

# A LITTLE QUANTUM MECHANICS:

$$\Psi_{\text{molecule vib}} = \Psi_1(n_1) \Psi_2(n_2) \dots \Psi_k(n_k) \quad k = 3N - 6$$

$n_i = 0$  ALL  $i$  GROUND STATE

FOCUS ONLY  
ON VIBRATIONAL  
TRANSITION.

$$\langle \mu_x \rangle_{nn'} = \int \Psi_{\text{molecule vib}}^{*(n)} \hat{\mu}_x \Psi_{\text{molecule vib}}^{(n')} d\tau$$

$$\hat{\mu}_x = \sum_j e_j \hat{x}_j$$

DIPOLE  
MOMENT  
OPERATOR

(X COMPONENT)

(236)

$\hat{\mu}_x$  CAN VARY AS MOLECULE  
VARIES DURING A NORMAL VIBRATION

$$\hat{\mu}_x = \mu_x^0 + \sum_k^{3N-6} \frac{\partial \mu_x}{\partial Q_k} Q_k + \dots$$

$\uparrow$  Equilibrium Value       $\frac{\Delta \mu}{\Delta Q}$   $\uparrow$   $\Delta Q$

ground state  $n=0$

$$\langle \mu_x \rangle_{0n'} = \frac{\mu_x^0 \int \Psi_{\text{molecule vib}}^{*(0)} \Psi_{\text{molecule vib}}^{(n')} d\tau + \int \Psi_{\text{molecule vib}}^{*(0)} \sum_k \frac{\partial \mu_x}{\partial Q_k} Q_k \Psi_{\text{molecule vib}}^{(n')} d\tau}{}$$

$$k = 3N - 6$$

$$\mu_x^0 \left[ \underbrace{\int \psi_1^*(0) \psi_1(n_1') d\tau}_{\text{ZERO UNLESS } n_1' = 0} \underbrace{\int \psi_2^*(0) \psi_2(n_2') d\tau \dots}_{\text{ZERO UNLESS } n_2' = 0} \dots \underbrace{\int \psi_k^*(0) \psi_k(n_k') d\tau}_{\text{ZERO UNLESS } n_k' = 0} \right]$$

DUE TO ORTHOGONALITY  
OF VIBRATIONAL WAVEFUNCTIONS.

DISCUSSING A TRANSITION SO  
NOT ALL  $n_i' = 0$  (NO TRANSITION IF  
THEY ARE ALL IN  
GROUND STATE)

FIRST  
TERM

$$\mu_x^0 \int \underbrace{\psi(0)}_{\text{molecule vib}} \underbrace{\psi(n')}_{\text{molecule vib}} d\tau = 0 \quad (237)$$

SECOND  
TERM

$$\sum_k \frac{\partial \mu_k}{\partial Q_k} \int \psi_1^*(0) \psi_1(n_1') d\tau \int \psi_2^*(0) \psi_2(n_2') d\tau$$

$$\sum_k \frac{\partial \mu_k}{\partial Q_k}$$

$$\dots \int \psi_k^*(0) \underbrace{Q_k}_{\text{vib}} \psi_k(n_k') d\tau$$

$n_1', n_2', \dots = 0$  OR TERM WILL BE ZERO

ONLY ONE VIBRATIONAL TRANSITION  
AT A TIME  $0 \quad n_k' = n$

$$\sum_k \frac{\partial \mu_k}{\partial Q_k} \underbrace{\int \psi_1^*(0) \psi_1(0) d\tau}_1 \underbrace{\int \psi_2^*(0) \psi_2(0) d\tau}_1$$

$$\dots \int \psi_k^*(0) Q_k \psi_k(n_k') d\tau$$

$$\frac{\partial \mu_x}{\partial Q_k} \int \psi_k^*(0) Q_k \psi_k(n_k') d\tau$$

↑  
CHANGE  
IN  
DIPOLE  
MOMENT  
WITH  
 $Q_k$   
IMPORTANT

↑  
SYMMETRY  
NORMAL  
COORDINATE  
IMPORTANT

(238)

$$\underbrace{\Gamma(\psi_k^*(0))}_{A_1} \otimes \underbrace{\Gamma(Q_k)}_{A_1} \otimes \underbrace{\Gamma(\psi_k(n_k'))}_{A_1} = A_1$$

$$\boxed{\mu_x \sim e x}$$

$$n_k' = 1 \quad \Gamma(\psi_k(n_k')) = \Gamma_{Q_k} \text{ (FUNDAMENTAL)}$$

$$\int \psi_k^*(0) x \psi_k(1) d\tau$$

$$\Gamma_{A_1} \otimes \Gamma_x \otimes \Gamma_{Q_1} = A_1$$

$$\Gamma_x \otimes \Gamma_{Q_1} = A_1$$

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# ELECTRONIC SPECTRA

## REVIEW

FRANCK-CONDON PRINCIPLE

Classical, Quantum Mechanical

## SPIN SELECTION RULE

"VIBRATIONLESS" TRANSITION

SYMMETRY SELECTION RULE

## ORBITALS AND STATES

VIBRONIC TRANSITIONS

SELECTION RULES

VIOLATIONS OF THE SPIN RULE

CLASSIFICATION OF ELECTRONIC SPECTRA

THE FATE OF ABSORBED ENERGY (JABLONSKI DIAGRAM)

VIBRATIONAL RELAXATION

INTERNAL CONVERSION

INTERSYSTEM CROSSING

} RADIATIONLESS  
TRANSITIONS

FLUORESCENCE

PHOSPHORESCENCE

} RADIATIVE  
TRANSITION

## EXAMPLES

FORMALDEHYDE

BUTADIENE

BENZENE

NAPHTHALENE

(PYRAZINE, ~~pyrazine~~, p-DIFLUOROBENZENE, ~~pyrazine~~)

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## ELECTRONIC SPECTRA

EXCITATION FROM ONE ELECTRONIC STATE TO ANOTHER.

SIMULTANEOUS PROMOTION OF VIBRATIONAL AND ROTATIONAL TRANSITIONS.

IN SOLUTION VIBRATIONAL AND ROTATIONAL STRUCTURE IS NOT RESOLVED.

IN THE GAS PHASE AT LOW TEMPERATURE VIBRATIONAL STRUCTURE OF AN ELECTRONIC TRANSITION CAN BE RESOLVED.

