{ g}.$$

Exact relation $M = \mathscr{A}/N_a$

$$M(^{208}\text{Pb}) = \frac{207.976652 \text{ g}}{6.022142 \times 10^{23}} = 3.4535 \times 10^{-22} \text{ g}.$$

Atomic masses are expressed in atomic mass units (u), based on the definition that the mass of a neutral atom of ¹²C is exactly 12 u. All other nuclides are assigned masses relative to ¹²C. The mass of a single atom can be computed from the fact that one mole of any substance contains 6.0221415×10^{23} atoms and has a mass equal to the atomic mass in grams. For ¹²C, 1 mole has a mass of 12 g, hence the mass of one atom is given by:

$$M(^{12}\text{C}) = \frac{12 \text{ g}}{6.0221415 \times 10^{23}} = 1.992647 \times 10^{-23} \text{ g}.$$

The atomic mass unit, u (also known as a dalton) is then

$$1 u = \frac{1.992647 \times 10^{-23} g}{12} = 1.660539 \times 10^{-24} g.$$

The energy equivalent of 1 u is $E = mc^2 = 931.494013$ MeV.

Atomic Number Density

A useful quantity in many calculations is the number density of atoms. By analogy with the basic relation between the mass and number of atoms, $N = (\mathcal{M}/\mathcal{A}) \cdot N_a$, the relation for the number density is given by

$$N(\text{atoms cm}^{-3}) = \frac{\rho}{\mathscr{A}} \cdot N_{\text{a}}$$

where ρ is the mass density (in g cm⁻³).

Relativistic Mechanics and Einstein's Mass/Energy Equivalence

The fundamental relation describing motion is that the force acting on a body will result in a change of momentum i.e.

$$\boldsymbol{F} = \frac{\mathrm{d}\,\boldsymbol{p}}{\mathrm{d}t}\,,$$

where p is the linear momentum mv and F the force. The quantities F, p, and v are all vectors. In classical mechanics, the mass of a body is constant, and the above relation reduces to F = mdv/dt = ma, the more familiar form of Newton's second law. In relativistic mechanics, the mass of a body changes with its speed v such that

$$\boldsymbol{F} = \frac{\mathrm{d}}{\mathrm{d}t}m\boldsymbol{v} = m\frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} + v\frac{\mathrm{d}m}{\mathrm{d}t}$$

From conservation of energy, the work done on a particle as it moves along a path of length *s* must equal the change in the kinetic energy ΔKE from the beginning to the end of the path. The work done by the force *F* on the particle as it moves through a displacement ds is given by $F \cdot ds$. The resulting change in the kinetic energy is then given by [3]

$$\Delta KE = \int_0^s \mathbf{F} \cdot d\mathbf{s} = \int_0^s \frac{d\mathbf{p}}{dt} \cdot d\mathbf{s} = \int_0^t \frac{dp}{dt} \cdot \frac{ds}{dt} \cdot dt = \int_0^{mv} \mathbf{v} \cdot d\mathbf{p},$$

where it is assumed that initially the particle is at rest v = 0. Using the expression for the relativistic mass

$$m = \frac{m_0}{(1 - v^2/c^2)^{1/2}}$$

and substituting in the relation for the change in kinetic energy gives

$$\Delta KE = m_0 \int_0^v v d \left[\frac{v}{(1 - v^2/c^2)^{1/2}} \right].$$

Differentiation of the term in square brackets leads to

$$\Delta KE = m_0 \int_0^v v \left[\frac{1}{(1 - v^2/c^2)^{1/2}} + \frac{v^2/c^2}{(1 - v^2/c^2)^{3/2}} \right] dv$$

= $m_0 \int_0^v \frac{v}{(1 - v^2/c^2)^{3/2}} dv = m_0 c^2 \frac{1}{(1 - v^2/c^2)^{1/2}} \Big|_0^v$
= $\frac{m_0 c^2}{(1 - v^2/c^2)^{1/2}} - m_0 c^2$

and finally,

 $\Delta KE = mc^2 - m_0 c^2 \,.$

This last expression can be rewritten in the form $mc^2 = m_0c^2 + \Delta KE$. The left hand side mc^2 can be regarded as the total energy of the particle consisting of the rest-mass energy m_0c^2 plus the kinetic energy of the particle. This expression for the total energy E, i.e. $E = mc^2$ shows the equivalence of mass and energy and one of The energy equivalent of the rest mass of an electron is

$$E = m_{\rm e}c^2 = (5.486 \times 10^{-4} \,\mathrm{u}) \times \frac{931.49 \,\mathrm{MeV}}{\mathrm{u}} = 0.511 \,\mathrm{MeV}$$

An interesting example is the direct conversion of mass to energy is the electron/positron annihilation $m_{e^-} + m_{e^+} \rightarrow 2\gamma$ in which the gamma photon each has an energy of 0.511 MeV.

