

ATOMS, MOLECULES & REACTIONS

QUANTUM MECHANICS, SPRING 2006, WEEK 6 HW

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$$\textcircled{1} \hat{P}_{12} \psi = \hat{P}_{12} \frac{1}{\sqrt{2} [2(s+1)]} \left\{ \begin{array}{l} \psi_A(1) \psi_A(2) + \psi_A(1) \psi_B(2) + \\ \psi_B(1) \psi_A(2) + \psi_B(1) \psi_B(2) \end{array} \right\} \left\{ \alpha(1) \beta(2) - \beta(1) \alpha(2) \right\}$$

$$= \frac{1}{\sqrt{2} [2(s+1)]} \left\{ \begin{array}{l} \psi_A(2) \psi_A(1) + \psi_A(2) \psi_B(1) + \psi_B(2) \psi_A(1) + \\ \psi_B(2) \psi_B(1) \end{array} \right\} \left[\alpha(2) \beta(1) - \beta(2) \alpha(1) \right]$$

↑
spatial part is the same as ψ

spin part is the negative of ψ

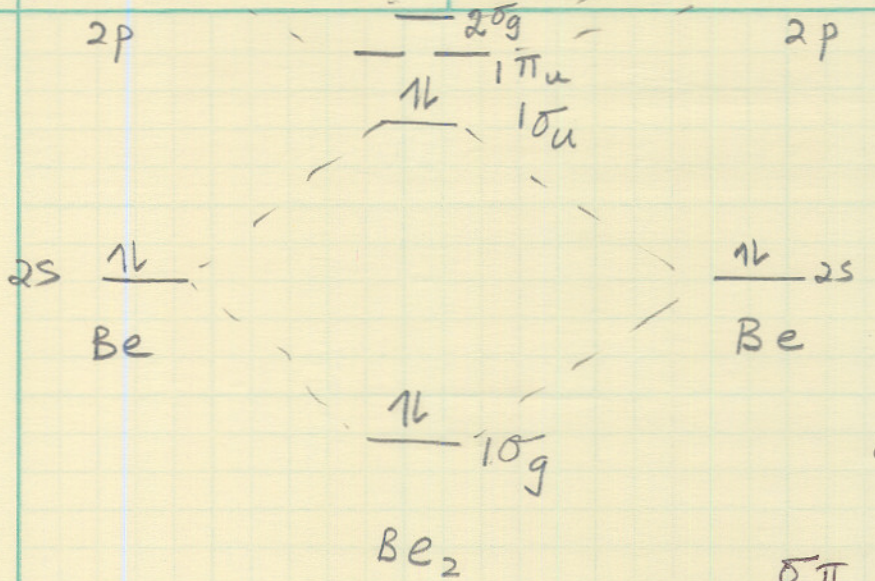
$$= -\psi$$

∴ ψ is antisymm. w.r.t. the permutation operator.

2/

Be₂

(2)



