

## Chapter 4.4 Lewis Structures

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Formal Charge ↗  
Octet Exceptions ↘

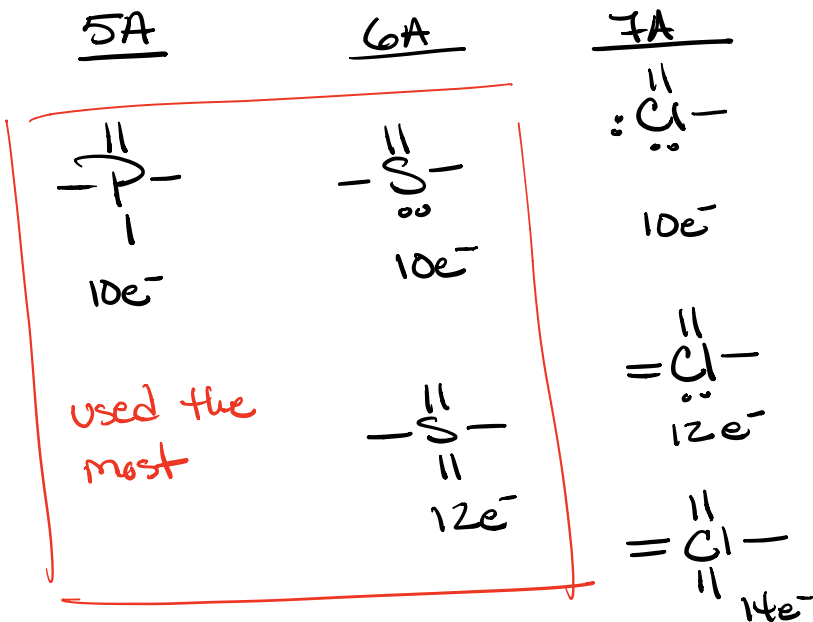
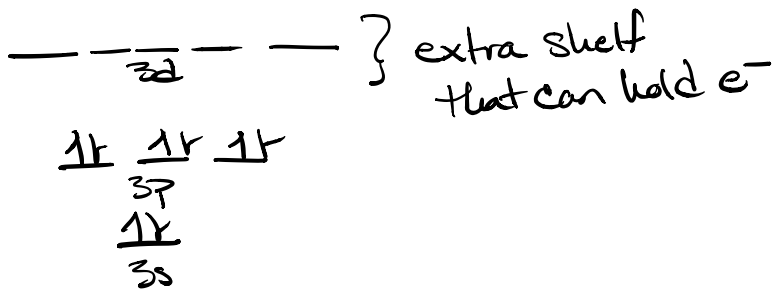
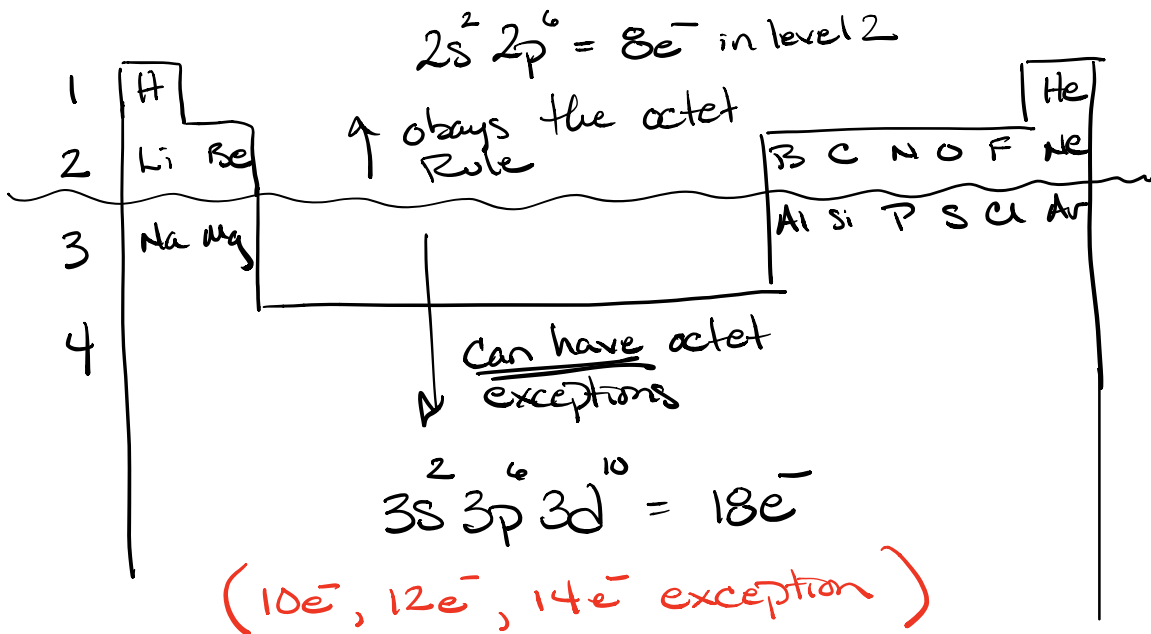
Goal is to reduce formal charges as much as possible in favor of octet exceptions.