The energy equivalent of 1 amu is

 $E = m_{\text{amu}}c^2 = (1 \text{ u}) \times \frac{931.49 \text{ MeV}}{\text{u}} = 931.49 \text{ MeV}.$

The energy equivalent of the rest mass of a proton is

 $E = m_{\rm p}c^2 = (1.007276\,{\rm u}) \times \frac{931.49\,{\rm MeV}}{{\rm u}} \cong 1\,{\rm GeV}\,.$

the most important expressions in nuclear physics. It will be seen later that in nuclear reactions, the mass is converted into energy and vice versa. Conversion of even small amounts of mass gives rise to considerable energies.

Binding Energy of the Nucleus

The binding energy, *BE*, of a nucleus is the energy which must be supplied to separate the nucleus into its constituent component nucleons. The sum of the masses of the constituents, m_c , of an isotope A_Z X is given by

$$m_{\rm c} = Zm_{\rm p} + (A - Z)m_{\rm n}\,,$$

where Z is the atomic number, A is the atomic mass number (number of nucleons in the nucleus), m_p is the mass of a proton atom and m_n is the mass of the neutron.

Mass Defect

The mass defect is the difference between the mass of the constituents m_c and the actual mass of the nucleus $m(^A_Z X)$, i.e.

mass defect =
$$m_c - m(^A_Z X) = Zm_p + (A - Z)m_n - m(^A_Z X) = \frac{BE}{c^2}$$

where *BE* is the binding energy of the nucleus and the mass defect is equivalent of the energy required (i.e. BE/c^2) to separate the components. It should be noted that the above expression for the mass defect involves the nuclear mass $m(^A_Z X)$. Since only atomic masses are available, the above relation should be expressed in atomic masses, i.e.

mass defect =
$$\frac{BE}{c^2} = Z \left[M(_1^1 \text{H}) - m_e + \frac{BE_{1e}}{c^2} \right] + (A - Z)m_n$$

- $\left[M(_Z^A X) - Zm_e + \frac{BE_{Ze}}{c^2} \right]$

or

Mass Defect and Binding Energy of ¹⁷/₈O

Using the atomic mass data in Appendix D, the mass defect is given by

mass defect =
$$\frac{BE}{c^2} = 8M(^1_1\text{H}) + 9m_n - M(^{17}_8\text{O})$$

= 8(1.0078250) + 9(1.0086649) - 16.9991317 = 0.1414524 u.

In energy units, the binding energy BE is given by

$$BE = mass \ defect \times \frac{931.5 \ MeV}{u} \approx 131.76 \ MeV$$
.

The average binding energy per nucleon $\langle BE \rangle = BE/A$ is then

$$\langle BE \rangle = \frac{131.76}{17} = 7.75 \,\mathrm{MeV} \,\mathrm{per} \,\mathrm{nucleon} \,.$$

mass defect =
$$\frac{BE}{c^2} = ZM(^{1}_{1}H) + (A - Z)m_n - M(^{A}_{Z}X) + \frac{1}{c^2} [ZBE_{1e} - BE_{Ze}].$$

The last term, $[ZBE_{1e} - BE_{Ze}]$, is the difference between the binding energies of Z hydrogen electrons and the Z electrons in the atom ${}^{A}_{Z}X$. It is orders of magnitude less than nuclear binding energies and hence to a very good approximation

$$BE(^{A}_{Z}\mathbf{X}) \cong \left[ZM(^{1}_{1}\mathbf{H}) + (A-Z)m_{n} - M(^{A}_{Z}\mathbf{X}) \right] c^{2}.$$

A plot of the binding energy per nucleon versus the atomic mass number shows a broad maximum in excess of 8 MeV per nucleon between mass numbers 50–100. The two dimensional plot is shown in Fig. 2.1. At lower and higher mass numbers,



Fig. 2.1. Average binding energy per nucleon versus mass number for stable nuclides

the binding energy per nucleon is less. It is for this reason that energy can be released by splitting heavy elements or by fusing light elements.

Notable departures from the smooth behaviour of the binding energy per nucleon vs. the mass number are provided by ⁴He, ¹²C, ¹⁶O. The binding energies per nucleon of these isotopes are higher than their immediate neighbours indicating that they are very strongly bound. These nuclei contain respectively one, three, and four sub-units of ⁴He. This tends to suggest that nucleons form stable sub-groups of two protons and two neutrons within the nucleus.

