

Diatomic molecule

Diatomic molecules are molecules composed of only two atoms, of the same or different chemical elements. The prefix *di-* is of Greek origin, meaning "two". If a diatomic molecule consists of two atoms of the same element, such as hydrogen (H₂) or oxygen (O₂), then it is said to be homonuclear. Otherwise, if a diatomic molecule consists of two different atoms, such as carbon monoxide (CO) or nitric oxide (NO), the molecule is said to be heteronuclear.

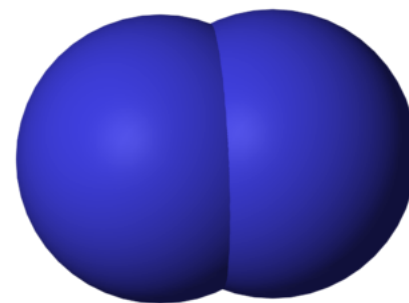
The only chemical elements that form stable homonuclear diatomic molecules at standard temperature and pressure (STP) (or typical laboratory conditions of 1 bar and 25 °C) are the gases hydrogen (H₂), nitrogen (N₂), oxygen (O₂), fluorine (F₂), and chlorine (Cl₂).^[1]

The noble gases (helium, neon, argon, krypton, xenon, and radon) are also gases at STP, but they are monatomic. The homonuclear diatomic gases and noble gases together are called "elemental gases" or "molecular gases", to distinguish them from other gases that are chemical compounds.^[2]

At slightly elevated temperatures, the halogens bromine (Br₂) and iodine (I₂) also form diatomic gases.^[3] All halogens have been observed as diatomic molecules, except for astatine, which is uncertain.

The mnemonics **BrINClHOF**, pronounced "Brinklehof", and **HONClBrIF**, pronounced "Honkelbrif",^[4] and HOFBrINCl (pronounced as Hofbrinkle) have been coined to aid recall of the list of diatomic elements.

Other elements form diatomic molecules when evaporated, but these diatomic species repolymerize when cooled. Heating ("cracking") elemental phosphorus gives diphosphorus, P₂. Sulfur vapor is mostly disulfur (S₂). Dilithium (Li₂) is known in the gas phase. Ditungsten (W₂) and dimolybdenum (Mo₂) form with sextuple bonds in the gas phase. The bond in a homonuclear diatomic molecule is non-polar. Dirubidium is diatomic.



A space-filling model of the diatomic molecule dinitrogen, N₂

Group →	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18							
↓ Period																									
1	1 H																		2 He						
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne							
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar							
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr							
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe							
6	55 Cs	56 Ba		72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn							
7	87 Fr	88 Ra		104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Fl	115 Uup	116 Lv	117 Uus	118 Uuo							
				Lanthanides							57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
				Actinides							89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

A periodic table showing the elements that exist as homonuclear diatomic molecules under typical laboratory conditions.

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Heteronuclear molecules

All other diatomic molecules are chemical compounds of two different elements. Many elements can combine to form heteronuclear diatomic molecules, depending on temperature and pressure.

Common examples include the gases carbon monoxide (CO), nitric oxide (NO), and hydrogen chloride (HCl).

Many 1:1 binary compounds are not normally considered diatomic because they are polymeric at room temperature, but they form diatomic molecules when evaporated, for example gaseous MgO, SiO, and many others.

Occurrence

Hundreds of diatomic molecules have been identified^[5] in the environment of the Earth, in the laboratory, and in interstellar space. About 99% of the Earth's atmosphere is composed of two species of diatomic molecules: nitrogen (78%) and oxygen (21%). The natural abundance of hydrogen (H₂) in the Earth's atmosphere is only of the order of parts per million, but H₂ is the most abundant diatomic molecule in the universe. The interstellar medium is, indeed, dominated by hydrogen atoms.

