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The Mole, Avogadro's Number and Albert Einstein*

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The mole[a] concept and Avogadro's number are discussed as sought by Albert Einstein in his PhD thesis of 1905. Einstein would probably have regarded the metric system of units based on centimetre-gram-second (cgs) preferable to today's SI system and specifically he would have rejected a recent SI suggestion to redefine Avogadro's constant as based on a nonatomistic continuum description of matter. He would probably also have preferred keeping a dualistic definition of mole able of bookkeeping both mass and number of particles: we advocate that here and call it the 'Einstein Definition' and as Avogadro's number we shall adopt an integer, the cube of 84446888 as suggested by Fox and Hill, providing also a definition of the kilogram based on the atomic mass of the carbon 12 isotope.

Einstein was the first to explain the microscopic movements of pollen grains reported by Robert Brown in 1828 and his explanation that the particles move as a result of an unequal number of water molecules bumping into them from opposite sides was what finally made the scientific world accept the atom theory in its modern shape. In a cosmic diffusion analogy, pollen or bacterial spores moving randomly in outer space driven by the solar winds between solar systems can be envisaged. Applying Einstein's diffusion theory, one can argue that life might have emerged from far outside of our planet from billions of solar systems, though not from outside of our Milky Way galaxy. As a curiosity we note that the number of solar systems (stars) in the Universe has been estimated to be of the order of Avogadro's number.

Keywords: Mole; Avogadro; Einstein Definitions; Einstein Diffusion; Problematic SI Units; Chemical Bond; Stellar Life; Kilogram Definition.

INTRODUCTION

What can *mole* (a concept most of us remember from school chemistry) have in common with Albert Einstein? We all know that Einstein was thinking deep on many things, but some may be surprised to hear that in 2005 when the Physics world celebrated the jubilee of his "miracle year" 1905, he was portrayed as a *chemist* because of his PhD thesis and discussions on atoms' and molecules' actual existence based on the Brownian molecular motions[1]. This work was the basis of his two fundamental publications in 1905 and several later[2–7].

Einstein realized that it is important, not least for chemistry, to quantify numbers and sizes of the microscopic particles that build up macroscopic systems. From the thermal motions of water molecules manifested through the jumpy movements of pollen particles, observed by biologist Robert Brown in microscope in 1828, Einstein also saw a possibility to determine Avogadro's number N_A (or Loschmidt's number

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[a] Etymology: "Mole" was derived from French Molécule (extremely small particle) or diminutive from Greek μολοσ (*molos* = substance). In analogy with atom, derived from Greek *atomos* or *atemnein*, uncleavable, we may thus interpret molecule as the smallest part that a substance can be divided into without losing its *chemical* character.

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as it was also called[8]). Einstein was the first to explain the random Brownian motions and his explanation that the pollen particles moved as a result of an unequal number of water molecules bumping into them from opposite sides was what finally made the scientific world accept the atom theory in its modern shape. We will return to how Einstein was thinking, which is important for understanding the origin of the mole concept, its use and what is exact and what is less exact, and connected educational challenges. In parenthesis, Einstein often complained about his school time and his teachers' inability to make knowledge interesting and understandable (but contrary to what is sometimes claimed Einstein was a top student). As for the *mole*, many educators have felt obliged to make their own "pedagogical" explanations of something that is really rather simple. Unfortunately, this may have the opposite effect and many clever students seem to have wondered what is all the fuss about? Without giving any examples how textbooks sometimes complicate things, let me relate to an instructor during my military service, a master sergeant saying when I had commented that something was in fact rather trivial: "Nordén may think this is simple, but wait until I have explained to Nordén!"

Below I will first comment on the recent (in 2019) redefinition of mole and Avogadro's constant suggested to be SI standard but point at problems that would make an earlier suggested alternative preferable. To a chemist the mole is a tool for handling amounts of chemical substances, and examples of the most important applications will be given. Here Avogadro's number, as sought by Albert Einstein, may be regarded a bridge between the palpable macroscopic world — where amounts of chemical substance are measured in number of moles — and the less palpable microscopic world — where 1 mole corresponds to a very large number of molecules, the Avogadro number. From a pedagogical point of view, one should emphasize the Avogadro number as an integer, as we are never speaking of halves of atoms. This is one reason why the SI mole is problematic.

Einstein's work is interesting from several angles, how he got inspiration from empirical laws for macroscopic properties, the thermodynamic laws and from work by contemporary giants like Planck, van't Hoff, and Boltzmann, whom he often cites less respectly. His mathematical derivations are sometimes more complicated than necessary, confusing or even wrong. However, his mathematical relations for the diffusion of microscopic particles were seminal and still form the fundamentals of modern computer-based methods for simulating molecular dynamics.

We shall finally consider the hypothetical "scaling up" of the Brownian motions of pollen grains in a droplet of water to cosmic dimensions, posing the question whether or not life could have emerged to planet Earth via "diffusion" through space from some other solar system or even galaxy?

Changing a problematic SI definition

The mole, symbol mol, is the SI unit of amount of substance. One mole contains exactly 6.022 140 76 $\times$ 10^{23} elementary entities. This number is the fixed numerical value of the Avogadro constant, N_A, when expressed in mol^{-1}, and is called the Avogadro number.

The new approach of defining Avogadro's number as a fixed constant, taken by SI in 2019, can be motivated because it will no longer depend on the experimentally determined mass (in grams) of an atom of each element. This calibration problem is true if N_A is considered the scaling factor between the gram and the respective atomic weight for each element. However, it would just move the problem how to accurately measure a mole of a substance as this will no longer be the mass in grams according to the numerical atomic or molecular mass but be numerically N_A multiplied by the average mass of its constituent particles, "a physical quantity whose precise value has to be determined experimentally for each substance."

The new SI definition has also been criticized as it is based on an obsolete (not fully atomistic) continuum description of matter. Other criticism can be raised due to problematic aspects of how colligative properties and other thermodynamic properties should be interpreted, due to inconsistencies related to how molar mass and molecular mass (both intensive properties) are defined.

But my own strongest objection against the SI definition of Avogadro's constant is pedagogical: it is no longer a number, answering to a question How many? A possibility to amend this problem would be to stress that N_A is an integer by adding a single particle to the SI definition:

N_A = 602214076000000000000001 particles/mole

That would make N_A an awkward number and hard to visualize in terms of a three-dimensional body, like a crystal, where a cubic relation would be more natural $N_A = n_A^3$ if n_A be the number of atoms lining each edge of a cube. In fact, this definition was recently suggested by Fox and Hill[9] as a way to let an exact value of N_A also be a way to define mass, in this way getting rid of the kilogram artifact, *Le Gran K*, which has been considered mechanically unstable and an obsolete way of defining mass. Just like the replacement of the *meter* artifact letting the length of *1 m* instead be defined by the fixed velocity of light in vacuum and length of a second, the **kilogram** can be defined by the mass of the carbon 12 isotope and Avogadro's number:

12 g = mass of N_A atoms of ^{12}C

This would define **1 kg as exactly (1000 N_A/12) $\times$ (mass of ^{12}C atom)** and thus be a strong argument for defining N_A an exact number. There is no physical or practical

benefit with an over 20 digits exact definition of N_A other than that it would emphasize that it is an integer, but the latter is conceptually important, as is also the volume description: an imaginary cube consisting of $n_A{}^3$ atoms. Let us therefore adopt the Fox–Hill definition of Avogadro's number (with the factor n_A being an integer too)[9]:

$$N_A = 602\ 214\ 141070\ 409\ 084\ 099\ 072$$
$$\text{elementary entities per mole} \qquad [1]$$
$$N_A = n_A{}^3 = (84\ 446\ 888)^3$$

Since carbon does not crystallize in a cubic arrangement of atoms, the cube consisting of N_A atoms of ^{12}C, with each side of the cube having 84 446 888 atoms, must be considered a purely hypothetical construction of a solid carbon mole. Still, it could be instructive as a model for the classroom for illustrating and comparing the macroscopic and microscopic dimensions. With a density of 2.26 a cube of carbon weighing 12 g is quite small: 5.31 cm^3, that is, having an edge of only 1.75 cm. For water, with density 1 and molecular weight 18, the mole cube is somewhat bigger: 18 cm^3, that is, a cube with the edge 2.6 cm.