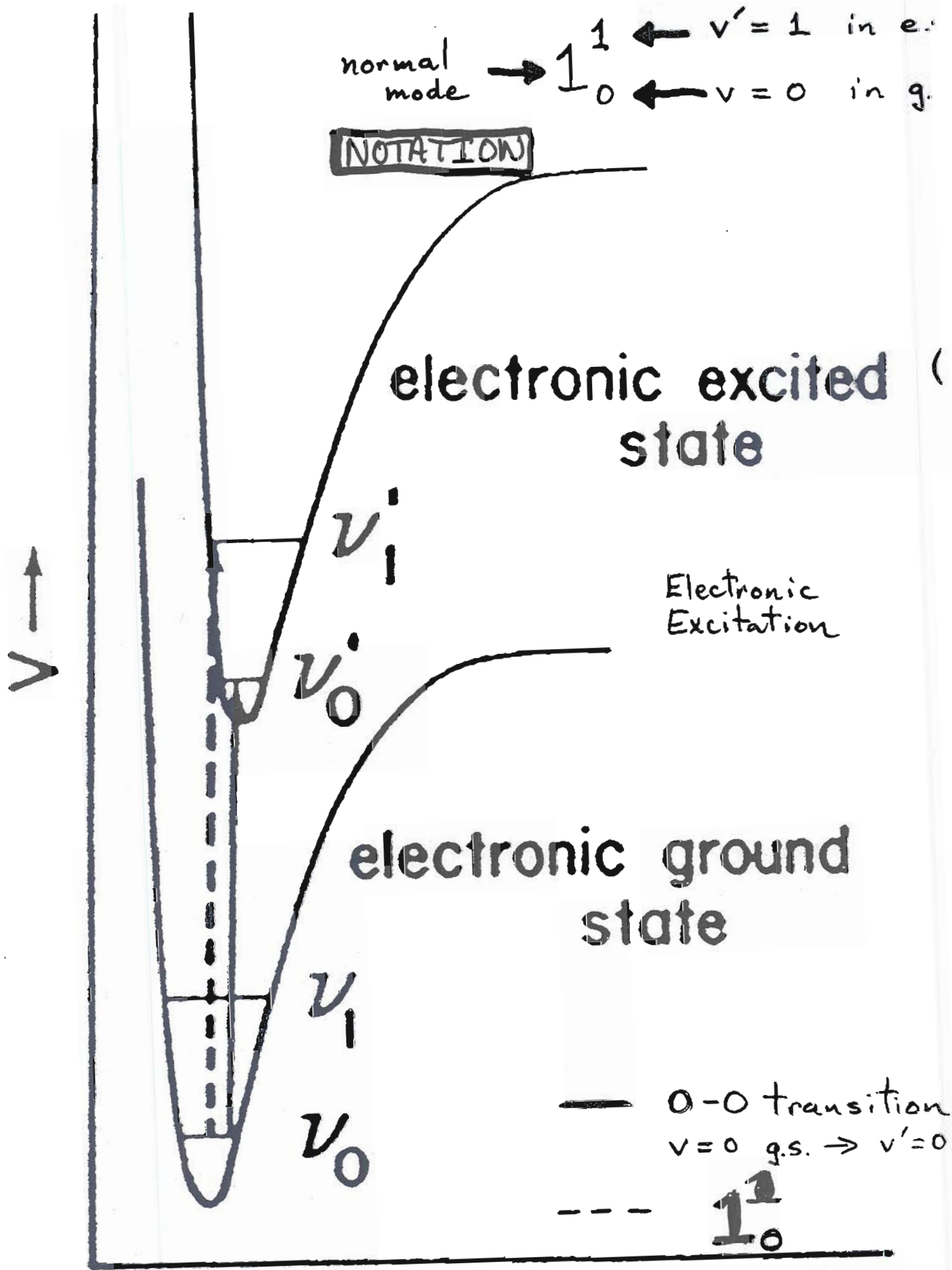
(ROTATIONAL FINE STRUCTURE IS NOT GENERALLY RESOLVED IN THE ELECTRONIC SPECTRA OF POLYATOMIC MOLECULES ..... WE WILL IGNORE THIS FEATURE.)

## ELECTRONIC SPECTROSCOPY

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- TRANSITIONS BETWEEN TWO DIFFERENT ELECTRONIC POTENTIAL ENERGY WELLS

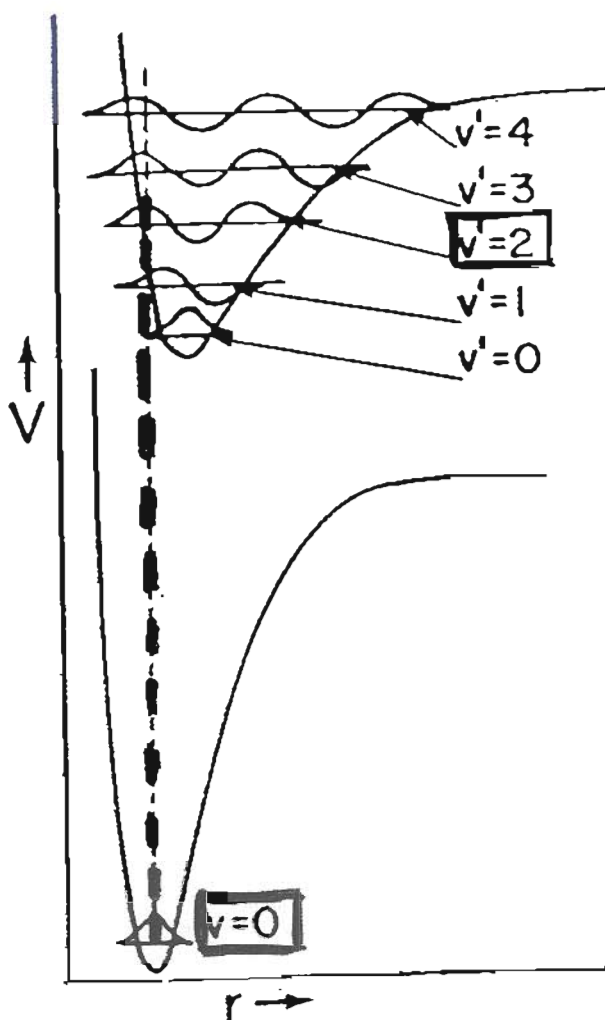
(CONTRAST WITH VIBRATIONAL SPECTRA  
- VIBRATIONAL LEVELS IN ONE WELL)



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~

q  $\rightarrow$

"vibronic"  
vibrational + electronic



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## FRANCK-CONDON PRINCIPLE

"Classically"

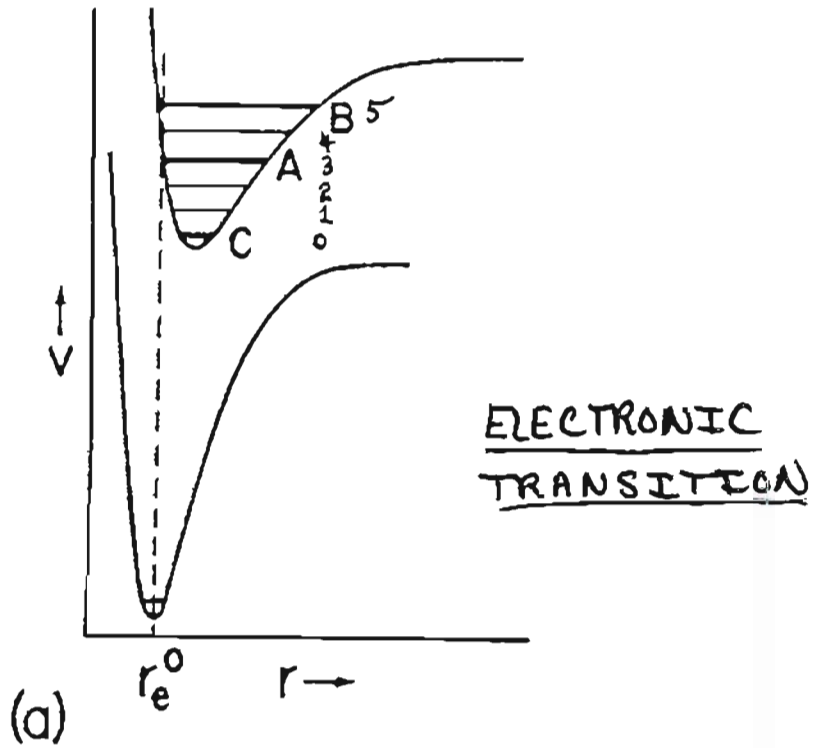
The electronic transition takes place so rapidly that the nuclei do not move. Thus a transition is a vertical line on a diagram showing the potential wells of the ground and excited states.

"Quantum Mechanically"

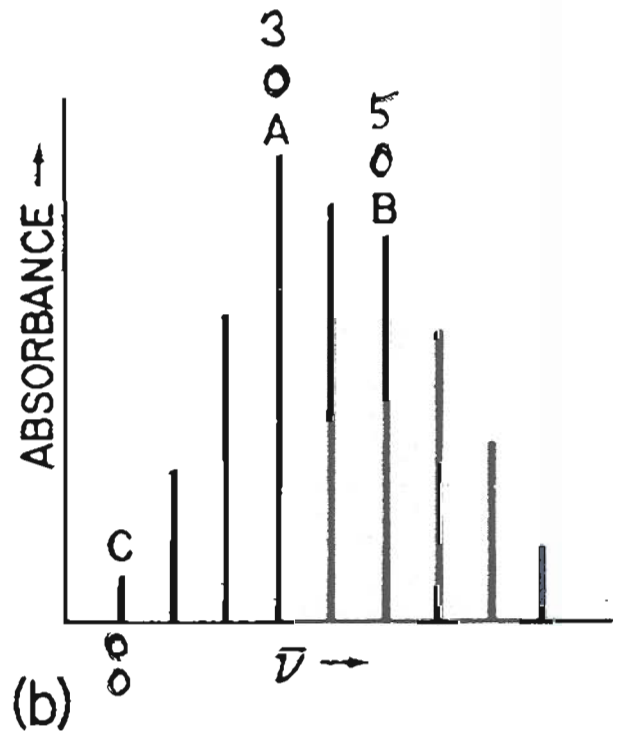
Add in the idea of overlap: the excited state vibrational wavefunction with that of the ground state vibrational wavefunction.  
 $v=0$  to  $v'=2$  BEST

FRANCK-CONDON FACTOR

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HOW THE FRANCK-CONDON PRINCIPLE MODIFIES THE APPEARANCE OF THE VIBRATIONAL STRUCTURE OF AN ELECTRONIC TRANSITION



FRANCK-CONDON FACTORS CHANGE INTENSITIES VIBRONIC TRANSITIONS.

