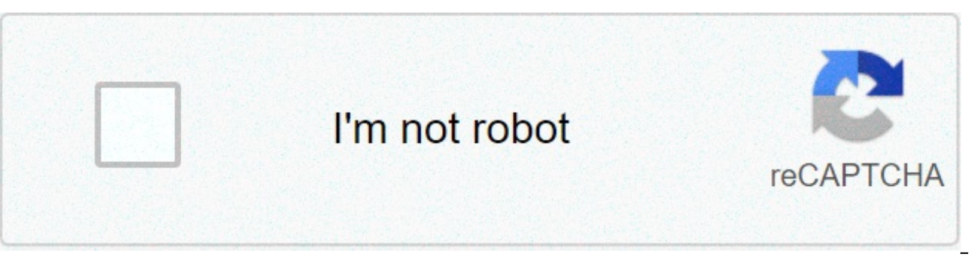

Continue

How many atoms are there in 16 gram of oxygen

The number of moles in a system can be determined using the atomic mass of an element, which can be found on the periodic table. This mass is usually an average of the abundant forms of that element found on earth. An element's mass is listed as the average of all its isotopes on earth. Avogadro's Constant One mole of oxygen atoms contains \(6.02214179 \times 10^{23}\) oxygen atoms. Also, one mole of nitrogen atoms contains \(6.02214179 \times 10^{23}\) nitrogen atoms. The number \(6.02214179 \times 10^{23}\) is called Avogadro's number (\(N_A\)) or Avogadro's constant, after the 19th century scientist Amedeo Avogadro. Each carbon-12 atom weighs about \(1.99265 \times 10^{-23}\; g\); therefore, \[(1.99265 \times 10^{-23}\; g) \times (6.02214179 \times 10^{23}\; atoms) = 12\; g\; \text{ of carbon-12} onumber \] The mass of a mole of substance is called the molar mass of that substance. The molar mass is used to convert grams of a substance to moles and is used often in chemistry. The molar mass of an element is found on the periodic table, and it is the element's atomic weight in grams/mole (g/mol). If the mass of a substance is known, the number of moles in the substance can be calculated. Converting the mass, in grams, of a substance to moles requires a conversion factor of (one mole of substance/molar mass of substance). The mole concept is also applicable to the composition of chemical compounds. For instance, consider methane, CH4. This molecule and its molecular formula indicate that per mole of methane there is 1 mole of carbon and 4 moles of hydrogen. In this case, the mole is used as a common unit that can be applied to a ratio as shown below: \[2 \text{ mol H } + 1 \text{ mol O }= 1 \text{ mol } \ce{H2O} onumber\] In this chemical reactions, the moles of H and O describe the number of atoms of each element that react to form 1 mol of \(\ce{H_2O}\). To think about what a mole means, one should relate it to quantities such as dozen or pair. Just as a pair can mean two shoes, two books, two pencils, two people, or two of anything else, a mole means 6.02214179×1023 of anything. Using the following relation: \[\text{1 mole} = 6.02214179 \times 10^{23}\] is analogous to saying: \[\text{1 Dozen} = \text{12 eggs}\] It is quite difficult to visualize a mole of something because Avogadro's constant is extremely large. For instance, consider the size of one single grain of wheat. If all the people who have existed in Earth's history did nothing but count individual wheat grains for their entire lives, the total number of wheat grains counted would still be much less than Avogadro's constant; the number of wheat grains produced throughout history does not even approach Avogadro's Number. Example \(\PageIndex{1}\): Converting Mass to Moles How many moles of potassium (\(\ce{K}\)) atoms are in 3.04 grams of pure potassium metal? Solution In this example, multiply the mass of \(\ce{K}\) by the conversion factor (inverse molar mass of potassium): \[\dfrac{1\; mol\; K}{39.10\; grams \;K} onumber \] 39.10 grams is the molar mass of one mole of \(\ce{K}\); cancel out grams, leaving the moles of \(\ce{K}\): \[3.04\; \cancel{g\; K} \left(\dfrac{1\; mol\; K}{39.10\; \cancel{g\; K}}\right) = 0.0778\; mol\; K onumber \] Similarly, if the moles of a substance are known, the number grams in the substance can be determined. Converting moles of a substance to grams requires a conversion factor of molar mass of substance/one mole of substance. One simply needs to follow the same method but in the opposite direction. Example \(\PageIndex{2}\): Converting Moles to mass How many grams are 10.78 moles of Calcium (\(\ce{Ca}\))? Solution Multiply moles of Ca by the conversion factor (molar mass of calcium) 40.08 g Ca/ 1 mol Ca, which then allows the cancelation of moles, leaving grams of Ca. \[10.78 \cancel{\;mol\; Ca} \left(\dfrac{40.08\; g\; Ca}{1\; \cancel{mol\; Ca}}\right) = 432.1\; g\; Ca onumber \] The total number of atoms in a substance can also be determined by using the relationship between grams, moles, and atoms. If given the mass of a substance and asked to find the number of atoms in the substance, one must first convert the mass of the substance, in grams, to moles, as in Example \(\PageIndex{1}\). Then the number of moles of the substance must be converted to atoms. Converting moles of a substance to atoms requires a conversion factor of Avogadro's constant (6.02214179×1023) / one mole of substance. Verifying that the units cancel properly is a good way to make sure the correct method is used. Example \(\PageIndex{3}\): Atoms to Mass How many atoms are in a 3.5 g sample of sodium (Na)? Solution \[3.5\; \cancel{g\; Na} \left(\dfrac{1\; mol\; Na}{22.98\; \cancel{g\; Na}}\right) = 0.152\; mol\; Na onumber \] \[0.152\; \cancel{mol\; Na} \left(\dfrac{6.02214179\times 10^{23}\; atoms\; Na}{1\;\cancel{ mol\; Na}}\right) = 9.15 \times 10^{22}\; atoms\; of\; Na onumber \] In this example, multiply the grams of Na by the conversion factor 1 mol Na/ 22.98 g Na, with 22.98g being the molar mass of one mole of Na, which then allows cancelation of grams, leaving moles of Na. Then, multiply the number of moles of Na by the conversion factor 6.02214179×1023 atoms Na/ 1 mol Na, with 6.02214179×1023 atoms being the number of atoms in one mole of Na (Avogadro's constant), which then allows the cancelation of moles, leaving the number of atoms of Na. Using Avogadro's constant, it is also easy to calculate the number of atoms or molecules present in a substance (Table \(\PageIndex{1}\)). By multiplying the number of moles by Avogadro's constant, the mol units cancel out, leaving the number of atoms. The following table provides a reference for the ways in which these various quantities can be manipulated: Table \(\PageIndex{1}\): Conversion Factors Known Information Multiply By Result Mass of substance (g) 1/ Molar mass (mol/g) Moles of substance Moles of substance (mol) Avogadro's constant (atoms/mol) Atoms (or molecules) Mass of substance (g) 1/Molar mass (mol/g) × Avogadro's constant (atoms/mol)) Atoms (or molecules) Example \(\PageIndex{4}\): Mass to Moles How many moles are in 3.00 grams of potassium (K)? Solution \[3.00 \; \cancel{g\; K} \left(\dfrac{1\; mol\; K}{39.10\; \cancel{g\; K}}\right) = 0.0767\; mol\; K onumber \] In this example, multiply the mass of K by the conversion factor: \[\dfrac{1\; mol\; K}{39.10\; grams\; K} onumber \] 39.10 grams is the molar mass of one mole of K. Grams can be canceled, leaving the moles of K. Example \(\PageIndex{5}\): Moles to Mass How many grams is in 10.00 moles of calcium (Ca)? Solution This is the calculation in Example \(\PageIndex{2}\) performed in reverse. Multiply moles of Ca by the conversion factor 40.08 g Ca/ 1 mol Ca, with 40.08 g being the molar mass of one mole of Ca. The moles cancel, leaving grams of Ca: \[10.00\; \cancel{mol\; Ca} \left(\dfrac{40.08\; g\; Ca}{1\;\cancel{ mol\; Ca}}\right) = 400.8\; grams \;of \;Ca onumber \] The number of atoms can also be calculated using Avogadro's Constant (6.02214179×1023) / one mole of substance. Example \(\PageIndex{6}\): Mass to Atoms How many atoms are in a 3.0 g sample of sodium (Na)? Solution Convert grams to moles \[3.0\; \cancel{g\; Na} \left(\dfrac{1\; mol\; Na}{22.98\; \cancel{g\; Na}}\right) = 0.130\; mol\; Na onumber \] Convert moles to atoms \[0.130548\; \cancel{ mol\; Na} \left(\dfrac{6.02214179 \times 10^{23}\; atoms \;Na}{1\; \cancel{ mol\; Na}}\right) = 7.8 \times 10^{22} \; atoms\; of\; \; Na onumber \] The mole, abbreviated mol, is an SI unit which measures the number of particles in a specific substance. One mole is equal to \(6.02214179 \times 10^{23}\) atoms, or other elementary units such as molecules. Question 2 1.008 g/mol 78.96 g/mol 20.18 g/mol 132.91g/mol 55.85 g/mol Question 2 2. 5.06g O (1mol/16.00g)= 0.316 mol of O 0.316 mols (6.022x1023 atoms/ 1mol) = 1.904x1023 atoms of O 3. 2.14g K (1mol/39.10g)= 0.055 mol of K 0.055 mols (6.022x1023 atoms/ 1mol) = 3.312x1022 atoms of K 4. 0.134kg Li (1000g/1kg)= 134g Li (1mol/6.941g)= 19.3 mols Li 19.3 (6.022x1023 atoms/ 1mol) = 1.16x1025 atoms of Li Question 3 4.5 mols of C (12.011g/1mol) = 54.05 g of C 7.1 mols of Al (26.98g/1mol) = 191.56 g of Al 2.2 mols of Mg (24.31g/1mol) = 53.48 g of MG Question 4 8. 6 mol H + 3 mol O → 3 mol H2O 9. 1 mol Cl + 1 mol Cl → 1 mol Cl2 10. 