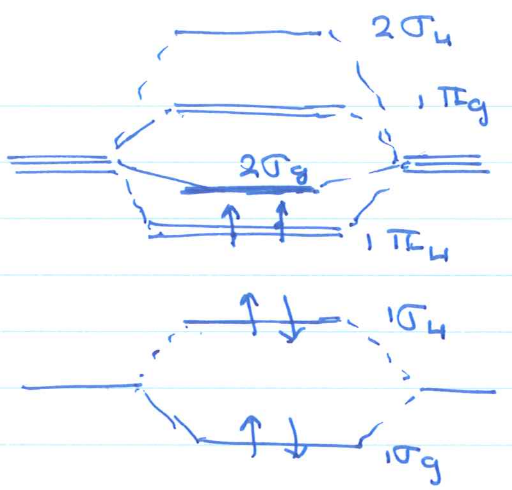
1) B_2



$B\ (1s^2 2s^2 2p)$.
$\overline{\ \ 3\ \ }$
$3 \times 2 = 6$

a)

b) B_2^- $+1$ el. (in $1\pi_u$) bonding $B = \frac{1}{2}(5-2) = \frac{3}{2}$
B_2 $= 1$
B_2^+ -1 el. $= \frac{1}{2}$.

c) $1\sigma_g^2 1\sigma_u^2 1\pi_u^2$

d) i) $\pi_u \longrightarrow \lambda = \pm 1$
triplet spin $m_{s_1} = m_{s_2}$ even under exchange.
fermions $\longrightarrow \lambda_1 \neq \lambda_2 \Longrightarrow \Lambda = -1+1 = 0 \Rightarrow \Sigma$

ii) inversion symm. $1\pi_u$ $\Big\} \Longrightarrow u \times u = g$.

iii) mirror plane symm. $+/-$?
$+ \times - \longrightarrow - \Longrightarrow {}^3\Sigma_g^-$

2 $\varphi = 3\phi_a + 2\phi_b$

$|\varphi|^2 = 1 = C^2 |\langle \varphi^* | \varphi \rangle|^2 = C^2 \{ \langle 3\phi_a + 2\phi_b | 3\phi_a + 2\phi_b \rangle|^2$

$C^2 \{ 9 |\phi_a|^2 + \cancel{12}\ 6 |\underbrace{\langle \phi_a | \phi_b \rangle}_{S'}|^2 + 6 |\underbrace{\langle \phi_b | \phi_a \rangle}_{S'}|^2 + 4 |\langle \phi_b \rangle|^2 \}$.

$C^2 (13 + 12 S') = 16 C^2 = \longrightarrow C = \frac{1}{4}$
$\Longrightarrow \varphi = \frac{3\phi_a + 2\phi_b}{4}$.

b $\frac{9}{16} - \frac{4}{16} = \frac{5}{16}$ $|\langle \phi_a | \varphi \rangle|^2 = \left|\frac{3}{4}\phi_a\right|^2 + \left|\frac{1}{2}\langle \phi_a | \phi_b \rangle\right|^2$

$= \frac{9}{16} + \frac{1}{4} S' = \frac{10}{16}$

$|\langle \phi_b | \varphi \rangle|^2 = \frac{3}{4} S' + \frac{1}{4} = \frac{3}{16} + \frac{4}{16} = \frac{7}{16}$

$P = |\langle \phi_a | \psi \rangle|^2 =$

$\langle \phi_a | \psi \rangle = \frac{3}{4}\phi_a^2 + \frac{1}{2}\phi_a\phi_b = \frac{3}{4} + \frac{1}{8} = \frac{7}{8} \Rightarrow \frac{49}{64}$

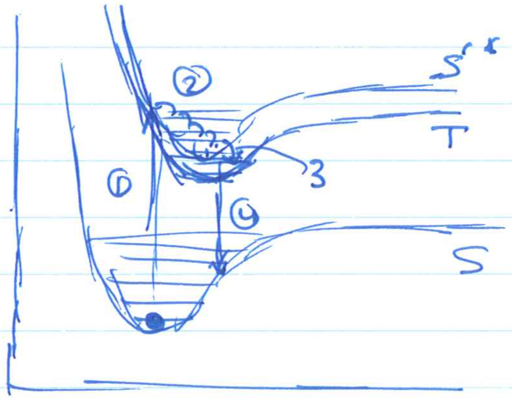
$\langle \phi_b | \psi \rangle = \frac{3}{4}\phi_b\phi_a + \frac{1}{2}\phi_b^2 = \frac{3}{16} + \frac{1}{2} = \frac{11}{16} \Rightarrow \frac{121}{256}$

$\frac{196}{256} - \frac{121}{256} = \frac{75}{256}$.

c $\psi = 3\phi_a + 2\phi_b$

orthoganal $\psi^* = 2\phi_a - 3\phi_b$.

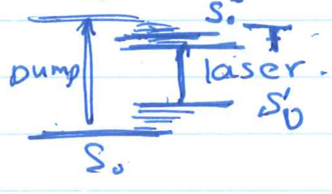
3.a)



① FC vertical.
② radiation less decay → vibr. ladda collisions
③ $S^* \to T$ ISC intersysten crossing. "spin-orbit"

4) phosphorescence. again FC.

b) long-lived upperlevel



4 XY_2. sp

linear

$E_{rot} = \tilde{B} J(J+1)$.