Molecular geometry

Historical significance

Diatomic elements played an important role in the elucidation of the concepts of element, atom, and molecule in the 19th century, because some of the most common elements, such as hydrogen, oxygen, and nitrogen, occur as diatomic molecules. John Dalton's original atomic hypothesis assumed that all elements were monatomic and that the atoms in compounds would normally have the simplest atomic ratios with respect to one another. For example, Dalton assumed

water's formula to be HO, giving the atomic weight of oxygen as eight times that of hydrogen^[6], instead of the modern value of about 16. As a consequence, confusion existed regarding atomic weights and molecular formulas for about half a century.

As early as 1805, [Gay-Lussac](#) and [von Humboldt](#) showed that water is formed of two volumes of hydrogen and one volume of oxygen, and by 1811 [Amedeo Avogadro](#) had arrived at the correct interpretation of water's composition, based on what is now called [Avogadro's law](#) and the assumption of diatomic elemental molecules. However, these results were mostly ignored until 1860, partly due to the belief that atoms of one element would have no [chemical affinity](#) toward atoms of the same element, and also partly due to apparent exceptions to Avogadro's law that were not explained until later in terms of dissociating molecules.

At the 1860 [Karlsruhe Congress](#) on atomic weights, [Cannizzaro](#) resurrected Avogadro's ideas and used them to produce a consistent table of atomic weights, which mostly agree with modern values. These weights were an important prerequisite for the discovery of the [periodic law](#) by [Dmitri Mendeleev](#) and [Lothar Meyer](#).^[7]

Excited electronic states

Diatomic molecules are normally in their lowest or ground state, which conventionally is also known as the **X** state. When a gas of diatomic molecules is bombarded by energetic electrons, some of the molecules may be excited to higher electronic states, as occurs, for example, in the natural aurora; high-altitude nuclear explosions; and rocket-borne electron gun experiments.^[8] Such excitation can also occur when the gas absorbs light or other electromagnetic radiation. The excited states are unstable and naturally relax back to the ground state. Over various short time scales after the excitation (typically a fraction of a second, or sometimes longer than a second if the excited state is [metastable](#)), transitions occur from higher to lower electronic states and ultimately to the ground state, and in each transition results a [photon](#) is emitted. This emission is known as [fluorescence](#). Successively higher electronic states are conventionally named **A**, **B**, **C**, etc. (but this convention is not always followed, and sometimes lower case letters and alphabetically out-of-sequence letters are used, as in the example given below). The excitation energy must be greater than or equal to the energy of the electronic state in order for the excitation to occur.

In quantum theory, an electronic state of a diatomic molecule is represented by

$$2S+1 \Lambda(v)$$

where **S** is the total electronic spin quantum number, **Λ** is the total electronic angular momentum quantum number along the internuclear axis, and **v** is the vibrational quantum number. **Λ** takes on values 0, 1, 2, ..., which are represented by the electronic state symbols **Σ**, **Π**, **Δ**,.... For example, the following table lists the common electronic states (without vibrational quantum numbers) along with the energy of the lowest vibrational level (**v** = **0**) of diatomic nitrogen (N₂), the most abundant gas in the Earth's atmosphere.^[9] In the table, the subscripts and superscripts after **Λ** give additional quantum mechanical details about the electronic state.

State	Energy (T_0 , cm^{-1}) See note below
$X^1\Sigma_g^+$	0.0
$A^3\Sigma_u^+$	49754.8
$B^3\Pi_g$	59306.8
$W^3\Delta_u$	59380.2
$B'^3\Sigma_u^-$	65851.3
$a^1\Sigma_u^-$	67739.3
$a^1\Pi_g$	68951.2
$w^1\Delta_u$	71698.4

Note: The "energy" units in the above table are actually the reciprocal of the wavelength of a photon emitted in a transition to the lowest energy state. The actual energy can be found by multiplying the given statistic by the product of c (the speed of light) and h (Planck's constant), i.e., about 1.99×10^{-25} Joule metres, and then multiplying by a further factor of 100 to convert from cm^{-1} to m^{-1} .