5 mol Na + 4 mol Cl → 4 mol NaCl + 1 mol Na (excess) The relative formula mass of a compound is calculated by adding together the relative atomic mass values for all the atoms in its formula. Moles are units used to measure substance amount. Something went wrong. Wait a moment and try again. Kwan Chi Kao, in Dielectric Phenomena in Solids, 2004The definition of Avogadro's number of 6.022 × 1023/mole is the number of atoms or molecules per one gram atomic weight. For one gram atomic weight of hydrogen with atomic weight of one gram, one mole of hydrogen contains 6.022 × 1023 hydrogen atoms. For one gram atomic weight of oxygen with atomic weight of 16 grams, one mole of oxygen also contains 6.022 × 1023 oxygen atoms. Similarly, for one gram atomic weight of silicon with atomic weight of 28 grams, one mole of silicon still contains 6.022 × 1023 silicon atoms. Thus, one mole of silicon oxide (SiO2) with a molecular weight of 28 + 2 × 16 = 60 grams contains 6.022 × 1023 SiO2 molecules.To transform this number into practical units in terms of the number of atoms or the number of molecules per cm3, we need to know the density of the material σ (grams per cm3). For example, the number of silicon atoms per cm3 isNSi=(6·022×1023mole−1/28grams mole−1)   ×2·33g cm−3=5×1022atoms/cm3Similarly, the number of SiO2 molecules per cm3 isNSiO2=(6·022×1023mole−1/60 grams mole−1)   ×2·22g cm−3=2·23 ×1022molecules/cm3where 2.33 g cm3 are, respectively, the densities of Si and SiO2.J O Bird BSc, CEng, MIEE, CMath, FIMA, FCollP, MIEIE, P J Chivers BSc, PhD, in Newnes Engineering and Physical Science Pocket Book, 19933The word 'mole' has been adopted to represent the Avogadro number of atoms of an element, that is, the relative atomic mass of an element. Thus, one mole of sodium weighs 23.0 g or one tenth of a mole of sodium weighs 2.3 g.4When applied to molecules, one mole of molecules is the relative molecular mass of that molecule, which is the summation of the individual relative atomic masses of the constituent atoms. For example, calcium carbonate contains calcium, carbon and oxygen in the ratio 1:1, 3 (i.e. CaCO3). The accurate relative atomic masses are Ca = 40.1, C = 12.01, O = 16.00, thus the relative molecular mass is 40.1 + 12.01 + (3 × 16.00) = 100.11. For many purposes the relative atomic masses are rounded up to the nearest whole number except for chlorine and copper which are 35.5 and 63.5 respectively.5When applied to solutions, a 1 molar, (1 M), solution is one in which 1 mole of a solute is dissolved in a solvent in order that the volume of the solution is 1000 cm3 (1 dm3 or 1 litre). This means that if the concentration of the solution is known in moles per dm3, the number of moles in any volume of solution can be determined. For example, to find how many moles of sodium hydroxide, NaOH, are contained in 200 cm3 of a 2 M, (2 molar), solution:1000 cm3 of the solution contains 2 moles of NaOHThus, 1 cm3 of the solution contains 21000 moles of NaOH and 200 cm3 of the solution contains 21000 × 200 moles of NaOH. That is, the number of moles of sodium hydroxide is 0.4.In order to find the mass of sodium hydroxide required to make 200 cm3 of 2 M solution:200 cm3 of a 2 M solution requires 21000 × 200 moles.0.4 moles of NaOH has a mass found by the equation:mass of NaOH = number of moles × relative molecular of NaOH mass of NaOH=0.4×(23+16+l)=0.4×40=16gThat is, the mass of sodium hydroxide required is 16 g.6When applied to gases, the molar volume of any gas is defined as occupying 22.4 dm3 at a temperature of 273 K and pressure 101.3 kPa (atmospheric pressure). Volumes of gases are easier to measure than masses. Using the molar volume definition, if the volume of a gas is known, the number of moles and hence the mass of the gas can be determined. For example, to find the number of moles of carbon dioxide gas which are contained in 100 cm3 of the gas measured at 273 K and 101.3 kPa. Use is made of the above definition that at 101.3 kPa and 273 K, 22400 cm3 of any gas is the volume of 1 mole of the gas.Thus, 22400 cm3 of CO2 are equivalent to 1 mole of CO2.and 1 cm3 of CO2 is equivalent to 122400 moles of CO2.Thus, 100 cm3 of CO2 are equivalent to12240 × 100 moles of CO2= 1224 or 0.00446 moles of carbon dioxide.In order to find the mass of carbon dioxide gas occupying 100 cm3 at 273 K and 101.3 kPa, use is made of the fact that 100 cm3 of CO2 is equivalent to 0.00446 moles.Mass of carbon dime = Number of moles of carbon dioxide× Relative molecular mass of carbon dioxide=0.00446× (12+2×16)=0.00466×44=0.196 g.The mass of carbon dioxide is 0.196 g.7If the temperature and pressure of the gas are different from the values stated, the volume must be converted to these values using the gas laws (see Chapter 46).J. Bevan Ott, Juliana Boerio-Goates, in Chemical Thermodynamics: Advanced Applications, 2000The calculation of the thermodynamic functions of a substance is based upon the uu Boltzmann distribution equation, which predicts the most probable distribution vv of molecules (or atoms) among a set of energy levels. The equation is(11.133)nigi=n0g0exp (−εikT),where ni is the number of molecules in the energy level εi and gi is the statistical weight factor (degeneracy) of that level, while n0 and g0 are the same quantities for the ground state.In the calculation of the thermodynamic properties of the ideal gas, the approximation is made that the energies can be separated into independent contributions from the various degrees of freedom. Translational and electronic energy levels are present in the ideal monatomic gas. ww For the molecular gas, rotational and vibrational energy levels are added. For some molecules, internal rotational energy levels are also present. The equations that relate these energy levels to the mass, moments of inertia, and vibrational frequencies are summarized in Appendix 6.Milton Ohring, in Engineering Materials Science, 1995It is universally accepted that atoms influence materials properties, but which subatomic portions or atoms (e.g., electrons, nuclei consisting or protons, neutrons) influence which properties is not so obvious. Before addressing this question it is necessary first to review several elementary concepts introduced in basic chemistry courses. Elements are identified by their atomic numbers and atomic weights. Within each atom is a nucleus containing a number of positively charged protons that is equal to the atomic number (Z). Circulating about the nucleus are Z electrons that maintain electrical neutrality in the atom. The nucleus also contains a number of neutrons; these are uncharged.Atomic weights (M) of atoms are related to the sum of the number of protons and neutrons. But this number physically corresponds to the actual weight of an atom. Experimentally, the weight of Avogadro's number (NA = 6.023 × 1023) of carbon atoms, each containing six protons and six neutrons, equals 12.00000 g, where 12.00000 is the atomic weight. One also speaks about atomic mass units (amu): 1 amu is one-twelfth the mass of the most common isotope of carbon, 12C. On this basis the weight of an electron is 5.4858 × 10−4 amu and protons and neutrons weigh 1.00728 and 1.00867 amu, respectively. Once the atomic weight of carbon is taken as the standard, M values for the other elements are ordered relative to it. A mole of a given element weighs M grams and contains 6.023 × 1023 atoms. Thus, if we had only 1023 atoms of copper, by a simple proportionality they would weigh 1/6.023 × 63.54 = 10.55 g (0.01055 kg). Note that the atomic weight of Cu, as well as most of the other elements in the Periodic Table including carbon, is not an integer. The reason for this is that elements exist as isotopes (some are radioactive, most are not), with nuclei having different numbers of neutrons. These naturally occurring isotopes are present in the earth's crust in differing abundances, and when a weighted average is taken, nonintegral values of M result. If compounds or molecules (e.g., SiO2, GaAs, N2) are considered, the same accounting scheme is adopted except that for atomic quantities we substitute the corresponding molecular ones.a.What weights of gallium and arsenic should be mixed together for the purpose of compounding 1.000 kg of gallium arsenide (GaAs) semiconductor?b.If each element has a purity of 99.99999 at.