Introduction to Reactor Physics

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By

Osvaldo Moreira
and María Laura Moreira

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Für meinen kleinen Sohn, Tatá genannt ...

An einem Tag im Winter, 2018.-

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The Atom

"Daher ist die Aufgabe nicht sowohl zu sehen, was noch Keiner gesehen hat, als, bei Dem, was jeder sieht, zu denken, was noch Keiner gedacht hat"

Arthur Schopenhauer

1.1 Chemical elements and sub-atomic particles

All the components of the universe are made up of various substances, the fundamental parts of which are called *molecules*. Molecules are the smallest part of substances that retain the same chemical properties as the substance they constitute. All existing molecules in the universe are made up of a relatively small number of fundamental components called *elements*. Many of these elements were already known in antiquity, such as iron, although at that time the concepts of element and substance were ignored and the elements (gold, silver, copper) were confused with alloys, mixtures and with the product of chemical reactions (such as fire).

From the 8th century onwards, alchemists managed to advance in the knowledge of materials by discovering new elements, substances and compounds, but without a scientific basis. In the 17th century, with the development of chemistry, the properties of the substances discovered by the alchemists were studied, but now applying the scientific method. In this stage of chemistry the concepts of substance, mixture, chemical reactions, etc. began to be understood.

Many years later, with chemistry already established as a science, a much clearer idea of the structure of substances (molecules and atoms) was developed. On March 6th, 1869 the Russian chemist Mendeleev[1] in his work "Principles of Chemistry" published the periodic system of the elements, under the title "The dependence of the chemical properties of the elements on the atomic weight"[2]. In this work, the 63 elements known up to that time were arranged in increasing order according to their atomic weight in seven groups with similar chemical properties. In 1871 Mendeleev was able to determine the properties of the previously undiscovered elements gallium, scandium and germanium. A few years later his thesis was confirmed: the element germanium was discovered in 1871, gallium in 1875 and scandium in 1879. Figure 1.1 shows the periodic table of the elements of the IUPAC (International Union of Pure and Applied Chemistry).

[1]Dmítriy Ivánovich Mendeléyev (*Tobolsk, Russia, 27.Jan.1834 - †Saint Petersburg, Russia, 20.Jan.1907) was a Russian chemist, famous for having discovered the underlying pattern in what is now known as the periodic table of the elements.

[2]Mendeleev D. "Sootnoshenie svoistv s atomnym vesom elementov" (*The Correlation of the Properties and Atomic Weights of the Elements*). *Zh. Russ. Khim. Obshch.*, **1**, No. 2/3, 60-77 (1869).

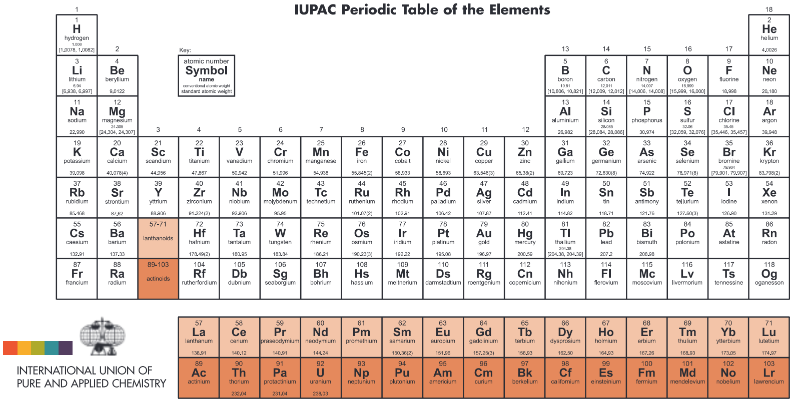

Figure 1.1: Periodic table of the elements of the IUPAC, November 28, 2016.

The smallest part of the elements that retains its chemical characteristics is called *atom*. Thus, the smallest particle of the elements oxygen, carbon or uranium is called oxygen atom, carbon atom or uranium atom, respectively. Molecules are arrangements (combinations) of atoms: the water molecule is an arrangement of 3 atoms, two atoms of the element hydrogen and one of the element oxygen: H_2O.