Mass Excess

The atomic masses are often described in terms of the mass excess ME defined by

 $ME(^{A}_{Z}X) = M(^{A}_{Z}X) - A,$

where the masses are expressed in atomic mass units (u). Hence, knowing the mass excess, the mass of any nuclide can be derived. Consider the example of 238 U. In the Nuclides.net database [5], the mass excess is given in units of keV, i.e. $ME(^{238}\text{U}) = 47308.9 \text{ keV}$. In a first step, this must be converted to atomic mass units using 1 u = 931.494013 MeV/ c^2 (see Appendix A), hence

 $ME(^{238}\mathrm{U}) = 0.0507882\,\mathrm{u}\,.$

The mass of ²³⁸U is then given by

$$M(^{238}\text{U}) = ME(^{A}_{7}\text{X}) + A = 0.0507882 \text{ u} + 238 \text{ u} = 238.0507882 \text{ u}$$

Nucleon Separation Energy

Another useful quantity, in addition to the binding energy, is the nucleon separation energy. Whereas the binding energy is the energy required to separate the nucleus into its constituent component nucleons, the nucleon separation is the energy required to remove a single nucleon from the nucleus according to the reaction i.e. (for a neutron removal):

 ${}^{A}_{Z}X \rightarrow {}^{A-1}_{Z}X + n$.

The energy required to remove this neutron, denoted $S_n(^A_Z X)$, is given by:

$$S_{n}({}^{A}_{Z}X) = \left[m({}^{A-1}_{Z}X) + m_{n} - m({}^{A}_{Z}X)\right]c^{2}$$

or

$$S_{\mathbf{n}}({}^{A}_{Z}\mathbf{X}) \cong \left[M({}^{A-1}_{Z}\mathbf{X}) + m_{\mathbf{n}} - M({}^{A}_{Z}\mathbf{X})\right]c^{2}.$$

Using the relation derived earlier for the binding energy i.e.

 $BE(^{A}_{Z}\mathbf{X}) \cong \left[ZM(^{1}_{1}\mathbf{H}) + (A - Z)m_{n} - M(^{A}_{Z}\mathbf{X}) \right] c^{2},$

the neutron separation energy can also be expressed as

$$S_{n}({}^{A}_{Z}X) = \left[BE({}^{A}_{Z}X) - BE({}^{A-1}_{Z}X)\right]c^{2}.$$

Similarly, the energy required to remove a single proton from the nucleus according to the reaction

$${}^{A}_{Z}X \rightarrow {}^{A-1}_{Z-1}Y + p$$
.

The energy required to remove this proton, denoted $S_p(^A_Z X)$, is given by:

$$S_{\rm p}(^{\rm A}_{Z}{\rm X}) = \left[m(^{\rm A-1}_{Z-1}{\rm Y}) + m_{\rm p} - m(^{\rm A}_{Z}{\rm X})\right]c^{2}$$

or

$$S_{\rm p}({}^{A}_{Z}{\rm X}) \cong \left[M({}^{A-1}_{Z-1}{\rm Y}) + M({}^{1}_{1}{\rm H}) - M({}^{A}_{Z}{\rm X}) \right] c^{2}.$$

Again using the relation for the binding energy, this can also be expressed as

$$S_{\mathrm{p}}({}^{A}_{Z}\mathrm{X}) = \left[BE({}^{A}_{Z}\mathrm{X}) - BE({}^{A-1}_{Z-1}\mathrm{Y})\right]c^{2}.$$

Table 2.1. Comparison of the binding energy per nucleon (BE/A) with the neutron and proton separation energies for selected nuclides

Nuclide	BE/A (MeV)	S _n (MeV)	S _p (MeV)
¹⁶ ₈ O	7.98	15.66	12.13
¹²⁹ ₅₃ I	8.44	8.83	6.80
⁹⁹ ₄₃ Tc	8.61	8.97	6.50



Fig. 2.2. The neutron separation energy as a function of the mass number

Some values of S_n and S_p are given in Table 2.1 and Fig. 2.2. The fact that the neutron and proton separation energies in ${}^{16}_{8}$ O are considerably higher than the average binding energy per nucleon, implies that this nuclide is particularly stable.

Q-Value for a Reaction

In a nuclear reaction, from conservation of energy, the total energy including the rest-mass energy must be the same before and after the reaction i.e.

$$\left(\sum_{i} \left[E_{i} + m_{i}c^{2}\right]\right)_{\text{before}} = \left(\sum_{i} \left[E_{i} + m_{i}c^{2}\right]\right)_{\text{after}}$$

where E_i and m_i are the kinetic energy and rest mass of particle respectively. Any change in the total kinetic energy before and after the reaction must be accompanied by an equivalent change in the total rest mass. Following [3], the *Q*-value of a reaction is defined the change in kinetic energy or rest mass in a reaction i.e.

$$Q = (kinetic \ energy)_{after} - (kinetic \ energy)_{before}$$

or
$$Q = (rest \ mass)_{after} \cdot c^2 - (rest \ mass)_{before} \cdot c^2.$$

If the kinetic energy of the products is greater than that of the reactants, the reaction is exothermic and Q is positive. If energy is required to induce a reaction, the reaction is endothermic and Q is negative. In such endothermic reactions a minimum kinetic energy of reactants is required for the reaction to proceed.

