THE MOLECULE: NOMENCLATURE

IONS AND IONIC COMPOUNDS

Atomic **CATIONS:** (positive ions)

Group IA, IIA and other main group cations where the **charge is equal to the group number**:

- element name followed by the word "ion"

e.g. Li^{+} : Lithium ion

Al^{3+} (aluminum is in group IIIA): Aluminum ion

Pb^{4+} (lead is in group IVA): Lead ion

I II III IV V VI VII

+1 +2 +3 -3 -2 -1

no roman numeral group number.

hydrogen 1 H 1.0079																		helium 2 He 4.0026
lithium 3 Li 6.941	beryllium 4 Be 9.0122												boron 5 B 10.811	carbon 6 C 12.011	nitrogen 7 N 14.007	oxygen 8 O 15.999	fluorine 9 F 18.998	neon 10 Ne 20.180
sodium 11 Na 22.990	magnesium 12 Mg 24.305												aluminium 13 Al 26.982	silicon 14 Si 28.086	phosphorus 15 P 30.974	sulfur 16 S 32.065	chlorine 17 Cl 35.453	argon 18 Ar 39.948
potassium 19 K 39.098	calcium 20 Ca 40.078		scandium 21 Sc 44.956	titanium 22 Ti 47.867	vanadium 23 V 50.942	chromium 24 Cr 51.996	manganese 25 Mn 54.938	iron 26 Fe 55.845	cobalt 27 Co 58.933	nickel 28 Ni 58.693	copper 29 Cu 63.546	zinc 30 Zn 65.38	gallium 31 Ga 69.723	germanium 32 Ge 72.61	arsenic 33 As 74.922	selenium 34 Se 78.96	bromine 35 Br 79.904	krypton 36 Kr 83.80
rubidium 37 Rb 85.468	strontium 38 Sr 87.62		yttrium 39 Y 88.906	zirconium 40 Zr 91.224	niobium 41 Nb 92.906	molybdenum 42 Mo 95.96	technetium 43 Tc [98]	ruthenium 44 Ru 101.07	rhodium 45 Rh 102.91	palladium 46 Pd 106.42	silver 47 Ag 107.87	cadmium 48 Cd 112.41	indium 49 In 114.82	tin 50 Sn 118.71	antimony 51 Sb 121.76	tellurium 52 Te 127.60	iodine 53 I 126.90	xenon 54 Xe 131.29
caesium 55 Cs 132.91	barium 56 Ba 137.33	57-70 *	lutetium 71 Lu 174.97	hafnium 72 Hf 178.49	tantalum 73 Ta 180.95	tungsten 74 W 183.84	rhenium 75 Re 186.21	osmium 76 Os 190.23	iridium 77 Ir 192.22	platinum 78 Pt 195.08	gold 79 Au 196.97	mercury 80 Hg 200.59	thallium 81 Tl 204.38	lead 82 Pb 207.2	bismuth 83 Bi 208.98	polonium 84 Po [209]	astatine 85 At [210]	radon 86 Rn [222]
francium 87 Fr [223]	radium 88 Ra [226]	89-102 **	lawrencium 103 Lr [262]	rutherfordium 104 Rf [267]	dubnium 105 Db [268]	seaborgium 106 Sg [271]	bohrium 107 Bh [272]	hassium 108 Hs [270]	meitnerium 109 Mt [276]	darmstadtium 110 Ds [281]	roentgenium 111 Rg [280]	ununbium 112 Uub [285]	ununtrium 113 Uut [284]	ununquadium 114 Uuq [289]	ununpentium 115 Uup [288]	ununhexium 116 Uuh [293]	ununseptium 117 Uus —	ununoctium 118 Uuo [294]

+3/+1 /+4/+2 /+3 /+4

Other Main Group cations, and d-block and f-block cations:

- element name
- followed by the charge on the ion, in roman numerals, in round brackets
- followed by the word "ion"

e.g. Mn^{2+} (d-block): Manganese (II) ion

Nd^{3+} (f-block): Neodymium (III) ion

Pb^{2+} (lead not in gr IIA: specify!): Lead (II) ion

group IV

The charge on the ion is specified for main group ions **ONLY** when it is not the same as the group number, and for d and f block cations at all times.

Molecular cations: (cations which consist of more than one atom; memorize!)

many exist. One needs to be memorized.

NH_4^+ : Ammonium ion

There are many others, but if you need those, I'll give you name and charge. The ammonium ion is common, and you need to know it.

Atomic **ANIONS:** (negative ions)

- Drop the last syllable (or last 2 syllables) from the element name
- Replace them with the syllable "ide"
- Followed by the word "ion"

e.g. Cl: Chlor*ine*

Cl^-: Chlor*ide ion*

e.g. Te: Tellu*rium*

Te^{2-}: Tellu*ride ion*

The charge on an anion is **never** specified. No element can form more than one type of anion (although some will form one type of anion and one or more type of cation.)

Molecular anions: (memorize)

only "ide" molecular ion.

OH^{-}	hydroxide ion
CH_3COO^{-}	acetate ion
NO_3^{-}	nitrate ion
CO_3^{2-}	carbonate ion
SO_4^{2-}	sulfate ion
PO_4^{3-}	phosphate ion

There are many others, but if you need those, I'll give you name and charge. The ammonium ion is common, and you need to know it.

IONIC COMPOUNDS: (metal + non-metal or any combination of the molecular ions/elemental ions; **Neutral by definition**)

- Name of the cation (with roman numeral included, if applicable) without the word "ion"
- Followed by Name of anion without the word "ion"

e.g. NaCl is made up of Na^+ and Cl^-
or sodium ion and chloride ion

called: **Sodium chloride**

e.g. $CrCl_3$ is made up of:

the "Cl" must be Cl^- (no choice for the anion!)

