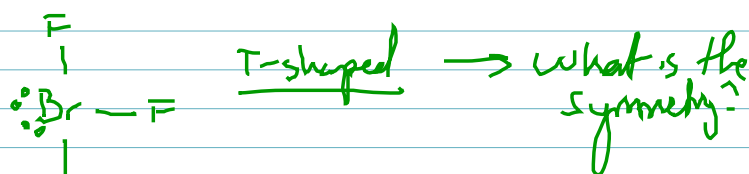
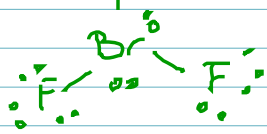
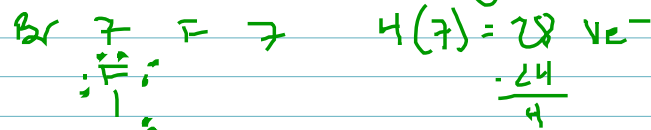


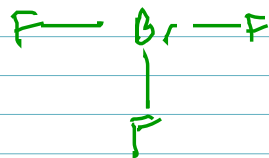
If not Roman - active modes for
bromine trifluoride

$\text{BrF}_3 \rightarrow$ Get geometry (Lewis Structure \rightarrow VSEPR)



Symmetry operations

C_{2v} C_2 E, σ, C_2



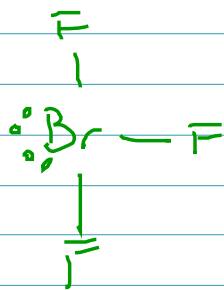
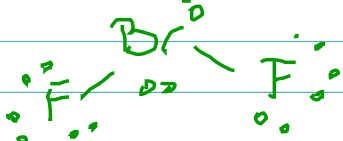
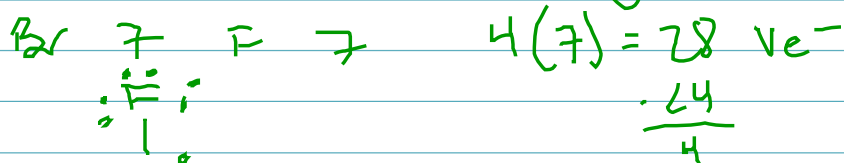
x, y, z axes on each atom and make a reducible representation (Γ) $4 \text{ atoms} \times 3 \text{ axes} = 12$

C_{2v}	E	C_2	$\sigma(xz)$	$\sigma(yz)$
Γ	12	-2	4	2

\rightarrow combine Br and 3 F
 \rightarrow 2 F move $y, z = 1, x = -1$
 \rightarrow 4 atoms, $x, z = 1, y = -1$
 \rightarrow 2 F move Br and 1 F $z = 1, x, y = -1$

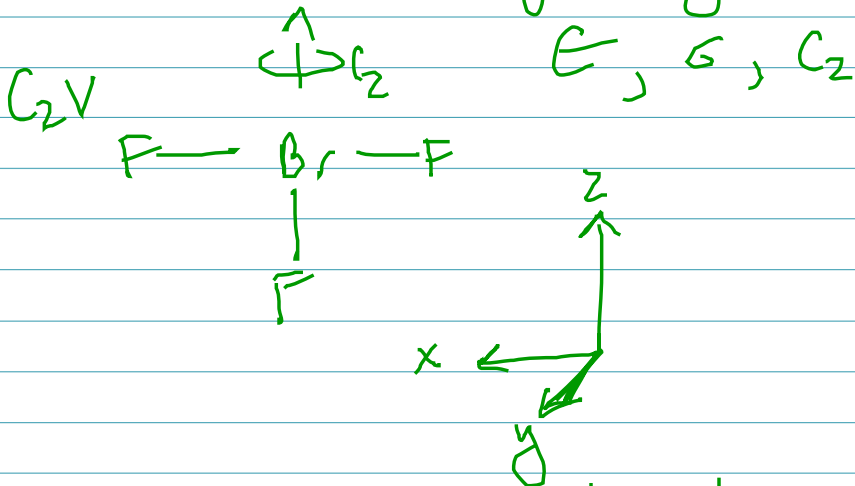
IR and Raman active modes for
bromine trifluoride

$\text{BrF}_3 \rightarrow$ Get geometry (Lewis Structure \rightarrow VSEPR)



T-shaped \rightarrow what is the symmetry?

