18.4 Performance characteristics of analytical processes

18.4.1 Introduction

The performance characteristics of the chemical analytical processes are those quantifiable terms, which may indicate the extent of quality of the processes. They include such terms, which are closely related to the method and to the analyte (like: sensitivity, selectivity, limit of detection, limit of determination, background and base-line, repeatability, reproducibility, etc.) and also those, which are concerned with the obtainable results. These latter are relevant also at the presentation of the analytical results (error, precision, standard deviation, systematic error, accuracy etc). See therefore also Chapter 2.

Effective communication among analytical scientists requires a consistent and uniform system of nomenclature and convention for specifying the performance characteristics of the chemical measurement processes. The *chemical measurement process* (*CMP*) is a fully specified analytical method that has achieved a state of statistical control. This measurement process, which may include substructure such as isolation of the analyte and instrumental sensing, lies between the other two components of the overall analytical system, namely Sampling (See section 18.3) and the Presentation of Results (See Chapter 2). Central to all three of these tasks are the issues of precision and accuracy. For this reason special attention is given to these statistical quantities in the discussion of Performance Characteristics of the CMP, in order to help prevent arbitrary and inappropriate usage of terminology among the three areas - e.g., "uncertainty" vs "inaccuracy" (See section 18.4.3).

Accepted statistical terminology and notation is used, even though this may occasionally lead to suggested changes from notation long popular with analytical chemists. A special effort will be made to distinguish between true (or asymptotic) values of parameters and observed or "estimated" values which necessarily exhibit the perturbations of random error. Also, the nature and validity of assumptions (such as normality) is emphasized; and an effort to minimize information loss is made by discouraging the use of ambiguous terms or incomplete reporting of data.

Measurable Quantity

The International Vocabulary of Basic and General Terms in Metrology defines the measurable quantity as "an attribute of a … substance which may be distinguished qualitatively and determined quantitatively" (See Section 18.2). In the context of Analytical Chemistry, the attribute may refer to a physical quantity such as *X*- or γ-ray energy, or it may refer to a measure of amount such as mass or concentration.

The general expression *qualitative analysis* thus refers to analyses in which substances are identified or classified on the basis of their chemical or physical properties, such as

chemical reactivity, solubility, molecular weight, melting point, radiative properties (emission, absorption), mass spectra, nuclear half-life, etc. *quantitative analysis* refers to analyses in which the amount or concentration of an analyte may be determined (estimated) and expressed as a numerical value in appropriate units. Qualitative Analysis may take place without Quantitative Analysis, but Quantitative Analysis requires the identification (qualification) of the analytes for which numerical estimates are given.

Analyte; Measurand

These terms, as well as the analog "determinand" are employed in Analytical Chemistry to indicate the chemical entity involved. The preferred term for Analytical Chemistry is *analyte*, defined as "the element [substance] sought or determined in a test portion…". The term *measurand*, as defined in section 18.2 is more encompassing: "the particular quantity subject to measurement."