%, how many impurity atoms will be introduced in the GaAs?Note: MGa = 69.72 g/mol, MAs = 74.92 g/mol, MGaAs = 144.64 g/mol.a.The amount of Ga required is 1000 × (69.72/144.64) = 482 g. This corresponds to 482/69.72 or 6.91 mol Ga or, equivalently, to 6.91 × 6.023 × 1023 = 4.16 × 1024 Ga atoms. Similarly, the amount of As needed is also 6.91 mol, or 518 g. The equiatomic stoichiometry of GaAs means that 4.16 × 1024 atoms of As are also required.b.Impurity atoms introduced by Ga + As atoms number 2 × (0.00001/100) × 6.91 × 6.023 × 1023 = 8.32 × 1017. Because the total number of Ga + As atoms is 8.32 × 1024, the impurity concentration corresponds to 10−7, or 1 part in 10 million.Returning to the subatomic particles, we note that electrons carry a negative charge of −1.602 × 10−19 coulombs (C); protons carry the same magnitude of charge, but are positive in sign. Furthermore, an electron weighs only 9.108 × 10−28 g, whereas protons and neutrons are about 1840 times heavier. In a typical atom in which M = 60, the weight of the electrons is not quite 0.03% of the total weight of the atom. Nevertheless, when atoms form solids, it is basically the electrons that control the nature of the bonds between the atoms, the electrical conduction behavior, the magnetic effects, the optical properties, and the chemical reactions between atoms. In contrast, the sub-nuclear particles and even nuclei, surprisingly, contribute very little to the story of this book. Radioactivity, the effects of radiation, and the role of high-energy ion beams in semiconductor processing (ion implantation) are exceptions. One reason is that nuclear energies and forces are enormous compared with what atoms experience during normal processing and use of materials. Another reason is that the nucleus is so very small compared with the extent to which electrons range. For example, in hydrogen, the smallest of the atoms (Fig. 2-1A), the single electron circulates around the proton in an orbit whose radius, known as the Bohr radius, is 0.059 nm long [1 nm = 10−9 m = 10 Å (angstroms)]. The radius of a proton is 1.3 × 10−6 nm, whereas nuclei, typically ~M1/3 times larger, are still very much smaller than the Bohr radius. Before a pair of atomic nuclei move close enough to interact, the outer electrons have long since electrostatically interacted and repelled each other. The preceding considerations make it clear why the next topic addressed is the atomic electrons.FIGURE 2-1. (A) Model of a hydrogen atom showing an electron executing a circular orbit around a proton. (B) De Broglie standing waves in a hydrogen atom for an electron orbit corresponding to n = 4.Joseph Feher, in Quantitative Human Physiology, 2012This chapter examines the concentration and kinetics in physiology. The concentration of a solute in solution is the amount of that solute per unit volume of solution. It can be expressed as the mass of the solute per unit volume or the number of moles of solute per unit volume. A mole of any substance is Avogadro's number of particles. The relationship among concentration, amount of solute, and volume of solution can be used to determine the volume of physiological fluids. Evans' Blue Dye is an example of a solute that can be used to estimate plasma volume, because the dye enters the plasma but cannot leave it easily. Elementary chemical reactions have forward and reverse rate constants that govern the rate of conversion in either the forward or reverse reaction. The rates of reaction have the units of moles per unit time per unit volume of solution. Enzymes speed chemical reactions by altering the path of the reaction by allowing it to proceed on the surface of the enzyme. Thus, enzymes convert homogeneous reactions in the fluid phase into heterogeneous reactions on the surface of the enzyme. It is found that the alternate path reduces the activation energy for the reaction, thereby allowing it to proceed quicker.Philip Kosky, ... George Wise, in Exploring Engineering (Third Edition), 2013Since molecules are extremely small entities, it takes enormous numbers of them to provide useful amounts of energy for powering automobiles or performing any macroscopic task. So rather than counting molecules by ones or twos, they are counted in very large units called mols,2 or even larger units called kmols3 (which are thousands of mols).The mol is defined to be the amount of substance containing as many "elementary entities" as there are atoms in exactly 0.012 kg of pure carbon-12. (The kmol is a factor 103 larger.)Just as a dozen eggs is a way of referring to exactly 12 eggs, a mol is a way of referring to 6.0221367 × 1023 molecules, which is the number of elementary entities in exactly 0.012 kg of carbon. This number of elementary entities is very large indeed and is referred to as Avogadro's Number, symbol NAv. Obviously, in a kmol, the number of elementary entities is 6.0221367 × 1026.Elementary entities may be such things as atoms, molecules, ions, electrons, or other well-defined particles or groups of such particles. The mole unit is therefore nothing but an alternate unit to counting individual elementary particles, and it is useful in the analysis of chemical reactions. Continuing our dozen-egg analogy, the elementary entities might consist of five individual chicken eggs and seven individual turkey eggs. If so, notice that not every egg has the same mass. The atomic masses4of some common elements correct to three significant figures are given in Table 6.1. They are measured relative to the mass of carbon–12 (written C12 or C-12), being exactly 12.0• (the superscript • means the zero reoccurs to infinite length). In addition, the number of mols n of a substance with mass m and a molecular mass M is given byTable 6.1. Atomic Masses of Some Common Elements to Three Significant FiguresHydrogen, H1.00Nitrogen, N14.0Oxygen, O16.0Helium, He4.00Carbon, C12.0Argon, Ar40.0Sulfur, S32.1Chlorine, Cl35.5Many gases are divalent (i.e., chemically combined as a paired set), such as hydrogen, oxygen, and nitrogen molecules, written H2, O2, and N2, respectively (and their molecular masses are 2.00, 32.0, and 28.0, respectively). Therefore, every kmol of water has a mass of 18.0 kg, since the atomic mass of every hydrogen atom is (approximately)* 1.00 kg/kmol, and the atomic mass of every oxygen atom is 16.0 kg/kmol.Example 6.1a.How many mols of water are in 10.0 kg of water?b.How many kmols of water are in 10.0 kg of water?Need: Number of mols, kmols in 10.0 kg of H2O.Know: Atomic masses of O and H are 16.0 and 1.00, respectively.How: The number of moles n of a substance with a mass m that has a molecular mass M is given by n = m/M.Solve: The molecular mass of water (H2O) is M = 2 × (1.00) + 1 × (16.0) = 18.0 kg/kmol = 18.0 g/mol.5 Then, for 10.0 kg of water,a.10.0kg=100.×102g,thenn=m/M=100.×102g/18.0g/mol=556mol.b.n=m/M=10.0kg/18.0kg/kmol=0.556kmol.Example 6.2Determine the effective molecular mass of air, assuming it is composed of 79% nitrogen and 21% oxygen.Need: Molar mass of air with 21% O2 and 79% N2. Therefore, the air is a mixture. A kmol of a mixture of "elementary entities" must still have Avogadro's Number of elementary particles, be they oxygen or nitrogen molecules. So, we need the combined mass of these two kinds of elementary entities in the correct ratio, each of which has a different mass.Know: Molar mass of O2 is 32.0 kg/kmol, and the molar mass of N2 is 28.0 kg/kmol.How: Proportion the masses of each constituent according to their concentration.Solve: Mair = %N2 × MN2 + %O2 × MO2 = 0.79 × 28.0 + 0.21 × 32.0 = 28.8 kg/kmol.Note: We have defined a kmol of air (even though "air" molecules per se do not exist), but in so doing, we preserved the notion that every mole should have Avogadro's Number of entities.Anna L. Smith, Rudy J.M. Konings, in Advances in Nuclear Fuel Chemistry, 2020The total energy of an assembly of N molecules is represented bywhich is identical to (1.101), with Ni the number of molecules having energy ϵi, but taking also into account E°0, the zero-point energy. According to the Boltzmann distribution law, Ni is proportional to the partition function Z:where NA is the number of Avogadro and gi is the statistical weight. Eq. (1.127) can now be rewritten as(1.129)E°=E°0+∑iεigie−εi/kBTZResolving this equation leads to(1.130)E°=E°0+RT2d(lnZ)dTThe molar enthalpy is the sum of E and the external energy, which is simply pV=RT in the case of an ideal gas. Thus(1.131)H=E°0+RT+RT2d(lnZ)dTfrom which the molar heat capacity at constant pressure follows as(1.132)C°p(T)=dH°(T)dT=R+RddT(T2d(lnZ)dT)The standard entropy is given by Bolzmann's equation aswhere Ω is the number of the arrangements of N molecules among the energy levels ϵi, with occupation Ni:Substituting Eq. (1.134) into Eq. (1.133), applying Stirling's approximation (i.e., ln N!