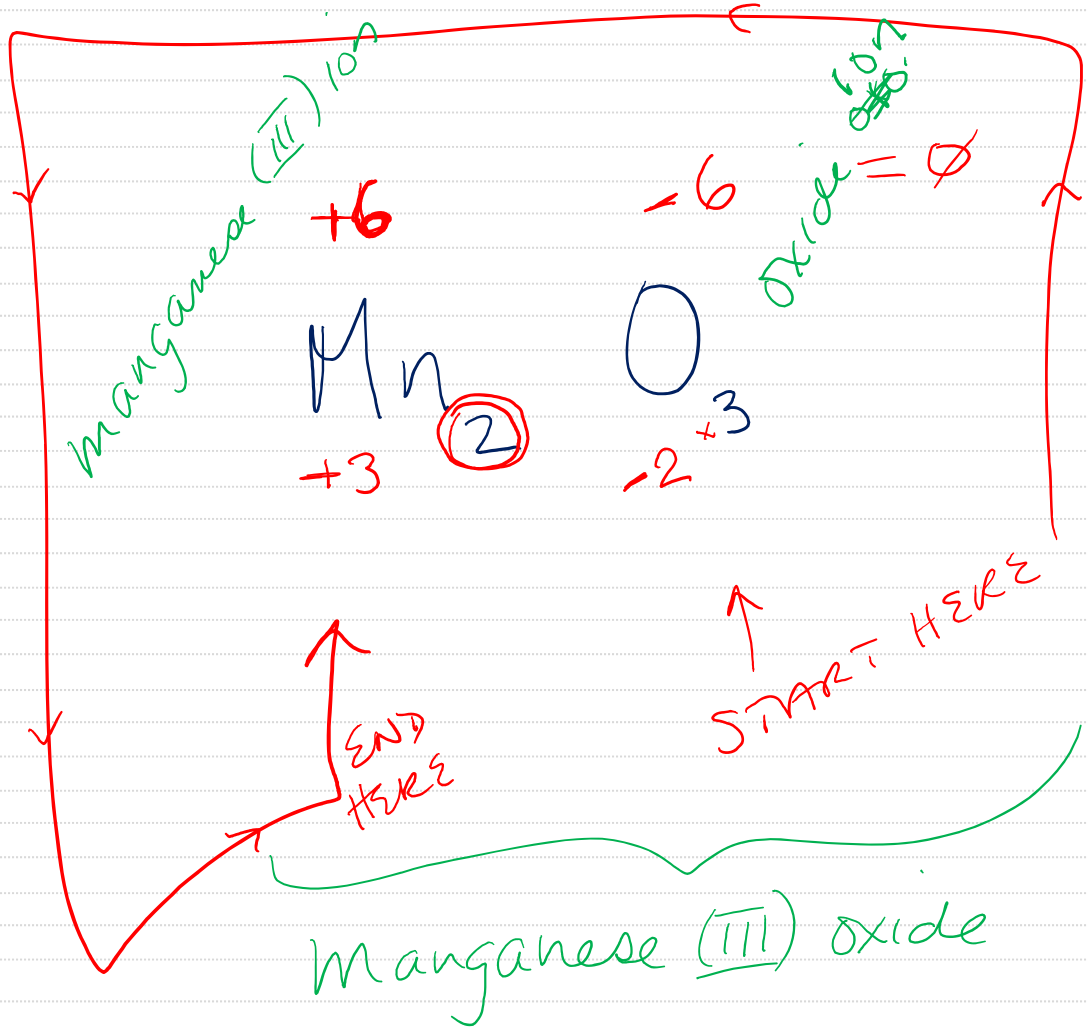
therefore, to give a neutral compound, and "balance"

the 3 Cl^- , the "Cr" must be Cr^{3+}.

The ions are therefore: Chromium (III) ion and Chloride ion

called: **Chromium (III) chloride**

e.g. Mn_2O_3 Name?



e.g. $Cu_3(PO_4)_2$

Copper (II) phosphate.

BINARY COVALENT COMPOUNDS: (2 non-metals)

You don't have electrical charges to dictate how many of each species may combine. Two elements may combine in ***several different ratios*** to form different covalent compounds.

The *words* used for the elements are the same as they were for ionic cpds :

- The less electronegative element is named first, using its element name
- The more electronegative is named second, with the last (or last 2) syllables replaced by "ide"

Prefixes are used to indicate how many of each element is used:

Mono/mon	1
di	2
tri	3
tetra/tetr	4
penta /pent	5
hexa/hex	6
hepta /hept	7
octa/oct	8
nona/non	9
deca/dec	10

Note: if only one of the less electronegative element (i.e. the first) is present, the prefix "mono" is left out. It is never left out for the more electronegative (second) however.

CO : Carbon monoxide (NOT monocarbon monoxide)

CO_2 : Carbon dioxide NOT carbon oxide e.g.

N_2O_5 : <u>di</u>nitrogen <u>pent</u>oxide

N_2O_4 : <u>di</u>nitrogen <u>tetr</u>oxide

N_2O : <u>di</u>nitrogen <u>mon</u>oxide (**not** dinitrogen oxide)

CO_2 : carbon <u>di</u>oxide (**not** monocarbon dioxide!)

THE MOLECULE: LEWIS STRUCTURES

A moderately reliable way of predicting the bonding and bond orders of atoms in a molecule.

It is based on observation.

It is not a theory – it isn't trying to explain anything

It is a model – within certain constraints, it makes accurate predictions

- It does not work well on ions or molecules with an odd number of electrons (radicals)
- It does not predict the magnetic properties of ions or molecules

THE MOLECULE: LEWIS STRUCTURES

"RECIPE"

1. Count the number of valence electrons on each atom.
    - Add 1 for each negative (-) charge
    - Subtract 1 for each positive (+) charge
2. Build the skeleton: Put the least electronegative element in the centre (never H in centre!)
    - If "acid", group all O and H into -O-H groups
    - If organic, you may have -CH2- groups or -CH3 groups & chains
    - Link each atom (or group, as above) directly to the central atom with 1 link, or single bond (S.B.)
3. Count the number of electrons used in the skeleton (2 for each bond)
    - Subtract this from the number of valence electrons counted in step 1 to get the number left over.
4. Use leftover electrons in step 3. To try to complete all octets (ie fill the valence s and p orbitals) (NB. H only gets a total of 2 (NOT 8!) therefore it is satisfied with 1 single bond.)

There are now 3 possible outcomes:

O. <u>EXACTLY ENOUGH ELECTRONS</u>

Stop! (for now)

I. NOT ENOUGH ELECTRONS TO COMPLETE THE OCTETS:

"do what?"

- You need 1 double bond (DB) for each 1 pair (2 electrons) missing
- OR You need 1 triple bond (TB) for each 2 pair (4 electrons) missing

"do it where?"

- O atoms often form DB's
- C atoms often form DB's, quite often form TB's
- N atoms often form TB's, quite often form DB's
- NEVER to a H atom
- Rarely to a halogen, Never to F atom
- Never have more than 4 bonds on a second row (Li ...Ne) atom

"do it how?"

- GO RIGHT BACK TO THE SKELETON!!!!
- Redraw skeleton with DB's/TB's as necessary
- Recalculate leftover electrons and re-do steps 3 and 4

II. YOU HAVE ELECTRONS LEFT OVER:

"expand the octet" of the central atom (as long as it is in row 3 or lower on the per. Table)

ie. Place the extra electrons, *in pairs*, on the *central atom*.

CORRECTING FOR FORMAL CHARGE

An atom, even in a molecule, has a "memory" of its original valence, and wants to maintain it.

1. Count the number of electrons "formally" assigned to each atom:
count all electrons in lone pairs

count 1 for each chemical bond touching the atom
2. Compare this against the original valence to get formal change, FC.
F.C. = {group #} - {(# lone electrons)+(# bonds)}

3. If, and only if:
The central atom is in row 3 or below on the periodic table
and
there are both **+** and **-** formal chages present in the molecule

MOVE A LONE PAIR OF ELECTRONS OFF THE ELEMENT WITH THE NEGATIVE FORMAL CHARGE AND INTO THE BOND JOINING IT TO THE ELEMENT WITH THE POSITIVE FORMAL CHARGE.

The net effect is that the formal charge that was negative goes up by one (eg. from -1 to 0, or from -3 to -2) and the formal charge that was positive goes down by one (eg from +3 to +2, or from +1 to 0)

WHEN THERE ARE NO LONGER **BOTH** POSITIVE AND NEGATIVE FORMAL CHARGES PRESENT, YOU **STOP** ADJUSTING THE MOLECULE.

RESONANCE

When a Lewis structure has fewer multiple bonds than there were **equivalent** positions where you could have placed the multiple bond(s) THE MULTIPLE BONDS ARE SHARED AMONG THE EQUIVALENT POSITIONS.

Draw enough "resonance structures" to show every possible position having every possible bond order. You do not need to show "permutations and combinations".