Ions  $\Rightarrow$  always have formal charges

$\text{PO}_4^{3-}$ ,  $\text{CO}_3^{2-}$ ,  $\text{SO}_4^{2-}$   $\Rightarrow$  will always have

formal charges  $\Rightarrow$   
but should have a min.  
# of charges  $\Rightarrow$  the  
same as the charge  
state

↑ Formal Charges  
Energy  
octet exceptions for  
period 3 & below in  
periodic table

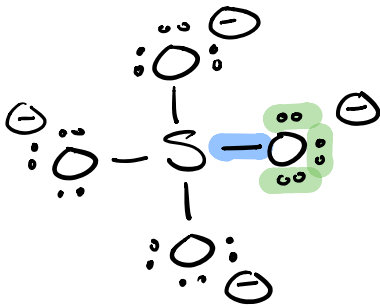




e<sup>-</sup> count  
 6A S  $1 \times 6e^- = 6e^-$   
 6A O  $4 \times 6e^- = 24e^-$   


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 $30e^-$



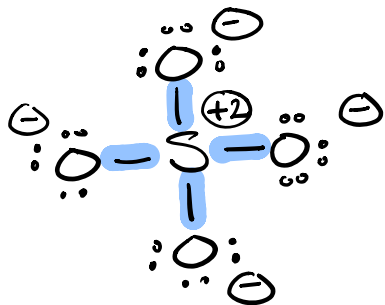
e<sup>-</sup> count  $32e^-$  ✓ → +2e<sup>-</sup>  
 $32e^-$

octet  
 oxygen ✓  
 sulfur ✓  
 formal charge

O 6A

formal charge = valence e<sup>-</sup> -  $\frac{1}{2}$ (bonding) - non bonding

=  $6 - \frac{1}{2}(2) - 6$   
 =  $6 - 1 - 6 = -1$

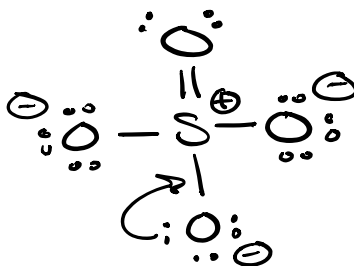
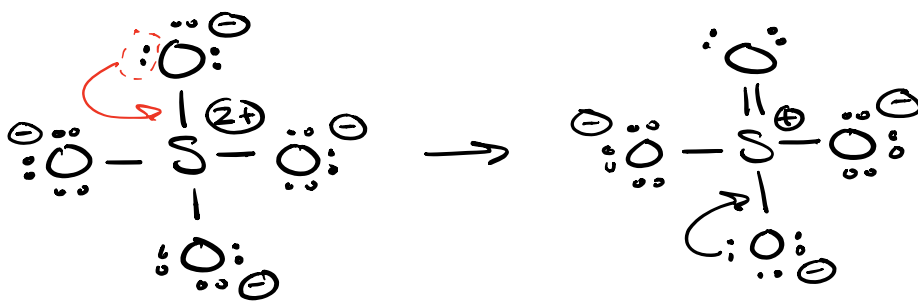


S 6A

fc =  $6 - \frac{1}{2}(8) - 0$   
 =  $6 - 4 = +2$

Too many formal charges ✗

To reduce formal charge make or break double bonds, usually take negatives & making double bond w/ positive.



