Index of Hydrogen Deficiency

The Index of Hydrogen Deficiency (IHD) provides a method to determine the number of double (π) bonds and/or rings in a compound from the molecular formula of the compound. A straightforward calculation to determine the Index of Hydrogen Deficiency (IHD) for a compound with the molecular formula \( \text{C}_n\text{H}_m\text{N}_x\text{X}_o \) where

\[
\begin{align*}
C &= \text{carbon and } n = \text{number of } \text{C’s} \\
H &= \text{hydrogen and } h = \text{number of } \text{H’s} \\
N &= \text{nitrogen and } m = \text{number of } \text{N’s} \\
X &= \text{halogen and } x = \text{number of } \text{X’s} \\
O &= \text{oxygen and } o = \text{number of } \text{O’s}
\end{align*}
\]

is to use the formula:

\[
\text{IHD} = \frac{2n + 2 - h + m - x}{2}
\]

Illustrative Example 1. \( \text{C}_8\text{H}_8\text{O}_2 \)

Using the formula to calculate the IHD:

\[
\text{IHD} = \frac{2(8) + 2 - 8 + 1 - 1}{2} = \frac{10}{2} = 5
\]

Therefore this compound contains total of 5 double bonds and/or rings.

Some possible structures for this molecule are:

Illustrative Example 2. \( \text{C}_7\text{H}_8\text{ClN} \)

\[
\text{IHD} = \frac{2(7) + 2 - 8 + 1 - 1}{2} = \frac{8}{2} = 4
\]

This compound has 4 DBs and/or rings.

Some possible structures for this molecule are: