

3-D Structures of Molecules

Skills to Develop

- List the common 3-D structures and their characteristics

Why do 3-D Structures Matter?

3D structures are important because they can have big effects on the properties of molecules. For instance, water has a dipole moment because it is bent, not linear. If it were linear, it would not be a great solvent for polar compounds, and all life would be completely different. In general, shapes of molecules will influence how they react, because they determine polarity (which can help pull molecules together to react) and fit (whether the reactive parts can get close to each other). Shapes of molecules can have other effects as well. Consider the following:

Formula	NaF	MgF ₂	AlF ₃	SiF ₄	PF ₅	SF ₆
Melting Point (°C)	980	1400	1040	-77	-83	-55

Notice that there is an abrupt change in the melt point between AlF₃ and SiF₄. You might take this as the change from an ionic compound to a covalent compound, but the difference in electronegativity between Al and Si isn't that large, and both are much less electronegative than F. We can explain the change better using molecular structure than bond type. In the first 3, the structure is typical of ionic compounds. Instead of clearly-defined molecules, there is an alternating lattice of positive and negative ions. Each cation is surrounded by 6 fluoride ions, and each fluoride ion is surrounded by 6, 3, or 2 cations (depending on the formula). All the ion-ion attractions must be loosened to melt the solid, which requires high temperature. In SiF₄, however, each Si is surrounded by 4 "fluoride ions" (because radius decreases across the periodic table) which naturally makes a tetrahedron, and thus clearly separated molecules. When the molecules pack in the solid, the F atoms touch other F atoms, not Si atoms, and are not attracted much at all. This is only more true for PF₅ and SF₆, in which the F atoms surround the central atom even more completely. Thus, these 3 compounds are molecular gases.

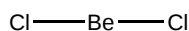
How do we Measure 3-D Structures?

We can measure 3D structures with several different techniques, but X-ray crystallography is probably the most common. For small molecules, it can usually tell you the exact positions of all the atoms as long as you can grow a good crystal. This data includes the bond lengths and bond angles.

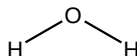
Describing 3-D Structures

You'll need to learn the names of the common geometries, which describe the shape of bonds around each atom. They are organized in the following diagram based on how many bonds the atom makes. If the molecule only has one central atom, the geometry of the molecule is the geometry of the central atom. If there are several atoms that have bonds to 2 or more atoms, we can describe the geometry at each.

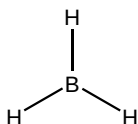
linear



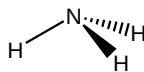
bent



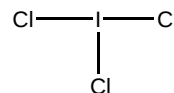
trigonal planar



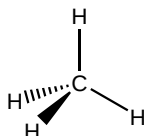
trigonal pyramidal



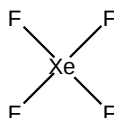
T-shaped



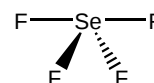
tetrahedral



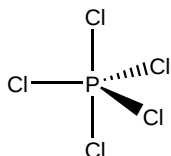
square planar



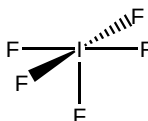
seesaw



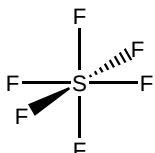
trigonal bipyramidal



square pyramidal



octahedral

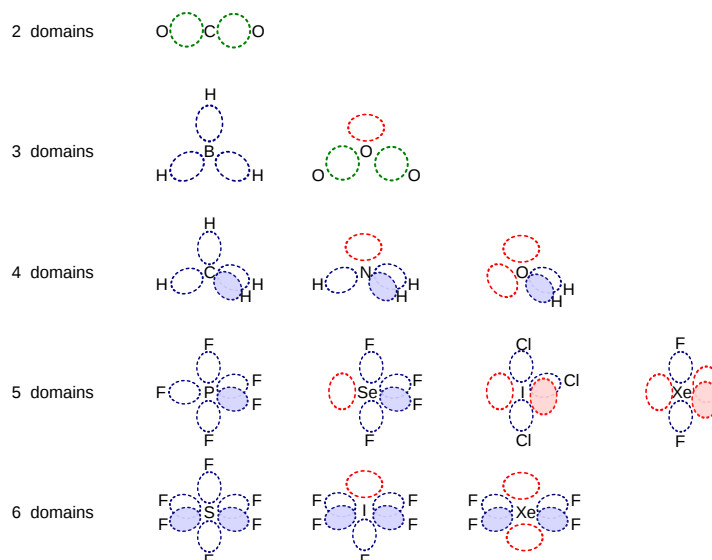


The names of different molecular shapes. Note that bonds shown with wedges are coming out of the page, and bonds shown dashed are going back behind the page.

Predicting Molecular Shapes (Bond Angles)

Lewis structures are a great way to predict the shapes of molecules. The basic idea is that while all electrons repel each other, electrons with the same spin repel each other even more. The 2 paired electrons with opposite spin that make up a bond can be in the same general area between the bonding nuclei (although they will still try to avoid each other within this area), but electrons with the same spin really have to give each other space. The result is that the bonding and non-bonding electron pairs each take up their own area and try to stay as far away from each other as they can. The area occupied by a lone pair or a bond is called a domain. (We only worry about the valence electrons. We can think of the core electrons having their own area closer to the nucleus, although it's actually a little more complicated than this.) For the same reason, the different parts of a molecule usually spread out also, so the different parts don't get too close and bump their electron pairs.

You can picture each pair of electrons as being a big soft balloon, as in the diagram. Bonding pairs are a little narrower because they are attracted to 2 nuclei and try to stay between them. Lone pairs are a little flatter and take up more space, because there's no other nucleus pulling them away in a specific direction. So we can expect bond angles are a little smaller than we might think, because lone pairs take up more space and push the bonds closer together. Multiple bonds also take up more space than single bonds, but still act like a single domain, because they are held by the same two atoms.



The electron domain model for predicting molecular shapes. Single bond domains are blue, multiple bond domains are green, and lone pair domains are red. Domains in front of other domains are shaded.

Bond Lengths

Bond lengths depend on the size of the atoms and the strength of the bonds. In general, bond length decreases going from single bond to double bond to triple bond.

Some Average Bond Lengths, in Å

Bond	r (Å)	Bond	r (Å)	Bond	r (Å)
C—C	1.54	C=C	1.34	C≡C	1.20
C—N	1.47	C=N	1.38	C≡N	1.16
N—N	1.45	N=N	1.25	N≡N	1.10
C—O	1.43	C=O	1.20	C≡O	1.13

Outside Links

- [CrashCourse Chemistry: Orbitals](#) (10 min)
- [Khan Academy: VSEPR I](#) (8 min)
- [Khan Academy: VSEPR III](#) (13 min)
- [Khan Academy: VSEPR IV](#) (15 min)
- [Khan Academy: VSEPR V](#) (11 min)
- [Khan Academy: VSEPR VI](#) (13 min)

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