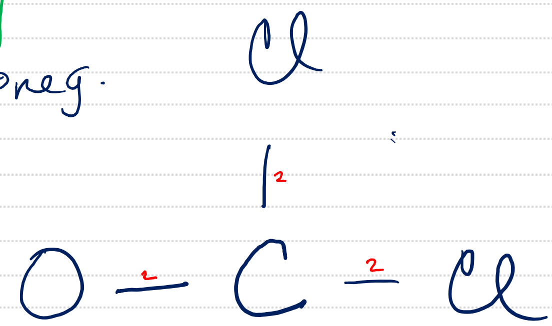
For example, it only takes two resonance structures to show that SO_4^{2-} has two double bonds, shared among 4 equivalent S to O bonds.

e.g. Cl_2CO Carbonyl dichloride

① Valence:

$2 * Cl : 2(7) = 14$
$1 * C : 1(4) = 4$
$1 * O : 1(6) = 6$ / 24 valence e^-

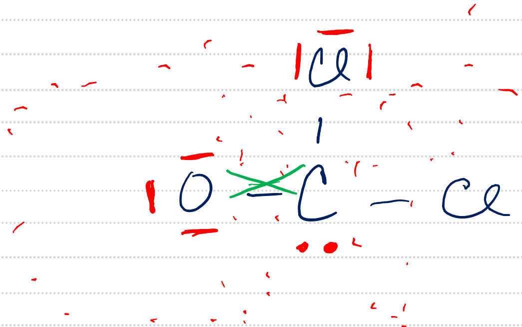
② least e^- neg.



skeleton

③ 24 valence
− 6 bonding / 18 left to use in completing octets.

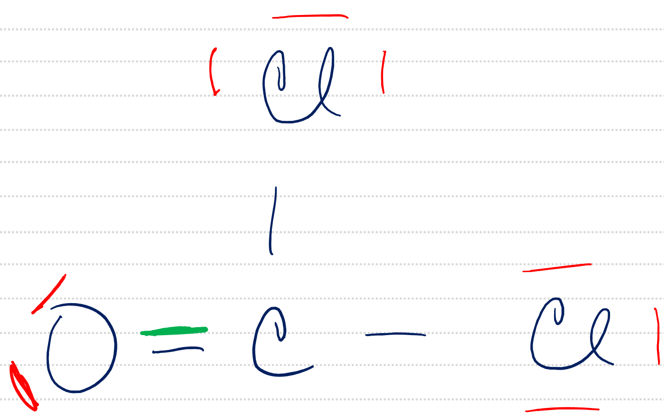
OCTETS ARE ABOUT SHARING



C : 2 − 2 / 18 16
− 6 (O)
10
− 6 Cl
4

Want? 6 more
have 4 more

MISSING ($2e^-$) 1 PAIR



new skeleton

24 valence

− 8 e^- in skeleton

16 left for:

− 0 (C)

− 4 (O)

12 − 12 = ∅ ✓

all octets (at least) complete

all e^-'s used.

STOP - for now

later - check for formal charge (none here)

check for resonance (none here)

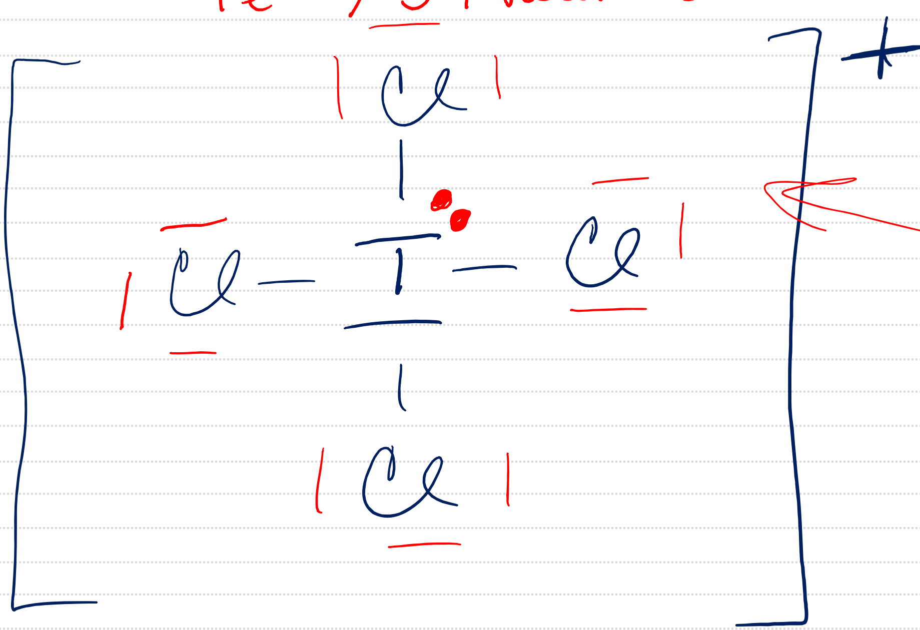
e.g. ICl_4^+ :

① I : 7

Cl : 4 × 7 = 28 (35)

+1   − 1 e⁻ / 34 valence e⁻

② :



③ 34 valence

− 8 e⁻ in skeleton

26 left.

− 24 e⁻ lone pairs

2 e⁻ LEFT OVER!

on central

CORRECTING FOR FORMAL CHARGE

An atom, even in a molecule, has a "memory" of its original valence, and wants to maintain it.

1. Count the number of electrons "formally" assigned to each atom:

- count all electrons in lone pairs

- count 1 for each chemical bond touching the atom

2. Compare this against the original valence to get formal change, FC.

F.C. = {group #} - {(# lone electrons)+(# bonds)}

3. If, and only if:

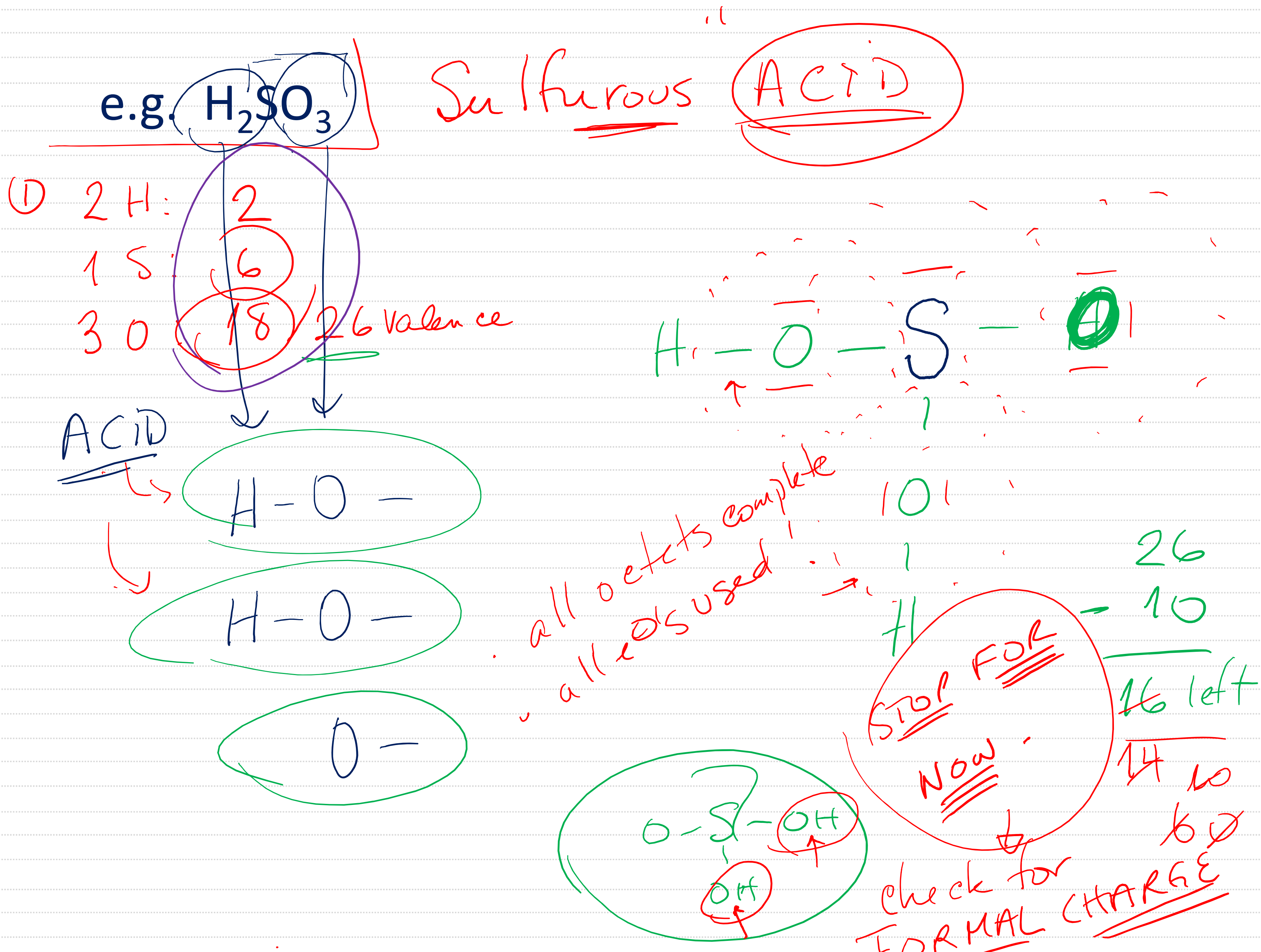
The central atom is in row 3 or below on the periodic table