Symmetry operations



x, y, z axes on each atom and make a reducible representation Γ $4 \text{ atoms} \times 3 \text{ axes} = 12$

C_{2v}	E	C_2	$\sigma(xz)$	$\sigma(yz)$
Γ	12	-2	4	2

\rightarrow containing Br and 1 F
 \rightarrow 2 F move $y, z = 1, x = -1$
 \rightarrow 4 atoms, $x, z = 1, y = -1$
 \rightarrow 2 F move Br and 1 F stay same. $z = 1, x, y = -1$

C_{2v}	E	C_2	$\sigma(xz)$	$\sigma(yz)$
Γ_1	12	-2	4	2

$3N - 6$ vibrational modes $(3(4) - 6) = 6$ modes

Decompose Γ , subtract translational, rotational modes

$$\#A_1 \text{ in } \Gamma = \frac{1}{4} \left[\underset{\substack{\text{red. rep} \\ \downarrow}}{(1)} \underset{12}{(12)} \underset{\substack{\text{irr. rep} \\ \downarrow}}{(1)} + \underset{-2}{(1)} \underset{-2}{(2)} \underset{1}{(1)} + \underset{4}{(1)} \underset{4}{(4)} \underset{1}{(1)} + \underset{2}{(4)} \underset{2}{(2)} \underset{1}{(1)} \right]$$

$$4A_1 \text{ in } \Gamma$$

$$\#A_2 \text{ in } \Gamma = \frac{1}{4} \left[\underset{12}{(1)} \underset{12}{(12)} \underset{4}{(4)} + \underset{-2}{(1)} \underset{-2}{(2)} \underset{1}{(1)} + \underset{-4}{(1)} \underset{4}{(4)} \underset{-1}{(-1)} + \underset{-2}{(1)} \underset{2}{(2)} \underset{-1}{(-1)} \right]$$

$$1A_2 \text{ in } \Gamma$$

$$\#B_1 \text{ in } \Gamma = \frac{1}{4} \left[\underset{12}{(1)} \underset{12}{(12)} \underset{1}{(1)} + \underset{2}{(1)} \underset{2}{(2)} \underset{1}{(1)} + \underset{4}{(1)} \underset{4}{(4)} \underset{1}{(1)} + \underset{-2}{(1)} \underset{2}{(2)} \underset{1}{(1)} \right]$$

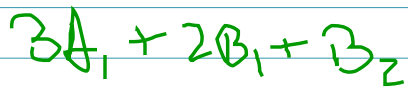
$$4B_1 \text{ in } \Gamma$$

$$\#B_2 \text{ in } \Gamma = \frac{1}{4} \left[\underset{12}{(1)} \underset{12}{(12)} \underset{1}{(1)} + \underset{2}{(1)} \underset{2}{(2)} \underset{1}{(1)} + \underset{-4}{(1)} \underset{4}{(4)} \underset{1}{(1)} + \underset{2}{(1)} \underset{2}{(2)} \underset{1}{(1)} \right]$$

$$3B_2 \text{ in } \Gamma$$

Translational $x \rightarrow \cancel{B_1}$ Rotational $R_x \rightarrow \cancel{B_2}$
 $y \rightarrow \cancel{B_2}$ $R_y \rightarrow \cancel{B_1}$
 $z \rightarrow \cancel{A_1}$ $R_z \rightarrow \cancel{A_2}$

$$\frac{4}{3}A_1 + \frac{1}{0}A_2 + \frac{4}{2}B_1 + \frac{3}{1}B_2 \rightarrow \text{Vibrational } \underline{3A_1 + 2B_1 + B_2}$$



$x, y, z \rightarrow IR \text{ active}$

$x^2, y^2, z^2, xz \text{ etc} \rightarrow Raman$

6 vibrations, all Raman active and IR active