At present, 118 elements are known, arranged according to their *atomic number* (noted Z), which are listed in Table 1.1. Elements from atomic number 95 (americium) and above do not occur naturally on Earth, but are produced artificially. The elements technetium ($Z = 43$), promethium ($Z = 61$), astatine ($Z = 85$), neptunium ($Z = 93$) and plutonium ($Z = 94$) (initially produced artificially, they had not been found on Earth) are found in trace form in uranium or thorium ores. The reason why there are only traces of the above elements is because they are decay products of the radioactive elements that make up these minerals. The most abundant elements in the Earth's crust are oxygen (49.2% w/w), silicon (25.7% w/w) and aluminium (7.5% w/w). The human being is made up of 65% by weight of oxygen, 18% by weight of carbon and 10% by weight of hydrogen.

The dimensions of an atom[3] are about 10^{-7} mm (0.1 nm). With special (non-optical) microscopes it is possible to obtain images representing atoms. Figure 1.2 shows an arrangement of dark dots representing the atoms that make up a molecule (an organic molecule, in this case copper chlorophthalocyanine), composed of 57 atoms: $CuN_8Cl_{16}C_{32}$.

Table 1.1: List of the chemical elements, ordered by atomic number Z (number of protons).

Element	Symbol	Z	Element	Symbol	Z	Element	Symbol	Z
Hydrogen	H	1	Niobium	Nb	41	Thallium	Tl	81
Helium	He	2	Molybdenum	Mo	42	Lead	Pb	82
Lithium	Li	3	Technetium	Tc	43	Bismuth	Bi	83
Beryllium	Be	4	Ruthenium	Ru	44	Polonium	Po	84
Boron	B	5	Rhodium	Rh	45	Astatine	At	85
Carbon	C	6	Palladium	Pd	46	Radon	Rn	86
Nitrogen	N	7	Silver	Ag	47	Francium	Fr	87
Oxygen	O	8	Cadmium	Cd	48	Radium	Ra	88
Fluorine	F	9	Indium	In	49	Actinium	Ac	89
Neon	Ne	10	Tin	Sn	50	Thorium	Th	90
Sodium	Na	11	Antimony	Sb	51	Protactinium	Pa	91
Magnesium	Mg	12	Tellurium	Te	52	Uranium	U	92
Aluminium	Al	13	Iodine	I	53	Neptunium	Np	93
Silicon	Si	14	Xenon	Xe	54	Plutonium	Pu	94
Phosphorus	P	15	Caesium	Cs	55	Americium	Am	95
Sulfur	S	16	Barium	Ba	56	Curium	Cm	96
Chlorine	Cl	17	Lanthanum	La	57	Berkelium	Bk	97
Argon	Ar	18	Cerium	Ce	58	Californium	Cf	98
Potassium	K	19	Praseodymium	Pr	59	Einsteinium	Es	99
Calcium	Ca	20	Neodymium	Nd	60	Fermium	Fm	100
Scandium	Sc	21	Promethium	Pm	61	Mendelevium	Md	101
Titanium	Ti	22	Samarium	Sm	62	Nobelium	No	102
Vanadium	V	23	Europium	Eu	63	Lawrencium	Lw	103
Chromium	Cr	24	Gadolinium	Gd	64	Rutherfordium	Rf	104
Manganese	Mn	25	Terbium	Tb	65	Dubnium	Db	105
Iron	Fe	26	Dysprosium	Dy	66	Seaborgium	Sb	106
Cobalt	Co	27	Holmium	Ho	67	Bohrium	Bh	107
Nickel	Ni	28	Erbium	Er	68	Hassium	Hs	108
Copper	Cu	29	Thulium	Tm	69	Meitnerium	Mt	109
Zinc	Zn	30	Ytterbium	Yb	70	Darmstadtium	Ds	110
Gallium	Ga	31	Lutetium	Lu	71	Roentgenium	Rg	111
Germanium	Ge	32	Hafnium	Hf	72	Copernicium	Ch	112
Arsenic	As	33	Tantalum	Ta	73	Nihonium	Nh	113
Selenium	Se	34	Tungsten	W	74	Flerovium	Fl	114
Bromine	Br	35	Rhenium	Re	75	Moscovium	Mc	115
Krypton	Kr	36	Osmium	Os	76	Livermorium	Lv	116
Rubidium	Rb	37	Iridium	Ir	77	Tennessine	Ts	117
Strontium	Sr	38	Platinum	Pt	78	Oganesson	Og	118
Yttrium	Y	39	Gold	Au	79			
Zirconium	Zr	40	Mercury	Hg	80			

It is not possible to obtain images of the internal structure of the atom

[3] The dimension of an atom or a sub-atomic particle refers to the spatial distribution of some physical magnitudes, such as electric charge or mass. Atoms, same as sub-atomic particles, have no geometrical dimensions in Newtonian sense.

with the same techniques used to observe the position of atoms in molecules (electron microscopy).

