Communication

A simple and general method to draw resonance forms

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Introduction

Knowledge of the most important resonance form(s) of covalent compounds of s- and p-block elements is essential for the application of the VSEPR model or for discussing in such compounds, at the basic level of the Valence Bond Model, bond distances, bond orders, relative bond strengths, dipole moments, orbital hybridization, reactivity, etc. This requires for every particular species: i) the knowledge of all its possible resonance forms and ii) some criteria to predict the most important resonance form(s).

At present there is no simple, systematic and general method to generate all resonance forms. Most reported methods apply only to simple molecules or require the use of mathematical formulae or complex rules. This communication reports a simple and general method to write resonance forms of any molecule or ion, simple or not, linear, branched or cyclic, containing any s– and p–block elements without using mathematical formulae or rules difficult to remember.

Fundamentals

It is necessary to accept some limitations when using any method of writing resonance forms:

1) Hydrogen and the elements of groups 1 and 2 only form σ bonds.
2) Li, Be (2s elements), B, C, N, O or F (2p elements) never exceed the octet. Although the expansion of the octet is a controversial matter, we will consider that the third and subsequent row elements of groups 13 to 18 (>2p elements) can expand the octet
3) π bonds between >2p elements are rare and very weak. Therefore, formation of a π bond requires 2p/2p or 2p/>2p pairs of elements.
4) Elements of the s- and p-block can only form single, double or triple bonds because formation of a quadruple bond requires the use of valence d orbitals (transition elements).
5) In molecules with an odd number of electrons (*e.g.* NO, NO_2) the unpaired electron is non-bonding, *i.e.*, it is a lone electron.

In some cases, it is necessary to calculate the formal charge of all atoms. The formal charge of an atom is the difference between the number of electrons it contributes to the molecule *(i.e.* its valence electrons) and the number of the electrons it 'owns' in the molecule. The latter can be calculated as the sum of its unshared electrons plus half of those it shares with its neighboring atoms (or plus the number of bonds this atom establishes with its connected atoms). The formal charges must always be considered with their mathematical signs. Consequently, the charge on a resonance form is always the algebraic sum of the formal charges of all atoms.

Before applying the method we need:

1) A sketch showing which atoms are bonded to which others (the σ skeleton).
2) To calculate **V** as the total number of pairs of electrons of the compound. This number is equal to the total number of valence electrons of all atoms less the charge (including the sign) of the species, if it is an ion, divided by two. For example for OH^-, V = [(6 + 1) - (-1)]/2=4; for NH_4^+, V = [(5 + 4x1) - (+1)]/2 = 4.
3) To count the number (**N**) of σ plus lone electron pairs (*leps*) of the octet representation. This representation is generated by the addition to each element of groups 13 to 18 (np elements) in the σ skeleton the necessary number of *leps* to attain the octet. With some experience, N can be deduced without drawing the octet representation. This is not a true electronic representation of the compound because often N≠V. Thus, for example, the octet representation of O_2 is the Lewis structure of O_2^{2-}.

The Method

Basic Resonance Forms.

We will first draw resonance forms trying to ensure, whenever possible, that each np element achieves its octet. We will call these the basic resonance forms. It is obvious that the octet representation will be a basic resonance form if V = N. This is the case for CF_4 because V = (4x7 + 4)/2 = 16 and N = 4 σ + 3x4 *leps* = 16.

Let's analyze the cases where N ≠ V.

***N* > *V*.**

It will be necessary to remove the excess, E = N – V pairs, from the octet representation. This must be done while maintaining the octet of all np elements. To illustrate the process with the simple case of O_2, we see that its octet representation has N = 1 σ + 3x2 *leps* = 7 pairs while V = (2x6)/2 = 6. Therefore, one pair must be removed from the octet representation. If one *lep* is eliminated from each oxygen and one π pair is added, the resulting representation will have 6 pairs and both oxygen atoms have an octet of electrons. Alternatively, this resonance form also results after establishing E = N – V = 1 π bond and completing the octet of both atoms. This observation can be generalized as a rule:

> *Add to the σ skeleton E = (N – V) π pairs between 2p/2p or 2p/>2p elements in all possible ways to form double or triple bonds without expanding the octet of any atom. Then complete the octet of all np elements.*

Some special cases.

In the absence of 2p elements to form π bonds (*e. g.*, $SnCl_2$) remove E *leps* from some bridging atom in the octet representation.

