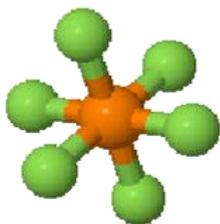


## I<sub>1</sub>- Using VSEPR to Predict Shapes of Molecules



Refcode: WINFAA

### TOP TIP!

If the central atom is positive, then subtract 1 electron from the overall electron total; if the central atom is negative, then add 1 electron to the overall electron total.



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The VSEPR predicted shapes of molecules can be found in a systematic way by using the number of electron pairs to determine the shape of the molecules.

To predict the shape of the molecules, first draw out the Lewis structure of the molecule. On the Lewis diagram, identify the central atom. For this molecule  $[\text{PF}_6]^-$  the central atom is Phosphorus (P).

### VSEPR Rules:

1. Identify the central atom
2. Count its valence electrons
3. Add one electron for each bonding atom
4. Add or subtract electrons for charge (see Top Tip)
5. Divide the total of these by 2 to find the total number of electron pairs
6. Use this number to predict the shape

To work out how many electrons are in the outer shell of the central atom phosphorus, just look at which group it is in and the group number is the number of electrons on the outer shell of the central atom. Phosphorus is in

group 5 so it has 5 electrons in its outer shell. Each atom that is bonded to the central atom will be contributing electrons to it; add the extra electrons to the number of valence shells. For the  $[\text{PF}_6]^-$  molecule there are 6 Fluorine atoms which contribute 1 electron each, so adding the 6 electrons to the valence shells totals 11 electrons. The Phosphorus has a negative charge so there is an extra electron. Add this extra electron to the other electrons and the final total should be 12 electrons. Divide the total number of electrons by 2, for  $[\text{PF}_6]^-$  the number is 6, giving the total number of electron pairs. Using the table in the next section and the total number of electron pairs, find the basic VSEPR shape which is assigned to the molecule. The VSEPR model for  $[\text{PF}_6]^-$  is Octahedral. The same method is applied to all molecules.

$[\text{PF}_6]^-$	To Summarise:
Central Atom	Phosphorus
Valence Electrons on Central Atom	5
6 [F] atoms (contributing 1 electron each)	6
+1 electron for negative charge on [P]	1
Total	12
Divide by 2 (number of electron pairs)	6
No. electron pairs gives base shape	<b>Octahedral</b> (VSEPR base shape for 6 e-pairs)

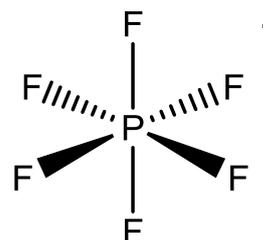
Check if the VSEPR shape of the molecule is correct by going to the database and examining the crystal structure (the refcode for the  $[\text{PF}_6]^-$  structure is WINFAA). Measure the bond angles on the structure comparing them to the ideal VSEPR model angles in the table in the next section. Measure the bond angles on the  $[\text{PF}_6]^-$  structure and compare them to the ideal bond angles on an octahedral structure.

### TOP TIP!

If the total number of electrons is an odd number, then that means the calculation has gone wrong. Try the calculation again.



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## Using VSEPR to Predict Shapes of Molecules

### Basic VSEPR Shapes:

Formula ( $EX_n$ )	Number of Electron Pairs	Shape	Spatial Arrangement	Theoretical Bond Angle
$EX_2$	2	Linear		$180^\circ$
$EX_3$	3	Trigonal Planar		$120^\circ$
$EX_4$	4	Tetrahedral		$109.5^\circ$
$EX_5$	5	Trigonal Bipyramidal		$90^\circ$ Axial-Equatorial and $120^\circ$ Equatorial-Equatorial
$EX_6$	6	Octahedral		$90^\circ$