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# Atoms and molecules book pdf

Introduction Context Born–Oppenheimer Approximation Approximate Methods Particle Model Independent Model Configuration Electron Interaction Electron Correlation Size-extensiveity and Size-Consistency Occupation Number Background Representation Creating and Annihilating Operators Number of Occupation Representation Number of Operators Assessment of Matrix Elements Normal-order product of ordinary operators Hole-particle formalism and vacuum Fermi Evaluation of Hamiltonian elements between reference states Normal control product for the Fermi vacuum Normal shape of the product of quantum mechanical operatorsGraphic representation of normal product operators Disruption Background theory Rayleigh–Schrödinger disturbance theory : traditional approachOperator-based prescription formulation of the disturbance theory Brillouin-Wigner disturbance theoryRayleigh-Schrödinger disturbance theoryOperator-based operator Sultura Val de Rayleigh-Schrödinger disturbance theory Factorization theorem and cancellation of unrelated terms Choice of order zero Hamiltonian H0 Intruder State Problems in Ray Disturbance Theory Leigh-Schrödinger Comparison of the Working Theory of Brillouin-Wigner and Rayleigh-Schrödinger Theories of Disruption Multi-Reference Theory Of Introduction Choice of Fermi Vacuum and Hole Particle States Self-Consistent Field Method Improved Configuration Method fully orbital active space improved Classification of formal disruptive methods multi-reference disturbance theory for complete model space Multi-reference disturbance theory for incomplete model space Hamiltonian intermediate methods, Ineffective valence methods Hamiltonian method State-Specific Disturbance Context Multi-reference Moller–Pleset Second Order Disturbance TheoryMulti-configuration quasi-degenerate theory disruption Complete active space second order disruption theory Multi-state complete active space second order disturbance theory coupled theory Method Introduction Single-reference coupled cluster method Extensive relationship with full configuration interaction ( FCI) method coupled cluster equation for double (CCD) and single and double (CCSD) approximations Evaluation of the element matrix for the pair of double equations of the group Chart representation of the elements of the matrix coupled with double clusters (CCD) Appearance of the theory of disturbance with more many bodies in the CC method Other variants of the CC Fock Space Multi-Reference Theory Coupled Cluster Method Background Choice of the waveoperator for multi-reference systems Connectivity of the actual Hamiltonian Fock space theory coupled for energy difference Systematic generation of cluster equations for different valence sectors Equation cluster method movement coupling Relationship between FSMRCC and EOMCC Intermediate numerical examples based Hamiltonian multi-reference cluster theory coupled Hilbert Space Coupled Cluster Theory Introduction universal multi-reference coupled cluster (SU-MRCC) theory Development of state-specific state-specific © 1996-2015, Amazon.com, Inc. or its affiliates PAGE 1 PAGE 2 Atoms and molecules describe the basic properties of atoms and molecules in terms of theoretical group methods in atomic and molecular physics. The book reviews mathematical concepts related to the properties of angular impulse, finite and continuous rotation groups, tensor operators, Wigner-Eckart theorem, vector fields and vector spherical harmonics. The text also explains quantum mechanics, including symmetry considerations, second quantification, density matrix, time-dependent and time-independent approximation methods. The book explains the atomic structure, in particular the Dirac equation in which its nonrelative approximation provides the basis for Hamiltonian derivation for all important interactions, such as spin-orbit, external fields, hyperphine. Together with multielectron atoms, the text discusses the theory of multiples, the formulation of Hartree-Fock, as well as the fields of electromagnetic radiation, their interactions with atoms in first and greater orders. The book explores molecules and complexes, including The Approximation of Born-Oppenheimer, Molecular Orbitals, Self-Consistent Field Method, Electronic States, Vibration and Rotation States, Molecular Spectra and Ligand Field Theory. The book can prove useful for graduate or advanced students and academics in the field of general and applied physics. This is Atoms, Molecules and Ions, Chapter 3 of the book Beginning of Chemistry (v. 1.0). For details about this (including licensing), click here. This book is licensed under a Creative Commons by-nc-sa 3.0 license. See the license for more details, but that means that essentially you can share this book as long as you credit the author (but see below), don't make money from it, and don't make it available to anyone else under the same conditions. This content has been accessible since 29 December 2012 and was then downloaded by Andy Schmitz in an effort to preserve the availability of this book. Normally, the author and publisher would be credited here. However, the publisher requested that the regular attribution of Creative Commons to the original publisher, authors, title and URI of the book be removed. In addition, at the request of the publisher, their names were removed in some passages. More information is available on the assignment page of this project. For more information on the source of this book, or why it is available free of charge, please refer to the project home page. You can browse or download additional books there. To download a .zip file that contains this book to use offline, simply click