VIBRATIONAL STRUCTURE ASSOCIATED WITH ABOVE ELECTRONIC TRANSITION

WHAT DETERMINES THE INTENSITY OF A SPECTRAL TRANSITION?

WE WILL CONSIDER ELECTRIC DIPOLE TRANSITIONS.

TRANSITION  
MOMENTS

$$M_x = \int \Psi_i \hat{\mu}_x \Psi_j d\tau$$

$$M_y = \int \Psi_i \hat{\mu}_y \Psi_j d\tau$$

$$M_z = \int \Psi_i \hat{\mu}_z \Psi_j d\tau$$

WAVEFUNCTIONS  
&  
OPERATORS

$\hat{\mu}_x$   
 $\hat{\mu}_y$   
 $\hat{\mu}_z$

COMPONENTS OF  
ELECTRIC DIPOLE  
MOMENT

$$\hat{\mu}_x = \sum_i e x_i$$

$\Psi_i$   
 $\Psi_j$

**TOTAL** WAVEFUNCTIONS OF  
THE TWO STATES  $i$  AND  $j$  CONNECTED  
BY THE TRANSITION.

## SPIN SELECTION RULES

IF RELATIVISTIC EFFECTS ARE NOT IMPORTANT THEN THE TOTAL WAVEFUNCTION CAN BE WRITTEN AS A PRODUCT OF A SPIN FUNCTION  $\chi$  AND A FUNCTION  $\phi$  OF ALL OTHER MOLECULAR COORDINATES (ELECTRONIC AND VIBRATIONAL):

$$\Psi_i = \underset{\substack{\downarrow \\ \text{SPIN}}}{\phi_i} \chi_i$$

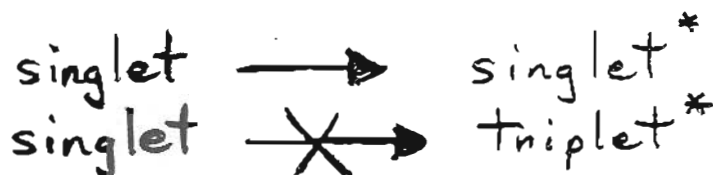
$\hat{\mu}_x$   
 $\hat{\mu}_y$   
 $\mu_z$

NO EFFECT ON SPIN FUNCTION  $\chi_i$

$$M_x = \int \Psi_i \mu_x \Psi_j^* d\tau = \int \phi_i \mu_x \phi_j^* d\tau \int \chi_i \chi_j^* d\tau$$

$$\int \chi_i \chi_j^* d\tau = \delta_{ij} \quad \text{ORTHONORMAL SET}$$

THUS THE TRANSITION MOMENTS ARE ALL ZERO UNLESS THE INITIAL AND FINAL STATES HAVE THE SAME SPIN.



ALTHOUGH WE HAVE SEEN THAT VIBRATIONS PLAY A ROLE IN ELECTRONIC SPECTRA LETS FOCUS INITIALLY ON THE ELECTRONIC PART OF THE ELECTRONIC TRANSITION.

$\phi_i$  electronic and nuclear coordinates  
(normal modes)

$$\phi_i = \underbrace{\bar{\Psi}_i(E)}_{\text{Electronic}} \underbrace{\bar{\Psi}_i(V)}_{\text{Vibrational}}$$

$$M_x = \int \bar{\Psi}_i(E) \bar{\Psi}_i(V) \hat{\mu}_x \bar{\Psi}_j(E) \bar{\Psi}_j(V) d\tau$$

different wells

$$= \underbrace{\int \bar{\Psi}_i(E) \hat{\mu}_x \bar{\Psi}_j(E) d\tau}_{\text{'electronic'}} \underbrace{\int \bar{\Psi}_i(V) \bar{\Psi}_j(V) d\tau}_{\text{'vibrational'}}$$

WHEN WILL THIS ELECTRONIC TERM BE NONZERO ?

LETS SUPPOSE THIS TERM IS NONZERO

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$$\Gamma(\bar{\Psi}_i) \otimes \Gamma_x \otimes \Gamma(\bar{\Psi}_j) = \Gamma(A_1)$$

(g)

HOW DO WE DESCRIBE ELECTRONS IN MOLECULES?

ELECTRONIC STATES.

WRITE ELECTRONIC STATES BY SPECIFYING ORBITALS THAT ARE OCCUPIED.

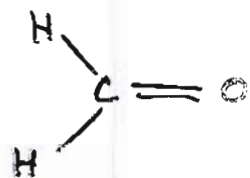
CAN WORK OUT THE SYMMETRIES OF VARIOUS ELECTRONIC STATES BY FOCUSING ON THE PARTIALLY OCCUPIED MO.

$( )^2 \rightarrow A_1$  totally symmetric  
NO DETAILED CONSIDERATION

e.g. FORMALDEHYDE

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STATES CAPS.  
orbitals lower case



$C_{2v}$

16 electrons

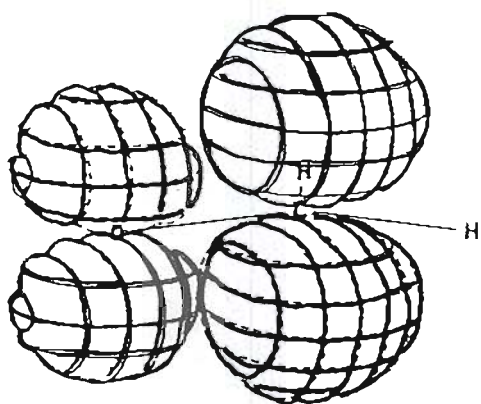
$(1a_1)^2 (2a_1)^2 (3a_1)^2 (4a_1)^2 (1b_1)^2 (5a_1)^2 (1b_2)^2 (2b_1)^2 (2b_2)^2$