The aforementioned fluorescence occurs in distinct regions of the electromagnetic spectrum, called "emission bands": each band corresponds to a particular transition from a higher electronic state and vibrational level to a lower electronic state and vibrational level (typically, many vibrational levels are involved in an excited gas of diatomic molecules). For example, N_2 **A-X** emission bands (a.k.a. Vegard-Kaplan bands) are present in the spectral range from 0.14 to 1.45 μm (micrometres).^[8] A given band can be spread out over several nanometers in electromagnetic wavelength space, owing to the various transitions that occur in the molecule's rotational quantum number, J . These are classified into distinct sub-band branches, depending on the change in J .^[10] The **R** branch corresponds to $\Delta J = +1$, the **P** branch to $\Delta J = -1$, and the **Q** branch to $\Delta J = 0$. Bands are spread out even further by the limited spectral resolution of the spectrometer that is used to measure the spectrum. The spectral resolution depends on the instrument's point spread function.

Energy levels

The molecular term symbol is a shorthand expression of the angular momenta that characterize the electronic quantum states of a diatomic molecule, which are eigenstates of the electronic molecular Hamiltonian. It is also convenient, and common, to represent a diatomic molecule as two point masses connected by a massless spring. The energies involved in the various motions of the molecule can then be broken down into three categories: the translational, rotational, and vibrational energies.

Translational energies

The translational energy of the molecule is given by the kinetic energy expression:

$$E_{trans} = \frac{1}{2}mv^2$$

where m is the mass of the molecule and \mathbf{v} is its velocity.

Rotational energies

Classically, the kinetic energy of rotation is

$$E_{rot} = \frac{L^2}{2I}$$

where

L is the angular momentum

I is the moment of inertia of the molecule

For microscopic, atomic-level systems like a molecule, angular momentum can only have specific discrete values given by

$$L^2 = l(l + 1)\hbar^2$$

where l is a non-negative integer and \hbar is the reduced Planck constant.

Also, for a diatomic molecule the moment of inertia is

$$I = \mu r_0^2$$

where

μ is the reduced mass of the molecule and

r_0 is the average distance between the centers of the two atoms in the molecule.

So, substituting the angular momentum and moment of inertia into E_{rot} , the rotational energy levels of a diatomic molecule are given by:

$$E_{rot} = \frac{l(l + 1)\hbar^2}{2\mu r_0^2} \quad l = 0, 1, 2, \dots$$

Vibrational energies

Another type of motion of a diatomic molecule is for each atom to oscillate—or vibrate—along the line connecting the two atoms. The vibrational energy is approximately that of a quantum harmonic oscillator:

$$E_{vib} = \left(n + \frac{1}{2} \right) \hbar\omega \quad n = 0, 1, 2, \dots$$

where

n is an integer

\hbar is the reduced Planck constant and

ω is the angular frequency of the vibration.

Comparison between rotational and vibrational energy spacings

The spacing, and the energy of a typical spectroscopic transition, between vibrational energy levels is about 100 times greater than that of a typical transition between rotational energy levels.

Hund's cases

The good quantum numbers for a diatomic molecule, as well as good approximations of rotational energy levels, can be obtained by modeling the molecule using Hund's cases.

See also

- Symmetry of diatomic molecules
- AXE method
- Octatomic element
- Covalent bond
- Industrial gas

References

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Further reading

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- Tipler, Paul (1998). *Physics For Scientists and Engineers: Vol. 1* (4th ed.). W. H. Freeman. ISBN 1-57259-491-8.

External links

- Hyperphysics (<http://hyperphysics.phy-astr.gsu.edu/hbase/molecule/rotrig.html#c3>) – Rotational Spectra of Rigid Rotor Molecules
 - Hyperphysics (<http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/hosc.html>) – Quantum Harmonic Oscillator
 - 3D Chem (<http://www.3dchem.com/>) – Chemistry, Structures, and 3D Molecules
 - IUMSC (<http://arquivo.pt/wayback/20160523113736/http://www.iumsc.indiana.edu/>) – Indiana University Molecular Structure Center
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