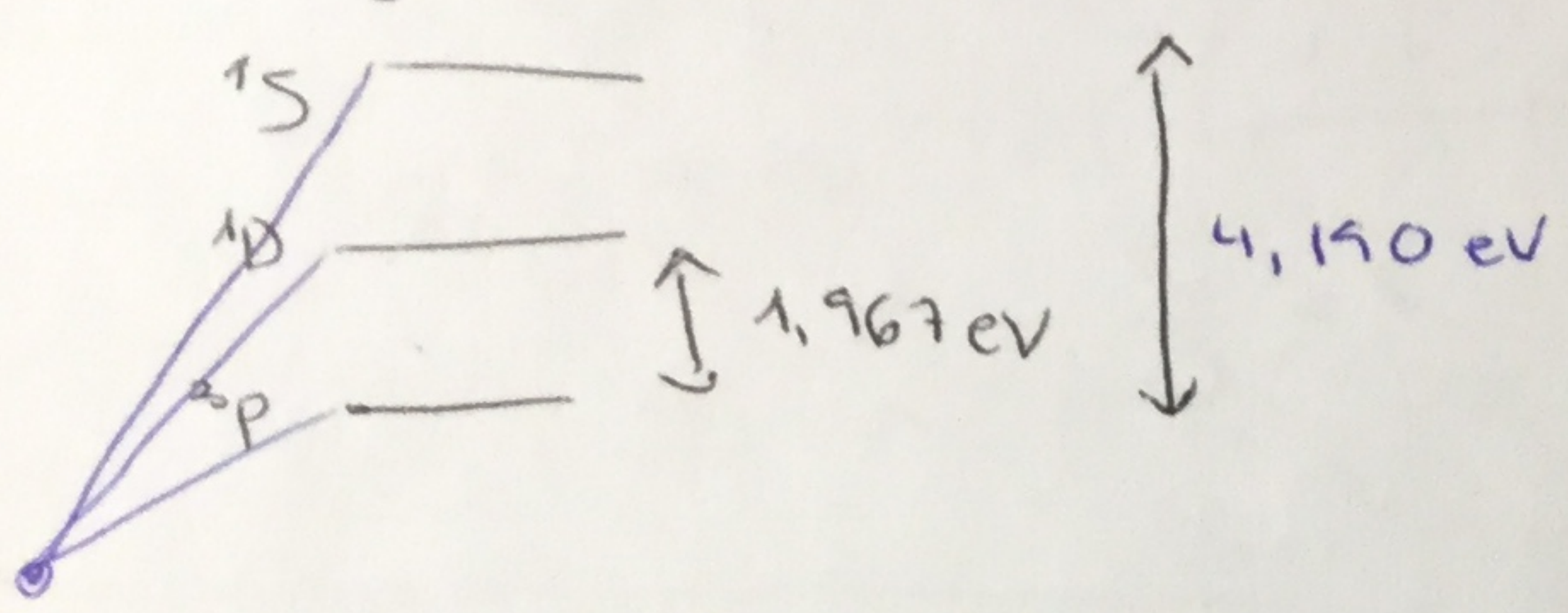


GENER 2016

3

a)  $T = 298,15 \text{ K}$   $\text{O}_2$   
 3 1° termes espectrals de més baixa E  $^3P < ^1D < ^1S$



$$d = (2S+1)(2L+1)$$

$$Z_{el} = g_{el,0}$$

$1S \rightarrow s=0, L=0 \quad d=1$

$1D \rightarrow s=0, L=2 \quad d=1(2(2)+1)=5$

$3P \rightarrow s=1, L=1 \quad d=(2+1) \cdot 3 = 9$

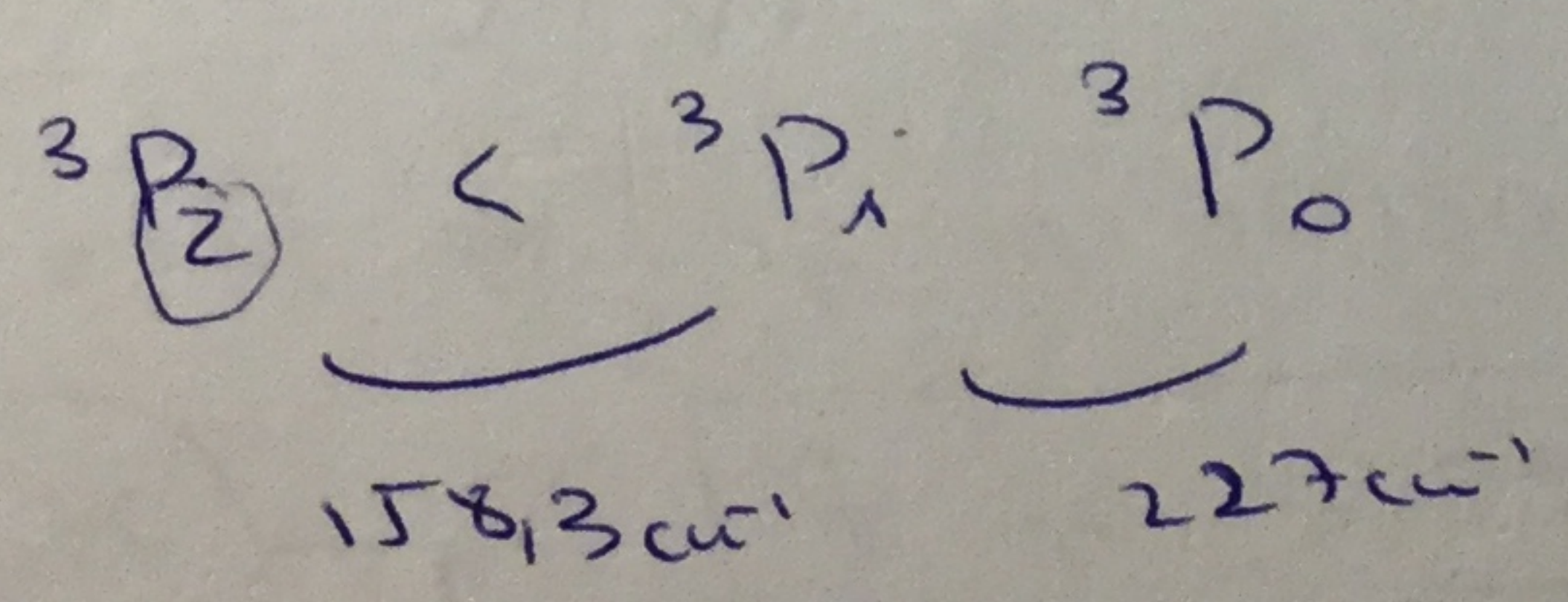
$1 \text{ eV} = 1,602177 \cdot 10^{-19} \text{ J}$

$$Z_{el} = \sum_{i=1} d_i e^{-E_i/kT} = 9 \cdot e^{-E_0/kT} + 5e^{-E_1/kT} + 1e^{-E_2/kT}$$

$$Z_{el} = 9 + 5e^{-\frac{1,967 \cdot 1,602177 \cdot 10^{-19}}{1,380658 \cdot 10^{-23} \cdot 298,15}} + e^{-\frac{4,15 \cdot 1,602177 \cdot 10^{-19}}{1,380658 \cdot 10^{-23} \cdot 298,15}}$$

