CONCLUSIONS:

(p_x, p_y) : BASIS FOR IRREDUCIBLE REPRESENTATION OF D_3 E (2.DIM.)

(p_z) : BASIS FOR IRREDUCIBLE REPRESENTATION OF D_3

A OR B ?

$C_3 p_z = p_z \Rightarrow$ 1DIM. REPR. A

SEPARATION OF ELEMENTS OF A GROUP INTO SMALLER SETS:

1. SUBGROUPS
2. CLASSES

SIMILARITY TRANSFORMATION

$A, X \in G$ $\qquad X^{-1} A X = B \in G$

B IS SIMILARITY TRANSFORM OF A BY X

A AND B ARE CONJUGATE

A COMPLETE SET OF ELEMENTS THAT ARE CONJUGATE TO ONE ANOTHER IS CALLED

A CLASS OF THE GROUP

(SIMILARITY RELATION FOR GIVEN A AND ALL $X \in G$!)

PROPERTIES:

1. THE ORDER OF ANY SUBGROUP g OF A GROUP OF ORDER h IS SUCH THAT

$$h/g = k \Rightarrow \text{INTEGER} \qquad (g \text{ IS DIVISOR OF } h)$$

2. THE ORDERS OF ALL CLASSES MUST BE INTEGRAL FACTORS OF THE ORDER OF THE GROUP

CHARACTER OF REPRESENTATION (IRREDUCIBLE)

IS A SUM OF DIAGONAL ELEMENTS
OF MATRIX REPRESENTATION (TRACE OF A MATRIX)

EXAMPLE: MATRIX REPRESENTATION OF D_3 IN (p_x, p_y, p_z)

$$\mathbb{D}(C_3^{+1}) = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} & 0 \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad -\tfrac{1}{2} - \tfrac{1}{2} + 1 = 0$$

FOR REDUCIBLE REPRESENTATION

$\chi(E) = 3, \quad \chi(C_3) = \chi(C_3^{-1}) = 0$

$\chi(C'_{2a}) = \chi(C'_{2b}) = \chi(C'_{2c}) = -1$

FOR IRREDUCIBLE REPRESENTATIONS OF D_3 IN $(p_x\, p_y\, p_z)$:

D_3	E	$2C_3$	$3C'_2$
$\chi_E(p_x p_y; \hat{R})$	2	−1	0
$\chi_A(p_z; \hat{R})$	1	1	−1

CHARACTER TABLE

FORMALISM

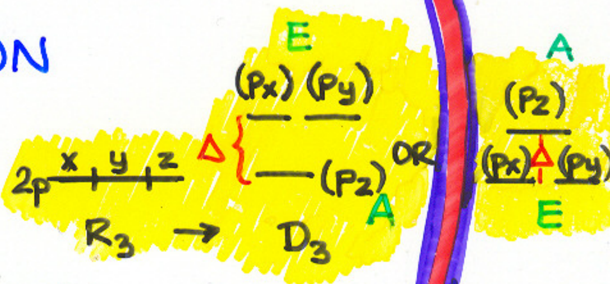
QUESTIONS ABOUT D_3:

1. WHAT IS THE GROUP ORDER?
2. HOW MANY CLASSES ARE IN D_3?
3. HOW MANY ELEMENTS IN EACH CLASS?
4. HOW MANY IRREDUCIBLE REPRESENTATIONS IS POSSIBLE TO CONSTRUCT?
5. WHAT ARE THE DIMENSIONS OF IRREDUCIBLE REPRESENTATIONS?

⋮

WHAT ARE THE TRANSFORMATION PROPERTIES OF $p_x\ p_y\ p_z$ UNDER SYMMETRY OPERATIONS OF D_3?

WHAT IS THE ENERGY SCHEME OF H ATOM IN EXCITED STATE OF SYMMETRY 2p IN A FIELD (EXTERNAL) OF D_3 SYMMETRY?



PHYSICS!

ANSWERS

GENERALIZATION

$\Gamma_i(R)_{mn}$: THE ELEMENT IN mTH ROW AND THE nTH COLUMN OF THE MATRIX REPRESENTATION OF $\hat{R}$ IN THE iTH IRREDUCIBLE REPRESENTATION

GREAT ORTHOGONALITY THEOREM

$$\sum_R [\Gamma_i(R)_{mn}][\Gamma_j(R)_{m'n'}]^* = \frac{h}{\sqrt{l_i l_j}} \delta_{ij} \delta_{mm'} \delta_{nn'}$$

l_i - DIMENSION OF Γ_i

TWO DIFFERENT VECTORS FROM h-DIMENSIONAL SPACE ARE ORTHOGONAL

AND

SQUARE OF THE LENGTH OF SUCH A VECTOR = h/l_i

FOR REAL NUMBERS:

$$\sum_R \Gamma_i(R)_{mn} \Gamma_j(R)_{mn} = 0 \quad \text{if } i \neq j$$

$$\sum_R \Gamma_i(R)_{mn} \Gamma_i(R)_{m'n'} = 0 \quad \text{if } m \neq m' \text{ or } n \neq n'$$

$$\sum_R \Gamma_i(R)_{mn} \Gamma_i(R)_{mn} = h/l_i$$

IMPORTANT RULES (PROPERTIES)