here. Did this book help you? Consider transmitting it: Creative Commons supports free culture from music to education. Their licenses helped to make this book available DonorsChoose.org helps people like you help teachers fund their classroom projects, from art materials to books to computers. Although it is not an SI unit, angstrom (Å) is a useful unit of length. This is one of the 1 meter, or 10−10 m. Why is it a useful drive? The final particles that make up all matter have a size of about 10-10 m or about 1 Å. This makes angstrom a natural unit, though not approved- for the description of these particles. The angstrom unit is named after Anders Jonas Ångström, a 19th-century Swedish physicist. Ångström's research dealt with the light emitted by bright objects, including the sun. Ångström studied the brightness of the different colors of light that the sun emitted and was able to infer that the sun is composed of the same types of matter that are present on earth. By extension, we now know that all matter in the universe is similar to the matter that exists on our planet. The basic block of matter is the atom. Curiously, the idea of atoms was first proposed in the 5th century î.Hr., when the Greek philosophers Leucippus and Democritus proposed their existence in a surprisingly modern way. However, their ideas did not take hold of their contemporaries, and it was not until the early 1800s that the evidence gathered to make scientists reconsider the idea. Today, the concept of atom is essential for the study of matter. The learning objectives of the modern atomic theory state. Find out the atoms are built. The smallest piece of an element that maintains the identity of that element is called the atomThe smallest piece of an element that maintains the identity of that element.. Individual atoms are extremely small. It would take about fifty million atoms in a row to make a line that is 1 cm long. The period at the end of a printed sentence has several million atoms in it. Atoms are so small that it's hard to believe that all matter is made of atoms, but it is. The concept that atoms play a fundamental role in chemistry is formalized by modern atomic theoryThe concept that atoms play a fundamental role in chemistry., first declared by John Dalton, an English scientist, in 1808. It consists of three parts: All matter is composed of atoms. The atoms of the same element are the same; atoms of different elements are different. Atoms combine in integer ratios to form compounds. These concepts form the basis of chemistry. Although the word atom comes from a Greek word that means indivisible, we now understand that the atoms themselves are composed of smaller parts called subatomic particles. The first part that was discovered was the subatomic particle electronA with a negative charge, a small subatomic particle with a negative charge. It is often represented as e−, with the right exponent showing the negative charge. Later, two larger particles were discovered. The proton subatomic particle with a positive charge. is a more massive (but still small) subatomic particle with a positive charge, represented as p+. Unladen neutron subatomic particle. is a subatomic with about the same mass as a proton, but without charge. It is represented either as n or n0. Now we know that the atoms of all elements are composed of electrons, protons and (with one exception) neutrons. Table 3.1 The properties of the three subatomic particles summarize the properties of these three subatomic particles. Table 3.1 Properties of the three subatomic particles Name of the Mass Symbol (approx.; kg) Pregnancy Proton p+ 1.6 × 10−27 1+ Neutron n, n0 1.6 × 10−27 none Electron e− 9.1 × 10−31 1− are these particles arranged in atoms? They're not randomly arranged. Ernest Rutherford's experiments in England in 1910 indicated a nuclear modelModel of an atom that has protons and neutrons in a central nucleus with electrons orbiting the nucleus. Atom. Relatively massive protons and neutrons are collected in the center of an atom, in a region called the nucleusThe center of an atom containing protons and neutrons. atom (plural nuclei). Electrons are outside the nucleus and spend their time orbiting in space around the nucleus. (See Figure 3.1 Structure of the atom.) Figure 3.1 The structure of the atom atoms has protons and neutrons in the center, making the nucleus, while electrons orbit the nucleus. Modern atomic theory states that the atoms of an element are the same, while the atoms of different elements are different. What makes atoms of different elements different? The fundamental characteristic that all atoms in the same element share is the number of protons. All hydrogen atoms have a single proton in the nucleus; all iron atoms have 26 protons in the nucleus. This number of protons is so important to the identity of an atom that it is called the atomic numberNumber of protons in an atom. Item. Thus, hydrogen has an atomic number of 1, while iron has an atomic number of 26. Each element has its own characteristic atomic number. Atoms of the same element may, however, have a different number of neutrons. Atoms of the same element (i.e. atoms with the same number of protons) with different neutron numbers are called isotopesAtoms of the same element that have different neutron numbers.. Most natural elements exist as isotopes. For example, most hydrogen atoms have a single proton in their nucleus. However, a small number (about one in a million) of hydrogen atoms have a proton and a neutron in their nuclei. This special isotope of hydrogen is called deuterium. A very rare form of hydrogen has a proton and two neutrons in the nucleus; this hydrogen isotope is called tritium. The sum of the number