

Molecular Geometry HOMEWORK

Section 8: Molecular

1. Complete the sentence below with the word "large" or "small."

Elements with large electronegativity differences form more ionic bonds.

2. What type of bond would form between these sets of elements – ionic or covalent?

a. P and H covalent because there are essentially no difference in electronegativity difference

b. Ca and F ionic because the small and essential would form a large electronegativity difference

3. Typically, covalent bonds form when two atoms EACH share 1 electron. However, there is a unique type of covalent bond in which ONE atom shares BOTH electrons to form that bond. This type of bond is called a coordinate covalent bond.

4. Imagine that you are asked to draw a Lewis dot structure for a newly discovered element that has been added to the bottom of the carbon family. What would you expect for its Lewis dot structure?

One pair and two lone dots (three total)



5. When drawing a Lewis dot structure for CHCl_3 , how do you determine which element goes in the middle?

the LEAST electronegative element goes in the middle

6. Large elements, which have energy levels that contain doublets, are capable of bonding with more than 4 bonds. These elements are found starting in a certain period on the Periodic Table. In which period would you find the smallest atoms that can accommodate more than 4 bonds?

In the third period

7. For the elements listed below, give the number of valence that are expected to form bonds around that element. If more than 2 electrons are possible, give your answer as "more than 2."

- Si
- Se
- As
- P more than 2
- Cl more than 2
- S more than 2

8. Draw the Lewis dot structure for the compounds below. Then, identify each Lewis dot structure as a traditional structure (all single bonds and a full octet with no special features), an expanded octet, a reduced octet, or a structure with a double/triple bond. Identifications may be used more than once or not at all.

Chlorine has an expanded octet

a. ClF_3

Cl: 7
F: $3 \times 7 = 21$
Total = 28



Chlorine has an expanded octet

b. BCl_3

B: 3
Cl: $3 \times 7 = 21$
Total = 24



Boron has a reduced octet

c. SF_6

S: 6
F: $6 \times 7 = 42$
Total = 48



d. NF_3

N: 5
F: $3 \times 7 = 21$
Total = 26



This is a traditional octet

e. COF_2

C: 4
O: 6
F: $2 \times 7 = 14$
Total = 24



Carbon has a double bond

f. BrF_5

Br: 7
F: $5 \times 7 = 35$
Total = 42



Bromine has an expanded octet

g. PCl_5

P: 5
Cl: $5 \times 7 = 35$
Total = 40



This is a traditional octet

h. BF_3

B: 3
F: $3 \times 7 = 21$
Total = 24



Boron has an expanded octet

Answer Key To Molecular Geometry Packet

J Dewey



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Multiscale Modeling of Complex Molecular Structure and Dynamics with MBN Explorer Ilia A. Solov'yov, Andrey V. Korol, Andrey V. Solov'yov, 2017-05-16 This book introduces readers to MesoBioNano MBN Explorer a multi purpose software package designed to model molecular systems at various levels of size and complexity In addition it presents a specially designed multi task toolkit and interface the MBN Studio which enables the set up of input files controls the simulations and supports the subsequent visualization and analysis of the results obtained The book subsequently provides a systematic description of the capabilities of this universal and powerful software package within the framework of computational molecular science and guides readers through its applications in numerous areas of research in bio and chemical physics and material science ranging from the nano to the mesoscale MBN Explorer is particularly suited to computing the system s energy to optimizing molecular structure and to exploring the various facets of molecular and random walk dynamics The package allows the use of a broad variety of interatomic potentials and can e g be configured to select any subset of a molecular system as rigid fragments whenever a significant reduction in the number of dynamical degrees of freedom is required for computational practicalities MBN Studio enables users to easily construct initial geometries for the molecular liquid crystalline gaseous and hybrid systems that serve as input for the subsequent simulations of their physical and chemical properties using MBN Explorer Despite its universality the computational efficiency of MBN Explorer is comparable to that of other more specialized software packages making it a viable multi purpose alternative for the computational modeling of complex molecular systems A number of detailed case studies presented in the second part of this book demonstrate MBN Explorer s usefulness and efficiency in the fields of atomic clusters and nanoparticles biomolecular systems nanostructured materials composite materials and hybrid systems crystals liquids and gases as well as in providing modeling support for novel and emerging technologies Last but not least with the release of the 3rd edition of MBN Explorer in spring 2017 a free trial version will be available from the MBN Research Center website mbnresearch.com

Pharmaceutical Crystals Tong Li, Alessandra Mattei, 2018-10-16 An important resource that puts the focus on understanding and handling of organic crystals in drug development Since a majority of pharmaceutical solid state materials are organic crystals their handling and processing are critical aspects of drug development Pharmaceutical Crystals Science and Engineering offers an introduction to and thorough coverage of organic crystals and explores the essential role they play in drug development and manufacturing Written contributions from leading researchers and practitioners in the field this vital resource provides the fundamental knowledge and explains the connection between pharmaceutically relevant properties and the structure of a crystal Comprehensive in scope the text covers a range of topics including crystallization molecular interactions polymorphism analytical methods processing and chemical stability The authors clearly show how to find solutions for pharmaceutical form selection and crystallization processes Designed to be an accessible guide this book

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