∼N ln N−N), and realizing that ΣNi=N, gives(1.135)S=−NkB∑i(NiN)ln(NiN)The ratio Ni/N is given by Eq. (1.128), and substitution yieldsIt is thus clear that all the thermal function of ideal gases can be derived from Z, becauseand thus(1.138)Z=ztrs·zvib·zrot·zelecN!To calculate thermodynamic functions, a detailed knowledge of the translational, rotational, vibrational, and electronic partition functions is thus required. It should be realized that the total energy of a molecule is composed of an external and an internal component. The external component is equal to the translational energy, the internal energy is the sum of electronic, rotational, and vibrational components, which can be separated (e.g., Born–Oppenheimer approximation).In Pergamon Materials Series, 2001The very gradual recognition that matter consists of atoms stretched over more than two millennia, and that recognition was linked for several centuries with the struggles of successive generations of scientists to understand the nature of crystals. This is why I am here combining sketches of the history of atoms and of the history of crystals, two huge subjects.The notion that matter had ultimate constituents which could not be further subdivided goes back to the Greeks (atom = Greek a-tomos, not capable of being cut). Democritus (circa 460 BC – circa 370 BC), probably leaning on the ideas of Epicurus, was a very early proponent of this idea; from the beginning, the amount of empty space associated with atoms and the question whether neighbouring atoms could actually be in contact was a source of difficulty, and Democritus suggested that solids with more circumatomic void space were in consequence softer. A century later, Aristotle praised Democritus and continued speculating about atoms, in connection with the problem of explaining how materials can change by combining with each other … mixtion, as the process came to be called (Emerton 1984).Even though Democritus and his contemporaries were only able to speculate about the nature of material reality, yet their role in the creation of modern science is more crucial than is generally recognised. That eminent physicist, Erwin Schrödinger, who in his little book on Nature and the Greeks (Schrödinger 1954, 1996) has an illuminating chapter about The Atomists, put the matter like this: "The grand idea that informed these men was that the world around them was something that could be understood, if only one took the trouble to observe it properly; that it was not the playground of gods and ghosts and spirits who acted on the spur of the moment and more or less arbitrarily, who were moved by passions, by wrath and love and desire for revenge, who vented their hatred, and could be propitiated by pious offerings. These men had freed themselves of superstition, they would have none of all this. They saw the world as a rather complicated mechanism, according to eternal innate laws, which they were curious to find out. This is of course the fundamental attitude of science to this day." In this sense, materials science and all other modern disciplines owe their origin to the great Greek philosophers.The next major atomist was the Roman Lucretius (95 BC – circa 55 BC), who is best known for his great poem, De rerum natura (Of the Nature of Things), in which the author presents a comprehensive atomic hypothesis, involving such aspects as the ceaseless motion of atoms through the associated void (Furley 1973). Lucretius thought that atoms were characterised by their shape, size and weight, and he dealt with the problem of their mutual attraction by visualising them as bearing hooks and eyes … a kind of primordial 'Velcro'. He was probably the last to set forth a detailed scientific position in the form of verse.After this there was a long pause until the time of the 'schoolmen' in the Middle Ages (roughly 1100–1500). People like Roger Bacon (1220–1292), Albertus Magnus (1200–1280) and also some Arab/Moorish scholars such as Averroes (1126–1198) took up the issue; some of them, notably Albertus, at this time already grappled with the problem of the nature of crystalline minerals. Averroes asserted that "the natural minimum … is that ultimate state in which the form is preserved in the division of a natural body". Thus, the smallest part of, say, alum would be a particle which in some sense had the form of alum. The alternative view, atomism proper, was that alum and all other substances are made up of a few basic building units none of which is specific to alum or to any other single chemical compound. This difference of opinion (in modern terms, the distinction between a molecule and an atom) ran through the centuries and the balance of dogma swung backwards and forwards. The notion of molecules as distinct from atoms was only revived seriously in the 17th century, by such scientists as the Dutchman Isaac Beeckman (1588–1637) (see Emerton 1984, p. 112). Another early atomist, who was inspired by Democritus and proposed a detailed model according to which atoms were in perpetual and intrinsic motion and because of this were able to collide and form molecules, was the French philosopher Pierre Gassendi (1592–1655). For the extremely involved history of these ideas in antiquity, the Middle Ages and the early scientific period, Emerton's excellent book should be consulted.From an early stage, as already mentioned, scholars grappled with the nature of crystals, which mostly meant naturally occurring minerals. This aspect of the history of science can be looked at from two distinct perspectives – one involves a focus on the appearance, classification and explanation of the forms of crystals (i.e., crystallography), the other, the role of mineralogy in giving birth to a proper science of the earth (i.e., geology). The first approach was taken, for instance, by Burke (1966) in an outstanding short account of the origins of crystallography, the second, in a more recent study by Laudan (1987).As the era of modern science approached and chemical analysis improved, some observers classified minerals in terms of their compositions, others in terms of their external appearance. The 'externalists' began by measuring angles between crystal faces; soon, crystal symmetry also began to be analysed. An influential early student of minerals – i.e., crystals – was the Dane Nicolaus Stenonius, generally known as Steno (1638–1686), who early recognised the constancy of interfacial angles and set out his observations in his book, The Podromus, A Dissertation on Solids Naturally Contained within Solids (see English translation in Scherz 1969). Here he also examines the juxtaposition of different minerals, hence the title. Steno accepted the possibility of the existence of atoms, as one of a number of rival hypotheses. The Swedish biologist Carolus Linnaeus (1707–1778) somewhat later attempted to extend his taxonomic system from plants and animals to minerals, basing himself on crystal shape; his classification also involved a theory of the genesis of minerals with a sexual component; his near-contemporaries, Romé de l'Isle and Haüy (see below) credited Linnaeus with being the true founder of crystallography, because of his many careful measurements of crystals; but his system did not last long, and he was not interested in speculations about atoms or molecules.From quite an early stage, some scientists realised that the existence of flat crystal faces could be interpreted in terms of the regular piling together of spherical or ellipsoidal atoms. Figure 3.1 shows some 17th-century drawings of postulated crystal structures due to the Englishman Robert Hooke (1635–1703) and the Dutchman Christiaan Huygens (1629–1695). The great astronomer, Johannes Kepler (1571–1630) had made similar suggestions some decades earlier. Both Kepler and Huygens were early analysts of crystal symmetries in terms of atomic packing. This use of undifferentiated atoms in regular arrays was very different from the influential corpuscular models of René Descartes (1596–1650), as outlined by Emerton (1984, p. 131 et seq.): Descartes proposed that crystals were built up of complicated units (star- or flower-shaped, for instance) in irregular packing; according to Emerton, this neglect of regularity was due to Descartes's emphasis on the motion of particles and partly because of his devotion to Lucretius's unsymmetrical hook-and-eye atoms.Figure 3.1. (from Emerson, p. 134) Possible arrangements of spherical particles, according to Hooke (left, from a republication in Micrographia Restaurata, London 1745) and Huygens (right, from Traité de la Lumière, Leiden 1690).In the 18th century, the role of simple, spherical atoms was once more in retreat. An eminent historian of metallurgy, Cyril Stanley Smith, in his review of Emerton's book (Smith 1985) comments: "… corpuscular thinking disappeared in the 18th century under the impact of Newtonian anti-Cartesianism. The new math was so useful because its smoothed functions could use empirical constants without attention to substructure, while simple symmetry sufficed for externals. Even the models of Kepler, Hooke and Huygens showing how the polyhedral form of crystals could arise from the stacking of spherical or spheroidal parts were forgotten." The great French crystallographers of that century, Romé de l'Isle and Haüy, thought once again in terms of non-spherical 'molecules' shaped like diminutive crystals, and not in terms of atoms.Jean-Baptiste Romé de l'Isle (1736–1790) and René Haüy (1743–1822), while they, as remarked, credited Linnaeus with the creation of quantitative crystallography, themselves really deserve this