If possible, avoid formation of π bonds with fluorine (*e. g.*, NSF); if not, consider also the resonance forms resulting after transforming the π pair into a *lep* on fluorine atoms, even if the octet of the donor atom is not complete (*e. g.*, BF_3).

In odd electron species, place the lone electron on any of the atoms in all possible ways, establish (E – 0.5) π pairs as above, and complete the octet of all the atoms except that with the lone electron, that will achieve only 7 electrons (*e. g.*, NO_2).

***N* < *V*.**

The octet representation will have fewer electrons than those contributed by all atoms. Therefore, to obtain the resonance forms we must add V – N *leps* to the octet representation. Since all atoms of this representation have at least four pairs of electrons, the V – N added pairs will expand the octet of some element(s) which must therefore be >2p elements (*e. g.*, BrF_5). In general, a bridging atom is always the acceptor of *leps* when they must be added to *(e. g.*, BrF_5, $[ICl_2]^-$) or removed from *(e.g.*, $SnCl_2$) the octet representation. The rule when N < V will be:

> *Add to the octet representation V – N* leps *on bridging >2p elements in all possible ways.*

***Extra Resonance Forms*.**

New resonance forms (called 'extra resonance forms') can be created from the basic ones by converting *leps* into π pairs. The new forms will have at least one atom with more than an octet as a consequence of such conversion. Therefore, the acceptor must be a >2p element, because it will need to expand its octet, and the donor atom must be a 2p element, because this is a requirement for the formation of a π bond (see limitation 3 above). This electron shift will result in the adding of one positive charge to the donor and one negative charge to the acceptor. Such a shift of electrons will be favoured *(i. e.*, the resulting resonance form will be more important) if in the basic resonance form the acceptor has formal positive charge and/or the donor a negative charge (SO_2 offers a very good example of this). The rule for drawing extra resonance forms will be:

> *From any basic resonance form, transform* leps *into π pairs in all possible ways to give double or triple bonds. The donor must be a 2p element and the acceptor a >2p element. This transfer of electrons should tend to annul, if possible, the formal charges of all atoms. If not, it should lead to place the negative formal charges into the most electronegative elements and the positive charges into the less electronegative ones.*

Final Remarks.

The reader must be aware that the valence bond model (**VBM**) is too simple to expect from it a description of the electronic structure of molecules as good as that of the molecular orbital model (**MOM**). In spite of this, from a pedagogical point of view, the utility of the VBM is superior to that of the MOM. It should be noted that if one is to describe qualitatively (*i.e.,* without using a computer) some simple molecules by means of the MOM, the knowledge of the best resonance form(s) is necessary, though the resonance forms of some molecules do not describe accurately their electronic structure. Thus, using our method we can only write one resonance form for F_3NO [V = (5 + 6 +3x7)/2 = 16, N = 4 σ + 3 x 4 *leps* = 16] in which the N–O and the three N–F bonds are single bonds because (N = V), while the N–O bond length (1.158 Å) suggests a N=O bond. To solve this problem it has been proposed that three ionic resonance forms $[F_2N{=}O]^+ F^-$ should also be considered.

For extensive illustrations with examples, including those mentioned here, and the complete set of references, the reader is invited to consult the full paper below.

Full paper corresponding to the Communication in
U. Chem. Ed. 2002, 7, 33

A Simple and General Method to Draw Resonance Forms

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Introduction

Knowledge of the most important resonance form(s) of covalent compounds of s- and p-block elements is essential for the application of the VSEPR model[1] or for discussing in such compounds at the basic level of the Valence Bond Model, bond distances, bond orders, relative bond strengths, dipole moments, orbital hybridization, reactivity, etc. This requires, for every particular species, i) knowledge of all its possible resonance forms and ii) some criteria to predict the most important. However, there is not a simple, systematic and general method to write all resonance forms.

Most reported methods apply only to simple molecules or require the use of mathematical formulae or rules difficult to remember.[2-16] This article reports a simple and general method to write the resonance forms of any molecule or ion, simple or not, linear, branched or cyclic, containing any s- and p-block element without using mathematical formulae or complex rules. Each rule is logically deduced to facilitate its comprehension and to make it easy to remember. There is not yet a general agreement about the criteria to order the resonance forms according to their importance, and this will not be discussed here; the reader is urged to read references 16-21.