and

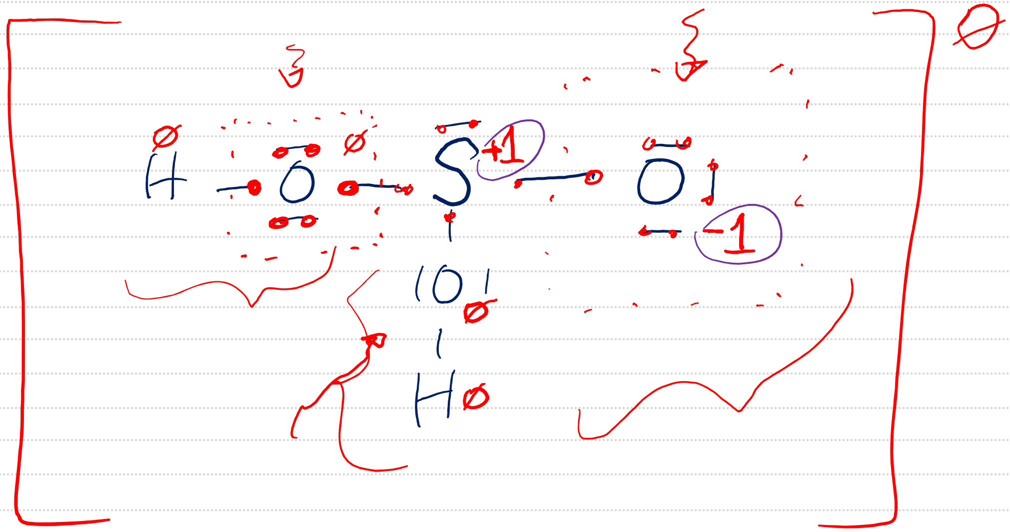
there are both **+** and **-** formal chages present in the molecule

MOVE A LONE PAIR OF ELECTRONS OFF THE ELEMENT WITH THE NEGATIVE FORMAL CHARGE AND INTO THE BOND JOINING IT TO THE ELEMENT WITH THE POSITIVE FORMAL CHARGE.

e.g. H_2SO_3


Sulfurous ACID
2 H: 2
1 S: 6
3 O: 18
26 valence
ACID
all octets complete
all e⁻s used
26
10
16 left
14
10
6
STOP FOR NOW
check for FORMAL CHARGE

e.g. H_2SO_3



F.C. (H): $1 - \{0 + 1\} = 0$

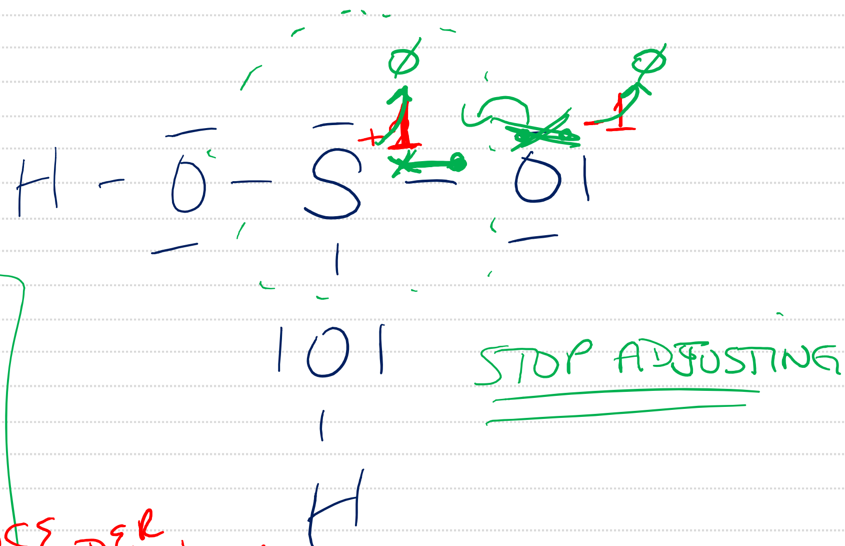
F.C. (−O−): $6 - \{4 + 2\} = 0$

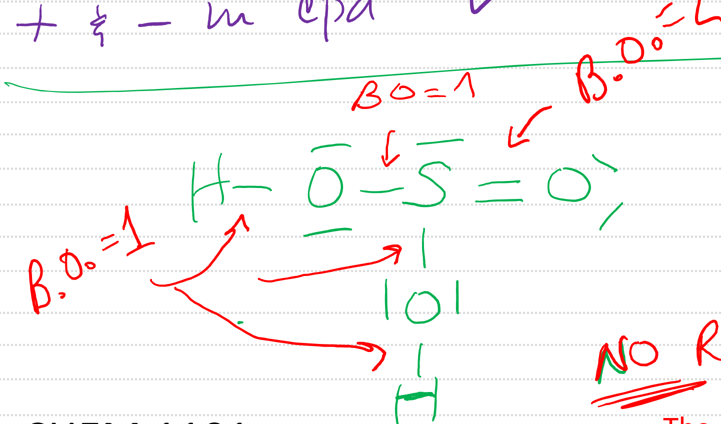
F.C. (−O|): $6 - \{6 + 1\} = -1$

F.C. (−S−): $6 - \{2 + 3\} = +1$

Central row 3 or lower ✓

+ & − in cpd ✓





NO RESONANCE

BOND ORDER GIVEN BY # lines.

