

CHEM 221
Instrumental Analysis
Problem Set #1 – Solutions
Spring 2005

Appendix 1

#1 a & b, #2 a & b.

$$\text{Mean} = \sum X_i / N = X_{\text{avg}}$$

$$\text{Standard Deviation} = \langle \text{use Std Dev calculator function} \rangle = s$$

$$\text{Relative Std Dev (RSD), ppt} = (s/X_{\text{avg}}) \times 1000$$

$$\text{Error} = X_{\text{avg}} - \mu$$

$$\% \text{-relative error} = (\text{error}/\mu) \times 100$$

	<u>A</u>	<u>B</u>	<u>C</u>	<u>D</u>
X_{avg}	61.43	3.25	12.10	2.6
s	0.11	0.02	0.06	0.2
RSD	1.7 ppt	6.0 ppt	4.7 ppt	79. ppt
μ	61.71	3.28	12.23	2.75
error	-0.28	-0.03	-0.13	-0.10
%-rel error	-0.45 %	-0.91 %	-1.1 %	-3.6 %

#3.

- a. $(-0.5 \text{ mg}/25 \text{ mg}) \times 100 = \underline{\underline{-2.0 \%}}$
- b. $(-0.5 \text{ mg}/100 \text{ mg}) \times 100 = \underline{\underline{-0.5 \%}}$
- c. $(-0.5 \text{ mg}/250 \text{ mg}) \times 100 = \underline{\underline{-0.2 \%}}$
- d. $(-0.5 \text{ mg}/500 \text{ mg}) \times 100 = \underline{\underline{-0.1 \%}}$

#4.

a. $0.5 \text{ mg}/x = 0.001 \rightarrow x = 500 \text{ mg Cu}$

$$\begin{aligned} (\text{sample mass}) \times 0.048 &= 0.500 \text{ g} \\ \text{sample mass} &= \underline{\underline{10. \text{ grams}}} \end{aligned}$$

b. $x = 100 \text{ mg Cu}$
sample mass = **2.1 grams**

c. $x = 62.5 \text{ mg Cu}$
sample mass = **1.3 grams**

d. $x = 41.67 \text{ mg Cu}$
sample mass = **0.87 grams**

#7.

$$(0.18)(0.400 \text{ g sample}) = 72.0 \text{ mg Cr}$$

$$\text{error} = -1.8 \text{ mg Cr} \rightarrow (-1.8 \text{ mg}/72.0 \text{ mg}) \times 1000 = \underline{\underline{-25. ppt}}$$

Chapter 1

#9. A plot of the data gives a straight line with a linear least squares determined equation: $S = 0.0670 c_x + 0.031$

a). The calibration sensitivity is simply the slope of the analytical curve:
0.0670

b). The analytical sensitivity (γ) is: m/s_s (where: m = slope of analytical curve and s_s = standard deviation of the signal). So, since s_s varies with the concentration, the analytical sensitivity will also vary with concentration giving:

<u>Conc (ppm)</u>	<u>γ</u>
2.00	7.1 (= 0.0670/0.0094)
6.00	8.0
10.00	8.0
14.00	7.9
18.0	6.1

c). The coefficient of variation (CV) = $(s_s/S) \times 100\%$ (this is also commonly referred to as the % relative standard deviation (%RSD). Since this varies with concentration also:

<u>Conc (ppm)</u>	<u>CV</u>
2.00	5.4% (= (0.0094/0.173) x 100%)
6.00	2.0%
10.00	1.2%
14.00	0.89%
18.00	0.88%

d). Recall equation 1-4 on page 13: $S_m = S_{avgbl} + 3s_{bl}$
Substituting in the values for this set of data gives:

$$S_m = 0.031 + 3(0.0079) = 0.0547$$

This is the *measured* signal at the detection limit.

We use the linear least squares equation to find the corresponding concentration at the detection limit:

$$S_m = 0.0670 c_m + 0.031$$

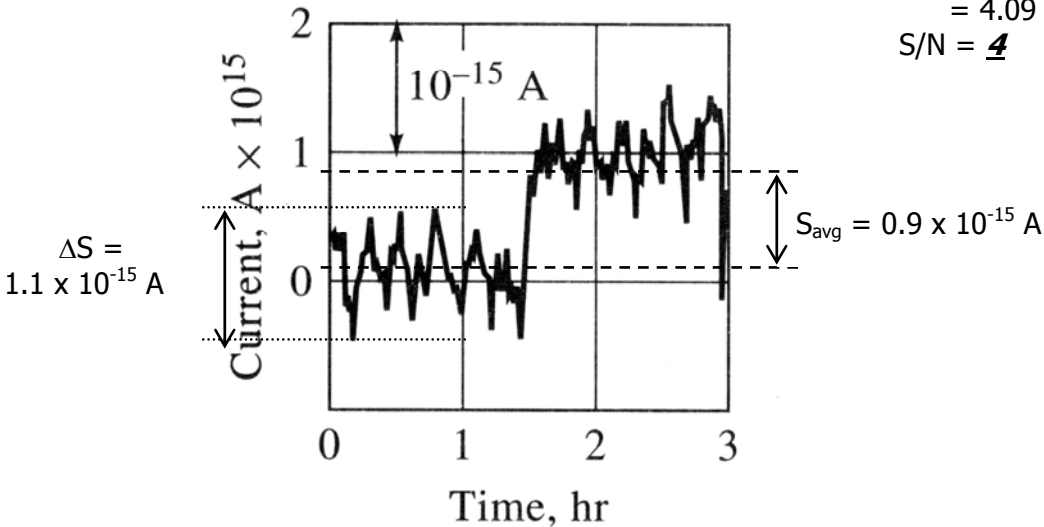
Solving for c_m gives: $c_m = (S_m - 0.031)/0.0670 = (0.0547 - 0.031)/0.0670$

$$c_m = \underline{\underline{0.35 \text{ ppm X}}}$$

Chapter 5

#6.

$$\begin{aligned} \text{So: } S/N &= 5 S_{\text{avg}}/\Delta S \\ &= \frac{5(0.9 \times 10^{-15} \text{ A})}{1.1 \times 10^{-15} \text{ A}} \\ &= 4.09 \\ S/N &= \underline{\underline{4}} \end{aligned}$$



#7.

- a.** From data set ($n=9$), we calculate: $\text{avg} = 1.002889 \text{ g} = \text{Signal}$
 $s = 0.002804 \text{ g} = \text{Noise}$

$$\text{So, } S/N = 1.002889/0.002804 = 357.7 \approx \underline{\underline{360}}$$

- b.** We know that: $(S/N)_n = (n)^{1/2}(S/N)_{n=1}$
 So, for $n=9$: $357.7 = (9)^{1/2}(S/N)_{n=1}$
 $(S/N)_{n=1} = 119.23$

$$\begin{aligned} \text{For } S/N = 500: \quad 500 &= (n)^{1/2}(119.23) \\ (n)^{1/2} &= 4.1935 \\ n &= 17.59 \approx \underline{\underline{18}} \end{aligned}$$

#8.

- a.** From data set ($n = 8$): $\text{avg} = \text{Signal} = 1.435$
 $S = \text{Noise} = 0.2707$ so: $S/N = \underline{\underline{5.3}}$
- b.** Using same method as in #7b, $(S/N)_{n=1} = 1.874$,
 so to get $S/N = 10$, need $n = 28.5 \approx \underline{\underline{29}}$