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Systematic Method for Constructing Lewis Representations

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Abstract

The systematic method for constructing Lewis representations is a method for representing chemical bonds between atoms in a molecule. It uses symbols to represent the valence electrons of the atoms involved in the bond. Using a number of rules in a defined order, it is often better suited to complicated cases than the Lewis representation of atoms. This method allows us to determine the formal charge and oxidation number of each atom in the edifice more efficiently than other methods.

Keywords

Systematic Method, Lewis Representation, Chemical Bond, Formal Charge, Oxidation Number

1. Introduction

Polyatomic structures are the result of interactions between the valence electrons of atoms that form chemical bonds [1]-[6].

In a Lewis diagram, atoms are represented by their chemical symbol, surrounded by one or more dots representing valence electrons. Covalent bonds are represented by a line connecting two atoms, with each atom sharing a pair of

electrons. Non-bonding electrons, also known as lone electrons, are represented by pairs of electrons located on a single atom.

The use of Lewis diagrams is useful for understanding the molecular geometry, chemical properties and reactivity of molecules [7]-[12].

The sequence of the eight rules of the systematic method for constructing Lewis representations of buildings are:

Step 1: Determine the total number of valence electrons ($n_{E.V}$) in the molecule, which is equal to the sum of the number of valence electrons $n_{E\,V}$ in each atom of the molecule minus the building block charge according to the following relationship:

$n_{E.V}(\text{building}) = \sum_{i}^{\text{number of atoms in the building}} n_{E.V}(\text{atom } i)$ – charge of the building (Relationship 1)

Step 2: Determine the number of binding and free doublets in the molecule (n_D):

n_D(building) = 1/2 total number of valence electrons of the building $n_{E\,V}$ (Relationship 2)

If the number of doublets is not integer but half-integer, we are dealing with a radical (single electron).

Step 3: Determine the number of anti-binding doublets in the molecule ($n_{D.A.L}$):

$n_{D.A.L}(\text{building}) = \sum_{i}^{\text{number of atoms in the building}} n_{D.A.L}(\text{atom } i)$ – charge of the building (Relationship 3)

Step 4: Determine the number of binding doublets in the molecule ($n_{D.L}$):

$n_{D.L}(\text{building}) = n_D(\text{building}) - n_{D.A.L}(\text{building})$ (Relationship 4)

Step 5: Determine the geometry according to Gillespie, which tells us about the spatial geometry of the species:

The geometry of a molecule around a given atom will be that for which the repulsions between the doublets are minimal.

Gillespie gave the rules for the orientation of bonds around the central atom of a molecule.

Gillespie postulate:

- All pairs of electrons (binding or non-binding) are at the same distance from the nucleus.

- These pairs are assumed to be located on the surface of a sphere with the nucleus at its center.

- These doublets repel each other, and are furthest apart to minimize electron repulsions.

- The V.S.E.P.R formulation is expressed as follows: AX_nE_n: (Relationship 5).

A: Central atom.

X: atoms or molecules covalently bonded to atom A and n their number.

E: free doublets or single electrons and n' their number on the valence layer of atom A.

Gillespie considers that multiple bonds behave like single bonds, to establish the V.S.E.P.R. formulation, it is necessary to establish the Lewis representation.

Step 6: Position any formal load(s).

The formal charge carried by an atom corresponds to the difference in valence electrons between the isolated atom and the atom when the edifice is formed, all bonds being considered purely covalent.

The sum of all formal charges is equal to the charge of the species.

C.F(atom) = $n_{E.V}$(atom in isolated state) – $n_{E.V}$(atom linked to the structure) (Relationship 6)

Step 7: Build the structure by positioning the doublets (binding—by single, double or triple bond—or non-binding), respecting the octet rule as far as possible and placing any single electron.

Step 8: Determine the oxidation number of each atom in the structure.

The oxidation number of an atom corresponds to the difference in valence electrons between the isolated atom and the atom when the structure is formed, all bonds being considered purely ionic.

The sum of the oxidation numbers is equal to the formal charge of the species

d.o(atom) = $n_{E.V}$(atom in isolated state) – $n_{E.V}$(atom bound to the structure) (Relationship 7)

2. Constructing Lewis Representations of Buildings Using the Systematic Method

In the following, we present the construction of Lewis representations according to the systematic method for some of the following molecules: NH_4^+; NH_2^-; NO_2^-; PCl_5; SO_2; H_2SO_3; $Cr_2O_7^{2-}$; Fe_3O_4; Pb_3O_4; H_2O_2.

2.1. The Building NH_4^+

Step 1:

Applying relation 1, we find: $n_{E.V}(NH_4^+) = n_{E.V}(N) + 4n_{E.V}(H) - 1$

Z(N) = 7 from where [He] $2s^2\ 2p^3 \rightarrow n_{E.V}(N) = 5$

and Z(H) = 1 from where $1s^1 \rightarrow n_{E.V}(H) = 1$

$n_{E.V}(NH_4^+) = 5 + 4 \times 1 - 1 = 8$

Step 2:

Applying relation 2, we find:

$n_D(NH_4^+) = 1/2 \times n_{E.V}(NH_4^+) = 8/2 = 4$ binding and non-binding doublets

Step 3:

Applying relation 3, we find: $n_{D.A.L}(NH_4^+) = n_{D.N.L}(N) + 4n_{D.N.L}(H) - 1$

Z(N) = 7 from where [He] $2s^2\ 2p^3 \rightarrow n_{D.N.L}(N) = 1$

and Z(H) = 1 from where $n_{D.N.L}(H) = 0$

$n_{D.A.L}(NH_4^+) = 1 + 4 \times 0 - 1 = 0$ free doublets

Step 4:

Applying relation 4, we find:

$n_{D.L}(NH_4^+) = n_D(NH_4^+) - n_{D.A.L}(NH_4^+)$

so $n_{D.L}(NH_4^+) = 4 - 0 = 4$ Bonding doublets

Step 5:

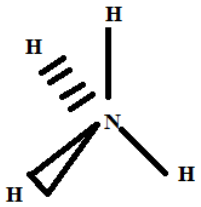
The V.S.E.P.R formulation is expressed as follows: $AX_nE_{n'}$:

N: central atom

Four hydrogen atoms covalently bonded to the nitrogen atom and n = 4 their number.