e.g. SO_4^{2-}

S : 6

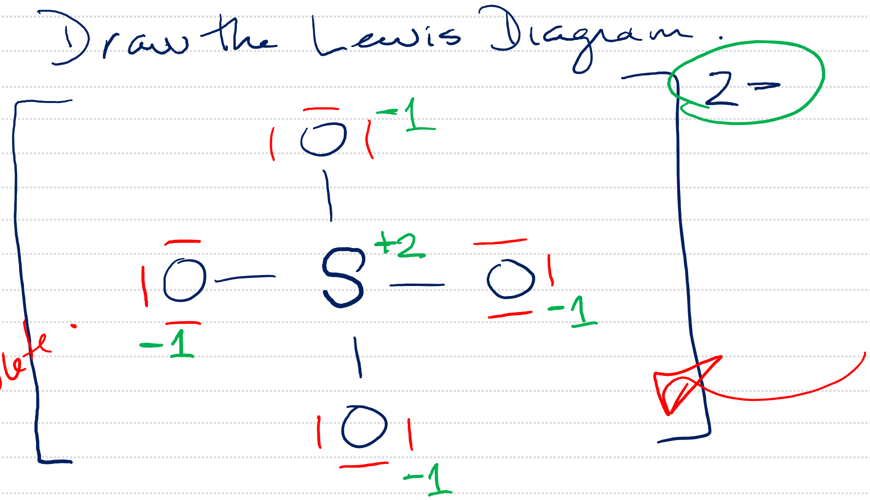
4 x O : 24

2− : 2 / 32.

−8

24

Draw the Lewis Diagram.

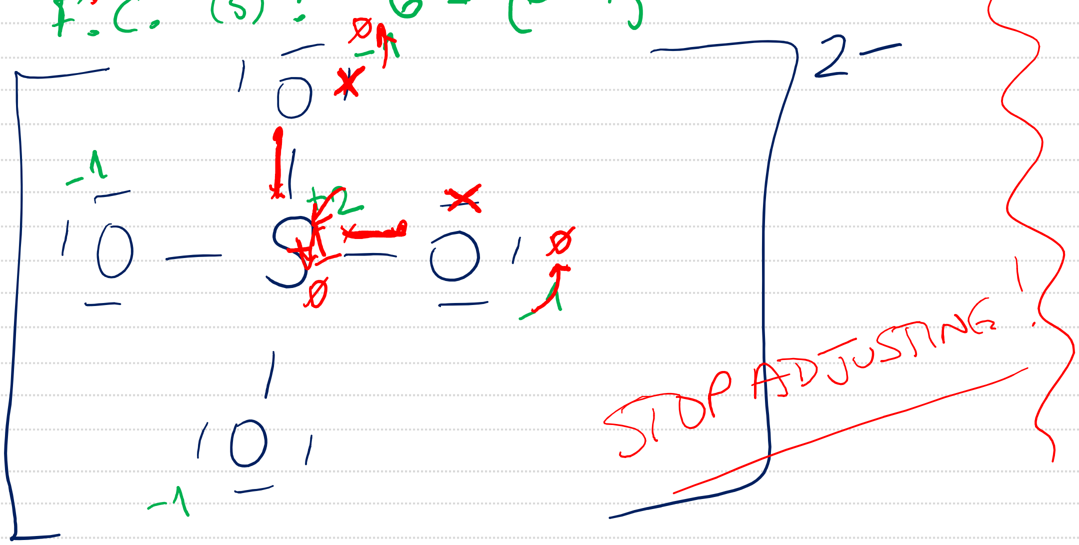


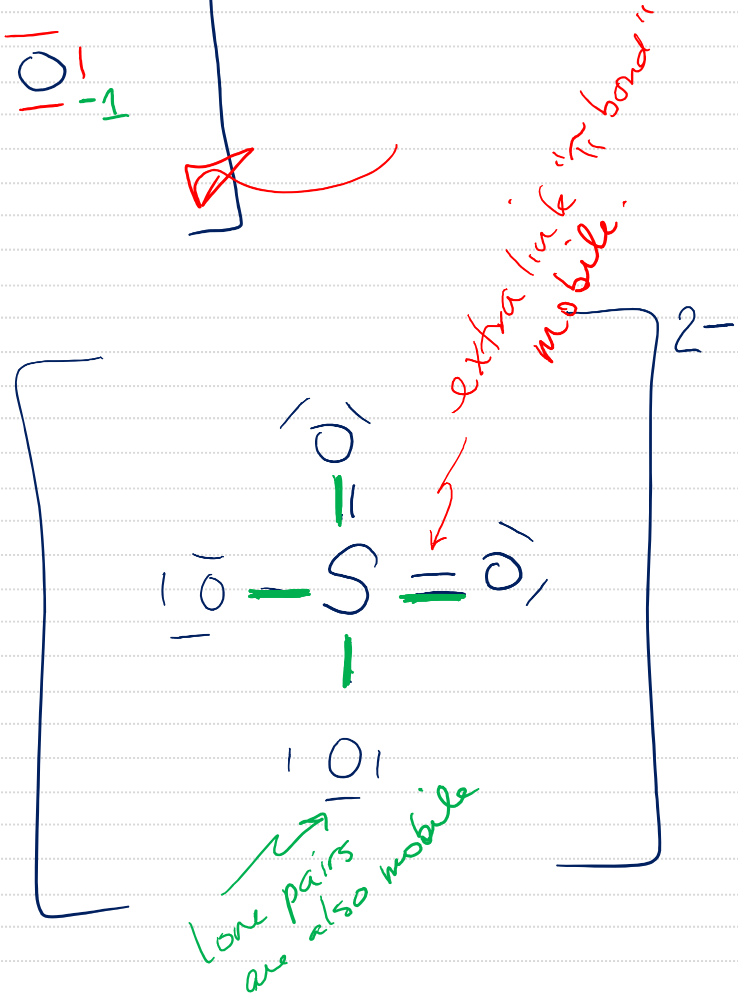
all e used

all octets complete.

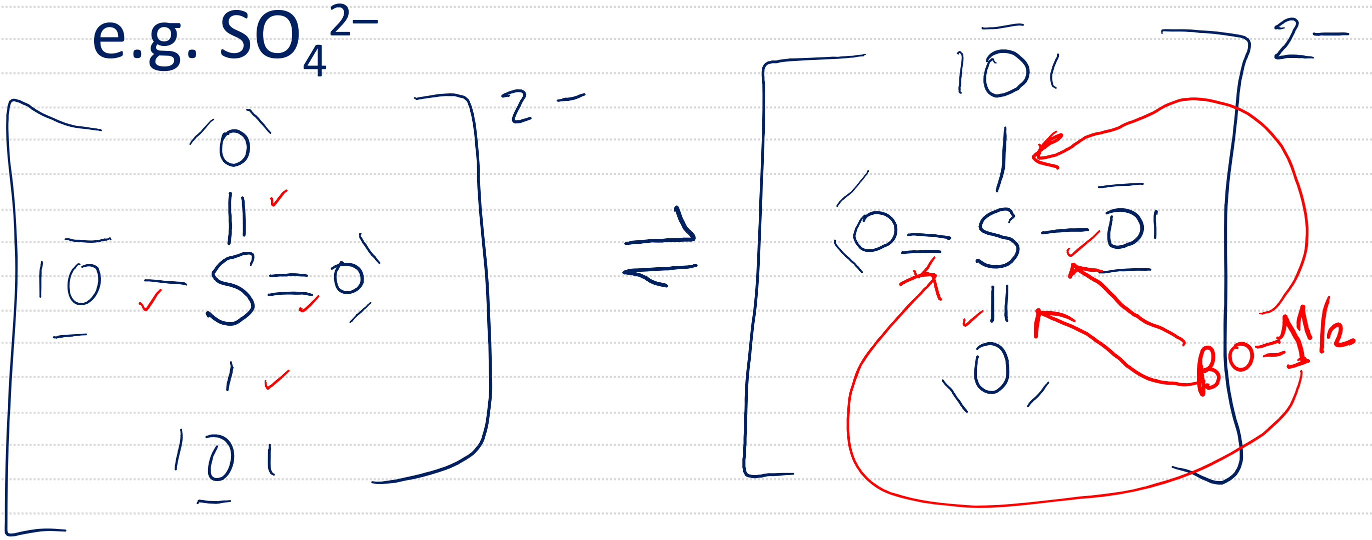
F.C. $\overline{O}$— : $6 - \{6 + 1\} = -1$

F.C. (S) : $6 - \{0 + 4\} = +2$





e.g. SO_4^{2-}



Bond order: single? B.O. = 1

fractional { double? B.O. = 2

triple : BO = 3

BOND ORDER AVERAGED

• B.O. : $\frac{\text{\# total chemical bonds}}{\text{\# positions in resonance}}$

count one structure.