In a binary nuclear reaction $a + X \rightarrow Y + b$, the Q-value is given by

$$Q = (E_{\rm Y} + E_{\rm b}) - (E_{\rm a} + E_{\rm X}) = \left[(m_{\rm a} + m_{\rm X}) - (m_{\rm Y} + m_{\rm b}) \right] c^2$$

In most binary reactions, the number of protons is conserved and the same number of electron masses can be added to both sides of the above reactions. Neglecting the differences in electron binding energies, the *Q*-value can be expressed in terms of

Q-Value for fusion [3]:

Consider the fusion reaction in which two protons fuse to form a deuteron i.e.

 $p+p \rightarrow d+\beta^++\nu\,.$

In this reaction, the number of protons is not conserved and care is required in the evaluation of the Q-value. To obtain the Q-value in terms of the atomic masses, add two electrons to both sides of the reaction i.e.

$${}^{1}_{1}H + {}^{1}_{1}H \rightarrow {}^{2}_{1}H + \beta^{+} + \beta^{-} + \nu$$

The *Q*-value is then obtained from:

$$Q = \left[2M(_1^1 \text{H}) - M(_1^2 \text{H}) - 2m_e - m_v\right]c^2$$

= (2 × 1.007825032 - 2.014101778 - 2 × 0.00054858) × $\frac{931.5 \text{ MeV}}{\text{u}}$
= 0.422 MeV,

where the rest mass of the neutrino has been assumed to be zero.

atomic masses i.e.

$$Q = (E_{\rm Y} + E_{\rm b}) - (E_{\rm a} + E_{\rm X}) = \left[(M_{\rm a} + M_{\rm X}) - (M_{\rm Y} + M_{\rm b}) \right] c^2.$$

In radioactive decay reactions (see Decay Energy) a parent nuclide decays to a daughter with the emission of a particle, i.e. $P \rightarrow D + d$.

The *Q*-value is given by $Q = (E_D + E_d)$ since the parent nuclide is at rest, hence $Q = (E_D + E_d) = [m_P - m_D - m_d]c^2 > 0$.

$$Q = (E_D + E_d) = [m_P - m_D - m_d]c^2 > 0.$$

It should be noted that in some types of radioactive decay, such as beta decay and electron capture, the number of protons is not conserved. In such cases the evaluation of the Q-value using atomic masses may be inaccurate. For more information on the calculation of Q-values using atomic masses, the reader is referred to [3].

Threshold Energy for a Nuclear Reaction

The actual amount of energy required to bring about a nuclear reaction is slightly greater than the Q-value. This is due to the fact that not only energy but also momentum must be conserved in any nuclear reaction. From conservation of momentum, a fraction $m_a/(m_a + M_X)$ of the kinetic energy of the incident particle a must be retained by the products. This implies that only a fraction $M_X/(m_a + M_X)$ of the incident particle is available for the reaction. It follows that the threshold energy is higher than the Q-value and is given by

$$E_{\rm th} = -\frac{Q(m_{\rm a}+M_{\rm X})}{M_{\rm X}}\,.$$

Energy Level Diagrams

Nuclear data can be displayed in the form of nuclear energy level diagrams. These diagrams are essentially a plot of the nuclear energy level versus the atomic number and are very useful for showing the nuclear transition corresponding to decay modes. From the basic decay data, energy level diagrams can be constructed according to the following procedure:

- The ground state of the daughter nucleus is chosen to have zero energy.
- If there is an increase in the atomic number (as in β^- decay), the daughter is shown to the right of the parent. The following is an example of the energy level diagram for the decay of ${}^{32}_{15}P$:



Fig. 2.3. Energy level diagram for the decay of ${}^{32}_{15}P$

• If the radioactive decay results in a decrease of the atomic number (e.g. alpha emission, positron emission, or electron capture) the daughter is shown to the left of the parent. The following is an example of the energy level diagram for the decay of ${}_{9}^{18}$ F. Since the decay energy is greater than $2m_ec^2(1.022 \text{ MeV})$ positron emission (β^+) competes with electron capture (ec) to the ground state.



