Next Tuesday: Midterm 1: Welch 1.316

- ~15 pts on orbitals
- ~15 pts on electronic configurations and periodic trends
- ~30 pts on determining point group (and drawing lewis structure)
- ~20 pts on symmetry operations
- ~20 pts on character tables

- Bring your student ID!
- You will be provided a periodic table
- You are allowed to bring three simple models from your model kit: octahedral, tetrahedral, and trigonal bipyramidal. Have these assembled before class, you will not have access to your full kit during the exam

Midterm 1 Office hours/Review Session

- My office hours in 4.314

Today: 4:30 pm – 5:30 pm

Monday: 4:30 pm – 6:30 pm

- Regular TA office hours:

Thursday: 12:30 pm – 1:30 pm (Spencer)

Friday: 4:00 pm – 5:00 pm (Rahul)

- Review session: Sunday night, 7:00 pm (for ~1.5h)

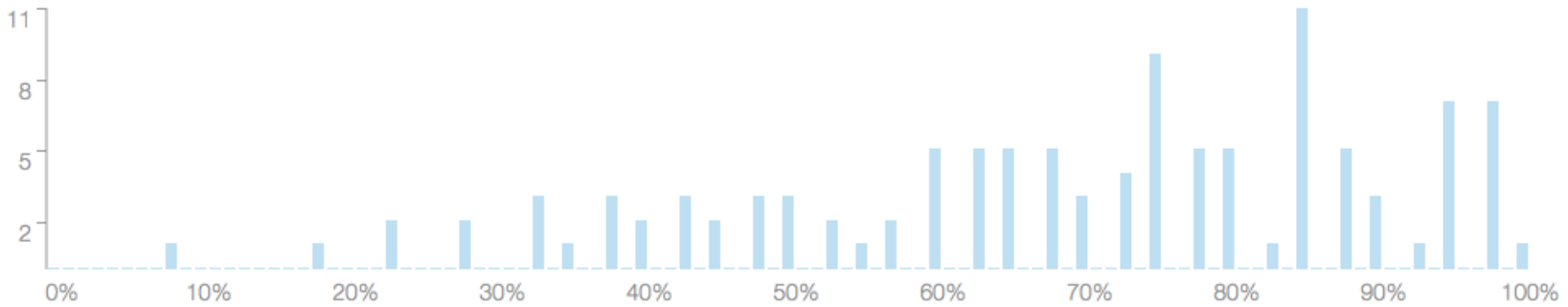
Welch 2.312

Led by Kanchan, with help from other TAs

Quiz 3

⊖ Average Score

68%

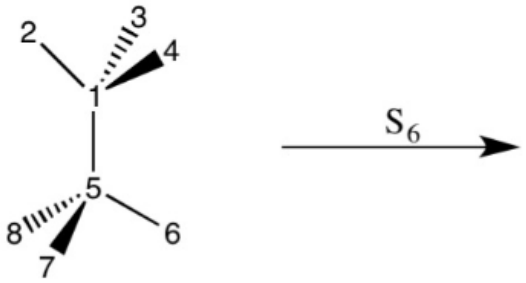


Attempts: 112 out of 113

+0.56

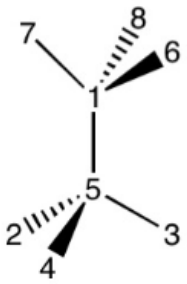
Discrimination Index

What is the product of the S_6 operation shown below?

