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## Chapter 1 structure and bonding answers

1 Chapter 1 Structure and Gluing 2 What is Organic Chemistry? Living things are made from organic chemicals Proteins that make up hair DNA, check genetic make-up foods, drugs examine structures in the right 3 Origins of Organic Chemistry Foundations for Organic Chemistry from the mid-1700s. Compounds obtained from plants, animals difficult to isolate and clean. Compounds also break down more easily. Torben Bergman (1770) first distinguishes between organic and inorganic chemistry. It was thought that organic compounds should contain some vital force because they were from living sources. 4 Origins of organic chemistry, because of their vital power, it was thought that organic compounds could not be synthesized in the laboratory as inorganic compounds. In 1816, Chevreul showed that this was not the case, he could prepare soap for animal fat and an alkaline and glycerin for a product in 1828, Woehler showed that it was possible to convert inorganic salt ammonium cyanide into organic matter urea 5 Origin of organic chemistry Organic chemistry study of carbon compounds. Why is it so special? 90% of the more than 30 million chemical compounds contain carbon. Examination of coal periodic chart answers some of these questions. Carbon can share group 4A, 4 valence electrons and form 4 covalent bonds. 6 Why this chapter? Review ideas for general chemistry: atoms, bonds, molecular geometry 7 1.1 Atom Positively loaded nucleus (very dense, protons and neutrons) and small (10<sup>-15</sup> m) Negatively charged electrons are in a cloud (10<sup>-10</sup> m) around the nucleus about 2 × 10<sup>-10</sup> m (200 picometers (pm)) [in Ångström unit (Å) m = 100 pm] 8 Atomic number and atomic mass The number of protons in the nucleus (A) and neutrons The same atomic numbers of atoms of each element are the same atoms, which are atoms of the same element that have different numbers of neutrons, and therefore with different mass numbers The atomic mass (atomic mass) of the element is the weighted average mass (amu) 9 1.2 : Orbitals Quantum mechanics: describes the electron energies and locations of a wave equation Wave function solution wave equation Each wave function is an orbital,  $\psi$  The plot  $\psi$  describes where electrons are most likely to electron cloud with no specific boundary so they show the most likely area. 10 Forms of atomic orbits of electrons Electrons Our different types of orbital orbits for electrons, which are derived from the hydrogen atom, p, d, and f s and p orbital key to organic and biological chemistry s orbital s orbital: spherical, nucleus mid-p orbital: dumbbell shape, core middle d orbital: elongated dumbbell shape, core mid 11 Orbitals and Clams (Continue) Orbitals are grouped into growing shell sizes and energies Different shells contain different numbers and the orbital orbits of each orbit can occupy two electrons 12 Orbitals and Shells (Continue) First shell contains one s orbital, denotes 1s, holds only two electrons Second shell contains one s orbital (2s) and three p orbital (2p), eight electrons Third shell contains one s orbital (3s), three p orbitals (3p), and five d orbitals (3d), 18 electrons 13 P-Orbitals Each shell has three perpendicular orbits, px, py, and pz, equal energy levels are a p orbital separated region with zero electron density, the node 14 1.3 Atomic structure: Electron Configurations Ground-state electron configuration (lowest energy arrangement) is an atom lists orbital occupied by electrons. Rules: 1. The lowest energy orbital fill first: 1s  $\rightarrow$  2s  $\rightarrow$  2p  $\rightarrow$  3s  $\rightarrow$  3p  $\rightarrow$  4s  $\rightarrow$  3d (Aufbau (build-up) principle) 2. Electrons act like they're spinning around an axis. Electron spin can be only in two directions, up  $\uparrow$  and down  $\downarrow$ . Only two electrons can occupy an orbital, and they must be opposite spin (Pauli exclusion principle) to unique wave equations 3. If two or more empty orbits of the same energy are available, electrons occupy parallel spins until all orbitals have one electron (Hund rule). 