Fundamentals

It is necessary to accept some limitations when using any method of writing resonance forms:

1. Hydrogen and the elements of groups 1 and 2 only form σ bonds.
2. Li, Be (2s elements), B, C, N, O or F (2p elements) never exceed the octet. Although the expansion of the octet is a controversial matter, we will consider that the third and subsequent row elements of groups 13 to 18 (>2p elements) can expand the octet
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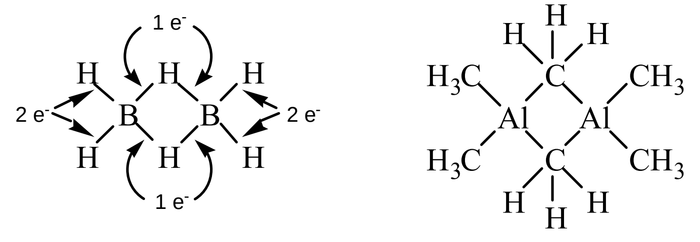
In some cases, it will be necessary to calculate the formal charge of all atoms. The formal charge of an atom is the difference between the number of electrons it contributes to the molecule (*i. e.*, its valence electrons) and the number of the electrons it owns in the molecule.

The latter can be calculated as the sum of its unshared electrons plus half of those it shares with its neighboring atoms (or plus the number of bonds this atom establishes with its connected atoms). The formal charges must always be considered with their mathematical signs. Consequently, the charge on a resonance form is always the algebraic sum of the formal charges of all atoms. In the discussion below there are several examples to illustrate this calculation.

Although hydrogen usually forms only one σ bond and 2p elements no more than four, in some molecules, H atoms can appear bonded to more than one atom, *e. g.,* the bridging H atoms in B_2H_4, or 2p elements bonded to more than four atoms, *e. g.,* the bridging C atoms in $[Al_2(CH_3)_6]$ (see Scheme 1). In such molecules, the lines that connect these 'special' H or 2p elements with others do not represent pairs of electrons. Thus, in B_2H_4 and $[Al_2(CH_3)_6]$, the four bridging bonds are electron deficient bonds formed with four electrons (2 from the H and 2 from the 2 B or Al), *i. e.*, one electron per bond. The terminal B–H, Al–C or C–H bonds are 'normal' two electrons σ bonds. Therefore, when counting the number of electrons in these electron deficient molecules, each bridging dash must be counted as one electron.

Scheme 1



Before applying the method we need:

1. Sketches showing which atoms are bonded to which others (the σ skeleton).
2. To calculate **V** as the total number of pair of electrons of the compound. This number is equal to the total number of valence electrons of all atoms, less the charge of the species (including the sign) if it is an ion, divided by two. For example, for OH^-, $V = [(6 + 1) – (–1)]/2 = 4$; NH_4^+, $V = [(5 + 4x1) - (+1)]/2 = 4$.
3. To count the number of σ plus lone electron pairs (*leps*) of the octet representation (**N**). This representation is generated by the addition to each atom of groups 13 to 18 (np elements) in the σ skeleton the necessary number of *leps* to attain the octet. With some experience, N can be deduced without drawing the octet representation. This is not a true electronic representation of the compound because often $N \neq V$. Thus, for example, the octet representation of O_2 is the Lewis structure of O_2^{2-} (see below Scheme 3).

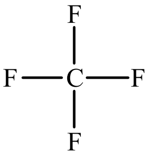
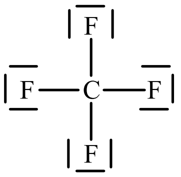
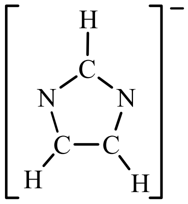
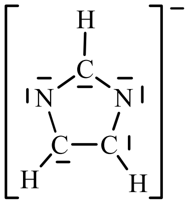
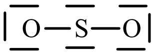
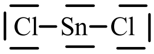
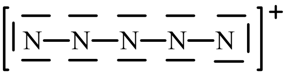
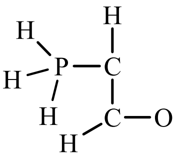
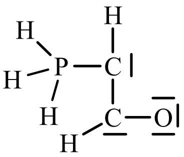
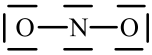
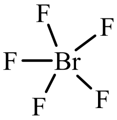
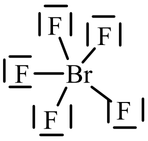
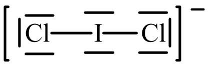
Discussion

Basic Resonance Forms.

