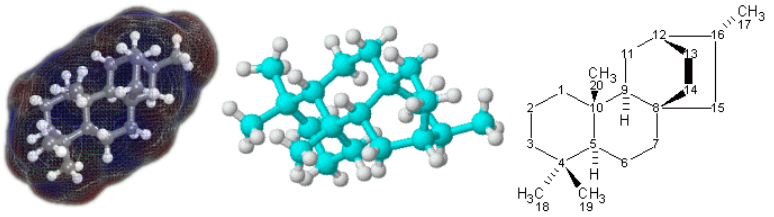
Molecule



3D (left and center) and 2D (right) representations of the terpenoid molecule atisane

A **molecule** (/ˈmɒlɪkjuːl/) is an electrically neutral group of at least two atoms held together by covalent chemical bonds.[1] [2] [3] [4] [5] [6] Molecules are distinguished from ions by their electrical charge. However, in quantum physics, organic chemistry, and biochemistry, the term *molecule* is often used less strictly and applied to polyatomic ions.

In the kinetic theory of gases, the term *molecule* is often used for any gaseous particle regardless of its composition. According to this definition noble gas atoms are considered molecules despite the fact that they are composed of a single non-bonded atom.[7]

A molecule may consist of atoms of a single chemical element, as with oxygen (O_2), or of different elements, as with water (H_2O). Atoms and complexes connected by non-covalent bonds such as hydrogen bonds or ionic bonds are generally not considered single molecules.[8]

Molecules as components of matter are common in organic substances (and therefore biochemistry). They also make up most of the oceans and atmosphere. A large number of familiar solid substances, however, including most of the minerals that make up the crust, mantle, and core of the Earth itself, contain many chemical bonds, but are *not* made of identifiable molecules. No typical molecule can be defined for ionic crystals (salts) and covalent crystals (network solids), although these are often composed of repeating unit cells that extend either in a plane (such as in graphene) or three-dimensionally (such as in diamond or sodium chloride). The theme of repeated unit-cellular-structure also holds for most condensed phases with metallic bonding. In glasses (solids that exist in a vitreous disordered state), atoms may also be held together by chemical bonds without any definable molecule, but also without any of the regularity of repeating units that characterises crystals.

Molecular science

The science of molecules is called *molecular chemistry* or *molecular physics*, depending on the focus. Molecular chemistry deals with the laws governing the interaction between molecules that results in the formation and breakage of chemical bonds, while molecular physics deals with the laws governing their structure and properties. In practice, however, this distinction is vague. In molecular sciences, a molecule consists of a stable system (bound state) comprising two or more atoms. Polyatomic ions may sometimes be usefully thought of as electrically charged molecules. The term *unstable molecule* is used for very reactive species, i.e., short-lived assemblies (resonances) of electrons and nuclei, such as radicals, molecular ions, Rydberg molecules, transition states, van der Waals complexes, or systems of colliding atoms as in Bose-Einstein condensate

History and etymology

According to Merriam-Webster and the Online Etymology Dictionary, the word "molecule" derives from the Latin "moles" or small unit of mass.

- **Molecule** (1794) – "extremely minute particle," from Fr. *molécule* (1678), from Mod.L. *molecula*, dim. of L. moles "mass, barrier". A vague meaning at first; the vogue for the word (used until late 18th century only in Latin form) can be traced to the philosophy of Descartes.

Although the existence of molecules has been accepted by many chemists since the early 19th century as a result of Dalton's laws of Definite and Multiple Proportions (1803–1808) and Avogadro's law (1811), there was some resistance among positivists and physicists such as Mach, Boltzmann, Maxwell, and Gibbs, who saw molecules merely as convenient mathematical constructs. The work of Perrin on Brownian motion (1911) is considered to be the final proof of the existence of molecules.

The definition of the molecule has evolved as knowledge of the structure of molecules has increased. Earlier definitions were less precise, defining molecules as the smallest particles of pure chemical substances that still retain their composition and chemical properties.[9] This definition often breaks down since many substances in ordinary experience, such as rocks, salts, and metals, are composed of large networks of chemically bonded atoms or ions, but are not made of discrete molecules.

Molecular size

Most molecules are far too small to be seen with the naked eye, but there are exceptions. DNA, a macromolecule, can reach macroscopic sizes, as can molecules of many polymers. The smallest molecule is the diatomic hydrogen (H_2), with a length of 0.74 Å.[10] Molecules commonly used as building blocks for organic synthesis have a dimension of a few Å to several dozen Å. Single molecules cannot usually be observed by light (as noted above), but small molecules and even the outlines of individual atoms may be traced in some circumstances by use of an atomic force microscope. Some of the largest molecules are macromolecules or supermolecules.