E: free doublets and n' = 0, zero their number on the valence layer of the nitrogen atom.

The type of molecule according to Gillespie is NH_4 and the basic geometry tetrahedral, as shown in the diagram opposite.



Step 6:

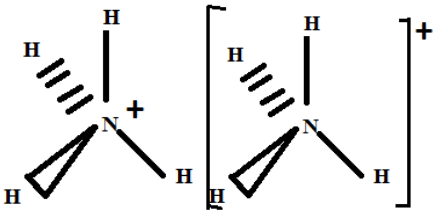
Applying relation 6, we find:

C.F(N) = $n_{E.V}$(N in isolated state) − $n_{E.V}$(N linked to the building) = 5 − 4 = + 1

C.F(H) = $n_{E.V}$(H in the isolated state) − $n_{E.V}$(H bound to the structure) = 1 − 1 = 0 no charge for the four hydrogens

Step 7:

Build the structure using the systematic method:



2.2. The Species NH_2^-

Step 1:

$n_{E.V}(NH_2^-) = n_{E.V}(N) + 2n_{E.V}(H) - (-1)$

Z(N) = 7 from where $n_{E.V}(N) = 5$ and Z(H) = 1 from where $n_{E.V}(H) = 1$

$n_{E.V}(NH_2^-) = 5 + 2 \times 1 + 1 = 8$

Step 2:

$n_D(NH_2^-) = 1/2 \times n_{E.V}(NH_2^-) = 8/2 = 4$ binding and non-binding doublets.

Step 3:

$n_{D.A.L}(NH_2^-) = n_{D.N.L}(N) + 2n_{D.N.L}(H) - (-1)$

Z(N) = 7 from where $n_{D.N.L}(N) = 1$ and Z(H) = 1 from where $n_{D.N.L}(H) = 0$

$n_{D.A.L}(NH_2^-) = 1 + 2 \times 0 + 1 = 2$ free doublets.

Step 4:

$n_{D.L}(NH_2^-) = n_D(NH_2^-) - n_{D.A.L}(NH_2^-)$

so $n_{D.L}(NH_2^-) = 4 - 2 = 2$ Bonding doublets.

Step 5:

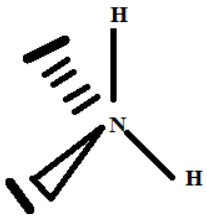
The V.S.E.P.R formulation is expressed as follows: $AX_nE_{n'}$:

N: central atom.

H: two atoms covalently bonded to the N atom and n = 2 is the number of covalent bonds that hydrogen can form with nitrogen.

E: two free doublets on the valence layer of the N atom.

So the Gillespie type of molecule is NH_2E_2 and the basic geometry tetrahedral, as shown in the diagram opposite.



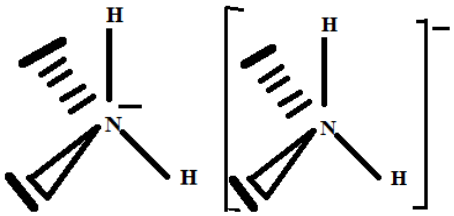
Step 6:

C.F(N) = $n_{E.V}$(N in isolated state) – $n_{E.V}$(N linked to the building) = 5 – 6 = –1

C.F(H) = $n_{E.V}$(H in the isolated state) – $n_{E.V}$(H bound to the structure) = 1 – 1 = 0 no charge for the two hydrogens.

Step 7:

Build the structure using the systematic method:



2.3. The Species NO_2^-

Step 1:

$n_{E.V}(NO_2^-) = n_{E.V}(N) + 2n_{E.V}(O) - (-1)$

Z(N) = 7 from where $n_{E.V}(N) = 5$ and Z(O) = 8 from where [He] $2s^2\ 2p^4 \rightarrow n_{E.V}(O) = 6$

$n_{E.V}(NO_2^-) = 5 + 2 \times 6 + 1 = 18$

Step 2:

$n_D(NO_2^-) = 1/2 \times n_{E.V}(NO_2^-) = 18/2 = 9$ binding and non-binding doublets.

Step 3:

$n_{D.A.L}(NO_2^-) = n_{D.N.L}(N) + 2n_{D.N.L}(O) - (-1)$

Z(N) = 7 from where $n_{D.N.L}(N) = 1$ and Z(O) = 8 from where $n_{D.N.L}(O) = 2$

$n_{D.A.L}(NO_2^-) = 1 + 2 \times 2 + 1 = 6$ free doublets.

Step 4:

$n_{D.L}(NO_2^-) = n_D(NO_2^-) - n_{D.A.L}(NO_2^-)$

so $n_{D.L}(NO_2^-) = 9 - 6 = 3$ bonding doublets.