Oxygen (6A)

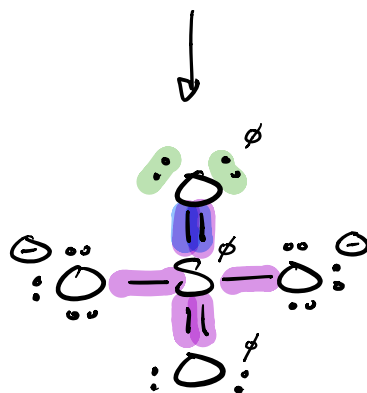
$$6 - \frac{1}{2}(4) - 4 =$$

$$6 - 2 - 4 = \emptyset$$

Sulfur (6A)

$$6 - \frac{1}{2}(12) - 0 =$$

$$6 - 6 = \emptyset$$



Best Structure

Lowest in energy

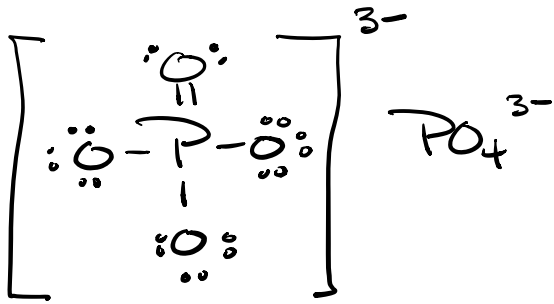
Consistent w/ experimentation



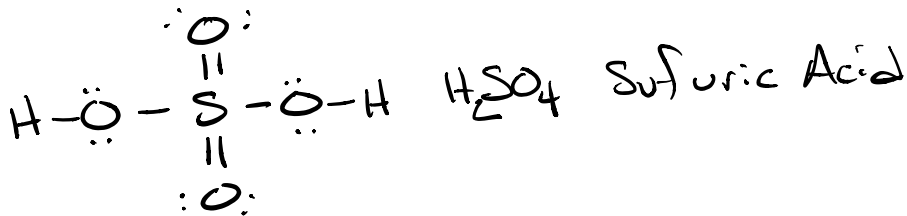
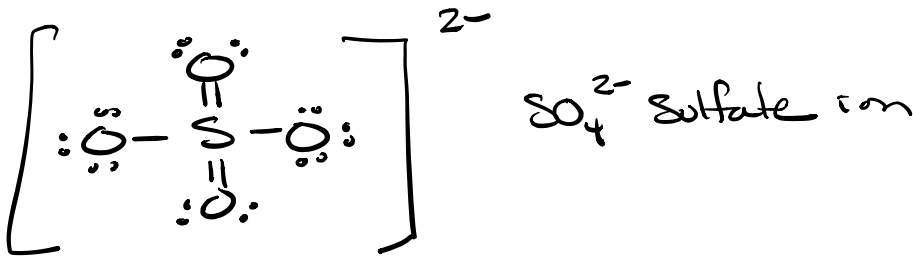
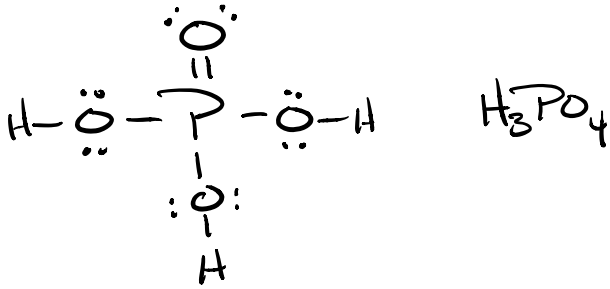
$e^-$  used  $32e^-$  ✓