Avogadro's and Loschmidt's numbers

Avogadro's number has been defined in a variety of ways during its long history. Its approximate value was first determined by Johann Loschmidt in 1865 from kinetic gas theory, based on an assumption that we shall call **Avogadro's postulate**, that *gasses at the same temperature and pressure have the same particle density irrespective of molecular size* (see definitions below). This made Einstein interested in making a more precise determination of the *number* of molecules per unit volume. Loschmidt's number, N_L, in early German literature identical to Avogadro's number, has later been redefined as the number of molecules per 1 cm^3 of an ideal gas at standard temperature and pressure. According to the ideal gas law, we obviously have at $P = 1$ atm (101325 Pa) and $T = 273.15$ K that

$$N_L = P\,N_A/RT = 2.686781 \times 10^{19}\ cm^{-3}.$$

Since $R/N_A = k_B$ we have here also a quantitative connection to Boltzmann's constant. Likewise, another important constant, Planck's constant h, is most accurately determined via Avogadro's number.

Should one call N_A a constant or a number? Einstein wrote about the size of molecules and the related problem of determining N_A (see below) in his PhD thesis. After Einstein, the first to derive a numerical value of N_A, was Jean Baptiste Perrin (in 1908) by considering the density distribution of Brownian particles in a vertical column subject to Earth gravitation and using Stokes–Einstein's formula for the diffusion of a spherical particle in a viscous medium. He obtained

values of both N_A and Boltzmann's constant, the latter through $k_B = R/N_A$, where the molar gas constant R was known with high precision. It was actually Perrin who coined the name Avogadro's constant with the motivation *Ce nombre invariable N est une constante universelle qu'il semble juste d'appeler constante d'Avogadro.* Also, seeing N_A as just a scaling parameter equal to the mass ratio between the *Gram* and the *Dalton* would make it logical to call it a *constant*.

However, for conceptual reasons, to stress that N_A be an integer, instead we shall choose to call N_A **Avogadro's number** then also honoring Albert Einstein who started the search for a number asking "How many?" We then also emphasize that Einstein's view was atomistic: a macroscopic system consists of minute, discrete particles, and the amount must therefore be possible to quantize in terms of a number, the amount of a mole of substance given by an integer, N_A telling the number of particles (thus my earlier rebelliously added single particle to the SI definition!). At the same time, we must recognize the fact that $N_A \times k_B = R$, where k_B and R both are universal constants, is an argument for calling Avogadro's number a universal constant. Einstein concludes from his expression for the molecular diffusion constant, Equation [17] below, that it only depends on "universellen Konstanten" (R and N_A), on the absolute temperature (T), on the viscosity of solvent (η), and on the size of the particles (Kugel Radius a).

How should we then best approach *mole* in an easily understandable and useful way? Let me to go back to how I was taught. My high school chemistry teacher, Dr Birger Adell, also a Professor of Physical Chemistry at the University of Lund and leading in education in Sweden, thought that for a concept to be both understandable and useful, it had to be defined stringently and worked for all situations, so any exceptions must be defined and taken care of from the beginning. For example, he worked out detailed rules how to determine the coefficients in redox reaction formulas, that is, involving electron transfer and changes in element valency. Let us, starting from Avogadro's number defined exactly by Equation [1], adopt the following definitions and notations [2] to [6], which were also those used by Einstein and which we denote as Einstein definitions to distinguish them from SI definitions.

THE EINSTEIN DEFINITIONS

One *gram atom* of an element is numerically identical to the same amount in grams as the atomic weight (atomic mass) indicates. Example:

1 *gram atom* of silver
(Ag with atomic weight 107,8682 u[b]) is 107.8682 g. [2]

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[b] Here u stands for "unified atomic mass unit" used to assign masses of atoms, molecules, and elementary particles. Within chemistry, often the alternative designation Dalton (**Da**) is used. 1 u = 1 **Da** = (exactly)

One *gram molecule* of a chemical substance is numerically identical to the same amount in grams as the molecular weight (molecular mass) indicates. Example:

1 *gram molecule* of hexane C_6H_{14} with molecular weight M
$$= 86.14 \ u \text{ is } 86.14 \text{ g } (6 \text{ C} + 14 \text{ H}$$
$$= 6 \times 12.00 \ u + 14 \times 1.01u = 86.14 \ u) \quad [3]$$

Henceforth, we shall call both gram atom and gram molecule *mole* with the definition:

1 mole of a substance of identical particles, atoms or molecules, of individual mass *A u* is of total mass *A* grams [4]

Mole is related to Avogadro's number (N_A), see [1], as follows:

1 mole of a substance contains exactly N_A particles of the substance, each particle with a particle mass *A u* [5]

The particles may be atoms, ions, or molecules (for electrons and photons, see below).

Note that [4] is not absolutely exact as it will depend on how accurately *A* has been determined for the elements that build up the substance.

Relation [5] also defines mole for electrons and photons: then it is N_A that defines the mole quantity as the number of electrons or photons.

For electrons and photons, this definition also provides equivalence relations with electrochemical and photochemical reactions *via* the *Faraday constant* and the photophysical *Quantum yield*, respectively.

From the kinetic gas theory, we have, according to the ideal gas law, for the volume of 1 mole: $V_{mol} = V/N_A = RT/P$, which means that:

The volume of 1 mole (the molar volume) of any ideal gas at STP is 22.414 l [6]

We shall call [6] **Avogadro's Postulate**. STP stands for "standard temperature and pressure," that is, 273.15 K and 1 atm (101325 Pa = 1.01325 bar). Note that [6] will be more or less exact depending on whether the gas is ideal or not; deviations are expected if there are interactions between the gas molecules. If they are attracted to each other, the molar volume will decrease (obviously to half if dimers form); more
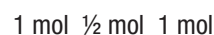
deviations are expected with higher density or lower pressure.