Radius

Effective molecular radius is the size a molecule displays in solution.[11] [12] The table of permselectivity for different substances contains examples.

Molecular formula

A compound's empirical formula is the **simplest** integer ratio of the chemical elements that constitute it. For example, water is always composed of a 2:1 ratio of hydrogen to oxygen atoms, and ethyl alcohol or ethanol is always composed of carbon, hydrogen, and oxygen in a 2:6:1 ratio. However, this does not determine the kind of molecule uniquely – dimethyl ether has the same ratios as ethanol, for instance. Molecules with the same atoms in different arrangements are called isomers. Also carbohydrates, for example, have the same ratio (carbon:hydrogen:oxygen = 1:2:1) (and thus the same empirical formula) but different total numbers of atoms in the molecule.

The molecular formula reflects the exact number of atoms that compose the molecule and so characterizes different molecules. However different isomers can have the same atomic composition while being different molecules.

The empirical formula is often the same as the molecular formula but not always. For example the molecule acetylene has molecular formula C_2H_2, but the simplest integer ratio of elements is CH.

The molecular mass can be calculated from the chemical formula and is expressed in conventional atomic mass units equal to 1/12th of the mass of a neutral carbon-12 (^{12}C isotope) atom. For network solids, the term formula unit is used in stoichiometric calculations.

Molecular geometry

Molecules have fixed equilibrium geometries—bond lengths and angles— about which they continuously oscillate through vibrational and rotational motions. A pure substance is composed of molecules with the same average geometrical structure. The chemical formula and the structure of a molecule are the two important factors that determine its properties, particularly its reactivity. Isomers share a chemical formula but normally have very different properties because of their different structures. Stereoisomers, a particular type of isomers, may have very similar physico-chemical properties and at the same time different biochemical activities.

Molecular spectroscopy

Molecular spectroscopy deals with the response (spectrum) of molecules interacting with probing signals of known energy (or frequency, according to Planck's formula). Molecules have quantized energy levels that can be analyzed by detecting the molecule's energy exchange through absorbance or emission.[13] Spectroscopy does not generally refer to diffraction studies where particles such as neutrons, electrons, or high energy X-rays interact with a regular arrangement of molecules (as in a crystal).

Theoretical aspects

The study of molecules by molecular physics and theoretical chemistry is largely based on quantum mechanics and is essential for the understanding of the chemical bond. The simplest of molecules is the hydrogen molecule-ion, H_2^+, and the simplest of all the chemical bonds is the one-electron bond. H_2^+ is composed of two positively charged protons and one negatively charged electron, which means that the Schrödinger equation for the system can be solved more easily due to the lack of electron–electron repulsion. With the development of fast digital computers, approximate solutions for more complicated molecules became possible and are one of the main aspects of computational chemistry.

When trying to define rigorously whether an arrangement of atoms is "sufficiently stable" to be considered a molecule, IUPAC suggests that it "must correspond to a depression on the potential energy surface that is deep enough to confine at least one vibrational state".[1] This definition does not depend on the nature of the interaction between the atoms, but only on the strength of the interaction. In fact, it includes weakly bound species that would not traditionally be considered molecules, such as the helium dimer, He_2, which has one vibrational bound state[14] and is so loosely bound that it is only likely to be observed at very low temperatures.

References

[1] IUPAC, *Compendium of Chemical Terminology*, 2nd ed. (the "Gold Book") (1997). Online corrected version: (1994) " molecule (http://goldbook.iupac.org/M04002.html)".

[2] Pauling, Linus (1970). *General Chemistry*. New York: Dover Publications, Inc.. ISBN 0-486-65622-5.

[3] Ebbin, Darrell, D. (1990). *General Chemistry, 3rd Ed.*. Boston: Houghton Mifflin Co.. ISBN 0-395-43302-9.

[4] Brown, T.L. (2003). *Chemistry – the Central Science, 9th Ed.*. New Jersey: Prentice Hall. ISBN 0-13-066997-0.

[5] Chang, Raymond (1998). *Chemistry, 6th Ed.*. New York: McGraw Hill. ISBN 0-07-115221-0.

[6] Zumdahl, Steven S. (1997). *Chemistry, 4th ed.*. Boston: Houghton Mifflin. ISBN 0-669-41794-7.