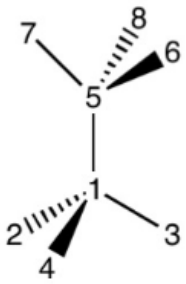


S_6

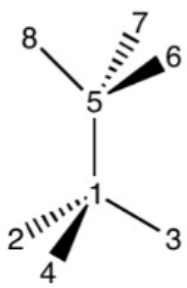
A



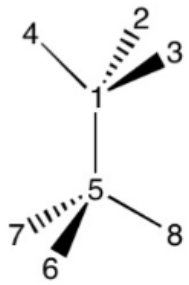
B



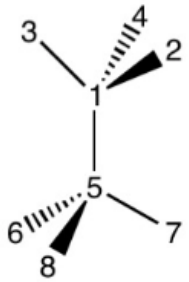
C



D



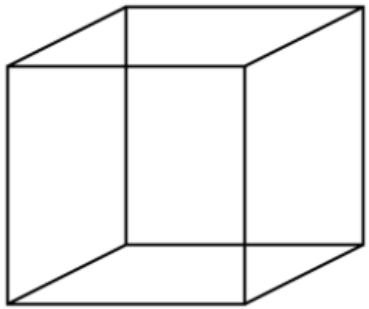
E



A	5 respondents	4 %	
B	97 respondents	**86 %**	✓
C	10 respondents	9 %	
D		0 %	
E		0 %	
No Answer	1 respondents	1 %	

Attempts: 113 out of 113

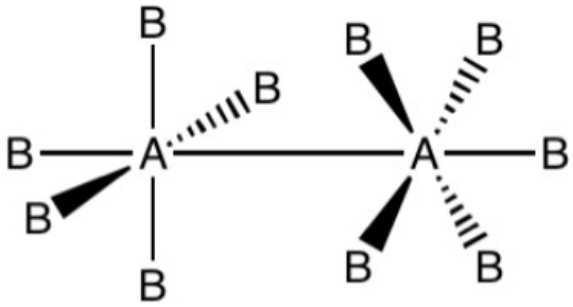
What rotation axes does a cube contain? Check all that apply.



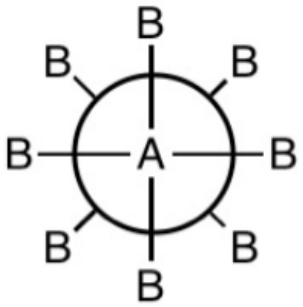
C1	83 respondents	**73** %	✔
C2	111 respondents	**98** %	✔
C3	91 respondents	**81** %	✔
C4	113 respondents	**100** %	✔
C5	1 respondents	1 %	
C6	4 respondents	4 %	
C7	1 respondents	1 %	
C8	4 respondents	4 %	
C9	1 respondents	1 %	
C10	1 respondents	1 %	

Attempts: 111 out of 113

What is the point group for the molecule below?