How *Mole* is used – three chemistry examples

Stoichiometric chemical reactions
Sodium metal (Na) reacts with chlorine gas (Cl_2)

$$Na + \tfrac{1}{2} \ Cl_2 \rightarrow NaCl \quad [7]$$

1 mol ½ mol 1 mol

"Stoichiometric"[c] here means that the reaction evens up exactly with respect to quantity of reacting species: with 1 mole sodium metal (23.0 g) burning in a bottle with ½ mole chlorine gas (22.4/2 = 11.2 l or, if we prefer to weigh, ½ × 35.4 × 2 = 35.4 g chlorine gas). In the bottle, we will find afterwards 1 mole of NaCl (table salt), that is, 23 + 35 = 48 g. The example shows how we may use mole, when designing experiments and syntheses of new compounds, by its simple relation to gram quantities. If we for some reason had only found, say, 43 g salt, it would have meant that the reaction had not proceeded to give full yield (only ca. 90%). One reason for incompletion could be that a thermodynamic chemical equilibrium is determining the effective yield as will be illustrated in the next example. Equilibrium reactions are normally written with double-headed arrows like in [8] below.

Chemical equilibrium
Chemical thermodynamics is a field of immense importance to all practical applications of chemistry and closely related to the theory of heat that so filled Einstein's mind in his PhD thesis work. We here give an example for the use of mole on a chemical equilibrium reaction.

An acid is a chemical compound that could produce protons (H^+) by dissociation. The monoprotic acid HA does this in the dissociation reaction [8].

$$\begin{array}{cccc} HA & \rightleftharpoons & H^+ & + & A^- \\ C_{HA}-x & & x & & x \end{array} \quad [8]$$
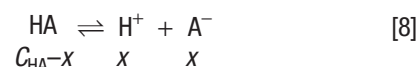
Under each species its respective concentration is noted, the total acid concentration from the beginning being C_{HA}. In a volume of 1000 ml, $N_A \, C_{HA}$ is thus the total number of molecules of HA before reaction.

1/12 of the mass of the carbon isotope $^{12}C \approx 1.6605402 \cdot 10^{-27}$ kg. For practical reasons, tabulated atom masses are often calculated as mean values of atom masses of the isotopes as abundant in nature. This has of course to be considered when calculating, for example, the molecular weight of a molecule containing pure ^{13}C-isotope. Henceforth, we shall use atomic weight and molecular weight for atomic mass and molecular mass.

[c]For "stoichiometric" compounds, the law of definite proportions holds so that a molecule has always a mass which is exactly the sum of the masses of elements occurring in definite proportions: for example, H_2O always consists of two parts of hydrogen and one part of oxygen. The law was suggested by Priestley and Lavoisier based on studies of combustion reactions very much like the one in reaction [8]. For certain so-called nonstoichiometric solid compounds, however, this is not the case. For nonstoichiometric ice, for example, if such a compound exists, it might be described as H_xO_y with x and y integers but with x/y different from 2 and thus not like in H_2O.

According to the thermodynamic "law of mass action" we have at equilibrium, with [A⁻] denoting the concentration of A⁻, [HA] denoting the concentration of HA, and so on, that

$$[A^-][H^+]/[HA] = K \qquad [9]$$

where the thermodynamic equilibrium constant K is called the acid's dissociation constant. If HA becomes fully dissociated, that is, $[A^-] = [H^+] = x = C_{HA}$, the acid is denoted as *strong* (K infinitely large), whereas it is said to be *weak* (K small) if only incompletely dissociated. If we may somehow determine the concentration x, knowing beforehand C_{HA} from how much acid we used to prepare the solution, we may calculate $K = x^2/(C_A-x)$. K has apparently dimension *concentration* (moles/liter = *molar* = *M*). Suppose we dissolve 0.1 mole HA in 1 l water, so that $C_{HA} = 100$ mM. If we somehow find out that $x = 1$ mM (by some physical–chemical measurement quantitating either the concentration [H⁺] or [HA]), we will know that the equilibrium constant $K = (0.001)^2/(0.1-0.001) = 10^{-5}$ M, a typical value for a weak acid like acetic acid ($10^{-4.7}$ M in water).

During my high school time, I once prepared a frightening large amount (100 g) of the extremely toxic liquid hydrogen cyanide (HCN) in my home, the laboratory that my mother had let me change her food cellar into. To my chemistry teacher I said I intended to determine the dissociation constant of the weak acid HCN using electric conductivity; only the charged ions H⁺ and CN⁻ are expected to conduct current. I never got a chance though, since my chemistry teacher called my mother saying: "dear Dr Nordén, I have now been unable to sleep for two nights because I know what your son has in your basement." She promised to make me neutralize the HCN by adding sodium hydroxide and flush out the product in the toilet. The "toilet reaction," HCN + NaOH → NaCN + H₂O, obviously required 100/27 moles of NaOH for 100 g HCN, that is, (100/27) × (23 + 16 + 1) = ca. 160 g NaOH.

But something else also would have prevented me from succeeding in determining the dissociation constant of HCN. For electrostatic reasons, the pure HCN does not dissociate at all, neither as a liquid nor as a gas. A strongly polar solvent, like water, is needed. In other words, reaction [8] is totally wrong and must be written instead:

$$HA + H_2O \rightleftharpoons H_3O^+ + A^- \qquad [10]$$
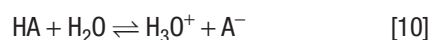
Note that this important relation holds generally! Also, for example, the very strong acid HCl (hydrochloric acid) does not dissociate at all if in absence of water or in a nonpolar solvent or in the gas phase. As it happens, I only recently discovered that HCl dissolves readily in a lipid bilayer and in fact provides a way by which chloride ions Cl⁻ could cross a biological membrane — ions otherwise normally believed to be prevented from crossing because of a very high Born energy barrier, like an isolated charge in vacuum. Such neutralization of ionic

groups may be exploited when designing "Cell Penetrating Peptides" to make them pass membranes and be used as drug-delivery systems in therapeutic contexts.

The equilibrium expression corresponding to reaction [10] will, instead of [9], thus be the following:

$$[A^-][H_3O^+]/[HA]\,[H_2O] = K´ \qquad [11]$$

where the concentration of water, [H₂O], for dilute solutions will be near that of pure water [H₂O] = 1000/18 = 55 M. We note that with this new definition the dissociation constant $K´$ is dimensionless and obviously numerically 55 times less than K.

Molecular weight determination

My third chemistry example is a method for molecular weight determination developed by Victor Meyer (1848–1897) based on Avogadro's postulate [6]. We connect to the hexane molecule mentioned in [3], a volatile liquid (boiling point 68.7°C). A glass ampoule containing a measured quantity, x g, of hexane is allowed to fall within a hermetically closed apparatus to the bottom of a long tube surrounded by boiling water where it breaks and the volatile hexane immediately evaporates. The expanded air is at the top of the apparatus collected in an upside-down turned measuring glass filled with water, and the gas volume V is measured. According to the gas law, we have

$$PV = n\,RT$$

where $T = 273 + 100$ K (boiling water) and the atmospheric pressure P is measured on a barometer, allowing the number of moles n to be determined. From $n = x/M_w$ the molecular weight M_w may now be calculated. Typically one obtains $M_w = 85 \pm 2$ Da, that is, in good agreement with the theoretical molecular weight 86.14.

How did Einstein really think?

