Chemistry 237 — Exam 1 2010

I. A. $\mathbf{A} = \begin{pmatrix} \sum x_i^2 & \sum x_i \exp(3x_i^2) \\ \sum x_i \exp(3x_i^2) & \sum \exp(6x_i^2) \end{pmatrix}$ $\quad \beta = \begin{pmatrix} a \\ b \end{pmatrix}$ $\quad \mathbf{z} = \begin{pmatrix} \sum x_i y_i \\ \sum y_i \exp(3x_i^2) \end{pmatrix}$

$\mathbf{A}\beta = \mathbf{z}$

B. $Y = y/x$; $\quad X = \exp(3x^2)/x$

C. s_y = constant (assumption for unwtd fit) → $w_{Yi} \quad x_i^2$

D. $s_y = 0.159$; $S \rightarrow 100\ S$ for 290 measurements; s_y ~ same.

II. A. $4.67(18) \times 10^{-4}$ mol/L

B. $A = 1.38$

C. 833.4 nm

III. A. $1s^2\,2s^2\,2p$; ground term = ^{2}P state = $^2P_{1/2}$

B. $1s^2\,2s\,2p^2$

C. For C, $2p^2$ yields ^{3}P, ^{1}D, and ^{1}S. Coupling an s electron gives ^{2}P, ^{4}P, ^{2}D, and ^{2}S.

D. There are $\binom{6}{2}$ = 15 states of $2p^2$; 2 $2s$ orbitals → 30.

(1) $(2S+1)(2L+1) = 6 + 12 + 10 + 2 = 30$

(2) $\Sigma\,(2J+1) = (2 + 4) + (2 + 4 + 6) + (4 + 6) + 2$

E. $\hat{S}^2\,\psi = S(S+1)\hbar^2\,\psi$ and $\hat{S}_z\,\psi = M_S\hbar\,\psi$ and similarly for the L and J operators. For each term, S and L are fixed (1 and 2 for ^{3}D), and M_S and M_L run over their allowed values (for ψ s appropriate for those values). There are 3 J values for ^{3}D (1, 2, and 3), and for each of these there are $(2J+1)$ M_J values.

IV. A. In the 2nd case, the two estimates agree roughly within their combined standard errors; in the first, the more uncertain first value is almost 6 σ away from the 2nd. That is statistically highly unlikely, so the values are inconsistent.

B. 28.51370(29); 0.001095(6); −2(5)

The last parameter is statistically insignificant.

V. 27690 cm^{-1} or 361.1 nm.