accolade. Romé de l'Isle was essentially a chemist and much concerned with the genesis of different sorts of crystal, but his real claim to fame is that he first clearly established the principle that the interfacial angles of a particular species of crystal were always the same, however different the shape of individual specimens might be, tabular, elongated or equiaxed – a principle foreshadowed a hundred years earlier by Steno. This insight was based on very exact measurements using contact goniometers; the even more exact optical goniometer was not invented until 1809 by William Wollaston (1766–1826). (Wollaston, incidentally, was yet another scientist who showed how the stacking of spherical atoms could generate crystal forms. He was also an early scientific metallurgist, who found out how to make malleable platinum and also discovered palladium and rhodium.)Haüy, a cleric turned experimental mineralogist, built on Romé's findings: he was the first to analyse in quantitative detail the relationship between the arrangement of building-blocks (which he called 'integrant molecules') and the position of crystal faces: he formulated what is now known as the law of rational intercepts, which is the mathematical expression of the regular pattern of 'treads and steps' illustrated in Figure 3.2(a), reproduced from his Traité de Cristallographie of 1822. The tale is often told how he was led to the idea of a crystal made up of integrant molecules shaped like the crystal itself, by an accident when he dropped a crystal of iceland spar and found that the small cleavage fragments all had the same shape as the original large crystal. "Tout est trouvé!" he is reputed to have exclaimed in triumph.Figure 3.2. (a) Treads and risers forming crystal faces of various kinds, starting from a cubic primitive form(after Haüy 1822). (b) Eilhardt Mitscherlich (1794–1863) (courtesy Deutsches Museum, Munich).From the 19th century onwards, chemists made much of the running in studying the relationship between atoms and crystals. The role of a German chemist, Eilhardt Mitscherlich (1794–1863, Figure 3.2(b)) was crucial (for a biography, see Schütt 1997). He was a man of unusual breadth who had studied oriental philology and history, became 'disillusioned with these disciplines' in the words of Burke (1966) and turned to medicine, and finally from that to chemistry. It was Mitscherlich who discovered, first, the phenomenon of isomorphism and, second, that of polymorphism. Many salts of related compositions, say, sodium carbonate and calcium carbonate, turned out to have similar crystal symmetries and axial ratios, and sometimes it was even possible to use the crystals of one species as nuclei for the growth of another species. It soon proved possible to use such isomorphous crystals for the determination of atomic weights: thus Mitscherlich used potassium selenite, isomorphous with potassium sulphate, to determine the atomic weight of selenium from the already known atomic weight of sulphur. Later, Mitscherlich established firmly that one and the same compound might have two or even more distinct crystal structures, stable (as was eventually recognised) in different ranges of temperature. (Calcite and aragonite, two quite different polymorphs of calcium carbonate, were for mineralogists the most important and puzzling example.) Finally, Wollaston and the French chemist François Beudant, at about the same time, established the existence of mixed crystals, what today we would in English call solid solutions (though Mischkristall is a term still used in German).These three findings – isomorphism, polymorphism, mixed crystals – spelled the doom of Haüy's central idea that each compound had one – and one only – integrant molecule the shape of which determined the shape of the consequent crystal and, again according to Cyril Smith (Smith 1960, p. 190), it was the molecule as the combination of atoms in fixed proportions – rather than the atoms themselves, or any integrant molecules – which now became the centre of chemical interest. When John Dalton (1766–1844) enunciated his atomic hypothesis in 1808, he did touch on the role of regularly combined and arranged atoms in generating crystals, but he was too modest to speculate about the constitution of molecules; he thought that "it seems premature to form any theory on this subject till we have discovered from other principles (my italics) the number and order of the primary elements" (Dalton 1808).The great Swedish chemist Jöns Berzelius (1779–1848) considered the findings of Mitscherlich, together with Dulong and Petit's discovery in 1819 that the specific heats of solids varied inversely as their atomic weights, to be the most important empirical proofs of the atomic hypothesis at that time. It is to be noted that one of these two cornerstones was based on crystallography, which thus became one of the foundations of modern atomic theory.Another 19th century scientist is one we have met before, in Chapter 2, Section 2.1.4. Thomas Graham (1805–1869), the originator of the concept of colloids, made a reputation by studying the diffusion of fluids (both gases and liquids) in each other in a quantitative way. As one recent commentator (Barr 1997) has put it, "the crucial point about Graham's law (of diffusion) is its quantitative nature and that it could be understood, if not completely explained, by the kinetic theory of gases developed by Maxwell and Clausius shortly after the middle of the nineteenth century. In this way the ideas of diffusion being connected with the random motion of molecules over a characteristic distance, the mean free path, entered science." Jean Perrin, whose crucial researches we examine next, could be said to be the inheritor of Graham's insights. Many years later, in 1900, William Roberts-Austen (1843–1905), a disciple of Graham, remarked of him (Barr 1997): "I doubt whether he would have wished any other recognition than that so universally accorded to him of being the leading atomist of his age".We move now to the late 19th century and the beginning of the 20th, a period during which a number of eminent chemists and some physicists were still resolutely sceptical concerning the existence of atoms, as late as hundred years after John Dalton's flowering. Ostwald's scepticism was briefly discussed in Section 2.1.1, as was his final conversion by Einstein's successful quantitative interpretation of Brownian motion in 1905 in terms of the collisions between molecules and small suspended particles, taken together with Jean Perrin's painstaking measurements of the Brownian motion of suspended colloidal gamboge particles, which together actually produced a good estimate of Avogadro's number. Perrin's remarkable experimental tour de force is the subject of an excellent historical book (Nye 1972); it is not unreasonable to give Perrin the credit for finally establishing the atomic hypothesis beyond cavil, and Nye even makes a case for Perrin as having preceded Rutherford in his recognition of the necessity of a compound atom. Perrin published his results in detail, first in a long paper (Perrin 1909) and then in a book (Perrin 1913). The scientific essayist Morowitz (1993) laments that "one of the truly great scientific books of this century gathers dust on library shelves and is missing from all libraries established after 1930". Morowitz shows a table from Perrin's 1913 book, reproduced here in the earlier form presented by Nye (1972), which gives values of Avogadro's number from 15 distinct kinds of experiment; given the experimental difficulties involved, these values cluster impressively just above the value accepted today, 60.22 × 1022. If no atoms … then no Avogadro's number. Perrin received the Nobel Prize for Physics in 1926. Phenomena observedN (Avogadro's Number)/1022Viscosity of gases (kinetic theory)62Vertical distribution in dilute emulsions68Vertical distribution in concentrated emulsions60Brownian movement (Perrin)Displacements69Rotations65Diffusion69Density fluctuation in concentrated emulsions60Critical opalescence75Blueness of the sky65Diffusion of light in argon69Blackbody spectrum61Charge on microscopic particles62RadioactivityHelium produced64Radium lost71Energy radiated60The detailed reasons for Ostwald's atomic scepticism when he gave a major lecture in Germany in 1895 are set out systematically in a book by Stehle (1994), who remarks: "The great obstacle faced by those trying to convince the sceptics of the reality of atoms and molecules was the lack of phenomena making apparent the graininess of matter. It was only by seeing individual constituents, either directly or indirectly through the observation of fluctuations about the mean behaviour predicted by kinetic theory, that the existence of these particles could be shown