ground state  $^1A_1$

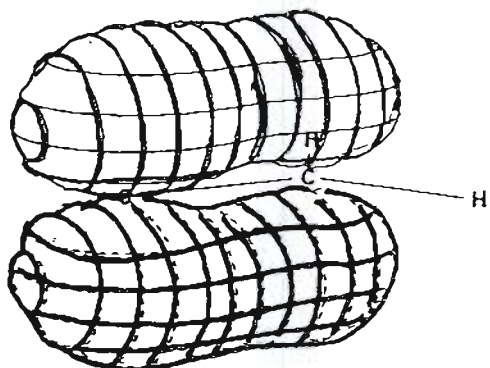
$\pi$   $n$   $\pi$

20. Formaldehyde

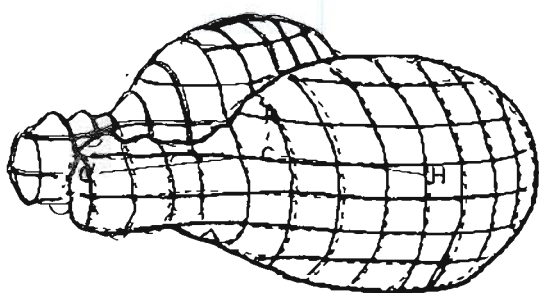
Symmetry:  $C_{2v}$



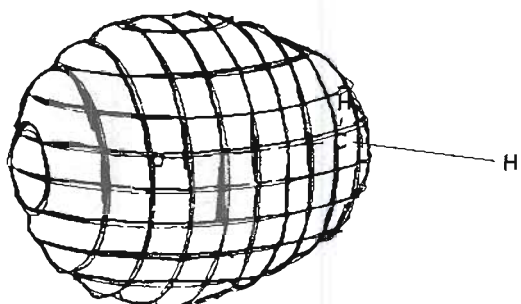
$2B_2$   $E = 0.2467 \pi^*_{CO}$



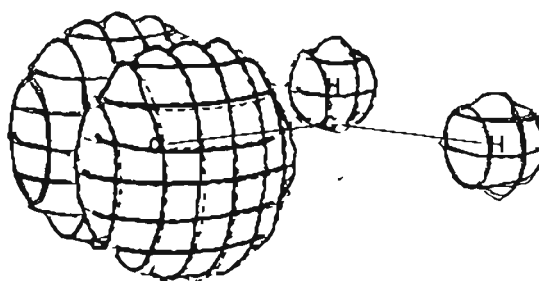
$1B_2$   $E = -0.4697 \pi_{CO}$



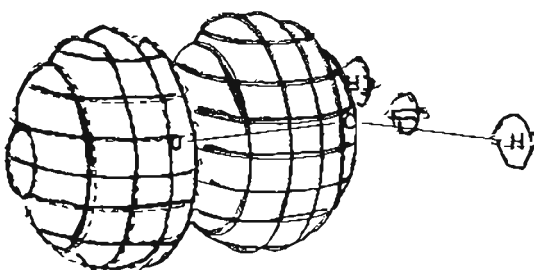
$1B_1$   $E = -0.6745 \pi_{CH_2}$



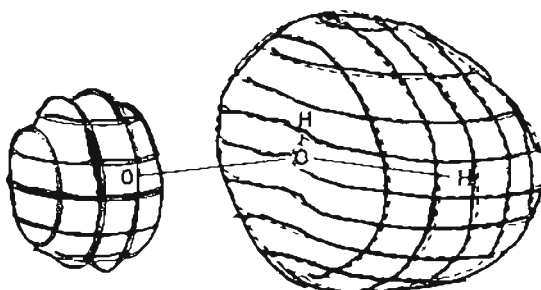
$3A_1$   $E = 1.3693 \sigma_{CO}$



$2B_1$   $E = -0.3853 \pi$

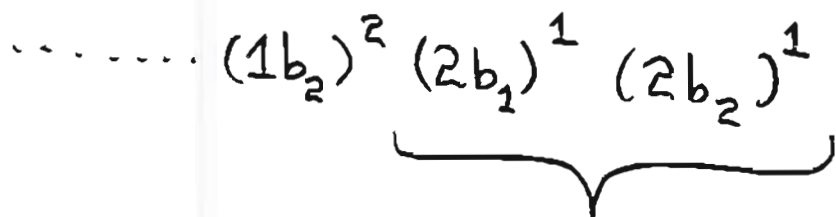


$5A_1$   $E = -0.5708 \pi_{CO}$  ( $\sigma_{CO}$ )

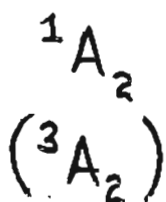


$4A_1$   $E = -0.8370 \sigma_{CH_2}$

WHAT STATE(S) WOULD ARISE FROM AN  $n \rightarrow \pi^*$  EXCITATION?

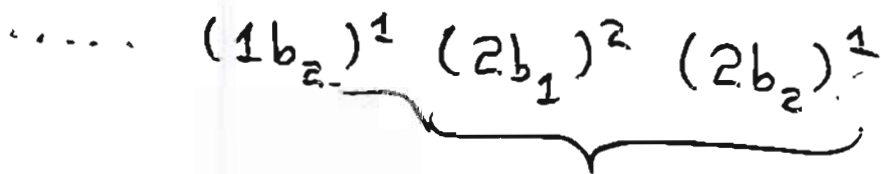


$C_{2v} \quad b_1 \otimes b_2 = a_2$

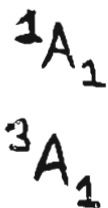


↑  $b_2 \pi^*$   
↑  $b_1 n$   
↑  $b_2 \pi^*$   
↑  $b_1 n$

WHAT STATE(S) WOULD ARISE FROM A  $\pi \rightarrow \pi^*$  EXCITATION?



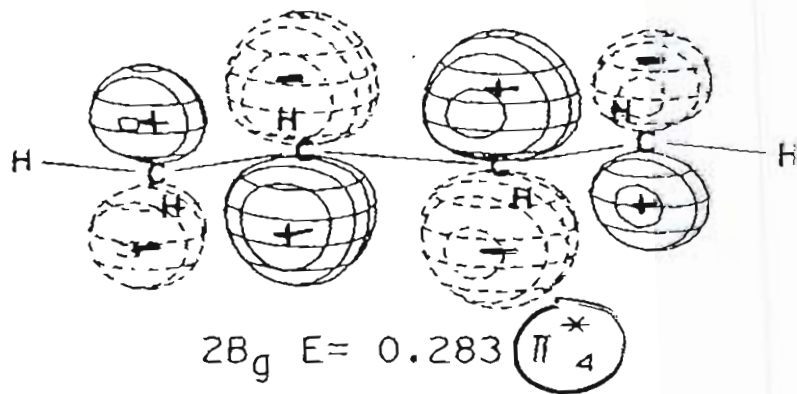
$C_{2v} \quad b_2 \otimes b_2 = a_1$



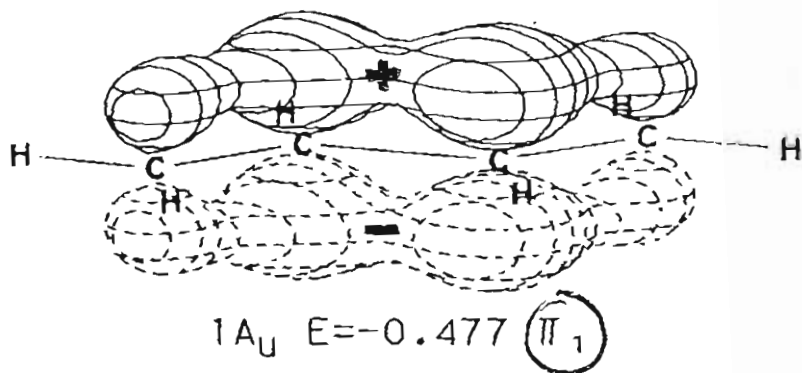
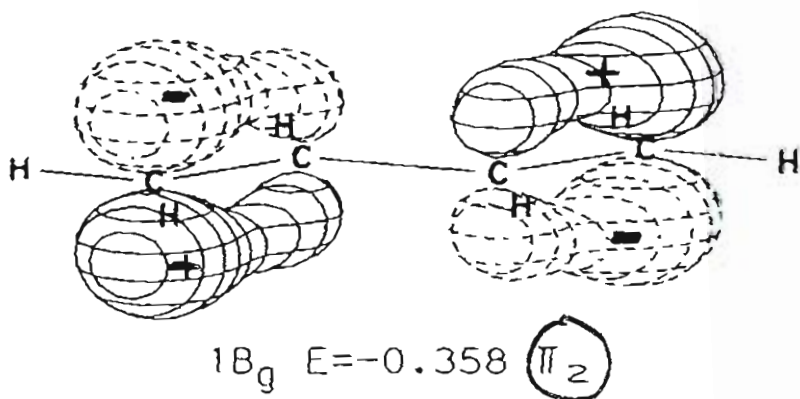
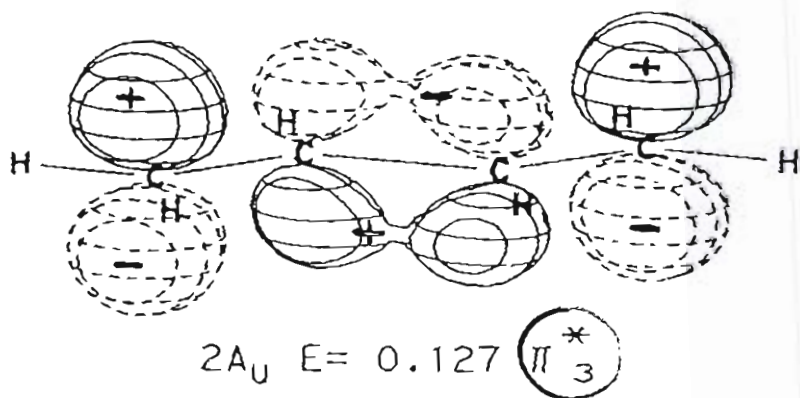
↑  $b_2 \pi^*$   
↑  $b_2 \pi$   
↑  $b_2 \pi$   
↑  $b_2 \pi$

