

Problem Set #11
Fall 2006
SOLUTIONS

12-6 (a) Recall that the mass absorption coefficients can be added in proportion to their mass contribution to the sample. It is easiest to split up the fraction of each molecular component and then sum the fraction for each molecule to the whole.

$$\mu_m = W_K \mu_{m,K} + W_I \mu_{m,I} + W_H \mu_{m,H} + W_O \mu_{m,O}$$

$$\mu_m = \frac{8.00}{100} \left(\frac{39.1}{166.0} \times 16.7 + \frac{126.9}{166.0} \times 39.2 \right) + \frac{92}{100} \left(0 + \frac{16.0}{18.0} \times 1.50 \right) = 3.94 \frac{\text{cm}^2}{\text{g}}$$

We just invoke Beer's Law, as altered for the x-ray field, wherein we use the sample density and the resultant mass absorption coefficient.

$$\ln\left(\frac{P_0}{P}\right) = \mu_m \rho x = 3.94 \times 1.05 \times 0.50 = 2.069$$

$$\frac{P}{P_0} = e^{-2.069} = 0.126$$

12-9 Here we just serially apply Bragg's Law. Look up the d-spacing for each of the crystals requested from the table 12-3.

$$n\lambda = 2d \sin\theta \Rightarrow \frac{\lambda}{2d} = \sin\theta \Rightarrow 2\theta = 2 \arcsin\left(\frac{\lambda}{2d}\right) = 2 \arcsin\left(\frac{1.76}{2(1.356)}\right) = 80.9^\circ$$

| | Topaz (d = 1.356 Å) | LiF (d = 2.014 Å) | NaCl (d = 2.820 Å) |
|--------------|------------------------------|----------------------------|-----------------------------|
| Fe (1.76 Å) | 80.9 ° | 51.8 ° | 36.4 ° |
| Se (0.992 Å) | 42.9 ° | 28.5 ° | 20.3 ° |
| Ag (0.497 Å) | 21.1 ° | 14.2 ° | 10.1 ° |

12-11 This is just turning the wavelength of the photon into its energy in eV. Equation 12-2 is a short cut to that