His early interest and work on the molecular nature of matter have been interpreted to indicate that Einstein in fact was a chemist![1] We will return and ask if this is really true by the end. His theoretical contributions have clearly had enormous importance for chemistry: from how to interpret the motion of molecules and flexible bio-macromolecules in chemical reactions to how to include relativistic effects of the motion of electrons in quantum chemical computations on compounds of heavy elements. Einstein's endeavor later in life to develop a universal theory for the fundamental forces may be viewed as an extension of his earliest thoughts about liquids and intermolecular forces, based on Newtonian kinetic theory of matter.

Einstein writes to a friend in May 1905 that he will soon send him four papers: *My second paper is on determination of the true size of atoms from diffusion and viscosity of dilute solutions of neutral substances. My third paper shows that,*

Figure 1. Albert Einstein at the time — 25 years old.

assuming the molecular kinetic heat theory, particles of size 1/1000 mm suspended in liquids will exhibit random thermal motion: indeed have physiologists observed (unexplained) motions that they call Brownian molecular motion.

If possible, one should read his early original work in German[2–7], where translators definitely cannot have tampered with text or math, to fully realize that Einstein despite his genius was probably at the time a fairly frustrated young man (age 25, Figure 1) who wanted desperately to make an impact. He could be quite arrogant when referring to the giants in science: in one of his papers on Brownian motion[5] he notices in passing that a formula he has just derived is identical to the one that Bolzmann (wrongly spelled!) typically uses: *Diese Bezeichung, welche dem von Bolzmann in seinem gas-theoretischen Untersuchungen vielfach benutzen Exponentialgesetz genau entspricht, ist für die molekulare Theorie der Wärme characteristisch.* Einstein criticized Boltzmann's fundamental relation for entropy $S = k \ln W$ which he means lacks proper dynamic basis showing how fixed he (Einstein) was on the thermal particle motion. One cannot completely exclude that Einstein might have misunderstood the proper statistical–mechanical meaning of W.[d]

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[d]The meaning of W, to denote number of accessible states, makes it possible to argue in defense of Einstein that regarding "accessible" it is not explained how often a state be populated and through what mechanism. This must somehow involve dynamics requiring some deeper ergodic analysis.

In the same Brownian-motion paper[5] Einstein also presented a formula (without proof but mentioned before[10]) which he in passing mentioned that Mr Planck's radiation formula turns over into for high temperatures T and low photon frequencies ν. The relation to Brownian dynamics is somewhat far-fetched but relevant to mention as Einstein here indicates yet another possibility to determine Avogadro's number. He argues as follows, presuming the Brownian motion may be approximated as an oscillating movement (which is wrong or at least unphysical!). He considers a particle as moving back and forth symmetrically relative to its equilibrium (average mass center) position. If subject to a very weak force proportional to $-M x$, the energy differential $dW = A'\exp[-(N/RT) M x^2/2]\, dx$, for a typical Brownian displacement measurement, with $(<x^2>)^{-1/2} = 10^{-4}$ cm and $T = 300$ K, should correspond to that M be ca. 5×10^{-6} g, and the force extremely weak: for "an elongation of 1 cm" (1 dyn cm = 1 erg in cgs, my comment) thus requiring only ca. 5×10^{-6} dyn. Einstein considers the possibility that such a "sinusoidal vibration," in case the particle carries an electric charge, would give rise to emission or absorption of radiation at frequency ν with intensity described by the formula:

$$\rho\nu = (R/N)\,(8\pi\nu^2/c^3)\,T$$

It is here Einstein says, *Die von Herrn Planck gegebene Strahlungsformel geht für kleine Periodenzahlen und hohe Temperaturen in diese Formel über.* He suggests that Avogadro's number and Planck's constant can then be obtained: *Aus dem Koeffizienten des Grenzgesetzes lässt sich die Grosse N bestimmen, und man erhält so die Plancksche Bestimmung der Elementarquanta.* Einstein ends the discussion by throwing a stone through the window: *Die Tatsache, dass man auf dem angedeuteten Wege nicht zu dem wahren Gesetz der Strahlung, sondern nur zu einem Grenzgesetz gelangt, scheint mir in einer elementaren Unvollkommenheit unserer physikalischen Anschauungen ihren Grund zu haben.* "The fact that one does not arrive at a true law of radiation, but only at a limiting law on the indicated path, seems to me to be based on an elementary imperfection of our physical conception." Despite this harsh outburst, Einstein later became a friend of Max Planck. Compare also Einstein's later claim (1935) of "incompleteness" of quantum mechanics and his debate about this with Bohr.

Now let us see how Einstein derives his famous diffusion equations for Brownian motion. He first adopts a model for thermal molecular motion in a liquid based on the relation for osmotic pressure which he considers a (empirically based) natural law the discovery for which Jacobus Henricus van't Hoff was awarded the first Nobel Prize in Chemistry, in 1901.

$$pV^* = RTz \qquad [12]$$

He assumes that V^* is a volume fraction containing z gram molecules (moles) of neutral, that is, nonionic particles (molecules)[2]. The volume could be a bubble with a semi-permeable membrane through which only solvent but not solute molecules may pass. p is the osmotic pressure, which Einstein shows, may be related thermodynamically as:

$$p = -(dF/dV^*) = (RT/V^*)(n/N) = (RT/N)\,v \qquad [13]$$

with F free energy and n number of dissolved particles per volume V^*, and $v = n/V^*$ number of particles per unit volume. N is the number of real molecules in 1 gram molecule. Einstein then presents a lengthy consistency proof of Equation [13] which he derives independently using thermodynamics and shows that the free energy $F = -(RT/N)[\lg J + n\lg V^*]$, where the function J is independent of the volume V^*, so that differentiation leads to the same Equation [13] that came from the osmotic pressure formula. Einstein triumphantly says: *Durch diese Betrachtung ist gezeigt, dass die Existenz des osmotischen Druckes eine Konsequenz des molekularkinetischen Theorie der Wärme ist.*

Next, Einstein considers suspended spherical particles, v per unit volume, and concludes that on a single particle a force K acts, which depends on position (x) but on average not on time. At thermodynamic equilibrium v is such a function on x, which for a small virtual displacement δx leads to a vanishingly small change in free energy. One has thus

$$0 = \delta F = \delta E - T\delta S \qquad [14]$$

with $\delta E = \int_0^l K v\, \delta x\, dx$

where K is the force over the cross section of a spherical particle between $x = 0$ and $x = l$ giving:

$$-Kv + (RT/N_A)(dv/dx) = 0 \qquad [15]$$

meaning also that $Kv - (dp/dx) = 0$.

