ABC CHEMISTRY

Mr. Aniket Bhardwaj · 15+ Years Mentorship

Group Theory

Premium CSIR-NET PYQ Book

41 Previous-Year Questions · 39 with verified answers · Distractor Analysis

3-Slide Solutions | Distractor Analysis | Exam Tricks | Revision Sheets

CSIR-NET · GATE · IIT-JAM — 3 Topics · 41 Real PYQs

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Course Contents

3 Topics · 41 PYQs

1 **Symmetry Elements Point Groups** — 39%
16 Qs E 8 · M 7 · H 1

2 **Character Tables** — 27%
11 Qs E 1 · M 8 · H 2

3 **Group Theory – General** — 34%
14 Qs E 7 · M 4 · H 3

Legend: **E** Easy **M** Medium **H** Hard · **%** = exam weightage (share of the chapter)

TOPIC 1

Symmetry Elements Point Groups

16 questions · Easy 8 | Medium 7 | Hard 1 · PYQ frequency: High

Q1

The molecule diborane belongs to the symmetry point group

A. C_{2v}

B. C_{2h}

C. D_2d

D. D_{2h}

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Symmetry Elements Point Groups

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'D needs the sideways C_2s'.

Symmetry Elements Point Groups

Correct Answer D D_{2h}

CONCEPT

Symmetry operations E, C_n, σ (v, h, d), i, S_n; a molecule's point group is assigned by a flow chart: linear ($C\infty v/D\infty h$), high symmetry (Td, Oh, Ih), then principal axis, perpendicular C_2s (D_n), σh (D_nh/C_nh), σv (C_nv/D_nd).

↓

LOGIC / WORKING

- Diborane: planar B_2H_4 frame with two bridging H in the perpendicular plane — three mutually perpendicular C_2 axes, three planes and an inversion centre → D_2h.
- Therefore the answer is (D).

FINAL: (D) D_{2h}

SHORTCUT / EXAM TRICK

Polar ⇒ C_n or C_nv or Cs; chiral ⇒ only proper rotations (C_n, D_n).

COMMON MISTAKE

Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

EXAM TIP

Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

MEMORY TRICK

'D needs the sideways C_2s'.

Why the Other Options Are Wrong

Correct answer: D

A C_{2v}

Why (D) is the key — Diborane: planar B_2H_4 frame with two bridging H in the perpendicular plane — three mutually perpendicular C_2 axes, three planes and an inversion centre → D_2h.

B C_{2h}

Ruled out: Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

C D_2d

Ruled out: Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

Q2

The symmetry point group of the most stable geometry of the following molecule mathrmCl(H)C=C=C(H)Cl is

A C_2

B C_1

C C_{2v}

D C_{2h}

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Symmetry Elements Point Groups

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'D needs the sideways C_2s'.

Correct Answer A C_2

CONCEPT

Symmetry operations E, C_n, σ (v, h, d), i, S_n; a molecule's point group is assigned by a flow chart: linear ($C\infty v/D\infty h$), high symmetry (Td, Oh, Ih), then principal axis, perpendicular C_2s (D_n), σh (D_nh/C_nh), σv (C_nv/D_nd).

↓

LOGIC / WORKING

- 1,3-Dichloroallene: the two CHCl planes are perpendicular; the only symmetry element is a C_2 through the central carbon — point group C_2 (chiral, axially dissymmetric).
- Therefore the answer is (A).

FINAL: (A) C_2

SHORTCUT / EXAM TRICK

Polar ⇒ C_n or C_nv or Cs; chiral ⇒ only proper rotations (C_n, D_n).

COMMON MISTAKE

Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

EXAM TIP

Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

MEMORY TRICK

'D needs the sideways C_2s'.

Why the Other Options Are Wrong

Correct answer: A

B — C_1

Why (A) is the key — 1,3-Dichloroallene: the two CHCl planes are perpendicular; the only symmetry element is a C_2 through the central carbon — point group C_2 (chiral, axially dissymmetric).

C — C_{2v}

Ruled out: Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

D — C_{2h}

Ruled out: Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

Q3

The product σ^xy.S₄^z (S₄^z is the four fold improper axis of rotation around the z-axis, and σ^xy is the reflection in the xy plane) is

A. C_4^z

B. C_4^z.i

C. C_4^y

D. C_2^z

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Symmetry Elements Point Groups

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'D needs the sideways C_2s'.

Correct Answer A C_4^z

CONCEPT

Symmetry operations E, C_n, σ (v, h, d), i, S_n; a molecule's point group is assigned by a flow chart: linear ($C\infty v/D\infty h$), high symmetry (Td, Oh, Ih), then principal axis, perpendicular C_2s (D_n), σh (D_nh/C_nh), σv (C_nv/D_nd).

↓

LOGIC / WORKING

- $S_4^z = C_4^z \cdot \sigma_{xy}$ by definition, so $\sigma_{xy} \cdot S_4^z = \sigma_{xy} \cdot \sigma_{xy} \cdot C_4^z = C_4^z$.
- Therefore the answer is (A).

FINAL: (A) C_4^z

SHORTCUT / EXAM TRICK

Polar ⇒ C_n or C_nv or Cs; chiral ⇒ only proper rotations (C_n, D_n).

COMMON MISTAKE

Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

EXAM TIP

Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

MEMORY TRICK

'D needs the sideways C_2s'.

Why the Other Options Are Wrong

Correct answer: A

B — **C_4^z.i**

Why (A) is the key — $S_4^z = C_4^z \cdot \sigma_{xy}$ by definition, so $\sigma_{xy} \cdot S_4^z = \sigma_{xy} \cdot \sigma_{xy} \cdot C_4^z = C_4^z$.

C — **C_4^y**

Ruled out: Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

D — **C_2^z**

Ruled out: Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

Q4

For every atom that is NOT shifted under C_4 and σ symmetry operations, the characters are respectively.

A. -1, -1

B. 0, 0

C. 1, 1

D. -1, 1

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Symmetry Elements Point Groups

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'D needs the sideways C_2s'.

Correct Answer C 1, 1

CONCEPT

Symmetry operations E, C_n, σ (v, h, d), i, S_n; a molecule's point group is assigned by a flow chart: linear ($C_\infty v/D_\infty h$), high symmetry (Td, Oh, Ih), then principal axis, perpendicular C_2s (D_n), σh (D_nh/C_nh), σv (C_nv/D_nd).

↓

LOGIC / WORKING

- Per unshifted atom $\chi(C_n) = 1 + 2\cos(2\pi/n)$: $C_4 \rightarrow 1 + 2\cos 90° = 1$; any reflection → 1.
- Therefore the answer is (C).

FINAL: (C) 1, 1

SHORTCUT / EXAM TRICK

Polar ⇒ C_n or C_nv or Cs; chiral ⇒ only proper rotations (C_n, D_n).