$\Delta E = \tilde{B}(J+1)(J+2) - \tilde{B}(J(J+1)$
$= 2(J+1)\tilde{B}$

$16 = 2(J+1)\tilde{B}$ $\qquad 18 = 2(J+2)\tilde{B} = 2J\tilde{B} + 4\tilde{B}$

$= 2JB + \tilde{B}$

$\Longrightarrow 2J\tilde{B} = 16 - 2\tilde{B}$ $\qquad \Longrightarrow 18 = 16 - 2\tilde{B} + 4\tilde{B}$

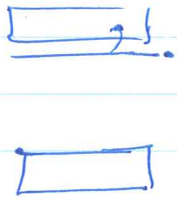
$2 = 2\tilde{B} \Longrightarrow \tilde{B} = 1$

$\Longrightarrow J(J+1) = 56 \Longrightarrow J = 7.$

c) there is a rot. spectr. thus its polar / dip. moment
XXY. isotope not necessary.

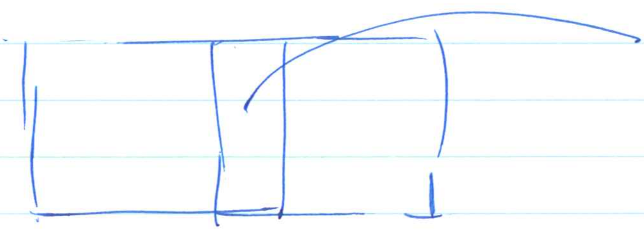
5 a) intrinsic pure.

b) donor

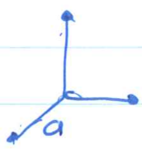


small fraction. with
$E_{ion} \sim$ bottom cond. band.

c)



6



a^3

$a_1 = a$
$a_2 = 2a$
$a_3 = 3a$

$b = \frac{2\pi}{a} = \left(\frac{2\pi}{a}\right)^3$

Miller indices normal of the planes.
smallest set of integers.

$\Longrightarrow d = \frac{2\pi}{|g|}$

$\sqrt{4+9+1} = \sqrt{14}\,a.$ $\qquad \bar{g} = n_1\hat{b}_1 + n_2\hat{b}_2 + n_3\hat{b}_3$

$b_i = \frac{2\pi}{a} \longrightarrow |\bar{g}| = \frac{2\pi}{a}\sqrt{14} \Longrightarrow d = a/\sqrt{14}$

7 $\psi = A e^{ik_x x} e^{ik_y y}$ $\longrightarrow$ $k_i = \frac{2\pi}{L} n_i$

per. B.-von K $\rightarrow$ $\psi(x+L) = \psi(x)$

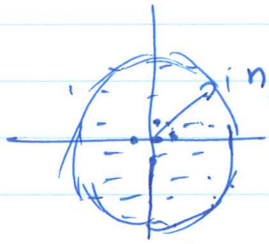
id. y.

a $\psi(x+L) = A e^{ik_x(x+L)} e^{ik_y y} = \psi(x) e^{ik_x L} = \psi(x) \underbrace{e^{i2\pi n_i}}_{=1}$

b $E\psi = \frac{-\hbar^2}{2m}\left\{\frac{\partial^2}{\partial x^2}\psi + \frac{\partial^2}{\partial y^2}\psi\right\} \Longrightarrow$

$= \frac{\hbar^2}{2m}(k_x^2 + k_y^2) = \frac{2\hbar^2\pi^2}{mL^2}(n_x^2 + n_y^2). = 2\frac{\hbar^2\pi^2}{mL^2} n^2$

c. traveling waves k_x and k_y $-\infty - \infty$



$2(4\pi n_F^2) = N.$

spin $\quad n_F^2 = \frac{N}{8\pi}$

$\Longrightarrow E_F = 2\frac{\hbar^2\pi^2}{mL^2}\frac{N}{8\pi} = \frac{\hbar^2\pi}{4mL^2} N.$

$L = 10^5 a \Longrightarrow$ ~~10^{10}~~

$N = 10^5 \cdot 5\times10^4 = 5\times10^9$ $\Bigg\} \frac{N}{L^2} = \frac{1}{2a^2}$

$\Longrightarrow E_F = \frac{\pi}{8} \cdot \frac{\hbar^2}{ma^2}$

d reciprocal lattice $k_x = \frac{2\pi}{a}$ $\quad k_y = \frac{2\pi}{2a}$

$\Longrightarrow k_y < k_x \quad E_{1y} = \frac{\hbar^2}{2m} k_{y1}^2 = \frac{\pi^2}{2}\frac{\hbar^2}{ma^2}$

$E_F / E_{1y} = \frac{\pi}{8}\frac{2}{\pi^2} = \frac{1}{4\pi}$! $\sim 8\%$

e $E_2 > E_F$ $\quad \frac{\hbar^2}{m}\frac{2\pi^2}{d^2} > \frac{\pi}{8}\frac{\hbar^2}{ma^2} \quad \frac{2\pi^2}{d^2} > \frac{\pi}{8a^2}$

$8\pi a^2 > d^2 \quad d < 2\sqrt{2\pi}\, a. \sim 5a.$