of protons and neutrons in the nucleus is called the mass numberThe sum of the number of protons and neutrons in a nucleus. isotope. Neutral atoms have the same number of electrons as protons, so their global load is zero. However, after we see later, this will not always be the case. The most common carbon atoms have six protons and six neutrons in their nuclei. What are the atomic number and mass number of these carbons A uranium isotope has an atomic number of 92 and a mass number of 235. What are the number of protons and neutrons in the nucleus of this atom? Solution If a carbon atom has six protons in the nucleus, its atomic number is 6. If it also has six neutrons in the nucleus, then the mass number is 6 + 6, or 12. If the atomic number of uranium is 92, then this is the number of protons in the nucleus. Because the mass number is 235, then the number of neutrons in the nucleus is 235 − 92, or 143. Test your number of protons in the nucleus of a tin atom is 50, while the number of neutrons in the nucleus is 68. What are the atomic number and mass number of this isotope? Response Atomic number = 50, mass number = 118 When we refer to an atom, we simply use the name of the element: the term sodium refers to the element, as well as to a sodium atom. But it can be cumbersome to use item names all the time. Instead, chemistry defines a symbol for each element. Atomic symbolA one or two letter representation of the name of an item. is a one- or two-letter abbreviation of the item name. By convention, the first letter of an item's symbol is always capitalized, while the second letter (if present) is lowercase. Thus, the symbol for hydrogen is H, the symbol for sodium is Na, and the symbol for nickel is Ni. Most symbols come from the English name of the element, although some symbols come from the Latin name of an element. (The symbol for sodium, Na, comes from its Latin name, natrium.) Table 3.2 The names and symbols of common elements list some common elements and their symbols. You should memorize the symbols in Table 3.2 Names and symbols of common elements, because this is how we will represent elements throughout chemistry. Table 3.2 Names and symbols of common elements Element Name Symbol Element Aluminum Name Al Mercury Hg Argon Ar Molibden Molibden Mo Arsenic Ca Neon Ne Bariu Ba Nichel Ni Beryllium Be Nitrogen N Bismuth Bi Oxygen O Bor b Pal Pd Brom Br Fosper P Calcium As Platinum Pt Carbon C Potassium K Chlorine Cl Radium Ra Crom Cr Radon Rn Cobalt Co Rubidium Rb Copper With Scandium Sc Fluor F Selenium Se Gallium Ga Silicon Si Germanium Ge Silver Ag Gold Au Sodium Na Helium He Str. Hydrogen H Sulf S Iodine I Ta Tantal Ta Iridium Ir Tin Sn Iron Fe Titanium Ti Krypton Kr Tungsten W Plumb Pb Uranium U Lithium Li Xenon Xe Magnesium Mg Zinc Zn Mangan Mn Zirconiu Zr Elements are grouped together in a special diagram called periodic tableA chart of all elements.. A simple periodic table is shown in Figure 3.2 A simple periodic table, while a larger one is shown in Chapter 17 Appendix: Periodic Table of Items. Items in the periodic table are listed in the order of the ascending atomic number. The periodic table has a special shape that will become important to us when the organization of electrons in atoms (see Chapter 8 Electronic structure). One One the use of the periodic table helps us to identify metals and non-metals. The nonmetals are located in the upper-right corner of the periodic table, on one side of the heavy line dividing the right side of the chart. All other elements are metals. Figure 3.2 A simple periodic table There is an easy way to represent isotopes using atomic symbols. We use the Construction of XZA where X is the symbol of the element, A is the mass number, and Z is the atomic number. Thus, for the carbon isotope which has 6 protons and 6 neutrons, the symbol is C612 where C is the symbol of the element, 6 represents the atomic number, and 12 represents the mass number. What is the symbol of a uranium isotope with an atomic number of 92 and a mass number of 235? How many protons and neutrons are in F2656e? Solution The symbol for this isotope is U92235 . This iron atom has 26 protons and 56 − 26 = 30 neutrons. Test Yourself How many protons are in N1123a? Response 11 protons It is also common to specify the mass number after the name of an element to indicate a specific isotope. Carbon-12 is a carbon isotope with 6 protons and 6 neutrons, while uranium-238 is a uranium isotope that has 146 neutrons. Key Runways Chemistry is based on modern atomic theory, which states that all matter is composed of atoms. The atoms themselves are composed of protons, neutrons and electrons. Each element has its own atomic number, which is equal to the number of protons in its nucleus. Isotopes of an element contain a different number of neutrons. The elements are represented by an atomic symbol. The periodic table is a chart that organizes all items. Exercises List the three statements that make up modern atomic theory. Explains the atoms are being combined. Which is bigger, a proton or an electron? Which is bigger, a neutron or an electron? What are the charges for each of the three subatomic particles? Where is most of the mass of an atom? Sketch a diagram of a boron atom, which has five protons and six neutrons in its nucleus. Sketch a diagram of a helium atom, which has two protons and two neutrons in its nucleus. Definition of atomic number. What is the atomic number for a boron atom? What's the atomic helium number? Define the isotope and give an example. What is the difference between deuterium and tritium? Which pair represents isotopes? H24e and H23e F2656e and M2556n S1428i and P1531 Which pair are isotopes? C2040a and K1940 F2656e and F2658e