

How do you determine the best Lewis structure? (individual atoms in a molecule)

Formal Charge: the difference between the # of valence e^- on the free atom & the # of valence e^- assigned to the atom in the molecule.

$$\text{Formal Charge} = \left(\begin{array}{l} \# \text{ valence } e^- \\ \text{in free atom} \end{array} \right) - \left(\begin{array}{l} \# \text{ valence } e^- \text{ assigned} \\ \text{to the atom in the} \\ \text{molecule} \end{array} \right)$$

Assigning valence e^- in a molecule:

- 1) lone pairs on an atom belong to the atom
- 2) shared (bonded) e^- are shared equally between the two atoms involved in the bond.



$\text{H} = 0 + \frac{1}{2}(2) = 1$
 $\text{O} = 4 + \frac{1}{2}(4) = 6$

$$\# \text{ assigned } e^- = \left(\begin{array}{l} \# \text{ lone} \\ \text{pair } e^- \end{array} \right) + \frac{1}{2} \left(\begin{array}{l} \# \text{ shared} \\ e^- \end{array} \right)$$

Rules: The sum of the formal charges in a molecule/ion must add up to the overall charge of the molecule or ion.

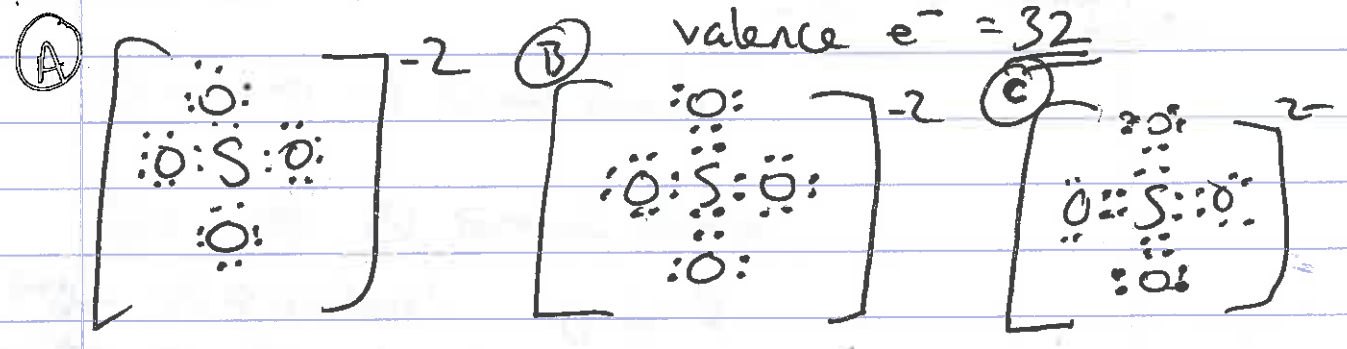
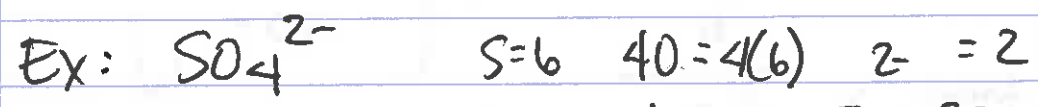
* follow these rules to determine the Best Lewis Structure(s) for a "more complex" ~~and~~ compound.

rules continued:

- if there is more than one Lewis Structure possible, the one w/ the ~~lowest~~ ^{negative formal} charges closest to zero & any negative formal charges on the more electronegative atoms is the better structure.