15 1.4 Development of chemical bonding Theory Kekulé and Couper independently noted that carbon is always four bonds van't Hoff and le Bel suggested that the four bonds of carbon dioxide have a specific spatial direction atoms around carbon corners in a tetrahedron on 16 Developing chemical bonding theory Atoms form bonds, because the compound that results in more stable than separate atoms of ion bindings in the form of salts as a result of electron transfers organic compounds covalent bonds sharing electrons (G. N. Lewis, 1916) 17 Development of chemical bonding Theory Lewis structures (electron point) show valence electrons in an atom as point hydrogen at a point, which makes the 1s electron Carbon four dots (2s<sup>2</sup> 2p<sup>2</sup>) Kekulé structures (line-bond structures) have a line drawn from two atoms indicating the 2 electron-covalent bond. Stable molecule results in completed shell, octet (eight points) of the main group of atoms (two hydrogen) 18 Developing chemical bonding theory Atoms of one, two, or three valence electrons to form one, two, or three bonds. Atoms of four or more chemically valued electrons form as many bonds as they need electrons to fill the s and p levels of the valence shells to reach a stable octet. The carbon has four valence electrons (2s<sup>2</sup> 2p<sup>2</sup>), which form four bonds (CH<sub>4</sub>). 19 Developing chemical bonding theory Nitrogenic five valence electrons (2s<sup>2</sup> 2p<sup>3</sup>), but forms only three bonds (NH<sub>3</sub>). Oxygen has six valence electrons (2s<sup>2</sup> 2p<sup>4</sup>), but forms two bonds (H<sub>2</sub>O) 20 Developing chemical bond theory 21 No bonding electrons not used to bond electrons is called nonbonding electrons, or solitary pairs of electrons nitrogen atom ammonia (NH<sub>3</sub>) Shares six valence electrons covalent bonds and the remaining two valence electrons lone pair 22 1.5 Description Chemical Bonds: Valence Bond Theory covalent bonding forms, when two atoms converge closely so that a uniquely occupied orbital one atom overlaps with one is merged into occupied orbital with the other atom two models to describe covalent bonding. Valence Bond Theory, Molecular Orbital Theory Valence Bond Theory: Electrons paired with the overlapping orbital and attracting the nuclei of both atom-H bond result from the overlap of two individually occupied hydrogen 1 orbitals H-H bond cylindrically symmetrical, sigma (s) bond 23 Bond Energy Reaction 2 H<sub>2</sub>  $\rightarrow$  H<sub>2</sub> emissions 436 kJ/mol Product 436 kJ/mol less energy than two atoms: H-H binding force 436 kJ/mol. (1 kJ = kcal; 1 kcal = kJ) 24 Bond Energy distance between the cores, which is the maximum stability If too close, it is repelled, because both are positively charged If they are too far apart, sticking weak 25 1.6 sp<sup>3</sup> Orbitals and the structure methane Arm 4 valence electrons (2s<sup>2</sup> 2p<sup>2</sup>) in CH<sub>4</sub>, all C-H bonds are identical (tetrahedral) sp<sup>3</sup> hybrid orbital: s orbital and three p orbital combine to form four equivalent, unsymmetrical, tetrahedral orbital (spp<sup>3</sup> = sp<sup>3</sup>), Pauling (1931) 26 methane sp<sup>3</sup> orbital structure of the C overlaps with 1s orbital 4 H atoms to form four identical C-H bonds Each C-H bond has a strength of 436 (439) kJ/mol and a length of 109 pm Bond angle: all H-C-H 109.5°, a tetrahedral angle. 27 1.7 sp<sup>3</sup> Orbitals and Ethane Two C intertangling structure from each of three sp<sup>3</sup> orbital orbits from each sp<sup>3</sup> orbital level that overlaps C, to form six C-H bonds in C-H bonds ethane 421 kJ/mol C-C-C in bond 154 pm long and strength 377 kJ / mol All bonding angles ethane tetrahedral 28 1.8 sp<sup>2</sup> Orbitals and structure ethylene Some representation of ethylene are given sp<sup>2</sup> hybrid orbital: 2s orbital combines two 2p orbital, Gives 3 orbital orbits (spp = sp<sup>2</sup>). This results in a double bond. Sp<sup>2</sup> orbitals are in a plane 120° angles Remaining p orbital perpendicular to plane 29 Bonds Sp<sup>2</sup> Hybrid Orbitals Two sp<sup>2</sup>-hybridized orbitals overlap form s bond p orbitals overlap side-to-side formation of pi (p) bond sp<sup>2</sup>-sp<sup>2</sup> s bond and 2 p-2p p bond result in the division of four electrons and formation of