unambiguously. Nothing of the kind had been seen as yet, as Ostwald so forcefully pointed out …". In fact, Johann Loschmidt (1821–1895) in 1866 had used Maxwell's kinetic theory of gases (which of course presupposes the reality of atoms, or rather molecules) together with a reasonable estimate of an atomic cross-section, to calculate a good value for Avogadro's Number, that longterm criterion of atomic respectability. Ostwald's resolute negation of the existence of atoms distressed some eminent scientists; thus, Ludwig Boltzmann's statistical version of thermodynamics (see Section 3.3.2), which was rooted in the reality of molecules, was attacked by opponents of atomism such as Ostwald, and it has been asserted by some historians that this (together with Ernst Mach's similarly implacable hostility) drove Boltzmann into a depression which in turn led to his suicide in 1906. Even today, the essential link between the atomic hypothesis and statistical thermodynamics provokes elaborate historical analyses such as a recent book by Diu (1997).Just after Ostwald made his sceptical speech in 1895, the avalanche of experiments that peaked a decade later made his doubts untenable. In the 4th (1908) edition of his textbook, Grundriss der physikalischen Chemie, he finally accepted, exactly a hundred years after Dalton enunciated his atomic theory and two years after Boltzmann's despairing suicide, that Thomson's discovery of the electron as well as Perrin's work on Brownian motion meant that "we arrived a short time ago at the possession of experimental proof for the discrete or particulate nature of matter – proof which the atomic hypothesis has vainly sought for a hundred years, even a thousand years" (Nye 1972, p. 151). Not only Einstein's 1905 paper and Perrin's 1909 overview of his researches (Perrin 1909), but the discovery of the electron by J.J. Thomson in 1897 and thereafter the photographs taken with Wilson's cloud-chamber (the 'grainiest' of experiments), Rutherford's long programme of experiments on radioactive atoms, scattering of subatomic projectiles and the consequent establishment of the planetary atom, followed by Moseley's measurement of atomic X-ray spectra in 1913 and the deductions that Bohr drew from these … all this established the atom to the satisfaction of most of the dyed-in-the-wool disbelievers. The early stages, centred around the electron, are beautifully set out in a very recent book (Dahl 1997). The physicist's modern atom in due course led to the chemist's modern atom, as perfected by Linus Pauling in his hugely influential book, The Nature of the Chemical Bond and the Structure of Molecules and Crystals, first published in 1939. Both the physicist's and the chemist's atoms were necessary precursors of modern materials science.Nevertheless, a very few eminent scientists held out to the end. Perhaps the most famous of these was the Austrian Ernst Mach (1838–1916), one of those who inspired Albert Einstein in his development of special relativity. As one brief biography puts it (Daintith et al. 1994), "he hoped to eliminate metaphysics – all those purely 'thought-things' which cannot be pointed to in experience – from science". Atoms, for him, were "economical ways of symbolising experience. But we have as little right to expect from them, as from the symbols of algebra, more than we have put into them". Not all, it is clear, accepted the legacy of the Greek philosophers, but it is appropriate to conclude with the words (Andrade 1923) of Edward Andrade (1887–1971): "The triumph of the atomic hypothesis is the epitome of modern physics".The most important episode of all in the history of crystallography was yet to come: the discovery that crystals can diffract X-rays and that this allows the investigator to establish just where the atoms are situated in the crystalline unit cell. But before that episode is outlined, it is necessary to mention the most remarkable episode in crystallographic theory – the working out of the 230 space groups. In the mid-19th century, and based on external appearances, the entire crystal kingdom was divided into 7 systems, 14 space lattices and 32 point-groups (the last being all the self-consistent ways of disposing a collection of symmetry elements passing through a single point), but none of these exhausted all the intrinsically different ways in which a motif (a repeated group of atoms) can in principle be distributed within a crystal's unit cell. This is far more complicated than the point-groups, because (1) new symmetry elements are possible which combine rotation or reflection with translation and (2) the various symmetry elements, including those just mentioned, can be situated in various positions within a unit cell and generally do not all pass through one point in the unit cell. This was recognised and analysed by three mathematically gifted theorists: E. Fedorov in Russia (in 1891), A. Schoenfliess in Germany (in 1891) and W. Barlow in England (in 1894). All the three independently established the existence of 230 distinct space groups (of symmetry elements in space), although there was some delay in settling the last three groups. Fedorov's work was not published in German until 1895 (Fedorov 1895), though it appeared in Russian in 1891, shortly before the other two published their versions. Fedorov found no comprehension in the Russia of his time, and so his priority is sometimes forgotten. Accounts of the circumstances as they affected Fedorov and Schoenfliess were published in 1962, in Fifty Years of X-ray Diffraction (Ewald 1962, pp. 341, 351), and a number of the earliest papers related to this theory are reprinted by Bijvoet et al. (1972). The remarkable feature of this piece of triplicated pure theory is that it was perfected 20 years before an experimental method was discovered for the analysis of actual crystal structures, and when such a method at length appeared, the theory of space groups turned out to be an indispensable aid to the process of interpreting the diffraction patterns, since it means that when one atom has been located in a unit cell, then many others are automatically located as well if the space group has been identified (which is not difficult to do from the diffraction pattern itself). The Swiss crystallographer P. Niggli asserted in 1928 that "every scientific structure analysis must begin with a determination of the space group", and indeed it had been Niggli (1917) who was the first to work out the systematics that would allow a space group to be identified from systematic absences in X-ray diffractograms.In 1912 Max von Laue (1879–1960), in Munich, instructed two assistants, Paul Knipping and Walter Friedrich, to send a beam of (polychromatic) X-rays through a crystal of copper sulphate and on to a photographic plate, and immediately afterwards they did the same with a zincblende crystal: they observed the first diffraction spots from a crystal. Laue had been inspired to set up this experiment by a conversation with Paul Ewald, who pointed out to him that atoms in a crystal had to be not only periodically arranged but much more closely spaced than a light wavelength. (This followed simply from a knowledge of Avogadro's Number and the measured density of a crystal.) At the time, no one knew whether X-rays were waves or particles, and certainly no one suspected that they were both. As he says in his posthumous autobiography (Von Laue 1962), he was impressed by the calculations of Arnold Sommerfeld, also in Munich, which were based on some recent experiments on the diffraction of X-rays at a wedge-shaped slit; it was this set of calculations, published earlier in 1912, that led von Laue to the idea that X-rays had a short wavelength and that crystals might work better than slits. So the experiments with copper sulphate and zincblende showed to von Laue's (and most other people's) satisfaction that X-rays were indeed waves, with wavelengths of the order of 0.1 nm. The crucial experiment was almost aborted before it could begin because Sommerfeld forbade his assistants, Friedrich and Knipping, to get involved with von Laue; Sommerfeld's reason was that he estimated that thermal vibrations in crystals would be so large at room temperature that the essential periodicity would be completely destroyed. He proved to be wrong (the periodicity is not destroyed, only the intensity of diffraction is reduced by thermal motion). Friedrich and Knipping ignored their master (a hard thing to do in those days) and helped von Laue, who as a pure theorist could not do the experiment by himself. Sommerfeld was gracious: he at once perceived the importance of what had been discovered and forgave his errant assistants.The crucial experiments that determined the structures of a number of very simple crystals, beginning with