$= \frac{6}{4} = 3/2$ or 1.5 or 1½ each

RESONANCE

When a Lewis structure has fewer multiple bonds than there were **equivalent** positions where you could have placed the multiple bond(s) THE MULTIPLE BONDS ARE SHARED AMONG THE EQUIVALENT POSITIONS.

Draw enough "resonance structures" to show every possible position having every possible bond order. You do not need to show "permutations and combinations".

For example, it only takes two resonance structures to show that SO_4^{2-} has two double bonds, shared among 4 equivalent S to O bonds.

Valence Shell Electron Pair Repulsion: VSEPR

All the electrons in one individual chemical bond (2 in a single bond, 4 in a double bond, 6 in a triple bond) have to stay in the same region of space. Each of these is a "bonding region".

Lone pair electrons and bonding electrons are each confined to their own "region of electron density".

"Regions of electron density" want to get as far apart from each other as possible.

RECIPE: "VSEPR geometries" or "molecular geometries"

1. Draw a Lewis Diagram

2. On the ***central atom***, count the number of regions of electron density

   - 1 for each lone pair (or, if an odd number of electrons, 1 for the lone electron)
   - 1 for each triple bond
   - 1 for each double bond
   - 1 for each single bond

RECIPE: "VSEPR geometries" or "molecular geometries"

3. Assign the "ideal shape" on which to base the geometry:
   - 2 regions: LINEAR
   - 3 regions: TRIANGULAR
   - 4 regions: TETRAHEDRAL
   - 5 regions: TRIGONAL BIPYRAMEDAL
   - 6 regions: OCTAHEDRAL

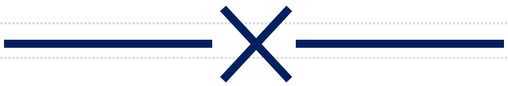
4. Position the lone pairs (or, if applicable, the lone electron)

5. Position the bonds and the outer atoms

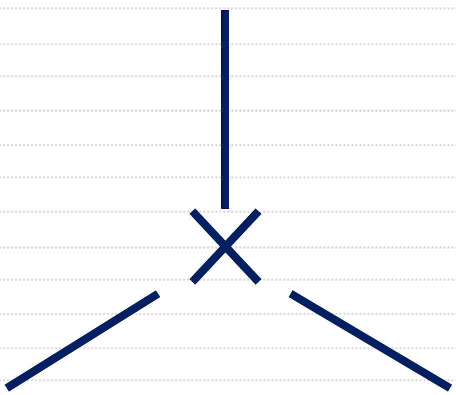
6. "Collapse" down the lone pairs (these dictate the shape, but are not part of the naming process)