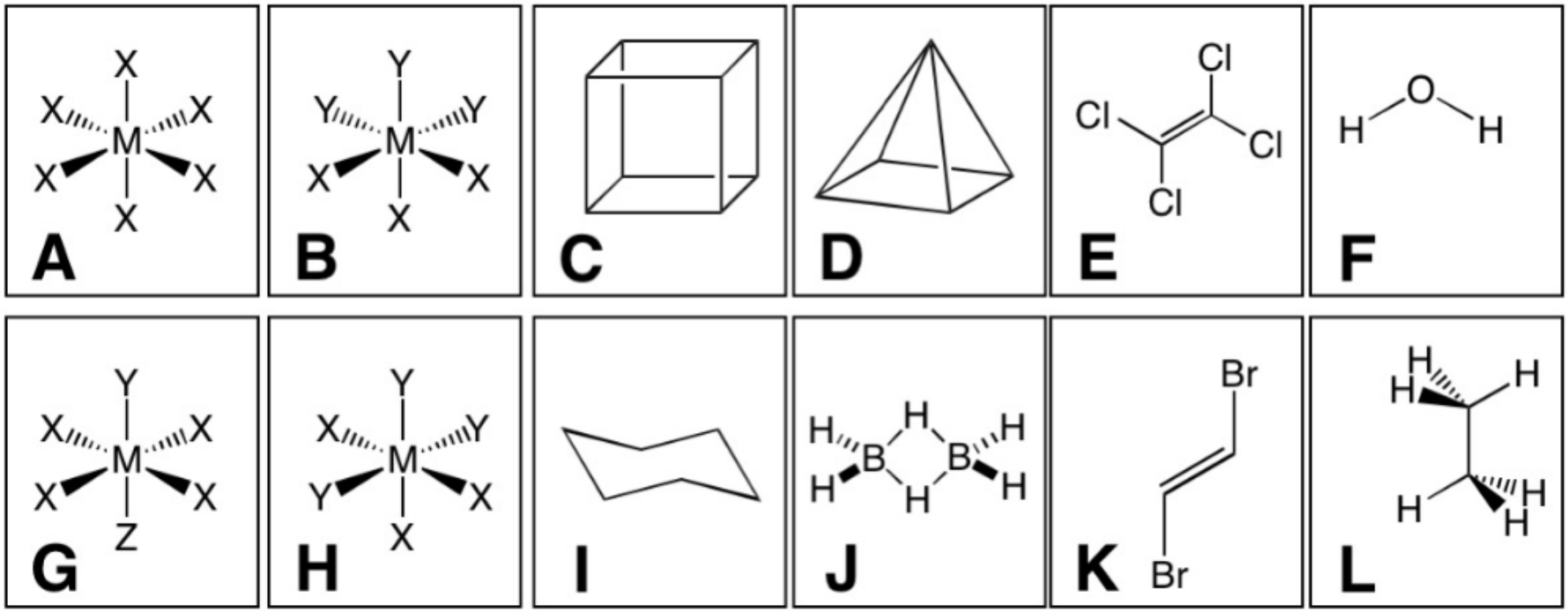
side view

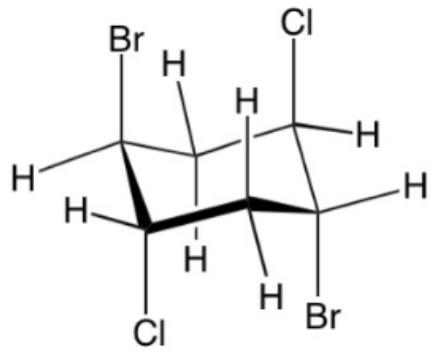


Newman projection

D4d	70 respondents	**62** %	✓
Something Else	41 respondents	36 %	
No Answer	2 respondents	2 %	

Match the following items with another item in the same point group. If there is no match indicate choose "no match" in the drop-down menu.



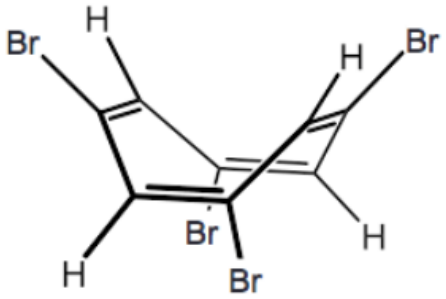
A) 

[answerA]