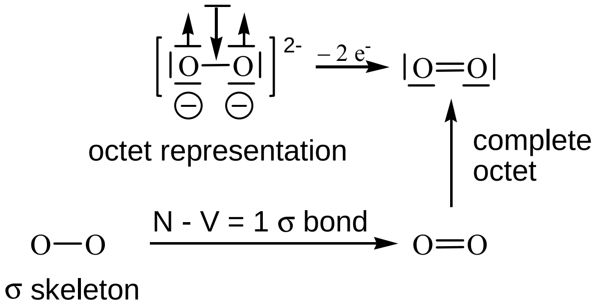
We will first draw resonance forms trying to ensure, whenever possible, that each np element achieves its octet. We will call these the basic resonance forms. It is obvious that the octet representation will be a basic resonance form if V = N. This is the case for CF_4 because $V = (4x7 + 4)/2 = 16$ and $N = 4\ \sigma + 3 \times 4$ *leps* = 16 (Scheme 2)

If N > V, it will be necessary to remove the excess, E = N – V pairs, from the octet representation. However, this must be done maintaining the octet of all np elements. Let us illustrate the process with the simple case of O_2. Its octet representation, corresponding to the peroxide ion, (see Scheme 3), has N = 7 pairs while, since each oxygen atom contributes 6

Scheme 2

	Sigma Skeleton	V	Octet Represetation	N	N-V
CF_4		(4x7 + 4)/2 = 16		16	0
$[C_3H_3N_2]^-$		(3x4 + 3x1 + 2x5 - (- 1))/2 = 13		15	2
SO_2	O—S—O	(3x6)/2 = 9		10	1
$SnCl_2$	Cl—Sn—Cl	(2x7 + 4)/2 = 9		10	1
N_5^+	[N—N—N—N—N]$^+$	(5x5 - 1)/2 = 12		16	4
C_2H_5OP		(2x4 + 5 + 6 + 5)/2 = 12		13	1
NO_2	O—N—O	(2x6 + 5)/2 = 8.5		10	1.5
BrF_5		(6x7)/2 = 21		20	-1
$[Cl_2I]^-$	[Cl—I—Cl]$^-$	(3x7- (- 1))/2 = 11		10	-1

Scheme 3

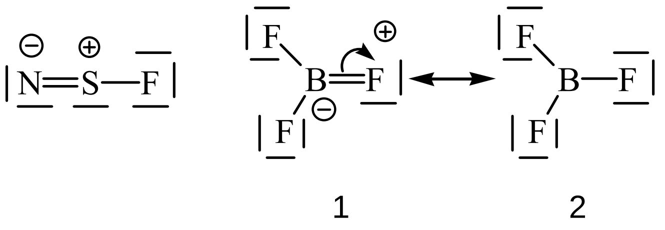


electrons, V = 6. Therefore, one pair must be removed from the octet representation. If two *leps* are eliminated and one pair is added as a π bond between the oxygen atoms, the resulting representation will have 6 pairs and both oxygen atoms an octet of electrons. Alternatively, this representation also results after adding E = N – V = 1 π bond to the σ skeleton and completing the octet of both atoms (see Scheme 3). This observation, and point 3) on page 1, allow the formulation of the following rule:

> *Add to the σ skeleton E = (N – V) π pairs between 2p/2p or 2p/>2p elements in all possible ways to form double or triple bonds without expanding the octet of any atom. Then, complete the octet of all np elements.*

When fluorine forms a double bond it attains a positive formal charge (see BF_3 in Scheme 4). This leads to a very unfavorable situation for the most electronegative element, this should be avoided by using other 2p elements, if available, to form the π bond(s). For example, in NSF (see Scheme 4) V = (5 + 6 + 7)/2 = 9, N = 10, therefore, the number of π bonds is E = N - V = 1. The π bond should be established only between S and N. If no other 2p element is available, as in BF_3 (see Scheme 4; V = (3 + 3x7)/2 = 12, N = 13; N - V = 1 π bond), resonance forms with fluorine forming a double bond (resonance form 1 in BF_3, Scheme 4) along with those in which the π pair is transformed into a fluorine *lep* (resonance form 2 in BF_3, Scheme 4), should also be considered. In this case the donor atom involved in the π bond (B in BF_3) will then have less than an octet.