sodium chloride, were done, not by von Laue and his helpers, but by the Braggs, William (1862–1942) and Lawrence (1890–1971), father and son, over the following two years (Figure 3.3). The irony was that, as von Laue declares in his autobiographical essay, Bragg senior had only shortly before declared his conviction that X-rays were particles! It was his own son's work which led Bragg senior to declare at the end of 1912 that "the problem becomes … not to decide between two theories of X-rays, but to find … one theory which possesses the capabilities of both", a prescient conclusion indeed. At a meeting in London in 1952 to celebrate the 40th anniversary of his famous experiment, von Laue remarked in public how frustrated he had felt afterwards that he had left it to the Braggs to make these epoch-making determinations; he had not made them himself because he was focused, not on the nature of crystals but on the nature of X-rays. By the time he had shifted his focus, it was too late. It has repeatedly happened in the history of science that a fiercely focused discoverer of some major insight does not see the further consequences that stare him in the face. The Ewald volume already cited sets out the minutiae of the events of 1912 and includes a fascinating account of the sequence of events by Lawrence Bragg himself (pp. 59–63), while the subtle relations between Bragg père and Bragg fils are memorably described in Gwendolen Caroe's memoir of her father, William H. Bragg (Caroe 1978). Recent research by an Australian historian (Jenkin 1995), partly based on W.L. Bragg's unpublished autobiography, has established that the six-year-old schoolboy Lawrence, in Adelaide, fell off his bicycle in 1896 and badly injured his elbow; his father, who had read about the discovery of X-rays by Wilhelm Röntgen at the end of 1895, had within a year of that discovery rigged up the first X-ray generator in Australia and so he was able to take a radiograph of his son's elbow – the first medical radiograph in Australia. This helped a surgeon to treat the boy's elbow properly over a period of time and thereby save its function. It is perhaps not so surprising that the thoughts of father and son turned to the use of X-rays in 1912.Figure 3.3. Portraits of the two Braggs(courtesy Mr. Stephen Bragg).Henry Lipson, a British crystallographer who knew both the Braggs has commented (Lipson 1990) that "W.H. and W.L. Bragg were quite different personalities. We can see how important the cooperation between people with different sorts of abilities is; W.H. was the good sound eminent physicist, whereas W.L. was the man with intuition. The idea of X-ray reflection came to him in the grounds of Trinity College, Cambridge, where he was a student of J.J. Thomson's and should not have been thinking of such things."Lawrence Bragg continued for the next 59 years to make one innovation after another in the practice of crystal structure analysis; right at the end of his long and productive life he wrote a book about his lifetime's experiences, The Development of X-ray Analysis (Bragg 1975, 1992), published posthumously. In it he gives a striking insight into the beginnings of X-ray analysis. In 1912, he was still a very young researcher with J.J. Thomson in the Cavendish Laboratory in Cambridge, and he decided to use the Laue diffraction technique (using polychromatic X-rays) to study ZnS, NaCl and other ionic crystals. "When I achieved the first X-ray reflections, I worked the Rumkorff coil too hard in my excitement and burnt out the platinum contact. Lincoln, the mechanic, was very annoyed as a contact cost 10 shillings, and refused to provide me with another one for a month. In these days (i.e., ≈1970) a researcher who discovered an effect of such novelty and importance would have very different treatment. I could never have exploited my ideas about X-ray diffraction under such conditions … In my father's laboratory (in Leeds) the facilities were on quite a different scale." In 1913 he moved to Leeds and he and his father began to use a newly designed X-ray spectrometer with essentially monochromatic X-rays. A 1913 paper on the structure of diamond, in his own words "may be said to represent the start of X-ray crystallography". By the time he moved back to Cambridge as Cavendish professor in 1938, the facilities there had distinctly improved.Though beaten in that race by the Braggs, von Laue received the Nobel Prize in 1914, one year before the Braggs did.In spite of these prompt Nobel awards, it is striking how long it took for the new technique for determining atomic arrangements in crystals – crystal structures – to spread in the scientific community. This is demonstrated very clearly by an editorial written by the German mineralogist P. Groth in the Zeitschrift für Kristallographie, a journal which he had guided for many years. Groth, who also taught in Munich, was the most influential mineralogist of his generation and published a renowned textbook, Chemische Kristallographie. In his 1928 editorial he sets out the genesis and development of his journal and writes about many of the great crystallographers he had known. Though he refers to Federov, the creator of space groups (whom he hails as one of the two greatest geniuses of crystallography in the preceding 50 years), Groth has nothing whatever to say about X-ray diffraction and crystal structure analysis, 16 years after the original discovery. Indeed, in 1928, crystal structure analysis was only beginning to get into its stride, and mineralogists like Groth had as yet derived very few insights from it; in particular, the structure analysis of silicates was not to arrive till a few years later.1 Metallurgists, also, were slow to feel at ease with the new techniques, and did not begin to exploit X-ray diffraction in any significant way until 1923. Michael Polanyi (1891–1976), in an account of his early days in research (Polanyi 1962) describes how he and Herman Mark determined the crystal structure of white tin from a single crystal in 1923; just after they had done this, they received a visit from a Dutch colleague who had independently determined the same structure. The visitor vehemently maintained that Polanyi's structure was wrong; in Polanyi's words, "only after hours of discussion did it become apparent that his structure was actually the same as ours, but looked different because he represented it with axes turned by 45° relative to ours".Even the originator was hesitant to blow his own trumpet. In 1917, the elder Bragg published an essay on "physical research and the way of its application", in a multiauthor book entitled "Science and the Nation" (Bragg 1917). Although he writes at some length on Röntgen and the discovery of X-rays, he includes not a word on X-ray diffraction, five years after the discoveries by his son and himself.This slow diffusion of a crucial new technique can be compared with the invention of the scanning tunnelling microscope (STM) by Binnig and Rohrer, first made public in 1983, like X-ray diffraction rewarded with the Nobel Prize 3 years later, but unlike X-ray diffraction quickly adopted throughout the world. That invention, of comparable importance to the discoveries of 1912, now (2 decades later) has sprouted numerous variants and has virtually created a new branch of surface science. With it, investigators can not only see individual surface atoms but they can also manipulate atoms singly (Eigler and Schweitzer 1990). This rapid adoption of the STM is of course partly due to much better communications, but it is certainly in part to be attributed to the ability of so many scientists to recognise very rapidly what could be done with the new technique, in distinction to what happened in 1912.In Sweden, a precocious school of crystallographic researchers developed who applied X-ray diffraction to the study of metallic phases. Their leaders were Arne Westgren and Gösta Phragmén. As early as 1922 (Westgren and Phragmén 1922) they performed a sophisticated analysis of the crystal structures of various phases in steels, and they were the first (from measurements of the changes of lattice parameter with solute concentration) to recognise that solutions of carbon in body-centred alpha-iron must be 'interstitial' – i.e., the carbon atoms take up positions between the regular lattice sites of iron. In a published discussion at the end of this paper, William Bragg pointed out that Sweden, having been spared the ravages of the War, was able to undertake these researches when the British could not, and appealed eloquently for investment in crystallography in Britain. The Swedish group also began to study intermetallic compounds, notably in alloy systems based on copper; Westgren found the unit cell dimensions of the compound Cu5Zn8 but could