Step 5:

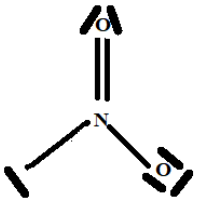
The V.S.E.P.R formulation is expressed as follows: $AX_nE_{n'}$:

N: central atom.

O: two atoms covalently bonded to the N atom and n = 2 is the number of covalent bonds oxygen can form with nitrogen.

E: one free doublet on the valence layer of the N atom.

So the Gillespie type of molecule is NO_2E_1 and the basic geometry triangular planar as shown in the diagram opposite.



Step 6:

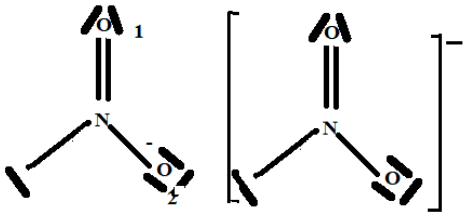
C.F(N) = $n_{E.V}$(N in isolated state) − $n_{E.V}$(N linked to the building) = 5 − 5 = O no formal charge on N.

C.F(O_1) = $n_{E.V}$(O_1 in the isolated state) − $n_{E.V}$(O_1 bound to the structure) = 6 − 6 = 0 no formal charge on O_1.

C.F(O_2) = $n_{E.V}$(O_2 in isolated state) − $n_{E.V}$(O_2 bound to the structure) = 6 − 7 = −1.

Step 7:

Build the structure using the systematic method:



2.4. The Species PCl_5

Step 1:

$n_{E\,V}(PCl_5) = n_{E.V}(P) + 5n_{E.V}(Cl) - 0$

Z(P) = 15 from where [Ne] $2s^2\ 2p^3 \rightarrow n_{E.V}(P) = 5$

and Z(Cl) = 17 from where [Ne] $2s^2\ 2p^5 \rightarrow n_{E.V}(Cl) = 7$

$n_{E\,V}(PCl_5) = 5 + 5 \times 7 - 0 = 40$

Step 2:

$n_D(PCl_5) = 1/2 \times n_{E\,V}(PCl_5) = 40/2 = 20$ binding and non-binding doublets.

Step 3:

$n_{D.A.L}(PCl_5) = n_{D.N.L}(P) + 5n_{D.N.L}(Cl) - 0$

Z(P) = 15 from where $n_{D.N.L}(P) = 1$ and Z(Cl) = 17 from where $n_{D.N.L}(Cl) = 3$

$n_{D.A.L}(PCl_5) = 1 + 5 \times 3 - 0 = 16$ free doublets.

Step 4:

$n_{D.L}(PCl_5) = n_D(PCl_5) - n_{D.A.L}(PCl_5)$

So $n_{D.L}(PCl_5) = 20 - 16 = 4$ Binding doublets.

Step 5:

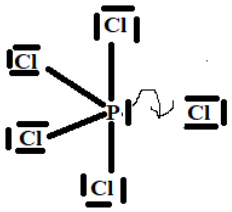
The V.S.E.P.R formulation is expressed as follows: AX_nE_n:

P: central atom.

Cl: four atoms covalently bonded to the P atom and n = 4 is the number of covalent bonds that chlorine can form with phosphorus.

E: one free doublet on the valence layer of atom P.

So the Gillespie type of molecule is PCl_4E and the basic geometry trigonal bi-pyramid, as shown in the diagram opposite.



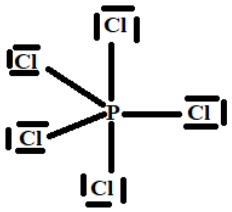
Step 6:

C.F(P) = $n_{E.V}$(P in isolated state) − $n_{E.V}$(P linked to the building) = 5 − 5 = 0 no formal charge on P.

C.F(Cl) = $n_{E.V}$(Cl in isolated state) − $n_{E.V}$(Cl bound to the structure) = 7 − 7 = 0 no formal charge on the five Cl atoms.

Step 7:

Build the structure using the systematic method:



2.5. The Species SO_2

Step 1:

$n_{E.V}(SO_2) = n_{E.V}(S) + 2n_{E.V}(O) - 0$

Z(S) = 16 hence [Ne] $2s^2\ 2p^4 \rightarrow n_{E.V}(S) = 6$ and Z(O) = 8 hence $n_{E.V}(O) = 6$

$n_{E.V}(SO_2) = 6 + 2 \times 6 - 0 = 18$

Step 2:

$n_D(SO_2) = 1/2 \times n_{E.V}(SO_2) = 18/2 = 9$ binding and non-binding doublets.

Step 3:

$n_{D.A.L}(SO_2) = n_{D.N.L}(S) + 2n_{D.N.L}(O) - 0$

Z(S) = 16 hence $n_{D.N.L}(S) = 2$ and Z(O) = 8 hence $n_{D.N.L}(O) = 2$

$n_{D.A.L}(SO_2) = 2 + 2 \times 2 - 0 = 6$ free doublets.

Step 4:

$n_{D.L}(SO_2) = n_D(SO_2) - n_{D.A.L}(SO_2)$

so $n_{D.L}(SO_2) = 9 - 6 = 3$ Binding doublets.

Step 5:

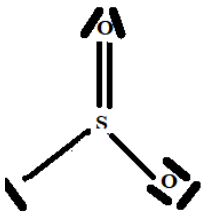
The V.S.E.P.R formulation is expressed as follows: $AX_nE_{n'}$:

S: central atom.

O: two atoms covalently bonded to the S atom and n = 2 is the number of covalent bonds oxygen can form with sulfur.

E: one free doublet on the valence layer of atom S.

So the Gillespie type of molecule is SO_2E and the basic geometry triangular planar, as shown in the diagram opposite.



