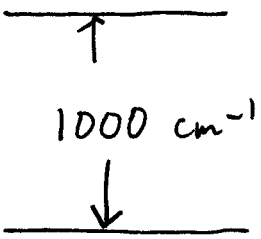
Practice Exam 780.04

1.



$A = 1\ s^{-1}$

FWHM absorption $\Delta\nu = 100\ MHz = 1.00 \times 10^{8}\ s^{-1}$

$K^{max} = ?$ $\quad K^{max} = \dfrac{8\pi^2 \nu_{ul}\, n_l}{3hc} |\mu_{ul}|^2$

$A = \dfrac{32\pi^3 \tilde{\nu}_{ul}^3}{3h} |\mu_{ul}|^2 = 1\ s^{-1}$

$|\mu_{ul}|^2 = 3.1884 \times 10^{-39}$ cgs units

$K^{max} = 1.2664 \times 10^{-16} n_l\ cm^{-1} = 0.12664\ cm^{-1}$

$I/I_0 = e^{-K^{max} l}$

$l = 1\ cm \quad I/I_0 = 0.88$

$l = 1\ m \quad I/I_0 = 0.28$

2. H ——— $1s + e^-$ $E_{1s} = -13.60\ eV$

↑ 0.76 eV

H^- ↓ ——— $1s^2$ $E_{1s^2} = -13.60\, Z_{eff}^2 \left[\frac{1}{1} + \frac{1}{1}\right]$

$E_{1s} - E_{1s^2} = 0.76\,eV = -13.60\left[1 - 2Z_{eff}^2\right]$

$-0.0559 = 1 - 2Z_{eff}^2$

$Z_{eff} = 0.7266$ Shielding $= 27.34\%$

3. a) B_2 10 electrons $KKLL(\pi_u 2p)^2$ $N = 1$

π_u^2 :

1	↑↓	—	↑	↑	↓	↓		
−1	—	↑↓	↑	↓	↓	↑		
Λ	2	−2	0	0	0	0		
Σ	0	0	1	0	−1	0		
			$^3\Sigma_g$			$^1\Sigma_g$		
$S = 0$ $\lvert\Lambda\rvert = 2$								
$^1\Delta_g$								

$u \times u = g$

~~S =~~

$^3\Sigma_g < {}^1\Delta_g < {}^1\Sigma_g$

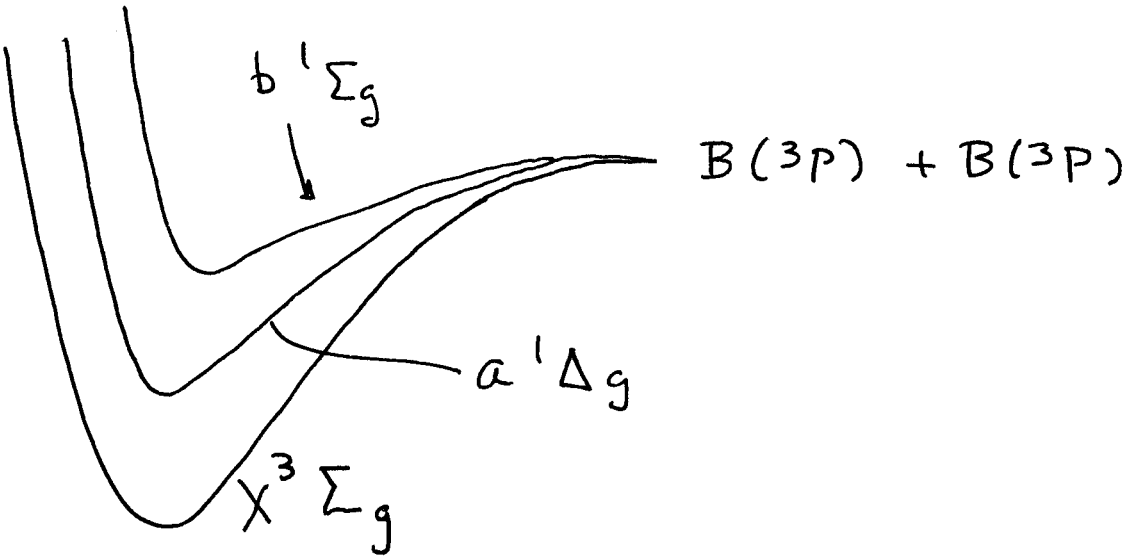
3 b) B $1s^2 2s^2 2p$ ^2P

^2P : $L' = 1$ $S' = 1/2$ $L'' = 1$ $S'' = 1/2$

$S = 1, 0$ "L" $= 2, 1, 0$ $^{1,3}\Delta$, $^{1,3}\Pi(2)$ $^{1,3}\Sigma(3)$

$\Lambda = \pm 2, \pm 1\,(2), 0(3)$

B_2



$^2P + {}^2P$ correlate with $^3\Sigma_g$, $^1\Sigma_g$, $^1\Delta_g$

4. D_2 $\psi_s = \psi_{rot}\,\psi_{ns}$ $\quad {}^1\Sigma_g^+$

$i_1 = 1 = i_2$

No. anti-symm spin states = 3 para J ODD

No. symm spin states = 6 ortho J EVEN

Ortho Para

J=2 ———

——— J=1

J=0 ———

$g_I = 6$ $\qquad$ $g_I = 3$

Equilibrium: $\dfrac{n(J=1)}{n(J=0)} = \dfrac{3 \cdot 3}{6 \cdot 1} e^{-2hB/kT}$

Normal: to 1ST approx. $\dfrac{n(J=1)}{n(J=0)} \approx \dfrac{1}{2} \left(\dfrac{g_I = 3}{g_I = 6} \right)$

5. $\tilde{\upsilon}_R(J) = \tilde{\upsilon}_0 + \tilde{B}_{v'}(J+1)(J+2) - \tilde{B}_{v''} J(J+1)$

$$\tilde{\upsilon}_R(J) = \tilde{\upsilon}_0 + (J+1)\left[\tilde{B}_{v'}(J+2) - \tilde{B}_{v''} J\right]$$

$$= \tilde{\upsilon}_0 + (J+1)\left[\tilde{B}_{v'} + \tilde{B}_{v'}(J+1) + \tilde{B}_{v''} - \tilde{B}_{v''}(J+1)\right]$$

$$\tilde{\upsilon}_R(J) = \tilde{\upsilon}_0 + (J+1)\left[\tilde{B}_{v'} + \tilde{B}_{v''}\right] + (J+1)^2\left[\tilde{B}_{v'} - \tilde{B}_{v''}\right]$$

(+) (−)

$\tilde{B}_{v'} < \tilde{B}_{v''}$

$$\frac{d\tilde{\upsilon}_R}{dJ} = (\tilde{B}_{v'} + \tilde{B}_{v''}) + 2(J+1)\left[\tilde{B}_{v'} - \tilde{B}_{v''}\right] = 0$$

$$2(J+1) = \frac{\tilde{B}_{v'} + \tilde{B}_{v''}}{\tilde{B}_{v''} - \tilde{B}_{v'}}$$

$$J \approx \frac{\tilde{B}_{v'} + \tilde{B}_{v''}}{2(\tilde{B}_{v''} - \tilde{B}_{v'})} - 1$$