The last equation means that the force K is exactly balanced by the (microscopic) osmotic pressure. Then taking the number of particles that move as a result of the force K, passing the cross section per time unit, $vK/6\pi\eta a$, to be just equal to the number moved by thermal diffusion, $D(\delta v/\delta x)$, where D is the diffusion coefficient, η the solvent viscosity, and a the radius of the spherical particles, Einstein gets the equation

$$vK/6\pi\eta a - D(\delta v/\delta x) = 0 \qquad [16]$$

From [15] and [16] he deduces that the diffusion coefficient D may be determined as:

$$D = (RT/N_A)(1/6\pi\eta a) \qquad [17]$$

and thus only depends on the universal gas constant R, Avogadro's number N_A, the temperature T, the viscosity η,

and the particle radius, a. Einstein then considers the space and time dependencies of the number of particles per unit volume $v = f(x, t)$ and derives the diffusion equation

$$(df/dt) = D(d^2f/dx^2)$$

by expanding $f(x + \Delta, t)$ into a series where only every second integral survives because of the probability symmetry $\phi(x) = \phi(-x)$, and Einstein notes: *Dies ist die bekannte Differentialgleichung der Diffusion, und man erkennt das D der Diffusionskoeffizient ist.*

He presents the solution as a probability distribution

$$P = \frac{e^{-x^2/4Dt}}{2\sqrt{\pi Dt}}. \qquad [18]$$

which shows the characteristic bell-shaped Gaussian error distribution profile. Einstein also derives an expression for the average distance λ_x that a small particle with diffusion coefficient D has moved in the time interval t:

$$\lambda_x = (\langle x^2\rangle)^{1/2} = (2Dt)^{1/2} = (t)^{1/2}[(RT/N_A)(1/3\pi\eta a)]^{1/2} \quad [19]$$

Here the last sign of equality is obtained by the insertion of D from Equation [17]. Using $N_A = 6\times10^{23}$, $t = 1$ s, and $\eta = 0.0135$, he gets for a particle of size $a = 0.001$ mm, that is, $\lambda_x = 8\times10^{-5}$ cm. With $t = 60$ s, he says, the average particle movement becomes instead 6×10^{-4} cm (compare with Figure 2). Finally, Einstein makes a reflection that reveals how focused he is on Avogadro's number: He says that the discovered relation vice versa offers a possibility to determine N. One gets:

$$N = t\,RT/\lambda_x^2\,3\pi\eta\,a \qquad [20]$$

He ends his paper by hoping that some researcher would soon manage to decide on this for the heat theory important question that he has here thrown up (maybe more correct: put forward). *Möge es bald einem Forscher gelingen, die hier aufgeworfene, für die Theorie der Wärme wichtige Frage zu entscheiden!*

Indeed, this inspired the French physicist Jean-Baptiste Perrin[11] using the recently invented "ultra-microscope" to study the Brownian motions (Figure 2) and sedimentation velocity of microscopic particles suspended in water. He could verify Einstein's explanation of the Brownian motions and also estimate the size of the water molecules, work for which he was awarded a Nobel Prize in Physics in 1926[11,12]. Besides Perrin, also the Polish physicist Smoluchowski had derived Einstein's diffusion formula (in 1906)[13]. A particularly simple and elegant derivation was presented by Langevin in 1908[14], who describes the motion of a particle in the x direction, in the absence of external forces, by two force terms: one viscous resistance according to Stoke's law (just as Einstein did) plus a fluctuating force, $F(t)$, independent of velocity, caused
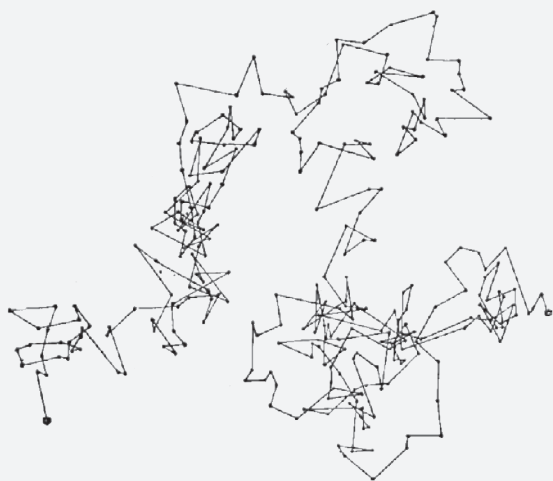
Figure 2. Brownian movements as reported by Perrin observed in ultra-microscope for mastics particles (ca. 1 μm) suspended in water. The time interval between two measurements is 1/3 s. The distance between the points from beginning to end is 0.035 mm. With tighter measuring intervals it is found that the movements between two points are as complicated as the whole picture. (From Perrin, J. B. Les Atoms (Paris: Libraire Félix, 1927).

by solvent collisions and having a vanishing time average $<F(t)> = 0$:

$$m\,(dv/dt) = 6\pi\eta\,av + F(t)$$

After integration and time averaging, Einstein's Equation [19] is obtained.

As mentioned earlier, Einstein wrote about the size of molecules in his PhD thesis[3] and the related problem of determining N_A. From experimental values of diffusion coefficients and viscosities of sugar solutions in water, Einstein used his diffusion equations to make a first estimate of Avogadro's number: $N_A = 2.1 \times 10^{23}$. In a later paper[4] he gave a value based on improved experimental data $N_A = 4.1 \times 10^{23}$ but when correcting for an algebraic error in his thesis, he got the value 6.6×10^{23}.[4]

Avogadro's number — more exact determinations

Perrin determined Avogadro's number, or constant, as he suggested it should be called in honor of Avogadro and his hypothesis of a fixed number of gas molecules per unit volume[12]. His most exact value 6.85×10^{23} is significantly bigger than the most exact value we know today, Equation [1]. Contemporary researchers studying diffusion of gold sol particles got values like 5.8×10^{23} (T. Svedberg), 6.55×10^{23} (A. Westgren). Millikan reported from extensive coulometric measurements (see *mole electrons*, below) what he then (in 1917) claimed to be the most exact value:

$N_A = (6.62 \pm 0.06) \times 10^{23}$. However, when his calculation was corrected for the difference between "international" Coulomb (0.99995 "absolute" C) and "international" volt (1.00045 "absolute" V), one gets instead $N_A = (6.064 \pm 0.06) \times 10^{23}$. In his classical oil drop experiment, Millikan determined the smallest charge (i.e., that of an electron) to be $1.5924(17) \times 10^{-19}$ C, which is only 0.6% smaller than the today established value $e = 1.602176634 \times 10^{-19}$ C, which in turn relates to Faraday's constant according to $F = N_A\,e$ (see below).

Another method for the determination of Avogadro's (Loschmidt's) number was developed by du Nouy[15], exploiting a mono-molecularly adsorbed layer of sodium oleate. When surface tension measurement shows that the whole surface is covered, one gets $N_A = (A^3 M \rho^2)/(V^3 c_1 c_2 c_3)$, where A is the adsorbed area, M the molecular weight of the adsorbed substance, and ρ its density (the other parameters refer to thickness of layer $L = V c_1 / A \rho$ with c concentrations at minima in surface tension curve). Nouy gets $N_A = (6.004 + 0.009) \times 10^{23}$, but correctly remarks that the value is probably too low as not all oleate molecules may have adsorbed — in fact he is only 0.3% too low.