Step 6:

$C.F(S) = n_{E.V}(S \text{ in isolated state}) - n_{E.V}(S \text{ linked to the building}) = 6 - 5 = +1$

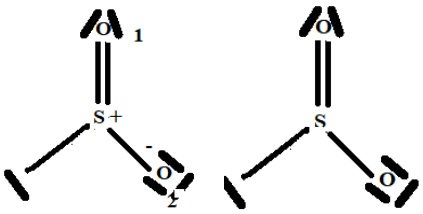
$C.F(O_1) = n_{E.V}(O_1 \text{ in isolated state}) - n_{E.V}(O_1 \text{ bound to the structure}) = 6 - 6 = 0$ no formal charge on O_1

$C.F(O_2) = n_{E.V}(O_2 \text{ in isolated state}) - n_{E.V}(O_2 \text{ bound to the structure}) = 6 - 7 = -1$

$C.F(SO_2) = C.F(S) + C.F(O_1) + C.F(O_2) = 1 + 0 - 1 = 0$

Step 7:

Build the structure using the systematic method:



2.6. The Species H_2SO_3

Step 1:

$n_{E.V}(H_2SO_3) = n_{E.V}(S) + 3n_{E.V}(O) + 2n_{E.V}(H) - 0$

$Z(S) = 16$ hence $n_{E.V}(S) = 6$; $Z(H) = 1$ hence $n_{E.V}(H) = 1$

and $Z(O) = 8$ hence $n_{E.V}(O) = 6$

$n_{E.V}(H_2SO_3) = 6 + 3 \times 6 + 2 \times 1 - 0 = 26$

Step 2:

$n_D(H_2SO_3) = 1/2 \times n_{E.V}(H_2SO_3) = 26/2 = 13$ binding and non-binding doublets.

Step 3:

$n_{D.A.L}(H_2SO_3) = n_{D.N.L}(S) + 3n_{D.N.L}(O) + 2n_{D.N.L}(H) - 0$

Z(S) = 16 hence $n_{D.N.L}(S) = 2$; Z(H) = 1 hence $n_{D.N.L}(H) = 0$

and Z(O) = 8 hence $n_{D.N.L}(O) = 2$

$n_{D.A.L}(H_2SO_3) = 2 + 3 \times 2 + 2 \times 0 - 0 = 8$ free doublets.

Step 4:

$n_{D.L}(H_2SO_3) = n_D(H_2SO_3) - n_{D.A.L}(H_2SO_3)$

so $n_{D.L}(H_2SO_3) = 13 - 8 = 5$ Bonding Doublets.

Step 5:

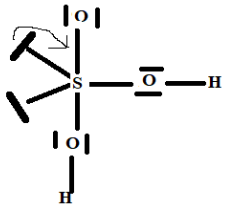
The V.S.E.P.R formulation is expressed as follows: $AX_nE_{n'}$:

S: central atom.

O: three oxygen atoms covalently bonded to the S atom and n = 3 is the number of covalent bonds that oxygen can form with sulfur.

E: two free doublets on the valence layer of atom S.

So the Gillespie type of molecule is $H_2SO_3E_2$ and the energetically most favorable trigonal bipyramid base geometry in T, as shown in the diagram opposite.



Step 6:

C.F(S) = $n_{E.V}$(S in isolated state) – $n_{E.V}$(S linked to the building) = 6 – 6 = 0

C.F(O_1) = $n_{E.V}$ (O_1 in isolated state) – $n_{E.V}$(O_1 bound to the structure) = 6 – 6 = 0 no formal charge on O_1

C.F(O_2) = $n_{E.V}$(O_2 in isolated state) – $n_{E.V}$(O_2 bound to the structure) = 6 – 6 = 0 no formal charge on O_2

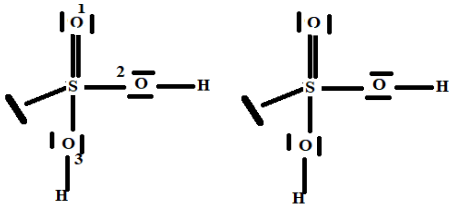
C.F(O_3) = $n_{E.V}$(O_3 in isolated state) – $n_{E.V}$(O_3 bound to the structure) = 6 – 6 = 0 no formal charge on O_3

C.F(H) = $n_{E.V}$(H in isolated state) – $n_{E.V}$(H linked to the building) = 1 – 1 = 0 no formal charge on twice H

C.F(H_2SO_3) = C.F(S) + C.F(O_1) + C.F(O_2) + C.F(O_3) + 2 C.F(H) = 0 + 3 × 0 + 2 × 0 = 0

Step 7:

Build the structure using the systematic method:



2.7. The Species $Cr_2O_7^{2-}$

Step 1:

$n_{E.V}(Cr_2O_7^{2-}) = 2n_{E.V}(Cr) + 7n_{E.V}(O) - (-2)$

Z(Cr) = 24 where Cr's valence layer is: [Ar] $3d^5\ 4s^1 \rightarrow n_{E.V}(Cr) = 6$;

Z(O) = 8 from which the valence layer of O is: [He] $2s^2\ 2p^4$ $n_{E.V}(O) = 6$;

$n_{E.V}(Cr_2O_7^{2-}) = 2 \times 6 + 7 \times 6 - (-2) = 56$

Step 2:

$n_D(Cr_2O_7^{2-}) = 1/2 \times n_{E.V}(Cr_2O_7^{2-}) = 56/2 = 28$ binding and non-binding doublets.