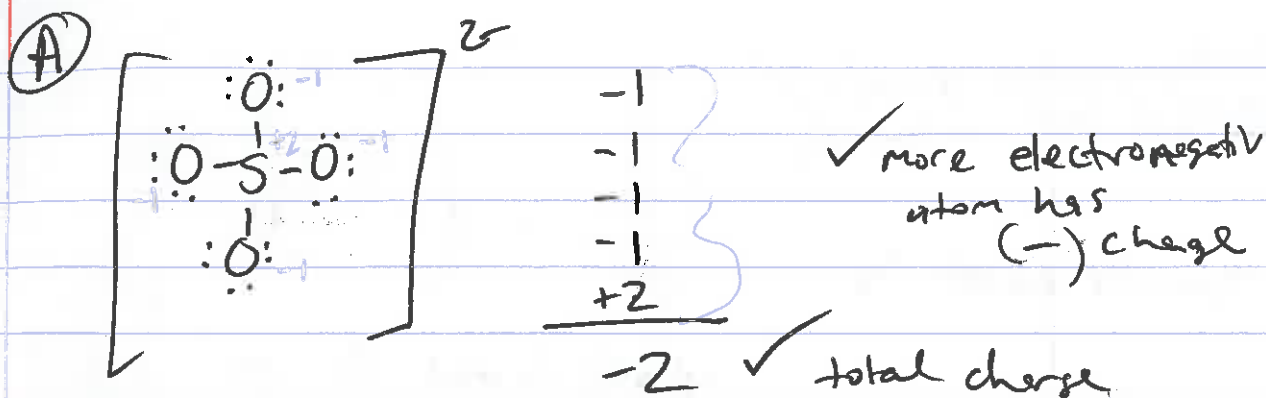
Better structures

- ① - formal charges closer to zero.
- ② - negative formal charges on more ~~etc~~ electronegative atoms.

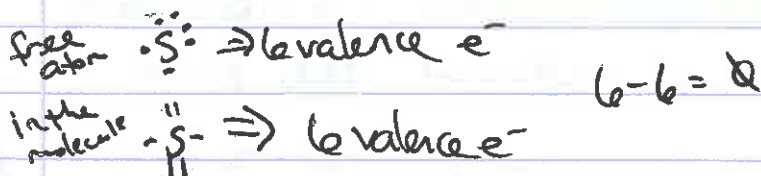
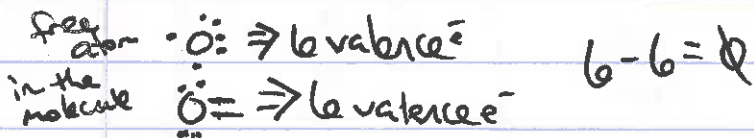
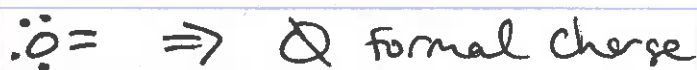
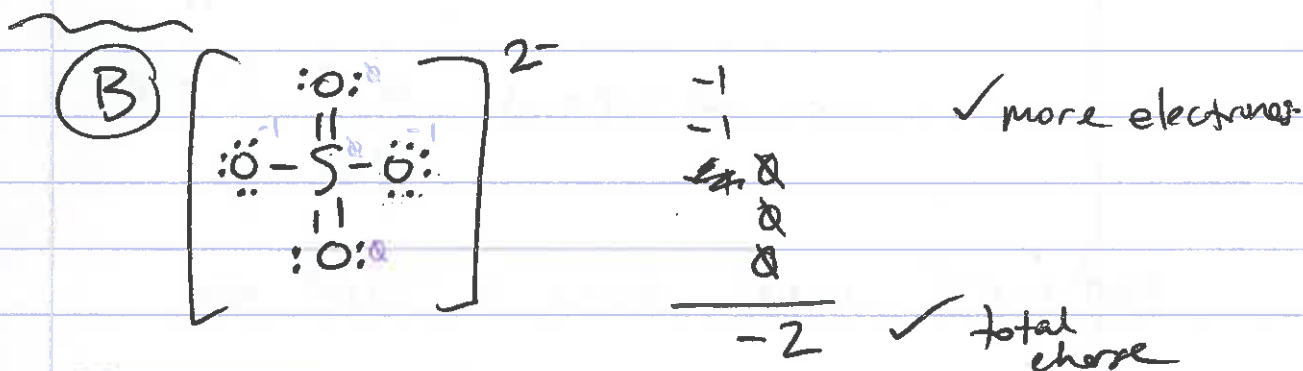


Formal Charges for A:

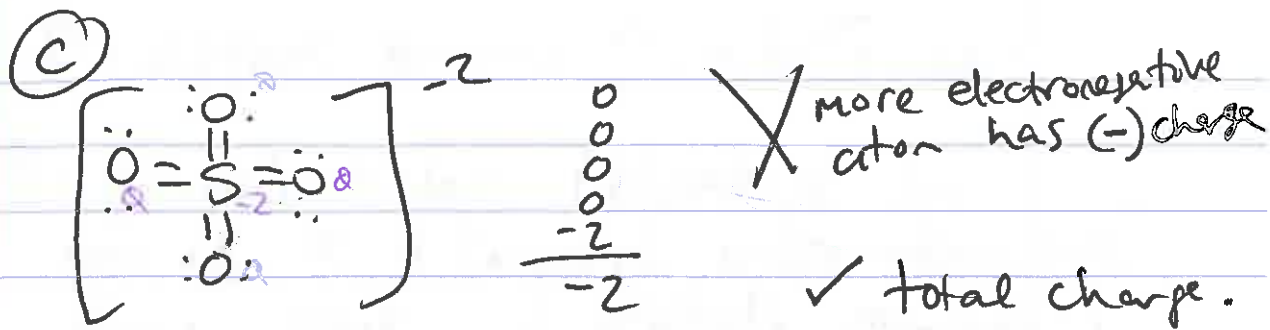
free atom	$\cdot\ddot{O}\cdot \Rightarrow 6$ valence e^-	Formal Charge $\ddot{O}- \Rightarrow 6 - 7 = -1$
in molecule	$\ddot{O}- \Rightarrow 7$ valence e^- <i>assigned</i>	
	$\ddot{S}\cdot \Rightarrow 6$ valence e^-	Formal Charge $-S- \Rightarrow 6 - 4 = +2$
	$-S- \Rightarrow 4$ valence e^- <i>assigned</i>	



★ valid Lewis dot structure.



★ Valid Lewis Dot Structure



$\ddot{\text{O}}\text{:} \Rightarrow 0$ formal charge.

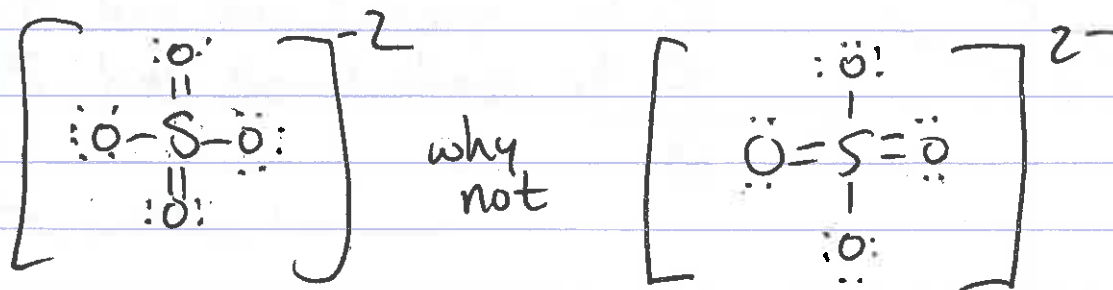
$\begin{array}{c} \text{S} \\ \text{=S=} \\ \text{=} \end{array} \Rightarrow -2$ formal charge.

free atom $\cdot\text{S}\cdot \Rightarrow 6$ $6 - 8 = -2$

$\begin{array}{c} \text{S} \\ \text{=S=} \\ \text{=} \end{array} \Rightarrow 8$

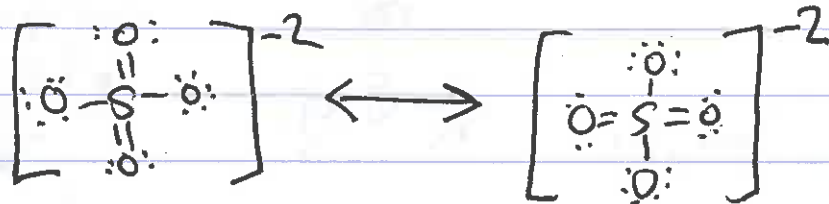
\Rightarrow Not a good Lewis Structure.

So... (B) is the Best



These Lewis structures are equivalent.

Resonance: more than one equivalent Lewis dot structure is possible.



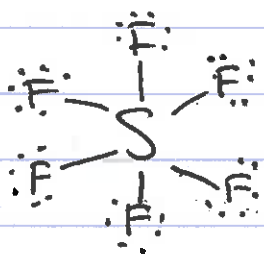
If resonance exists you must show it!

Exceptions to the Octet Rule.

Expanded Octet: (elements in period 3 & beyond only - because they have d orbitals available -)

• The central atom has more than 8 e⁻ around it.

ex: SF₆ 48 valence e⁻



bonded e⁻ = 12 e⁻

6 F: = 36 e⁻

48 e⁻ ✓

F has formal charge of 0

S has formal charge of 0

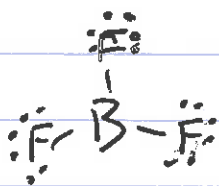
0 ✓

e⁻ deficient: some atoms will commonly form compounds where they have fewer than 8 valence e⁻.

E. Boron

BF₃

24 e⁻



24 e⁻ ✓