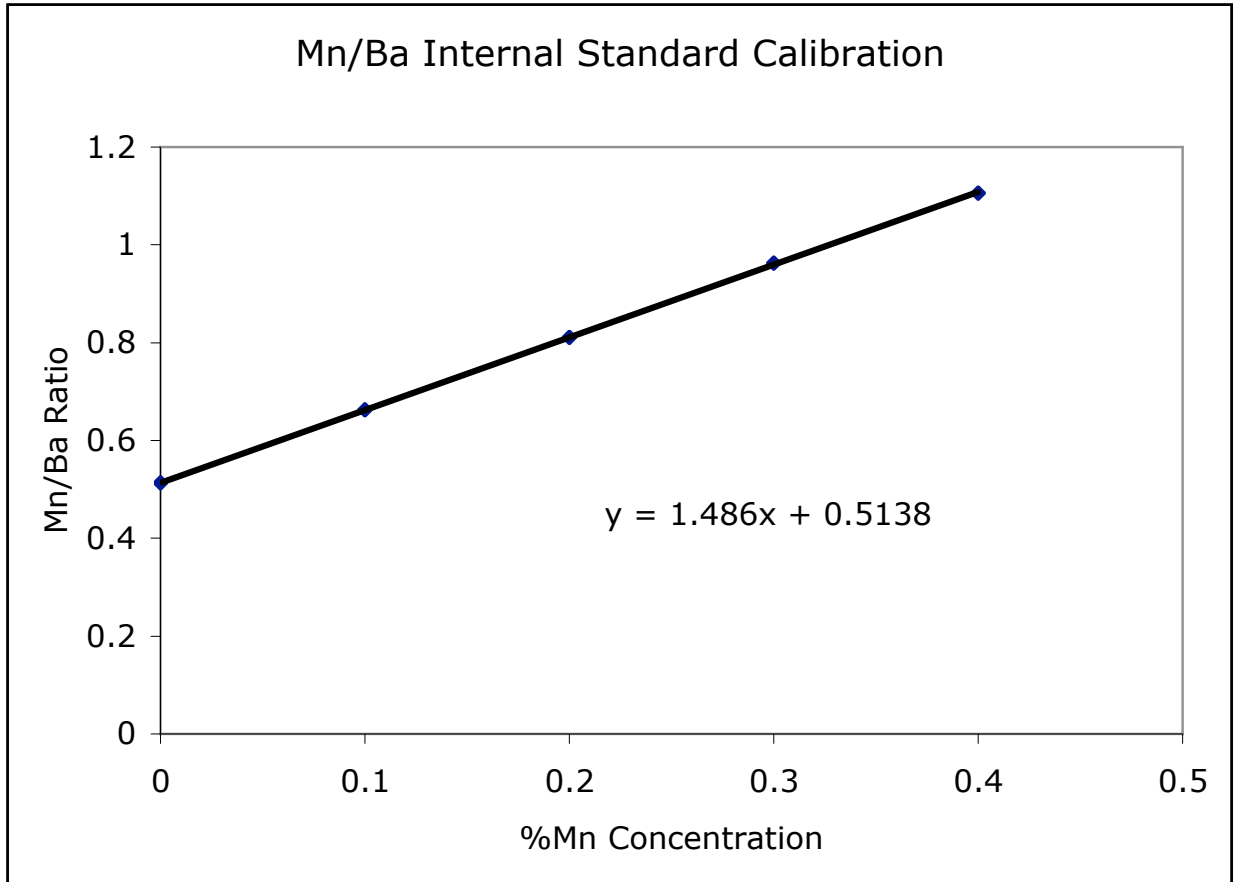
$$V_0 = \frac{hc}{e} \left(\frac{1}{\lambda_0} \right) = \frac{(6.626 \times 10^{-34})(2.9979 \times 10^8)}{1.602 \times 10^{-19}} \times 10^{10} \frac{\text{Å}}{\text{m}} \left(\frac{1}{\lambda_0} \right) = 12399.6 \left(\frac{1}{\lambda_0} \right)$$

$$= 12399.6 \left(\frac{1}{3.064 \text{ Å}} \right) = 4046.9 \text{ V}$$

- (a) 4.046 kV (b) 1.323 kV (c) 20.94 kV (d) 25.00 kV

12-12 Calculate the Mn/Ba ratio for each concentration sample. Use a least square routine to fit it to a straight line. Use that calibration curve to determine the unknown sample's Mn concentration.

| Weight% Mn | Barium (cps) | Manganese (cps) | Mn/Ba Ratio |
|------------|--------------|-----------------|-------------|
| 0.00 | 156 | 80 | 0.513 |
| 0.10 | 160 | 106 | 0.6625 |
| 0.20 | 159 | 129 | 0.811 |
| 0.30 | 160 | 154 | 0.9625 |
| 0.40 | 151 | 167 | 1.106 |



The curve is an excellent fit. Slope $m = 1.486$ and Intercept $b = 0.5138$. We invert the linear equation to solve for the unknown's ratio of 0.886.

$$y = mx + b \quad x = \frac{y - b}{m} = \frac{0.886 - 0.5138}{1.486} = 0.2504$$

The unknown sample therefore has a Mn concentration of 0.250%. We can take the variance of the fit from the LINEST function in Excel (which gives the error of the fit so we square it). We have $\text{var}(\text{fit}) = 0.002153^2 = 4.633 \times 10^{-6}$. We need the sum of the x's and the squares and the determinant.

$$\Sigma x = 1.00 \quad \Sigma x^2 = 0.300 \quad \text{Det} = 0.500$$

With this we can find the variance of the interpolated unknown. We have

$$s_{x_{\text{int}}}^2 = \frac{S_{\text{fit}}^2}{D m^2} (n x_{\text{int}}^2 - 2 x_{\text{int}} \sum x_i + \sum x_i^2)$$

Standard Deviation of the unknown = 0.00069.

Note: The question did not specifically ask for error information, so I did not grade for it, but I include it here for completeness.