

Section 4.2: Three-Dimensional Structure

Mini Investigation: Balloon Model of Electron Repulsion, page 210

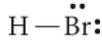
Answers may vary. Sample answers:

- A.** The two balloons tied together orient themselves in a straight line, as far from one another as possible.
- B.** The three balloons tied together orient themselves in the triangular arrangement called trigonal planar.
- C.** The four balloons tied together orient themselves in a tetrahedral arrangement.
- D.** Yes, the balloons are good models of valence shell electron-pair repulsions. The balloons move as far apart as possible in the same way that electrons in valence shell orbitals move as far apart as possible.
- E.** In any of the modes, if I pushed the balloons together and let go, the balloons would quickly move back to their original orientation.
- F.** If one balloon in 4 balloons tied together was a lone pair, the three-dimensional structure would be a trigonal pyramid. If 2 balloons in the 4 were lone pairs, the three-dimensional structure would be a trigonal planar.

Tutorial 1 Practice, page 212

1. (a) Geometry of HBr predicted using VSEPR theory:

Step 1. Draw the simplified Lewis structure.



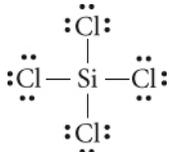
Step 2. The hydrogen bromide molecule has 1 pair of bonding electrons. The only possible structure is linear.

Step 3. Draw the three-dimensional structure.



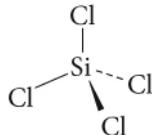
(b) Geometry of SiCl₄ predicted using VSEPR theory:

Step 1. Draw the simplified Lewis structure.



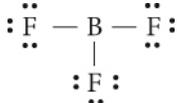
Step 2. The silicon tetrachloride molecule has 4 pairs of bonding electrons around the central atom. There are no lone electron pairs on the silicon atom. The best arrangement of the 4 bonding electron pairs around the central atom to minimize electron-pair repulsion is a tetrahedral structure.

Step 3. Draw the three-dimensional structure.



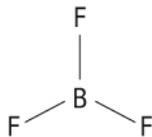
(c) Geometry of BF₃ predicted using VSEPR theory:

Step 1. Draw the simplified Lewis structure.



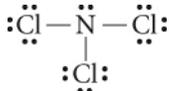
Step 2. The boron trifluoride molecule has 3 pairs of bonding electrons around the central atom. There are no lone electron pairs on the boron atom. The best arrangement of the 3 bonding electron pairs around the central atom to minimize electron-pair repulsion is a trigonal planar structure.

Step 3. Draw the three-dimensional structure.



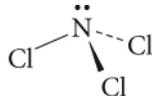
(d) Geometry of NCl_3 predicted using VSEPR theory:

Step 1. Draw the simplified Lewis structure.



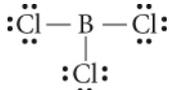
Step 2. The nitrogen trichloride molecule has 3 pairs of bonding electrons around the central atom. There is 1 lone electron pair on the nitrogen atom. The best arrangement of the 4 electron pairs (3 bonding and 1 lone pair) around the central atom to minimize electron-pair repulsion is a trigonal pyramidal structure.

Step 3. Draw the three-dimensional structure.



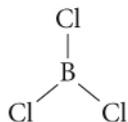
2. (a) Geometry of BCl_3 predicted using VSEPR theory:

Step 1. Draw the simplified Lewis structure.



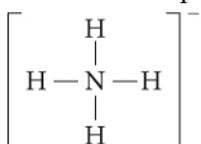
Step 2. The boron trichloride molecule has 3 pairs of bonding electrons around the central atom. There are no lone electron pairs on the boron atom. The best arrangement of the 3 bonding electron pairs around the central atom to minimize electron-pair repulsion is a trigonal planar structure.

Step 3. Draw the three-dimensional structure.



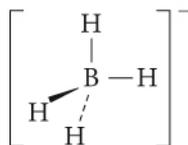
(b) Geometry of BH_4^- predicted using VSEPR theory:

Step 1. Draw the simplified Lewis structure.



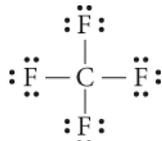
Step 2. The tetrahydroborate ion has 4 pairs of bonding electrons around the central atom. There are no lone electron pairs on the boron atom. The best arrangement of the 4 bonding electron pairs around the central atom to minimize electron-pair repulsion is a tetrahedral structure.

