Electron Pair Repulsion Theory
(Stretch & Challenge - shapes of molecul

Learning Outcomes *Specification ref*

- use electron pair repulsion theory to predict shape
- explain distortions to standard geometric shapes b repulsion between bonding and non-bonding pairs

Electron Pair Repulsion Theory

- Identify how many groups of electrons surround th

  This will determine the shape "in essence", but this will be d there are non-bonding/lone pairs involved.
- Identify how many of those electron groups are:
  - bonding pairs of electrons,
  - non-bonding/lone pairs of electrons,
  - if multiple bonds are constraining two or mor
- This will determine the actual molecular shape (*w*

Q1. Use electron pair repulsion theory to deduce the sha
ammonia, NH_3.

There are ___ electron groups around the centra
Since electron pairs repel, they will try to move
[So the best shape for them to adopt, "in essenc

Those electron groups consist of ___ bonding pa
and ___ non-bondir

*So the actual **molecular shape** is __________*
with b

<u>Extra comment</u> *wrt bond angle chosen?*

1. **Identify Electron Groups:**
- **Central Atom:** Nitrogen N is the central atom in ammo
- **Valence Electrons:** Nitrogen has 5 valence electrons.
- **Hydrogen Atoms:** Each hydrogen contributes 1 electron
- **Electron Pairs:** The total number of valence electron
electron pairs.

Hence there are **4 electron groups** around the central n

2. **Electron Pair Repulsion:**
- According to VSEPR theory electron pairs repel each
repulsion.
- For 4 electron pairs the arrangement that minimizes

3. **Bonding and Lone Pairs:**
- Among the 4 electron groups there are 3 bonding pairs
- There is 1 lone pair of electrons on the nitrogen ato

4. **Molecular Shape:**
- While the electron pair geometry is tetrahedral the p
bonding pairs more strongly than the bonding pairs repe
- This results in a **trigonal pyramidal** shape for the mo

5. **Bond Angles:**
- In a perfect tetrahedral arrangement the bond angles
- However the lone pair-bond pair repulsion is stronger
ammonia.
- The bond angle in ammonia is approximately **107 degree**

Q2a. Use electron pair repulsion theory to deduce the
tetrachlorophosphonium(V) ion, PCl_4^+.

There are ___ electron groups around the cent
Since electron pairs repel, they will try to mo
[So the best shape for them to adopt, "in essen

Those electron groups consist of ___ bonding p
and ___ non-bond

*So the actual **molecular shape** is ________*
with

Filling in the Blanks:

There are **4** electron groups around the central N ato

Since electron pairs repel they will try to move as fa
$So the best shape for them to adopt "in essence" is t

Those electron groups consist of **3** bonding pairs of el
and **1** non-bonding/lone pairs of electrons. $1 mark$

So the actual molecular shape is **trigonal pyramidal** 1
with bond angles of **107 degrees**. $1 mark$

Extra Comment on Bond Angle:

The bond angle is slightly less than 109.5° due to the
thus compressing the bond angle to approximately 107°

Summary:

- **Electron Groups:** 4
- **Electron Pair Geometry:** Tetrahedral
- **Molecular Shape:** Trigonal Pyramidal
- **Bond Angles:** ~107 degrees

Q2b. Use electron pair repulsion theory to deduce the sh
tetrachlorophosphonium(III) ion, PCl_4^- .

There are ___ electron groups around the centra
Since electron pairs repel, they will try to move
[So the best shape for them to adopt, "in essence

Those electron groups consist of ___ bonding pa
and ___ non-bondin

So the actual ***molecular shape*** *is a "sees*
with bond angles

Answer

Q2a: Tetrachlorophosphonium(V) ion, PCl_4^+

1. Identify the number of electron groups around the central phosphorus (P) atom. The PCl_4^+ ion has 4 chlorine atoms bonded to the phosphorus atom. Therefore, there are 4 bonding pairs of electrons and no lone pairs
2. Since there are 4 electron groups, they will arrange themselves to minimize repulsion. The best shape for them to adopt is a **tetrahedral** arrangement
3. The electron groups consist of **4 bonding pairs of electrons** and **0 non-bonding/lone pairs of electrons**
4. The actual molecular shape is **tetrahedral**
5. In a tetrahedral arrangement, the bond angles are approximately **109.5 degrees**

Answer: There are 4 electron groups around the central P atom. The best shape for them to adopt is tetrahedral. Those electron groups consist of 4 bonding pairs of electrons and 0 non-bonding/lone pairs of electrons. So the actual molecular shape is tetrahedral with bond angles of 109.5 degrees