As mentioned, Loschmidt was the first to make a successful determination (in 1865) of the number of atoms or molecules in a mole. From kinetic gas theory, Maxwell had derived a relation between viscosity η, density ρ, average molecular velocity v, and mean free path x between two molecule collisions:

$$\eta = (1/3)\,\rho\,v\,x \qquad [21]$$

The molecules were pictured as hard elastic spheres with diameter d. Loschmidt found a relation that allowed the determination of $N_L = V/d^2(2)^{1/2}\pi\,x$, with V the volume of 1 mole gas. He could only show a lower limit though: $N_L = N_A \geq 4.4 \times 10^{23}$.[8]

The most exact determinations of N_A are today made by X-ray diffraction[16]. First the density is determined at a macroscopic level for an ultra-pure crystalline sample, for example, of silicon or silver. Then the geometric distances defining the unit cell are determined, and the number of atoms in the unit cell is calculated. The X-ray crystallographic method of determining Avogadro's number also shows a precise determination of Planck's constant, h, which is considered one of the fundamental constants that are hardest to determine very exactly.
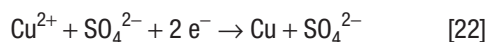
Mole electrons

Electrochemistry and redox chemistry are about chemical reactions involving electron transfer such as created by electrolysis. In fact, almost all important chemistries around us involve electron transfer reactions: the photosynthesis in plants, most of the important reactions in our life processes, degradation of metals by corrosion, combustion, and so on.

They all involve redox reactions where transfer of electrons between atoms or molecules leads to changes in valence of participating elements.

Let us consider a simple electrochemical experiment in the laboratory: the precipitation of a metal from a metal-salt solution onto an electrode during electrolysis. One speaks of *coulometry*, meaning an electrochemical analytical method in which quantitative reduction or oxidation of a substance is used for the determination of the amount of it. The amount of electrical current charge is exactly related to the amount of converted substance (e.g., precipitated metal on the electrode).

Due to that different redox reactions are generally associated with different free energy changes, and corresponding different limiting voltages, a scan of the current (A) versus a ramped voltage (V), provides a spectrum with information of the various species that are present in a mixture. This so-called polarography (or voltammetry) is an important analytical method for which Jaroslav Heyrovský was awarded the Chemistry Nobel Prize in 1959.

Suppose we apply a voltage across two platinum electrodes dipping into an aqueous solution of copper sulfate ($CuSO_4$) and the voltage is high enough to drive the electrolytic reduction reaction[e]:

$$Cu^{2+} + SO_4^{2-} + 2\ e^- \rightarrow Cu + SO_4^{2-} \qquad [22]$$

with metallic copper precipitating on the cathode (which delivers electrons to the copper ions). Weighing the electrode before and after the experiment will tell how much (x g) copper corresponds to the delivered electric charge: current I (Ampere) times time t (seconds). With the atom weight A of copper, x g means x/A moles of Cu. Since every Cu according the reaction [22] requires two electrons, we have the equation:

$$I\,t = 2\ (x/A)\ F \qquad [23]$$

_____

[e]A beautiful relation that connects chemistry (molecules) and physics (electricity) is Nernst's formula, which gives the limiting voltage needed to drive an electrochemical reaction or the resting voltage of a fuel cell or battery:

$$E = E^\circ - (RT/zF)\ \ln\{[red]/[ox]\}$$

Here E is the resting voltage of an electrochemical cell, for example, in a battery, at equilibrium, that is, no current is flowing. z is the number of electrons in the reaction, $z = 2$ in formula [22], and [red]/[ox] is the ratio of the concentrations (or "activities") of the reduced and oxidized electrode reaction species. But it should be for the complete electrochemical reaction — [22] being only half of it, here the reaction at the cathode. Nernst formula can be seen as composed of two parts like the free energy change $\Delta G = \Delta H - T\Delta S$, where the entropy part $T\Delta S$ is the second (negative) term where in a battery the concentration difference is the driving force. For definition of F, see Equations [23] and [24].

where F is a conversion constant (called **Faraday's constant**) and identical to the charge of one mole of electrons:

$$F = 96485.33212...\ C\ mol^{-1}. \qquad [24]$$

If we divide by the number of particles in one mole, i.e. Avogadro's number, we get the charge of the electron

$$e = 96485.33212/(6.02214078 \times 10^{23})$$
$$= 1.602\ 176\ 634\ 10^{-19}\ C. \qquad [25]$$

This is today the fixed definition of electron charge according to SI (in 2019).

One mole of stars and a definition duality

Although being just a curious coincidence, we may note that the number of stars in the whole of the Universe has in fact been estimated to be approximately 10^{24},[17] thus similar to Avogadro's number, giving us also a feeling for the enormous size of the number of molecules in a mole.

Accepting the duality of the mole, according to our non-SI definitions [1] to [6], it would be appropriate to speak of one mole of stars, in the same way as we may speak of one mole of *photons* or one mole of *electrons*, meaning the Avogadro number of particles could be extended to any other countable entities.

While it is reasonable and very convenient to make the speed of light a fixed constant, this way defining the length of a *meter*, it is not advisable to lock too many fundamental constants that may be mathematically correlated to other 'constants' some of which can be expected to be more exactly determined in the future with the advent of new and more precise methodology. However, the Fox–Hill definition of Avogadro's number, Equation [1] — in contrast to the SI definition as a universal constant — has the advantage that being an integer N_A will not be in conflict with modern atomistic theory with discrete countable particles, for which Einstein's attempts to determine the Avogadro number and estimating the size of molecules constitute epoch-making history.

From where did life originate?

At a so-called Alfred Nobel Symposium, an international meeting arranged jointly by the three scientific Nobel Prize Committees (Physics, Chemistry, and Physiology or medicine), on the theme *Energy in Cosmos, Molecules and Life* in June 2005 at Sånga Säby outside Stockholm, I ventured to speculate about the possibility that life might not have had its origin on our planet but somewhere else and possibly much earlier than usually assumed (even before the cooling down of planet Earth). The Panspermia hypothesis was put forward on a scientific basis by the first Swedish Nobel Laureate, Svante Arrhenius[18]. Panspermia was however disregarded as a rather uninteresting hypothesis since it was argued only to move the problem to a different place and, furthermore, be neither

plausible nor possible as it would involve the challenge of cosmic radiation which no living organism would survive the exposure of for any longer time. However, if birth of life could have occurred at some time before the birth of the Earth, new exciting scenarios could be envisaged, including the possibility that spores of life be spread over a bigger stellar space.

It has been shown that certain microorganisms (e.g., *Deinococcus radiodurans*) have unique ability of repairing both single- and double-stranded DNA or RNA, meaning that they might in fact survive a longer space voyage after which a whole organism can put itself together correctly, to survive and reproduce when having reached a habitable surrounding. The radiation protection could also be anticipated to be significantly improved due to shielding by soil or ice for a spore incapsulated inside a comet, asteroid, or meteoroid. In fact, since water appears a necessity for all life forms we know of, one could envisage the first organisms arising in the melt water on the "sunny side" of a comet, alternatively in the sea on an Earth-like planet from which the spores could have been ejected into space by a down-flopping meteor.

