The Thiocyano-iron (III) Complex Ion or Molecule

1. Data table and sample calculations:

Reaction 1: $Fe^{+3} + SCN^- \longleftrightarrow Fe(SCN)^{+2}$

Test Tube No.	Solution Depth		Initial Concentrations		Equilibrium Concentrations			K_{eq}
	Tube No. 1	Other Tube	Fe^{+3}	SCN^-	$Fe(SCN)^{+2}$	Fe^{+3}	SCN^-	
1	-	-	0.02 M	0.001 M	0.001 M	-	-	n/a
2	6.70 cm	8.20 cm	0.01 M	0.001 M	0.000817 M	0.00918 M	0.000183 M	4.86E+02
3	5.00 cm	8.20 cm	0.005 M	0.001 M	0.000610 M	0.00439 M	0.000390 M	3.56E+02
4	2.50 cm	8.00 cm	0.0025 M	0.001 M	0.000313 M	0.00219 M	0.000688 M	2.08E+02
5	1.40 cm	8.10 cm	0.00125 M	0.001 M	0.000173 M	0.000827 M	0.000827 M	1.94E+02

Sample calculation:
For test tube 2: $A_1 = A_2$; $ec_1l_1 = ec_2l_2$
(6.70 cm)(0.001 M Fe(SCN)$^{+2}$) = (8.20 cm) x   x = (6.70 cm)(0.001 M Fe(SCN)$^{+2}$)/ (8.20 cm) = 0.000817 M Fe(SCN)$^{+2}$
$[Fe^{+3}]_{eq} = [Fe^{+3}]_{initial} - [Fe(SCN)^{+2}]_{eq} = 0.01$ M - 0.000817 M = 0.009183 M
$[SCN^-]_{eq} = [SCN^-]_{initial} - [Fe(SCN)^{+2}]_{eq} = 0.001$ M – 0.000817 M = 1.83 x 10^{-4} M
$K_{eq} = [Fe(SCN)^{+2}]/ ([Fe^{+3}][SCN^-]) = 0.000817/ (0.00918 * 0.000183) = 4.86$ x 10^2

Reaction 2: $Fe^{+3} + 3 SCN^- \longleftrightarrow Fe(SCN)_3$

Test Tube No.	Solution Depth		Initial Concentrations		Equilibrium Concentrations			K_{eq}
	Tube No. 1	Other Tube	Fe^{+3}	SCN^-	$Fe(SCN)^{+2}$	Fe^{+3}	SCN^-	
1	-	-	0.02 M	0.001 M	0.001 M	-	-	n/a
2	6.70 cm	8.20 cm	0.01 M	0.001 M	0.000817 M	0.00918 M	-0.00145 M	-2.91E+07
3	5.00 cm	8.20 cm	0.005 M	0.001 M	0.000610 M	0.00439 M	-0.000829 M	-2.44E+08
4	2.50 cm	8.00 cm	0.0025 M	0.001 M	0.000313 M	0.00219 M	0.0000625 M	5.85E+11
5	1.40 cm	8.10 cm	0.00125 M	0.001 M	0.000173 M	0.000827 M	0.000481 M	1.44E+09

Sample calculation:
For test tube 2: $A_1 = A_2$; $ec_1l_1 = ec_2l_2$
(6.70 cm)(0.001 M Fe(SCN)$_3$) = (8.20 cm) x   x = (6.70 cm)(0.001 M Fe(SCN)$_3$)/ (8.20 cm) = 0.000817 M Fe(SCN)$^{+2}$
$[Fe^{+3}]_{eq} = [Fe^{+3}]_{initial} - [Fe(SCN)_3]_{eq} = 0.01$ M - 0.000817 M = 0.00918 M
$[SCN^-]_{eq} = [SCN^-]_{initial} - 3[Fe(SCN)_3]_{eq} = 0.001$ M – 3(0.000817 M) = - 0.00145 M
$K_{eq} = [Fe(SCN)_3]/ ([Fe^{+3}][SCN^-]^3) = 0.000817/ (0.00918 * (-0.00145)^3) = -2.91$ x 10^7

2. Correct values are for reaction 1: Relative deviation calculation

Average K_{eq} value = (486 + 356 +208 +194)/4 = 311
Standard deviation =Square root { [(486-311)^2 + (356-311)^2 +(208-311)^2 + (194-311)^2]/ (4-1)} = 137.8
Relative standard deviation = 137.8/ 311 = 44.3%

3. Beer's law is a law that directly relates concentration and pathlength with absorbance for a solution. It is $A = ecl$, where
   e = extinction coefficient or molar absorbtivity constant for a given colored substance
   c = molar concentration of the substance
   l = pathlength of the substance through which the light travels.

4. Beer's law was applied in this laboratory experiment qualitatively. A reference solution (test tube no. 1) of known concentration was compared against a solution of unknown concentration. The amount of liquid in the test tube in the referent test tube (related to the height of the liquid or pathlength, l) was varied until the color intensity was equal to that of the unknown concentration solution. At this point, the absorbances of each solution could be considered equal. If the height of liquid in each tube, or pathlength, were measured, one could determine the unknown solutions concentration via calculations. Thus,

$A_{reference} = A_{unknown}$ so that
$ec_{referent}l_{referent} = ec_{unknown}l_{unknown}$ (where e is the same because the substance is the same and l is equivalent to the height of liquid in each test tube)
$c_{unknown} = c_{referent}l_{referent} / l_{unknown}$

5. A. The solution must absorb light in the visible spectrum to analyze it using a visible spectrophotometer or visible colorimeter.
   B. One could determine the wavelength setting for use in the analysis by measuring the absorbance of a set (constant) concentration solution across varying wavelengths. The wavelength that showed the strongest absorbance would be the λ_{max}, or the optimal wavelength for use in the analysis.
   C. You could use Beer's law to determine the unknown concentration by creating an absorbance-concentration calibration curve with the known concentration solutions and then testing the unknown concentration solution against the curve:
   First, measuring the absorbance of the solutions of known concentration, keeping the pathlength constant (using the same sample tube).
   Second, creating a graph of absorbance (y-axis) versus concentration (x-axis) with the results from the known concentration solutions and fitting a best fit linear regression line to it. The line $y=mx+b$ would be equivalent to $A=(el)c + correction$.
   Third, measuring the absorbance of the unknown concentration and then plugging it into the regression line equation to determine the concentration: $(A-correction)/el=c$ or $A-b/m =x$, which would be the concentration.

6. If one of the reactants is in high excess, it would drive the limiting reactant to be completely used up such that the initial concentration of limiting reactant (in a 1:1 molar ratio reaction, as in the iron-thiocyanate equilibrium) would be equal to the concentration of Fe-SCN complex formed.

   Therefore, in this lab, if I were to create solutions of known Fe-SCN concentration, I would create them by making the limiting reactant [SCN^-] equal to 0.0001M, 0.0002, 0.0004M, 0.0006M, 0.0008M, and 0.001M (whatever concentration of product I desire to make the calibration curve with) and consistently mixing them with 0.02M or higher concentrations of Fe^{+3} (well in excess of what is needed).

   The equilibrium mixture of Fe-SCN to be tested would be produced by mixing a concentration of SCN^- and Fe^{+3} that were closer in magnitude to each other.