Ground state = $^1\Sigma_g^+$

First excited state
config: = $1\sigma_u^1 1\pi_u^1$

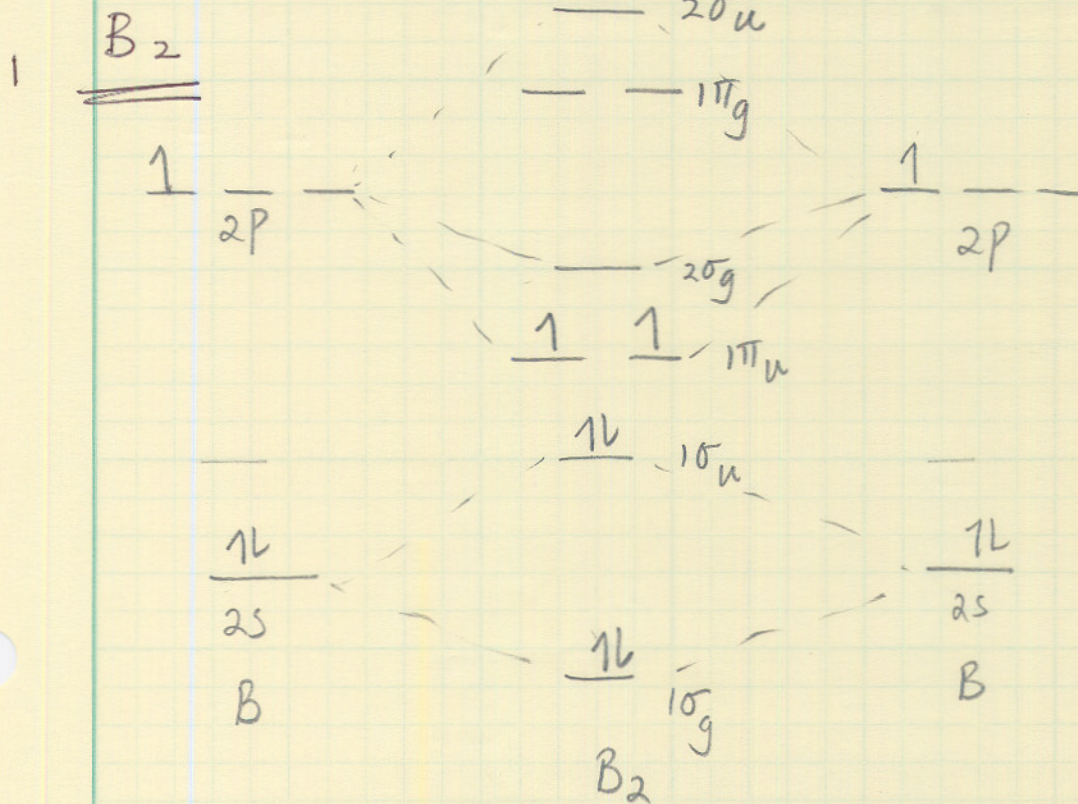
$\sigma\pi \Rightarrow M_L = \pm 1$

$\Lambda = 1$

$S = 0, 1$

$^1\Pi_g$ $^3\Pi_g$ $u \times u = g$

$^3\Pi_g$ is first excited state



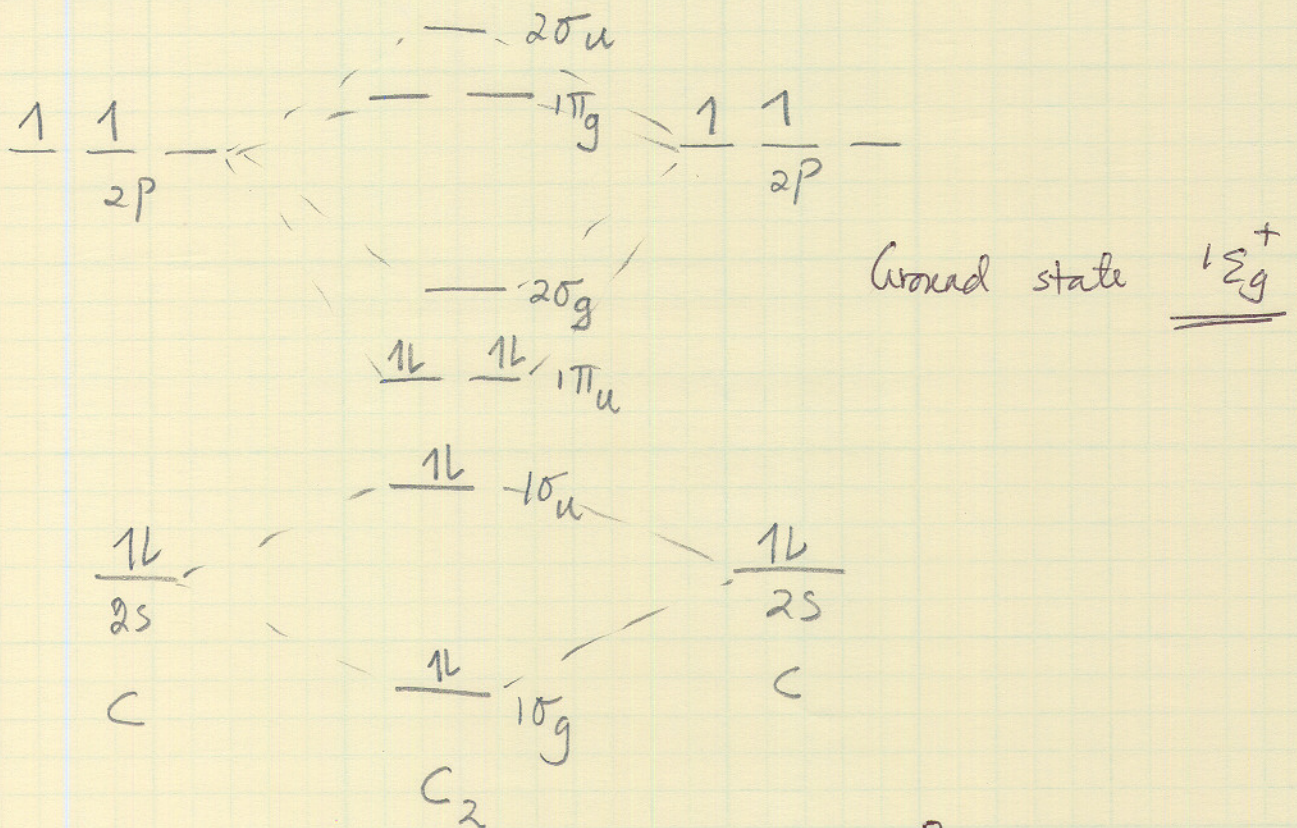
π^2 config: ${}^1\Delta$ $({}^3\Sigma^-)$ ${}^1\Delta^+$ $u \times u = g$