octets ✓  $12e^-$  ✓

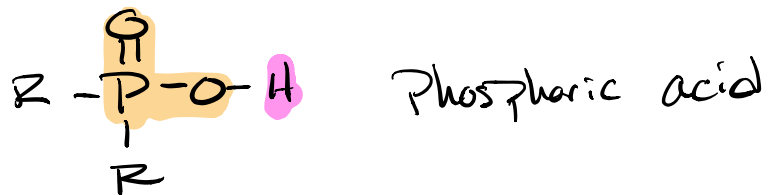
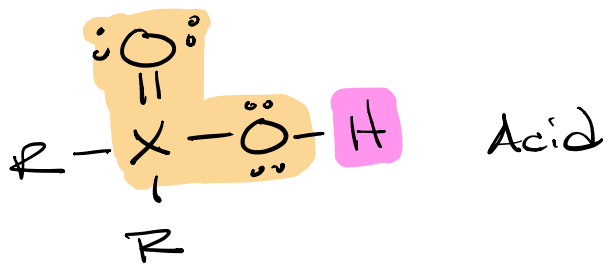
formal charge ✓



Find in  
 $\text{ATP}$ ,  $\text{DNA}$ ,  $\text{RNA}$   
 ↑  
 phosphate backbone

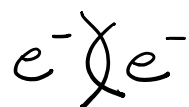


# Acid



# VSEPR Theory

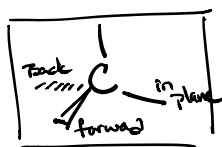
## Valence Shell Electron Pair Repulsion Theory



Valence Shell  $e^-$  pair repel on another leading to 3-D Geometry.



- ▶ wedge Coming out towards you
- |||| Hash going back away in space
- line In plane



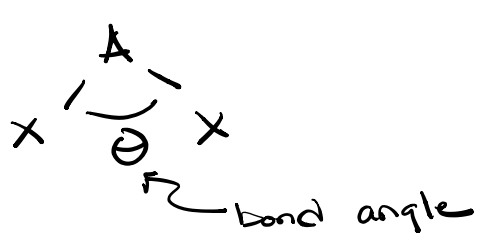
A = Central Atom

X = atom attached to Central

E = lone pair e<sup>-</sup>

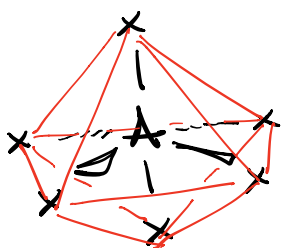
### Families of geometries

# of groups attached to Central	Possible Geometries					Chem 1A
octahedral 6	AX <sub>6</sub>	AX <sub>5</sub> E	AX <sub>4</sub> E <sub>2</sub>	AX <sub>3</sub> E <sub>3</sub>	AX <sub>2</sub> E <sub>4</sub>	↑
Trigonal bipyramid 5	AX <sub>5</sub>	AX <sub>4</sub> E	AX <sub>3</sub> E <sub>2</sub>	AX <sub>2</sub> E <sub>3</sub>		
Tetrahedral 4		AX <sub>4</sub>	AX <sub>3</sub> E	AX <sub>2</sub> E <sub>2</sub>		↓
Trigonal planar 3			AX <sub>3</sub>	AX <sub>2</sub> E		
linear 2				AX <sub>2</sub>		