In order to have a representation of the internal structure of the atoms, physical models have been developed based on the concepts of quantum mechanics. These models make it possible to describe and understand the observations and measurements of atomic systems. It should be noted that these physical models can only partially describe the results of the experiments.

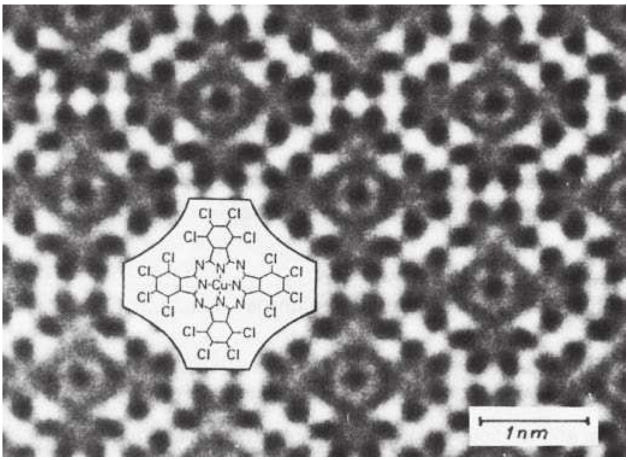

Figure 1.2: Atoms in a copper chlorophthalocyanine crystal. Credit: Kernenergie Basiswissen, M. Volkmer.

At the beginning of the 20th century, the atomic models proposed by Rutherford[4] and Bohr[5] indicated that the atom is composed of a very small nucleus (compared to the atomic size) that concentrates almost all the atomic

[4]Ernest Rutherford (*Spring Grove, New Zealand, 30.Aug.1871 - †Cambridge, England, 19.Oct.1937) was a New Zealand physicist who became Nobel Laureate in chemistry in 1908. Rutherford is considered one of the leading experimental physicists.

[5]Niels Henrik David Bohr (*Copenhagen, 7.Oct.1885 - †ibid., 18.Nov.1962) was a Danish physicist. In 1921 he received the Hughes Medal and in 1922 the Nobel Prize in physics for the advances in the structure of the atom and the radiation emitted by it.

mass and a shell that surrounds it.

The nucleus of the atom is composed of particles called protons (with positive charge), denoted p, and neutrons (with zero charge[6]), noted n. These particles are also called nucleons, because they constitute the atomic nucleus. The atoms of each element have a certain number of protons in the nucleus (see Table 1.1). Each element is determined by the number of protons. Up to the element calcium ($Z = 20$) approximately the numbers of protons Z and neutrons N in the nucleus are almost equal: $Z \sim N$. From this element onwards the number of neutrons exceeds the number of protons.

In the atomic shell are particles called electrons, denoted e, (negatively charged), and in general equal in number to the number of protons in the nucleus. Thus, the atom is electrically neutral. If the atom loses an electron, the positive charges in the nucleus outnumber the negative charges; then we have a positive ion. If the atom picks up an electron, the negative charges outnumber the positive charges and we have a negative ion.

1.2 Structure of the electronic shell and nucleus

Since protons have a positive charge, in a nucleus they should in principle repel each other and thus destroy the atomic nucleus. Since there are stable nuclei with many protons, it follows that there must be some other interaction that manages to keep the protons together. This interaction, stronger than electrostatic repulsion, is called the *nuclear force*.

As has been said, the shell of atoms is made up of electrons. Graphically we can think that around the nucleus there is a cloud of electrons. Electrons and protons attract each other, as a result of an electrical attraction. In principle, the electrons should collapse on the atomic nucleus. Since this does not happen, it follows there must be an interaction that prevents the electrons

[6]It is important to note that the neutron is a sub-atomic particle with zero charge, unlike other sub-atomic particles, such as the photon, which have no charge.

from collapsing onto the nucleus. This interaction is explained by applying the hypotheses of quantum mechanics. The fact that the electrons do not collapse on the nucleus is a quantum effect.