[7] Chandra, Sulekh. *Comprehensive Inorganic Chemistry*. New Age Publishers. ISBN 8122415121.

[8] Molecule (http://www.britannica.com/EBchecked/topic/388236/molecule), Encyclopaedia Britannica on-line

[9] Molecule Definition (http://antoine.frostburg.edu/chem/senese/101/glossary/m.shtml#molecule) (Frostburg State University)

[10] Roger L. DeKock, Harry B. Gray (1989). *Chemical structure and bonding* (http://books.google.com/?id=q77rPHP5fWMC&pg=PA199). University Science Books. p. 199. ISBN 093570261X. .

[11] Chang RL, Deen WM, Robertson CR, Brenner BM. (1975). "Permselectivity of the glomerular capillary wall: III. Restricted transport of polyanions". *Kidney Int.* **8** (4): 212–218. doi:10.1038/ki.1975.104. PMID 1202253.

[12] Chang RL, Ueki IF, Troy JL, Deen WM, Robertson CR, Brenner BM. (1975). "Permselectivity of the glomerular capillary wall to macromolecules. II. Experimental studies in rats using neutral dextran" (http://www.pubmedcentral.nih.gov/articlerender.fcgi?tool=pmcentrez&artid=1334749). *Biophys J.* **15** (9): 887–906. doi:10.1016/S0006-3495(75)85863-2. PMID 1182263. PMC 1334749.

[13] IUPAC, *Compendium of Chemical Terminology*, 2nd ed. (the "Gold Book") (1997). Online corrected version: (1997,2006) " spectroscopy (http://goldbook.iupac.org/{{{file}}}.html)".

[14] Anderson JB (May 2004). "Comment on "An exact quantum Monte Carlo calculation of the helium-helium intermolecular potential" [J. Chem. Phys. 115, 4546 (2001)]". *J Chem Phys* **120** (20): 9886–7. doi:10.1063/1.1704638. PMID 15268005.

External links

- Molecule of the Month (http://www.chm.bris.ac.uk/motm/motm.htm) – School of Chemistry, University of Bristol