Fig. 2.4. Energy level diagram for the decay of ${}^{18}_{9}$ F

In addition to showing the decay modes and energies, these diagrams can also be used to show half-lives, branching ratios, nuclear isomerism, etc. as in the above examples.

Nuclear Spin and Parity

Protons and neutrons have half integral spin i.e. $+\frac{1}{2}$ or $-\frac{1}{2}$. Spin, which can be loosely associated with the picture of a particle spinning, is inherently quantum mechanical in nature and related to the intrinsic angular momentum associated with the subatomic particle. Spin is a vector quantity, with a total spin and a component of spin in a specified direction. The total spin has a spin quantum number (symbol *s*) with value equal to an integer for a boson, and a half-integer for a fermion and the word 'spin' is often used to mean this quantum number.

The overall spin of an atomic nucleus is by virtue of the spin of each nucleon within it. The hydrogen nucleus, for example, contains one proton with a spin quan-

Number of protons	Number of neutrons	Spin quantum number	Examples
Even	Even	0	¹² C, ¹⁶ O, ³² S
Odd	Even	1/2	¹ H, ¹⁹ F, ³¹ P
"	"	3/2	¹¹ B, ³⁵ Cl, ⁷⁹ Br
Even	Odd	1/2	¹³ C
"	"	3/2	¹²⁷ I
"	"	5/2	¹⁷ O
Odd	Odd	1	² H, ¹⁴ N

Table 2.2. Spin quantum number for various nuclei

tum number of $\frac{1}{2}$, and this gives rise to a spin of $\frac{1}{2}$ for a hydrogen atom. The spin produces a magnetic moment, and this forms the basis of the technique of nuclear magnetic resonance.

Within a nucleus, nucleons (protons and neutrons) have a strong tendency to pair i.e. neutron with neutron or proton with proton so that their spins cancel (spins pair anti-parallel). Hence for all even-*Z* even-*N* nuclei such as ${}^{12}C$, ${}^{16}O$, ${}^{32}S$, the ground state spin is always zero as shown in Table 2.2.

Nuclei with an odd number of protons, neutrons, or both, will have an intrinsic nuclear spin. Although there is the tendency for nucleons to pair up spins anti-parallel to become spin-0, the total spin is not necessarily the lowest value after pairing off – some nucleons remain unpaired and result in spins as high as $\frac{11}{2}$.

The parity of a nucleus is the sign of the spin and is either odd (-) or even (+). Parity is important due to the fact that it is conserved in nuclear processes (in the case of weak interactions, however, such as in beta decay, parity conservation is weakly broken).

Nuclear Isomerism

Nuclei usually exist in their ground state with the individual nucleons paired up subject to energy constraints. In some nuclides, for example resulting from radioactive decay, one or more nucleons can be excited into one or more higher spin states. These nuclei can revert back to the ground state by the emission of gamma radiation. If this emission is delayed by more than 1 μ s, the nucleus is said to be a nuclear isomer and the process of releasing energy is known as isomeric transition.

There are two very different ways that such nuclei can possess spin. Either the nucleus rotates as a whole, or several nucleons can orbit the nucleus independently in a non-collective rotation. The latter case can result in the nucleons being trapped in high spin states such that they have much higher lifetimes. Nuclides with even-Z and even-N (i.e. with a whole number of ⁴He nuclei) can also have high excess rotational spin due to alpha particles rotating independently around the nucleus. Examples here are ¹²C, ¹⁶O, ²⁰Ne, and ²⁴Mg.

^{212m}Po is an example where the isomer has a much longer half-life than the ground state. With a spin of 18, the half-life of 45 s is very much longer than the ground state half-life of 300 ns. The isomer can be considered as two neutrons and two protons orbiting around the doubly magic ²⁰⁸Pb nucleus. The high spin state decays by alpha emission which carries off the 18 units of spin.

Other examples are 178n Hf (spin 16 due to 4 of the 78 nucleons orbiting the nucleus), 178 W (spin 25 due to 8 unpaired nucleons orbiting the nucleus).

Nuclide Charts

The origin of the nuclide chart is somewhat uncertain. In his autobiography [6], Segrè mentions the "Segrè Chart" compiled with the help of his wife at Los Alamos in 1945. After the war it was declassified and published, selling more than 50,000 copies. Segrè also mentions that the "first modest table of isotopes was published by a student in our Rome group in the 1930s", see G. Fea [7]. One of the earliest



Fig. 2.5. Nuclide stability diagram. Stable nuclides (*black*) fall in a narrow range of neutron to proton ratio. Unstable nuclides (*white*) have neutron to proton ratios outside this range. Also shown are the proton and neutron magic numbers represented by the horizontal and vertical lines

nuclides charts was complied by G. Friedlander and M. Perlman and published by the General Electric Company in 1946. In contrast to the earlier charts by Fea and Segrè, this chart had the proton number as the vertical axis and the neutron number as the horizontal axis. The current version of this chart is the 16th edition [8].