Step 3:

$n_{D.A.L}(Cr_2O_7^{2-}) = 2n_{D.N.L}(Cr) + 7n_{D.N.L}(O) - (-2)$

Z(Cr) = 24 hence $n_{D.N.L}(Cr) = 1$ and Z(O) = 8 hence $n_{D.N.L}(O) = 2$

$n_{D\,A\,L}(Cr_2O_7^{2-}) = 2 \times 1 + 7 \times 2 - (-2) = 18$ free doublets.

Step 4:

$n_{D.L}(Cr_2O_7^{2-}) = n_D(Cr_2O_7^{2-}) - n_{D.A.L}(Cr_2O_7^{2-})$

so $n_{D.L}(Cr_2O_7^{2-}) = 28 - 18 = 10$ Bonding Doublets.

Step 5:

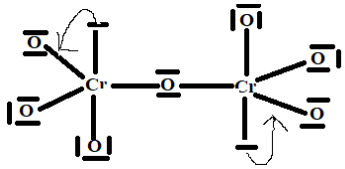
The V.S.E.P.R formulation is expressed as follows: $AX_nE_{n'}$:

Cr: central atom.

O: four oxygen atoms covalently bonded to the Cr atom and n = 4 is the number of covalent bonds that oxygen can form with chromium.

E: one free doublet on the valence layer of the Cr atom.

The Gillespie type of molecule is therefore CrO_4E and the basic geometry trigonal bipyramid, as shown in the diagram opposite.



Step 6:

C.F(Cr) = $n_{E.V}$(Cr in isolated state) − $n_{E.V}$(Cr bound to the structure) = 6 − 5 = +1

C.F(O_1) = $n_{E.V}$(O_1 in isolated state) − $n_{E.V}$(O_1 bound to the structure) = 6 − 6 = 0 no formal charge on O_1

C.F(O_2) = $n_{E.V}$(O_2 in isolated state) − $n_{E.V}$(O_2 bound to the structure) = 6 − 6 = 0 no formal charge on O_2

C.F(O_3) = $n_{E.V}$(O_3 in isolated state) − $n_{E.V}$(O_3 bound to the structure) = 6 − 7 = −1

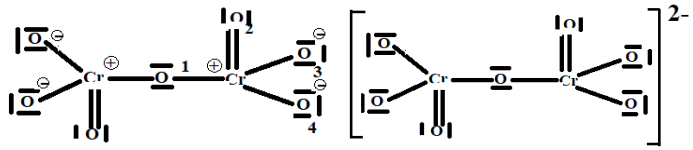
C.F(O_4) = $n_{E.V}$(O_4 in isolated state) − $n_{E.V}$(O_4 bound to the structure) = 6 − 7 = −1

$C.F(Cr_2O_7^{2-}) = 2C.F(Cr) + C.F(O_1) + 2C.F(O_2) + 2C.F(O_3) + 2C.F(O_4) = 2 \times 1 + 1 \times 0 + 2 \times 0 + 2 \times (-1) + 2 \times (-1)$

$C.F(Cr_2O_7^{2-}) = -2$

Step 7:

Build the structure using the systematic method:



2.8. The Species Fe_3O_4

Step 1:

$n_{E.V}(Fe_3O_4) = 3n_{E.V}(Fe) + 4n_{E.V}(O) - 0$

$Z(Fe) = 26$ from which the valence layer of Fe is: [Ar] $3d^6\ 4s^2 \rightarrow n_{E.V}(Cr) = 8$;

$Z(O) = 8$ from which the valence layer of O is: [He] $2s^2\ 2p^4 \rightarrow n_{E.V}(O) = 6$;

$n_{E.V}(Fe_3O_4) = 3 \times 8 + 4 \times 6 - 0 = 48$

Step 2:

$n_D(Fe_3O_4) = 1/2 \times n_{E.V}(Fe_3O_4) = 48/2 = 24$ binding and non-binding doublets.

Step 3:

$n_{D.A.L}(Fe_3O_4) = 3n_{D.N.L}(Fe) + 4n_{D.N.L}(O) - 0$

$Z(Fe) = 26$ from where $n_{D.N.L}(Fe) = 2$ and $Z(O) = 8$ from where $n_{D.N.L}(O) = 2$

$n_{D.A.L}(Fe_3O_4) = 3 \times 2 + 4 \times 2 - 0 = 14$ free doublets.

Step 4:

$n_{D.L}(Fe_3O_4) = n_D(Fe_3O_4) - n_{D.A.L}(Fe_3O_4)$

Therefore $n_{D.L}(Fe_3O_4) = 24 - 14 = 10$ Bonding doublets.

Step 5:

The V.S.E.P.R formulation is expressed as follows: $AX_nE_{n'}$:

Fe_1: central atom

Two oxygen atoms and one Fe_2 atom covalently bonded to the Fe_1 atom and n = 3 is their number.

E: two free doublets on the valence layer of the Fe_1 atom.

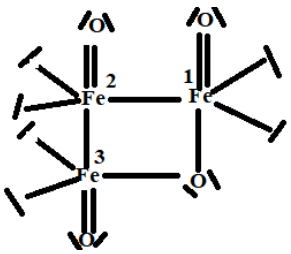
The Gillespie type of molecule is therefore $Fe_1O_2Fe_2E_2$ and the basic geometry trigonal bipyramid.

Fe_2: central atom

Two iron atoms and one oxygen atom covalently bonded to the central Fe_2 atom and n = 3 their number.

E: two free doublets on the valence shell of the central Fe atom.

