

Research Methodology in Chemistry

Edited by
Fiona N.-F. How, Ph.D



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RESEARCH METHODOLOGY IN CHEMISTRY

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CHAPTER – 2

GOOD CHEMISTRY RESEARCH

Fiona N.-F. How

General type of chemistry research

Quantitative research is based on the measurement of any quantity and amount. It is applicable to experiment or method that can be expressed in terms of quantity. Whereas, qualitative research is based upon qualitative observation, i.e., methodology that relates with feature, kind or class. Data analyses from carbon, hydrogen, nitrogen and sulfur (CHNS) elemental analyses can be of qualitative and quantitative. The qualitative aspect of the elemental analyses are the type of the element that are present in the compound can be known and identify. The quantitative aspect determines the exact amount of each element present in the compound using mass fractions calculation that represents the sample. Both qualitative and quantitative feature of elemental analyses are essential to determine the structure of the unknown compound.

IR spectra also exhibit data capable to provide qualitative and semiquantitative features the data analysis process. The qualitative features for IR spectra are to identify the functional groups present in the compound. IR spectra are also use for identification and classification of the unknown sample compound through matching spectrum with reference. The semiquantitative aspect relies on the Beer's law.

For any single compound in a homogeneous medium, the absorbance at any frequency is expressed as $A = abc$, where

A is the measured sample absorbance at the given wavenumber.

a is the molecular absorptivity at the wavenumber.

b is the path length of source beam in the sample,

c is the concentration of the sample.

From the expression above, the intensities of absorption bands are directly proportional to the concentration of each component in a homogeneous mixture or solution. Therefore the absorbance of the peaks or bands obtained is corresponded to the concentration of sample in molarity.