Nuclide charts are based upon the proton-neutron model of the nucleus and are essentially a plot of the number of protons versus the number of neutrons in stable and unstable nuclei. In these charts, the vertical and horizontal axes represent the number of protons and neutrons respectively in the nucleus as shown in Fig. 2.5.

The charts contain information on the basic nuclear properties of known nuclides. Each nuclide is represented by a box containing basic nuclear data. This data consists of the half-life, neutron cross-sections, main gamma lines etc. of that nuclide. An important characteristic of the charts is the use of colour to denote the mode of decay, half-life, or cross-sections. If the nuclide has one or more metastable states, the box is subdivided into smaller boxes for each state. The main nuclide charts in use world-wide are the Karlsruhe (Germany) [9], Strasbourg (France) [10], General Electric or KAPL (US) [8], and the JAERI (Japan) [11] charts.

It can be seen that stable isotopes lie within a relatively narrow range indicating that the neutron to proton ratio must have a certain value or range of values to be stable. Radioactive nuclei (white squares in Fig. 2.5) mostly lie outside this range. The plot also shows that for low atomic numbers, the neutron to proton ratio is unity.

At higher atomic numbers, this value increases indicating a higher ratio of neutrons to protons in heavy atoms.

The extremities of the white regions above and below the region of stability are known as the proton and neutron "drip-lines" beyond which nuclei are extremely unstable (i.e. if a nucleon is added it will "drip" out again). As nucleons are successively added to a nucleus on the stability line, the binding energy of the last nucleon decreases steadily until it is no longer bound and the nucleus decays by either neutron or proton emission.

Nuclei with even numbers of protons and neutrons are more stable than nuclei with other combinations of neutrons and protons. For uneven numbers of protons and neutrons, there are only very few stable nuclides. The stability of nuclei is extremely significant for special numbers of protons and neutrons. These (magic) numbers are 2, 8, 20, 28, 50, 82 and 126 and correspond to full shells in the shell model of the nucleus. The element tin with the proton number Z = 50, for example, has 10 stable isotopes, more than all other elements.

When the proton and neutron numbers both have magic values, the nucleus is said to be "doubly magic". Doubly magic, stable nuclides are for example ⁴He, the alpha particle, as well as the nuclide ²⁰⁸Pb, which is reached in several decay processes, for example in the decay chain of ²³²Th.

In addition to providing the most important basic nuclear data, the charts allow one to trace out radioactive decay processes and neutron reaction paths. This feature is described in more detail in the following section.

The Karlsruhe Nuclide Chart [9] is described in detail at the end of this chapter. The Strasbourg Nuclide Chart [10] was developed by Dr. Mariasusai Antony from the Louis Pasteur University of Strasbourg. Approximately 5000 copies of the 1992 version were sold in more than 40 countries. This original version contained data on approximately 2550 ground states and 571 isomers. An updated version was published in 2002. The new chart displays about 2900 isotopes in the ground states and about 700 isomers. The chart is a booklet of 44 A4 formatted pages. The front cover page exhibits a stork, symbol of the region of Alsace for which Strasbourg is the capital. The colours blue, white and red (actually reddish-brown) were chosen to indicate the tri-colours of France.

Continuing a half-century tradition, Knolls Atomic Power Laboratory (KAPL) has recently published the 16th edition (2003) of its Chart of the Nuclides in both wallchart and textbook versions [8]. The first edition was published by the General Electric Company in 1946. Evaluated nuclear data is given for about 3100 known nuclides and 580 known isomers. For each nuclide the half-life, atomic mass, decay modes, relative abundances, nuclear cross-section, and other nuclear properties are detailed. The updated chart includes approximately 300 new nuclides and 100 new isomers not found in the 15th (1996) edition. There has been at least one change in more than 95% of the squares on the chart.

The first edition of the JAERI nuclide chart was published in February 1977. Since then the chart has been revised every 4 years, i.e. 1980, 1984, 1988, 1992, 1996, with the most recent edition appearing in 2000 [11]. In total, seven editions have been published. Approximately 2000 copies of each edition were printed, most



Revised 6th edition of the "Karslruher Nuklidkarte"

Strasbourg nuclide chart



KAPL nuclide chart

Japanese (JAERI) nuclide chart

Fig. 2.6. Main paper-based nuclide charts

of which are distributed to the Japanese nuclear data community and international organisations. The chart comes as an A4-sized booklet.