To extract an electron from the electron cloud surrounding the nucleus it is necessary to supply it with energy. From this it follows that to extract each of the electrons from this cloud it is necessary to deliver different amounts of energy. This fact indicates that the electrons of an atom are not bound to the nucleus in the same way (different binding energy). The values of this binding energy of the electrons differ from each other discretely. This discretization in the values of the binding energy of the electrons is called *energy levels*. These energy levels are named with capital letters (starting with the level closest to the nucleus): K, L, M, N, O, P and Q levels.

The most bound electrons (highest binding energy) are found in the shells closest to the nucleus, while the electrons with the lowest binding energy are found in the higher shells. These layers are not really shells (or orbitals, as they used to be called). They only indicate the energy levels and the distribution of electrons in these levels. It makes no physical sense to talk about the position or velocity of an electron. The most accurate description of the electrons in the atom is a spatial distribution of negative charge, more or less symmetrical, with a center of symmetry at the center of the atomic nucleus; this is, graphically, an electron cloud, as mentioned.

The ratio of dimensions (spatial distribution) between the electron cloud and the nucleus is of the order of 10^4. In other words: if the average radius of the electron cloud is 100 m, the average radius of the atomic nucleus (taken also as the positive charge density) is only 1 cm. Protons and neutrons have a very similar mass, while that of electrons is about 1836 times smaller than the mass of nucleons. For this reason it can be considered that the mass of an atom is practically given by the nucleons. In Table 1.2 we have the values of mass and charge for nucleons and electrons[7].

The proton, neutron and electron are the so-called elementary particles. They are the particles that constitute matter and originate from radioactive

[7]National Institute of Standards and Technology (NIST), Fundamental Physical Constants: https://physics.nist.gov/cuu/Constants/index.html

Table 1.2: Mass and charge of nucleons and electrons (NIST, Fundamental Physical Constants). The numbers in parentheses indicate the standard deviation.

Elementary particle	Symbol	Mass	Charge	
		[kg]	[C]	Elementary
Electron	e	$9.109\,383\,7015(28) \times 10^{-31}$	$-1.602\,176\,634 \times 10^{-19}$	-1
Proton	p	$1.672\,621\,923\,69(51) \times 10^{-27}$	$1.602\,176\,634 \times 10^{-19}$	$+1$
Neutron	n	$1.674\,927\,498\,04(95) \times 10^{-27}$	0	0

decays[8] or cosmic radiation. They are also generated artificially in nuclear reactions[9]. These elementary particles are not immutable, but can be transformed, generated or destroyed in different ways.

Given the radial dimensions of the electron cloud and the nucleus, it follows that the atom is essentially empty space. If we imagine compressing all the matter in an ocean liner so that the electrons are compacted around the atomic nucleus, the entire mass of the ocean liner would occupy the volume of a pinhead.

Since all the mass of the atom is practically concentrated in the nucleus, it is useful to indicate the number of nucleons that a nucleus possesses. This number is called the *mass number* and is noted $A = Z + N$. In addition to the mass of the atom, another very important property is the charge of the nucleus. Each proton has the minimum unit of positive charge, equal in absolute value to that of the electron and of opposite sign. The number of protons is then equal to the number of elementary charges in the nucleus. The number of protons is the atomic number Z, as already mentioned. The mass number is written to the left and above the element symbol, left superscript. The atomic number to the left and below, left subscript. In general the atomic number Z is omitted, since it is determined by the element symbol. For example ^{4}He (instead of $^{4}_{2}$He), ^{238}U (instead of $^{238}_{92}$U).

[8] Radioactive decay is the natural transformation of a nucleus into a different one. This concept will be discussed in detail in Chapter 2.

[9] Nuclear reactions are the reactions that take place in the atomic nucleus and generally involve sub-atomic particles. See Chapter 2.