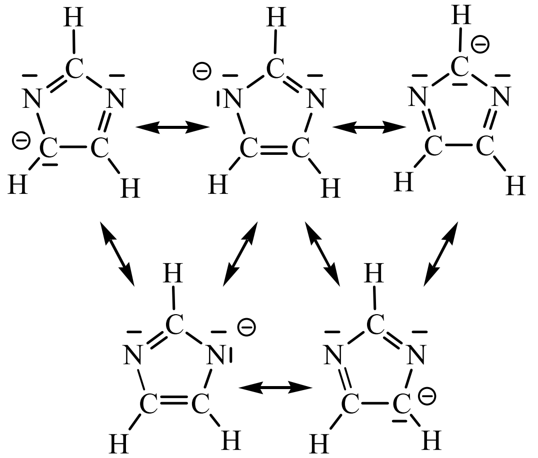
Scheme 4



The species $C_3H_3N_2^-$, SO_2, $SnCl_2$, C_6H_6, N_5^+, C_2H_5OP and NO_2 (Scheme 2) satisfy the condition N > V. Schemes 5–11 show the basic resonance forms of these species. The formal charges are indicated.

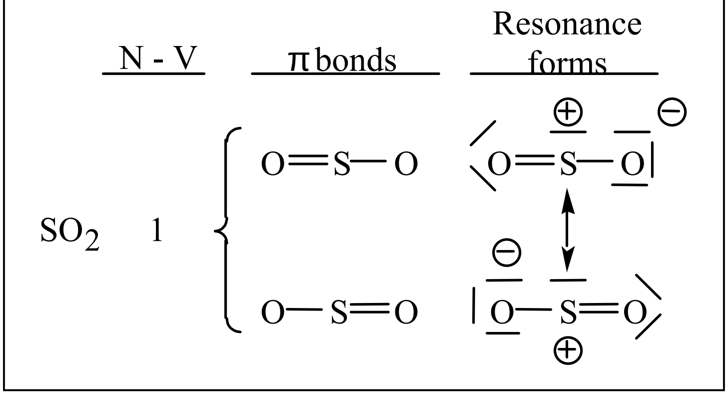
In the anion $C_3H_3N_2^-$, the two π pairs cannot be placed adjacent or in the form of a triple bond because these situations would require three or four atoms being almost linear which would produce too great a strain in the ring. The five possible ways for placing two alternate double bonds are shown in Scheme 5. Five resonance forms result after *leps* are added to satisfy the octet of each atom.

Scheme 5



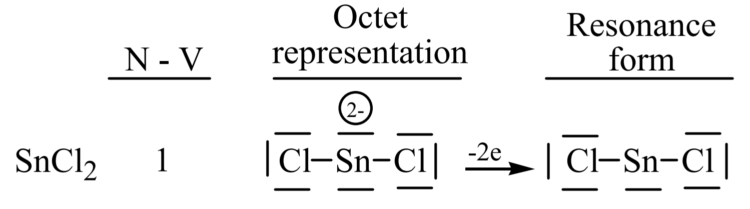
There are two different ways to locate one π bond in SO_2 ($E = N - V = 1$) each involving the S (3p element) and one of the O (2p element) atoms (Scheme 6). The two resonance forms result after completing the octet of all atoms. Note that the sum of the formal charges of all atoms is equal to the charge of the species (0) and that both resonance forms have $V = 9$ pairs, which supports the correct application of the method.

Scheme 6



In the case of $SnCl_2$ (Scheme 7) no 2p element is available to form the π bond. In this case, the pair of electrons to be removed from the octet representation is eliminated from the atom that has the more negative formal charge, *i. e.*, Sn. In general, when it is required to remove *leps* from the octet representation, it must be eliminated from some bridging atom(s). In such a case, such atom(s) (Sn, in the case of $SnCl_2$) will not achieve the octet.

