Lewis Structures

Lewis structures are *models* for molecules.
A model must to some degree represent the item for which it is a model. A good model will, in certain ways, accurately represent, even mimic, the behavior of the item for which it is a model; it may even allow predictions concerning the behavior of the item.

If Lewis structures are good models of the molecules they represent, they will accurately represent the molecules in certain ways, but, very likely, not in all ways. If the Lewis model is to be useful, we should be aware of the strengths and weaknesses of this model.

At the outset we should state that the Lewis structures we draw are planar and are not meant to be accurate

3-dimensional

images of the 3-dimensional molecules they represent. Rather they are meant to convey information about bonding and valence shell electron distribution.

Drawing Lewis Structures

1. Draw the molecular skeleton joining connected atoms by single bonds (single bonds corresponding to one pair of electrons in a bond are represented as a dash,), and only rarely as a pair of dots, :).

2. Determine the number of valence electrons in the structure.
   Number of VE = total number of atomic VE, plus negative charge or minus positive charge, if an ion.

3. Distribute the valence electrons on the structure in accord with the following rules:

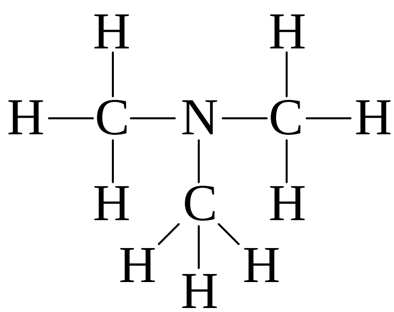
   (a) *Valence shell occupancy* for atoms: H=2; other atoms ≥ 8, if possible. VSO may not exceed 8 for second row atoms, may be 10 or 12 for third and higher rows.

   (b) Maximize the number of bonds consistent with (a).

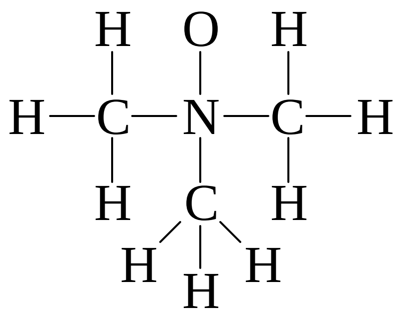
4. Calculate the formal charge for each atom.

   Formal charge = core charge - valence electron ownership.
   Core charge = charge on isolated atom if stripped of its valence electrons.
   Valence electron ownership = All unshared valence electrons held by the atom in the structure and 1/2 the electrons in bonds to the atom.

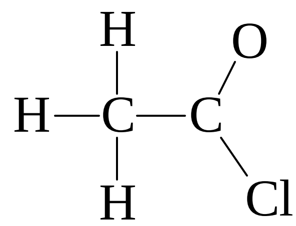
Some examples —



trimethylamine



trimethylamine oxide

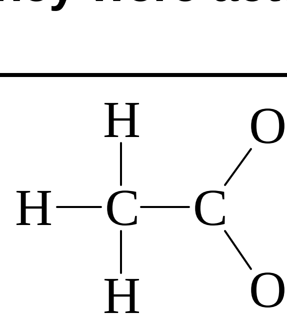


acetyl chloride

Lewis model failure: For a given skeleton structure the electronic structure will not always be uniquely defined. (It's time to jump ship or patch the leak.)

If one can draw more than one reasonable Lewis structure for a molecule, then that molecule is a hybrid of the structures which may be drawn. Each contributing Lewis structure is a *resonance* or *canonical* structure. The hybrid (the molecule) is more stable than any of the contributing structures would be **if they were actual molecules**.

One more example, acetate $^{-1}$ ion —



acetate ion (-1)

Resonance Rules —

1. All nuclei must be in the same location in every resonance structure; they cannot move.

2. Each resonance structure must have the same number of unpaired electrons (*eg*, 0, 1, 2, *etc.*).

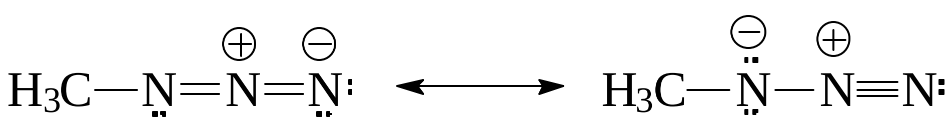
Molecular Geometry From Lewis Structures

Electron-pair repulsion model —

Count the number of "electron groups" around the atom. Each unshared pair counts as one group, as does each bond **whether single or multiple**.

# of Electron Groups	Geometry Around Atom (Including Unshared Pairs)
2	Linear (digonal)
3	Trigonal, planar
4	Tetrahedral

If there is more than one resonance structure, use the one with the greater number of bonds attached to the atom in question.



Hybridization from molecular geometry –

If the atom is –	the hybridization is –
tetrahedral	sp^3
trigonal	sp^2
linear	sp