Step 3. Draw the three-dimensional structure.



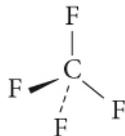
(c) Geometry of CF₄ predicted using VSEPR theory:

Step 1. Draw the simplified Lewis structure.



Step 2. The tetrafluoromethane molecule has 4 pairs of bonding electrons around the central atom. There are no lone electron pairs on the boron atom. The best arrangement of the 4 bonding electron pairs around the central atom to minimize electron-pair repulsion is a tetrahedral structure.

Step 3. Draw the three-dimensional structure.



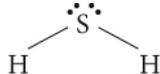
(d) Geometry of H₂S predicted using VSEPR theory:

Step 1. Draw the simplified Lewis structure.



Step 2. The hydrogen sulfide molecule has 2 pairs of bonding electrons around the central atom. There are 2 lone electron pairs on the sulfur atom. The best arrangement of the 4 electron pairs (2 bonding and 2 lone pairs) around the central atom to minimize electron-pair repulsion is a bent structure.

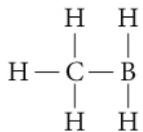
Step 3. Draw the three-dimensional structure.



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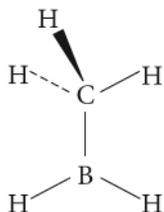
1. (a) Geometry of CH₃BH₂ predicted using VSEPR theory:

Step 1. Draw the simplified Lewis structure. There are two central atoms, carbon and boron.



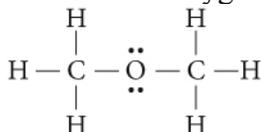
Step 2. The methylborane molecule has 4 pairs of bonding electrons around the central carbon atom and 3 pairs of bonding electrons around the central boron atom. There are no lone electron pairs on either central atom. To minimize electron-pair repulsion, the best arrangement of the 4 bonding electron pairs around the carbon atom is a tetrahedral structure, and the best arrangement of the 3 bonding electron pairs around the boron atom is a trigonal planar structure.

Step 3. Draw the three-dimensional structure.



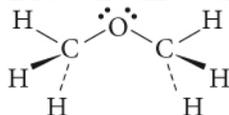
(b) Geometry of CH₃OCH₃ predicted using VSEPR theory:

Step 1. Draw the simplified Lewis structure. There are three central atoms, 2 carbon atoms and 1 oxygen atom.



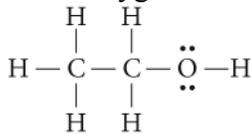
Step 2. The methoxymethane molecule has 4 pairs of bonding electrons around each central carbon atom. There are 2 pairs of bonding electrons around the oxygen atom, and it has 2 lone pairs. To minimize electron-pair repulsion, the best arrangement of the 4 bonding electron pairs around each carbon atom is a tetrahedral structure. The best arrangement of the 4 electron pairs (2 bonding pairs and 2 lone pairs) around the oxygen atom is a bent structure.

Step 3. Draw the three-dimensional structure.



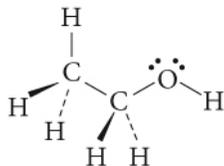
(c) Geometry of CH₃CH₂OH predicted using VSEPR theory:

Step 1. Draw the simplified Lewis structure. There are 3 central atoms, 2 carbon atoms and 1 oxygen atom.



Step 2. The ethanol molecule has 4 pairs of bonding electrons around each central carbon atom. There are 2 pairs of bonding electrons around the oxygen atom, and it has 2 lone pairs. To minimize electron-pair repulsion, the best arrangement of the 4 bonding electron pairs around each carbon atom is a tetrahedral structure. The best arrangement of the 4 electron pairs (2 bonding pairs and 2 lone pairs) around the oxygen atom is a bent structure.

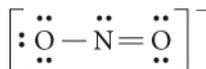
Step 3. Draw the three-dimensional structure.



Tutorial 3 Practice, page 215

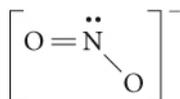
1. Geometry of NO_2^- predicted using VSEPR theory:

Step 1. Draw the simplified Lewis structure. Nitrogen is the central atom.



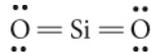
Step 2. The nitrite ion has 3 groups of electrons (a single bond, a double bond, and 1 lone pair) around the central nitrogen atom. To minimize electron-pair repulsion, the best arrangement of the 3 electron groups around the nitrogen atom is a bent structure.