U92238 and U92235 Give complete symbols of each atom, including atomic number and mass number. an oxygen atom with 8 protons and 8 neutrons a potassium atom with 19 protons and 20 neutrons a lithium atom with 3 protons and 4 neutrons Give complete symbols of each atom, including atomic number and mass number. a magnesium atom with 12 protons and 12 neutrons a magnesium atom with 12 protons and 13 neutrons a xenon atom with 54 protons and 77 neutrons Americiu-241 is an isotope used in smoke What is the complete symbol for this isotope? Carbon-14 is an isotope used to perform radioactive dating tests on previous living material. What is the complete symbol for this isotope? Give atomic symbols for each element. sodium argon radon Give atomic symbols for each element. silver gold mercury iodine Give the name of the element. Give the name of the item. Answers All matter is composed of atoms; the atoms of the same element are the same, and the atoms of different elements are different; atoms combine in integer ratios to form compounds. A proton is larger than an electron. proton: 1+; electron: 1−; neutron: 0 Atomic number is the number of protons in a nucleus. The boron has an atomic number of five. Isotopes are atoms of the same element, but with different neutron numbers. H11 and H12 are examples. isotopes no isotopes silicon manganese iron chromium Learning Learning Objectives Define the molecule. Name simple molecules based on their formulas. Determine a formula of a molecule based on its name. There are many substances that exist as two or more atoms connected together so strongly that they behave as a single particle. These multiatom combinations are called moleculesThe smallest part of a substance that has the physical and chemical properties of that substance.. A molecule is the smallest part of a substance that has the physical and chemical properties of that substance. In some respects, a molecule is similar to an atom. A molecule, however, is composed of more than one atom. Some elements naturally exist as molecules. For example, hydrogen and oxygen exist as molecules with two atoms. Other elements also exist naturally as diatomic moleculesO molecule with only two atoms. (see Table 3.3 Elements that exist as diatomic molecules). Like any molecule, these elements are labeled with a molecular formulaA formal list of what and how many atoms are in a molecule., a formal list of what and how many atoms are in a molecule. (Sometimes only the word formula is used, and its meaning is inferred from context.) For example, the molecular formula for elemental hydrogen is H2, H being the symbol for hydrogen and index 2 implying that there are two atoms of this element in the molecule. Other diatomatic elements have similar formulas: O2, N2 and so on. Other elements exist as molecules — for example, sulfur normally exists as an eight-atom molecule, S8, while phosphorus exists as a molecule with four atoms, P4 (see Figure 3.3 Molecular art of S). Otherwise, we assume that the elements exist as individual atoms rather than molecules. It is assumed that there is only one atom in a formula if there is no numeric index on the right side of an item's symbol. Table 3.3 Elements that exist as diatomic molecules Hydrogen oxygen nitrogen fluoride chlorine bromine iodine Figure The molecular art of the molecules S8 and P4 If each green represents a sulfur atom, then the diagram on the left represents a Molecule. The molecule on the right shows that there is a form of elemental phosphorus, like a molecule with four atoms. Figure 3.3 The molecular art of S presents two examples of how we will represent molecules in this text. An atom is represented by a small ball or sphere, which generally indicates if the nucleus is in the molecule. A cylindrical line connecting the balls represents the connection between the atoms that make this collection of atoms a molecule. This bond is called the chemical bondConcorda between two atoms in a molecule. In Chapter 9 Chemical Links, we explore the origin of chemical bonds. You will see other examples of this and cylinder representation of molecules throughout this book. Many compounds exist as molecules. In particular, when nonmetals connect with other nonmetals, the compound usually exists as molecules. (The compounds between a metal and a non-metal are different and will be taken into account in point 3.4 Ion and ion compounds.) In addition, in some cases, there are many different types of molecules that can be formed between any given elements, with all different molecules having different chemical and physical properties. Do I distinguish them? The answer is a very specific system of naming compounds, called chemical nomenclatureA very specific system for naming compounds, in which single substances obtain unique names.. Following the rules of the nomenclature, each compound has its own unique name, and each name refers to a single compound. Here, we start with relatively simple molecules that have only two elements in them, the so-called binary compounds: Identify the molecule elements in its formula. This is why you need to know the names and symbols of the elements in Table 3.2 Names and symbols of common elements. Start the name with the name of the item of the first item. If there is more than one atom of this element in the molecular formula, use a numeric prefix to indicate the number of atoms, so is listed in Table 3.4 Numeric prefixes used in the name of molecular compounds. Do not use the mono-prefix if there is only one atom of the first element. Table 3.4 Numerical prefixes used in the name of molecular compounds Number of atoms of an element Prefix 1 mono- 2 di- 3 tri- 4 tetra- 5 penta- 6 hexa- 7 hepta- 8 octa- 9 nona- 10 deca- Name