COMMON MISTAKE

Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

EXAM TIP

Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

MEMORY TRICK

'D needs the sideways C_2s'.

Why the Other Options Are Wrong

Correct answer: C

A **-1, -1**

Why (C) is the key — Per unshifted atom $\chi(C_n) = 1 + 2\cos(2\pi/n)$: $C_4 \rightarrow 1 + 2\cos 90° = 1$; any reflection $\rightarrow 1$.

B **0, 0**

Ruled out: Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

D **-1, 1**

Ruled out: Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

Q5

The equivalent symmetry operations for S_6^3 and S_3^6 are, respectively

A. C_3 and C_2

B. σ_h and I

C. σ_h and E

D. i and E

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Symmetry Elements Point Groups

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'D needs the sideways C_2s'.

Correct Answer D i and E

CONCEPT

Symmetry operations E, C_n, σ (v, h, d), i, S_n; a molecule's point group is assigned by a flow chart: linear ($C\infty v/D\infty h$), high symmetry (Td, Oh, Ih), then principal axis, perpendicular C_2s (D_n), σh (D_nh/C_nh), σv (C_nv/D_nd).

↓

LOGIC / WORKING

- $S_6^3 = C_2 \cdot \sigma_h = i$; $S_3^6 = C_3^6 \cdot \sigma_h^6 = E \cdot E = E$.
- Therefore the answer is (D).

FINAL: (D) i and E

SHORTCUT / EXAM TRICK

Polar ⇒ C_n or C_nv or Cs; chiral ⇒ only proper rotations (C_n, D_n).

COMMON MISTAKE

Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

EXAM TIP

Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

MEMORY TRICK

'D needs the sideways C_2s'.

Why the Other Options Are Wrong

Correct answer: D

A — **C_3 and C_2**

Why (D) is the key — $S_6^3 = C_2 \cdot \sigma_h = i$; $S_3^6 = C_3^6 \cdot \sigma_h^6 = E \cdot E = E$.

B — **σ_h and I**

Ruled out: Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

C — **σ_h and E**

Ruled out: Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

Q6

A cube does not have the symmetry element

A. C_2

B. C_3

C. C_4

D. C_6

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Symmetry Elements Point Groups

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'D needs the sideways C_2s'.

Correct Answer D C_6

CONCEPT

Symmetry operations E, C_n, σ (v, h, d), i, S_n; a molecule's point group is assigned by a flow chart: linear ($C\infty v/D\infty h$), high symmetry (Td, Oh, Ih), then principal axis, perpendicular C_2s (D_n), σh (D_nh/C_nh), σv (C_nv/D_nd).

↓

LOGIC / WORKING

- A cube (O_h) has C_4 (through face centres), C_3 (body diagonals) and C_2 (edge midpoints) but no C_6.
- Therefore the answer is (D).

FINAL: (D) C_6

SHORTCUT / EXAM TRICK

Polar ⇒ C_n or C_nv or Cs; chiral ⇒ only proper rotations (C_n, D_n).

COMMON MISTAKE

Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

EXAM TIP

Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

MEMORY TRICK

'D needs the sideways C_2s'.

Why the Other Options Are Wrong

Correct answer: D

A C_2

Why (D) is the key — A cube (O_h) has C_4 (through face centres), C_3 (body diagonals) and C_2 (edge midpoints) but no C_6.

B C_3

Ruled out: Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

C C_4

Ruled out: Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

Q7

Among the following, the CORRECT statement is:

A. The number of irreducible representations is equal to classes of symmetry operations

B. The number of irreducible representations is equal to the order of the symmetry point group

C. The irreducible representations contained in any point group are always of one dimension

D. A symmetry point group may not contain a totally symmetric irreducible representation

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Symmetry Elements Point Groups

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'D needs the sideways C_2s'.

Correct Answer A The number of irreducible representations is equal to classes of symmetry operations

CONCEPT

Symmetry operations E, C_n, σ (v, h, d), i, S_n; a molecule's point group is assigned by a flow chart: linear ($C\infty v/D\infty h$), high symmetry (Td, Oh, Ih), then principal axis, perpendicular C_2s (D_n), σh (D_nh/C_nh), σv (C_nv/D_nd).

↓

LOGIC / WORKING

- Number of irreducible representations = number of classes (a). Σ(dimension)² = order, irreps may be 1-, 2- or 3-dimensional, and every group has the totally symmetric representation.
- Therefore the answer is (A).

FINAL: (A) The number of irreducible representations is equal to classes of symmetry operations

SHORTCUT / EXAM TRICK

Polar ⇒ C_n or C_nv or Cs; chiral ⇒ only proper rotations (C_n, D_n).

COMMON MISTAKE

Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

EXAM TIP

Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

MEMORY TRICK

'D needs the sideways C_2s'.

Why the Other Options Are Wrong

Correct answer: A

B — **The number of irreducible representations is equal to the order of the symmetry point group**

Why (A) is the key — Number of irreducible representations = number of classes (a). Σ(dimension)² = order, irreps may be 1-, 2- or 3-dimensional, and every group has the totally symmetric representation.

C — **The irreducible representations contained in any point group are always of one dimension**

Ruled out: Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

D — **A symmetry point group may not contain a totally symmetric irreducible representation**

Ruled out: Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

Q8

A square pyramidal, MX_4, molecule belongs to C_{4v} point group. The symmetry operations are: E, $2C_4$, C_2, $2\sigma_v$ and 2σ_d. The trace for the reducible representation, when symmetry operations of C_{4v} applied to MX_4, is: (c) 5 1 1 1 1 (a) 5 1 1 1 3 (b) 1 1 1 1 1 (d) 4 1 1 1 3

SELF-PRACTICE answer on record: (A) — options were not printed in the source.

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Symmetry Elements Point Groups

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'D needs the sideways C_2s'.

Q9

A molecules contains the following symmetry operations: E, $2C_6$, $2C_3$, C_2, $3\sigma_d$, $3\sigma_v$. The number of classes and order of the symmetry point group is:

(A) 3, 12

(B) 5, 12

(C) 6, 12

(D) 6, 6

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Symmetry Elements Point Groups

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
'D needs the sideways C_2s'.

Correct Answer C 6, 12

CONCEPT

Symmetry operations E, C_n, σ (v, h, d), i, S_n; a molecule's point group is assigned by a flow chart: linear ($C\infty v/D\infty h$), high symmetry (Td, Oh, Ih), then principal axis, perpendicular C_2s (D_n), σh (D_nh/C_nh), σv (C_nv/D_nd).

↓

LOGIC / WORKING

- E, $2C_6$, $2C_3$, C_2, 3σ_d, $3\sigma_v$ are six classes containing 1+2+2+1+3+3 = 12 operations — C_6v, order 12.
- Therefore the answer is (C).