Step 3. Draw the three-dimensional structure.



2. (a) Geometry of SiO_2 predicted using VSEPR theory:

Step 1. Draw the simplified Lewis structure. The central atom is silicon.



Step 2. The silicon dioxide molecule has 2 double bonds and no lone electron pairs around the central atom. To minimize electron-pair repulsion, the best arrangement of the 2 groups of electrons around the silicon atom is a linear structure.

Step 3. Draw the three-dimensional structure.



(b) Geometry of HCN predicted using VSEPR theory:

Step 1. Draw the simplified Lewis structure. The central atom is carbon.



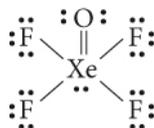
Step 2. The hydrogen cyanide molecule has 2 groups of electrons (a single bond and a triple bond) around the central carbon atom, and no lone pairs. To minimize electron-pair repulsion, the best arrangement of the 2 groups of electrons around the carbon atom is a linear structure.

Step 3. Draw the three-dimensional structure.



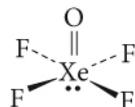
(c) Geometry of XeOF_4 predicted using VSEPR theory:

Step 1. Draw the simplified Lewis structure. The central atom is Xe.



Step 2. The xenon oxytetrafluoride molecule has 6 groups of electrons around the central xenon atom (4 single bonds, 1 double bond, and 1 lone pair). To minimize electron-pair repulsion, the best arrangement of the 6 groups of electrons around the xenon atom is a square pyramidal structure.

Step 3. Draw the three-dimensional structure.

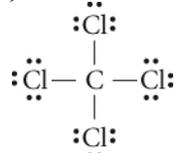


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1. The words that make up the initialism “VSEPR”—valence shell electron-pair repulsion—describe the concept of the theory very well. The main concept of the theory is that pairs of electrons, both bonding and non-bonding, will repel one another and maximize the distance between themselves around an atom. This can be used to predict geometric structures for most molecules and ionic substances that contain non-metallic elements. There are some exceptions in which the VSEPR theory does not accurately describe the structure of a pure substance.

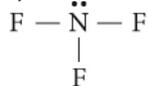
2. Prediction of the three-dimensional structure and bond angles:

(a) CCl_4 molecule:



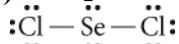
The central atom has 4 bonding pairs and no lone pairs, so CCl_4 has a tetrahedral structure. The bond angles are 109.5° .

(b) NF_3 molecule:



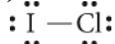
The central atom has 4 pairs of electrons (3 bonding pairs and 1 lone pair), so NF_3 has a trigonal pyramidal structure. The bond angles are 107° .

(c) SeCl_2 molecule:



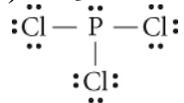
The central atom has 4 pairs of electrons (2 bonding pairs and 2 lone pairs), so SeCl_2 has a bent or V-shaped structure. The bond angles are 104.5° .

(d) ICl molecule:



There is 1 bonding pair between the iodine and chlorine atoms, so ICl has a linear structure. The bond angles are 180° .

(e) PCl_3 molecule:



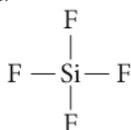
The central atom has 4 pairs of electrons (3 bonding pairs and 1 lone pair), so PCl_3 has a trigonal pyramidal structure. The bond angles are 107° .

(f) SCl_2 molecule:



The central atom has 4 pairs of electrons (2 bonding pairs and 2 lone pairs), so SCl_2 has a bent or V-shaped structure. The bond angles are 104.5° .

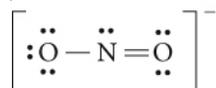
(g) SiF_4 molecule:



The central atom has 4 bonding pairs and no lone pairs, so SiF_4 has a tetrahedral structure. The bond angles are 109.5° .

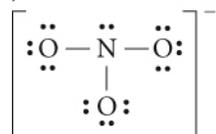
3. Prediction of the three-dimensional structure and bond angles:

(a) NO_2^- ion:



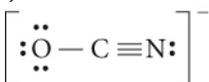
The central atom has 3 electron groups (1 single bond, 1 double bond, and 1 lone pair), so NO_2^- has a bent or V-shaped structure. The bond angle is 120° .