7. Name and draw the resulting shape

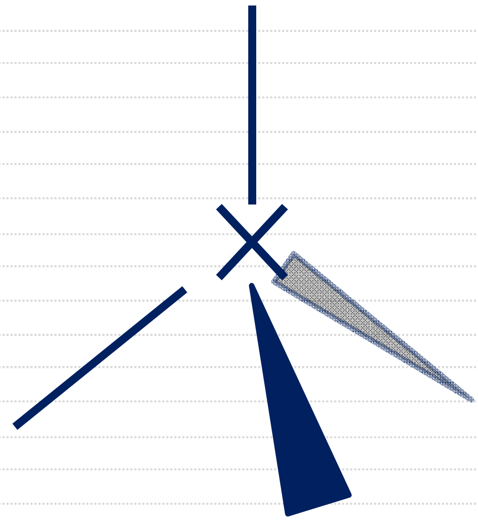
2 regions: linear

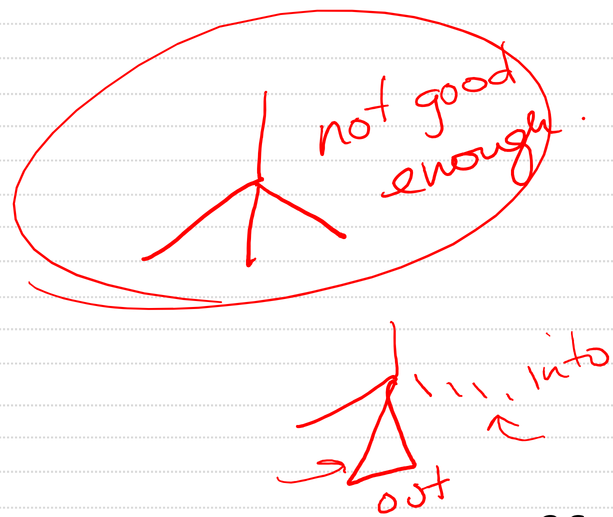


3 regions: triangular

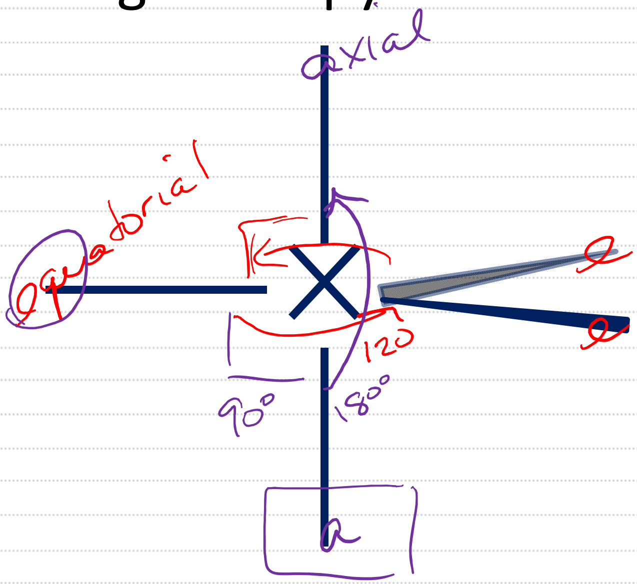


4 regions: tetrahedral

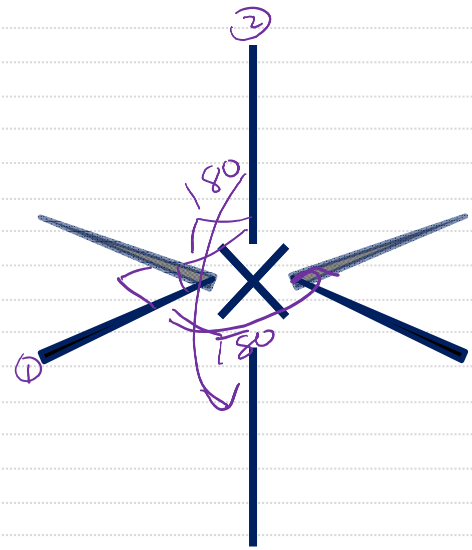




5 regions:
trigonal bipyramedal



6 regions: octahedral



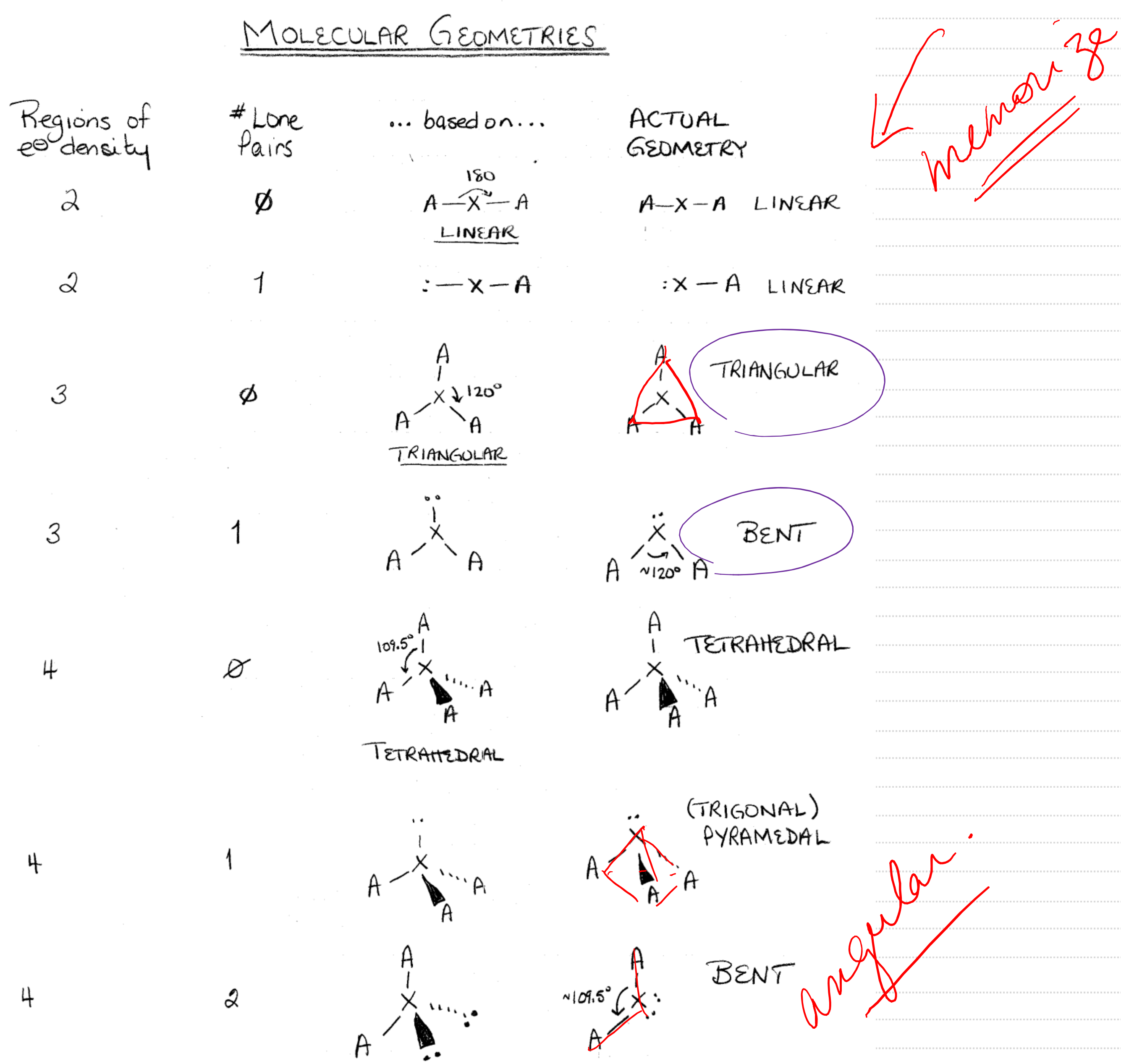
roomier? a?

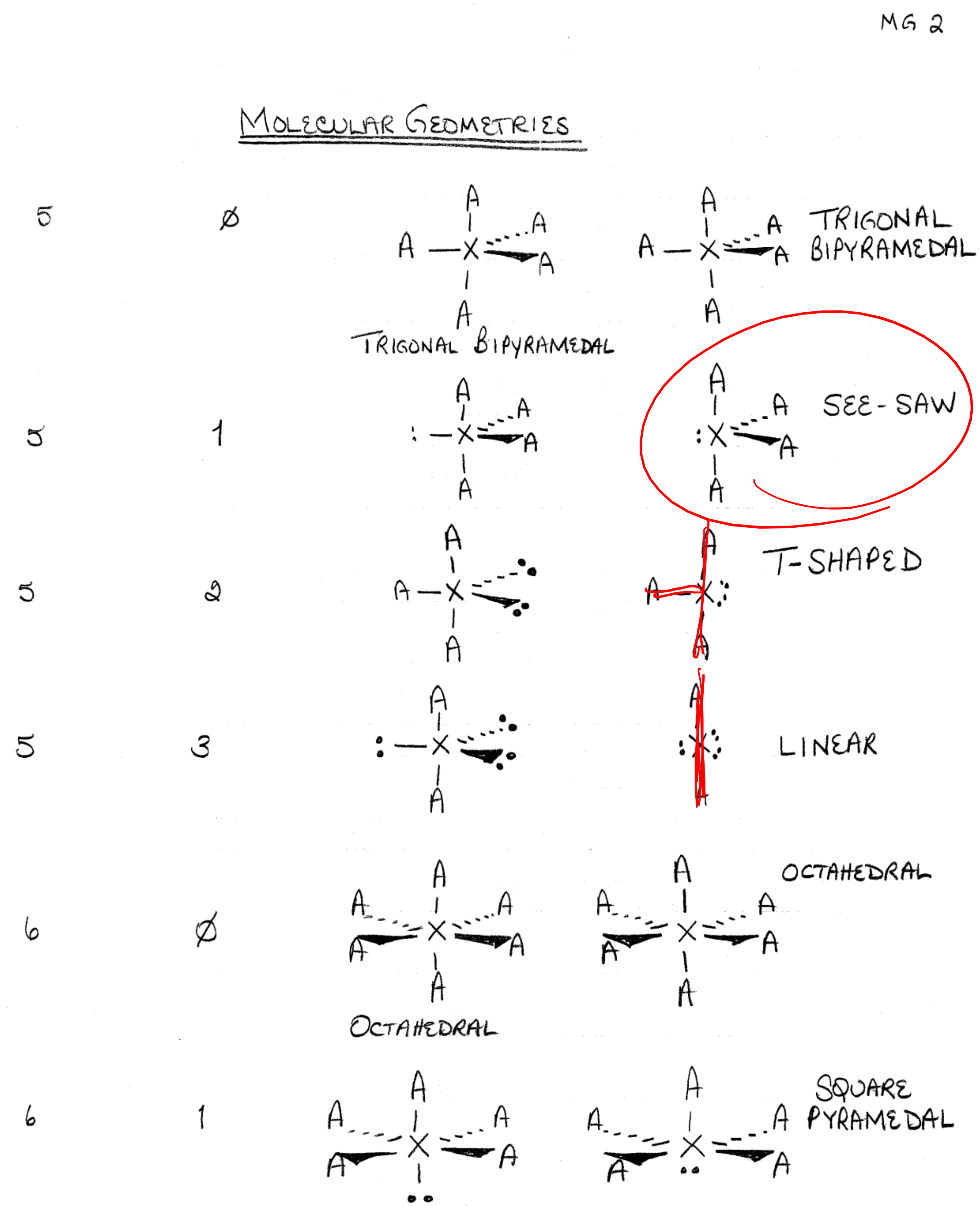
e?

more space!!