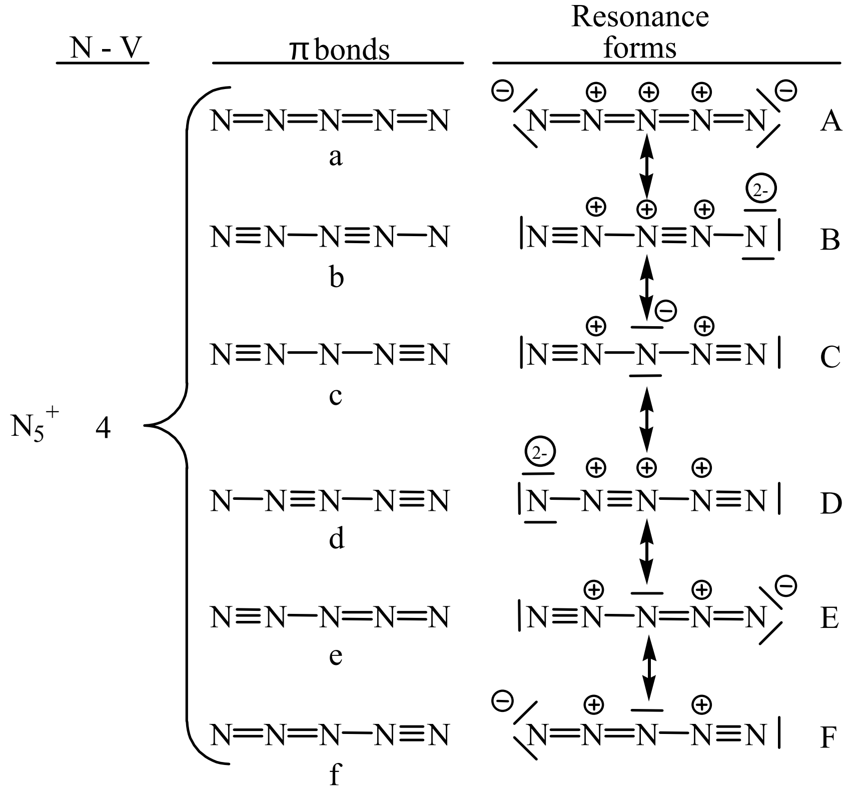
Scheme 7



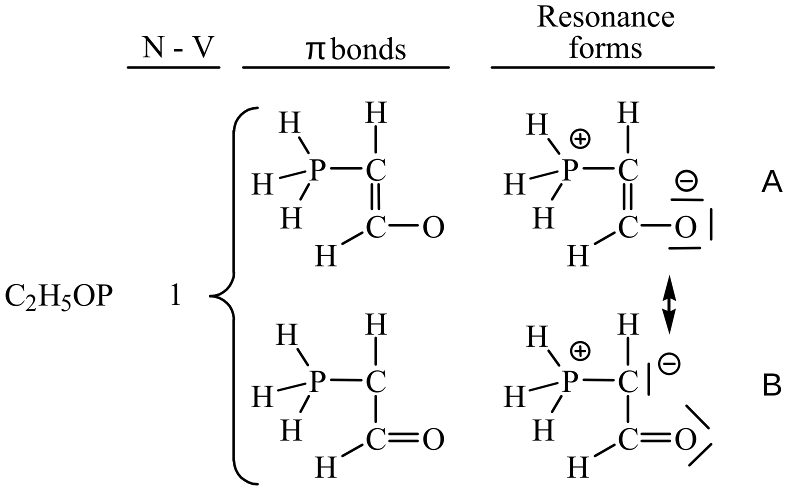
The four π bonds, which must be present in the N_5^+ cation ($E = N - V = 4$, see Scheme 2), can form four double, two triple or one triple and two double bonds. Only one possibility exists for the former case (‘a’ in Scheme 8). In an octet representation, an atom cannot form two triple or one triple and one double bonds because that would expand the octet. Therefore, two triple bonds can only be placed as shown in ‘b’, ‘c’ or ‘d’. Similarly, one triple bond and two double bonds can only be positioned as shown in ‘e’ and ‘f’. Six resonance forms are obtained after *leps* are added to satisfy the octet of each atom. For all resonance forms, the sum of the formal charges is equal to the charge of the ion, +1.[22, 23]

In the ylide $H_3PCHCHO$ one π bond has to be placed (Scheme 2). This cannot be located between C and P to generate a basic resonance form, because the P would then expand the octet. Therefore, the only possible positions are between the two C or between the C and O atoms (Scheme 9). After completing the octet of all the np elements, two basic resonance forms result. The sum of formal charges is zero in both cases, as expected for a neutral species.