(b) NO_3^- ion:



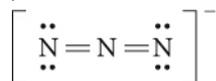
The central atom has 3 bonding electron pairs and no lone pairs, so NO_3^- has a trigonal planar structure. The bond angles are 120° .

(c) OCN^- ion:



The central atom has 2 groups of electrons (1 single bond, and 1 triple bond) and no lone pairs, so OCN^- has a linear structure. The bond angles are 180° .

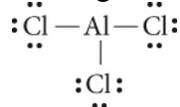
(d) N_3^- ion:



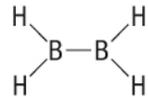
The central atom has 2 groups of electrons (2 double bonds) and no lone pairs, so N_3^- has a linear structure. The bond angles are 180° .

4. Molecules such as ICl and HBr are linear. You can tell because only 2 atoms participate in the bonding and there are no unpaired electrons, so the molecule has a linear shape.

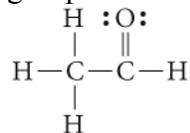
5. (a) The AlCl_3 molecule has a trigonal planar structure, because the central atom has 3 bonding electron pairs and no lone pairs:



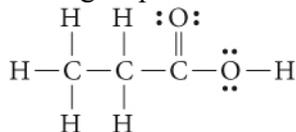
(b) Both of the boron atoms in B_2H_4 have a trigonal planar arrangement of atoms, because each boron atom has 3 bonding electron pairs and no lone pairs.



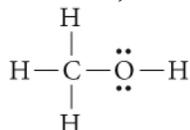
(c) In the CH_3COH molecule, the carbon atom in COH is trigonal planar, because it has 3 groups of electrons (1 double bond and 2 single bonds) and no lone pairs.



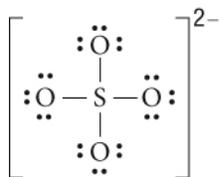
(d) In the $\text{CH}_3\text{CH}_2\text{COOH}$ molecule, the carbon atom in COO is trigonal planar, because it has 3 groups of electrons (1 double bond and 2 single bonds) and no lone pairs.



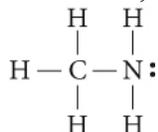
6. (a) In the CH_3OH molecule, the arrangement of atoms around the carbon atom is tetrahedral, because there are 4 bonding pairs of electrons and no lone pairs.



(b) The SO_4^{2-} ion has a tetrahedral arrangement of atoms around the central sulfur atom, because there are 4 bonding pairs of electrons and no lone pairs.



(c) The CH_3NH_2 molecule has a tetrahedral arrangement of atoms around the central carbon atom, because there are 4 bonding pairs of electrons and no lone pairs.

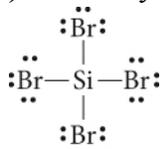


7. (a) Geometry of BeI_2 predicted using VSEPR theory, and drawing of structure:

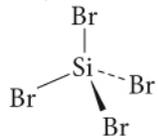


The central atom has 2 bonding pairs of electrons and no lone pairs, so BeI_2 has a linear structure, as shown above.

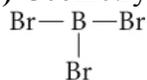
(b) Geometry of SiBr_4 predicted using VSEPR theory, and drawing of structure:



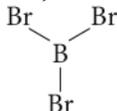
The SiBr_4 molecule has a tetrahedral arrangement of atoms around the central carbon atom, because there are 4 bonding pairs of electrons and no lone pairs.



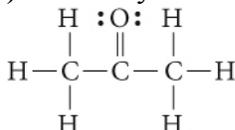
(c) Geometry of BBr_3 predicted using VSEPR theory, and drawing of structure:



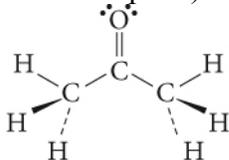
The BBr_3 molecule has a trigonal planar arrangement of atoms around the central boron atom, because there are 3 bonding pairs of electrons and no lone pairs.



(d) Geometry of CH_3COCH_3 predicted using VSEPR theory, and drawing of structure:

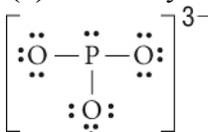


In the CH_3COCH_3 molecule, the two carbon atoms bonded to the central carbon have a tetrahedral arrangement of atoms, because there are 4 bonding pairs of electrons and no lone pairs. The central carbon has a trigonal planar arrangement of atoms, because there are 3 groups of electrons around the C atom (2 single bonds, and 1 double bond along with 2 lone pairs).