${}^3\Sigma_g^-$ ground state

First excited state: ${}^1\Pi_u$ ${}^2\sigma_g$ ${}^1\Pi_u$ ${}^3\Pi_u$ terms

${}^3\Pi_u$ first excited state

C_2



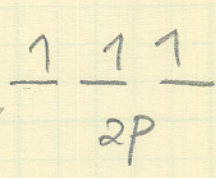
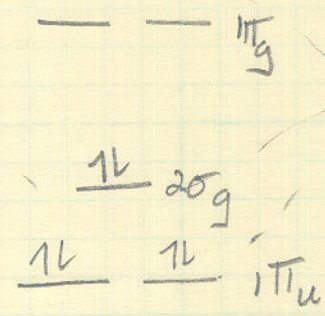
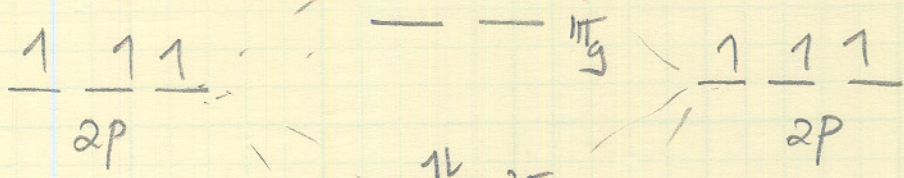
First ex. state: ${}^1\Pi_u$ ${}^3\sigma_g$

$$\left. \begin{array}{l} m_{l_1} = \pm 1 \\ m_{l_2} = -1 \\ m_{l_3} = \pm 1 \end{array} \right\} \Rightarrow M_L = \pm 1$$

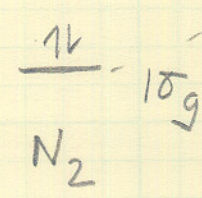
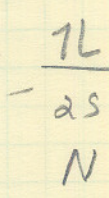
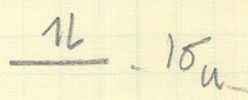
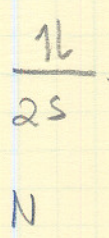
$$S = 0, 1$$

$\Lambda = 1, S = 0, 1$

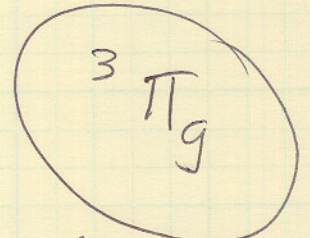
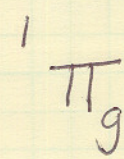
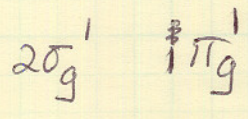
${}^1\Pi_u$ $({}^3\Pi_u)$ ← first excited state



gr. state = $^1\Sigma_g^+$

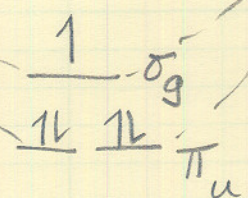
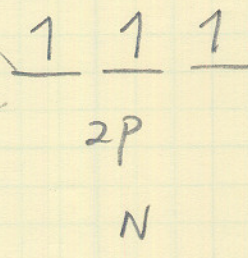
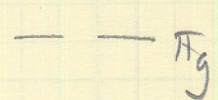
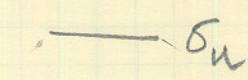
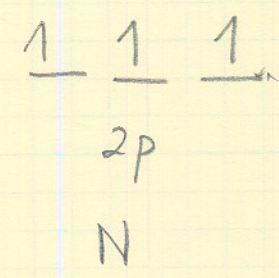