Scheme 8



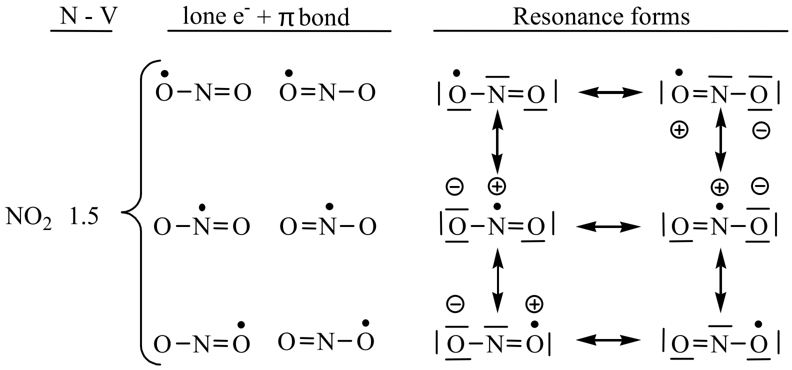
Scheme 9



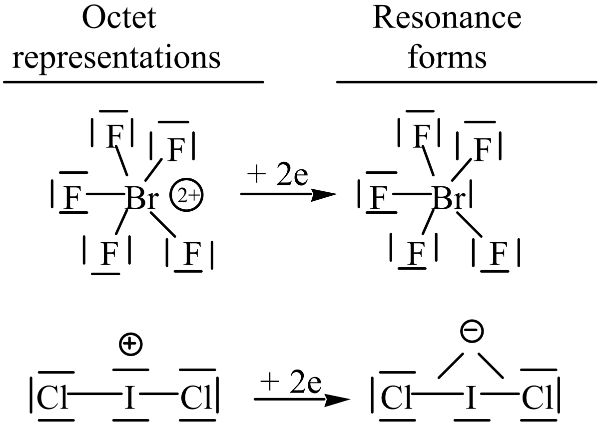
NO_2 is an odd electron species with E = N – V = 1.5 (Scheme 2). Therefore, starting from the σ skeleton we have to locate an unpaired electron on one of the atoms (see limitation 5, above), to form one π bond, and complete the octet of all atoms, except the one with the unpaired electron, which will only have 7 electrons. Scheme 10 shows all resonance forms of NO_2.

In BrF_5 and $[ICl_2]^-$, N < V (see Scheme 2), *i. e.*, the octet representations have fewer electrons than those contributed by all atoms. Therefore, to obtain the resonance forms we must add to each octet representation, V – N = 1 pair. Since all atoms of this representation have at least

Scheme 10



Scheme 11



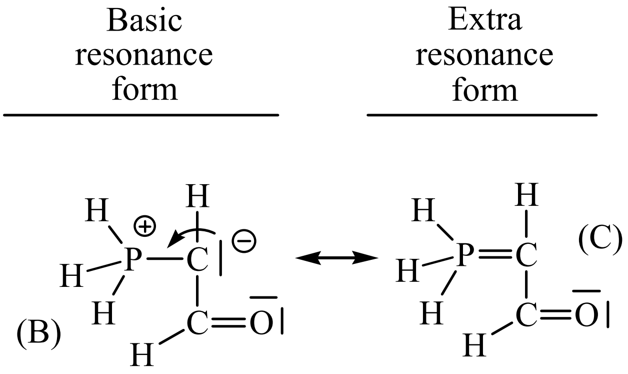
four pairs of electrons, the V – N added pairs will expand the octet of some atom(s) which must therefore be of >2p elements. Thus, in BrF_5, the pair to be added to the octet representation can only be placed on the central bromine atom. Scheme 11 shows the formal charges of the atoms in the octet representations of BrF_5 and $[ICl_2]^-$. Note that the charges of both octet representations are equal to those of the species plus 2 positive charges. Therefore, the addition of a pair of electrons to the octet representations is required, as previously established. In addition, because the central atoms bear the highest positive charge it is to these atoms that such pairs of electrons should be added. In general, when N < V, the N – V pairs to be added must be located on bridging atoms. In general, a bridging atom is the acceptor or the donor of pairs of electrons when they must be removed from (*e. g.*, $SnCl_2$) or added to (*e. g.*, BrF_5, $[ICl_2]^-$) the octet representation.

***Extra Resonance Forms*.**

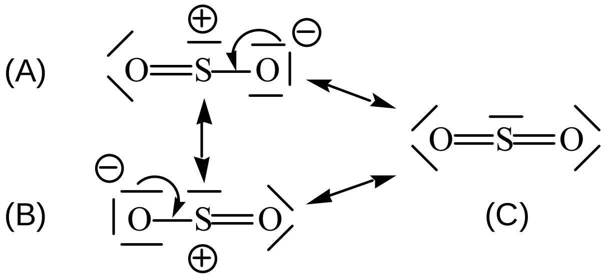
From the basic resonances forms new ones can be created by converting *leps* into π pairs. We will call these extra resonance forms. Scheme 12 shows an example of this transformation starting from the resonance form B (Scheme 9) of the ylide $H_3PCHCHO$ to give the extra resonance form C. After such conversion the donor atom (Carbon) maintains the octet while the acceptor (Phosphorus) reaches the decet. Therefore, the acceptor must be a >2p element. This impedes the generation of a new resonance form from A (Scheme 9) because the only *leps* are on the oxygen atom and the acceptor could only be the carbon atom which is not a >2p element. In addition, the donor atom must be a 2p element because one such atom is required for the formation of a π bond (see limitation 3 above). This electron shift will result in the adding of one positive charge to the donor and one negative charge to the acceptor.