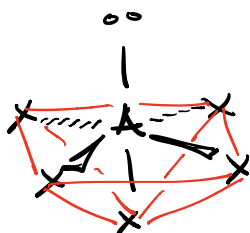




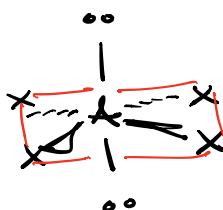
# Octahedral Family



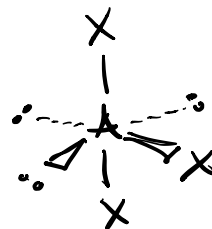
octahedral  
 $AX_6$



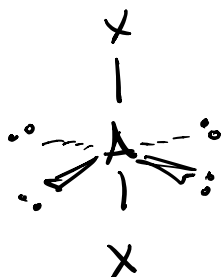
Square pyramidal  
 $AX_5E$



Square planar  
 $AX_4E_2$

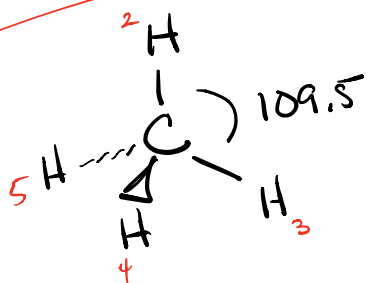


T-shaped  
 $AX_3E_3$

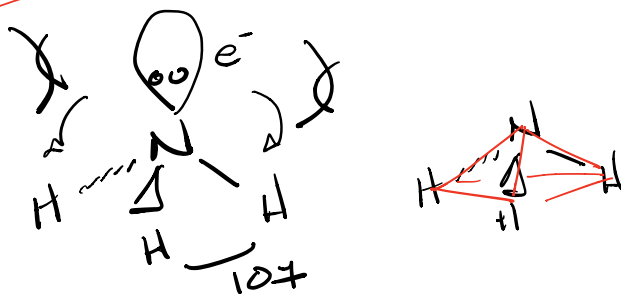


Linear  
 $AX_2E_4$

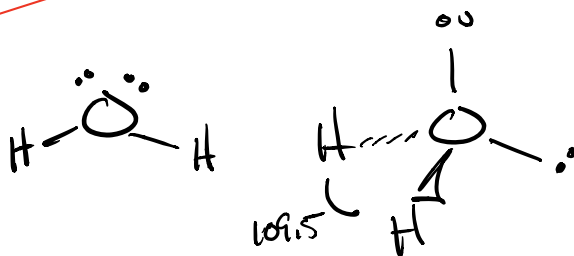
Abbreviation	Molecule	Electronic Structure <i>See e<sup>-</sup></i> "Parent"	Molecular Structure <i>e<sup>-</sup> invisible</i>	Bond Angle
<u>AX<sub>4</sub></u> 4	CH <sub>4</sub>	Tetrahedral	Tetrahedral	109.5°