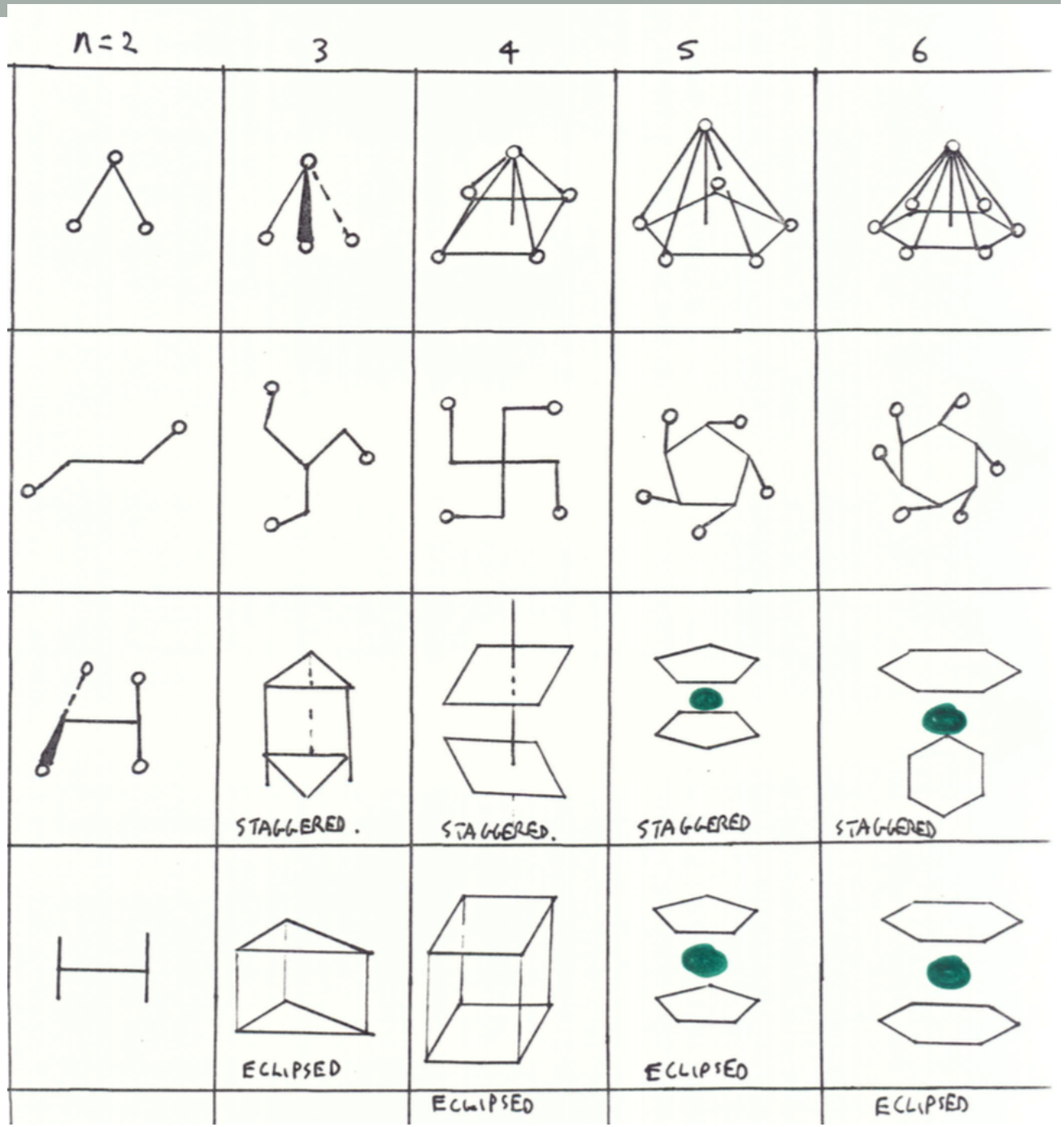
B) Fluoroacetylene, C2HF [answerB]

C) A dx2-y2 orbital [answerC]

D) Br_4cyclooctatetraene (pictured below) [answerD]



Point group short cuts



CHARACTER TABLES, POINT GROUPS, AND THEIR APPLICATIONS

MFT section 4.4

Mulliken symbols

A: singly degenerate (1 under E operation), sym w.r.t. C_n

B: singly degenerate (1 under E operation), antisym w.r.t. C_n

E: doubly degenerate (2 under E operation)

T: triply degenerate (3 under E operation)

$_1$: sym w.r.t. σ_v or a perpendicular C_2

$_2$: antisym w.r.t. σ_v or a perpendicular C_2

$_g$: sym w.r.t. inversion center

$_u$: antisym w.r.t. inversion center

‘ : sym w.r.t. σ_h

“ : antisym w.r.t. σ_h

Characters:
+ values = symmetric
- values = antisymmetric

Properties of characters and irreducible representations (Table 4.7)

- Order (h) = sum of coefficients on symmetry operations
- Number of classes = number of columns
- Number of irreducible representations = number of classes
- Sum of square of dimensions (characters in the ‘E’ column) equals order (h)
- Within an irreducible representation (row), sum of square of characters multiplied by coefficient of the class equals order of group (h)
- Irreducible represntations are orthodonal
- There is always a totally symmetric representation (all characters = 1)

A bit more explanation on the functions on the right hand side of character tables:

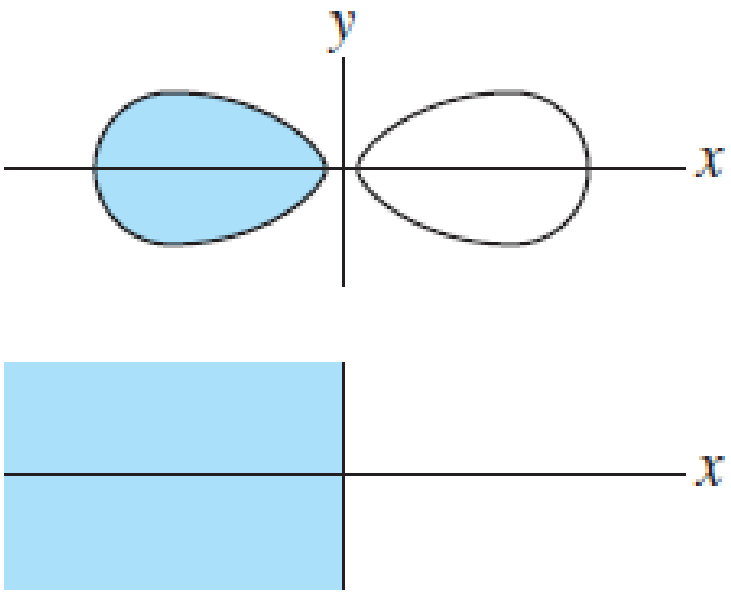
Character table for C_{4v} point group

	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)

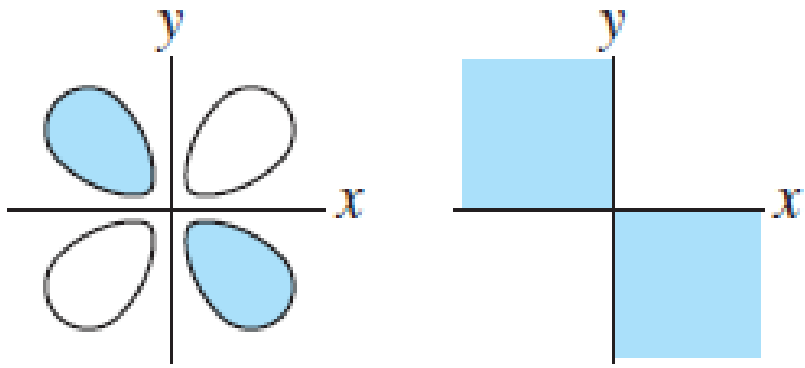
This portion of the table represents how rotations and different orbitals behave w.r.t. symmetry operations in this point group.

$z = p_z$, $xy = d_{xy}$ etc.

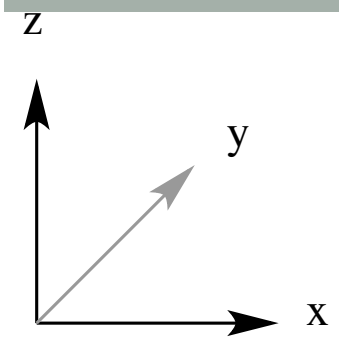
Note: s orbital is always going to be in the group where all characters are 1's

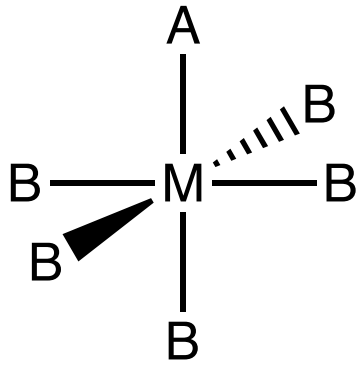


p_x orbitals have the same symmetry as x (positive in half the quadrants, negative in the other half).



d_{xy} orbitals have the same symmetry as the function xy (sign of the function in the four quadrants).





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A_1	1	1	1	1	1	z	x^2+y^2, z^2
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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)

1) Why is a specific orbital associated with a specific irreducible representation?
2) Why is a specific rotation associated with a specific irreducible representation?
3) What does (x,y) mean?