Figure 3 shows a fuzzy photo of myself in an inspired moment (notice the wine glass!) with a calculation I presented on the white board, and literally had done on the back of an envelope, then exactly 100 years after Albert Einstein delivered his PhD thesis on Brownian motion and the theory for diffusion. At the reasonable assumption that life arose *after* Big Bang, the earliest time would be some 10^{10} years ago when the first planets had formed and cooled down. We may then apply Einstein's key Equations [18] and [19] to make an estimate of how far from our planet a live spore may have migrated and reached the Earth, assuming the same kind of random walk diffusion dance that Robert Brown once observed the spores do in a microscopic water volume, but now with giant leaps in outer space. But instead of beginning from a planet far away, we do the opposite tracking, starting the random walk trajectory from the Earth. We clearly need some time, even a "one-step hop" of 4.2 light-years to our closest solar system Proxima Centauri, hosting the nearest potentially habitable exoplanets, would take at least some 1000 years assuming driven by the solar wind from that sun, that is, the pollen grain moving with a velocity of some 10^5 m/s or 10^{13} m/year. If the transport vehicle be a comet, some two orders of magnitude slower than the solar wind, the jump will take correspondingly longer time. The solar wind, by changing direction always directed radially from a sun, would fulfill the criterion of a true random walk. What is interesting is that when stretching the travel time from 1000 years to the maximum conceivable 10^{10} years, random diffusion can bring us via many (several billion) of the 200 billion suns of our galaxy, but with a total travel distance of 10^{23} m still not significantly far outside the Milky Way. In fact, since diffusion is very ineffective for large distances, the origin can be said to be only in our "immediate surrounding."*

One may thus conclude that life could have originated outside the Earth and migrated by the solar wind diffusion as I propose from any of some billion Earth-sized habitable planets in the "immediate surrounding" of our solar system (40 billion such planets have been estimated to exist in the Milky Way) or originated in the melt water of a comet, but could not have come from another galaxy!

Concluding remark – was Einstein a chemist?

After having now travelled many horizons, I would like to conclude with a view of the mole concept and

Foto: Anja Verena Mudring

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*A reviewer remarked that a more effective transport mechanism than the solar wind, which due to that it changes direction between the suns, which will provide a true random walk "diffusion" and thus work poorly for longer distances, would be cosmic "Taylor dispersion," that is, an apparent diffusive transport due to shear flow of the solar systems, for example, as evidenced from the whirl arms of a galaxy. Still, this mechanism seems not to contradict our conclusion that the travelling spores could not possibly have entered from outside our galaxy.
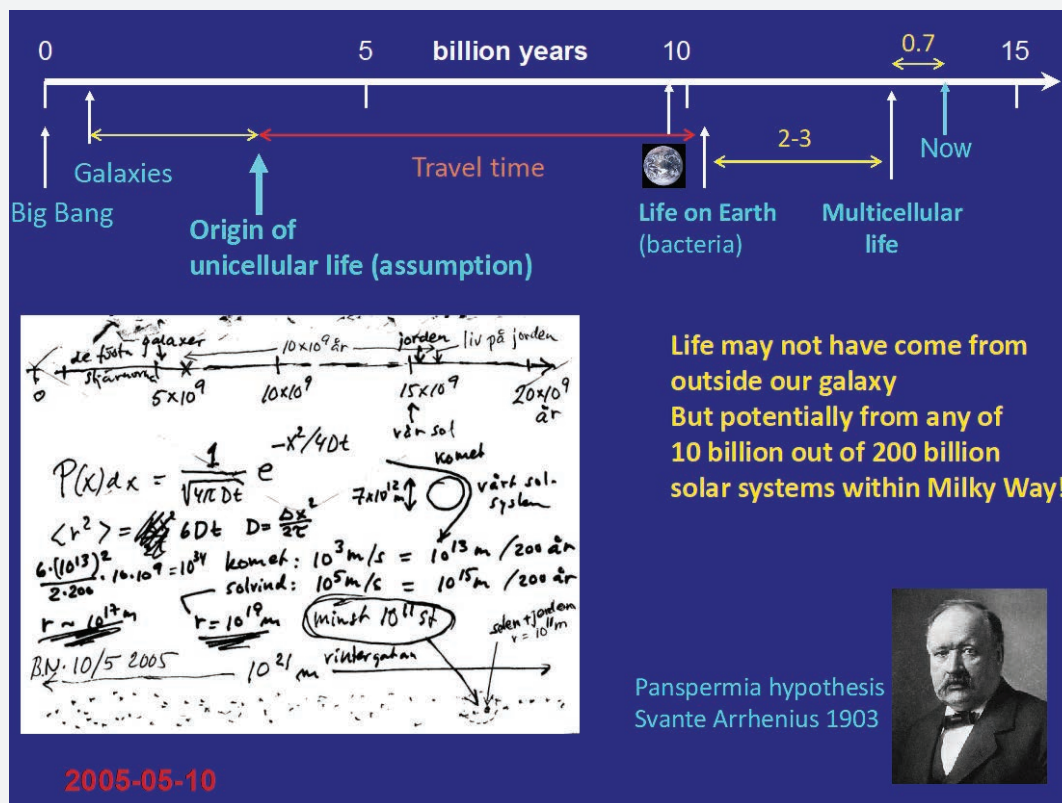
Figure 3. At the Alfred Nobel Symposium: "Energy in Cosmos, Molecules and Life" at Sånga Säby in 2005, the author presents a speculation on the possibility that life might have begun elsewhere than on our planet Earth (see text). An estimate made literally on the back of an envelope, exactly 100 years after that Albert Einstein submitted PhD thesis, using his diffusion theory, Equations [18] and [19], estimates how far a bacterium spore or pollen grain might have travelled if driven stochastically by the solar winds between different solar systems. With 10^{10} years' travel time (the maximum time conceivable after the cooling of the first planets in our galaxy) many billion planets in the "near neighborhood" of Earth might have been possible sources of origin, however no place outside our galaxy. With shorter travel times closer exoplanets become possible, the closest some 1000 years away.

Avogadro's number as bridges between the palpable macroscopic and the less palpable microscopic worlds, and with thermodynamics in the center. I will also ask whether or not Einstein was a true chemist? My answer is "no!" simply based on the fact that Einstein never considered what is central to chemistry, namely chemical reactions and chemical bonds between atoms. However, we might envisage by just extrapolating his thermodynamic views and imagination a little further, to quantum mechanics, that he could have!

Obviously, to a chemist the mole is instrumental for handling macroscopic ensembles of molecules in the contexts of stoichiometric chemical reactions, equilibria, and expressing concentrations, that is, number densities of molecules, as we have illustrated by a few examples. This is due to the law of definite proportions, meaning that a chemical compound's stoichiometric composition (its formula) exactly regulates the masses of the elements. Take the combustion of hydrogen as an example, in air or in pure oxygen, the latter probably

the cleanest conceivable combustion reaction one could ever design, or the same reaction if run as "cold combustion" in a fuel cell converting chemical energy into electrical power, both described by the reaction formula:

$$2\,H_2 + O_2 \rightarrow 2\,H_2O \qquad [26]$$
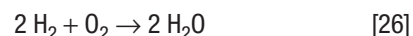
The reaction, whether occurring in a flame or in a fuel cell, is pure because the exhaust is only just water (with air a complication adds due to the presence of nitrogen, which at high temperature reacts with oxygen to form undesirable nitric oxides as byproducts). The reaction formula [26] thus tells us that exactly two molecules of hydrogen will react with exactly one molecule of oxygen to form exactly two water molecules. However, it does not tell us anything about dynamics or about how the reacting molecules and various possible intermediate radicals may dance around and collide with each other along the complex path of the reaction — things Albert Einstein certainly would have been interested in

knowing more about. The practical chemist can easily design the gas proportions, for example, by weighing, to optimize the reaction knowing that 1 mole of oxygen gas is equal to 32.0 g (2×16.0 g) and 2 moles of hydrogen 4 g ($2 \times 2 \times 1.0$ g), to get a stoichiometric perfect reaction. The example is good from an educational point of view, visualizing the differences in molecular masses, in turn reflecting corresponding differences in size of the atoms.