The Gillespie type of molecule is therefore $Fe_2Fe_1Fe_3OE_2$ and the basic geometry trigonal bipyramid, as shown in the diagram opposite.



Step 6:

$C.F(Fe_1) = n_{E.V}(Fe1 \text{ in isolated state}) - n_{E.V}(Fe_1 \text{ bound to the structure}) = 8 - 8$

= 0

C.F(Fe_2) = $n_{E.V}$(Fe2 in isolated state) − $n_{E.V}$(Fe_2 bound to the structure) = 8 − 8 = 0

C.F(Fe_3) = $n_{E.V}$(Fe3 in isolated state) − $n_{E.V}$(Fe_3 bound to the structure) = 8 − 8 = 0

C.F(O) = $n_{E.V}$(O in isolated state) − $n_{E.V}$(O bound to the structure) = 6 − 6 = 0 no formal charge on the three O.

C.F(Fe_3O_4) = 3C.F(Fe) + 4C.F(O) = 3 × 0 + 4 × 0

C.F(Fe_3O_4) = 0

Step 7:

Build the structure using the systematic method: same layout as described for geometry.

2.9. The Species Pb_3O_4

Step 1:

$n_{E.V}(Pb_3O_4) = 3\ n_{E.V}(Pb) + 4n_{E.V}(O) - 0$

Z(Pb) = 82 from which the valence layer of Pb is [Xe] $4f^{14}\ 5d^{10}\ 6s^2 6p^2$ → $n_{E.V}$(Pb) = 4;

Z(O) = 8 from which the valence layer of O is: [He] $2s^2\ 2p^4$ → $n_{E.V}$(O) = 6;

$n_{E.V}(Pb_3O_4) = 3 \times 4 + 4 \times 6 - 0 = 36$

Step 2:

$n_D(Pb_3O_4) = 1/2 \times n_{E.V}(Pb_3O_4) = 36/2 = 18$ binding and non-binding doublets.

Step 3:

$n_{D.A.L}(Pb_3O_4) = 3n_{D.N.L}(Pb) + 4n_{D.N.L}(O) - 0$

Z(Pb) = 82 from where $n_{D.N.L}$(Pb) = 1 and Z(O) = 8 from where $n_{D.N.L}$(O) = 2

$n_{D.A.L}(Pb_3O_4) = 3 \times 1 + 4 \times 2 - 0 = 11$ free doublets.

Step 4:

$n_{D.L}(Pb_3O_4) = n_D(Pb_3O_4) - n_{D.A.L}(Pb_3O_4)$

so $n_{D.L}(Pb_3O_4) = 18 - 11 = 7$ Bonding Doublets.

Step 5:

The V.S.E.P.R formulation is expressed as follows: $AX_nE_{n'}$:

Pb_1: central atom

two oxygen atoms and one Pb_2 atom covalently bonded to the

central Pb_1 atom and n = 3 in number.

E: zero free doublet on the valence layer of the central atom Pb_1.

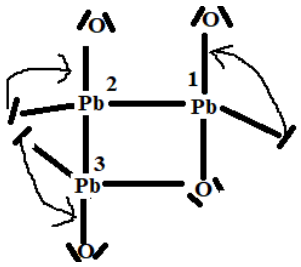
So the Gillespie type of molecule is $Pb_1O_2Pb_2$ and the basic geometry triangular planar.

Pb_2: central atom

two lead atoms and one oxygen atom covalently bonded to the central Pb_2 atom and n = 3 their number.

E: zero free doublets on the valence layer of the central atom Pb_2.

So the Gillespie type of molecule is $Pb_2Pb_1Pb_3O$ and the basic geometry triangular planar, as shown in the diagram opposite.



Step 6:

C.F(Pb_1) = $n_{E.V}$(Pb_1 in isolated state) − $n_{E.V}$(Pb_1 linked to the building) = 4 − 4 = 0

C.F(Pb_2) = $n_{E.V}$(Pb_2 in isolated state) − $n_{E.V}$(Pb_2 linked to the building) = 4 − 4 = 0

C.F(Pb_3) = $n_{E.V}$(Pb_3 in isolated state) − $n_{E.V}$(Pb_3 linked to the building) = 4 − 4 = 0

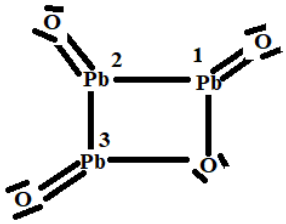
C.F(O) = $n_{E.V}$(O in isolated state) − $n_{E.V}$(O bound to the structure) = 6 − 6 = 0 no formal charge on the three O

C.F(Pb_3O_4) = 3C.F(Pb) + 4 C.F(O) = 3 × 0 + 4 × 0

C.F(Pb_3O_4) = 0

Step 7:

Build the structure using the systematic method:



2.10. The Species H_2O_2

Step 1:

$n_{E.V}(H_2O_2) = 2n_{E.V}(O) + 2n_{E.V}(H) - 0$

Z(O) = 8 from where $n_{E.V}(O) = 6$ and Z(H) = 1 from where $n_{E.V}(H) = 1$

$n_{E.V}(H_2O_2) = 2 \times 6 + 2 \times 1 - 0 = 14$

Step 2:

$n_D(H_2O_2) = 1/2 \times n_{E.V}(H_2O_2) = 14/2 = 7$ binding and non-binding doublets.

Step 3:

$n_{D.A.L}(H_2O_2) = 2n_{D.N.L}(O) + 2n_{D.N.L}(H) - 0$

Z(O) = 8 from where $n_{D.N.L}(O) = 2$ and Z(H) = 1 from where $n_{D.N.L}(H) = 0$

$n_{D.A.L}(H_2O_2) = 2 \times 2 + 2 \times 0 - 0 = 4$ free doublets.