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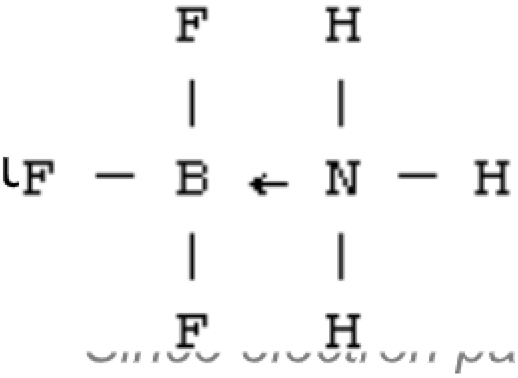
Q2b: Tetrachlorophosphonium(III) ion, PCl_3

1. Identify the number of electron groups around the central phosphorus (P) atom. The PCl_3 ion has 3 chlorine atoms bonded to the phosphorus atom and 1 lone pair. Therefore, there are 4 electron groups in total (3 bonding pairs and 1 lone pair)
2. Since there are 4 electron groups, they will arrange themselves to minimize repulsion. The best shape for them to adopt is a **tetrahedral** arrangement, but the presence of the lone pair will affect the molecular geometry
3. The electron groups consist of **3 bonding pairs of electrons** and **1 non-bonding/lone pair of electrons**
4. The actual molecular shape is a **trigonal pyramidal** shape due to the presence of the lone pair
5. In a trigonal pyramidal arrangement, the bond angles are slightly less than **109.5 degrees**, typically around **107 degrees** due to the lone pair-bonding pair repulsion

Answer: There are 4 electron groups around the central P atom. The best shape for them to adopt is tetrahedral. Those electron groups consist of 3 bonding pairs of electrons and 1 non-bonding/lone pair of electrons. So the actual molecular shape is trigonal pyramidal with bond angles of approximately 107 degrees

Q3. Use electron pair repulsion theory to deduce the s



a Su ond angles if B is the ce

groups around the centr

Since electron pairs ________, they will try to

[So the best shape for them to adopt, "in essenc

Those electron groups consist of ___ bonding p

and ___ non-bond

*So the actual **molecular shape** is __________*

with

b Suggest the shape and bond angle if N is the centra

There are around the central

Since electron pairs ________, they will try to

[So the best shape for them to adopt, "in essence"

Those electron groups consist of

*So the actual **molecular shape** is ____________*

with b

Final Answer:

For BF_3: trigonal planar shape with bond angles of 120°;

For NH_3: trigonal pyramidal shape with bond angles of approximately 107°

Explanation

To analyze the shapes of BF_3 and NH_3 using electron pair repulsion theory (VSEPR theory), we will follow the steps outlined in the question

Part a: Analyzing BF_3

1. Identify the central atom and its electron groups
   - The central atom is Boron (B), which has 3 bonding pairs of electrons with the three Fluorine (F) atoms
2. Determine the arrangement of electron groups
   - Since there are 3 bonding pairs and no lone pairs around the central B atom, the electron groups will arrange themselves to minimize repulsion
3. Deduce the shape based on the arrangement
   - The best shape for them to adopt, "in essence", is **trigonal planar**
4. Identify the types of electron groups
   - Those electron groups consist of **3 bonding pairs of electrons** and **0 non-bonding/lone pairs of electrons**
5. Determine the actual molecular shape and bond angles
   - So the actual molecular shape is **trigonal planar**, with bond angles of **120°**

Part b: Analyzing NH_3

1. Identify the central atom and its electron groups
   - The central atom is Nitrogen (N), which has 3 bonding pairs of electrons with the three Hydrogen (H) atoms and 1 lone pair of electrons
2. Determine the arrangement of electron groups
   - Since there are 3 bonding pairs and 1 lone pair around the central N atom, the electron groups will arrange themselves to minimize repulsion
3. Deduce the shape based on the arrangement
   - The best shape for them to adopt, "in essence", is **tetrahedral** (considering the arrangement of all electron groups)
4. Identify the types of electron groups
   - Those electron groups consist of **3 bonding pairs of electrons** and **1 non-bonding/lone pair of electrons**
5. Determine the actual molecular shape and bond angles
   - So the actual molecular shape is **trigonal pyramidal**, with bond angles of **approximately 107°** (due to the presence of the lone pair)

Q4. There are very few noble gas compounds, due to group of elements. However, xenon tetrafluoride c between the two elemental gases:

a Use electron pair repulsion theory to suggest the
Assume that xenon has eight electrons in its outer shell.

There are around the central

Since electron pairs _______, they will try to

[So the best shape for them to adopt, "in essence", i

Those electron groups consist of

*So the actual **molecular shape** is ____________*

with bon

b i Draw a diagram of this molecule:

b ii Explain why you have chosen this orientation of th
central atom (i.e. there is more than one orientatio
which is best and **why**?)