$Z_{el} = 9$  Novenèr nivell poblat el  $^3P$

b)  $\text{FP}_{el}$   $3P$  es desdoble interacció spin-orbita



- $^3P_2 \rightarrow$  Rotació  $2J+1 \rightarrow d=5$
- $^3P_1 \rightarrow$  Rotació  $2J+1 \rightarrow d=3$
- $^3P_0 \rightarrow$  Rotació  $2J+1 \rightarrow d=1$

$$Z = 5 \cdot e^0 + 3 \cdot e^{-\frac{15813 \text{ cm}^{-1} \cdot 3 \cdot 10^8 \text{ cm} \cdot 100 \cdot h}{5 \cdot kT}}$$

$$+ 1e^{-\frac{22700 \cdot 3 \cdot 10^8 \cdot h}{kT}}$$

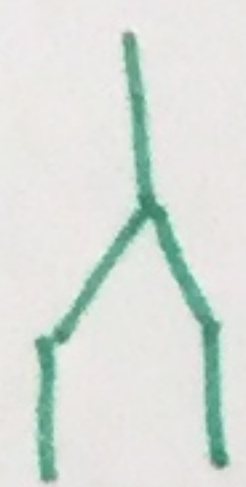
$$Z = 5 + 3e^{-0,76445} + e^{-1,0955}$$

$Z = 6,73$   $Be^-$

Està poblat el  $P_2$  i  $P_1/2$

8 July 2015

2



Emission

$J+1$

$J$

OK

$J$

$(J-1)$

$\lambda_1 = 588,996 \text{ nm}$   
 $\lambda_2 = 589,593 \text{ nm}$

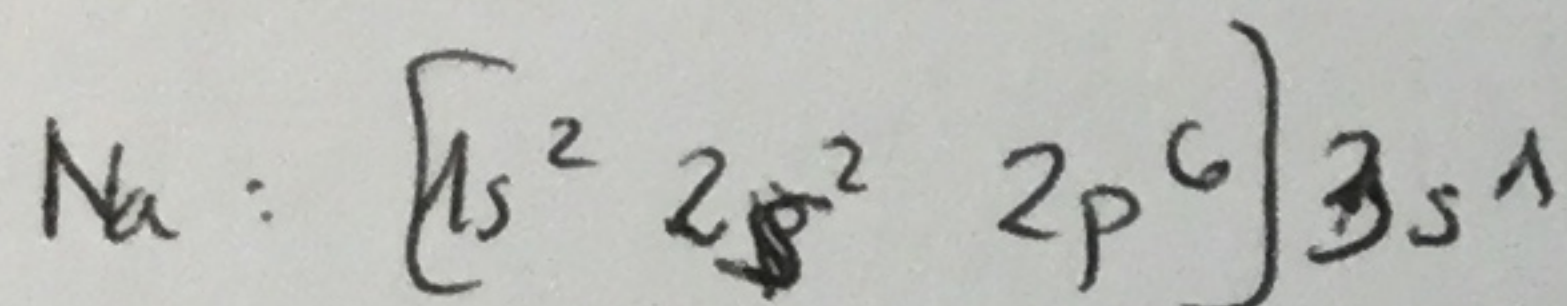
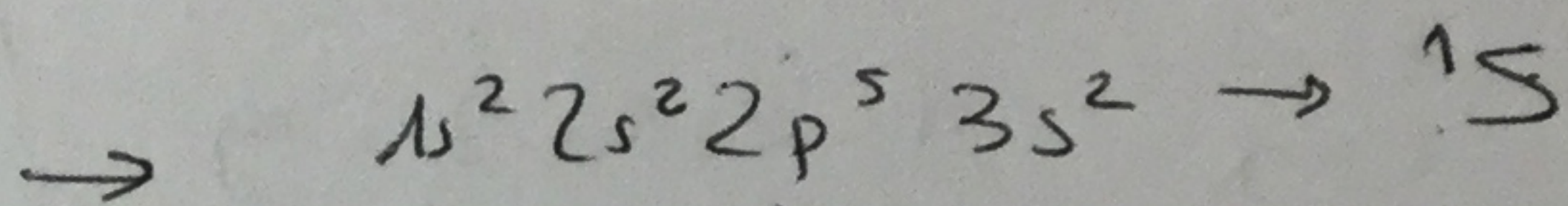
$c = \lambda \cdot \nu$        $\nu = \frac{c}{\lambda}$        $\bar{\nu} = \frac{\nu}{c} = \frac{1}{\lambda}$

$\nu = c \bar{\nu}$

$\bar{\nu} = \frac{1}{588,996 \text{ nm}} \cdot \frac{10^7 \text{ nm}}{1 \text{ cm}} = 16978 \text{ cm}^{-1}$

+J + E

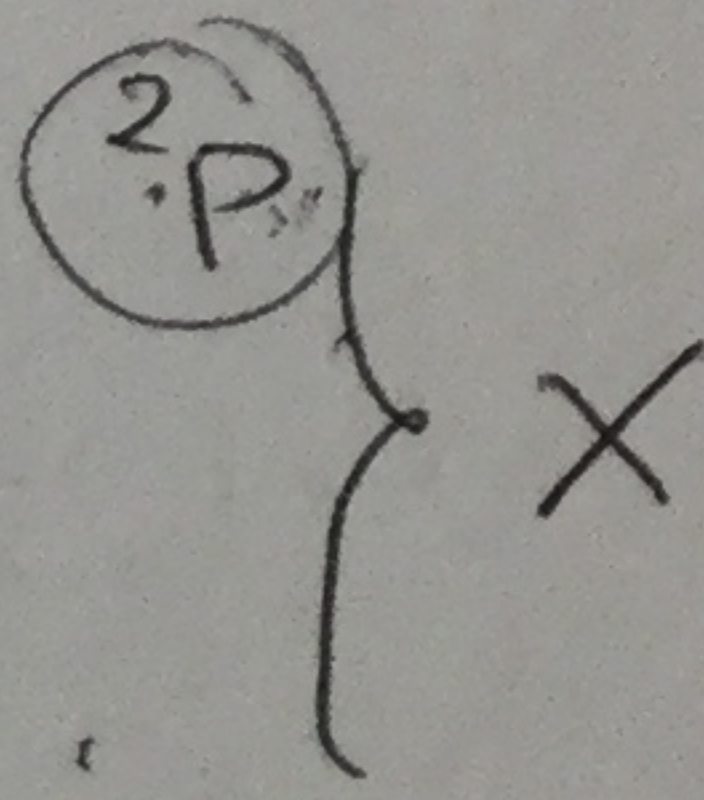
$\frac{\bar{\nu}}{2} = 16960,8 \text{ cm}^{-1}$



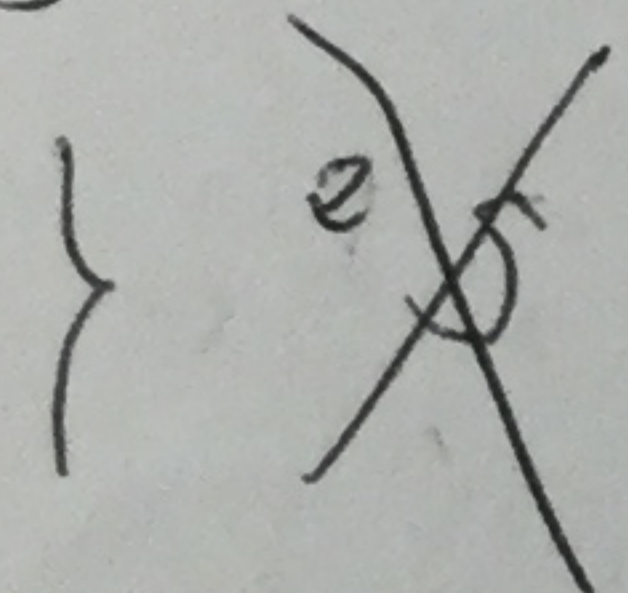
Inversión configuración  $p^5 = p^1$

$s = 1/2$

$L = 1$

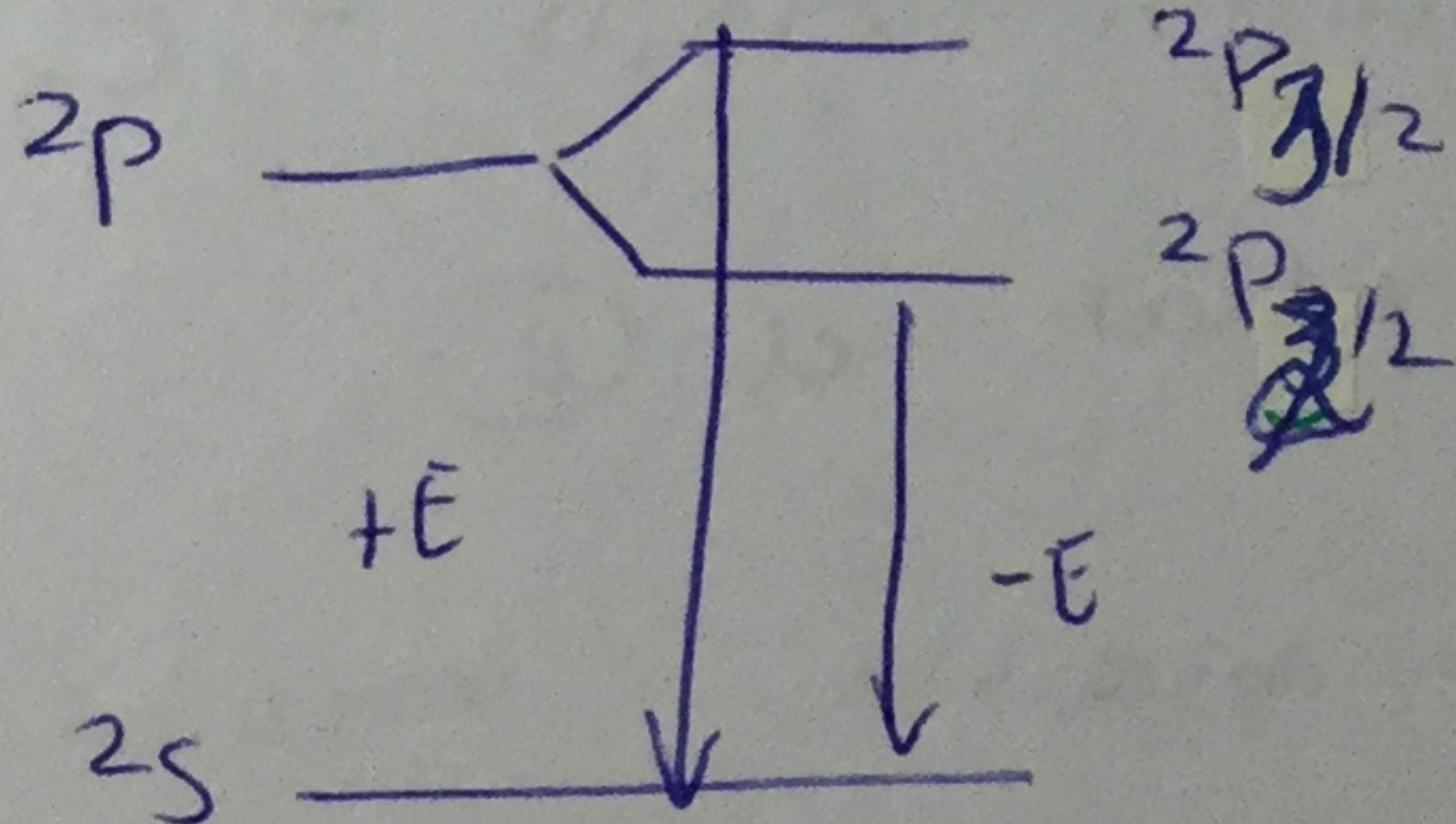
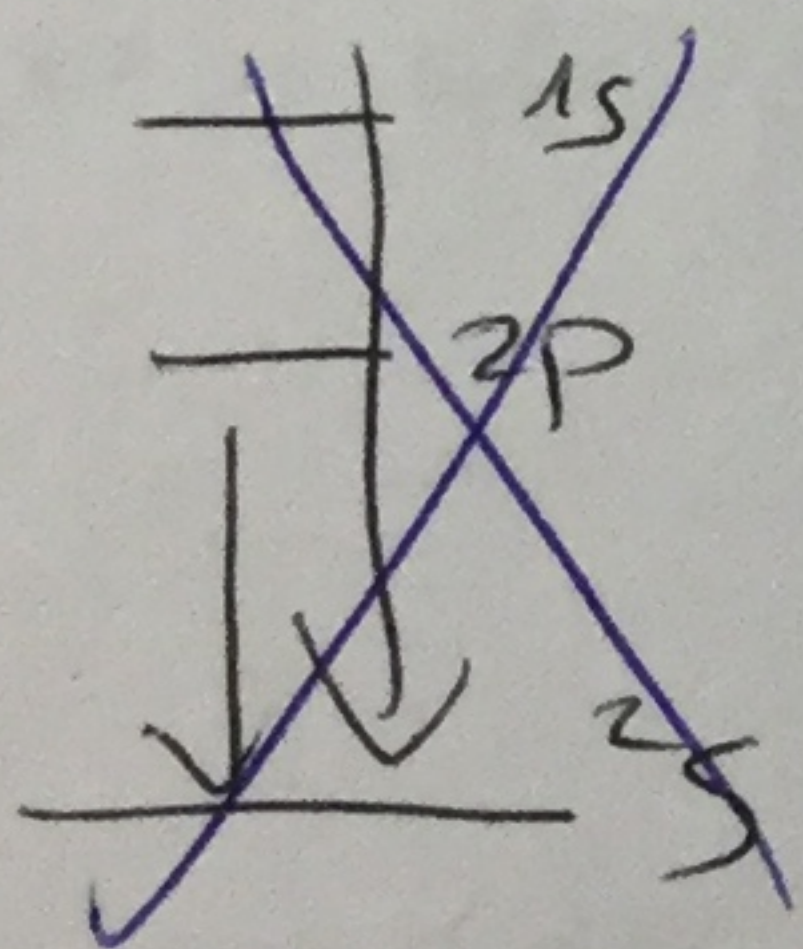


$1S$      $s = 1/2$   
 $L = 0$



$1S$      $s = 0$   
 $L = 0$

Termos esp.  $2P < 1S$



$S_T = 1/2$

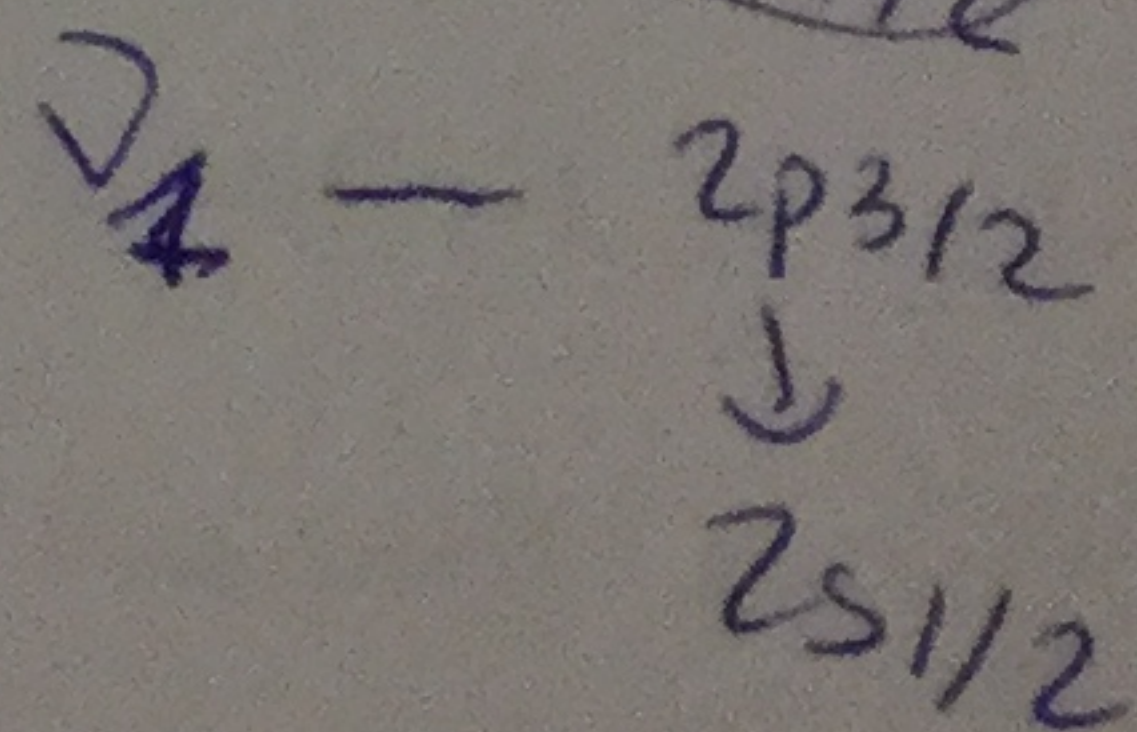
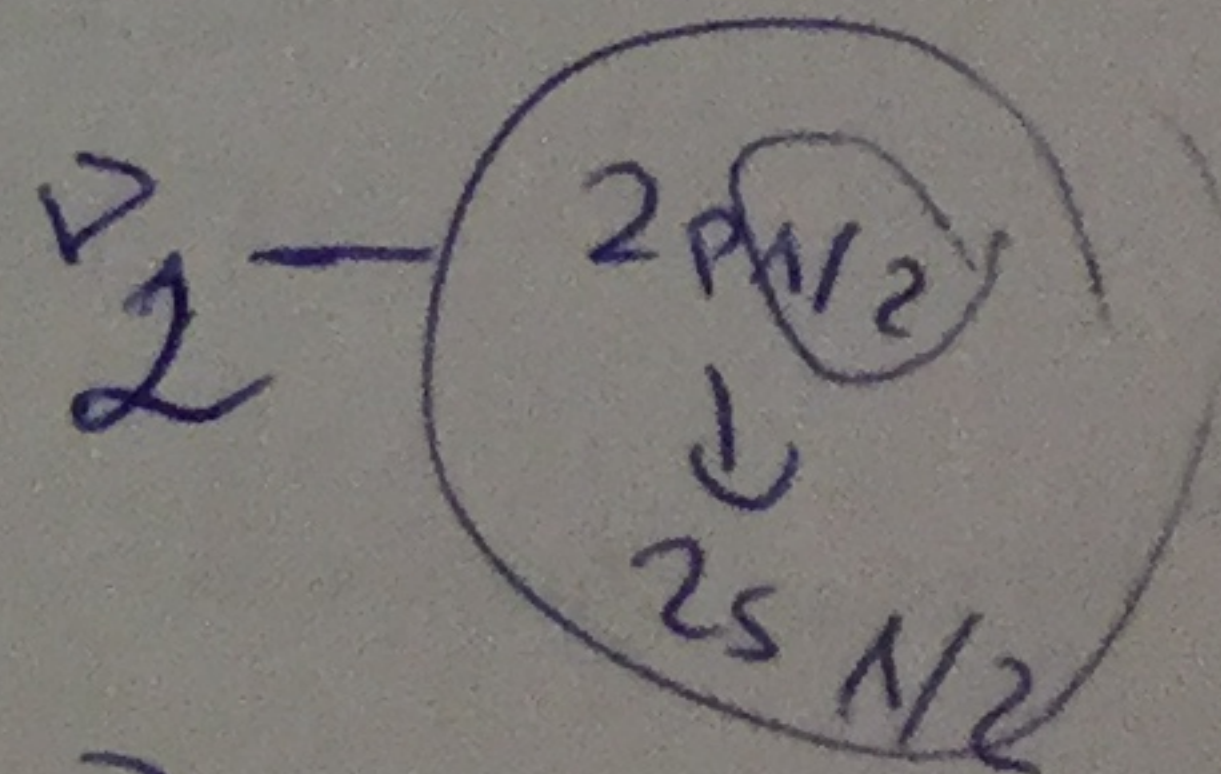
$L = 1$

$J = 3/2, 1/2$

+nu + E

$A = \frac{2 \Delta E_{so}}{[J(J+1) - L(L+1) - S(S+1)]}$

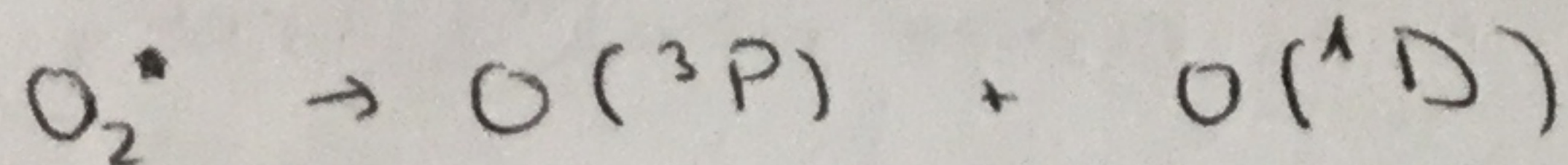
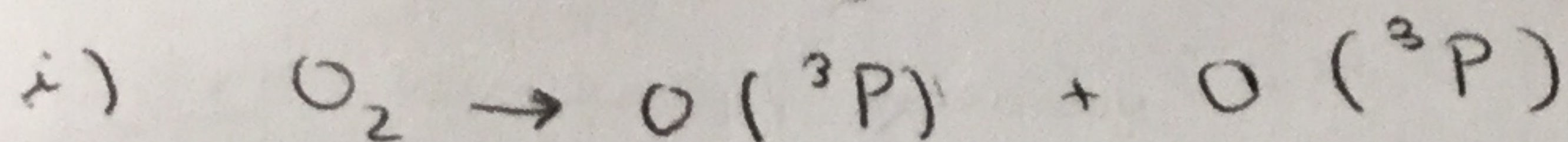
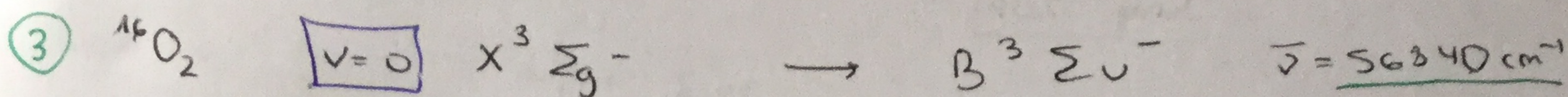
$A = \frac{2 \cdot h c \bar{\nu}}{\frac{1}{2}(3/2) - 1(2) - \frac{1}{2}(3/2)}$



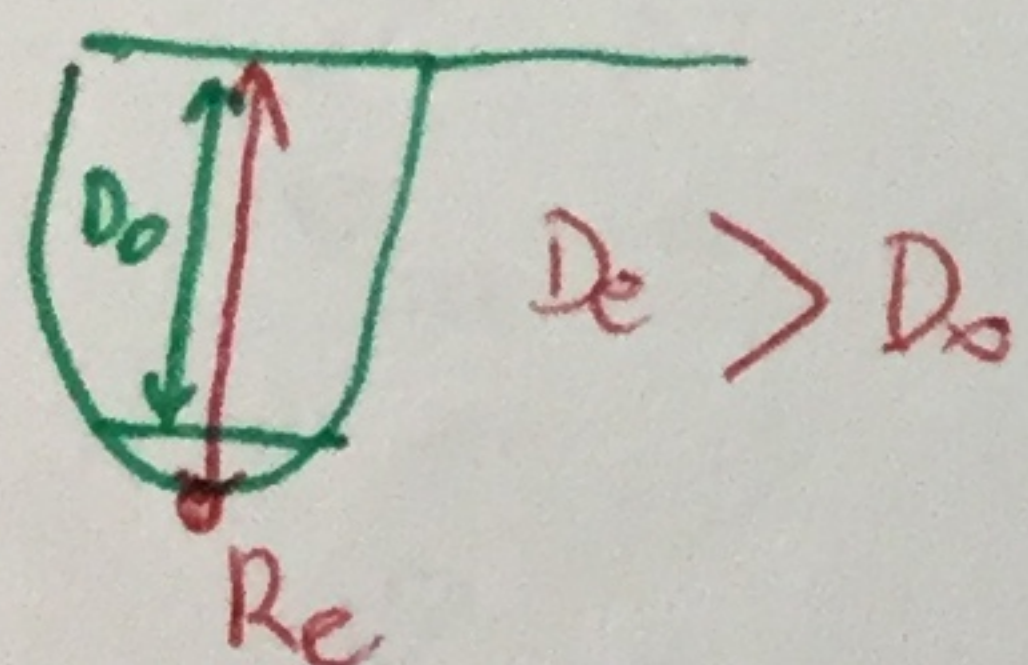
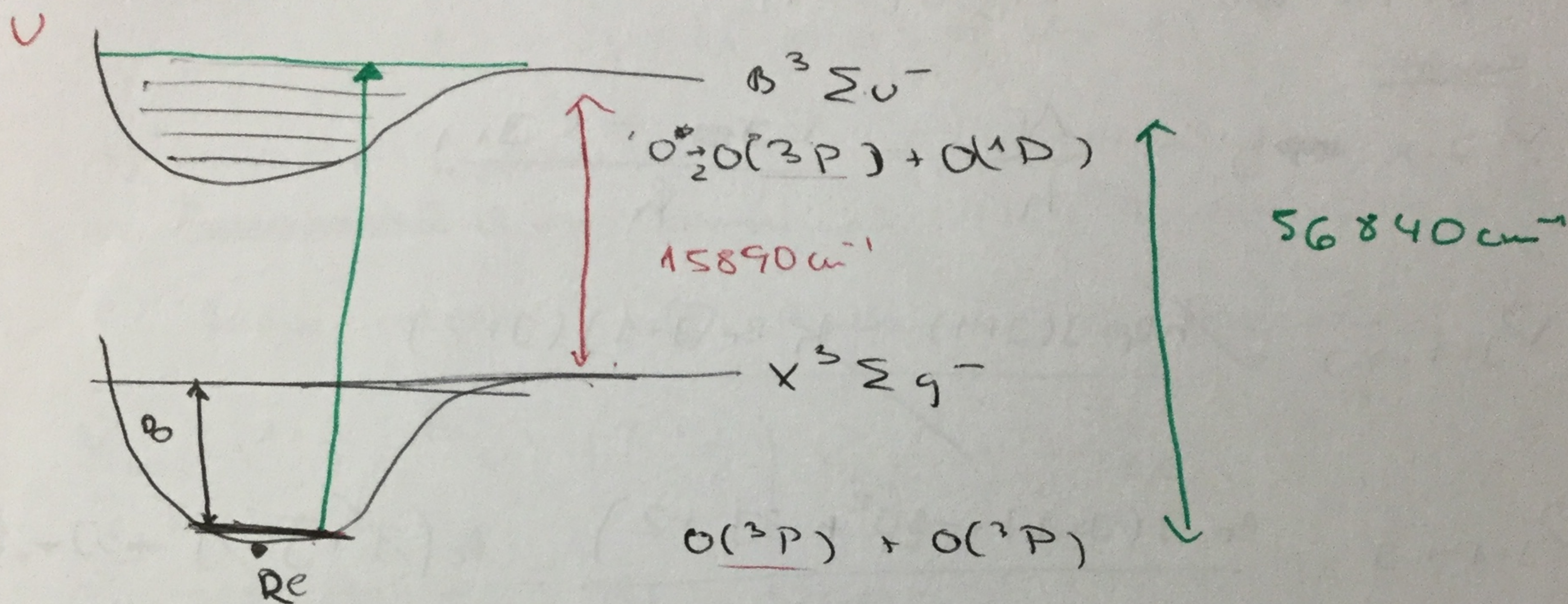
~~$A = h c \bar{\nu}$~~

$A = \frac{2 h c \bar{\nu}}{\frac{3}{2}(5/2) - 1(2) - \frac{1}{2}(3/2)} = \frac{2 h c \bar{\nu}}{\frac{15}{4} - 2 - \frac{3}{4}} = 1$

Enero 2015



$\Delta E (^1\text{D}; ^3\text{P}) = 15890 \text{ cm}^{-1}$



$D_0 = U_\infty - U(v=0)$

$D_0 = \Delta E (B^3\Sigma_u^- \rightarrow X^3\Sigma_g^-) - \Delta E (^1\text{D}; ^3\text{P})$

$D_0 = 40950 \text{ cm}^{-1} \rightarrow \text{J}$

b)  $1580,2 \text{ cm}^{-1} = \bar{\nu}_e$

$D_e = D_0 + \frac{1}{2} \bar{\nu}_e = 40950 \text{ cm}^{-1} + \frac{1}{2} (1580,2 \text{ cm}^{-1})$

$D_e = 40959,9 \text{ cm}^{-1}$

$41740,1 \text{ cm}^{-1}$

July 2014

$^{36}\text{Ar } ^1\text{H}^+$

$v=0$

③ Espectre rotacional d'emissió  
 $\nu_2 = 1234,786 \text{ GHz}$   
 $\nu_1 = 617,554 \text{ GHz}$

Vibració fundamental  $\underline{\underline{v=0}}$   
 Sòlo nivell ③ (rot)

a) Assignar línies:

$$\frac{1234,786 \text{ GHz}}{617,554 \text{ GHz}} = \frac{-2B_e J(J+1)}{-2B_e J(J+1)}$$

Emissió

$$\nu_{J+1 \rightarrow J} = \frac{\Delta E}{h} = \frac{E_J - E_{J+1}}{h}$$

$$\nu_{J+1 \rightarrow J} = \frac{hB_e J(J+1) - hB_e (J+1)(J+2)}{h}$$

$$\nu_{J+1 \rightarrow J} = \frac{B_e J(J+1) - B_e (J^2 + 3J + 2)}{h} = B_e (J^2 + J - J^2 - 3J - 2)$$

$$\nu_{J+1 \rightarrow J} = B_e (-2J - 2) = -2B_e (J+1)$$

$$\nu_{J+1 \rightarrow J} = -2B_e (J+1)$$

$$\nu_{J+2 \rightarrow J+1} = B_e (J+1)(J+2) - B_e (J+2)(J+3)$$

$$\nu_{J+2 \rightarrow J+1} = B_e (J^2 + 3J + 2 - (J^2 + 6J + 6))$$

$$\nu_{J+2 \rightarrow J+1} = B_e (-3J - 4) = -2B_e (J+2)$$

$$\frac{1234,786 \text{ GHz}}{617,554 \text{ GHz}} = \frac{-2B_e (J+2)}{-2B_e (J+1)}$$

$$2 = \frac{J+2}{J+1}$$

$$2J+2 = J+2$$

$$\boxed{J=0}$$

GEN 2014

3. m.n.v.  $\underline{3N-6} = 3 \text{ m.n.v}$

no lineal  
 $\bar{\nu}_{1e} = 1304 \text{ cm}^{-1}$   
 $\bar{\nu}_{2e} = 981 \text{ cm}^{-1}$   
 $\bar{\nu}_{3e} = 512 \text{ cm}^{-1}$

- a)  $(1, 2, 0) \leftarrow (0, 0, 0)$
- b)  $(0, 1, 1) \leftarrow (0, 0, 0)$   $f_{15} / c / ca$
- c)  $(1, 0, 0) \leftarrow (0, 0, 0)$
- d)  $(0, 2, 0) \leftarrow (0, 0, 0)$
- e)  $(0, 0, 2) \leftarrow (0, 0, 0)$
- f)  $(1, 0, 0) \leftarrow (0, 0, 1)$

- a) Banda de combinación
- b) ~~fundamental~~ Banda combinación
- c)  $\bar{\nu}_{2e}$  fundamental
- d) 1<sup>o</sup> overtone
- e) Banda caliente
- f) Banda de combinación

$$\bar{\nu}_{120} = \left(1 + \frac{1}{2}\right) \bar{\nu}_{1e} + \left(2 + \frac{1}{2}\right) \bar{\nu}_{2e} + \frac{1}{2} \bar{\nu}_{3e}$$

$$\bar{\nu}_{120} = 1.5 \cdot 1304 + 2.5 \cdot 981 = 3266 \text{ cm}^{-1}$$

$$\bar{\nu}_{011} = 981 + 512 = 1493 \text{ cm}^{-1}$$

$$\bar{\nu}_{100} = 1304 \text{ cm}^{-1}$$

$$\bar{\nu}_{020} = 1962 \text{ cm}^{-1}$$

$$\bar{\nu}_{002} = 512 \text{ cm}^{-1}$$

$$f) \bar{\nu}_{100} \leftarrow 001 = 1304 - 512 = \underline{792 \text{ cm}^{-1}}$$

July 2015

$\nu = 1$  poblat!!

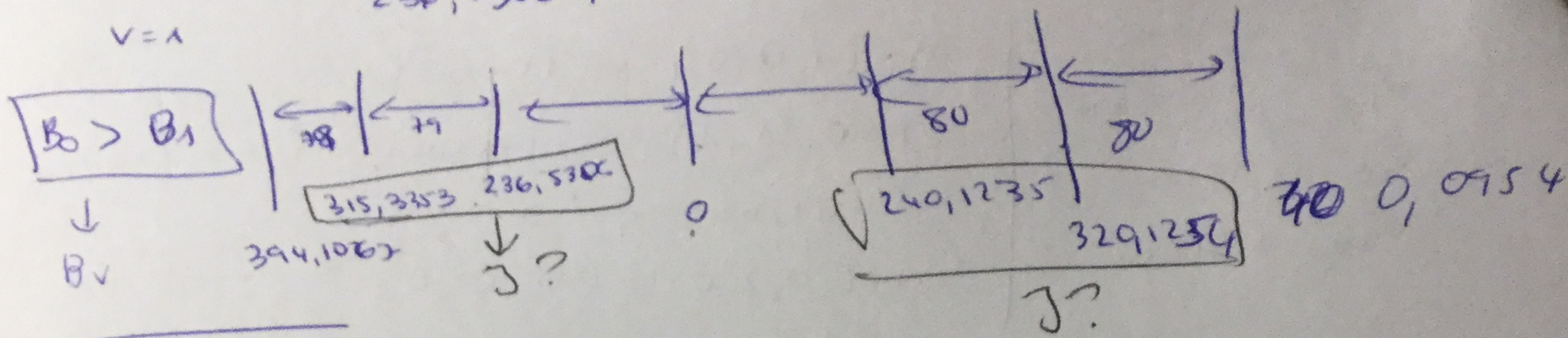
3

Rotació per

$7L$  19 F

236,5306, 240,1235, 315,3353

$v = 1$



$$\frac{315,3353}{236,5306} = \frac{hBe(J+2)(J+3) - hBe(J+1)(J+2)}{hBe(J+1)(J+2) - hBe(J)(J+1)}$$