Step 4:

$n_{D.L}(H_2O_2) = n_D(H_2O_2) - n_{D.A.L}(H_2O_2)$

Therefore $n_{D.L}(H_2O_2) = 7 - 4 = 3$ Bonding Doublets.

Step 5:

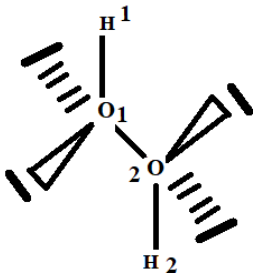
The V.S.E.P.R formulation is expressed as follows: $AX_nE_{n'}$:

O: central atom.

An oxygen atom and a hydrogen atom covalently bonded to the O atom and n = 2 is the number of covalent bonds that oxygen 1 can form with oxygen 2 and hydrogen.

E: free doublets and 2 their number on the valence layer of the O_1 atom.

So the Gillespie type of molecule is $O_1H_1E_2$ and the basic geometry is tetrahedral angled, as shown in the diagram opposite.



Step 6:

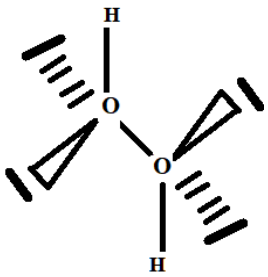
C.F(O) = $n_{E.V}$(O in isolated state) − $n_{E.V}$(O bound to the structure) = 6 − 6 = 0 no charge for both oxygens

C.F(H) = $n_{E.V}$(H in the isolated state) − $n_{E.V}$(H bound to the structure) = 1 − 1 = 0 no charge for the two hydrogens

C.F(H_2O_2) = 2C.F(O) + 2C.F(H) = 2 × 0 + 2 × 0 = 0

Step 7:

Build the structure using the systematic method:



3. Oxidation Number of Atoms in Buildings Using the Systematic Method

We determine the degree of oxidation of the various atoms in the structure using the systematic method for some of the following molecules: NH_4^+; NH_2^-; NO_2^-; PCl_5; SO_2; H_2SO_3; $Cr_2O_7^{2-}$; Fe_3O_4; Pb_3O_4; H_2O_2.

3.1. The Species NH_4^+

Step 8:

We have χ(N) > χ(H), so the nitrogen atom will attract towards itself the electrons involved with hydrogen.

d.o(N) = $n_{E.V}$(N atom in isolated state) − $n_{E.V}$(N atom bound to the structure) = 5 − 8 = −3

d.o(H) = $n_{E.V}$(H atom in isolated state) − $n_{E.V}$(H atom bound to the structure) = 1 − 0 = 1

C.F(NH_4^+) = d.o(N) + 4d.o(H) = −3 + 4 × 1 = +1

3.2. The Species NH_2^-

Step 8:

We have χ(N) > χ(H), so the nitrogen atom will attract towards itself the electrons involved with hydrogen.

d.o (N) = $n_{E.V}$ (N atom in isolated state) − $n_{E.V}$ (N atom bound to the structure) = 5 − 8 = −3

d.o (H) = $n_{E.V}$ (H atom in isolated state) − $n_{E.V}$ (H atom bound to the structure) = 1 − 0 = 1

C.F (NH_2^-) = d.o (N) + d.o (H_1) + d.o (H_2) = −3 + 2 × 1 = −1

3.3. The Species NO_2^-

We have χ(O) > χ(N), so the oxygen atom will attract to itself the electrons involved with nitrogen.

d.o(N) = $n_{E.V}$(N atom in isolated state) − $n_{E.V}$(N atom bound to the structure) = 5 − 2 = 3

d.o(O_1) = $n_{E.V}$(O atom1 in isolated state) − $n_{E.V}$(O atom1 bound to the edifice) = 6 − 8 = −2

d.o(O_2) = $n_{E.V}$(O atom2 in isolated state) − $n_{E.V}$(O atom2 bound to the edifice) = 6 - 8 = - 2

C.F(NO_2^-) = d.o(N) + d.o(O_1) + d.o(O_2) = 3 + 2 × (−2) = −1

3.4. The Species PCl_5

We have χ(Cl) > χ(P), so the chlorine atom will attract to itself the electrons involved with the phosphorus.

d.o(Cl) = $n_{E.V}$(Cl atom in isolated state) − $n_{E.V}$(Cl atom bound to the structure) = 7 − 8 = −1

d.o(P) = $n_{E.V}$(P atom in isolated state) − $n_{E.V}$(P atom bound to the structure) = 5 − 0 = +5

C.F(PCl_5) = d.o(S) + 5d.o(Cl) = 5 + 5 × (−1) = 0

3.5. The Species SO_2

We have χ(O) > χ(S), so the oxygen atom will attract to itself the electrons involved with sulfur.

d.o(S) = $n_{E.V}$(S atom in isolated state) − $n_{E.V}$(S atom bound to the structure) = 6 − 2 = +4

d.o(O_1) = $n_{E.V}$(O atom1 in isolated state) − $n_{E.V}$(O atom1 bound to the edifice) = 6 − 8 = −2

d.o(O_2) = $n_{E.V}$(O atom2 in isolated state) − $n_{E.V}$(O atom2 bound to the edifice) = 6 − 8 = −2

C.F(SO_2) = d.o(S) + d.o(O_1) + d.o(O_2) = 4 + 2 × (−2) = 0

3.6. The Species H_2SO_3

We have χ(O) > χ(S) and χ(O) > χ(S), so the oxygen atom will attract the electrons involved with sulfur and hydrogen.