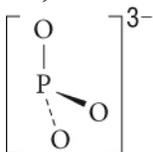


(e) Geometry of CH_2H_4 predicted using VSEPR theory, and drawing of structure:

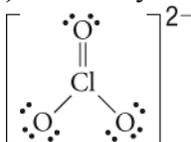
8. (a) Geometry of PO_3^{3-} predicted using VSEPR theory, and drawing of structure:



The PO_3^{3-} ion has a trigonal pyramidal arrangement of atoms around the central boron atom, because there are 3 bonding pairs of electrons on the boron atom and 1 lone pair.

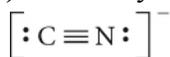


(b) Geometry of CO_3^{2-} predicted using VSEPR theory, and drawing of structure:



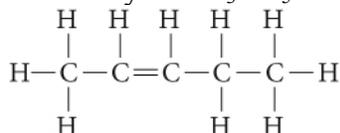
The CO_3^{2-} ion has a trigonal planar arrangement of atoms around the central carbon atom, because there are 3 groups of electrons around the carbon atom (2 single bonds and 1 double bond) and no lone pairs, as shown above.

(c) Geometry of CN^- predicted using VSEPR theory, and drawing of structure:



The CN^- ion has only two atoms, so the only possibility is a linear structure.

9. Geometry of $\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2\text{CH}_3$ predicted using VSEPR theory:



This molecule will have tetrahedral geometry around the first, fourth, and fifth carbons, because each of these carbons has 4 bonding pairs and no lone pairs. It will have trigonal planar geometry around the second and third carbons, because each of these carbon atoms has 3 groups of surrounding electrons (2 single bonds and 1 double bond).

10.

Compound	Number of pairs of electrons on central atom	Number of lone pairs	Name of shape	Diagram of shape
NBr_3	4	1	trigonal pyramidal	
CS_2	4 (2 double bonds)	0	linear	$\text{S} - \text{C} - \text{S}$
SeH_4	5	1	seesaw	
SeF_6	6	0	octahedral	
ICl_4^-	6	2	square planar	
ICl	4	3	linear	$\text{I} - \text{Cl}$
CH_3Cl	4	0	tetrahedral	
BrCl_5	6	1	square pyramidal	

BrF_3	5	2	T-shaped	$\begin{array}{c} \cdot\cdot \\ \text{F} - \text{Br} - \text{F} \\ \cdot\cdot \\ \\ \text{F} \end{array}$
XeI_3^-	6	3	T-shaped	$\left[\begin{array}{c} \cdot\cdot \\ \text{I} - \text{Xe} - \text{I} \\ \cdot\cdot \\ \\ \text{I} \end{array} \right]^-$
SBr_4	6	2	square planar	$\begin{array}{c} \text{Br} \quad \text{Br} \\ \diagdown \quad / \\ \text{S} \\ / \quad \diagdown \\ \text{Br} \quad \text{Br} \end{array}$ <p style="text-align: center;">90°</p>
BrO_2^-	4	2	bent	$\left[\begin{array}{c} \cdot\cdot \\ \text{O} \quad \text{Br} \quad \text{O} \\ \cdot\cdot \\ \diagdown \quad / \\ \text{O} \end{array} \right]^-$
OF_2	4	2	bent	$\begin{array}{c} \cdot\cdot \\ \text{F} \quad \text{O} \quad \text{F} \\ \cdot\cdot \end{array}$
CF_2Cl_2	4	0	tetrahedral	$\begin{array}{c} \text{Cl} \\ \\ \text{C} \\ / \quad \backslash \\ \text{F} \quad \text{Cl} \\ \backslash \quad / \\ \text{F} \end{array}$
H_2Se	4	2	bent	$\begin{array}{c} \cdot\cdot \\ \text{H} \quad \text{Se} \quad \text{H} \\ \cdot\cdot \end{array}$
PBr_6^-	6	0	octahedral	$\left[\begin{array}{c} \text{Br} \\ \cdot\cdot \quad \quad \cdot\cdot \\ \text{Br} \quad \text{P} \quad \text{Br} \\ \cdot\cdot \quad \quad \cdot\cdot \\ \text{Br} \end{array} \right]^-$