

## Compilation of Definitions “van der Waals interaction”

Definition a) Excludes Electrostatic Interactions and Short Range Repulsion

Definition b) Excludes Electrostatic Interactions, Short Range Repulsion and Hydrogen Bonds

Definition c) Includes London Dispersion only

Definition d) Includes London Dispersion and Short Range Repulsion

*This list was compiled by students of CHEM 6572 (Macromolecular Structure) at Georgia Tech, Fall of 2020.*

Definition a) Excludes Electrostatic Interactions and Short Range Repulsion

“All of the attractive forces discussed (dipole-dipole, dipole-induced dipole, and instantaneous dipole-induced dipole) are collectively called van der Waals forces. -Reger, D. L., Goode, S. R., & Ball, D. W. (2010). Chemistry: Principles and Practice (3rd ed.). Belmont, CA: Mary Finch. Pg. 440.

These intermolecular forces, collectively called van der Waals forces, are all electrical in nature. We will focus our attention on three types: 1. Dipole-dipole forces 2. Hydrogen bonds 3. Dispersion forces. -Solomons T. W. G., Fryhle C. B. (2011). Organic Chemistry (10th ed.). Petra Recter. Pg. 75.

“Van der Waals bonds arise from the interaction between two permanent or induced electric dipole moments in a pair of atoms or molecules.” - Sears and Zemansky’s University Physics with Modern Physics, 13th Edition by Hugh D. Young, Roger A. Freedman and A. Lewis Ford, ISBN 13: 978-0321696861, Addison-Wesley, Pg. 1437.

“The noncovalent associations between electrically neutral molecules, collectively known as van der Waals forces, arise from the electrostatic interactions among permanent and/or induced dipoles.” - Biochemistry, 4th Edition, by Donald Voet and Judith G. Voet, ISBN-13: 978-0470570951, John Wiley & Sons, Pg. 260.

“the van der Waals bond, is an interaction between the electric dipole moments of atoms or molecules; typical energies are 0.1 eV or less.” - Sears and Zemansky’s University Physics with Modern Physics, 13th Edition by Hugh D. Young, Roger A. Freedman and A. Lewis Ford, ISBN 13: 978-0321696861, Addison-Wesley, Pg. 1407.

“The van der Waals equation,  $(P + \frac{n^2a}{V^2})(V - nb) = nRT$ , more accurately relates the pressure, volume, and temperature of a real gas because the pressure correction term,  $\frac{n^2a}{V^2}$ , accounts for interactions between atoms or molecules in the gas phase. Because these interactions are considered in the van der Waals equation, the term van der Waals forces is frequently used collectively to indicate all types of attractive forces possible between molecules: dipole-dipole interactions, induced dipole interactions, and dispersion forces.” - Gilbert, Kirss, Foster, Davies. Chemistry (Third Edition). Pg. 477.

The attractive or repulsive forces between molecular entities (or between groups within the same molecular entity) other than those due to bond formation or to the electrostatic interaction of ions or of ionic groups with one another or with neutral molecules. The term includes: dipole–dipole, dipole-induced dipole and London (instantaneous induced dipole-induced dipole) forces. The term is sometimes used loosely for the totality of nonspecific attractive or repulsive intermolecular forces. IUPAC. Compendium of Chemical Terminology, 2nd ed. (the "Gold Book"). Compiled by A. D. McNaught and A. Wilkinson. Blackwell Scientific Publications, Oxford (1997). Online version (2019-) created by S. J. Chalk. ISBN 0-9678550-9-8. <https://doi.org/10.1351/goldbook>.

Van der Waals forces may arise from three sources. First, the molecules of some materials, although electrically neutral, may be permanent electric dipoles. Because of fixed distortion in the distribution of electric charge in the very structure of some molecules, one side of a molecule is always somewhat positive and the opposite side somewhat negative. The tendency of such permanent dipoles to align with each other results in a net attractive force. Second, the presence of molecules that are permanent dipoles temporarily distorts the electron charge in other nearby polar or nonpolar molecules, thereby inducing further polarization. An additional attractive force results from the interaction of a permanent dipole with a neighbouring induced dipole. Third, even though no molecules of a material are permanent dipoles (e.g., in the noble gas argon or the organic liquid benzene), a force of attraction exists between the molecules, accounting for condensing to the liquid state at sufficiently low temperatures.