FINAL: (C) 6, 12

SHORTCUT / EXAM TRICK

Polar ⇒ C_n or C_nv or Cs; chiral ⇒ only proper rotations (C_n, D_n).

COMMON MISTAKE

Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

EXAM TIP

Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

MEMORY TRICK

'D needs the sideways C_2s'.

Why the Other Options Are Wrong

Correct answer: C

A **3, 12**

Why (C) is the key — E, $2C_6$, $2C_3$, C_2, $3\sigma_d$, $3\sigma_v$ are six classes containing 1+2+2+1+3+3 = 12 operations — C_6v, order 12.

B **5, 12**

Ruled out: Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

D **6, 6**

Ruled out: Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

Q10

The symmetry point group of propyne is

A C_3

B C_{3v}

C D_3

D D_3d

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Symmetry Elements Point Groups

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'D needs the sideways C_2s'.

Correct Answer B C_{3v}

CONCEPT

Symmetry operations E, C_n, σ (v, h, d), i, S_n; a molecule's point group is assigned by a flow chart: linear ($C\infty v/D\infty h$), high symmetry (Td, Oh, Ih), then principal axis, perpendicular C_2s (D_n), σh (D_nh/C_nh), σv (C_nv/D_nd).

↓

LOGIC / WORKING

- Propyne $CH_3–C\equiv C–H$: a C_3 axis along the chain and three σ_v planes, no C_2 perpendicular and no $\sigma_h \rightarrow C_3v$.
- Therefore the answer is (B).

FINAL: (B) C_{3v}

SHORTCUT / EXAM TRICK

Polar ⇒ C_n or C_nv or Cs; chiral ⇒ only proper rotations (C_n, D_n).

COMMON MISTAKE

Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

EXAM TIP

Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

MEMORY TRICK

'D needs the sideways C_2s'.

Why the Other Options Are Wrong

Correct answer: B

A — **C_3**

Why (B) is the key — Propyne $CH_3–C\equiv C–H$: a C_3 axis along the chain and three σ_v planes, no C_2 perpendicular and no $\sigma_h \rightarrow C_3v$.

C — **D_3**

Ruled out: Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

D — **D_3d**

Ruled out: Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

Q11

The point group obtained by adding symmetry operation σ_h to the point group C_4 is

A. S_4

B. C_{4h}

C. D_{2h}

D. D_4

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Symmetry Elements Point Groups

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'D needs the sideways C_2s'.

Correct Answer B C_{4h}

CONCEPT

Symmetry operations E, C_n, σ (v, h, d), i, S_n; a molecule's point group is assigned by a flow chart: linear ($C_{\infty}v/D_{\infty}h$), high symmetry (Td, Oh, Ih), then principal axis, perpendicular C_2s (D_n), σh (D_nh/C_nh), σv (C_nv/D_nd).

↓

LOGIC / WORKING

- Adding σ_h to C_n generates C_nh: $C_4 + \sigma_h = C_4h$ (which also contains S_4 and i).
- Therefore the answer is (B).

FINAL: (B) C_{4h}

SHORTCUT / EXAM TRICK

Polar ⇒ C_n or C_nv or Cs; chiral ⇒ only proper rotations (C_n, D_n).

COMMON MISTAKE

Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

EXAM TIP

Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

MEMORY TRICK

'D needs the sideways C_2s'.

Why the Other Options Are Wrong

Correct answer: B

A S_4

Why (B) is the key — Adding σ_h to C_n generates C_nh: $C_4 + \sigma_h = C_4h$ (which also contains S_4 and i).

C D_{2h}

Ruled out: Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

D D_4

Ruled out: Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

Q12

The correct relation involving symmetry operations

A $S_4^2=S_2$

B $\sigma(xz).\sigma(yz)=C_2(x)$

C $S_4^3=C_4^3$

D $S_6^3=S_2$

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Symmetry Elements Point Groups

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'D needs the sideways C_2s'.

Correct Answer D $S_6^3=S_2$

CONCEPT

Symmetry operations E, C_n, σ (v, h, d), i, S_n; a molecule's point group is assigned by a flow chart: linear (C∞v/D∞h), high symmetry (Td, Oh, Ih), then principal axis, perpendicular C_2s (D_n), σh (D_nh/C_nh), σv (C_nv/D_nd).

↓

LOGIC / WORKING

- $S_6^3 = C_2\sigma_h = S_2$ = i (d) is correct. $S_4^2 = C_2$ (not S_2); σ(xz)σ(yz) = C_2(z); $S_4^3 = C_4^3\sigma_h \neq C_4^3$.
- Therefore the answer is (D).

FINAL: (D) $S_6^3=S_2$

SHORTCUT / EXAM TRICK

Polar ⇒ C_n or C_nv or Cs; chiral ⇒ only proper rotations (C_n, D_n).

COMMON MISTAKE

Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

EXAM TIP

Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

MEMORY TRICK

'D needs the sideways C_2s'.

Why the Other Options Are Wrong

Correct answer: D

A $S_4^2=S_2$

Why (D) is the key — $S_6^3 = C_2\sigma_h = S_2 = i$ (d) is correct. $S_4^2 = C_2$ (not S_2); $\sigma(xz)\sigma(yz) = C_2(z)$; $S_4^3 = C_4^3\sigma_h \neq C_4^3$.

B $\sigma(xz).\sigma(yz)=C_2(x)$

Ruled out: Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

C $S_4^3=C_4^3$

Ruled out: Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

Q13

The symmetry point group of ethane in its staggered conformation is

A C_{3v}

B D_3d

C D_{3h}

D S_6

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Symmetry Elements Point Groups

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'D needs the sideways C_2s'.

Correct Answer B D_3d

CONCEPT

Symmetry operations E, C_n, σ (v, h, d), i, S_n; a molecule's point group is assigned by a flow chart: linear ($C\infty v/D\infty h$), high symmetry (Td, Oh, Ih), then principal axis, perpendicular C_2s (D_n), σh (D_nh/C_nh), σv (C_nv/D_nd).

↓

LOGIC / WORKING

- Staggered ethane: C_3, three perpendicular C_2, three σ_d, S_6 and i → D_3d (eclipsed would be D_3h).
- Therefore the answer is (B).

FINAL: (B) D_3d

SHORTCUT / EXAM TRICK

Polar ⇒ C_n or C_nv or Cs; chiral ⇒ only proper rotations (C_n, D_n).

COMMON MISTAKE

Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

EXAM TIP

Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

MEMORY TRICK

'D needs the sideways C_2s'.

Why the Other Options Are Wrong

Correct answer: B

A C_{3v}

Why (B) is the key — Staggered ethane: C_3, three perpendicular C_2, three σ_d, S_6 and i → D_3d (eclipsed would be D_3h).