$$1,333 = \frac{J^2 + 5J + 6 - J^2 - 3J - 2}{2J + 2} = \frac{2J + 4}{2J + 2}$$

~~$$J^2 + 1,333J + 1,333J - 2J - 2 = 0$$

$$1,333J - 0,666J - 2 = 0$$

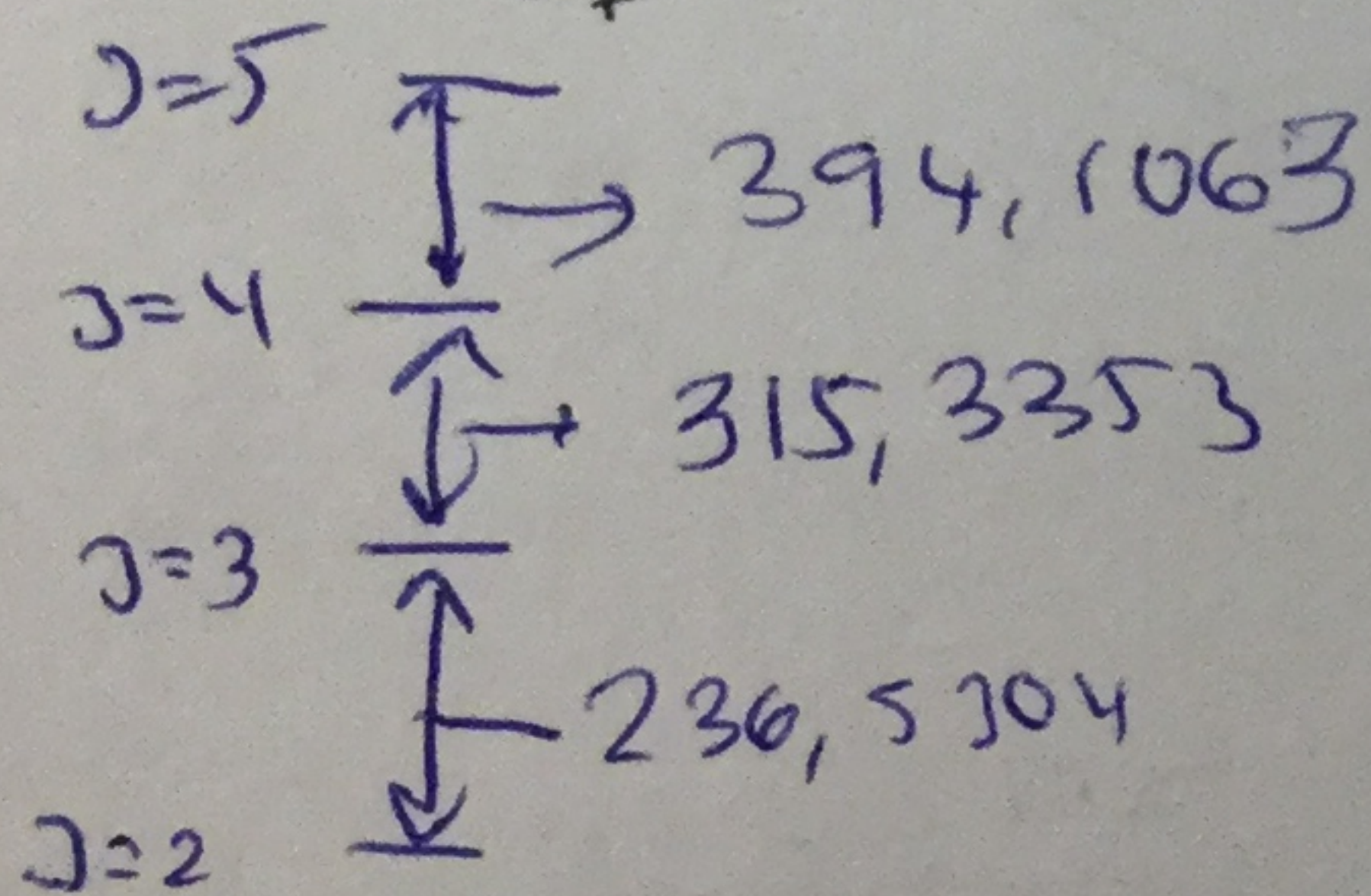
$$J = 1,5$$~~

$$1,333 \cdot 2J + 2 \cdot 1,333 = 2J + 4$$

$$1,333J + 1,333 = J + 2$$

~~$$0,333J = 0,666$$~~

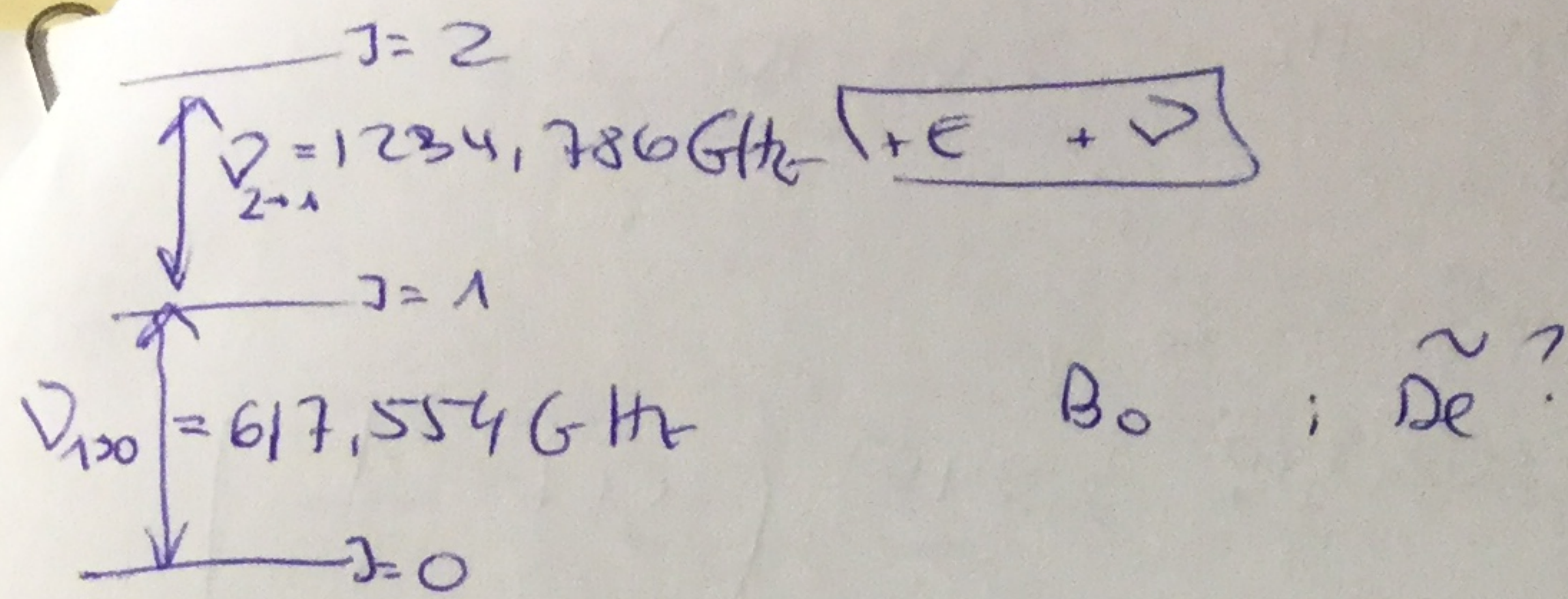
$$J = 2$$



$$B_v = 39,43 \text{ cm}^{-1}$$

$$B_{De} = 3,461 \cdot 10^{-4} \text{ cm}^{-1}$$

Calcular J:



$$E_{rot}(v, J) = h B_0 J(J+1) - h \tilde{D}_e J^2(J+1)^2$$

$$\begin{aligned} \nu_{2 \rightarrow 1} &= 1234,786 \text{ GHz} = \frac{h B_0 (2) - h \tilde{D}_e 1(2)^2}{h} - \frac{h B_0 (1) + h \tilde{D}_e 4 \cdot 9}{h} \\ \nu_{1 \rightarrow 0} &= 617,554 \text{ GHz} = \frac{h B_0 (1) - h \tilde{D}_e 1(1)^2}{h} - \frac{h B_0 (0) + h \tilde{D}_e 0}{h} \end{aligned}$$

$$2 = \frac{2B_0 - 4\tilde{D}_e - B_0 + 36\tilde{D}_e}{4\tilde{D}_e - 2B_0} = \frac{-B_0 + 32\tilde{D}_e}{4\tilde{D}_e - 2B_0}$$

$$1 = \frac{-B_0 + 16\tilde{D}_e}{-2B_0 + 4\tilde{D}_e} \rightarrow 4\tilde{D}_e - 2B_0 = +16\tilde{D}_e - B_0$$

$$\begin{cases} 1234,786 = 32\tilde{D}_e - 4B_0 \\ 617,554 = 4\tilde{D}_e - 2B_0 \end{cases} \rightarrow \begin{cases} 617,552 = 16\tilde{D}_e - 2B_0 \\ 617,554 = 4\tilde{D}_e - 2B_0 \end{cases} \rightarrow B_0 = \frac{16\tilde{D}_e - 617,552}{2}$$

~~$$B_0 = \frac{617,554 + 2B_0}{4} = \frac{617,554 + 32\tilde{D}_e - 2(617,554)}{4}$$

$$4\tilde{D}_e = -617,554 + 16\tilde{D}_e \rightarrow \tilde{D}_e = \frac{617,554}{28} = 22,06$$~~

$$\begin{aligned} x = \tilde{D}_e &= -0,013 \rightarrow y = 0,013 \\ y = B_0 &= -309,8 = 308,8 \end{aligned}$$

$\bar{\nu} < 0 \rightarrow \tilde{D}_e > 0$   
 $B_e$

$$\alpha = 3,0 \text{ GHz} = 3,0 \cdot 10^9 \text{ Hz}$$

$$n_e? \quad B_V = 308,8$$

$$B_e = 308,8 \cdot 10^3 + 3,0 \cdot 10^9 \left( \alpha + \frac{1}{2} \right)$$

$$B_e = 3,103 \cdot 10^{11} \text{ Hz}$$

$$r_e = \sqrt{\frac{h}{8 \pi^2 \mu B_e}} = 1,289 \cdot 10^{-10} \text{ m}$$

$$= 1,29 \text{ \AA}$$

$$\mu = \frac{36}{37}$$



GEN 2013

3

