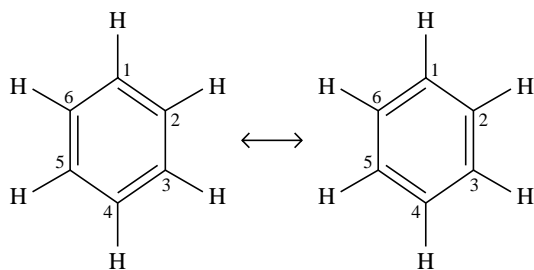


- Kekulé initially proposed that a benzene molecule is a ring of six carbon atoms with alternating single and double covalent bonds. However, he later realized that the chemical reactivity of benzene could be better explained as two possible structures with their double bonds in different locations. Kekulé suggested that these two structures are in a very rapid equilibrium so that there is no fixed location for a particular double bond.



- (g) According to modern theory, each carbon atom in benzene is bonded to two adjacent carbons (in the ring) and one hydrogen using the three sp^2 hybrid orbitals to form sigma bonds. Each of the six carbon atoms has a half-filled p orbital (perpendicular to the plane of the ring) which overlaps with adjacent p orbitals. The six p orbitals overlap above and below the plane of the carbon atoms. In modern terms, the p electrons are delocalized around the ring. This is a particularly stable arrangement. (This description actually describes only one of three molecular orbitals for benzene, each containing two paired electrons.)

4.3 VSEPR THEORY

Try This Activity: Electrostatic Repulsion Model

(Page 242)

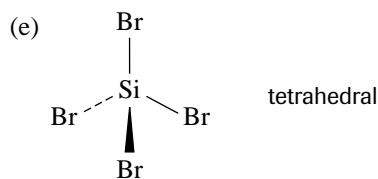
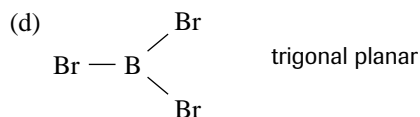
- Two balloons are at about 180° to each other (a linear arrangement).
- Three balloons are at about 120° to each other and all in one plane (a trigonal planar arrangement).
- Four balloons are at about 109° to each other with each one pointing to one corner of a tetrahedron (a tetrahedral arrangement).
- Balloons let you visualize electron orbitals and how they might be arranged. The electrostatic repulsion is modelled by the balloons pushing equally against each other. A disadvantage of the balloon model is that electron orbitals are not physical objects of a fixed size. A balloon only contacts or “repels” where it touches another balloon. Electrostatic repulsion occurs to varying extents between all electrons in the two nearby orbitals. In other words, the repulsion is much more complicated than implied by the two touching balloons.

PRACTICE

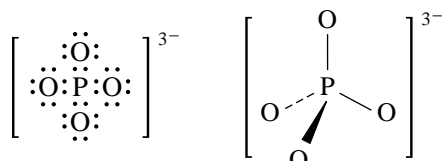
(Page 246)

Understanding Concepts

- VSEPR is an acronym for valence shell electron pair repulsion — a theory that predicts molecular shape by assuming that repulsion between all pairs of electrons in the valence shell of an atom controls the direction of those pairs formed by bonding, and thus determines the shapes of molecules.
- $\text{I} - \text{Be} - \text{I}$ linear
 - pyramidal
 - V-shape



3. (a) PO_4^{3-} will be tetrahedral in shape because it has four bond pairs around the P atom.



- (b) IO_3^- will be pyramidal in shape, having three bond pairs and one lone pair around the I atom.



4. (a) According to VSEPR theory, the shape around each carbon atom in cubane should be tetrahedral, since there are four bond pairs around each.
 (b) If we assume an ideal cubic shape, three of the bond angles around each carbon have to be 90° .
 (c) The normal tetrahedral angle is about 109° . To make these bonding orbitals bend to about 90° would greatly increase the repulsion of the electron pairs. This stress likely makes this molecule very unstable.

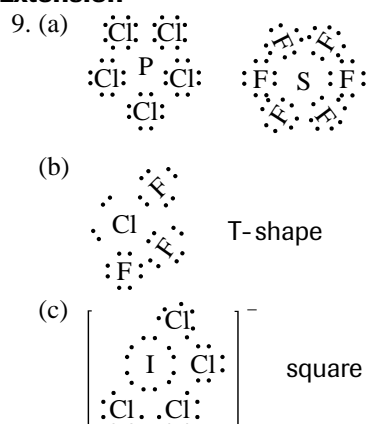
Applying Inquiry Skills

5. VSEPR theory was created to explain known molecular shapes. It provided a simpler way to explain shapes and also to predict molecular shapes.
 6. (Student reports may use a variety of criteria to evaluate sites. Typical criteria would involve the completeness of information, the opportunity for interaction, and the clarity and conciseness of information provided.)