Like a magician, Einstein repeatedly uses *die Theorie der Wärme,* that is thermodynamics, to pull useful relations out of a hat. The balance between energy and entropy is recurrent, such as in his consideration of osmotic pressure as an effect of random microscopic motion (diffusion) of molecules balanced by a macroscopic hydrostatic pressure. We conclude that the relation for free energy (we use G for free energy, Einstein F)

$$\Delta G = \Delta H - T \times \Delta S \qquad [27]$$

applies to a variety of very different contexts, and to characterizing conditions at equilibrium, when $\Delta G = 0$ and $\Delta H = T\Delta S$. From electrochemical — in an electrolysis cell, a battery or in a fuel cell — and to various other chemical reactions at equilibrium, it is characteristic how the electric potential energy (enthalpy) $\Delta H = q \times U$ for an ion with charge q crossing a membrane spanned by the voltage U may be exactly balanced in an ion channel by a free energy, entropic term $T \times \Delta S = RT \times \ln\{[c_1]/[c_2]\}$, where c_1 and c_2 denote concentrations of diffusing ions at opposite sides of the membrane, for example, showing how the voltage and ion concentration gradient of a nerve cell are related to each other (several Nobel Prizes, both in Chemistry and Physiology or medicine). The same relation (Nernst formula) also determines the electrochemistry of both a battery and a fuel cell (Walther Nernst, Nobel Prize in Chemistry 1920).

Einstein and others have considered entropy also in many other contexts, both very macroscopic such as cosmological and also very microscopic such as quantum mechanical treatment of molecules. We may here discuss a case of chemical relevance, that is, the balance between potential and kinetic energy of the electrons in a molecule and the fundamental mechanism of chemical bonding — which obviously lies at the true heart of chemistry. If we consider the hydrogen molecule in our reaction [26] it could be described with the formula

H:H

meaning that the molecule consists of two hydrogen atoms sharing two electrons (the dots). A popular (though incorrect) way of explaining the chemical bond between the two hydrogen atoms is to say that the negatively charged electrons act as an electrostatic glue between the two positively charged protons. Here Einstein could have made a contribution that would have qualified him to call himself a chemist. The total energy of the hydrogen molecule may be described as $E = V + T$, the sum of the potential (V) and the kinetic energy (T). V is the energy of electrostatic attractions of the electrons to the protons minus the repulsions between the electrons and repulsion between the protons. For the time average potential energy $<V>$ one might think it easy to see that it will be dominated by localization of the electrons in a region between the two protons, contributing to attractive parts of the potential and thus the chemical bonding. The kinetic energy $<T>$, however, is also important though less obvious to envisage the mechanistic role of.

Here Einstein might have come up with a theory using the Virial theorem suggested by Clausius in 1870 ("virial" Latin for force or energy) holding for both classical and quantum systems, for both macroscopic heavenly bodies and microscopic particles like electrons. The force may be gravitation between planets or Coulombic electrostatic forces between atomic particles. As an example, let us consider a boy swinging on a swing. He reaches the highest potential energy V_{max} at the highest point, the swing's turning point, $V_{max} = mgh_{max}$, with m his mass, g the gravitation constant, and h_{max} the height above the bottom point. At the bottom point of the pendulum motion, where $h = 0$ and potential energy minimum $V = 0$, instead his kinetic energy is at maximum, $T_{max} = \frac{1}{2} m v_{max}^2$. But the total energy $E = V + T$ must be conserved, meaning that it be equal to V_{max} as well as to T_{max}, so we have $E = mgh_{max} = \frac{1}{2} m v_{max}^2$. For any h and v we thus have: $mgh + \frac{1}{2} m v^2 = E = mgh_{max}$. Forming averages, if we assume $<mgh> = \frac{1}{2} mgh_{max}$, that is, the potential energy at half-height $h_{max}/2$, we have $\frac{1}{2}mgh_{max} + <T> = mgh_{max}$, that is, $<T> = <V>$. However, this is wrong because the boy spends more time over $h_{max}/2$, where the swing moves more slowly than under the mid-point so his average potential energy must be bigger, in fact it is $<V> = mg(2/3)h_{max}$, giving instead $<T> = \frac{1}{2}<V>$. This is the virial theorem which although seemingly simple is at center stage of many cosmological as well as quantum contexts. For the case of the hydrogen molecule, due to a sign convention (V of a bound electron is negative), the virial theorem reads: $<T> = -\frac{1}{2}<V>$.

Although difficult to say how far "chemist Einstein" could have drawn the parallel with the swinging boy, there are a few qualitative conclusions he might have made about the hydrogen molecule based on the virial theorem when comparing it to the free, isolated hydrogen atoms. In the latter, very likely T is largest for an electron when, like the boy at the bottom point, it is closest to the proton. While in the molecule too, T will be very large when the electrons are close to the protons, their average $<T>$ is not as big as in the isolated atom, because the electron has more space in the molecule to move around in. That in turn would mean that $<V>$ is not as negative as for the electrons on the isolated hydrogen atoms.

Still, the fact that bonding is stable means that the total energy $E = <V> + <T>$ must have decreased when forming the H_2 molecule. Einstein might have tried to apply Equation [27] although the entropy of an electron is not defined, nor is temperature, he might have reasoned as follows: going to a bound state must be a spontaneous process so ΔG is negative. But if $<V>$ is not as negative for the electrons in H_2 as in the separate H atoms it means that ΔH is positive (endothermic reaction) and it would as compensation require a positive ΔS. Einstein would interpret that in terms of an increased liberation of movement of the electrons (expanding electron cloud). This picture of bonding caused by delocalization of electrons (decrease of $<T>$) is counter-intuitive but holds for many molecular systems. An electron delocalization is also the reason for the strong bonding between atoms in a metal.

But Einstein never asked how atoms were held together in molecules. He only asked about their number and motions. As we have concluded one might regard Avogadro's number just a scaling parameter, equal to the ratio between the gram and the unified atomic mass unit u ($= Da$). But it may also, from a more philosophical as well as educational point of view, be valuable to apprehend it as a countable number, a number that illustrates the size and number density of the particles in our microscopic universe. With the advent of single-molecule methods in various new fields of chemistry and physics, it is indeed becoming increasingly relevant to count and handle isolated molecules and even atoms. Therefore, we have here revolted against SI and adopted the definition suggested by Fox and Hill, Equation [1], which solves some irate problems and closes the circle.

It is said that the old Chemistry professor of the University of Lund, Christian Wilhelm Blomstrand, for some time also its President, one night was found by a colleague and friend roaming silently weeping the dark corridors of the old Chemistry building. When asked what was wrong, Professor Blomstrand told his friend that he had got so immensely sad when he thought about the atoms: "I am crying because they are so tiny!" Blomstrand lived in 1826–1897 and had obviously before Einstein got a feeling for the size of the particles that build up matter, insight that had dramatically changed his world picture.

CONFLICT OF INTEREST

Bengt Nordén declares that he has no conflict of interest relating to the content of this article.

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