C D_{3h}

Ruled out: Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

D S_6

Ruled out: Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

Q14

A molecule has a 2-fold axis and a mirror plane perpendicular to that. The point group must have a

A. C_2 axis

B. Centre of inversion

C. σ_h plane

D. σ_v plane

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Symmetry Elements Point Groups

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'D needs the sideways C_2s'.

Correct Answer B Centre of inversion

CONCEPT

Symmetry operations E, C_n, σ (v, h, d), i, S_n; a molecule's point group is assigned by a flow chart: linear ($C\infty v/D\infty h$), high symmetry (Td, Oh, Ih), then principal axis, perpendicular C_2s (D_n), σh (D_nh/C_nh), σv (C_nv/D_nd).

↓

LOGIC / WORKING

- C_2 and a perpendicular σ_h generate S_2 = i: the group must contain a centre of inversion (C_2h).
- Therefore the answer is (B).

FINAL: (B) Centre of inversion

SHORTCUT / EXAM TRICK

Polar ⇒ C_n or C_nv or Cs; chiral ⇒ only proper rotations (C_n, D_n).

COMMON MISTAKE

Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

EXAM TIP

Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

MEMORY TRICK

'D needs the sideways C_2s'.

Why the Other Options Are Wrong

Correct answer: B

A — **C_2 axis**

Why (B) is the key — C_2 and a perpendicular σ_h generate S_2 = i: the group must contain a centre of inversion (C_2h).

C — **σ_h plane**

Ruled out: Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

D — **σ_v plane**

Ruled out: Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

Q15

The symmetry elements that are present in BF_3 are

A. C_3, σ_v, σ_h, $3C_2$

B. C_3, $3C_2$, S_2, σ_v

C. C_3, $3C_2$, σ_h, S_2

D. C_3, σ_h, σ_v, i

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Symmetry Elements Point Groups

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'D needs the sideways C_2s'.

Correct Answer A $C_3, \sigma_v, \sigma_h, 3C_2$

CONCEPT

Symmetry operations E, C_n, σ (v, h, d), i, S_n; a molecule's point group is assigned by a flow chart: linear ($C\infty v/D\infty h$), high symmetry (Td, Oh, Ih), then principal axis, perpendicular C_2s (D_n), σh (D_nh/C_nh), σv (C_nv/D_nd).

↓

LOGIC / WORKING

- BF_3 (D_3h): C_3, three C_2 perpendicular to it, σ_h (molecular plane), three σ_v, S_3 — no i, no S_2.
- Therefore the answer is (A).

FINAL: (A) $C_3, \sigma_v, \sigma_h, 3C_2$

SHORTCUT / EXAM TRICK

Polar ⇒ C_n or C_nv or Cs; chiral ⇒ only proper rotations (C_n, D_n).

COMMON MISTAKE

Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

EXAM TIP

Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

MEMORY TRICK

'D needs the sideways C_2s'.

Why the Other Options Are Wrong

Correct answer: A

B C_3, $3C_2$, S_2, σ_v

Why (A) is the key — BF_3 (D_3h): C_3, three C_2 perpendicular to it, σ_h (molecular plane), three σ_v, S_3 — no i, no S_2.

C C_3, $3C_2$, σ_h, S_2

Ruled out: Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

D C_3, σ_h, σ_v, i

Ruled out: Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

Q16

The point group of NSF_3 is:

A. D_3d

B. C_{3h}

C. D_{3h}

D. C_{3v}

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Symmetry Elements Point Groups

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'D needs the sideways C_2s'.

Correct Answer D C_{3v}

CONCEPT

Symmetry operations E, C_n, σ (v, h, d), i, S_n; a molecule's point group is assigned by a flow chart: linear ($C_\infty v/D_\infty h$), high symmetry (Td, Oh, Ih), then principal axis, perpendicular C_2s (D_n), σh (D_nh/C_nh), σv (C_nv/D_nd).

↓

LOGIC / WORKING

- NSF_3 is a tetrahedral-type molecule with N≡S on the C_3 axis and three F: C_3 and three σ_v, nothing else → C_3v.
- Therefore the answer is (D).

FINAL: (D) C_{3v}

SHORTCUT / EXAM TRICK

Polar ⇒ C_n or C_nv or Cs; chiral ⇒ only proper rotations (C_n, D_n).

COMMON MISTAKE

Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

EXAM TIP

Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

MEMORY TRICK

'D needs the sideways C_2s'.

Why the Other Options Are Wrong

Correct answer: D

A — **D_3d**

Why (D) is the key — NSF_3 is a tetrahedral-type molecule with N≡S on the C_3 axis and three F: C_3 and three σ_v, nothing else → C_3v.

B — **C_{3h}**

Ruled out: Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).

C — **D_{3h}**

Ruled out: Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

TOPIC REVISION

Symmetry Elements Point Groups

16 PYQs · Last-minute revision

TOPIC SUMMARY

Symmetry operations E, C_n, σ (v, h, d), i, S_n; a molecule's point group is assigned by a flow chart: linear ($C\infty v/D\infty h$), high symmetry (Td, Oh, Ih), then principal axis, perpendicular C_2s (D_n), σh (D_nh/C_nh), σv (C_nv/D_nd).

IMPORTANT FORMULA SHEET

- Order h = number of operations
- $S_2 = i$, $S_1 = \sigma$
- C_nv: n σv; D_nh: $nC_2 \perp$ + σh
- Chirality: no S_n (no σ, i)

FREQUENTLY ASKED CONCEPTS

- Point group of NH_3 (C_3v), H_2O (C_2v), BF_3 (D_3h), CH_4 (Td), SF_6 (Oh), ferrocene staggered (D_5d)
- Polar and chiral criteria
- Number of symmetry operations

COMMON MISTAKES & QUICK NOTES

Watch out:
Missing the perpendicular C_2 axes in planar molecules (BF_3 is D_3h, not C_3v).
Allene is D_2d, staggered ethane D_3d, eclipsed ethane D_3h, trans-N_2F_2 C_2h.

MOST-REPEATED PYQs & EXPECTED IN EXAM

PYQs in this topic: Q1 Q2 Q3 Q4 Q5 Q6 Q7 Q8 Q9 Q10 Q11 Q12 Q13 Q14 Q15 Q16

Expect 2 question(s) next session on Symmetry Elements Point Groups.

TOPIC 2

Character Tables

11 questions · Easy 1 | Medium 8 | Hard 2 · PYQ frequency: High

Q17

The character table of the C_{2v} point group is given below: The two functions varphi = $p_1 + 2p_2 + 2p_3 + p_4$ and varphi = $p_1 - 2p_2 - 2p_3 + p_4$ (where p_k is the p- orbital on the k^th atom of cis-butadiene and σ_v is the molecular plane) belong to

A. A_1 and A_2 respectively

B. Both A_2

C. Both B_2

D. B_1 and B_2 respectively

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Character Tables

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
'Unmoved atoms × contribution per atom'.