1. THE SUM OF THE SQUARES OF THE DIMENSIONS OF THE IRREDUCIBLE REPRESENTATIONS IS EQUAL TO THE ORDER OF THE GROUP

$$l_1^2 + l_2^2 + \dots + l_s^2 = h$$

2. THE SUM OF THE SQUARES OF THE CHARACTERS IN ANY IRREDUCIBLE REPRESENTATION EQUALS TO h

$$\sum_R [\chi_i(R)]^2 = h$$

3. (THE VECTORS WHOSE COMPONENTS ARE) THE CHARACTERS OF TWO DIFFERENT IRREDUCIBLE REPRESENTATIONS ARE ORTHOGONAL

$$\sum_R \chi_i(R)\chi_j(R) = 0 \quad \text{WHEN } i \neq j$$

AT THE SAME TIME THE SQUARE OF THE LENGTH OF SUCH VECTOR

$$\sum_R [\chi_i(R)]^2 = h$$

4. THE CHARACTERS OF REPRESENTATION OF ALL OPERATIONS BELONGING TO THE SAME CLASS ARE IDENTICAL

5. THE NUMBER OF IRREDUCIBLE REPRESENTATIONS OF A GROUP IS EQUAL TO THE NUMBER OF CLASSES IN THE GROUP

6. AMONG THE IRREDUCIBLE REPRESENTATIONS OF A GROUP ALWAYS THERE IS FULLY-SYMMETRIC REPRESENTATION A_1 FOR WHICH ALL CHARACTERS ARE EQUAL 1 (TRANSFORMATION PROPERTIES OF SCALARS)

7. THE CHARACTERS OF REPRESENTATION ARE INDEPENDENT OF BASIS FUNCTIONS

CONCLUSION: COMPLETE CHARACTER TABLE FOR D_3

D_3	E	$2C_3$	$3C_2'$
$\chi_{A_1}(\hat{R})$	1	1	1
$\chi_E(\hat{R})$	2	−1	0
$\chi_{A_2}(\hat{R})$	1	1	−1

CHARACTER TABLE

4.

		D_2	$\hat{E}$	$\hat{C}_2^z$	$\hat{C}_2^y$	$\hat{C}_2^x$
		C_{2v}	$\hat{E}$	$\hat{C}_2$	$\hat{\sigma}_v$	$\hat{\sigma}_v$
Γ_1	A_1	A_1	1	1	1	1
Γ_2	B_1	A_2	1	1	-1	-1
Γ_3	B_2	B_1	1	-1	1	-1
Γ_4	B_3	B_2	1	-1	-1	1

D_2: $x^2, y^2, z^2 \in A_1$
$xy, z, R_z \in B_1$
$xz, y, R_y \in B_2$
$yz, x, R_x \in B_3$
C_{2v}: $z, x^2, y^2, z^2 \in A_1$; $xy, R_z \in A_2$
$xz, x, R_y \in B_1$; $yz, y, R_x \in B_2$

5. D_3

		D_3	$\hat{E}$	$2\hat{C}_3$	$3\hat{C}_2'$
		C_{3v}	$\hat{E}$	,,	$3\hat{\sigma}_v$
(p_z)	Γ_1	A_1	1	1	1
	Γ_2	A_2	1	1	-1
$(p_x p_y)$	Γ_2	E	2	-1	0

D_3: $x^2+y^2, z^2 \in A_1$; $z, R_z \in A_2$
$\left.\begin{array}{l}(xz, yz), (x^2-y^2, xy), (x, y)\\ (R_x, R_y)\end{array}\right\} \in E$
C_{3v}: $x^2+y^2, z^2, z \in A_1$; $R_z \in A_2$
$(x^2-y^2, xy), (xz, yz), (x, y)$,
$(R_x, R_y) \in E$

6.

	D_4	$\hat{E}$	$\hat{C}_2$	$2\hat{C}_4$	$2\hat{C}_2'$	$2\hat{C}_2''$
	C_{4v}	$\hat{E}$	,,	,,	$2\hat{\sigma}_v$	$2\hat{\sigma}_v'$
	D_{2d}	$\hat{E}$	,,	$2\hat{S}_4$	$2\hat{C}_2$	$2\hat{\sigma}_d$
Γ_1	A_1	1	1	1	1	1
Γ_2	A_2	1	1	1	-1	-1
Γ_3	B_1	1	1	-1	1	-1
Γ_4	B_2	1	1	-1	-1	1
Γ_5	E	2	-2	0	0	0

D_4: $x^2+y^2, z^2 \in A_1$; $z, R_z \in A_2$
$(x, y), (xz, yz), (R_x, R_y) \in E$
$(x^2-y^2) \in B_1$ $xy \in B_2$
C_{4v}: $x^2+y^2, z^2, z \in A_1$; $R_z \in A_2$;
$x^2-y^2 \in B_1$; $xy \in B_2$;
$(xz, yz), (x, y), (R_x, R_y) \in E$
D_{2d}: $x^2+y^2, z^2 \in A_1$; $R_z \in A_2$;
$x^2-y^2 \in B_1$; $xy, z \in B_2$,
$(xz, yz), (x, y), (R_x, R_y) \in E$

7.

