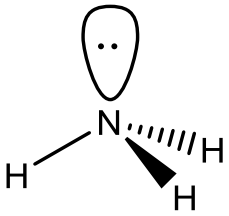
Some molecular shapes have bonding pairs, lone pairs or both lone and bonding pairs of electrons. So how does the existence of lone pairs affect the molecular shape and the VSEPR model of crystal molecules?

To see how the existence of lone pairs affects the molecular shape and the VSEPR model of crystal molecules, work out the basic shape of the crystal molecule first and then apply the lone pairs. $[XeF_5]^-$: Xenon is in group 8 so it has 8 electrons in its valence shell. There are 5 fluorine atoms bonded to xenon, each contribute 1 electron, so in total they contribute 5 electrons. Xenon is negatively charged so an extra electron is added. The total number of all the electrons is 14. We divide 14 by 2 to get 7 which is the total number of electron pairs. Therefore the shape of the molecule $[XeF_5]^-$ therefore is pentagonal bipyramidal.

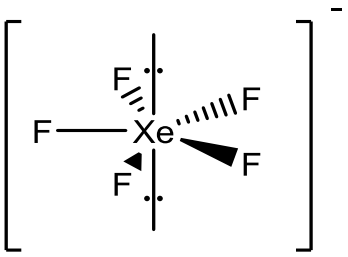
To see the effect of the lone pairs on the molecules, a few adjustments have to be made, showing the difference between the electrostatic repulsion between bonding pairs and lone pairs.



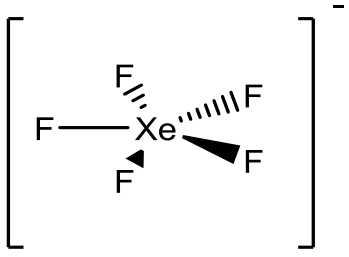
Lone pair/lone pair > lone pair/bonding pair > bonding

Lone pairs have the greatest repelling effect because they are closer to the nucleus of the central atom compared to the bonding pairs, therefore they repel other lone pairs greater compared to bonding pairs. Bonding pairs have a bond between the nucleus of the central atom and the nucleus of a bonding atom therefore are further away from the nucleus, so they do not repel other electrons as much as lone pairs.

For $[XeF_5]^-$ the basic shape is pentagonal bipyramidal with the lone pairs opposite each other to minimise the repulsions of the lone pair/lone pair repulsions. Therefore the $[XeF_5]^-$ molecule is a pentagonal planar shape without the lone pairs. To work out the new shape of the molecule take the basic shape with the lone pairs and cover up the lone pairs. Count how many bonding pairs remain and using the table below work out what shape has that many bonding pairs – find the basic shape, then find the shape that has the number of bonding pairs you are looking for. The $[XeF_5]^-$ has 5 bonding pairs and the basic shape is pentagonal bipyramidal so the shape with 5 bonding pairs is pentagonal planar.