Decay and Reaction Processes

A small section of a nuclide chart is shown in Fig. 2.7. The central box, with coordinates Z, N represents a nuclide with Z protons and N neutrons. When this "parent" nuclide decays, it results in a "daughter" nuclide with co-ordinates Z', N' depending on the decay process. In Fig. 2.7, the position of the daughter nuclide is shown following decay by α , β^- , ε/β^+ , n, and p decay processes. These decay processes are explained in detail in Chap. 4. With this information, the radioactive decay chain can be traced out. Starting with a parent nuclide, the position of the daughter can be found from the decay mode (given in the parent box) and the information given in Fig. 2.7. If the daughter is radioactive, it then becomes the parent for the next decay process etc. In this way the full decay chain may be traced out starting from a parent nuclide.

Similarly the nuclide chart may be used to trace out activation and nuclear reactions. In Fig. 2.8, a small section of the chart is shown with the nuclide Z, N at its centre.

A target nuclide of element X, with Z protons and N neutrons will transform through reaction with a particle a to an element Y, with Z' protons and N' neutrons, through the emission of a particle b.

The reaction can be written:

 $a + {}^{Z+N}X \rightarrow {}^{Z'+N'}Y + b$,

or more compactly in the form



Fig. 2.7 (*left*). Nuclear decay processes on the nuclide chart. A nuclide with "co-ordinates" Z, N transforms to the nuclide Z', N' through the decay processes shown

Fig. 2.8 (*right*). Activation processes and nuclear reactions on the nuclide chart. A target nuclide with co-ordinates Z, N transforms to the nuclide Z', N' through the processes shown

 $^{Z+N}$ X(a, b) $^{Z'+N'}$ Y.

The result of interaction of a variety of particles a (neutrons, alpha particles, deuterons, gamma radiation, protons etc.) with a target nuclide with co-ordinates Z, N is shown in Fig. 2.8.

Electronic Nuclide Charts

There are a variety of "electronic" nuclide charts available on the internet. Each of these resources has its own particular tool for navigating the nuclide chart efficiently and displaying the data once a particlur nuclide has been selected. These internet resources are restriced, however, to only displaying nuclear data. The main ones are shown below.



Fig. 2.9 *Table of Nuclides* Korea Atomic Energy Research Institute KAERI http://atom.kaeri.re.kr/



Fig. 2.10 *Table of the Nuclides* Japanese Atomic Energy Research Institute (JAERI) http://sutekh.nd.rl.ac.uk/ CoN/

Each horizontal row represents one element; the coloured dots indicate the known isotopes of that element. A vertical column represents the nuclides with same neutron numbers. Heavy lines on the Chart occur for Z and N equal to 2, 8, 20, 28, 50, 82, and 126. These are the so-called "magic numbers"



Fig. 2.11 WWW Chart of the Nuclides Japan Atomic Energy Research Institute (JAERI) http://wwwndc.tokai. jaeri.go.jp/CN00/

The latest version of "Chart of the Nuclides 2000" was made by T. Horiguchi, T. Tachibana, H. Koura and J. Katakura, and published by the Japanese Nuclear Data Committee (JNDC) and the JAERI Nuclear Data Center.

"WWW Chart of the Nuclides" here is based on the most recent compilation of experimental data by T. Horiguchi (Hiroshima International University) (2000)



Fig. 2.12 *The Lund/LBNL Nuclear Data Search* http://nucleardata. nuclear.lu.se/ Database/toi/

The handbook "Table of Isotopes" has for many years been the most widely used source of information for nuclear structure and decay data. This service is intended to give convenient Web access to the Table of Isotopes data. At present only part of the decay data is implemented, but the service will eventually include search facilities, table generators, charts and drawings of all nuclear structure and decay data in the ToI book



Fig. 2.13. IAEA's Nuclear Data Centre, http://www-nds.iaea.or.at/

Nuclides.net [5]

The Institute for Transuranium Elements, http://www.nuclides.net/

The main user interface, Nuclide Explorer, provides access to nuclide information (data on approximately 3650 ground states and isomers, from internationally recognised sources) through nuclide charts. In addition to displaying nuclear data, various applications/calculations can be launched.

There are six main applications:

- Decay Engine a software module for decay calculations.
- Dosimetry and Shielding a module that allows the calculation of dose rates from both unshielded and shielded point sources. A choice of 10 shield materials is available.
- Virtual Nuclides allow the user to do decay and dosimetry and shielding calculations on mixtures of nuclides.
- Fission Yield the module gives the user access to fission products and yields for 36 fissioning nuclides (data for spontaneous fission and neutron induced fission with thermal, fast, and 14 MeV neutrons) from the main international data-files.
- Cross-Sections give averaged neutron cross sections from the main international datafiles. Data include the cross sections for room temperature, Maxwell averaged, resonance integral, fission averaged, and 14 MeV neutrons.
- The Universal Nuclide Chart shows the most important basic data. It can also be used to simulate decay processes and reaction paths in nuclear reactors.