of the second element using three parts: a numerical prefix indicating the number of atoms of the second element, plus the strain of the element name (for example. , ox for oxygen, chlorine for chlorine, etc.), plus the suffix -ide. Combines the two words, leaving a space between them. Let's see these steps work for a molecule whose molecular formula is SO2, which has one sulfur atom and two oxygen atoms - this completes step 1. According to step 2, we start with the name of the first element – sulfur. Remember, we don't use the mono prefix for the first item. Now, for step 3, we combine numeric di- (see Table Table Numerical prefixes used in the name of molecular compounds) with the stem- and suffix -ide, to make dioxide. By bringing these two words together, we have the unique name for this compound - sulfur dioxide. Why all this trouble? There is another common compound consisting of sulfur and oxygen whose molecular formula is SO3, so the compounds must be distinguished. SO3 has three oxygen atoms in it, so it's a different compound with different chemical and physical properties. The chemical nomenclature system is designed to give this compound its own unique name. Its name, if you go through all the steps, is sulfur trioxide. Different compounds have different names. In some cases, when a prefix ends in a or a or a and the item name starts with a drop of or one on the prefix. So we see monoxide or pentoxide rather than monooxide or pentaoxide in the name of molecules. A great thing about this system is that it works both ways. From the name of a compound, you should be able to determine the molecular formula. Simply list the symbols of the element, with a numeric index if there is more than one atom of that element, in the order of the name (we do not use an index 1 if there is only one atom of the present element; 1 is the default). From the name of nitrogen trichloride, you should be able to get NCl3 as the formula for this molecule. From the name of penoxide diphosphorus, you should be able to get the formula P2O5 (note the numeric prefix on the first element, indicating that there is more than one phosphorus atom in the formula). Name each molecule. Solution A molecule with a single phosphorus atom and three fluoride atoms is called phosphorus trifluoride. A compound with a carbon atom and an oxygen atom is appropriately called carbon monoxide, not carbon monooxide. There are two atoms in each element, selenium and bromine. According to the rules, the correct name here is dibromide of divincion. Test Your Name Each Molecule. Sulfur tetrafluoride responses diphosphorus pentasulfur Give formula for each molecule. Carbon tetrachloride silicon dioxide trisilicon tetranitre Solution The name of carbon tetrachloride implies one carbon atom and four chlorine atoms, so the formula is CCl4. The name of silicon dioxide implies one silicon atom and two oxygen atoms, so the formula is SiO2. We have a name that has numeric prefixes on both elements. Tri- means three, and tetra- means four, so the formula for this compound is Si3N4. Test your Yes formula for each molecule. disulfur difluoride iodine pentabrorid Answers Some simple molecules have common names that we use as part of the formal chemical nomenclature system. For example, H2O is given the name water, not dihydrogen monoxide. NH3 is called ammonia, while CH4 is called methane. We will occasionally see other molecules that have common names; we'll show them as they come. Key Takeaways Molecules are groups of atoms that as a single unit. Some elements exist as molecules: molecules: oxygen, sulfur, and so on. There are rules that can express a unique name for any given molecule, and a unique formula for any given name. Exercises Which of these formulas represent molecules? Tell me how many atoms are in each molecule. Which of these formulas are molecules? Tell me how many atoms are in each molecule. What is the difference between CO and Co? What is the difference between H2O and H2O2 (hydrogen peroxide)? The correct formula is given for each diatomic element. In 1986, when Halley's comet last passed by Earth, astronomers detected the presence of S2 in their telescopes. Why is sulfur not considered a diatomic element? What is the fluoride strain used in the name of molecules? CF4 is an example. What is the selenium strain used in the name of molecules? SiSe2 is an example. Give the right name for each molecule. Give the right name for each molecule. Give the right name for each molecule. Give the right name for each molecule. Give the right name for each molecule. Give the correct formula for each name. dinitrogen pentoxide tetraboron tricarbid phosphorus pentachloride Gives the correct formula for each name. triiodide nitrogen diarsenic trisulphide of trichloride iodine Gives the correct formula for each name. dioxigen dichloride dithrogen trisulfur of xenon tetrafluoride Gives the correct formula for each name. chlorine dioxide selenium dibrodice dinitrogen trioxide Gives the correct formula for each name. iodine trifluoride xenon trioxide disulfur decapitar Gives the correct formula for each name. germanium dioxide dibolid carbon dibromide Responses not a molecule a molecule; four atoms total a molecule; four total atoms not a CO molecule is a carbon and oxygen compound; Co is the cobalt element. H2, O2, N2, F2, Cl2, Br2, I2 phosphorus trifluoride tellur dichloride dithrogen trioxide xenon difluoride dioxigen difluoride sulfur hexafluoride dinitrogen dinitrogen titrox dinitrogen pentoxide learning Objective express edit masses of atoms and molecules. Since matter is defined as anything that has mass and takes up space, it shouldnot be surprising to learn that atoms and molecules have mass. Individual