eg 2 determine the empirical formula for a compound that is 19.93 % C, 1.68 % H and 78.43 % Cl by mass.

In a 100 g sample:

C: $19.93\ g \times \frac{1\ mol}{12.01\ g} = 1.659\ mol$

H: $1.68\ g \times \frac{1\ mol}{1.01\ g} = 1.663\ mol$

Same

Cl: $78.43\ g \times \frac{1\ mol}{35.45\ g} = 2.212\ mol$

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In a 100 g sample:

$$\text{C: } 19.93\text{ g} \times \frac{1\text{ mol}}{12.01\text{ g}} = 1.659\text{ mol} \div 1.659\text{ mol} = 1.000$$

$$\text{H: } 1.68\text{ g} \times \frac{1\text{ mol}}{1.01\text{ g}} = 1.663\text{ mol} \div 1.659\text{ mol} = 1.002$$

$$\text{Cl: } 78.43\text{ g} \times \frac{1\text{ mol}}{35.45\text{ g}} = 2.212\text{ mol} \div 1.659\text{ mol} = 1.333$$

Problem! This number is no where near 1. You should not be satisfied with rounding this, instead you will need to multiple to obtain a whole number (or close to a whole number). Here are some guidelines

- .500 (or close to) => multiply by 2
- .333 or .666 => multiply by 3
- .250 or .750 => multiply by 4

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In a 100 g sample:

C: $19.93 \text{ g} \times \dfrac{1 \text{ mol}}{12.01 \text{ g}} = 1.659 \text{ mol} \div 1.659 \text{ mol} = 1.000 \times 3^{*} = 3.000 \simeq 3$

H: $1.68 \text{ g} \times \dfrac{1 \text{ mol}}{1.01 \text{ g}} = 1.663 \text{ mol} \div 1.659 \text{ mol} = 1.002 \times 3 = 3.006 \simeq 3$

Cl: $78.43 \text{ g} \times \dfrac{1 \text{ mol}}{35.45 \text{ g}} = 2.212 \text{ mol} \div 1.659 \text{ mol} = 1.333 \times 3 = 4.000 \simeq 4$

Therefore the empirical formula is $C_3H_3Cl_4$

* an extra multiplication step is required to create whole number ratios (rounding to whole numbers in the last step must always be close)

Numbers are now roundable!

This extra step can occur in an empirical formula calculation and/or a molecular formula calculation. Look for it!!