

Character tables

point group | Symmetry operations separated into functions

Names of irreducible representations (Mulliken) | #s characters
 (+) symmetric
 (-) antisymmetric
 (0) (zero) no overlap

* R_x, R_y, R_z

↳ rotational movement of molecule along x, y, z axes

* functions that correspond to d orbitals (quadratic)

Simplest cases ± 1

More complicated values of 0
 numbers $\neq \pm 1$

→ often occurs when two functions have to transform together

A, B, E, T
 ↓ singly degenerate character under E operation = 1
 ↓ doubly degenerate character under E operation = 2
 ↓ triply degenerate character under E operation = 3

Character table for C_{4v} point group

	E	$2C_4(z)$	C_2	$2\sigma_v$	$2\sigma_d$	linear, rotations	quadratic
A_1	1	1	1	1	1	z	x^2+y^2, z^2
A_2	1	1	1	-1	-1	R_z	
B_1	1	-1	1	1	-1		x^2-y^2
B_2	1	-1	1	-1	1		xy
E	2	0	-2	0	0	(x, y) (R_x, R_y)	(xz, yz)

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p_x, p_y, p_z
 → determine
 their
 characters

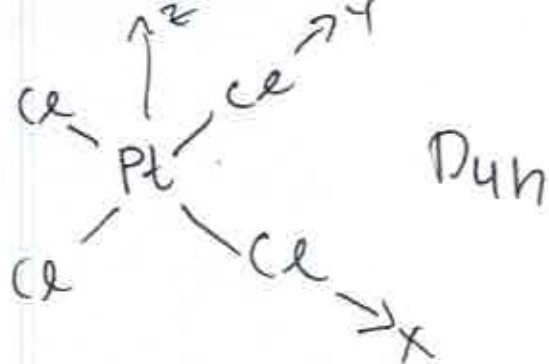
Character table for D_{4h} point group

	E	$2C_4(z)$	C_2	$2C'_2$	$2C''_2$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$	linears, rotations	quadratic
A_{1g}	1	1	1	1	1	1	1	1	1	1		x^2+y^2, z^2
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1	R_z	
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1		x^2-y^2
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1		xy
E_g	2	0	-2	0	0	2	0	-2	0	0	(R_x, R_y)	(xz, yz)
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1		
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1	z	
B_{1u}	1	-1	1	1	-1	-1	1	-1	-1	1		
B_{2u}	1	-1	1	-1	1	-1	1	-1	1	-1		
E_u	2	0	-2	0	0	-2	0	2	0	0	(x, y)	

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$$\text{order } 1 + 2 + 1 + 2 + 2 + 1 + 2 + 1 + 2 + 2 = \boxed{16 = h}$$

Sum of coefficients on
operations (top row)

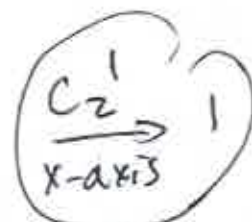


d_{z^2}



$E \rightarrow$

1



$i \rightarrow$

1



$S_4 \rightarrow$

1

$C_4 \rightarrow$

1

axis in between x & y axes

$\sigma_h \rightarrow$

1

$C_2 \rightarrow$

1

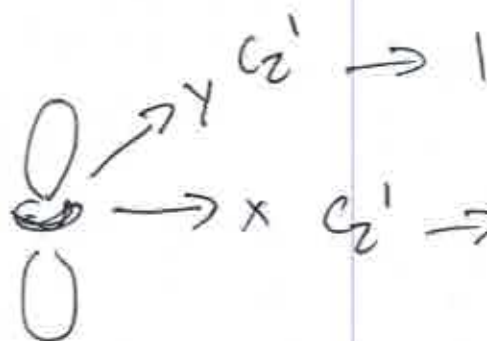
z-axis

$\sigma_v \rightarrow$

1

$\sigma_d \rightarrow$

1



character = 1
for both

$$\frac{(1+1)}{2} = 1$$

Characters: all 1's