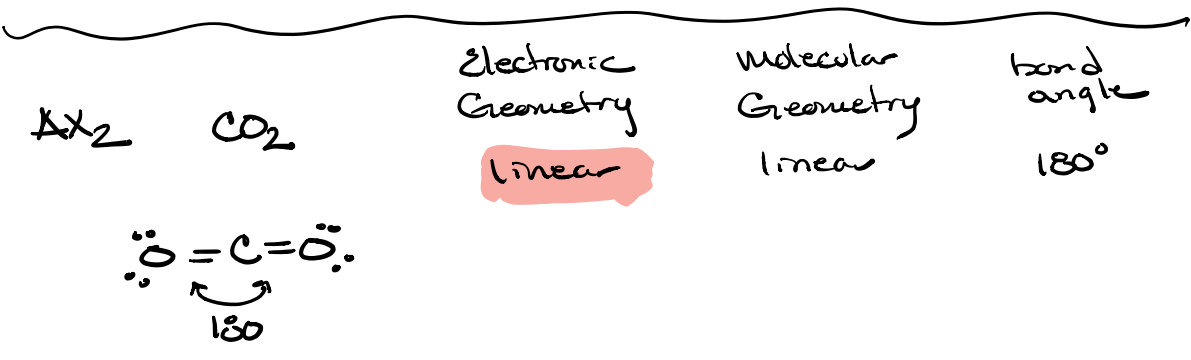
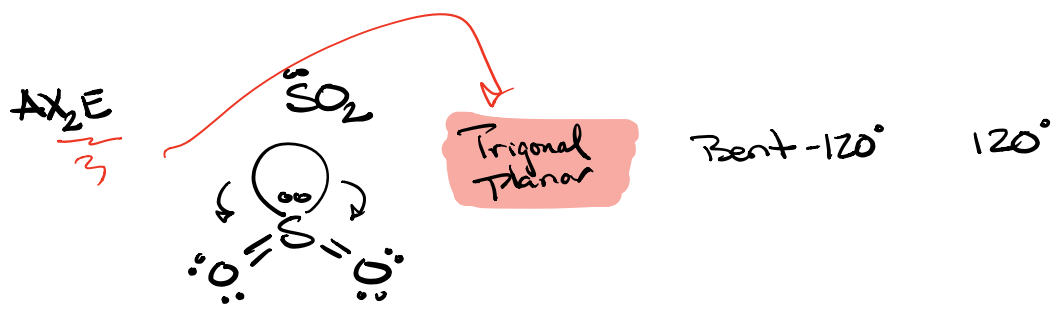
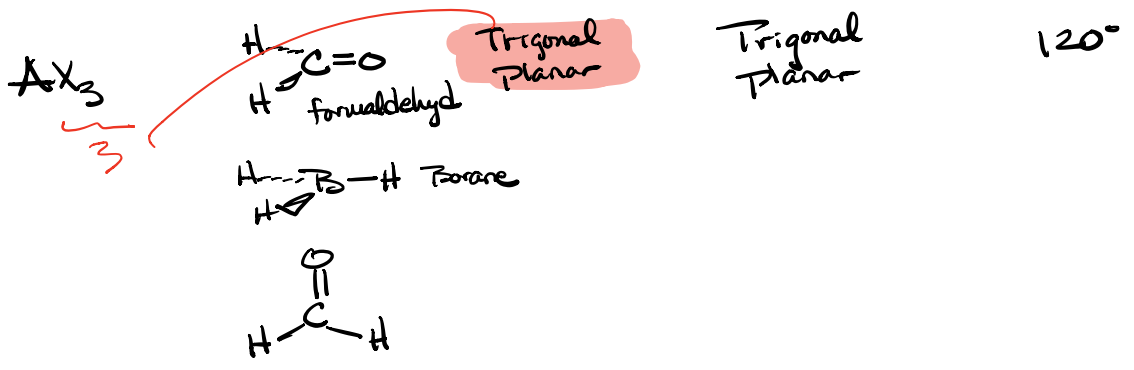
<u>AX<sub>3</sub>E</u> 4	NH <sub>3</sub>	Tetrahedral	Trigonal Pyramidal	109.5°
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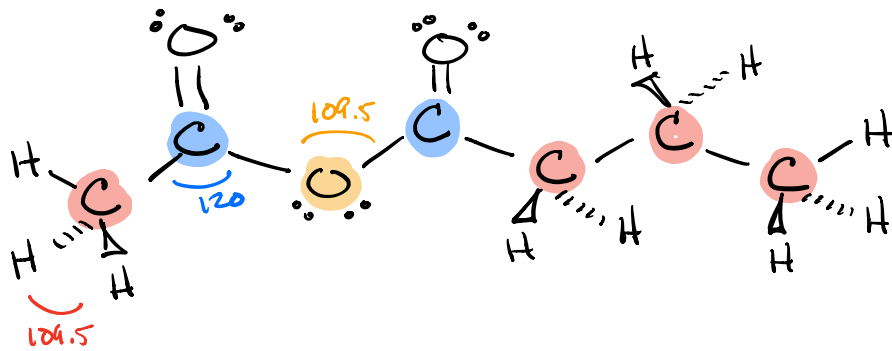
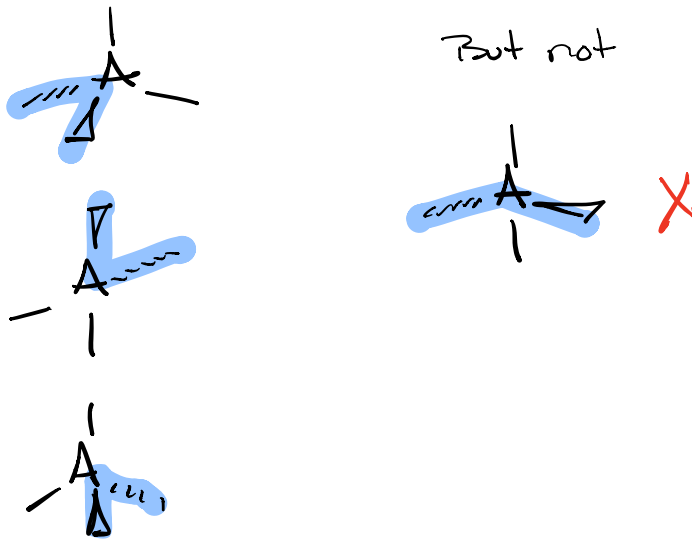


<u>AX<sub>2</sub>E<sub>2</sub></u> 4	H <sub>2</sub> O	Tetrahedral	Bent-109.5	109.5°
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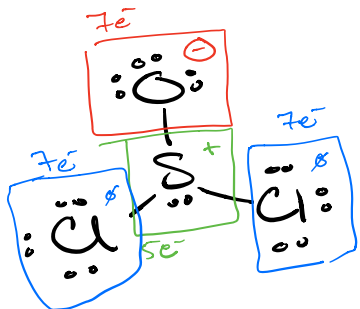
<u>Abbreviation</u>	<u>Molecule</u>	<u>Parent electronic</u>	<u>Molecular geometry</u>	<u>bond angle</u>
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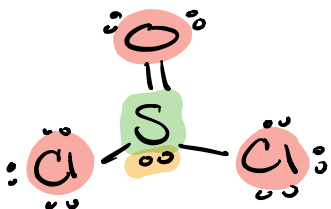
- Tetrahedral  $AX_4$
- Trigonal planar  $AX_3$
- Bent  $109.5$   $AX_2E_2$

Draw the structure of  $\underline{\text{SOCl}}_2$  and give its shape.

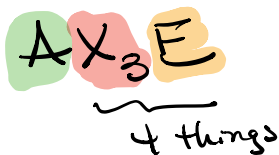


$$\begin{array}{r}
 6A \text{ S } 1 \times 6 = 6 \\
 6A \text{ O } 1 \times 6 = 6 \\
 7A \text{ Cl } 2 \times 7 = 14 \\
 \hline
 26e^-
 \end{array}$$

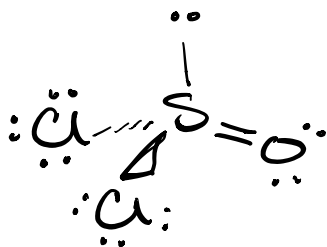
26e<sup>-</sup> ✓  
 octet ✓  
 formal charge ✗

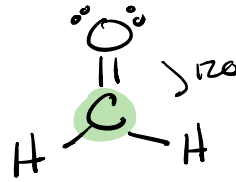
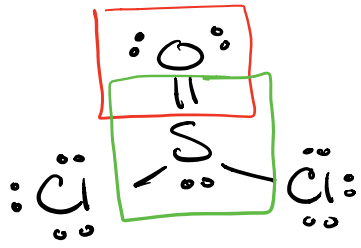


26e<sup>-</sup> ✓  
 octet ✓  
 O ✓  
 S 10e<sup>-</sup> ✓  
 Cl ✓  
 formal charge ✓



Geometry Electronic	Geometry Molecular	
Tetrahedral	Trigonal Pyramidal	109.5°





$$\begin{array}{r}
 \text{O} \quad 1 \times 6 = 6 \\
 \text{C} \quad 1 \times 4 = 4 \\
 \text{H} \quad 2 \times 1 = 2 \\
 \hline
 12
 \end{array}$$

AX<sub>3</sub>

Trigonal planar