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1,3-Butadiene, Transoid (Continued)

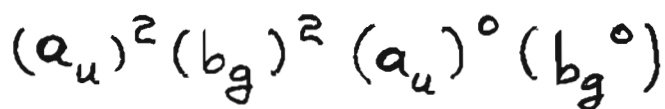
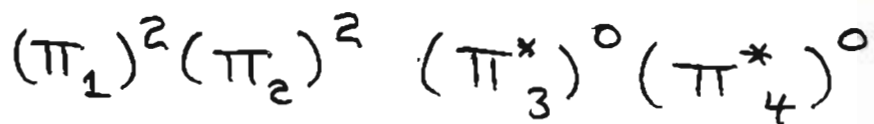


$\pi$  ORBITALS  
TRANS - BUTADIENE  
 $C_{2h}$

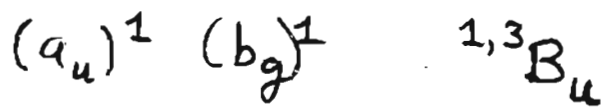
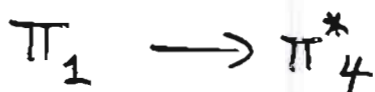
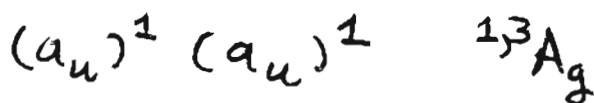
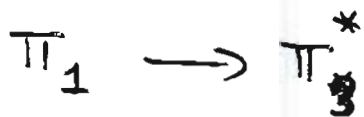
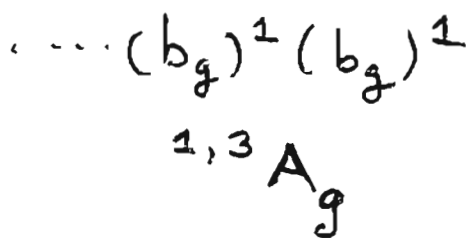
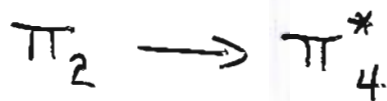
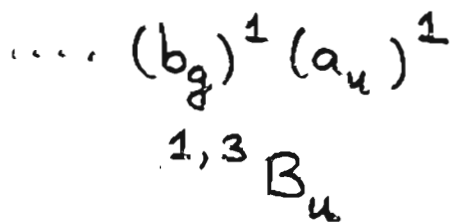


# TRANS-BUTADIENE

WHAT IS THE SYMMETRY OF THE GROUND STATE



${}^1A_g$



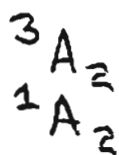
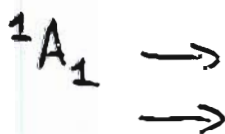
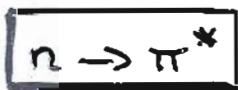
CONTINUING TO FOCUS ON :

$$M_x = \int \Psi_i(E) \mu_x \Psi_j(E) d\tau$$

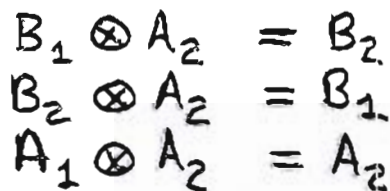
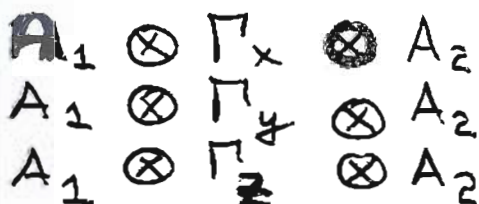
WHICH OF THE TRANSITIONS IN FORMALDEHYDE (~~FORMALDEHYDE~~) WILL BE ALLOWED AND WHICH FORBIDDEN?

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H<sub>2</sub>CO



SPIN FORBIDDEN



FORBIDDEN



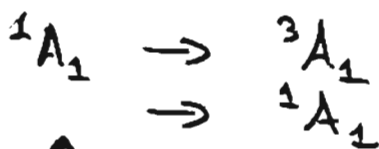
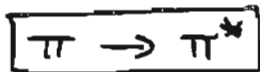
(Why is it seen?)

IT IS MAGNETIC DIPOLE ALLOWED.

MORE IMPORTANTLY, H<sub>2</sub>CO DOES NOT BELONG TO C<sub>2v</sub> POINT GROUP IN EXCITED STATE.)

H<sub>2</sub>CO

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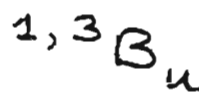
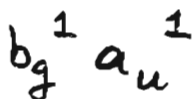
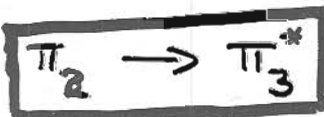


SPIW FORBIDDEN

	<b>Yes.</b>		<b>Yes.</b>		
x	A <sub>1</sub> ⊗	B <sub>1</sub>	⊗	A <sub>2</sub>	= B <sub>1</sub>
y	A <sub>1</sub> ⊗	B <sub>2</sub>	⊗	A <sub>1</sub>	= B <sub>2</sub>
z	A <sub>1</sub> ⊗	A <sub>1</sub>	⊗	A <sub>1</sub>	= A <sub>1</sub>

ALLOWED  
z. polarization

TRANS-BUTADIENE



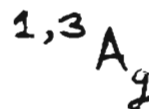
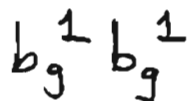
C<sub>2h</sub>

x, y  
z

A <sub>g</sub>	⊗	B <sub>u</sub>	⊗	B <sub>u</sub>
A <sub>g</sub>	⊗	A <sub>u</sub>	⊗	B <sub>u</sub>

A<sub>g</sub>  
B<sub>g</sub>

ALLOWED x,  
FORBIDDEN z

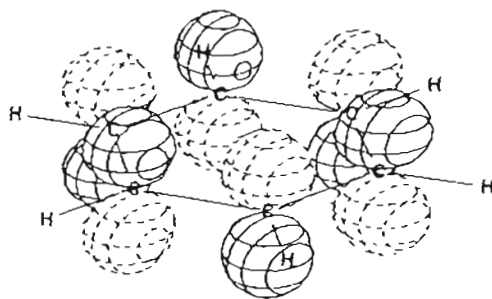


x, y  
z

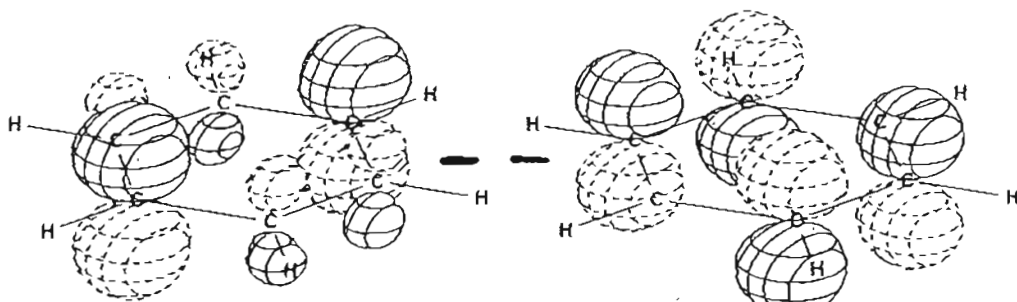
A <sub>g</sub>	⊗	B <sub>u</sub>	⊗	B <sub>g</sub>
A <sub>g</sub>	⊗	A <sub>u</sub>	⊗	B <sub>u</sub>