Article Sources and Contributors

Molecule *Source*: http://en.wikipedia.org/w/index.php?oldid=410702187 *Contributors*: -Midorihana-, 194.200.130.xxx, 2D, 4lex, AUG, Abecedare, Abrech, Academic Challenger, Accurizer, Addshore, Admp, AeonicOmega, Agent Smith (The Matrix), Ahoerstemeier, Akendall, Akmkgp, Alansohn, Alarics, Alchemist Jack, AlexiusHoratius, American Eagle, Amplitude101, AnakngAraw, Andel, Andonic, Andre Engels, Andres, Animum, Anna Lincoln, Anonymous editor, Antixt, Arkuat, Art LaPella, Atrip, Avicennasis, Azazell0, BMunage, Barras, Bart133, Bduke, Ben-Zin, Bensaccount, Bernarddb, Bihco, Binary TSO, Bluemask, Bluestar232, Bobblewik, Bobo The Ninja, Bobo192, BodyTag, Bomac, Bongwarrior, BoxingWear3, Brandmeister, Burntsauce, Cacycle, Caknuck, Callmarcus, Can't sleep, clown will eat me, CanonLawJunkie, Capricorn42, Captain538, CarbonCopy, CardinalDan, CattleGirl, Cburnett, Centrx, ChemGardener, ChemNerd, Christian List, Christian75, CiTrusD, Conversion script, Coren, Cosmic Latte, Crohnie, Ctbolt, Ctjf83, Curps, Cursayer, DMacks, DR.smallprick, DVD R W, Daveberos, David Shear, Dbenbenn, Dcandy, Ddoherty, DeadEyeArrow, Deglr6328, Deor, DerHexer, Deryck Chan, Disavian, Discospinster, DivineAlpha, Droll, E. Fokker, EdGl, Edgar181, Edguy99, Ehrenkater, Elipongo, Enviroboy, Epbr123, Erajda, Eric Forste, Eric-Wester, Erik9, Everard Proudfoot, Everyking, Evil saltine, Excirial, Explicit, Exzakin, Favonian, Fishhead15, Fleminra, Flowerpotman, FlyingToaster, Footballfan190, Fred Bauder, Fredrik, Funnybunny123456789, Fusion7, GB fan, GMiranda, Gakrivas, Galoubet, Gawaxay, Gentgeen, Giftlite, Gilliam, Gnowor, Gogo Dodo, Golnazfotohabadi, Graham87, Greg L, Gsmgm, Guoguo12, Gurch, Guy Peters, Gökhan, Hadal, Hallenrm, Halsall, Hans Dunkelberg, HappyCamper, Happysailor, Headbomb, Heimstern, Hetar, HexaChord, Husond, Hydrogen Iodide, Ian Pitchford, Icairns, Icseaturtles, Ignatzmice, Insanity Incarnate, Iridescent, IronGargoyle, Ironist, Itub, Ivan Akira, Izzymello, J.delanoy, JAn Dudík, JForget, JaGa, Jackfork, Jade Knight, James A. Stewart, Jason Leach, Jauhienij, Jayg101, Jaytoneypwnz, Jclemens, Jcwf, Jebba, Jimmywolfe100, Jmnbpt, JoanneB, John, John W. Kennedy, JohnArmagh, JohnCD, Johnbibby, Jolt76, Jorge Stolfi, Joshua Issac, Juliobryant24, Jusdafax, Justinashley, KBlott, KPH2293, Kagredon, Karol Langner, Katimawan2005, Kendal Ozzel, Ketsuekigata, Kingkamata, KnightLago, Kyle Barbour, KyleRGiggs, L Kensington, LAX, Landon1980, LeaveSleaves, Liftarn, Lightmouse, Ligulem, Linas, Linshukun, Lir, Littlealien182, Livajo, LizardJr8, Locumele, Lolimgay, Looie496, Looxix, Lowzeewee, Lradrama, Lsy098, Lucinos, M stone, Mannafredo, Marc Venot, Marek69, MarkSutton, Materialscientist, Mattdj2, McDogm, Mclparker, Mcpazzo, Mermaid from the Baltic Sea, Merovingian, Michael Hardy, Michaelas10, Middayexpress, MightyWarrior, Mikael Häggström, Mike Dill, Mike Rosoft, Mileycyrushater9, Miquonranger03, Moreschi, Moshe Constantine Hassan Al-Silverburg, Munita Prasad, Muttenjeff, Mykej, Mythealias, N5iln, Nanobug, Ncmvocalist, Negovori, Nikai, Noctibus, Nono64, Numbo3, Nunquam Dormio, OSt, Obradovic Goran, Ohnoitsjamie, Omicronpersei8, Ospalh, Otisjimmy1, Otvaltak, P99am, Patrick, Pedro, Phaldo, Phil Boswell, PhilKnight, Philip Trueman, Pietdesomere, Pill, Piolinfax, Pokeman, Postdlf, Prodego, Qxz, RJHall, Range125, Recognizance, Res2216firestar, Restre419, RexNL, Rgoodermote, Rifleman 82, Rmiller8, Road Wizard, Ron Ritzman, Rrburke, Russellboyd, SDC, Sadi Carnot, Sahuagin, Samuel, Sander123, SasukeX, Sbharris, Scarian, Scientizzle, Scjessey, Shizhao, Shoeofdeath, Shortydude3630, Sionus, Skynet1216, Smalljim, Sodium, Someguy1221, SonicAD, Sophus Bie, SpaceFlight89, SpeedyGonsales, Starkiller88, SteveLower, Steven Zhang, Strangey0, Suntag, SuperHamster, THB, Tarquin, Template namespace initialisation script, The High Fin Sperm Whale, The Rambling Man, The Thing That Should Not Be, Thebigbendizzle, Thecheesykid, Tide rolls, TigerShark, TimonyCrickets, TomasBat, TotoBaggins, TravisAF, Troy 07, Tygar, Tyler, Unconcerned, Unschool, Useight, V8rik, Vb, Versus22, Viriditas, Vsmith, Vulcan Hephaestus, Walkerma, Wavelength, Whiskey in the Jar, WillWare, Wireless Keyboard, Wk muriithi, Wysprgr2005, Yamaguchi先生, Yyy, Zandperl, ZooFari, Zzuuzz, Ásgeir IV., Ævar Arnfjörð Bjarmason, Александър, 824 anonymous edits

Image Sources, Licenses and Contributors

Image:Atisane3.png *Source*: http://en.wikipedia.org/w/index.php?title=File:Atisane3.png *License*: GNU Free Documentation License *Contributors*: ,

File:Loudspeaker.svg *Source*: http://en.wikipedia.org/w/index.php?title=File:Loudspeaker.svg *License*: Public Domain *Contributors*: Bayo, Gmaxwell, Husky, Iamunknown, Myself488, Nethac DIU, Omegatron, Rocket000, The Evil IP address, Wouterhagens, 7 anonymous edits

License