1st ex. state:



first ex. state

N_2^+



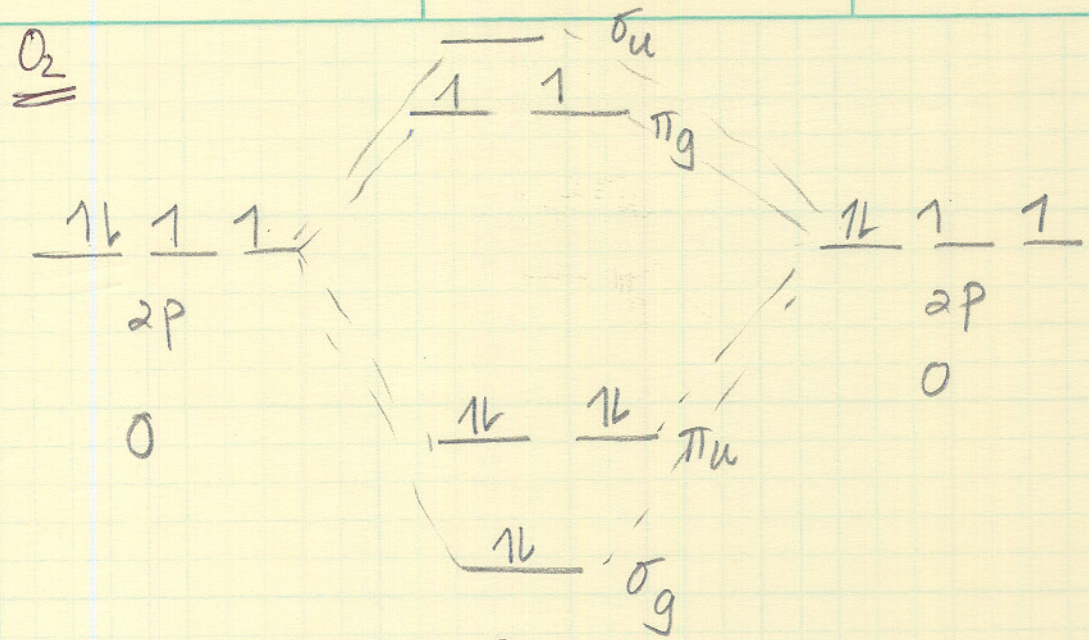
N_2^+

$^2\Sigma_g^+$

ground state

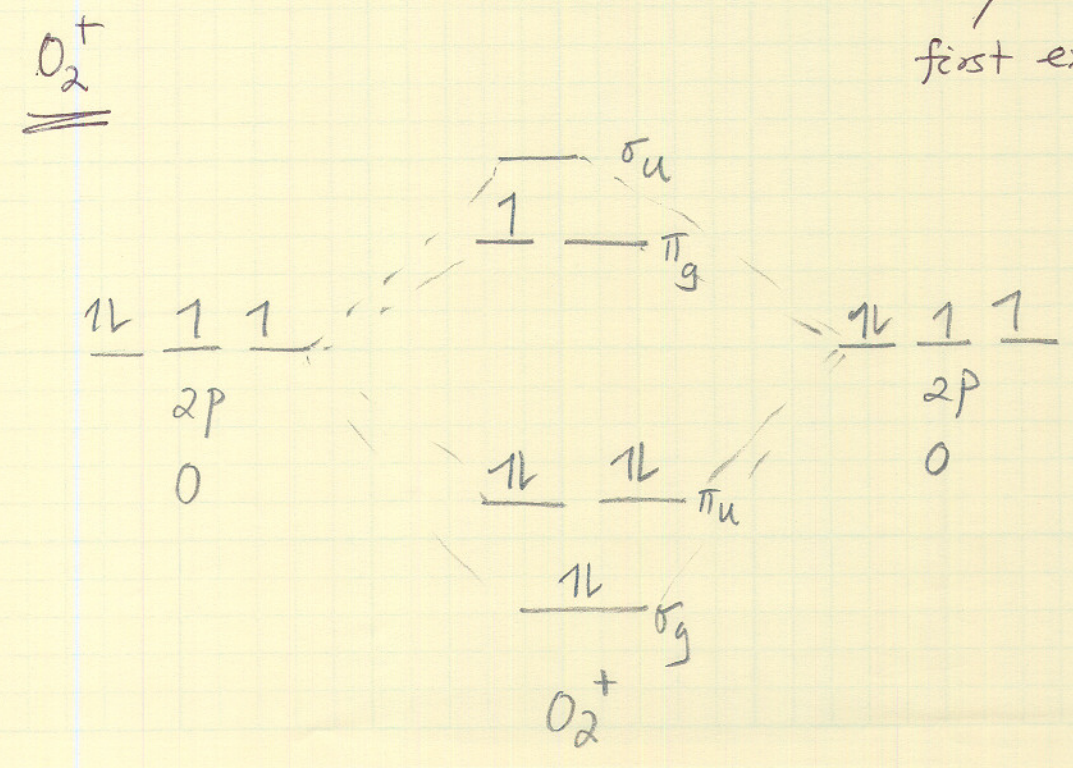
$^2\Pi_g$

excited state

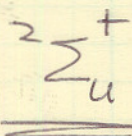


Ground state π_g^2 $^1\Delta_g$ $3\Sigma_g^-$ $^1\Sigma_g^+$
 ↓
 ground state

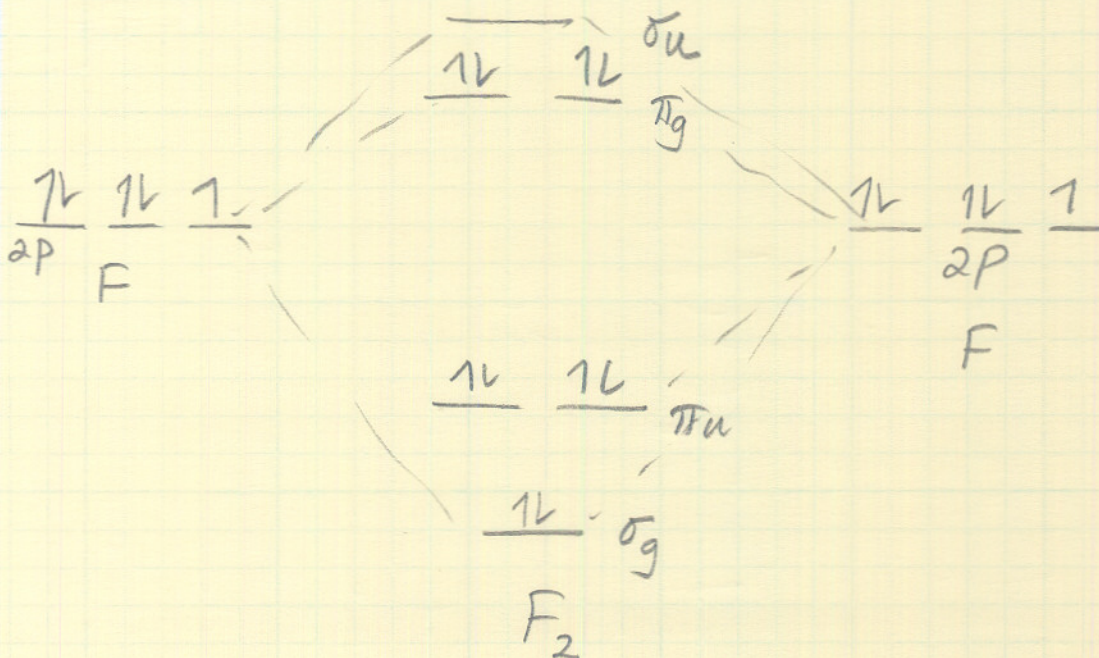
first ex-state $\pi_g^1 \sigma_u^1$ $^1\pi_u$ $3\pi_u$
 first ex-state



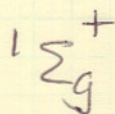
First ex. state:



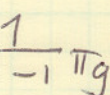
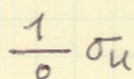
F₂



gr. state

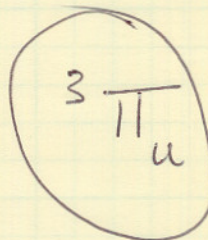
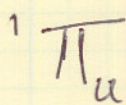