d.o(S) = $n_{E.V}$(S atom in isolated state) − $n_{E.V}$(S atom bound to the structure) = 6 − 2 = +4

d.o(O_1) = $n_{E.V}$(O atom1 in isolated state) − $n_{E.V}$(O atom1 bound to the edifice) = 6 − 8 = −2

d.o(O_2) = $n_{E.V}$(O atom2 in isolated state) − $n_{E.V}$(O atom2 bound to the edifice) = 6 − 8 = −2

d.o(O_3) = $n_{E.V}$ (O atom3 in isolated state) − $n_{E.V}$(O atom3 bound to the edifice) = 6 − 8 = −2

d.o(H) = $n_{E.V}$ (H atom in isolated state) − $n_{E.V}$(H atom bound to the structure) = 1 − 0 = +1

C.F(H_2SO_3) = d.o(S) + d.o(O_1) + d.o(O_2) + d.o(O_3) + 2d.o(H) = 4 + 3 × (−2) + 2 × 1 = 0

3.7. The Species $Cr_2O_7^{2-}$

We have χ(O) > χ(Cr), so the oxygen atom will draw the electrons involved with chromium towards itself.

d.o(Cr) = $n_{E.V}$(Cr atom in the isolated state) − $n_{E.V}$(Cr atom bound to the structure) = 6 − 0 = + 6

d.o(O_1) = $n_{E.V}$(O atom1 in isolated state) - $n_{E.V}$(O atom1 bound to the edifice) = 6 − 8 = −2

d.o(O_2) = $n_{E.V}$(O atom2 in isolated state) − $n_{E.V}$(O atom2 bound to the edifice) = 6 − 8 = −2

d.o(O_3) = $n_{E.V}$(O atom3 in isolated state) − $n_{E.V}$(O atom3 bound to the edifice) = 6 − 8 = −2

d.o(O_4) = $n_{E.V}$(O atom4 in isolated state) − $n_{E.V}$(O atom4 bound to the edifice) = 6 − 8 = −2

C.F($Cr_2O_7^{2-}$) = 2d.o(Cr) + d.o(O_1) + 2d.o(O_2) + 2d.o(O_3) + 2d.o(O_4) = 2 × 6 + 1 × (−2) + 2 × (−2) + 2 × (−2)

C.F($Cr_2O_7^{2-}$) = −2

3.8. The Species Fe_3O_4

We have χ(O) > χ(Fe), so the oxygen atom will attract towards itself the electrons involved with the iron.

d.o(Fe_1) = $n_{E.V}$(Fe atom1 in isolated state) − $n_{E.V}$(Fe atom1 bound to the structure) = 8 − 5 = +3

d.o(Fe_2) = $n_{E.V}$(Fe atom2 in isolated state) − $n_{E.V}$(Fe atom2 bound to the struc-

ture) = 8 − 6 = +2

d.o(Fe_3) = $n_{E.V}$(Fe atom3 in isolated state) − $n_{E.V}$(Fe atom3 bound to the structure) = 8 − 5 = +3

d.o(O) = $n_{E.V}$(O atom in isolated state) − $n_{E.V}$(O atom bound to the structure) = 6 − 8 = −2

C.F(Fe_3O_4) = d.o(Fe_1) + d.o(Fe_2) + d.o(Fe_3) + 4d.o(O) = 3 + 2 + 3 + 4 × (−2) C.F(Fe_3O_4) = 0

3.9. The Species Pb_3O_4

We have χ(O) > χ(Pb), so the oxygen atom will attract towards itself the electrons involved with lead.

d.o(Pb_1) = $n_{E.V}$(Pb atom1 in isolated state) − $n_{E.V}$(Pb atom1 bound to the structure) = 4 − 1 = +3

d.o(Pb_2) = $n_{E.V}$(Pb atom2 in isolated state) − $n_{E.V}$(Pb atom2 bound to the structure) = 4 − 2 = +2

d.o(Pb_3) = $n_{E.V}$(Pb atom3 in isolated state) − $n_{E.V}$(Pb atom3 bound to the structure) = 4 − 1 = +3

d.o(O) = $n_{E.V}$(O atom in isolated state) − $n_{E.V}$(O atom bound to the structure) = 6 − 8 = −2

C.F(Pb_3O_4) = d.o(Pb_1) + d.o(Pb_2) + d.o(Pb_3) + 4d.o(O) = 3 + 2 + 3 + 4 × (−2) C.F(Pb_3O_4) = 0

3.10. The Species H_2O_2

We have χ(O) > χ(H), so the oxygen atom will attract towards itself the electrons brought into play with hydrogen.

d.o(O_1) = d.o(O_2) = $n_{E.V}$(O atom in isolated state) - $n_{E.V}$(O atom bound to the structure) = 6 − 7 = −1

d.o(H_1) = d.o(H_2) = $n_{E.V}$(H atom in isolated state) − $n_{E.V}$(H atom bound to the structure) = 1 − 0 = +1

C.F(H_2O_2) = 2d.o(O) + 2d.o(H) = 2 × (−1) + 2 × 1 = 0

The importance of this systematic method for the Lewis representation of molecules lies in determining the oxidation state of each atom in the structure [7]-[12].

4. Conclusion

The systematic method for constructing Lewis representations of molecules is an excellent method for simultaneously determining the Gillespie geometry, formal charge and oxidation state of molecules, and is better than the other methods Lewis representations of atoms as well as the linear combination method of atomic orbitals [1]-[6].

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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