

SPECTROPHOTOMETRIC DETERMINATION OF AN EQUILIBRIUM CONSTANT (#2.4)

The CCLI Initiative Computers in Chemistry Laboratory Instruction

Learning Objectives

The objective of this experiment is to determine the equilibrium constant governing the formation of $Fe(SCN)^{2+}$ from iron(III) and thiocyanic acid by using the *MicroLAB* Colorimeter to measure the concentration of $Fe(SCN)^{2+}$.

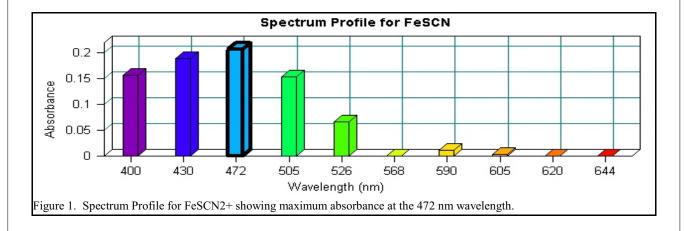
Background

Every chemical reaction is subject to equilibrium conditions that govern the concentrations of the products and reactants. In this experiment, known quantities of iron(III) and thiocyanic acid are mixed to form a dark red iron-thiocyanate complex. At equilibrium the concentrations of the products and reactants are governed by the law of mass action where the equilibrium constant K_f is not a true constant in that it depends on temperature, and it is more exact to use "activities" in place of concentrations.

 $Fe(SCN)^{2+}$ is a dark red cation that absorbs light most effectively at 447 nm. Thus, a spectrophotometer can be used to measure the equilibrium concentration of the $Fe(SCN)^{2+}$ cation. The equilibrium concentrations of H^+ , HSCN, and Fe^{3+} can be calculated from the initial quantities, stoichiometry, and the equilibrium concentration of $Fe(SCN)^{2+}$.

The Colorimeter

The MicroLAB Colorimeter is described and its operation explained. The output resulting from the scan of the ten LEDs is seen in Figure 1, and is a colored bar graph where the colors are representative of the color of that wavelength of light and the height is representative of the absorbance at that wavelength.



Beer's Law relates the absorption of light by a colored species to its concentration in the solution, given by the expression:

$$A = \log \left(\left| I_0 \right| / \left| I_1 \right| \right) = \epsilon bc \tag{1}$$

 I_0 represents the current reading for the cell *without* an absorbing species in the path, i.e., the blank, and I_t is the current reading through the cell *with* an absorbing species, i.e., the sample, ϵ is the molar absorptivity (in units of cm⁻¹), b is the path length for the light through solution (in cm) and c is the concentration of the species of interest, $[Fe(SCN)^{2+}]$.

The absorbance of each solution is plotted versus the molar concentration of Fe(SCN)²⁺; this establishes a calibration curve (see Figure 2) from which the unknown concentrations of Fe(SCN)²⁺ are determined by means of a calibration equation similar to equation (2)

Abs =
$$k*[Fe(SCN)^{2+}] + b$$
 (2)

Procedure

- 1. Measurement of absorbance for each solution from the transmission data.
- 2. Calculation of the equilibrium concentration of Fe(SCN)²⁺, using the calibration equation (2)
- 3. Calculation of the equilibrium concentrations of Fe ³⁺, HSCN and H⁺ using the Table of Equations.
- 4. Calculation of the equilibrium constant K_f.

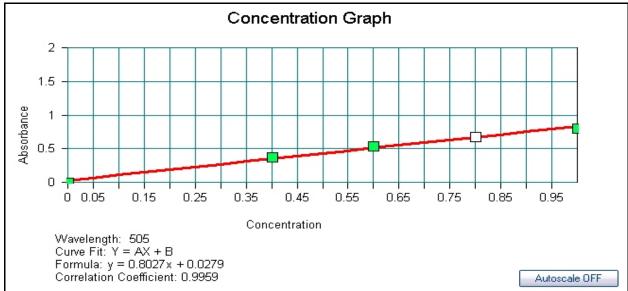


Figure 2. Sample Absorbance versus concentration graph for an $Fe(SCN)^{2+}$ solution at 470 nm wavelength. Using the coefficient of the X term in the formula, k, we can calculate the molar absorptivity for that wavelength.

Data Analysis: Guidance is provided for making the measurements and doing the calculations.

Instructor Resources Provided

- 1. Sample Report Sheets providing the format to organize the data collection with sample data.
- 2. Questions to consider, answer and turn-in with suggested answers.
- 3. Tips and Traps section to assist the instructor with potential problems and solutions.
- 4. Sample *MicroLAB* screen shots and graphs.
- 5. Laboratory preparation per student station.

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