A<sub>u</sub>  
B<sub>g</sub>

FORBIDDEN x  
FORBIDDEN



$1B_{2g} \quad E = 0.4803 \pi_{cc}^*$

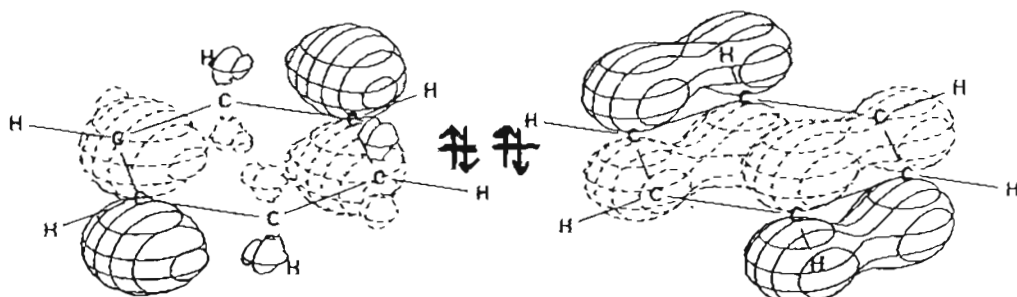


$1E_{2u} \quad E = 0.2478 \pi_{cc}^*$

$1E_{2u} \quad E = 0.2478 \pi_{cc}^*$

**MOS**

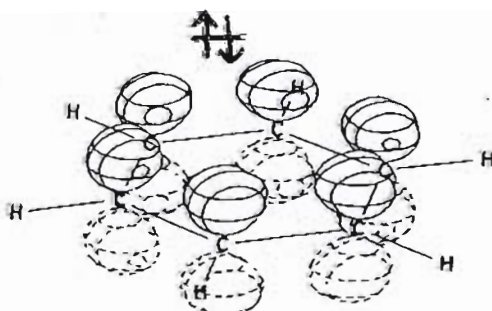
**$\pi$ -MOLECULAR ORBITALS  
BENZENE  
 $D_{6h}$**



$1E_{1g} \quad E = -0.2937 \pi_{cc}$

$1E_{1g} \quad E = -0.2937 \pi_{cc}$

**FUN  
WITH  
DEGENERACY!**



$1A_{2u} \quad E = -0.4676 \pi_{cc}$

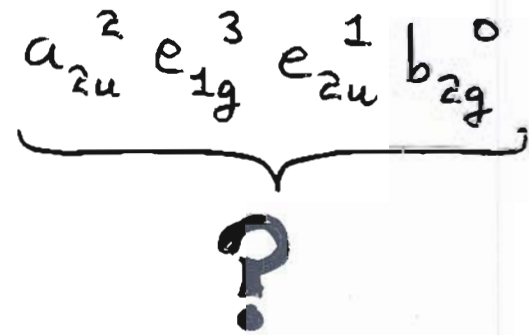
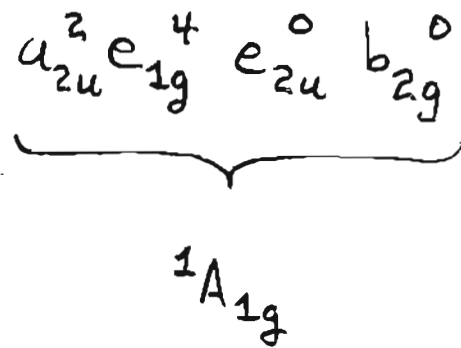
**254**

$b_{2g}$		—	$\pi^*$
$e_{2u}$	—	—	$\pi^*$
$e_{1g}$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\pi$
$a_{2u}$		$\uparrow\downarrow$	$\pi$