Making Connections

7. Enzymes catalyze reactions. Their shape is critical, because they fit into precise spaces on the surface of other molecules to alter bond strengths—like a key fits precisely into a lock to allow it to operate.
 8. Optical isomers are molecular structures that are identical except for their 3-D orientation. They are so named because the two isomeric structures of such a substance will rotate the plane of polarized light in opposite directions—called levorotary (counterclockwise), and dextrorotary (clockwise). Any central atom (such as carbon) to which are bonded four different atoms (or side groups) always has a “left-handed” and a “right-handed” orientation, which are mirror images of each other. That terminology, of course, comes from describing the human hand—which has a front, back, thumb side, and little finger side that can be arranged in space in two ways that are mirror images.

Extension

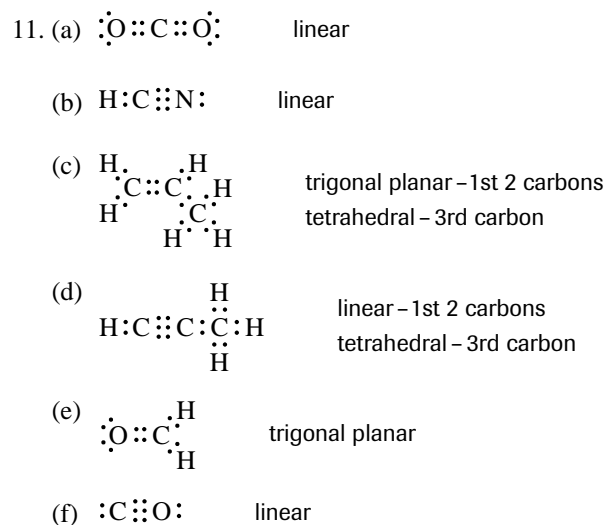


PRACTICE

(Page 249)

Understanding Concepts

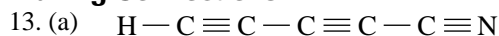
10. To make the rules of VSEPR theory work, multiple bonds must be treated just like single bonds—that is, they are considered to be one bond, which involves 4 or 6 electrons.



Applying Inquiry Skills

12. VSEPR is a very successful scientific theory. It successfully predicts the shapes of most molecular structures with a minimum of complexity—both being criteria for a “good” theory.

Making Connections



linear shape

- (b) Astronomers detect molecules in space by spectroscopic analysis of electromagnetic radiation (light) absorbed and emitted by regions of space.

Explore an Issue: Take a Stand: Linus Pauling and the Vitamin C Controversy

(Page 250)

- (a) It is claimed that large doses of vitamin C:
- reduce occurrence and severity of common cold,
 - lower the risk of heart disease and stroke,
 - reduce risk for most common types of cancer,
 - increase survival time and improve quality of life in terminal cancer patients,
 - improve blood vessel dilation, and
 - lower blood lead (Pb) levels.
- (b) The main criticism of Pauling's claims for the benefits of large doses of vitamin C are:
- The results of Pauling's studies using vitamin C to prevent the common cold are not reproducible. Numerous well-designed studies have shown that vitamin C does not prevent common colds; at best, vitamin C may slightly reduce cold symptoms.
 - Pauling's analyses of vitamin C therapy for the prevention and treatment of cancer is flawed. Independent analyses of the same studies show no significant effect.
 - The Linus Pauling Institute of Medicine is largely funded by the pharmaceutical company that produces most of the world's supply of vitamin C.
 - Pauling has lost scientific credibility by his association with the health food industry, which is notorious for making unsubstantiated claims.
- (c) To be scientifically valid, a claim must be experimentally testable. Then there must exist empirical evidence from well-designed experiments that have suitable controls and controlled variables. Finally, the evidence must be reproducible by independent investigators.
- (d) Pauling's fame was very likely a large factor in influencing public and scientific opinion about the benefits of vitamin C. Pauling's two Nobel Prizes represented significant achievements, and both involved contradicting conventional thinking of the time. It seemed plausible that once again Pauling knew more than his contemporaries.

A person unknown to the public and with no scientific training would not be taken seriously if he/she made the same claims about vitamin C, because the public would have no basis to believe the claims.

Reproducible evidence from well-designed studies provides the most reliable basis for deciding which claims to believe. When the empirical evidence is unclear or contradictory, the claim is inconclusive or shown to be false.

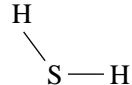

- (e) A scientist who goes against the rest of the scientific community risks his career and reputation, if independent research proves his claim to be wrong. On the other hand, if independent research supports his claim, he may enhance his career and receive much recognition.

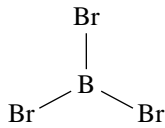
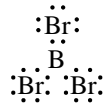
The practice and work of science is not always completely objective, especially when new theories are proposed that contradict accepted knowledge. However, if continuing research consistently shows that the new theory is better than the old theory at explaining and predicting experimental evidence, the new theory will eventually be accepted (although this may occasionally take a long time).