Correct Answer C Both B_2

CONCEPT

Rows are irreducible representations (A/B singly, E doubly, T triply degenerate; 1/2 and g/u labels), columns are classes; the right-hand columns list how x, y, z, Rx…, and quadratic functions transform — the key to IR/Raman activity and hybridisation.

↓

LOGIC / WORKING

- The p orbitals are perpendicular to the molecular plane (σ_v), so σ_v gives −1; C_2 exchanges atoms 1↔4, 2↔3 and inverts each p → both functions give −1; the perpendicular plane exchanges the same atoms without inversion → +1. Characters (1, −1, −1, 1) = B_2 for both.
- Therefore the answer is (C).

FINAL: (C) Both B_2

SHORTCUT / EXAM TRICK

χ per unmoved atom: E 3, σ 1, i −3, C_2 −1, C_3 0, C_4 1, S_4 −1, S_6 −2.

COMMON MISTAKE

Counting atoms moved by the operation as contributing to the character.

EXAM TIP

Total number of vibrational modes must equal 3N−6 (3N−5 linear) — use it to check the reduction.

MEMORY TRICK

'Unmoved atoms × contribution per atom'.

Why the Other Options Are Wrong

Correct answer: C

A — **A_1 and A_2 respectively**

Why (C) is the key — The p orbitals are perpendicular to the molecular plane (σ_v), so σ_v gives −1; C_2 exchanges atoms 1 ↔ 4, 2 ↔ 3 and inverts each p → both functions give −1; the perpendicular plane exchanges the same atoms without inversion → +1. Characters (1, −1, −1, 1) = B_2 for both.

B — **Both A_2**

Ruled out: Counting atoms moved by the operation as contributing to the character.

D — **B_1 and B_2 respectively**

Ruled out: Total number of vibrational modes must equal 3N−6 (3N−5 linear) — use it to check the reduction.

Q18

The irreducible representations of C_{2h} are A_g, B_g, A_u and B_u. The Raman active modes of trans-1,3-butadiene belong to the irreducible representations

A. A_g and B_g

B. A_g and A_u

C. A_u and B_g

D. B_g and B_u

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Character Tables

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'Unmoved atoms × contribution per atom'.

Correct Answer A A_g and B_g

CONCEPT

Rows are irreducible representations (A/B singly, E doubly, T triply degenerate; 1/2 and g/u labels), columns are classes; the right-hand columns list how x, y, z, Rx…, and quadratic functions transform — the key to IR/Raman activity and hybridisation.

↓

LOGIC / WORKING

- Raman activity needs a quadratic function (x^2, xy …), which in a centrosymmetric group is always g: A_g and B_g (rule of mutual exclusion: IR modes are A_u, B_u).
- Therefore the answer is (A).

FINAL: (A) A_g and B_g

SHORTCUT / EXAM TRICK

χ per unmoved atom: E 3, σ 1, i −3, C_2 −1, C_3 0, C_4 1, S_4 −1, S_6 −2.

COMMON MISTAKE

Counting atoms moved by the operation as contributing to the character.

EXAM TIP

Total number of vibrational modes must equal 3N−6 (3N−5 linear) — use it to check the reduction.

MEMORY TRICK

'Unmoved atoms × contribution per atom'.

Why the Other Options Are Wrong

Correct answer: A

B — **A_g and A_u**

Why (A) is the key — Raman activity needs a quadratic function (x^2, xy …), which in a centrosymmetric group is always g: A_g and B_g (rule of mutual exclusion: IR modes are A_u, B_u).

C — **A_u and B_g**

Ruled out: Counting atoms moved by the operation as contributing to the character.

D — **B_g and B_u**

Ruled out: Total number of vibrational modes must equal 3N−6 (3N−5 linear) — use it to check the reduction.

Q19

The character table for the D_4 point group is provided below: D_3 E 2 C_3 3C A_1 1 1 1 x^2+y^2 . z^2 A_2 1 1 -1 z. R_2 E 2 -1 0 (x, y),(R_x, R_y) (.x^2-y^2-xy), (xz, yz) For this point group, the correct statement among the following is:

A it is possible to have a totally symmetric normal mode of vibration which is IR-active

B all IR-active normal modes are necessarily Raman inactive

C all Raman-active normal modes are necessarily IR-active

D it is possible to have a pair of IR-active normal modes that are degenerate

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Character Tables

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
'Unmoved atoms × contribution per atom'.

Correct Answer D it is possible to have a pair of IR-active normal modes that are degenerate

CONCEPT

Rows are irreducible representations (A/B singly, E doubly, T triply degenerate; 1/2 and g/u labels), columns are classes; the right-hand columns list how x, y, z, Rx…, and quadratic functions transform — the key to IR/Raman activity and hybridisation.

↓

LOGIC / WORKING

- In D_3 the doubly degenerate E representation spans (x, y), so a degenerate pair of IR-active modes is possible (d). A_1 is Raman-only (no x, y, z), so (a) is false; E modes are both IR and Raman active, so (b) and (c) are false.
- Therefore the answer is (D).

FINAL: (D) it is possible to have a pair of IR-active normal modes that are degenerate

SHORTCUT / EXAM TRICK

χ per unmoved atom: E 3, σ 1, i −3, C_2 −1, C_3 0, C_4 1, S_4 −1, S_6 −2.

COMMON MISTAKE

Counting atoms moved by the operation as contributing to the character.

EXAM TIP

Total number of vibrational modes must equal 3N−6 (3N−5 linear) — use it to check the reduction.

MEMORY TRICK

'Unmoved atoms × contribution per atom'.

Why the Other Options Are Wrong

Correct answer: D

A **it is possible to have a totally symmetric normal mode of vibration which is IR-active**

Why (D) is the key — In D_3 the doubly degenerate E representation spans (x, y), so a degenerate pair of IR-active modes is possible (d). A_1 is Raman-only (no x, y, z), so (a) is false; E modes are both IR and Raman active, so (b) and (c) are false.

B **all IR-active normal modes are necessarily Raman inactive**

Ruled out: Counting atoms moved by the operation as contributing to the character.

C **all Raman-active normal modes are necessarily IR-active**

Ruled out: Total number of vibrational modes must equal 3N−6 (3N−5 linear) — use it to check the reduction.

Q20

IR active normal modes of methane belong to the irreducible representation: T_d E 8 C_3 3 C_2 6 S_4 6 σ_a A_1 1 1 1 1 1 $x^2+y^2+z^2$ A_2 1 1 1 -1 -1 E 2 -1 2 0 0 2 $x^2-x^2-y^2$, x^2-y^2 T_1 3 0 -1 1 -1 R_v, R_v, R_v T_2 3 0 -1 -1 1 x, y, z, x y, y z, z x

A. $E + A_1$

B. $E + A_2$

C. T_1

D. T_2

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Character Tables

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'Unmoved atoms × contribution per atom'.