First ex. state

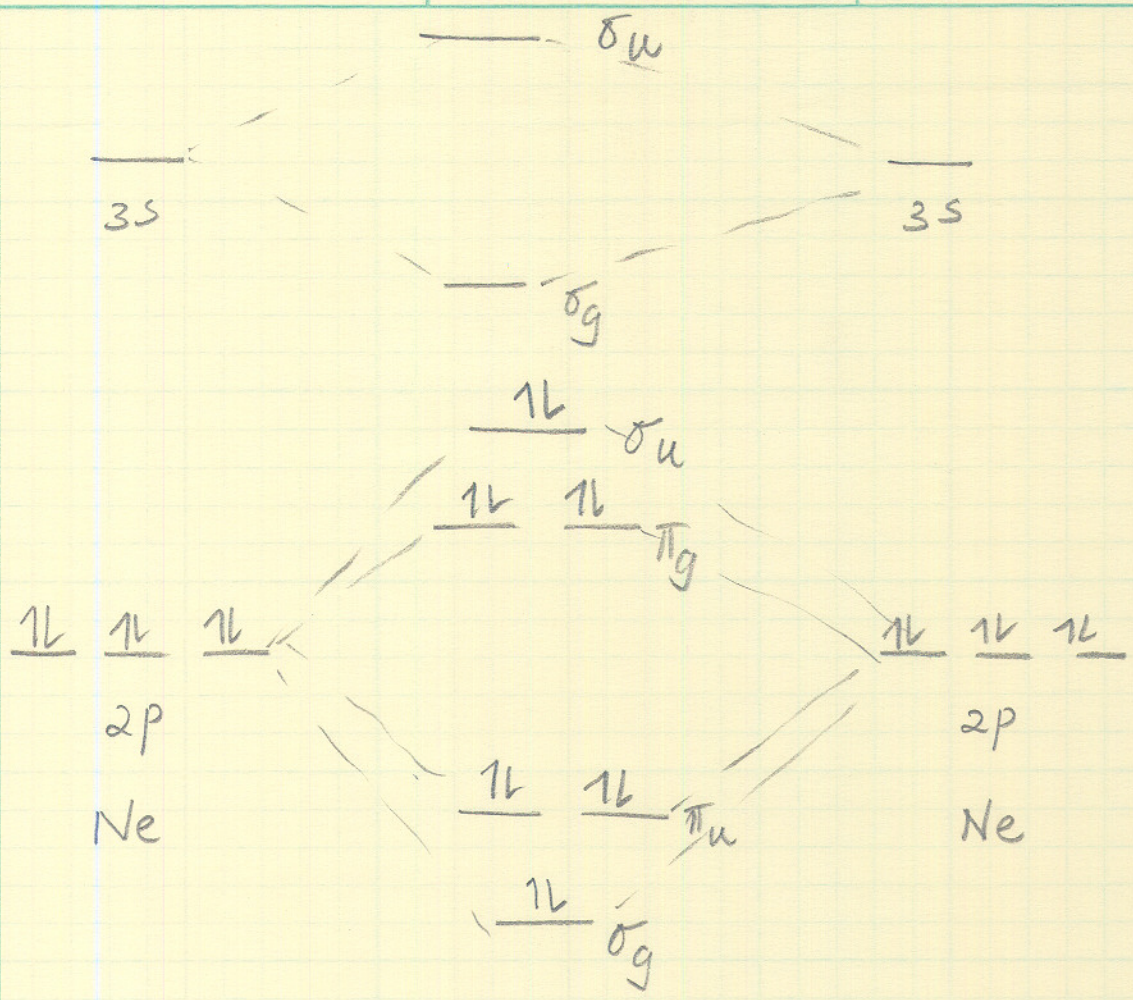


$$\left. \begin{array}{l} m_{l_1} = +1 \\ m_{l_2} = +1 \\ m_{l_3} = \pm 1 \\ m_{l_4} = 0 \end{array} \right\} \begin{array}{l} M_L = \pm 1 \\ \Lambda = 1 \end{array}$$

$$S = 0, 1$$



← first ex. state.



gr. state $1\Sigma_g^+$

1st ex. state $\sigma_u^1 \sigma_g^1$

$1\Sigma_u^+$ $3\Sigma_u^+$
 1st ex. state -