Part a:

1. Xenon (Xe) has 8 electrons in its outer shell. In xenon tetrafluorid
xenon is the central atom surrounded by four fluorine atoms
2. According to the electron pair repulsion theory (VSEPR theory), e
pairs around a central atom will arrange themselves to minimize
3. Since xenon has 4 bonded pairs (from the four fluorine atoms) ar
pairs (due to the octet rule), the best shape for them to adopt, "in
is octahedral
4. The electron groups consist of 4 bonding pairs (Xe-F bonds) and
5. The actual molecular shape is square planar, as the lone pairs occ
positions opposite each other in the octahedral arrangement, res
planar structure with the fluorine atoms in the same plane
6. The bond angles in a square planar geometry are 90 degrees

Answer: The geometry of xenon tetrafluoride is square planar with bo
of 90 degrees

Part b

```
        F
        |
  F  -  Xe  -  F
        |
        F
```

Part b ii:

1. I have chosen this orientation of the electron pairs around the central at
   because the square planar shape minimizes the repulsion between the
   bonding pairs and the lone pairs

2. In this configuration, the two lone pairs are positioned opposite each oth
   which allows the four fluorine atoms to be as far apart as possible, thus
   reducing electron pair repulsion and stabilizing the molecular structure

Answer: The orientation is chosen to minimize repulsion, leading to a square planar shape with lone pairs opposite each other

Q5. a Use electron pair repulsion theory to deduce the

b Show the bond angles on a diagram of the ethene

Part a-

Answer

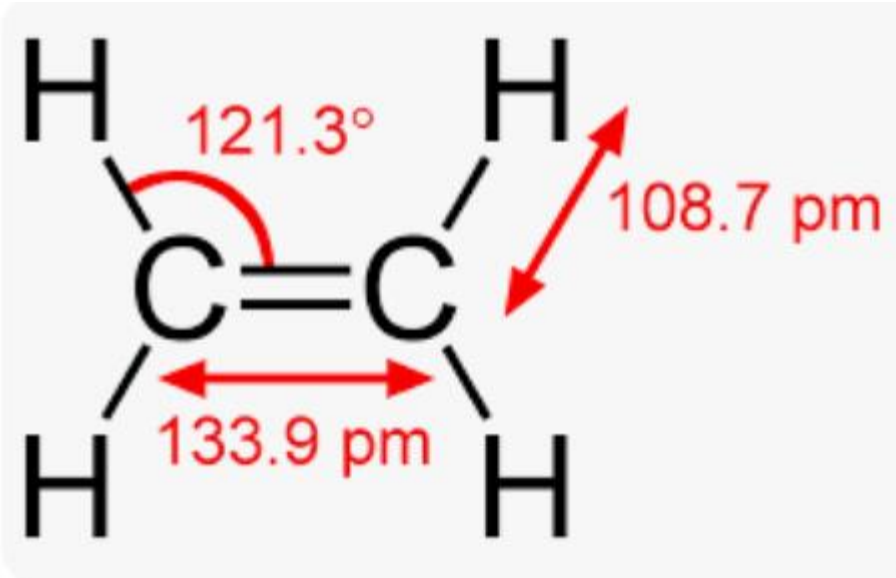
The shape of ethene ($H_2C=CH_2$) is trigonal planar around each carbon atom, witl bond angles of approximately 120 degrees

Explanation

1. Identify the central atoms in ethene ($H_2C=CH_2$). The central atoms are the carbon atoms (C)
2. Determine the number of electron pairs around each carbon atom. Each carbon in ethene forms three sigma bonds (two with hydrogen and one witl the other carbon) and has one pi bond (the double bond with the other carbon). Therefore, each carbon has three regions of electron density
3. Apply the VSEPR (Valence Shell Electron Pair Repulsion) theory. According t VSEPR theory, regions of electron density will arrange themselves to minimize repulsion. Three regions of electron density around a central atom will adopt a trigonal planar geometry
4. Since the carbon atoms in ethene are bonded to two hydrogen atoms and one other carbon atom, the shape around each carbon atom is trigonal planar
5. The bond angles in a trigonal planar arrangement are approximately 120 degrees

a-

part b



H
H
121.3°
108.7 pm
C
C
133.9 pm
H
H

Q6. a Use electron pair repulsion theory to deduce th

b Explain why you have chosen this bond angle.

Answer

1. Identify the central atom
central atom that is bond

2. Determine the number of
Assuming T is a Group 1
electrons

3. Count the bonding pairs
each forming a single bo
electrons

4. Determine the number of
valence electrons and is
remaining

5. Apply the VSEPR (Valenc
arrangement of 2 bondin
corresponds to a tetrahe
the molecule is determin
leads to a bent molecula

6. Calculate the bond angle
angle is 109.5°. However,
strongly than bonding pa
H_2T will be slightly less