Correct Answer D T_2

CONCEPT

Rows are irreducible representations (A/B singly, E doubly, T triply degenerate; 1/2 and g/u labels), columns are classes; the right-hand columns list how x, y, z, Rx…, and quadratic functions transform — the key to IR/Raman activity and hybridisation.

↓

LOGIC / WORKING

- IR activity requires the mode to transform as x, y or z; in T_d these span T_2, so the IR-active modes are the two T_2 sets (ν_3, ν_4).
- Therefore the answer is (D).

FINAL: (D) T_2

SHORTCUT / EXAM TRICK

χ per unmoved atom: E 3, σ 1, i −3, C_2 −1, C_3 0, C_4 1, S_4 −1, S_6 −2.

COMMON MISTAKE

Counting atoms moved by the operation as contributing to the character.

EXAM TIP

Total number of vibrational modes must equal 3N−6 (3N−5 linear) — use it to check the reduction.

MEMORY TRICK

'Unmoved atoms × contribution per atom'.

Why the Other Options Are Wrong

Correct answer: D

A — **E + A_1**

Why (D) is the key — IR activity requires the mode to transform as x, y or z; in T_d these span T_2, so the IR-active modes are the two T_2 sets (ν_3, ν_4).

B — **E + A_2**

Ruled out: Counting atoms moved by the operation as contributing to the character.

C — **T_1**

Ruled out: Total number of vibrational modes must equal 3N−6 (3N−5 linear) — use it to check the reduction.

Q21

The reducible representation Gamma, in the table is equal to the following superposition of the irreducible representation of C_{2v} point group. $C_{2\ v}$ E C_2 σ_v σ_v ^′ A_1 1 1 1 1 A_2 1 1 -1 -1 B_1 1 -1 1 -1 B_2 1 -1 -1 1 Ð 8 -2 -6 4

A $A_1 + 2A_2 + 5B_1$

B $A_1 + 2A_2 + 5B_2$

C $5A_1 + A_2 + 2B_1$

D $A_1 + 5A_2 + 2B_1$

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Character Tables

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'Unmoved atoms × contribution per atom'.

Correct Answer B $A_1 + 2A_2 + 5B_2$

CONCEPT

Rows are irreducible representations (A/B singly, E doubly, T triply degenerate; 1/2 and g/u labels), columns are classes; the right-hand columns list how x, y, z, Rx…, and quadratic functions transform — the key to IR/Raman activity and hybridisation.

↓

LOGIC / WORKING

- $n(A_1) = (8 - 2 - 6 + 4)/4 = 1$; $n(A_2) = (8 - 2 + 6 - 4)/4 = 2$; $n(B_1) = (8 + 2 - 6 - 4)/4 = 0$; $n(B_2) = (8 + 2 + 6 + 4)/4 = 5$.
- Therefore the answer is (B).

FINAL: (B) $A_1 + 2A_2 + 5B_2$

SHORTCUT / EXAM TRICK

χ per unmoved atom: E 3, σ 1, i −3, C_2 −1, C_3 0, C_4 1, S_4 −1, S_6 −2.

COMMON MISTAKE

Counting atoms moved by the operation as contributing to the character.

EXAM TIP

Total number of vibrational modes must equal 3N−6 (3N−5 linear) — use it to check the reduction.

MEMORY TRICK

'Unmoved atoms × contribution per atom'.

Why the Other Options Are Wrong

Correct answer: B

A $A_1 + 2A_2 + 5B_1$

Why (B) is the key — $n(A_1) = (8 - 2 - 6 + 4)/4 = 1$; $n(A_2) = (8 - 2 + 6 - 4)/4 = 2$; $n(B_1) = (8 + 2 - 6 - 4)/4 = 0$; $n(B_2) = (8 + 2 + 6 + 4)/4 = 5$.

C $5A_1 + A_2 + 2B_1$

Ruled out: Counting atoms moved by the operation as contributing to the character.

D $A_1 + 5A_2 + 2B_1$

Ruled out: Total number of vibrational modes must equal 3N−6 (3N−5 linear) — use it to check the reduction.

Q22

Refer to the character table of the point group C_{3v} given above. Find which of the following transition is forbidden

A $a_1 \rightleftharpoons a_1$

B $a_1 \rightleftharpoons e$

C $a_2 \rightleftharpoons e$

D $a_1 \rightleftharpoons a_2$

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Character Tables

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'Unmoved atoms × contribution per atom'.

Correct Answer D $a_1 \rightleftharpoons a_2$

CONCEPT

Rows are irreducible representations (A/B singly, E doubly, T triply degenerate; 1/2 and g/u labels), columns are classes; the right-hand columns list how x, y, z, Rx…, and quadratic functions transform — the key to IR/Raman activity and hybridisation.

↓

LOGIC / WORKING

- A transition is allowed if Γ_i × Γ_dipole × Γ_f contains A_1. Dipole spans A_1 (z) and E (x, y). $a_1 \times a_2 = A_2 \neq A_1$ and $A_2 \times E = E \neq A_1$, so $a_1 \leftrightarrow a_2$ is forbidden; the others contain A_1.
- Therefore the answer is (D).

FINAL: (D) $a_1 \rightleftharpoons a_2$

SHORTCUT / EXAM TRICK

χ per unmoved atom: E 3, σ 1, i −3, C_2 −1, C_3 0, C_4 1, S_4 −1, S_6 −2.

COMMON MISTAKE

Counting atoms moved by the operation as contributing to the character.

EXAM TIP

Total number of vibrational modes must equal 3N−6 (3N−5 linear) — use it to check the reduction.

MEMORY TRICK

'Unmoved atoms × contribution per atom'.

Why the Other Options Are Wrong

Correct answer: D

A $a_1 \rightleftharpoons a_1$

Why (D) is the key — A transition is allowed if Γ_i × Γ_dipole × Γ_f contains A_1. Dipole spans A_1 (z) and E (x, y). $a_1 \times a_2 = A_2 \neq A_1$ and $A_2 \times E = E \neq A_1$, so $a_1 \leftrightarrow a_2$ is forbidden; the others contain A_1.

B $a_1 \rightleftharpoons e$

Ruled out: Counting atoms moved by the operation as contributing to the character.

C $a_2 \rightleftharpoons e$

Ruled out: Total number of vibrational modes must equal 3N−6 (3N−5 linear) — use it to check the reduction.