Pentagonal Bipyramidal



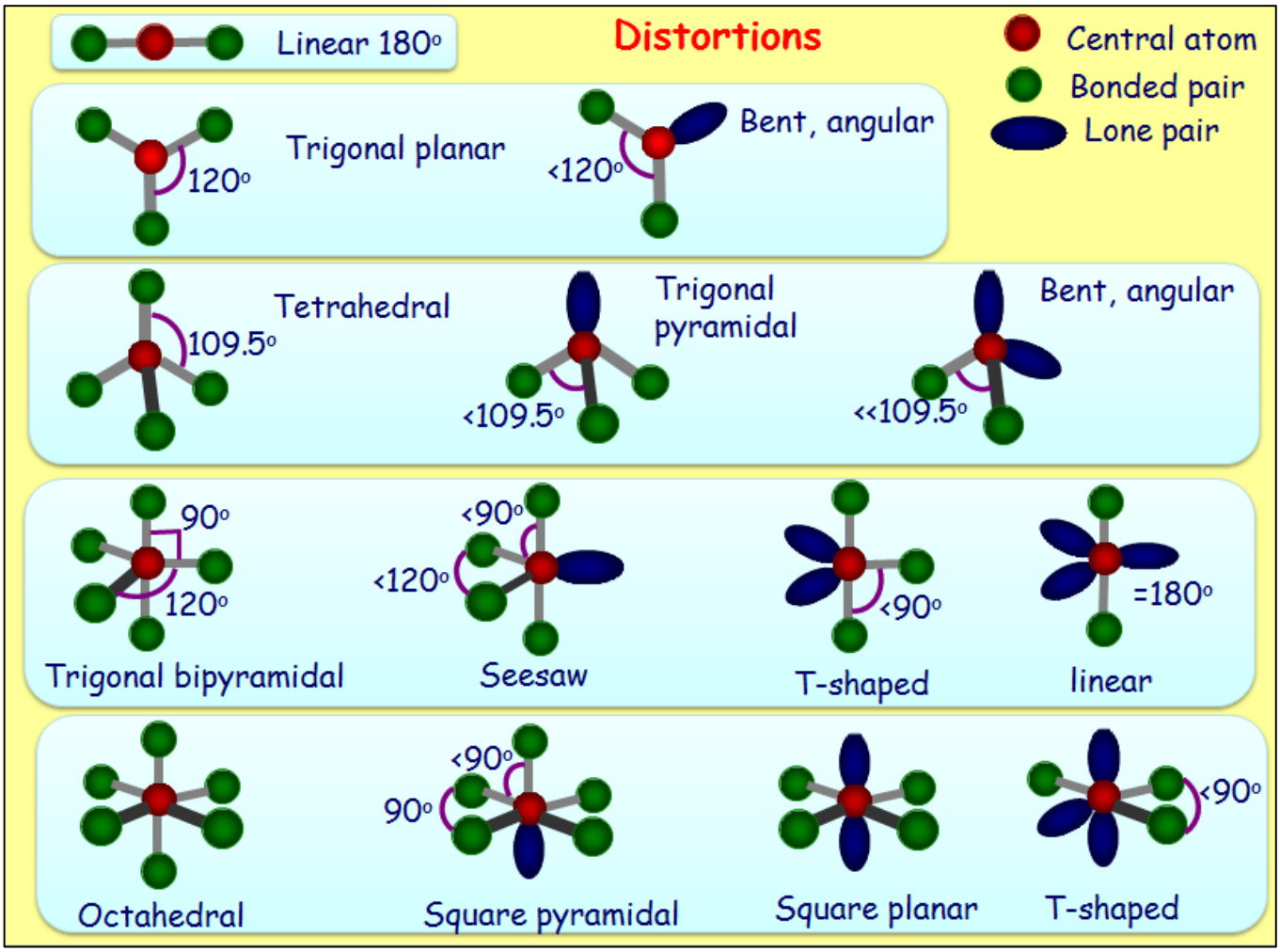
Pentagonal Planar

Check if the new shape of the molecule is correct by examining the crystal structure of the molecule on the WebCSD database. Measure the bond angles on the molecule and see how they compare to the ideal bond angles on the VSEPR shape. Check if the new shape of the molecule $[XeF_5]^-$ is correct by examining the crystal structure on the WebCSD database (Refcode: *SOBWAH*).

Produced by Mumena Ali at Newcastle University as part of a Nuffield Bursary Project.
Edited by Steven Carman as part of an MChem Project.

I6- VSEPR- Effect of Lone Pairs

The table below give the names of the different VSEPR shapes and their names including lone pairs.



Thanks to Dr Simon Doherty, School of Chemistry, Newcastle University, for permission to use his VSEPR lecture slide

TOP TIP!
Remember not to include the lone pairs when naming the shape of the molecule. Just look at the shape defined by the covalent bonds!

www.flickr.com/photos

TOP TIP!
Remember lone pairs require the most space. This means they prefer equatorial positions in the trigonal bipyramidal shape.

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