All the possible geometries up to six regions.

Reason them out rather than memorizing them!

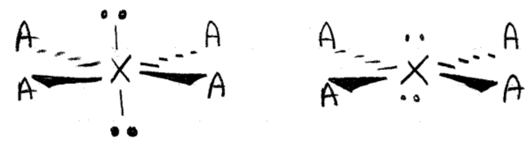




NOTE: lone pairs are always axial on the trigonal bipyramid

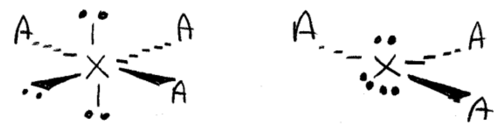
MOLECULAR GEOMETRIES

6 2



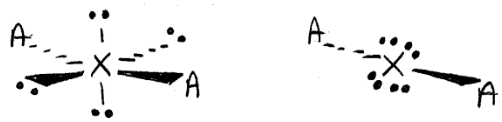
SQUARE PLANAR

6 3



T-SHAPED

6 4

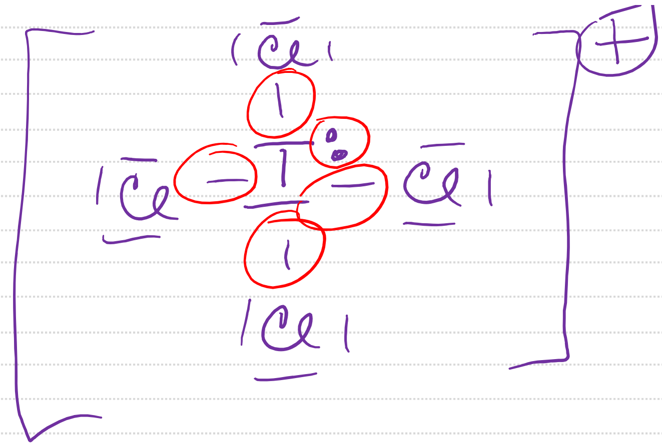


LINEAR

NOTE: Any time you have only 1 bonding region, the molecule is linear!

ie	2	regions	1	lone	pair	⇒ 1	bonding	region	- linear
	3	"	2	"	"	⇒ 1	"	"	"
	4	"	3	"	"	⇒ 1	"	"	"
	5	"	4	"	"	⇒ 1	"	"	"
	6	"	5	"	"	⇒ 1	"	"	"

Remember ICl_4^+



1. Draw a Lewis Diagram

2. On the ***central atom***, count the number of regions of electron density

   L.P.: 1
   T.B.: 0
   D.B.: 0
   S.B.: 4

   5 Regions

3. Assign the "ideal shape" on which to base the geometry:

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- 3 regions: TRIANGULAR
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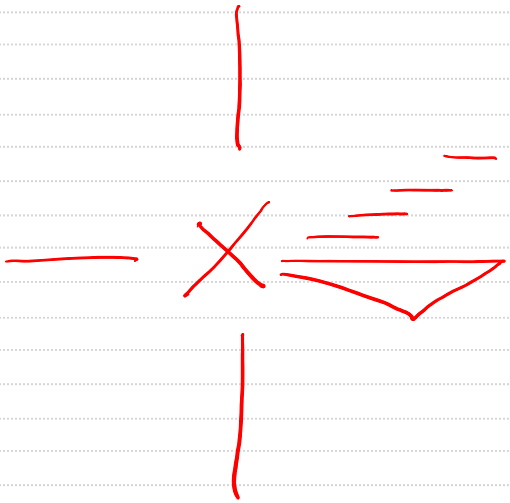
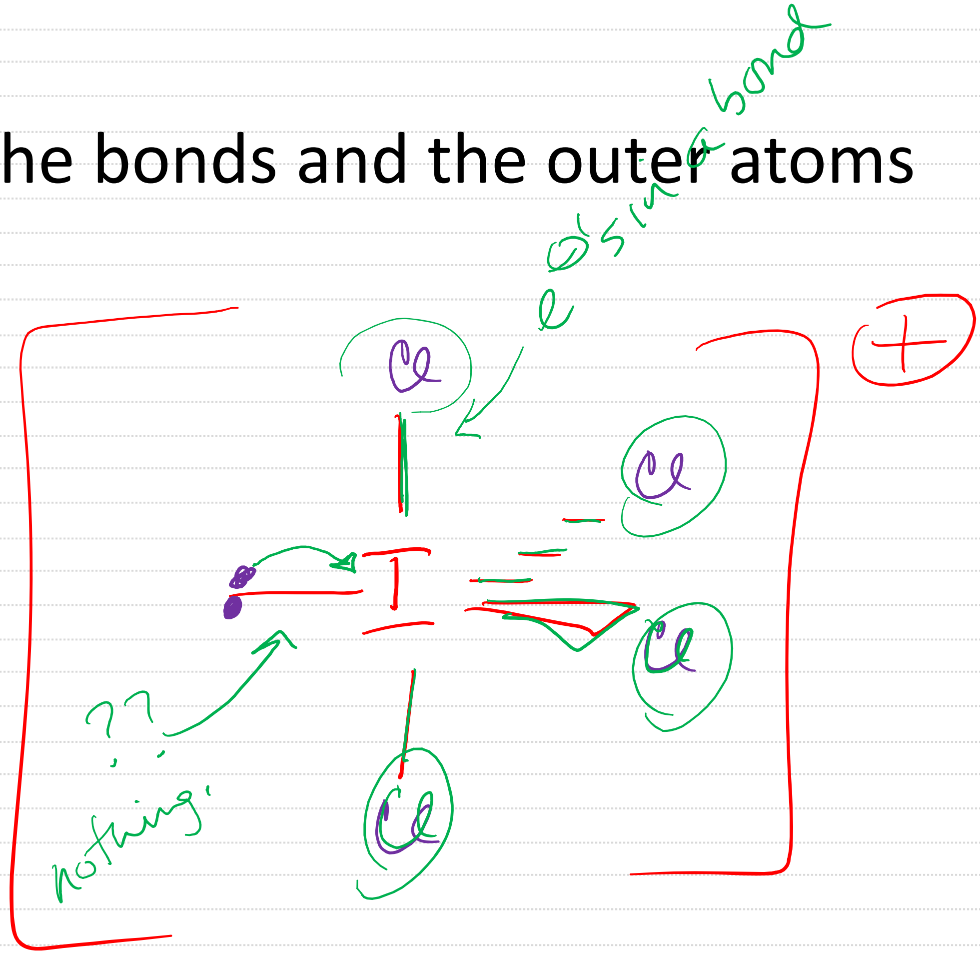


4. Position the lone pairs (or, if applicable, the lone electron)

5. Position the bonds and the outer atoms



6. "Collapse" down the lone pairs (these dictate the shape, but are not part of the naming process)

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