atoms and molecules, however, are very small, and the masses of individual atoms and molecules are also very small. For macroscopic objects, we use units such as grams and kilograms to specify their masses, but these units are far too large to comfortably describe the masses of individual atoms and molecules. It takes another ladder. Atomic mass unitA twelfth of the mass of a carbon-12 atom. (u; some texts use amu, but this older style is no longer accepted) is defined as a twelfth of the mass of a carbon-12 atom, a carbon isotope that has six protons and six neutrons in its nucleus. By this scale, the mass of a proton 1,00728 u, the mass of a neutron is 1,00866 u, and the mass of an electron is 0,000549 u. There will be much error if you estimate the mass an atom by simply counting the total number of protons and neutrons in the nucleus (i.e. identifying its mass number) and ignoring electrons. Thus, the mass of carbon-12 is about 12 u, the mass of oxygen-16 is about 16 u, and the mass of uranium-238 is about 238 u. More accurate masses are found in scientific references- for example, the exact mass of uranium-238 is 238.050788 u, so you can see that we are not far away by using the value of the whole number as the mass of the atom. What is the mass of an item? This is somewhat more complicated because most elements exist as a mixture of isotopes, each of which has its own mass. Thus, although it is easy to talk about the mass of an atom, when talking about the mass of an element, we must consider the isotopic mixture. Atomic massA weighted averages of the isotope masses that make up an element. an element is a weighted average of the isotope masses that make up an element. What do we mean by a weighted average? Well, consider an element that consists of two isotopes, 50% with mass 10 you and 50% with mass 11 u. A weighted average is found multiplying each mass with fractional appearance (in decimal form) and then adding all products. The amount is the weighted average and serves as the formal atomic mass of the element. In this example, we have the following: Note that no atom in our hypothetical element has a mass of 10.5 u; rather, this is the average mass of atoms, weighted by their percentage occurrence. This example is similar to a real item. Boron exists as about 20% boron-10 (five protons and five neutrons in nuclei) and about 80% boron-11 (five protons and six neutrons in nuclei). The atomic mass of boron is calculated in a similar way to what we did for our hypothetical example, but the percentages are different: Thus, we use 10.8 u for the atomic mass of the boron. Virtually all elements exist as isotope mixtures, so atomic masses can vary significantly from integers. Table 3.5 Selected atomic masses of some elements list the atomic masses of some elements; a more expansive table is in Chapter 17 Appendix: Periodic Table of Items. Atomic masses in Table 3.5 Selected atomic masses of some elements are listed with three decimal places where possible, but in most cases only one or two decimal places are required. Note that many of the atomic masses, especially the larger ones, are not very close to integers. This is, in part, the effect of an increasing number of isotopes as atoms grow in size. (The record number is 10 isotopes for tin.) Table 3.5 Selected atomic masses of elements Name element Atomic mass (u) Name element Atomic mass (u) Aluminum 26.981 Molybdenum 95.94 Argon 39.948 Neon 20.180 Arsenic 74.922 Nickel 58.693 Barium 137.327 Nitrogen 14.00 7 Beryllium 9.012 Oxygen 15.999 208.980 Palladium 106.42 Bor 10.811 Phosphorus 30.974 Brom 79.904 Platinum 195.084 Calcium 40.078 Potassium 39.098 Carbon Radium n/a Chlor 35.453 Radon n/a Cobalt 58.933 Rubidium 85.468 Copper 63.546 Scandium 44.956 Fluor 18.998 Selenium 78.96 Galiu 69.723 Silicium 2 8.086 Germanium 72.64 Silver 107.86 8 Gold 196.967 Sodium 22.990 Helium 4.003 Stronium 87.62 Hydrogen 1.008 Sulf 32.065 Iodine 126.904 Tanta 180.948 Iridium 192.217 Tin 118.710 Iron 55.845 Titan 4 7.867 Krypton 83.798 Tungsten 183.84 Lead 207.2 Uranium 238.029 Lithium 183.84 Lead 207.2 Uranium 238.029 Lithium 207.029 Lithium 207.029 Lithium 207.029 Lithium 207.029 Lithium 207.029 Lithium 207.029 Lithium 20 6.941 Xenon 131.293 Magnesium 24.305 Zinc 65.409 Mangan 54.938 Zirconium 91.224 Mercury 200.59 Molybdenum 95.94 Note: The atomic mass is given at three decimal places, if known. Now that we understand that atoms have mass, it's easy to extend the concept to the mass of molecules. Molecular massThe sum of the masses of atoms in a molecule. is the sum of the masses of atoms in a molecule. This may seem like a trivial extension of the concept, but it is important to count the number of each type of atom in the molecular formula. Also, although each atom in a molecule is a specific isotope, we use the weighted average, or atomic mass, for each atom in the molecule. For example, if we were to determine the molecular mass of dinitrogen trioxide, N2O3, we would have to add the atomic mass of nitrogen twice with the atomic mass of oxygen three times: We would not be far away if we limited our number to one or even two decimal places. What is the molecular mass of each substance? Solution Add an atomic nitrogen mass and three atomic bromine masses: Add two atomic carbon masses and six atomic hydrogen masses: Compound C2H6 also has a common name – ethane. Test yourself What is the molecular mass of each substance? Answers On March 20, 1995, the Japanese terrorist group Aum Shinrikyo (Sanskrit for the Supreme Truth) launched some sarin gas into the Tokyo subway system; twelve people were killed, and thousands were injured (part (a) of the accompanying figure) Sarin (molecular formula C4H10FPO2) is a nerve toxin that was