The nature of this attractive force in molecules, which requires quantum mechanics for its correct description, was first recognized (1930) by the Polish-born physicist Fritz London, who traced it to electron motion within molecules. London pointed out that at any instant the centre of negative charge of the electrons and the centre of positive charge of the atomic nuclei would not be likely to coincide. Thus, the fluctuation of electrons makes molecules time-varying dipoles, even though the average of this instantaneous polarization over a brief time interval may be zero. Such time-varying dipoles, or instantaneous dipoles, cannot orient themselves into alignment to account for the actual force of attraction, but they do induce properly aligned polarization in adjacent molecules, resulting in attractive forces. These specific interactions, or forces, arising from electron fluctuations in molecules (known as London forces, or dispersion forces) are present even between permanently polar molecules and produce, generally, the largest of the three contributions to intermolecular forces. Gregersen, Erik. "Van Der Waals Forces." Encyclopedia Britannica , [www.britannica.com/science/van-der-Waals-forces](http://www.britannica.com/science/van-der-Waals-forces).

"Van der Waals forces - the relatively weak attractive forces that act on neutral atoms and molecules that arise because of the electric polarization induced in each of the particles by the presence of other particles" "Van der Waals forces." "Van der Waals forces." Merriam-Webster.com Dictionary, Merriam-Webster, <https://www.merriam-webster.com/dictionary/van%20der%20Waals%20forces>.

Definition b) Excludes Electrostatic Interactions, Short Range Repulsion and Hydrogen Bonds

Other electrostatic interactions occur between particles that are polar but not actually charged, for example, two carbonyl groups: These forces, called van der Waals interactions, are usually weaker than hydrogen bonds. The interaction between two strongly polar groups is known as a dipole–dipole interaction and has a strength of about  $9 \text{ kJ} \cdot \text{mol}^{-1}$ . Very weak van der Waals interactions, called London dispersion forces, occur between nonpolar molecules as a result of small fluctuations in their distribution of electrons that create a temporary separation of charge. Nonpolar groups such as methyl groups can therefore experience a small-attractive force, in this case about  $0.3 \text{ kJ} \cdot \text{mol}^{-1}$ : Pratt, C.W. and Cornely, K. Essential Biochemistry, 4th ed. Wiley, 2018. Pg. 27

Definition c) Includes London Dispersion only

Random variations in the positions of the electrons around one nucleus may create a transient electric dipole, which induces a transient, opposite electric dipole in the nearby atom. The two dipoles weakly attract each other, bringing the two nuclei closer. These weak attractions are called van der Waals interactions. As the two nuclei draw closer together, their electron clouds begin to repel each other. At the point where the van der Waals attraction exactly balances this repulsive force, the nuclei are said to be in van der Waals contact.” - Lehninger Principles of Biochemistry, 6th Edition by David L. Nelson and Michael M. Cox, ISBN-13: 978-1429234146, W.H. Freeman, Pg. 54.

“When any two atoms approach each other closely, they create a weak, nonspecific attractive force called a van der Waals interaction. These nonspecific interactions result from the momentary random fluctuations in the distribution of electrons of any atom, which gives rise to transient unequal distribution of electrons.” -Molecular Cell Biology, 8th Edition, by Lodish et al., ISBN-13: 978-1-4641-8339-3, W.H. Freeman and Company, Pg. 38.

The basis of a van der Waals interaction is that the distribution of electronic charge around an atom fluctuates with time. At any instant, the charge distribution is not perfectly symmetric. This transient asymmetry in the electronic charge about an atom acts through ionic interactions to induce a complementary asymmetry in the electron distribution within its neighboring atoms. The atom and its neighbors then attract one another. This attraction increases as two atoms come closer to each other, until they are separated by the van der Waals contact distance." Biochemistry (Eight Edition). Jeremy M. Berg, John Tymoczko, Gregory J. Gatto Jr., Lubert Streyer, Pg. 8.

van der Waals interactions - a weak electrical attraction between two nonpolar molecules that have been brought together through hydrophobic interactions (LDW: wrong), which occur due to the constant motion of electrons giving molecules a tiny asymmetry in charge that changes with time. -Freeman et al.; Biological Science, 5th Edition; Pearson, 2014. ISBN-13: 978-0321841803.