C-C double bonding Electrons in the s bond between the centered nuclei of Electrons in the p bond occupy regions on each side of a line of ethylene H atoms structure between the ethane E in a single bond shorter and stronger than the ethane bond shorter and stronger, as the single-bond e-bond stronger ethane-bound double bond c-c binding length 134 pm (C-C 154 pm) 31 1.9 sp Orbitals and Acetylene C-C structure of a three-electron Carbon 2s orbital hybridized into a single orbital sp hybridized two p orbitals remain unchanged sp orbitals linear, 180° apart x-axis Two p orbitals perpendicular to the y-axis and z-axis 32 Orbitals acetylene 2 the hybrid orbits of each C-form sp-sp s bond pz orbitals form a pz-pz p bond from each C in lateral overlap, and the binding of p orbitals overlap in 33 Acetylene by sharing six electrons C-C Two sp orbitals s bonds of hydrogen 34 A Methane C-C and C-H bonds, Hybridization of ethane, ethylene and acetylene 35 1.10 Hybridization of nitrogen and oxygen elements other than C may enter a hybridized orbit H-N-H bonding angle ammonia (NH<sub>3</sub>) 107.3° C-N-H binding angle \* N orbital (spp<sup>3</sup>) hybridization four sp<sup>3</sup> orbital is a sp<sup>3</sup> orbital occupied by two nonbonding electrons, and three sp<sup>3</sup> orbital one electron each, forming bonds H and CH<sub>3</sub>. 36 1.11 Description of chemical bonds: Molecular orbital theory molecular orbital (MO): where electrons are most likely (specific energy and general shape) in a molecular additive combination (bond) in MO energy extractor (bond inhibitor) MO lower higher energy 37 Molecular Orbitals of ethylene p knitting MO in the blk lonic lonic lye combining the same algebraic signal the p antibonding MO with the lye combining opposite marks Only knitting MO contained in 38 1.12 Drawing Structures Drawing all knitting organic molecules can become boring. A number of shorthand methods have been developed to write structures. Condensed structures do not have a single bond of c-h or C-C. We understand them. e.g. 39 drawing structures (continuation) 3 General rules: 1) Carbonates are not usually displayed. Instead, the carbon atom is assumed to be at each intersection of two lines (bonds) and the end of each line. 2) Carbon-bound hydrogen atoms do not appear. 3) Atoms other than carbon and hydrogen are displayed (see Table 1.3). 40 Summary of electrons occupy orbital around the nucleus. Organic chemistry - chemistry of carbon compounds: Atom: charged nuclei containing positively charged protons and neutrally filled neutrons surrounded by negatively charged electrons Electronic structure of atoms described by the wave equation Electrons occupy orbital around the nucleus. Different orbital levels have different energy levels, and different forms are secular, the p orbital of the dumbbell-shaped spheroid - the pair of electrons divided between atoms Valence bond theory - the electron division occurs by overlapping two atomic orbital (AO) theories, which belong to the entire molecule 41 Summary (Continuation) Sigma (s) bonds - Circle cross-section, and form the head-on interaction Pi (p) bonds - dumbbell-shaped sideways interaction A p orbitals Carbon uses hybrid orbital materials to form bonds in organic molecules. The tetrahedral geometry with a single bond of carbon in four sp<sup>3</sup> hybrid orbitals double bonds with flat geometry, carbon use three equivalent sp<sup>2</sup> hybrid orbital and one non-hybridized p orbital carbon uses two equivalent sp hybrid orbitals to form triple bond linear geometry, two hybridized p orbital atoms like nitrogen and oxygen are hybridized to form strong, oriented bonds of nitrogen atom ammonia and oxygen atom in water sp<sup>3</sup>-hybridized 42 Let's Work on Problem Draw is an electron-point structure acetonitrile, C<sub>2</sub>H<sub>3</sub>N, which contains a carbon-nitrogen triple bond. How many electrons are in the outer shell of the nitrogen atom? How many are knitted and how many are not knitted? 43 Answer In order to answer this question, it must be recognized that nitrogen contains 8 electrons in its outer shell. Six will be used for C-N triple bond (shielded box) and two non-bonding non-bonding

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