first synthesized in 1938. It is considered to be one of the deadliest known toxins, estimated to be about 500 times stronger than cyanide. Scientists and engineers studying the spread of chemical weapons, would be sarin (yes, there are such scientists) would like to have a less dangerous chemical, indeed, one that is nontoxic, so they are not threatening themselves. Sulfur hexafluoride is used as a model compound for sarin. SF6 (a molecular model that is shown in part (b) in the accompanying figure) has a similar molecular mass (approximately 146 u) as sarin (approximately 140 u), so it has similar physical properties in the vapor phase. Sulphur hexafluoride is also very easy to detect accurately, even at low levels, and is not a normal part of the atmosphere, so there is a potential contamination from natural sources. Therefore, SF6 is also used as an air tracer for ventilation systems in buildings. It is non-toxic and very chemically inert, so workers should not take special precautions than watching for asphyxiation. Figure 3.4 Sarin and sulphur hexafluoride (a) Properly protected workers release the Tokyo metro after the sarin nerve toxin has been released. (b) A molecular model of SF6. (c) A set of high-voltage electric switches that would be filled with SF6 as a spark suppressor. Sulfur hexafluoride also has another interesting use: a spark suppressor in high voltage electrical equipment. High-pressure SF6 gas is used instead of older oils that may have contaminants that are environmentally friendly (part (c) of the accompanying figure). Key Takeaways Atomic Mass Unit (u) is a unit that describes the masses of individual atoms and molecules. Atomic mass is the weighted average of the masses of all isotopes of an element. Molecular mass is the sum of the masses of atoms in a molecule. Exercises Define the atomic mass unit. What is his abbreviation? Defines atomic mass. What's his unit? Estimate the mass, in whole numbers, of each isotope. hydrogen-1 hydrogen-3 iron-56 Estimate the mass, in whole numbers, of each isotope. phosphorus-31 carbon-14 americium-241 Determine the atomic mass of each element, taking into account the isotopic composition. lithium, which is 92.4% lithium-7 (mass 7,016 u) and 7,60% lithium-6 (mass 6,015 u) oxygen, which is 99.76% oxygen-16 (mass 15.995 u), 0.038% oxygen-17 (mass 16.999 u), and 0.205% oxygen-18 (mass 17.999 u) Determine the atomic mass of each element, taking into account the isotopic composition. neon, which is 90.48% neon-20 (mass 19.992 u), 0.27% neon-21 (mass 20.994 u), and 9.25% neon-22 (mass 21.991 u) uranium, which is 99.27% uranium-238 (mass 238.051 u) and 0.720% uranium-235 (mass 235.044 u) How far would your response from Exercise 5a be if you used whole-number masses for individual lithium isotopes? How far would your 6b exercise response be if you used integer masses for individual uranium isotopes? What is the atomic mass of an oxygen atom? What is the molecular mass of oxygen in its elemental form? What is the atomic mass of bromine? What is the molecular mass of bromine in its elemental form? Determine the mass of each substance. Determine the mass of each substance. Determine the mass of each substance. Determine the mass of each substance. Determine the mass of each substance. Determine the mass of each substance. Determine the mass of each substance. Responses Atomic mass unit is defined as a twelfth of the mass of a carbon-12 atom. Its abbreviation is u. 37.996 u 28.010 u 44.009 u 22.990 u 69.619 u 135.036 u 104.64 u 183.898 u 245.281 u Learning objectives I know form ions. Learn the characteristic charges that ions have. Build a suitable formula for an ion compound. Generates a suitable name for an ion compound. So far, we have discussed elements and compounds that are electrically neutral. Have the same number of as protons, so that the negative charges of electrons are balanced by the positive loads of protons. However, this is not always the case. Electrons can from one atom to another; when they do, species with global electrical loads are formed. Such species are called ionA species with a global electrical charge.. Species with global positive taxes are called cationiA species with a global positive load., while species with global negative charges are called anioniA species with a global negative load.. Remember that ions form only when electrons move from one atom to another; a proton never moves from one atom to another. Compounds formed from positive and negative ions are called ionial compoundcompound compounds consisting of positive and negative ions.. Individual atoms can gain or lose electrons. When they do, they become monatomic ions. When atoms gain or lose electrons, they usually gain or lose a characteristic number of electrons and thus take on a characteristic global charge. Table 3.6 The monatomic ions of the various charges list how many common ions they lose (making cations) or gain (making anions). There are several things to observe about the ions in Table 3.6 Monatomic ions of various charges. First, each cation-forming element is a metal, except one (hydrogen), while each element that forms anions is a nonmetal. This is actually one of the chemical properties of metals and nonmetals: metals tend to form cations, while nonmetals tend to form anions. Second, most atoms form ions of a single characteristic charge. When sodium atoms form ions, they always form a load of 1+, never a load of 2+ or 3+ or even 1−. Thus, if you commit the information in Table 3.6 Monatomic ions of different taxes in memory, you will always know what most atoms load. (In Chapter 9 Chemical Links, we'll discuss why atoms make up the taxes they make.) Table 3.6 Monatomic ions of various loads Ioni formed