		D_6	$\hat{E}$	$\hat{C}_2$	$2\hat{C}_3$	$2\hat{C}_6$	$3\hat{C}_2'$	$3\hat{C}_2''$
		C_{6v}	$\hat{E}$	,,	,,	,,	$3\hat{\sigma}_v$	$3\hat{\sigma}_d$
		D_{3h}	$\hat{E}$	$\hat{\sigma}_h$	,,	$2S_3$	$3\hat{C}_2'$	$3\hat{\sigma}_v$
Γ_1	A_1	A_1'	1	1	1	1	1	1
Γ_2	A_2	A_2'	1	1	1	1	-1	-1
Γ_3	B_1	A_1''	1	-1	1	-1	1	-1
Γ_4	B_2	A_2''	1	-1	1	-1	-1	1
Γ_5	E_1	E''	2	-2	-1	1	0	0
Γ_6	E_2	E'	2	2	-1	-1	0	0

D_6: $(x^2+y)^2, z^2 \in A_1$
$z, R_z \in A_2$;
$(x, y)(xz, yz)$,
$(R_x, R_y) \in E_1$
$(x^2-y^2, xy) \in E_2$
C_{6v}: $x^2+y^2, z^2, z \in A_1$
$R_z \in A_2$
$(x, y), (xz, yz)$,
$(R_x, R_y) \in E_1$
$(x^2-y^2, xy) \in E_2$
D_{3h}: $x^2+y^2, z^2 \in A_1'$
$R_z \in A_2'$; $z \in A_2''$;
$(x^2-y^2, xy), (x, y) \in E'$
$(xz, yz), (R_x, R_y) \in E''$

APPLICATIONS:

Tablica VI.2. Rozkład termów atomowych $(d^n)^{2S+1}L$ na reprezentacje nieprzywiedlne

Term R_3	Elementy symetrii T_d: / Elementy symetrii O:	$\hat{E}$ / $\hat{E}$	$8\hat{C}_3$ / $8\hat{C}_3$	$3\hat{C}_2$ / $3\hat{C}_2$	$6\sigma_d$ / $6\hat{C}'_2$	$6\hat{S}_4$ / $6\hat{C}_4$	Rozkład
S		1	1	1	1	1	A_1
P	SPECTROSCOPIC	3	0	−1	−1	1	T_1
D	TERMS ⟹	5	−1	1	1	−1	$E+T_2$
F		7	1	−1	−1	−1	$A_2+T_1+T_2$
G		9	0	1	1	1	$A_1+E+T_1+T_2$
H		11	−1	−1	−1	1	$E+2T_1+T_2$

SPLITTING OF ENERGY LEVELS →

CHARACTER TABLE

8.	O / T_d	$\hat{E}$ / $\hat{E}$	$8\hat{C}_3$ / „	$3\hat{C}_2$ / „	$6\hat{C}_2$ / $6\sigma_d$	$6\hat{C}_4$ / $6\hat{S}_4$	
Γ_1	A_1	1	1	1	1	1	$O: (x^2-y^2, xy) \in E;$ $(x, y, z), (R_x, R_y, R_z) \in T_1$
Γ_2	A_2	1	1	1	−1	−1	$(xy, xz, yz) \in T_2$
Γ_3	E	2	−1	2	0	0	$T_d: (x^2-y^2, z^2) \in E;$
Γ_4	T_1	3	0	−1	−1	1	$(R_x, R_y, R_z) \in T_1$
Γ_5	T_2	3	0	−1	1	−1	$(x, y, z), (xy, xz, yz) \in T_2$

9. $C_{\infty v}$	$\hat{E}$	$2\hat{C}(\varphi)$	$\hat{\sigma}_v$	
$A_1 = \Sigma^+$	1	1	1	x^2+y^2, z^2, z
$A_2 = \Sigma^-$	1	1	−1	R_z
$E_1 = \Pi$	2	$2\cos\varphi$	0	$(x, y), (xz, yz), (R_x, R_y)$
$E_2 = \Delta$	2	$2\cos 2\varphi$	0	(x^2-y^2, xy)
$E_3 = \Phi$	2	$2\cos 3\varphi$	0	
...	.	...	.	