Designation: E 158 – 86 (Reapproved 1996)$^{\varepsilon 1}$

Standard Practice for
Fundamental Calculations to Convert Intensities into Concentrations in Optical Emission Spectrochemical Analysis[1]

This standard is issued under the fixed designation E 158; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

ε^1 Note—Keywords were added editorially in June 1996.

1. Scope

1.1 This practice covers fundamental forms of plots, used to convert measured intensities into concentrations in both photographic and direct reading analysis. It includes equations suitable for use with calculators or computers for such conversions, and methods for making background corrections and corrections for interferences from other elements.

1.2 A previous issue of this practice attempted to treat optical emission and X-ray fluorescence as one field, employing similar calculations to convert measured radiation intensities into concentrations. In fact, quite different procedures are used in the two fields. This practice confines itself to optical emission spectrochemical analysis. A separate practice will be devoted to calculations in X-ray fluorescence spectroscopy.

1.3 This practice is related to but should be distinguished from:

1.3.1 Practice E 116E 116, which describes procedures for converting either transmittance or optical density of lines on a photographic emulsion into intensities or relative intensities. This step is required in photographic analysis before the present practice can be applied.

1.3.2 Practice E 305E 305, which describes the procedures for fitting a curve to a group of plotted points, and for standardizing the equipment, in order to obtain optimum accuracy, guided by sound statistical practice.

1.3.3 Practice E 876E 876 discusses the statistical treatment commonly applied to spectrochemical data, such as calculating the standard deviation and the relative standard deviation.

1.4 This practice includes the following sections:

1.5 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to use.*

2. Referenced Documents

2.1 *ASTM Standards:*

E 116 Practice for Photographic Photometry in Spectrochemical Analysis[2]

E 135 Terminology Relating to Analytical Chemistry for Metals, Ores, and Related Materials[2]

E 305 Practice for Establishing and Controlling Spectrochemical Analytical Curves[2]

E 876 Practice for the Use of Statistics in the Evaluation of Spectrometric Data[3]

3. Terminology

3.1 For definitions of terms used in this practice, refer to Terminology E 135E 135.

4. Significance and Use

4.1 Over the years, many workers have developed improved methods for plotting the measured intensities obtained from chemically analyzed specimens ("standards"), and for calculating concentrations of unknowns from the "analytical" curves obtained. This practice describes the methods of plotting and the calculation techniques which have been found to produce superior results.

---

[1] This practice is under the jurisdiction of ASTM Committee E-1 on Analytical Chemistry for Metals, Ores and Related Materials and is the direct responsibility of Subcommittee E01.22 on Statistics and Quality Control.

Current edition approved Oct. 31, 1986. Published December 1986. Originally published as E 158 – 60 T. Last previous edition E 158 – 83.

[2] *Annual Book of ASTM Standards*, Vol 03.05.

[3] *Annual Book of ASTM Standards*, Vol 03.06.

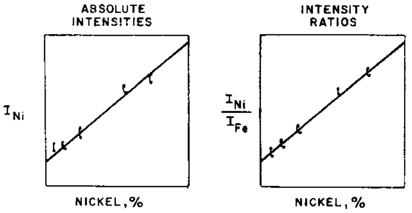

FIG. 1 The Advantage of Using an Internal Standard

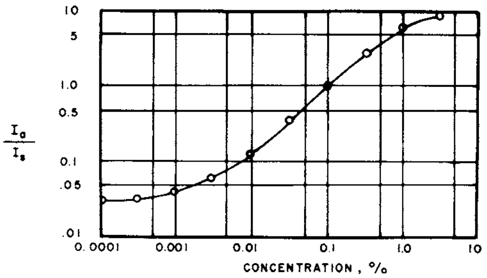

FIG. 2 Log-Log Plot

5. Fundamental Theory

5.1 In optical emission spectrochemical analysis, there are relatively few interferences from other elements, for materials with spectra of normal complexity, provided that a spectrograph or spectrometer with adequate dispersion and resolution is used, and that analytical lines are selected carefully. In general, the intensity of an analytical line is a function only of the concentration of the element that produces it. Therefore, it is common practice to employ an individual analytical curve for each element in a matrix. Observed intensities are converted into concentrations directly from this curve, without any correction for other elements. However, at times, it may be desirable to apply corrections for background or for interferences from other elements, as discussed later in this practice.