Fig. 2.14. Nuclides.net: The Nuclide Explorer



Fig. 2.15. Nuclides.net: Universal Nuclide Chart

A Short History of the Karlsruhe Nuclide Chart

The *Karlsruhe Chart of the Nuclides* was initiated by Professor Walter Seelmann-Eggebert from the Technische Hochschule (TH) Karlsruhe to display basic nuclear data (half-lives, decay modes, particle energies, and most probable gamma energies) [9, 12]. The Karlsruhe chart of the nuclides was based on an earlier chart by G. Friedlander and M. L. Pearlman in the *General Electric Chart of the Nuclides* [13].

1st Edition, 1958: The first edition appeared as a wall chart in DIN A0 format. Coloured boxes were used to indicate the decay modes (black = stable nuclide, red = β^+ decay or electron capture, blue = β^- decay, yellow = alpha decay, white = isomeric transition). In addition a DIN A4 version was available as a collection of sheets with an explanatory brochure for desktop use. It was prepared by W. Seelmann-Eggebert and G. Pfennig both from the Institute of Radiochemistry in the Karlsruhe Research Centre and the TH Karlsruhe. The data used in the chart was from the Nuclear Data Sheets of the National Research Council and the Table of Isotopes by D. Strominger, J. M. Hollander, G.T. Seaborg. The original chart contained data on 267 stable and 1030 unstable nuclides and more than 220 isomeric states from the, at that time, 102 known elements from hydrogen to nobelium.

2nd Edition, 1961: Following on the interest shown in the first edition, a second edition was published in 1961 with additional authors H. Münzel and G. Zundel – also from the Institute of Radiochemistry. A new feature was the introduction of coloured



Fig. 2.16. Original Karlsruhe Chart of the Nuclides from 1958



Fig. 2.17. *Left:* Prof. W. Seelmann-Eggebert with the original 1st edition (1958) of the Karlsruhe Chart of the Nuclides. *Right:* The co-authors H. Klewe-Nebenius (*left*), G. Pfennig (*centre*), H. Münzel (*right*) with the revised 6th edition (1998/2001).

corners of different size to indicate the branching ratio of the decay mode. The second edition contained information on 103 elements, and data on approximately 70 new unstable nuclides.

3rd Edition, 1968: Due to the increasing use of the Karlsruhe chart of the nuclides worldwide, a third edition was produced in 1968 with explanatory text in four languages – German, English, French and Spanish. The colour green was introduced to indicate spontaneous fission, and atomic masses were based on 12 C. Instead of single DIN A4 sheets, the desktop version was printed in a special arrangement in a strip folded to DIN A4 format. The third edition contained information on 105 elements and more than 1600 nuclides – an increase of 250 over the 2nd edition.

4th Edition, 1974: Much of the data in the 3rd edition had to be revised to reflect the higher accuracy data obtained from the use of Ge detectors. Owing to the improved experimental technique, new data had become available for many short-lived fission products. The 4th edition contained data on more than 1900 nuclides.

5th Edition, 1981: The fifth edition was authored by W. Seelmann-Eggebert, G. Pfennig, H. Münzel, and H. Klewe-Nebenius. New decay modes of double beta decay $(2\beta^{-})$ and proton decay (p, colour orange) were introduced. To discriminate between direct and β -delayed particle emission, new notations for the latter ($\beta p, \beta n, \beta 2n, \beta sf$, etc.) were introduced. The 5th edition contained data on more than 2220 nuclides.

6th Edition, 1995: The sixth edition was published in 1995 – more than a decade after the 5th edition – by G. Pfennig and H. Klewe-Nebenius and dedicated to Professor W. Seelmann-Eggebert who died in 1988. In the meantime, four new heavy elements (108–111) had been discovered at the Gesellschaft für Schwerionenforschung (GSI) at Darmstadt. New decay modes of cluster emission e. g. C-14, O-20, Ne-24 etc. indicated by the colour violet) were added. The 6th edition contained data on approximately 2690 nuclides from 111 elements.

Revised 6th Edition, 1998/2001: the sixth edition was revised in 1998 to include data on the newly discovered element 112, new names for elements 104–108, new decay data for some transuranics and 150 mostly short-lived nuclides far from the line of stability.

Since the introduction of the Karlsruhe Chart of Nuclides, over 150,000 copies of the wall chart and 203,000 copies of the brochure with the folded chart have been printed. For the sixth edition more than 15,000 wall charts and 45,000 brochures were printed.