not work out the structure; that feat was left to one of Bragg's young research students, Albert Bradley, who was the first to determine such a complicated structure (with 52 atoms in the unit cell) from diffraction patterns made from a powder instead of a single crystal (Bradley and Thewlis 1926); this work was begun during a visit by Bradley to Sweden. This research was a direct precursor of the crucial researches of William Hume-Rothery in the 1920s and 1930s (see Section 3.3.1.1).In spite of the slow development of crystal structure analysis, once it did 'take off' it involved a huge number of investigators: tens of thousands of crystal structures were determined, and as experimental and interpretational techniques became more sophisticated, the technique was extended to extremely complex biological molecules. The most notable early achievement was the structure analysis, in 1949, of crystalline penicillin by Dorothy Crowfoot-Hodgkin and Charles Bunn; this analysis achieved something that traditional chemical examination had not been able to do. By this time, the crystal structure, and crystal chemistry, of a huge variety of inorganic compounds had been established, and that was most certainly a prerequisite for the creation of modern materials science.Crystallography is a very broad science, stretching from crystal-structure determination to crystal physics (especially the systematic study and mathematical analysis of anisotropy), crystal chemistry and the geometrical study of phase transitions in the solid state, and stretching to the prediction of crystal structures from first principles; this last is very active nowadays and is entirely dependent on recent advances in the electron theory of solids. There is also a flourishing field of applied crystallography, encompassing such skills as the determination of preferred orientations, alias textures, in polycrystalline assemblies. It would be fair to say that within this broad church, those who determine crystal structures regard themselves as being members of an aristocracy, and indeed they feature prominently among the recipients of the 26 Nobel Prizes that have gone to scientists best described as crystallographers; some of these double up as chemists, some as physicists, increasing numbers as biochemists, and the prizes were awarded in physics, chemistry or medicine. It is doubtful whether any of them would describe themselves as materials scientists!2 Crystallography is one of those fields where physics and chemistry have become inextricably commingled; it is however also a field that has evinced more than its fair share of quarrelsomeness, since some physicists resolutely regard crystallography as a technique rather than as a science. (Thus an undergraduate specialisation in crystallography at Cambridge University was killed off some years ago, apparently at the instigation of physicists.) What all this shows is that scientists go on arguing about terminology as though this were an argument about the real world, and cannot it seems be cured of an urge to rank each other into categories of relative superiority and inferiority. Crystallography is further discussed below, in Section 4.2.4.A. BERMAN, in Total Pressure Measurements in Vacuum Technology, 1985Small particles suspended in a fluid medium exhibit random motion due to collisions with the surrounding molecules. This effect, known as Brownian motion, occurs in all fluids and at all pressures and can be used as a measure of the number density of molecules in a gas. A pressure gauge using this principle can be considered a primary pressure standard since its calibration can be predicted only from the knowledge of the particle dimension and density. An outstanding feature is that it can determine pressures down to the lowest degree of rarefaction attainable under laboratory conditions.Kappler (1931) used the Brownian motion of a mirror suspended in gas for the determination of Avogadro's number. He indirectly deduced the molecular collision rate since experimental conditions did not permit recording each molecular impact.Morimura et al. (1974) measured the random fashion in which a small mirror suspended on a fine quartz fiber was deflected in a rarefied gas environment. They showed that the damping moment acting on the mirror is proportional to gas pressure provided that the mean free path of gas molecules is larger than the mirror size. The damping ratio varies almost linearly with pressure in the range 10−1–1 Pa (10−3–10−2 Torr) and is almost independent of pressure from 1 to 1066.6 Pa (10−2–8 Torr). Morimura et al. assumed that nonlinearity in this region results from molecular viscosity. The gauge needs a complex electronic system and does not permit determinations below 10−1 Pa (10−3 Torr), because of the mirror suspension and vibrations imparted to the instrument by the vacuum system.Kendall (1970) suggested the use of Brownian motion as a possible basis for a vacuum gauge by utilizing very small particles suspended in gas. Such a gauge is feasible if problems such as the particle suspension, damping of oscillations, and illumination and counting of particle collisions could be adequately solved.Particles of 1-μm radius are launched from a vibrating surface mechanically or electrically in a levitation region (Butler et al., 1977). Suspension of particles in the earth's gravitational field can be achieved electromagnetically (for conducting particles), magnetically (for diamagnetic particles), or electrostatically (for charged particles). It is essential to obtain three-axis stabilization of levitated particles and damping of their oscillation after disturbances in order to keep them in the field of observation and to comply with stability requirements. Particles can be illuminated either by conventional methods or by laser, provided that heating and diffraction effects are maintained at a minimum. A medium-power microscope is sufficient for the observation of the movement of particles.The major drawbacks to the method are clustering of particles mainly when the pressure which is to be determined is below 10−1 Pa (10−3 Torr), mechanical vibrations, and radiation-induced desorption.The Brownian gauge has not yet left the research laboratory.PETER B. VOSE, in Introduction to Nuclear Techniques in Agronomy and Plant Biology, 1980Practical work with radioisotopes is continuously requiring the calculation of specific activity, weights of reacting substances, amount of activity remaining at a given time, minimum detectable amounts of radioactivity etc. Table 1.2 gives some basic numerical data often required in such calculations. Equations (1)TABLE 1.2. Basic numerical data for calculations of specific activity, half-life, attenuation and other functionsAvogadro's numberN = 6.025 × 1023atoms / g atom, or molecules/g moleBase of natural logarithmse = 2.71828ln 2 = 0.693ln x = 2.3026 log xlog e = 0.4343Conversion dataHoursMinutesSeconds1 year=8.760 × 1035.525 × 1053.154 × 1071 day=241.440 × 1038.640 × 1041 hour=1603.600 × 103and (9) provide the foundation of many of these calculations.The total number of radioactive atoms, N, in a carrier-free radioactive isotope, i.e. one not containing any stable isotope, can be calculated by means of Avogadro's number (6.025 × 1023) which is defined as the number of atoms in the atomic weight of an element expressed in grams, or in the case of a compound the number of molecules in the gram molecular weight. Thus N for 1 g of a pure radioisotope will be Avogadro's number divided by the mass number, e.g. for 32P, N=6.025×102332 atoms/g.Example: Calculate the specific activity of (a) a sample of pure 35S, and (b) a sample with 75% stable S, (half-life 35S = 87 days).∴λ=0.69387d−1=0.69387×1.44×103min−1note: conversion to minutes, as it is necessary later to express d.p.m. as Ciand N=6.025×102335∴Sp A∗=0.69387×1.44×103×6.025×102335d.p.m./g=0.693×6.025×102387×1.44×103×35×12.22×1012Ci/g=4.9×104Ci/g Sand a sample with 75% stable S would clearly only have 25% of the activity per gram total SExample: Calculate the weight of 5 mCi of pure 32P (half-life 32P = 14 days).∴A*=5×3.7×107d.p.s.λ=0.69314×8.640×104sec−1but N=A*λ=5×3.7×107×14×8.640×1040.693atoms=5×3.7×107×14×8.640×1040.693×326.025×1023g=17×10−9g=17 nanogramsExample: Assuming a minimum statistically correct detectable count rate of 10 c.p.m. above background, and a counting efficiency of 25%, calculate the minimal detectable amount of 3H, (half-life 3H = 12.26 years). A* = λN can be used to calculate the number of 3H atoms giving this activity.The minimum detectable disintegration rate will beA*=100.25=40d.p.m.=4060d.p.s.andλ=0.69312.26×3.154×107sec−1∴N=Aλ=40×12.26×3.154×10760×0.693atoms=40×12.26×3.154×10760×0.693×36.025×1023g=17.7×10−16g3H

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