Such a shift of electrons will be favoured *(i. e.*, the resulting resonance form will be more important) if in the basic resonance form the acceptor has formal positive charge and/or the donor a negative charge. Fluorine should be excluded from consideration as the donor atom because it would acquire a positive charge in such a structure.

Scheme 12



Scheme 13



Amongst the other molecules for which basic resonance forms have been deduced above, only for SO_2 can one formulate an extra resonance form. From any of its basic resonance forms the conversion of a *lep* of the negatively charged oxygen into a π pair leads to an extra resonance form (C) with zero formal charge on all atoms (Scheme 13). If the donor atom was the other oxygen atom, the resulting resonance form would result in a triple S–O bond and a positive charge on the very electronegative oxygen atom, which would make the corresponding resonance form highly disfavoured. The conversion of another *lep* into a π bond in (C) would have the same effect.

Summary of the method.

Basic Resonance Forms

If N = V, the octet representation is a resonance form.

If N > V, add to the σ skeleton $E = (N - V)$ π pairs between 2p/2p or 2p/>2p elements in all possible ways to form double or triple bonds without expanding the octet of any atom. Then, complete the octet of all np elements. If there are not 2p elements to form π bonds, remove E *leps* from some bridging atom(s) in the octet representation. If possible, avoid formation of π bonds with fluorine; if not, consider also the forms resulting after transforming each π pair into one *lep* on the fluorine atom, even if the octet of the donor atom is not complete. In odd electron species, locate the lone electron on any of the atoms in all possible ways, establish $E - 0.5$ π pairs, as above, and complete the octet of all the atoms except the one with the lone electron, that will achieve only 7 electrons.

If N < V, add to the octet representation V – N pairs on bridging >2p elements in all possible ways.

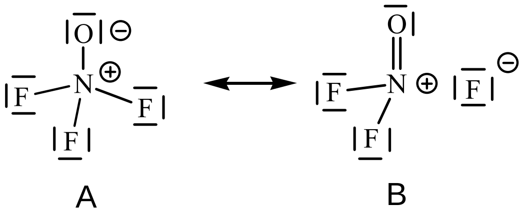
Extra Resonance Forms

From any basic resonance form, transform *leps* into π pairs in all possible ways to give double or triple bonds. The donor must be a 2p element and the acceptor a >2p element. This transfer of electrons should tend to annul, if possible, the formal charges of all atoms. If not, it should lead to place the negative formal charges on the most electronegative elements and the positive charges on the least electronegative ones.

Final Remarks

The reader must be aware that the Valence Bond Model (**VBM**) is too simple to expect from it a description of the electronic structure of molecules as good as that of the Molecular Orbital Model (**MOM**). In spite of this, from a pedagogical point of view, the utility of the VBM is very superior to that of the MOM. It should be noted that if one is to describe qualitatively (*i.e.,* without using a computer) some simple molecules by means of the MOM, the knowledge of the best resonance form(s) is necessary. In addition, just using a paper and a pencil one can deduce the resonance forms of a molecule and from them to propose the structure (using the VSEPR model[1]) and make predictions about the reactivity, the formal charges, some physical properties (*e.g.*, IR spectra of the studied ylide[24]), etc. However, not surprisingly, the resonance forms of some molecules do not describe accurately its electronic structure. Thus, using our method we can only write one resonance form for F_3NO [V = (5 + 6 +3x7)/2 = 16; N = 4 σ + 3 x 4 *leps* =16] in which the N–O and the three N–F bonds are single bonds because N = V (see A in Scheme 14), while the N–O bond length (1.158 Å) suggests a N=O bond. To solve this problem it has been proposed that three ionic resonance forms [$(F_2N{=}O)^+\ F^-$, for example B in Scheme 14] should also be considered.[21]

Scheme 14



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