Q23

Character table of C_{2v} point group is: C_2, E C_2 σ, σ_v A_1 1 1 1 1 z A_2 1 1 -1 -1 1 B_1 1 -1 1 -1 x B_2 1 -1 -1 1 y If the initial and final states belong to A_1 and B_1 irreducible representation respectively, the allowed electronic transition from A_1 to B_1 is:

A. z-polarized

B. y-polarized

C. x-polarized

D. x, z-polarized

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Character Tables

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'Unmoved atoms × contribution per atom'.

Correct Answer C x-polarized

CONCEPT

Rows are irreducible representations (A/B singly, E doubly, T triply degenerate; 1/2 and g/u labels), columns are classes; the right-hand columns list how x, y, z, Rx…, and quadratic functions transform — the key to IR/Raman activity and hybridisation.

↓

LOGIC / WORKING

- $A_1 \times \Gamma(\mu) \times B_1 \supset A_1$ requires $\Gamma(\mu) = B_1$, and x spans $B_1 \rightarrow$ x-polarised.
- Therefore the answer is (C).

FINAL: (C) x-polarized

SHORTCUT / EXAM TRICK

χ per unmoved atom: E 3, σ 1, i −3, C_2 −1, C_3 0, C_4 1, S_4 −1, S_6 −2.

COMMON MISTAKE

Counting atoms moved by the operation as contributing to the character.

EXAM TIP

Total number of vibrational modes must equal 3N−6 (3N−5 linear) — use it to check the reduction.

MEMORY TRICK

'Unmoved atoms × contribution per atom'.

Why the Other Options Are Wrong

Correct answer: C

A **z-polarized**

Why (C) is the key — $A_1 \times \Gamma(\mu) \times B_1 \supset A_1$ requires $\Gamma(\mu) = B_1$, and x spans B_1 → x-polarised.

B **y-polarized**

Ruled out: Counting atoms moved by the operation as contributing to the character.

D **x, z-polarized**

Ruled out: Total number of vibrational modes must equal 3N−6 (3N−5 linear) — use it to check the reduction.

Q24

The E × E direct product in D_3 point group contains the irreducible representations D_3 E 2 C_3 3 C_2 A_1 1 1 -1 A_2 1 1 -1 E_2 2 -1 0

A. $A_1 + A_2 + E$

B. $2A_1 + E$

C. $2A_2 + E$

D. $2A_1 + 2A_2$

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Character Tables

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'Unmoved atoms × contribution per atom'.

Correct Answer A $A_1 + A_2 + E$

CONCEPT

Rows are irreducible representations (A/B singly, E doubly, T triply degenerate; 1/2 and g/u labels), columns are classes; the right-hand columns list how x, y, z, Rx…, and quadratic functions transform — the key to IR/Raman activity and hybridisation.

↓

LOGIC / WORKING

- E × E characters: (4, 1, 0) = $A_1(1,1,1) + A_2(1,1,-1) + E(2,-1,0)$.
- Therefore the answer is (A).

FINAL: (A) $A_1 + A_2 + E$

SHORTCUT / EXAM TRICK

χ per unmoved atom: E 3, σ 1, i −3, C_2 −1, C_3 0, C_4 1, S_4 −1, S_6 −2.

COMMON MISTAKE

Counting atoms moved by the operation as contributing to the character.

EXAM TIP

Total number of vibrational modes must equal 3N−6 (3N−5 linear) — use it to check the reduction.

MEMORY TRICK

'Unmoved atoms × contribution per atom'.

Why the Other Options Are Wrong

Correct answer: A

B $2A_1 + E$

Why (A) is the key — E × E characters: (4, 1, 0) = $A_1(1,1,1) + A_2(1,1,-1) + E(2,-1,0)$.

C $2A_2 + E$

Ruled out: Counting atoms moved by the operation as contributing to the character.

D $2A_1 + 2A_2$

Ruled out: Total number of vibrational modes must equal 3N−6 (3N−5 linear) — use it to check the reduction.

Q25

Identify the Mulliken notation for the following irreducible representation E C_n nC_2 i σ_h 1 1 -1 -1 -1

A. A'_{1u}

B. A''_{2u}

C. B'_{2u}

D. A'_{2u}

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Character Tables

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'Unmoved atoms × contribution per atom'.

Correct Answer B A''$_{2u}$

CONCEPT

Rows are irreducible representations (A/B singly, E doubly, T triply degenerate; 1/2 and g/u labels), columns are classes; the right-hand columns list how x, y, z, Rx…, and quadratic functions transform — the key to IR/Raman activity and hybridisation.

↓

LOGIC / WORKING

- $\chi(C_n) = +1 \rightarrow$ A; $\chi(C_2') = -1 \rightarrow$ subscript 2; $\chi(i) = -1 \rightarrow$ u; $\chi(\sigma_h) = -1 \rightarrow$ double prime: $A_2''_u$ (option b).
- Therefore the answer is (B).

FINAL: (B) A''$_{2u}$

SHORTCUT / EXAM TRICK

χ per unmoved atom: E 3, σ 1, i −3, C_2 −1, C_3 0, C_4 1, S_4 −1, S_6 −2.

COMMON MISTAKE

Counting atoms moved by the operation as contributing to the character.

EXAM TIP

Total number of vibrational modes must equal 3N−6 (3N−5 linear) — use it to check the reduction.

MEMORY TRICK

'Unmoved atoms × contribution per atom'.

Why the Other Options Are Wrong

Correct answer: B

A — **A'_{1u}**

Why (B) is the key — $\chi(C_n) = +1 \rightarrow A$; $\chi(C_2') = -1 \rightarrow$ subscript 2; $\chi(i) = -1 \rightarrow u$; $\chi(\sigma_h) = -1 \rightarrow$ double prime: $A_2''_u$ (option b).

C — **B'_{2u}**

Ruled out: Counting atoms moved by the operation as contributing to the character.

D — **A'_{2u}**

Ruled out: Total number of vibrational modes must equal 3N−6 (3N−5 linear) — use it to check the reduction.

Q26

The π-orbital $p_1 + p_2 - p_3 - p_4$ of cis-butadiene belongs to the irreducible representation $C_{2\ v}$ E C_2 σ_v σ_v ^′ A_1 1 1 1 1 A_2 1 1 -1 -1 B_1 1 -1 1 -1 B_2 1 -1 -1 1

A A_1

B A_2

C B_1

D B_2

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Character Tables

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'Unmoved atoms × contribution per atom'.

Correct Answer B A_2

CONCEPT

Rows are irreducible representations (A/B singly, E doubly, T triply degenerate; 1/2 and g/u labels), columns are classes; the right-hand columns list how x, y, z, Rx…, and quadratic functions transform — the key to IR/Raman activity and hybridisation.

