H-Rule

What is the H-Rule?

\[ H = 2C + N + 2 \]

*Hydrogen-Halogen! This is NOT just Hydrogen

What does it calculate?

The maximum number of monovalent atoms \( H \), less may be present. However this rule only applies to compounds that contain hydrogen, carbon, oxygen, nitrogen, fluorine, chlorine, bromine, and iodine. If other elements are present, this rule may not apply. (Glossary)

Example:

Use the H-Rule to find the maximum number of H’s

1. \( m/z = 102 \ (M; \ 100\%), \ M+1=156 \ (6.95\%), \ M+2= (0.38\%) \)

\[ \frac{6.95}{1.1} = 6.318 \rightarrow 6 \text{ Carbons} \]
\[ 102-(12)6 = 30 \rightarrow C_6H_{30}? \ NO \]

From the H-Rule, we get: \( 2(6)+0+2 = 14 \)

14 is MAX number of H’s we can have in our structure so:

\( C_6H_{30} \) is NOT a viable option

The H-Rule can help you find the right the formula by minimizing the numbers of the available formulas! Yay!

What? Another Example:

2. \( m/z = 132 \ (M; \ 100\%), \ M+1=133 \ (7.9\%), \ M+2= (30\%) \)

\[ \frac{7.9}{1.1} = 7.18 \rightarrow 7 \text{ Carbons} \]
\[ 132-12(7) = 48- 35 = 13 \rightarrow C_7H_{13}? \ YES \]

From the H-Rule we get: \( 2(7)+0+2 = 16 \)
16 is the MAX number of H’s we can have and since 13 H’s are less than 16, $C_7H_{13}$ is a viable option for the molecular formula

Why did we subtract 35 from the m/z?

Since the M+2 was 30%, that corresponds to the natural abundance of Chlorine (Cl) which has a mass of 35.

YOUR TURN!

Practice Problems:

Which molecular formula(s) fit the Mass Spectrum data?

Eliminate your options by using the H-Rule.

1) $m/z = 220$ (M; 100%), M+1 = 221 (9.43%), M+2 = 222 (0.4%)
   a) $C_8H_{124}$
   b) $C_8H_{12}O_7$
   c) $C_9H_{20}N_2O_4$
   d) $C_9H_{11}2$

2) $m/z = 142$ (M; 100%), M+1 = 143 (8.9%), M+2 = 144 (0.26%)
   a) $C_8H_{46}$
   b) $C_9H_{2}O_2$
   c) $C_8H_{14}O_2$
   d) $C_8H_{18}N_2$

3) $m/z = 136$ (M; 100%), M+1 = 137 (6.89%), M+2 = 138 (32%)
   Please write down possible formulas (up to 3):

*Practice Problems solutions are on next page*
Practice Problems Solutions:

1) b and c
2) c and d; b would be unlikely however it is still an option
3) Any formula that follows the H-Rule and has a Cl

Did you do well? YAY!

On to the next topic, which is the...

N-Rule

What is the N-Rule?

If the m/z of a formula is odd then there is an odd number of N’s. If the m/z is even there is an even number of N’s.

REMEMBER: Even includes the number 0! (Lecture Supplement)

Woohoo! The N-Rule is pretty simple to calculate. Just look at the m/z and depending on whether it is odd or even, it will tell you whether there is an N present.

Examples:

1) m/z = 132
   ^ even number → even number of N’s
   This includes 0! So, possibly no N’s

2) m/z = 145
   ^ odd number → odd number of N’s
   There is DEFINITELY an N present!

This rule can help narrow down even more options! Combine this rule with the H-Rule and BAM, you will be even closer to finding the correct molecular formula! Remember to take into consideration the M+2 abundance as well.

Thank You 😊 I hope this tutorial helped!
Works Cited