5.2 *Internal Standard Method*—In the early days of quantitative optical emission spectrochemical analysis, Gerlach and Schweitzer[4] found that when they measured the "blacknesses" of lines produced on photographic emulsion by a series of chemically analyzed materials and plotted them against their known concentrations, quite erratic results were obtained. A single specimen gave different "blacknesses" when run repeatedly. These variations were ascribed to erratic excitation and to variations in illumination. If they measured a line of an "internal standard element" that had the same concentration in all their materials, they could measure these exposure variations. Ratios determined by dividing the "blackness" of an analytical line by the "blackness" of an internal standard line, gave more repeatable results when the same material was burned repeatedly. Plots of "blackness" ratios versus concentration produced analytical curves with a better fit of points. Fig. 1 illustrates the advantages in precision and fit of points to a curve obtained by the internal standard technique, when applied to the determination of nickel in low-alloy steels. Curves plotted on linear graph paper are used for illustration.

5.2.1 Over the years, power supplies for sampling and exciting materials have become much more stable, and exposure variations have been reduced, but in general, the internal standard procedure still produces better results than the use of absolute intensities. Accordingly, the method is employed almost universally.

6. Plotting Analytical Curves with a Constant Internal Standard

6.1 *Log-Log, Linear, and Log-Linear Plots*—Different plotting methods produce analytical curves of widely different appearance. Each has its own advantages. Fig. 2, Fig. 3, and Fig. 4 illustrate the curves most commonly employed. The characteristics of each are listed. It should be emphasized that a knowledge of the theoretical shape of a curve can assist in deciding how best to fit a curve to an array of plotted points.

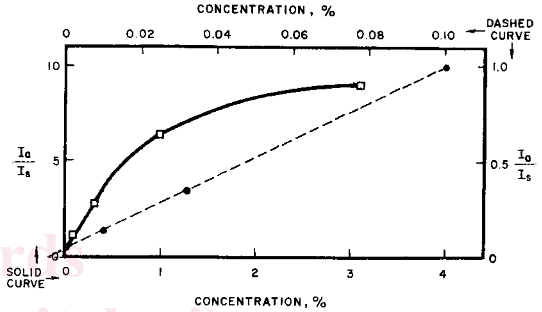

FIG. 3 Linear Plot

6.2 *Theoretical Data*—The theoretical data used to plot the curves are presented in Table 1. It is assumed that throughout the series of measurements the ratio of the intensity of the background to the intensity of the internal standard line remains constant, at 0.030. At low concentrations, the ratio of the intensity of the analytical line to the intensity of the internal standard line (I_a/I_s) is assumed to vary in direct proportion to the concentration. At 0.01 %, (Column 2), it is assumed to measure 0.100 (Column 3); therefore at 0.0032 %, it will measure 0.032, etc. The total signal is the sum of the intensity ratios of the background and line. Thus, at 0.01 %, it is 0.130; at 0.0032 %, it is 0.062, etc. The table first lists concentrations down to 0.0001 %, where the line signal is 0.001, and the background, 0.030. Then the table lists increasing concentrations. At 0.32 %, it is assumed that self-absorption is significant, so that the line response is not as great as the increase in concentration. The data tabulated in Column 5 are explained later in 6.5.1.

6.3 *Characteristics of Log-Log Plots*—Fig. 2 shows the appearance and major features of a log-log plot. The intensity ratios of the total signal (Column 4, Table 1) are plotted against concentrations (Column 2), using log-log graph paper. In the illustration, intensity ratios are plotted vertically, since these are measured, and concentrations horizontally, since they are known (at the time of plotting the curve). However, some workers prefer to reverse the scales.

6.3.1 Below the detection limit, the curve starts as a horizontal line, corresponding to the spectral background. The curve rises slowly as the line signal can be distinguished above

---

[4] Gerlach, W., and Schweitzer, E., *Foundations and Methods of Chemical Analysis by the Emission Spectrum*, Adam Hilger, Ltd., London, 1929.