**SEXTET**

$\pi \rightarrow \pi^*$



$e_{1g}^1 \otimes e_{2u}^1 = b_{1u} + b_{2u} + e_{1u}$

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IN  
 $D_{6h}$

**STATES**

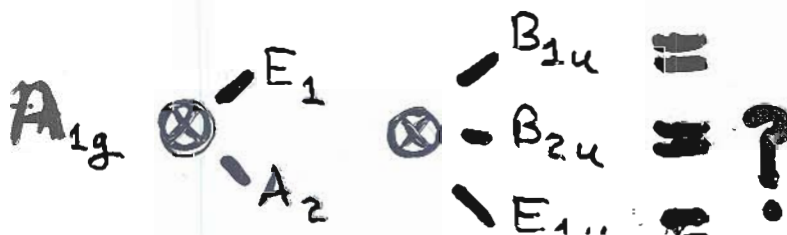
STATES

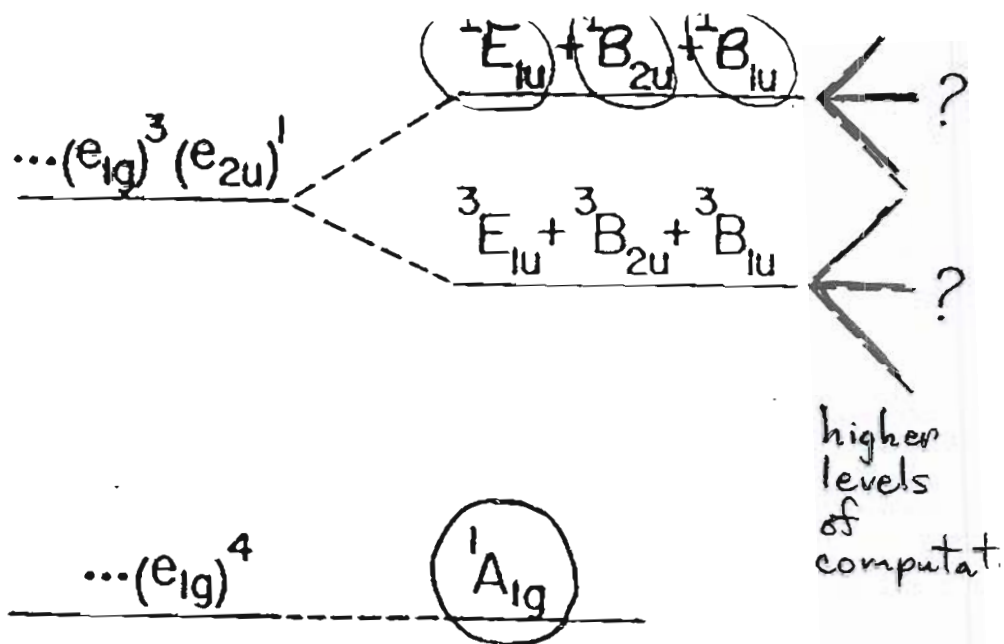
$^{1,3}B_{1u}$

$^{1,3}B_{2u}$

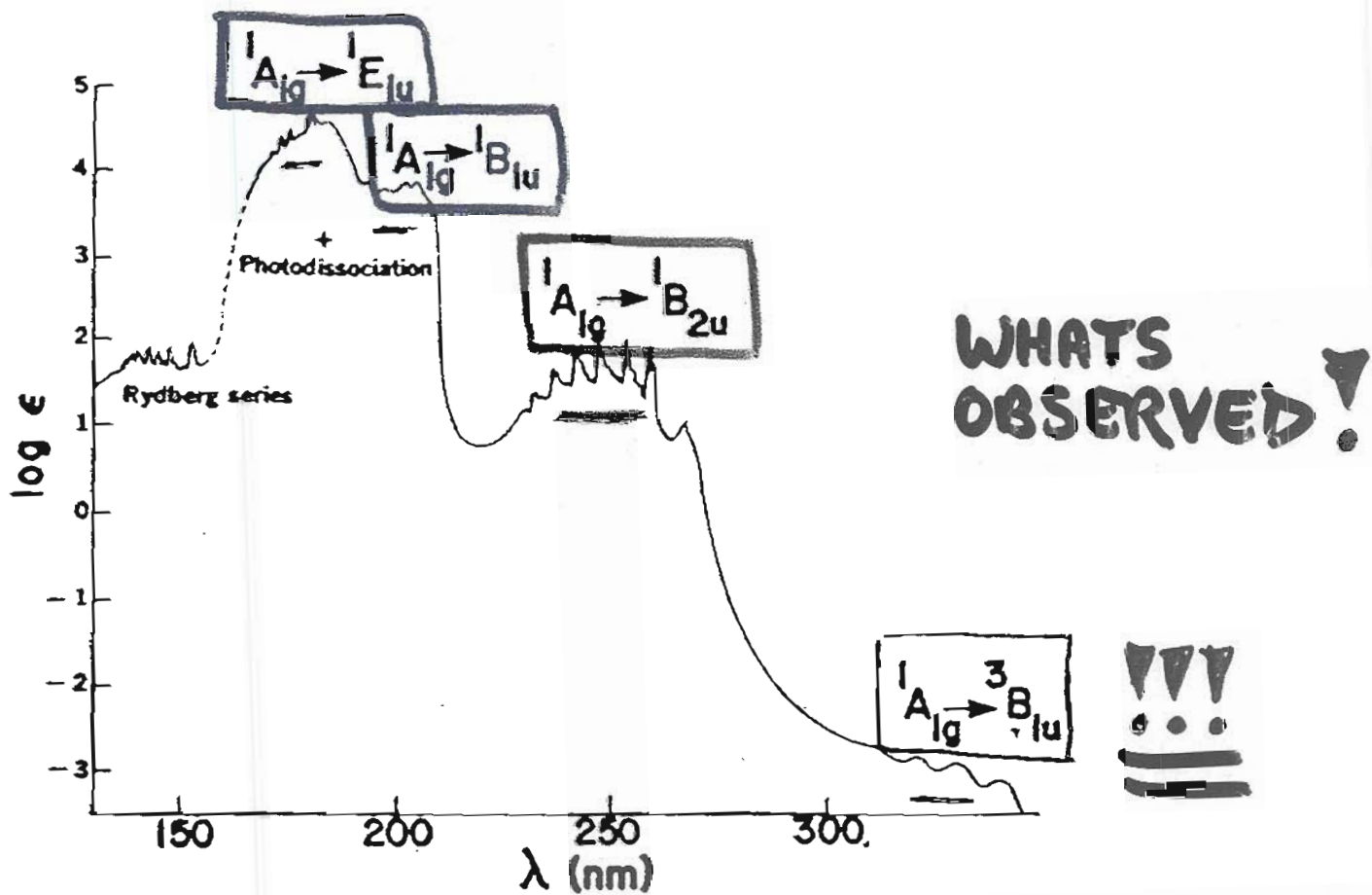
$^{1,3}E_{1u}$

ALLOWED OR FORBIDDEN?





Partial state diagram of benzene.



Low resolution spectrum of benzene

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# WORKING OUT (OR LOOKING UP) DIRECT PRODUCTS.



Allowed x, y Polarization



FORBIDDEN YET SEEN! WHY?



"DOUBLY FORBIDDEN" YET SEEN! WHY?

HOW CAN THE FORBIDDEN TRANSITIONS OCCUR ?

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## VIBRONIC TRANSITIONS

TO THIS POINT WE HAVE BEEN CONSIDERING ONLY THE ELECTRONIC WAVEFUNCTIONS.

$$M_x^{el} = \int \bar{\Psi}_i \hat{\mu}_x \Psi_j d\tau$$

ELECTRONICALLY FORBIDDEN TRANSITIONS ARE SEEN (USUALLY WEAK) DUE TO INTERACTIONS WITH VIBRATIONS.

AN EXCITATION OF AN ASYMMETRIC NORMAL MODE EFFECTIVELY LOWERS THE MOLECULAR SYMMETRY.

EXCITATION OF THIS NORMAL MODE WOULD ACCOMPANY THE ELECTRONIC EXCITATION.

SO FAR

$$M_x = \underbrace{\int \bar{\Psi}_i \hat{\mu}_x \Psi_j d\tau}_{M_x^{el} \text{ electronic}} \underbrace{\int \Psi_i^v(v) \bar{\Psi}_j^v(v) d\tau}_{\text{FRANK-CONDON FACTOR}} \\ \left. \begin{array}{l} \text{vibrational} \\ \text{overlap} \\ \text{integral} \end{array} \right\}$$

UP TO NOW LOOKED AT THIS TERM AND WHEN IT IS NONZERO BY SYMMETRY.

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IF  $M^{el} = 0$  WE MUST CONSIDER THE NONSEPARABILITY OF VIBRATIONS AND ELECTRONIC MOTION.

$$\Psi_i = \Psi_i(E) \Psi_i(V)$$

electronic      vibrational

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$$M_x = \int \bar{\Psi}_i(E) \bar{\Psi}_i(V) \mu_x \Psi_j(E) \Psi_j(V) d\tau$$

CANNOT SEPARATE INTO ELECTRONIC AND VIBRATIONAL PORTIONS AS BEFORE.

$\bar{\Psi}_i(E)$	ELECTRONIC GROUND STATE <u>USUALLY</u> TOTALLY SYMMETRIC	$A_1$
$\bar{\Psi}_i(V)$	$v=0$ , TOTALLY SYMMETRIC VIBRATIONAL GROUND STATE	$A_1$

$$\Gamma(\bar{\Psi}_i(E)) \otimes \Gamma(\bar{\Psi}_i(v=0)) \otimes \Gamma(\mu_x) \otimes \Gamma(\bar{\Psi}_j(E)) \otimes \Gamma(\Psi_j(V))$$

$$A_1 \otimes A_1 \otimes \Gamma\left(\begin{matrix} x \\ y \\ z \end{matrix}\right) \otimes \Gamma(\bar{\Psi}_j(E)) \otimes \Gamma(\Psi_j(V))$$


---

TO BE NONZERO

$$\Gamma\left(\begin{matrix} x \\ y \\ z \end{matrix}\right) = \Gamma(\bar{\Psi}_j(E)) \otimes \Gamma(\Psi_j(V))$$

FOR A TRANSITION TO BE VIBRONICALLY ALLOWED

$$\Gamma \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \Gamma(\Psi_i(E)) \otimes \Gamma(\Psi_j(v))$$

excited state

TALKING ABOUT TRANSITIONS THAT ARE NOT ELECTRONICALLY ALLOWED SO WE KNOW THAT

$$\Gamma \begin{pmatrix} x \\ y \\ z \end{pmatrix} \neq \Gamma(\Psi_j(E))$$

(WOULD LEAD TO  $\int \Psi_i(E) \mu_x \Psi_j(E)$  BEING NONZERO)

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IF  $\Psi_j(v=0)$  THEN  $\Gamma(\Psi_j(v=0)) = A_1$

AND SINCE  $\Gamma \begin{pmatrix} x \\ y \\ z \end{pmatrix} \neq \Gamma(\Psi_j(E))$

A 0-0 BAND IS NOT VIBRONICALLY ALLOWED.

$v=0$  g.s.       $v=0$  e.s.

$$A_1 \otimes A_1 \otimes \underbrace{\Gamma \begin{pmatrix} x \\ y \\ z \end{pmatrix} \otimes \Gamma(\Psi_j(E))}_{\text{NOT } A_1} \otimes A_1$$

g.s.       $v=0$  g.s.       $v=0$  e.s.



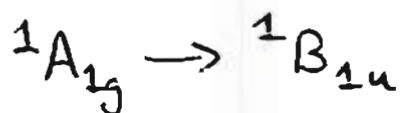
CONSIDER  $z \sim A_{2u}$

$$\Gamma(\text{vib})_{v=1} \otimes B_{1u} = A_{2u}$$



$$\Gamma(\text{vib})_{v=1} = B_{1u} \otimes A_{2u} = B_{2g}$$

AS YOU "KNOW" ~~THESE MODES ARE~~ THERE ARE 2  $B_{2g}$  MODES IN BENZENE.



