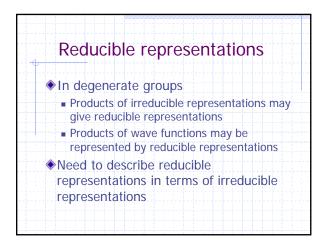
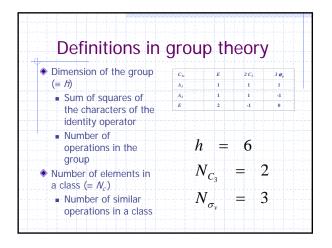
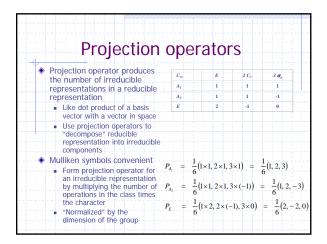
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resentations	
	(
	stry resentations



Direct	I2	Im	nc				
DIICCI	. 31	лц	13				
♦ A reducible							
representation is	Dith	E	2 C3	3 C2	<b>a</b> h	2.53	3.0
expressible as a direct	A, 1	1.	1			1	11
sum of irreducible	A2"	1		-1	- 1	1	-1
representations	-E'	2	-1	0	2	-1	- 0
• A direct sum is given by	A, *	1	1	1	-1	-1	
the representation with	A2"	1	1	-1	-1	-1	1
characters that are sum	E	2	-1	0	-2	1	0
of characters							
E2C,		3 C,	σ		2.5,	3 00	
A,'@A,' 2 2		0	2		2		<del>]  </del>
		-1-1	3				++
A <sub>1</sub> '@E' 3 0		1	3		0	1	

Direct	produ	ct		
Direct products are	C <sub>3v</sub>	E	2 C3	3 σ.
expressible as direct	A	1	1	1
sums of irreducible	A2	1	1	-1
representations	E	2	-1	0
$\clubsuit$ Examples in $C_{3\nu}$				
<ul> <li>Important in determining the representation of a</li> </ul>	$E \otimes .$	E =	$A_1 \oplus A$	$A_2 \oplus E$
multi-electron wave	C <sub>b</sub>	E	2 C,	3 <b>σ</b> .,
function	EØE	4	1	0
<ul> <li>Gives a means to decompose a multi- electron wave function into terms</li> </ul>	A <sub>1</sub> @ A <sub>2</sub> @ E	4		0 -





Reducing a re with projecti		
• Inner product of the projection operator with the reducible representation gives the number of representations present in the reducible representation • Example in $C_3v$ $E \otimes E = A_1 \oplus A_2 \oplus E$	$P_{A_{1}} \bullet (E \otimes E) =$ $P_{E} \bullet (E \otimes E) =$	$= \frac{1}{6}(1, 2, 3) \bullet (4, 1, 0)$ $= \frac{1}{6}(1 \bullet 4 + 2 \bullet 1 + 3 \bullet 0)$ $= \frac{1}{6}(1 \bullet 4 + 2 \bullet 1 + 3 \bullet 0)$ $= \frac{1}{6}(1, 2, -3) \bullet (4, 1, 0)$ $= \frac{1}{6}(1 \bullet 4 + 2 \bullet 1 - 3 \bullet 0)$ $= \frac{1}{6}(2 - 2, 0) \bullet (4, 1, 0)$ $= \frac{1}{6}(2 - 2 \bullet 1 + 0 \bullet 0)$

	to H <sub>2</sub> O wave tions
<ul> <li>Configuration results in a direct product of one- electron wave functions</li> <li>Want multi-electron wave functions that conform to known symmetry</li> <li>Perform a direct product to find the term</li> </ul>	Filling order 1a <sub>1</sub> 2a <sub>1</sub> 1b <sub>2</sub> 3a <sub>1</sub> 1b <sub>1</sub> 4a <sub>1</sub> 2b <sub>2</sub>
<ul> <li>Reduce the direct product to a direct sum         <ul> <li>Gives all terms arising from that configutation</li> </ul> </li> <li>Example: ground term of H<sub>2</sub>O         <ul> <li>10 electrons</li> </ul> </li> </ul>	$(1a_1)^2 (2a_1)^2 (1b_2)^2 (3a_1)^2 (1b_1)^2$ $\otimes A_1 \otimes A_1 \otimes B_2 \otimes B_2 \otimes A_1 \otimes A_1 \otimes B_1 \otimes B_1$

Excited state	$H_2U$
<ul> <li>Find first excited state by promoting a single electron</li> <li>Consider only partially filled shells</li> <li>Filled shells give totally symmetric representation as a product</li> <li>Spins of the two electrons may be paired or unpaired</li> <li>Singlet</li> <li>Triplet</li> </ul>	$\cdots (1b_1)^l (4a_1)^l$ $\Gamma = B_1 \otimes A_1$ $= B_1$ $^1B_1 \qquad ^3B_1$

	Summary
۲	Multi-electron wave functions found as direct products of one-electron wave functions Can be classified as reducible or irreducible representations
	Reducible representations can be expressed as a
ľ	direct sum of irreducible representations
	Use projection operators to determine the direct sum
۲	The direct sum gives the terms that arise from a configuration
۲	Use Pauli's principle to determine possible spin of wave functions
۲	Terms symbols use irreducible representations of the group