Chemguide – answers

SHAPES OF MOLECULES AND IONS (single bonds only)

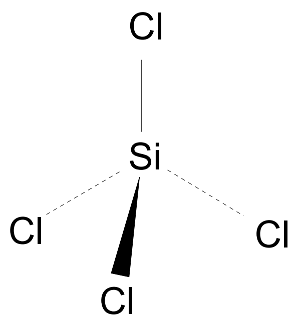
1. a) Silicon is in Group 4 of the Periodic Table, and so has 4 outer electrons. There is no need to work out the whole electronic structure.

   b) Since we are talking about single covalent bonds, each chlorine is going to contribute 1 electron to each bond. That gives a total of 8 electrons.

   c) 4

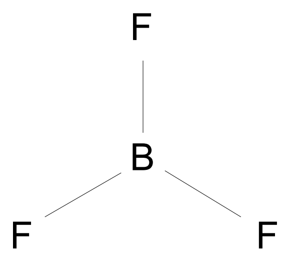
   d) There are 4 pairs of electrons and 4 bonds. So there are 4 bond pairs and no lone pairs.

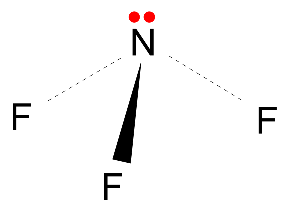
   e) The bonds will take up a tetrahedral arrangement to minimise repulsion. So:



You *must* show clearly the difference between the bonds in the plane of the paper (ordinary lines), going into the paper (dotted lines) and coming out towards you (wedges). The exact pattern of these that you draw doesn't matter, but get into the habit of always doing it the same way. In my case, for a tetrahedral arrangement, I always use the pattern shown here – with one bond in the plane, two going back in, and one coming out.

2.





The boron has only 3 electrons in its outer level, and is forming 3 bonds with fluorine. There are therefore only three bond pairs and no lone pairs. The bond pairs arrange themselves in a trigonal planar way.

In NF_3 there are also three bond pairs, but the nitrogen has a lone pair as well. The four pairs of electrons arrange themselves tetrahedrally, but the description of the shape only takes account of the atoms. NF_3 is pyramidal.

3. In methane, the four bond pairs get as far apart as possible in a tetrahedral arrangement. All the repulsions are identical, and the bond angle is that found in a pure tetrahedron.

   In ammonia, one of the electron pairs is a lone pair. The repulsion between a lone pair and a bond pair is greater than between two bond pairs, and that squeezes the bond pairs very slightly closer together.

   In water, with two lone pairs, that effect is even greater.

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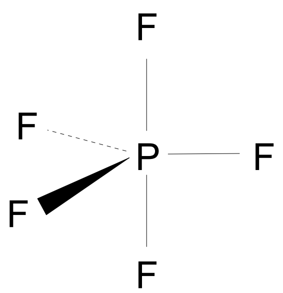
4. a) the ion PH_4^+

Phosphorus has 5 electrons in its bonding level.
The four bonds to the hydrogens add another 4 electrons to that bonding level, making 9.
The single positive charge reduces that by 1 – giving 8 electrons in 4 pairs.
These must all be bonding pairs because of the four bonds to hydrogens.
The shape will be tetrahedral with a bond angle of 109.5°.

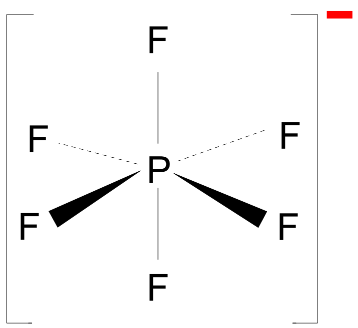
b) the molecule PF_5

Phosphorus has 5 electrons in its bonding level.
The five bonds to the fluorines add another 5 electrons to that bonding level, making 10 – in 5 pairs.
These must all be bonding pairs because of the five bonds to fluorines.
The shape will be a trigonal bipyramid with bond angles of 120° and 90°.



c) the ion PF_6^-

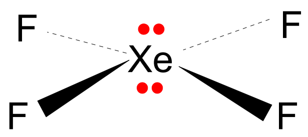
Phosphorus has 5 electrons in its bonding level.
The six bonds to the fluorines add another 6 electrons to that bonding level, making 11.
The negative charge adds another electron, making 12 – in 6 pairs.
These must all be bonding pairs because of the six bonds to fluorines.
The shape will be octahedral with bond angles of 90°.



d) the molecule XeF_4

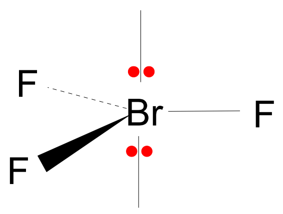
Xenon has 8 electrons in its bonding level.
The four bonds to the fluorines add another 4 electrons to that bonding level, making 12 – in 6 pairs.
These are only four fluorines and therefore 4 covalent bonds. That means that there must be 2 lone pairs as well.

The pairs will arrange themselves in an octahedral shape.
Lone pair-lone pair repulsions are greater than lone pair-bond pair repulsions and bond pair-bond pair repulsions, so the lone pairs will get as far apart as possible at 180°.
That leads to a square planar structure for the atoms with bond angles of 90°. Any other arrangement would have lone pairs at 90° to each other, and there would be more repulsion.

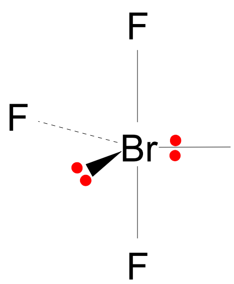


5. BrF_3

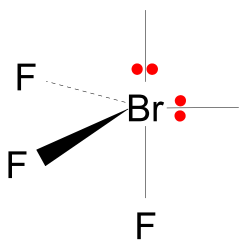
Bromine has 7 electrons in its bonding level.
The three bonds with the fluorines add another 3 electrons to that bonding level, making 10 – in 5 pairs.
These are only three fluorines and therefore 3 covalent bonds. That means that there must be 2 lone pairs as well.
The pairs will arrange themselves in a trigonal bipyramid.
The problem is now to work out where the two lone pairs are.
The possible structures are:



1



2



3

Count the various repulsions in each structure, remembering that you can ignore any repulsions where the angle is greater than 90°:

structure	lone pair-lone pair	lone pair-bond pair	bond pair-bond pair
1	0	6	0
2	0	4	2
3	1	3	2

(Refer back to the ClF_3 case on the Chemguide page if you need help in working this table out. The one which isn't discussed fully is structure 3, when I discarded this one simply because it has a lone pair-lone-pair repulsion. The lone pair pointing upwards is responsible for 2 lone pair-bond pair repulsions with the fluorines on the left. The lone pair on the right is only repelling the downward pointing fluorine bond. The bottom fluorine bond is repelling the other two fluorine bonds.)

The least repulsions are in structure 2. The molecule is T-shaped.

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The bond angles will be approximately 90° and 180°. (It is difficult to work these out exactly. For reasons beyond the level I am aiming at, it isn't quite as simple to work out when you have fluorines attached than when you have hydrogens. The high electronegativity of the fluorines distorts the arrangement of electrons in the bonds, and that affects the amount of repulsions.)