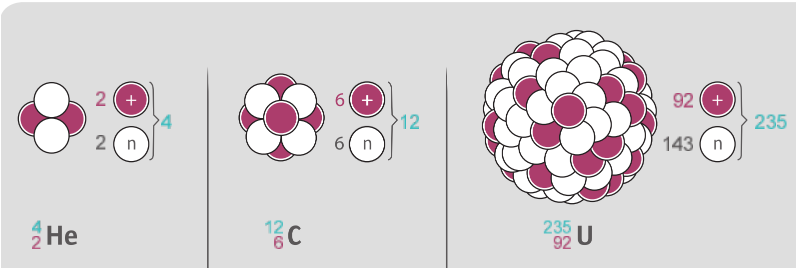

Figure 1.3: Model of the structure of the atomic nucleus. The superscript number on the left (in blue) indicates the mass number (total number of protons and neutrons); the left subscript (in red) indicates the atomic number (number of protons). Credit: Kernenergie Basiswissen, M. Volkmer.

For the elementary particles the same notation can be extended. Then we have for the proton $^1_1$p, for the neutron $^1_0$n, and in the case of the electron $^{\ 0}_{-1}$e. This notation is only used for explanatory purposes. An atomic species that has been characterized with the number of protons and neutrons is called a *nuclide*.

Atoms of an element can have different numbers of neutrons for the same number of protons. These atoms with the same number of positive charges in the nucleus (atomic number) but with different mass numbers are called *isotopes*. Isotopes do not differ in their chemical properties, but in the physical properties of the atomic nucleus. As the 118 elements have many isotopes, there are approximately 2900 nuclides. In nature there are 256 stable isotopes and 80 decaying isotopes. Nuclides that decay (whether natural or artificial) are called *radionuclides*.

Natural hydrogen has three isotopes: ^{1}H, ^{2}H and ^{3}H. The most abundant of these is ^{1}H, called hydrogen, which has the lowest mass. The nucleus of this nuclide consists of a single proton. The abundance of this isotope in the natural isotopic mixture is 99.9885(70)% at. The second isotope, called heavy hydrogen or deuterium (^{2}H $\equiv$ D) is found in nature in the proportion 0.0115(70)% at. Its nucleus consists of one proton and one neutron. Finally, the isotope of hydrogen existing in nature that has the highest mass is called tritium (^{3}H $\equiv$ T). Its nucleus consists of one proton and two neutrons. Tritium is constantly generated in the upper layers of the atmosphere due to cosmic radiation. It is also found in nuclear power plants, especially in power plants whose nuclear reactor uses natural uranium to produce energy. Tritium is a radioactive isotope.

A water molecule possessing the isotopes ^{1}H and ^{3}H (T) is written HTO accordingly. If the water molecule possesses only the isotope ^{2}H (deuterium) it is written D_2O, also called heavy water.

Figure 1.4 shows the isotopes of the first 10 elements. The complete table is called the radionuclide table, similar to the periodic table of the elements.

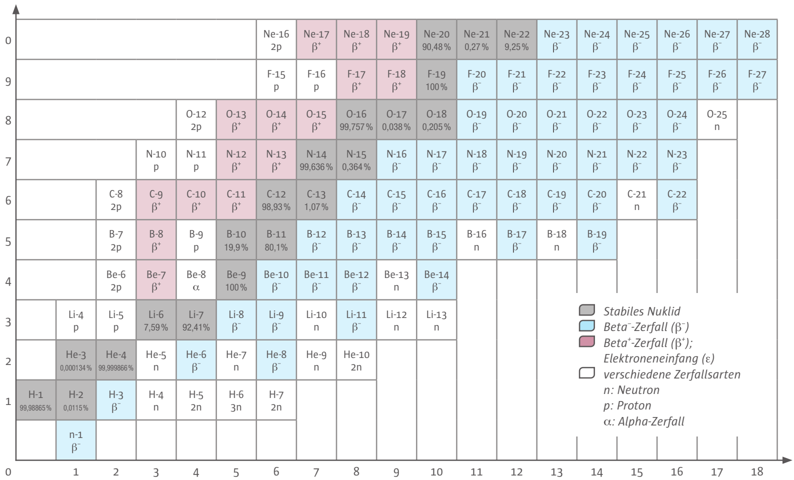

Figure 1.4: Isotopes of elements with atomic number 1 to 10. The x-axis shows the number of neutrons N while the y-axis shows the atomic number Z. Although the neutron is not an element in the periodic table, it is generally included in the radionuclide table. The nuclides in grey represent stable nuclei, where for $Z \lesssim 20$ we have $Z \sim N$. Credit: Kernenergie Basiswissen, M. Volkmer.