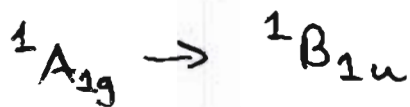
VIBRONICALLY ALLOWED  
Z POLARIZED  
 $B_{2g}$  VIBRATION EXCITED  $v=1$

CONSIDER  $(x, y) \sim E_{1u}$

$$\Gamma(\text{vib})_{v=1} \otimes B_{1u} = E_{1u}$$

$$\Gamma(\text{vib})_{v=1} = B_{1u} \otimes E_{1u} = E_{2g}$$

THERE ARE 4  $E_{2g}$  MODES IN BENZENE.



VIBRONICALLY ALLOWED  
(x, y) POLARIZED  
 $E_{2g}$  VIBRATION EXCITED  $v=1$



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$$z \sim A_{2u}$$

$$\Gamma_{v=1}^{(vib)} \otimes A_{2u} = B_{2u}$$

$$\Gamma_{v=1}^{(vib)} = B_{2u} \otimes A_{2u} = B_{1g}$$

BUT THERE ARE NO  $B_{1g}$  VIBRATIONAL MODES  
IN BENZENE



VIBRONICALLY FORBIDDEN  
WITH Z. POLARIZATION

$$(x, y) \sim E_{1u}$$

$$\Gamma_{v=1}^{(vib)} \otimes E_{1u} = B_{2u}$$

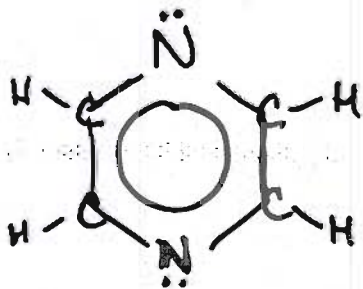
$$\Gamma_{v=1}^{(vib)} = E_{1u} \otimes B_{2u} = E_{2g}$$

THERE ARE 4  $E_{2g}$  MODES IN BENZENE.



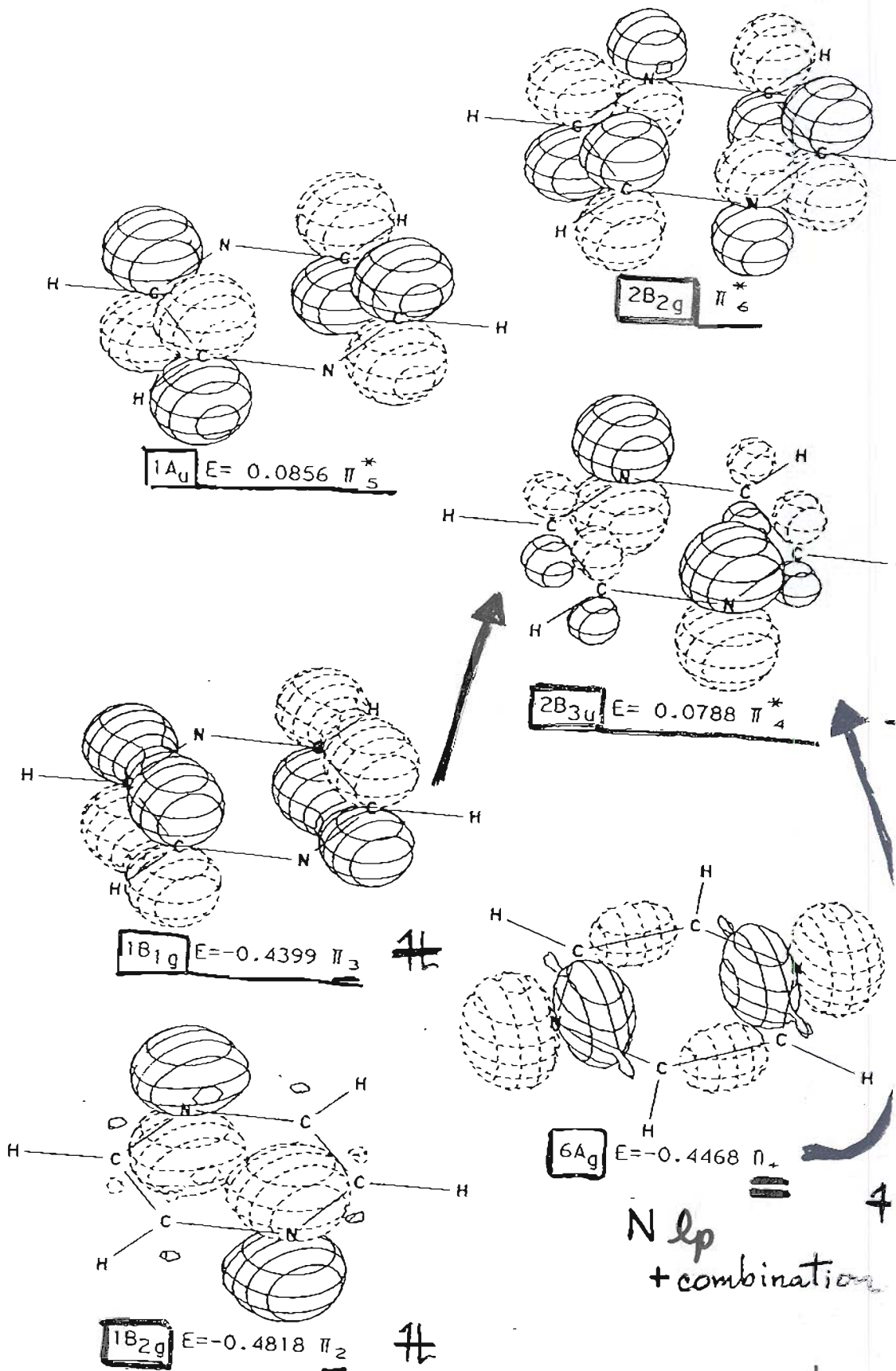
VIBRONICALLY ALLOWED  
(x, y) POLARIZATION  
 $E_{2g}$  VIBRATIONAL,  $v=1$   
EXCITATION

# PYRAZINE



$D_{2h}$

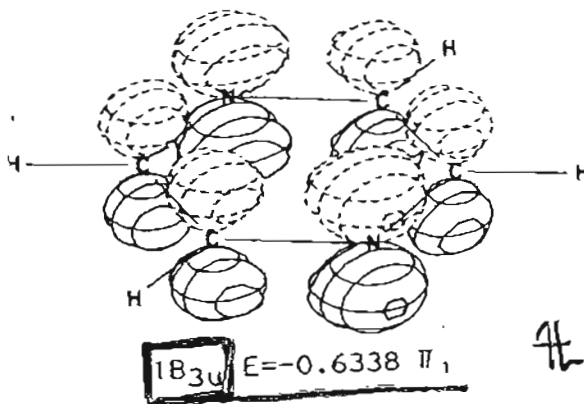
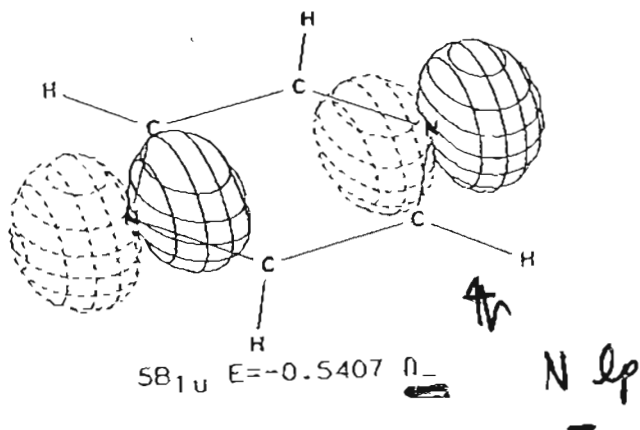
264



N lp + combination = 4

$B_{1g} \rightarrow B_{3u}$   
 $A_g \rightarrow B_{3u}$

ALLOWED?	STATE	x B
$b_{1g} \otimes b_{3u}$	$1,3 B_{2u}$	y f
$a_g \otimes b_{3u}$	$1,3 B_{3u}$	z f



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