What's the shape of that molecule?
Part 1. A VSEPR short-cut

Robert Perkins and Claude Lassigne
Kwantlen College
P.O. Box 9300
Surrey, B.C. V3T 5H8

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The VSEPR model proposed by Gillespie[1] in 1963 has proved to be extremely useful as a starting point for the discussion of molecular geometry. A recent review article[2] describes recent reformulations of the basic ideas, along with examples of new applications of the model.

The starting point for the VSEPR analysis has always been the Lewis structure of the molecule, cation, or anion under consideration. Since many introductory chemistry students often have difficulties assigning correct Lewis structures, we have for several years now been using a VSEPR short-cut method. The students can perform the analysis to check whether or not they have the same structure as that suffested from the Lewis structure. If the VSEPR short-cut method described in this paper does not give the same structure as suggested from the Lewis structure, then the student is encouraged to try again. The aim of the method (which becomes extremely fast once the student has tried several examples) is to arrive at a structure which has the correct molecular shape. The method also does away with Lewis structures when they are not required.

VSEPR short-cut steps

1. Determine the number of valence electrons on the central atom, adding electrons if the species is an anion, subtracting electrons if it is a cation.
2. Add one electron for every hydrogen or halogen atom attached to the central atom. Add nothing for a Group 6 atom (oxygen, sulfur, or selenium) attached to the central atom. Subtract one electron for every Group 5 atom (nitrogen, phosphorous, or arsenic) attached to the central atom. Subtract two electrons for every Group 4 atom (carbon, silicon, or germanium) attached to the central atom.
3. Divide the total number of electrons determined in step 2 by two, this will be the **coordination number** (CN) of the central atom.
4. From the CN subtract the number of attached atoms. This number will equal the number of **lone pairs** (LP) of electrons surrounding the central atom. The difference between the CN and LP will be the number of **bonding pairs** (BP) of electrons surrounding the central atom. The BP will correspond to the number of **sigma bonds** present in the molecule.
5. The resulting shape of the molecule can be determined from the combination of BP and LP. For example:

   if CN = 4 = 3 BP + 1 LP ---> AX_3E (trigonal pyramidal)
   if CN = 5 = 3 BP + 2 LP ---> AX_3E_2 (T-shaped)
6. The octet on the central atom (if it is in Period 2) may have to be completed by proposing π bonds if atoms from Group 6 (oxygen family), Group 5 (nitrogen family), or Group 4 (carbon family) are attached to the central atom.
7. If the central atom is in Period 3, 4, or more; it may be able to expand its octet and accommodate more than 8 electrons.
8. Resonance structures may be necessary to account for experimentally measured bond lengths and bond angles.

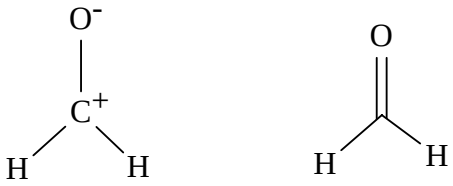
Example 1 **BrF_3**

*Br has 7 valence electrons	7e
*add 1 electron for each F (a halogen)	3e
*total electrons around Br (central atom)	10e
*divide by 2e for the coordination number	5
*subtract the attached atoms	5 - 3 = 2
*assign the bonding type	AX_3E_2 (T-shaped)

Example 2 **CH_2O**

*C has 4 valence electrons	4e
*add 1 electron for each H (nothing for O)	2e
*total electrons around C (central atom)	6e
*divide by 2e for the coordination number	3
*subtract the attached atoms	3 - 3 = 0
*assign the bonding type	AX_3 (trigonal planar)

With only single bonds present, this structure places 6 electrons around C and 8 electrons around O (with formal charges on each atom). One can achieve a completed octet around each atom by proposing a double bond between the two atoms (C and O). Notice that the shape of the molecule will be the same for each resonance structure.



Example 3 **SCN^-**

*C (central atom) has 4 valence electrons	4e
*subtract 1 electron for the N (0 for S)	-1e
*add 1 electrron for the charge on the species	1e
*total electrons around C	4e
*didvide by 2e for the coordination number	2
*subtract the attached atoms	2 - 2 = 0
*assign the bonding type	AX_2 (linear)

With only single bonds present, this structure places 6 electrons around C, 8 electrons around S, and 6 electrons around N (with formal charges on each atom). One can achieve a completed octet around each atom by proposing a double bond betwen C and S and between C and N. Two other resonance structures are possible in which we have one single bond and one triple bond. Note that all structures will have the same linear shape.

$^+S{\equiv}C\text{-}N^{2-}$ $S{=}C{=}N^-$ $^-S\text{-}C{\equiv}N$

Example 4 **ICl_2^+**

*I(central atom) has 7 valence electrons	7e
*add 1 electron for each Cl	2e
*subtract 1 electron for the charge	-1e
*total electrons around I(central atom)	8e
*divide by 2e for the coordination number	4
*subtract the attached atoms	4 - 2 = 2

*assign the bonding type AX_2E_2 (V-shape)

The above procedure will work for any even electron compound. With practice, a student can take the formula for any compound and determine its shape in under a minute. Once the shape has been determined, any resonance structures proposed must have the same shape.

References:

1. R. J. Gillespie, *Journal of Chemical Education*, **40**, 295(1963)
2. R. J. Gillespie, *Chemical Society Reviews*, 59(1992).