1.3 Binding energy and mass defect

The intensity of the nuclear interaction can be estimated by calculating the binding energy of the nucleons. For this we will analyse the nucleus of the helium atom ^{4}He. Since helium has two protons, $Z = 2$, we deduce that $N = 4 - Z = 2$, *i.e.* it also has 2 neutrons. Next, we calculate the mass of the nucleus of ^{4}He (NIST) from its constituents (see Table 1.2)[10]:

$$\begin{aligned} m(^4\mathrm{He}) &= 2m(\mathrm{p}) + 2m(\mathrm{n}) \\ &= 2(1.67262192369 \times 10^{-27}\ \mathrm{kg} + 1.67492749804 \times 10^{-27}\ \mathrm{kg}) \\ &= 6.69509884346 \times 10^{-27}\ \mathrm{kg} \end{aligned}$$

Now, the mass of the nucleus ^{4}He is $m(^4\mathrm{He}) = 6.6446573357 \times 10^{-27}$ kg. That is, the mass of the nuclide is less than the sum of its constituents by the amount $\Delta m = 0.05044150776 \times 10^{-27}$ kg.

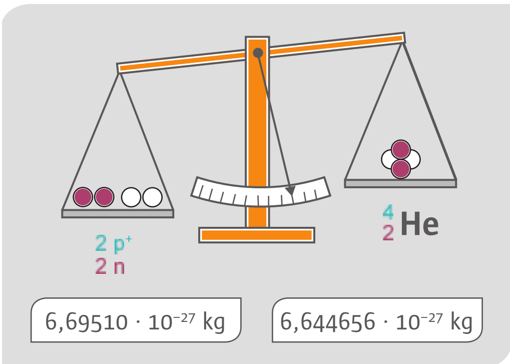

Figure 1.5: In the formation of a nucleus from the original nucleons there is a loss of mass. Credit: Kernenergie Basiswissen, M. Volkmer.

Mass loss (also called mass defect) arises because when protons and

[10] In this text, the mass of a sub-atomic particle (p, e, etc.) or of the nucleus of an atom is denoted by the letter m. Thus, $m(^4\mathrm{He})$ indicates the mass of the nucleus of ^{4}He (2 p and 2 n). The atomic mass, noted ω, refers to the total mass of the atom, *i.e.*, the nucleus plus the electrons. Obviously $\omega > m$.

neutrons join together to form a nucleus, some of the rest mass of the nucleus is converted into energy. This energy is released in the form of electromagnetic radiation (called γ-radiation). In order to obtain the original components of the ^{4}He it is necessary to give it exactly the energy released in the formation process. The loss of mass (and with it the energy released) is responsible for keeping the particles together in the nucleus. This process of forming an atomic nucleus (also called nucleosynthesis) can be explained by a mechanical model, such as the one shown in Figure 1.6.

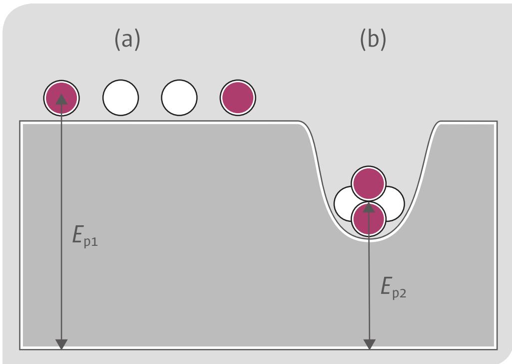

Figure 1.6: Union of spheres (a) into a stable unit (b) by the release of energy, a process comparable to the formation of a nucleus from the elementary particles protons and neutrons. Credit: Kernenergie Basiswissen, M. Volkmer.

In this comparison we have:

(a) Four spheres are in indifferent equilibrium in one plane, not interacting with each other. These have a potential energy denoted E_{p1}, with respect to the plane below. These four spheres refer to the two protons and the two neutrons.

(b) When the four spheres fall into the well, all four are now confined and in equilibrium. Since the four spheres are now in a lower position than initially, they have lost potential energy, *i.e.*, they have released