by the loss of a single electron H + Na + K + Rb + Ag + Au + Ions formed by the loss of two electrons Mg2 + Ca2 + Sr2 + Fe2 + Co2 + Ni2 + Cu2 + Zn2 + Sn2 + Hg2 + Pb2 + Ions formed by the loss of three electrons Sc3+ Fe3+ Co3+ Ni3+ Au3+ Al3+ Cr3+ Ions formed by the loss of four electrons Ti4+ Sn4+ Pb4+ Ions formed by obtaining a single electron F− Cl− Br− I− Ions formed by obtaining two electrons O2− S2− Se2− Ions formed by obtaining three electrons N3− P3− Third, there are some exceptions to the previous point. A few elements, all metals, can form more than one possible task. For example, iron atoms can form 2+ cations or 3+ cations. Cobalt is another element that can form more than one possible charged ion (2+ and 3+), while lead can form 2+ or 4+ cations. Unfortunately, there is little understanding that two charges a metal atom can take, so it is best to memorize only the possible charges a particular item can have. Write down the convention to indicate a The magnitude of the cargo is listed as an exponent right next to the item symbol. If the fee is positive or negative, number 1 is not written; if the magnitude of the load is greater than 1, then is written before the + or − sign. An item symbol without a task written next to it is supposed to be the unladen atom. The name of an ion is simple. For a cation, simply use the item name and add the ion word (or, if you want it to be more specific, add cation) after the item name. So Na+ is sodium ion; Ca2+ is calcium ion. If the item has more than one charge possible, the tax amount comes after the item name and before the ion word. Thus, Fe2+ is iron two ions, while Fe3+ is iron three ions. In print, we use Roman numerals in parentheses to represent the load on the ion, so that these two iron ions would be represented as iron (II) cation and iron (III) cation, respectively. For a monatomic anion, use the element name strain and add the suffix -ide to it, and then add ion. This is similar to how we called molecular compounds. Thus, Cl− is the chloride ion, and N3− is the nitride ion. Name each species. Solution This species has a load of 2− on it, so it is an anion. Anions are named using the element name strain with the added suffix -ide. This is anion oxide. Because this species has no toll, it is an atom in its elemental form. That's cobalt. In this case, there is a load of 2+ per atom, so it is a cation. We observe from Table 3.6 The monatomic ions of the various charges that cobalt cations can have two possible loads, so that the ion name must specify what charge the ion has. This is cobalt cation (II). Test your name each species. Responses to the anion of the phosphorus cation phosphide, the chemical formulas for ion compounds are called ionic formulasChemical formula for an ion compound.. An appropriate ion formula has a cation and anion in it; an ion compound is never formed only between two cations or only two anions. The key to writing appropriate ion formulas is simple: the total positive charge must balance the total negative load. Because ion charges are characteristic, sometimes we need to have more than one of a cation or anion to balance positive and negative global charges. It is conventional to use the lowest ratio of ions that are needed to balance charges. For example, consider the ion compound between Na+ and Cl−. Each ion has a single charge, a positive one and a negative one, so we need only one ion from each to balance the overall load. When writing the ion formula, we follow two additional conventions: (1) we write the formula for the first cation and the formula for the following anion, but (2) do not write the charges on the ion. Thus, for the compound between Na+ and Cl−, we have the NaCl ion formula (Figure 3.5 NaCl = Mass salt). The Na2Cl2 formula also has balanced charges, but the convention is to use the lowest ion ratio, which would be one of each. (Remember to our conventions to write formulas that do not write an index 1 where there is only one atom of a certain element present.) For the ionic compound magnesium cations (Mg2+) and oxide anions (O2−), again we only need one of each ion to balance the charges. By convention, the formula is MgO. Figure 3.5 NaCl = Table salt The NaCl ionic compound is very common. For the ion compound between Mg2+ and Cl− ions, we now consider that the charges have different magnitudes, 2+ on magnesium ions and 1− on chloride ions. To balance the charges with the lowest number of ions possible, we need two chloride ions to balance the load on a magnesium ion. Rather than write the mgClCl formula, we combine the two chloride ions and write it with an index 2: MgCl2. What is the formula MgCl2 tells us? There are two chloride ions in the formula. Although chlorine as an element is a diatomic molecule, Cl2, elemental chlorine is not part of this ion compound. Chlorine is in the form of a negatively charged ion, not the neutral element. Index 2 is in the ion formula because we need two Cl− ions to balance the load on an Mg2+ ion. Write the appropriate ion formula for each of the two ions given. Ca2+ and Cl− Al3+ and F− Al3+ and O2− Solution We need two Cl− ions to balance the load on a Ca2+ ion, so that the appropriate ion formula is CaCl2. We need three F− ions to balance the load on the Al3+ ion, so the correct ion formula is AlF3. With Al3+ and O2−, keep in mind that none of the fees is a perfect multiple of the other. That means we have to move on to the least common multiple, which in this case will be six. To get a total of 6+, we need two Al3+ ions; to get 6−, we need three O2− ions. Therefore, the correct ion formula is Al2O3. Test Write the appropriate ion formulas for each of the two ions given. Fe2+ and S2− Fe3+ and S2− Answers The name of