“When two uncharged atoms are brought very close together, their surrounding electron clouds influence each other. Random variations in the positions of the electrons around one

nucleus may create a transient electric dipole, which induces a transient, opposite electric dipole in the nearby atom. The two dipoles weakly attract each other, bringing the two nuclei closer. These weak attractions are called van der Waals interactions (also known as London forces). As the two nuclei draw closer together, their electron clouds begin to repel each other. At the point where the net attraction is maximal, the nuclei are said to be in van der Waals contact.”-Lehninger PRINCIPLES of BIOCHEMISTRY, 7th Edition by David L. Nelson and Michael M. Cox, ISBN-13: 978-1-4641-2611-6, W. H. Freeman and Company.

When any two atoms approach each other closely, they create a weak, nonspecific attractive force called a van der Waals interaction. These nonspecific interactions result from the momentary random fluctuations in the distribution of the electrons of any atom, which give rise to a transient unequal distribution of electrons. Van der Waals interactions, involving either transiently induced or permanent electric dipoles, occur in all types of molecules, both polar and nonpolar. In particular, van der Waals interactions are responsible for the cohesion between nonpolar molecules such as heptane,  $\text{CH}_3\text{-(CH}_2\text{)}_5\text{-CH}_3$ , that cannot form hydrogen bonds or ionic interactions with each other. -Lodish, Harvey F. Molecular Cell Biology. New York: W.H. Freeman and Co, 2013. Print. Pg.30

When two neutral atoms approach each other, transient fluctuations in the electron clouds of each atom set up transient dipoles, leading to an attractive force between the atoms. This attractive force is called the London Force, or the van der Waals attraction. Kuriyan, J; Konforti, B; Wemmer, D. The Molecules of Life: Physical and Chemical Principles; Garland Science: New York, NY, 2013. Print. p. 964.

Interactions resulting from ever-changing regions of positive and negative charge that enable all atoms and molecules to stick together (Reece, Jane B., and Neil A. Campbell. Biology. Pearson Benjamin Cummings, 2008.)

“The molecules of an alkane are held together by these induced-dipole--induced dipole interactions, which are known as van der Waals forces. Van der Wals forces are the weakest of all the attractive forces.” -Organic Chemistry, Seventh Edition by Paula Yurkanis Bruice, ISBN 13: 978-0-321-80322-1. Pearson, pg 114.

“Van der Waals forces are the result of induced electrical interactions between closely approaching atoms or molecules as their negatively charged electron clouds fluctuate instantaneously in time. These fluctuations allow attractions to occur between the positively charged nuclei and the electrons of nearby atoms. Van der Waals attractions operate only over a very limited interatomic distance (0.3 to 0.6 nm) and are an effective bonding interaction at physiological temperatures only when a number of atoms in a molecule can interact with several atoms in a neighboring molecule. For this to occur, the atoms on interacting molecules must pack together neatly. That is, their molecular surfaces must possess a degree of structural complementarity.” - Biochemistry, 5th Edition by Reginald H. Garrett and Charles M. Grisham, ISBN-13: 978-1133106296, Cengage Learning, Pg. 12.

Definition d) Includes London Dispersion plus Short Range Repulsion

Random variations in the positions of the electrons around one nucleus may create a transient electric dipole, which induces a transient, opposite electric dipole in the nearby atom. The two dipoles weakly attract each other, bringing the two nuclei closer. These weak attractions are called van der Waals interactions. As the two nuclei draw closer together, their electron clouds begin to repel each other. At the point where the van der Waals attraction exactly balances this repulsive force, the nuclei are said to be in van der Waals contact.” - Lehninger Principles of Biochemistry, 6th Edition by David L. Nelson and Michael M. Cox, ISBN-13: 978-1429234146, W.H. Freeman, Pg. 54.

“The van der Waals force is an electromagnetic interaction between correlated fluctuating charges on two electrically neutral surfaces. As the surfaces approach more closely, the force increases as fluctuations of shorter and shorter length scale come into play, but ultimately the force will saturate when the surfaces are so close that the even shortest wavelength charge fluctuations are included.” -Luo, Y.; Zhao, R.; Pendry, J. B. Proceedings of the National Academy of Sciences 2014, 111 (52), 18422. <https://doi.org/10.1073/pnas.1420551111>.