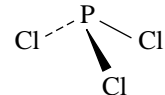
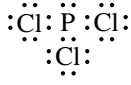
SECTION 4.3 QUESTIONS

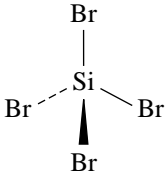
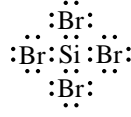
(Page 250)

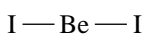
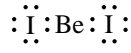

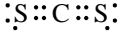
Understanding Concepts

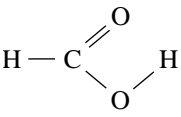
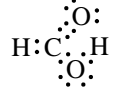
- (a)  V-shape 

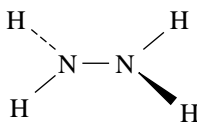
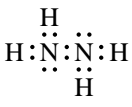
(b)  trigonal planar 

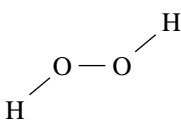

(c)  pyramidal 

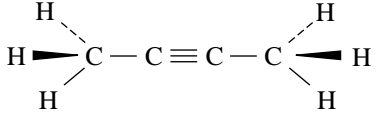
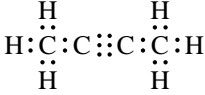
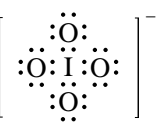
(d)  tetrahedral 

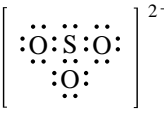
(e)  linear 
- (a)  linear 

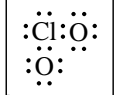
(b)  linear (C)
V-shape (O) 

(c)  pyramidal
(both Ns) 

(d)  V-shape
(both Os) 

(e)  linear (central Cs)
tetrahedral (end Cs) 
- (a)  tetrahedral

(b)  pyramidal

(c)  V-shape

Making Connections

- Dr. Bader's work has added to our understanding of molecules by applying quantum mechanics to the overall structure of a molecule. This gives a more comprehensive understanding of the structure and bonding, thus allowing for better predictions of molecular structures and ultimately, new substance properties.

5. Dr. Ronald Gillespie, the co-creator of VSEPR theory, is currently Professor Emeritus at McMaster University. He holds B.Sc. and Ph.D. degrees in science, and a D.Sc. from London University. He has won many significant awards, including the Chemical Institute of Canada Medal, the Henry Marshall Tory Medal of the Royal Society of Canada, and the Izaak Walter Killam Memorial Prize of the Canada Council for Pure Science, to name just a few. He is a visiting professor at nine international universities in Europe, Australia, and Asia, and has been awarded four honorary doctorates. His major topic of research, in cooperation with Dr. Richard Bader, is using calculated electron probability distributions to better understand the VSEPR model.
6. The sense of taste seems to be essentially built around the ability of taste receptors to form hydrogen bonds at specific locations with certain molecules. Thus, artificial sweeteners like saccharin and cyclamate and acesulfame-K are non-nutritive molecules with structural similarities to natural sugars. The molecular structure for sweetness involves part of the molecule being a small pentagon or hexagon of atom with the ability to hydrogen bond at a specific spot on the ring. Similarly, artificial compounds like Bitrex®—added as a safety precaution to many medications to make the taste extremely bitter—are structured to a shape that triggers human taste receptors for bitterness to react strongly.

4.4 POLAR MOLECULES

PRACTICE

(Page 253)

Understanding Concepts

- $\begin{array}{ccc} \delta^+ & & \delta^- \\ \text{H} & \text{---} & \text{Cl} \\ 2.1 & & 3.0 \end{array}$

polar covalent
 - $\begin{array}{ccc} \delta^- & & \delta^+ \\ \text{C} & \text{---} & \text{H} \\ 2.5 & & 2.1 \end{array}$

polar covalent
 - $\begin{array}{ccc} \delta^+ & & \delta^- \\ \text{N} & \text{---} & \text{O} \\ 3.0 & & 3.5 \end{array}$

polar covalent
 - $\begin{array}{ccc} \delta^+ & & \delta^- \\ \text{I} & \text{---} & \text{Br} \\ 2.5 & & 2.8 \end{array}$

polar covalent
 - $\begin{array}{ccc} + & & - \\ \text{Mg} & \text{---} & \text{S} \\ 1.2 & & 2.5 \end{array}$

ionic
 - $\begin{array}{ccc} & & \\ \text{P} & \text{---} & \text{H} \\ 2.1 & & 2.1 \end{array}$

nonpolar covalent
- polar covalent
 - ionic
 - nonpolar covalent
- The list of the bonds in order of increasing bond polarity is assumed to be the same as the order of increasing difference in electronegativity of the bonded atoms. Thus, the orders are as follows:
 - H—H, C—H, Be—H, N—H, Li—H, O—H, F—H
 - I—I, I—Cl, P—Cl, (Li—I, Al—Cl), Rb—F (Note: Li—I and Al—Cl have equal dipoles.)
 - C—H, C—O, O—H
 - C—H, C—Cl, C—F