↓

LOGIC / WORKING

- C_2 swaps $1 \leftrightarrow 4$, $2 \leftrightarrow 3$ and inverts each p: $p_1+p_2-p_3-p_4 \rightarrow -p_4-p_3+p_2+p_1$ = same → +1; σ_v (molecular plane) → −1; σ_v' swaps $1 \leftrightarrow 4$, $2 \leftrightarrow 3$ without inversion → −1. (1, 1, −1, −1) = A_2.
- Therefore the answer is (B).

FINAL: (B) A_2

SHORTCUT / EXAM TRICK

χ per unmoved atom: E 3, σ 1, i −3, C_2 −1, C_3 0, C_4 1, S_4 −1, S_6 −2.

COMMON MISTAKE

Counting atoms moved by the operation as contributing to the character.

EXAM TIP

Total number of vibrational modes must equal 3N−6 (3N−5 linear) — use it to check the reduction.

MEMORY TRICK

'Unmoved atoms × contribution per atom'.

Why the Other Options Are Wrong

Correct answer: B

A — **A_1**

Why (B) is the key — C_2 swaps $1 \leftrightarrow 4$, $2 \leftrightarrow 3$ and inverts each p: $p_1+p_2-p_3-p_4 \rightarrow -p_4-p_3+p_2+p_1$ = same → +1; σ_v (molecular plane) → −1; σ_v' swaps $1 \leftrightarrow 4$, $2 \leftrightarrow 3$ without inversion → −1. (1, 1, −1, −1) = A_2.

C — **B_1**

Ruled out: Counting atoms moved by the operation as contributing to the character.

D — **B_2**

Ruled out: Total number of vibrational modes must equal 3N−6 (3N−5 linear) — use it to check the reduction.

Q27

The point group of ClF_3 molecule and its corresponding number of irreducible representation are respectively.

A. C_{3v} and 4

B. C_{2v} and 4

C. C_{3v} and 4

D. C_{2v} and 3

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Character Tables

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'Unmoved atoms × contribution per atom'.

Correct Answer B C_{2v} and 4

CONCEPT

Rows are irreducible representations (A/B singly, E doubly, T triply degenerate; 1/2 and g/u labels), columns are classes; the right-hand columns list how x, y, z, Rx…, and quadratic functions transform — the key to IR/Raman activity and hybridisation.

↓

LOGIC / WORKING

- ClF_3 is T-shaped (C_2v); C_2v has four classes and therefore four irreducible representations (A_1, A_2, B_1, B_2).
- Therefore the answer is (B).

FINAL: (B) C_{2v} and 4

SHORTCUT / EXAM TRICK

χ per unmoved atom: E 3, σ 1, i −3, C_2 −1, C_3 0, C_4 1, S_4 −1, S_6 −2.

COMMON MISTAKE

Counting atoms moved by the operation as contributing to the character.

EXAM TIP

Total number of vibrational modes must equal 3N−6 (3N−5 linear) — use it to check the reduction.

MEMORY TRICK

'Unmoved atoms × contribution per atom'.

Why the Other Options Are Wrong

Correct answer: B

A — **C_{3v} and 4**

Why (B) is the key — ClF_3 is T-shaped (C_2v); C_2v has four classes and therefore four irreducible representations (A_1, A_2, B_1, B_2).

C — **C_{3v} and 4**

Ruled out: Counting atoms moved by the operation as contributing to the character.

D — **C_{2v} and 3**

Ruled out: Total number of vibrational modes must equal 3N−6 (3N−5 linear) — use it to check the reduction.

TOPIC REVISION

Character Tables

11 PYQs · Last-minute revision

TOPIC SUMMARY

Rows are irreducible representations (A/B singly, E doubly, T triply degenerate; 1/2 and g/u labels), columns are classes; the right-hand columns list how x, y, z, Rx…, and quadratic functions transform — the key to IR/Raman activity and hybridisation.

IMPORTANT FORMULA SHEET

- Γ_{3N}: $\chi(E) = 3N$, $\chi(C_2) = -1\times$(unmoved atoms), $\chi(\sigma) = +1\times$(unmoved atoms), $\chi(i) = -3\times$(unmoved)
- $\chi(C_n)$ per unmoved atom $= 1 + 2\cos(2\pi/n)$
- $\Gamma_{vib} = \Gamma_{3N} - \Gamma_{trans} - \Gamma_{rot}$

FREQUENTLY ASKED CONCEPTS

- Γ_{vib} of H_2O ($2A_1 + B_2$), NH_3 ($2A_1 + 2E$)
- Hybrid orbitals from Γ_{σ}
- Degeneracy from the E/T label
- Which irreps are IR/Raman active

COMMON MISTAKES & QUICK NOTES

Watch out:
Counting atoms moved by the operation as contributing to the character.
Total number of vibrational modes must equal 3N−6 (3N−5 linear) — use it to check the reduction.

MOST-REPEATED PYQs & EXPECTED IN EXAM

PYQs in this topic: Q17 Q18 Q19 Q20 Q21 Q22 Q23 Q24 Q25 Q26 Q27

Expect 2 question(s) next session on Character Tables.

TOPIC 3

Group Theory – General

14 questions · Easy 7 | Medium 4 | Hard 3 · PYQ frequency: High

Q28

The character table of C_{3v} point group is provided below, along with an additional reducible representation, Gamma E 2 C_3 3 σ_v A_1 1 1 1 A_2 1 1 -1 E 2 -1 0 Đ 6 0 2 Gamma is given by

A $A_1 + A_2 + E$

B $2A_1 + 2E$

C $2A_2 + 2E$

D $2A_1 + 2A_2 + E$

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Group Theory – General

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
'Rule of mutual exclusion lives with i'.

Correct Answer B $2A_1 + 2E$

CONCEPT

Operations form a group (closure, identity, inverse, associativity); classes of operations; representations (matrices) and characters; reduction formula $n_i = (1/h)\ \Sigma\ \chi_R\ \chi_i\ g$; direct products decide selection rules and orbital overlap.

↓

LOGIC / WORKING

- Reduction formula, h = 6: $n(A_1) = (6\cdot1 + 2\cdot0\cdot1 + 3\cdot2\cdot1)/6 = 2$; $n(A_2) = (6 + 0 - 6)/6 = 0$; $n(E) = (12 + 0 + 0)/6 = 2 \rightarrow \Gamma = 2A_1 + 2E$ (dimension check 2 + 4 = 6).
- Therefore the answer is (B).

FINAL: (B) $2A_1 + 2E$

SHORTCUT / EXAM TRICK

A mode is IR-active if its irrep transforms as x, y or z; Raman-active if as x^2, xy, etc.

COMMON MISTAKE

Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

EXAM TIP

Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

MEMORY TRICK

'Rule of mutual exclusion lives with i'.

Why the Other Options Are Wrong

Correct answer: B

A — **$A_1 + A_2 + E$**

Why (B) is the key — Reduction formula, h = 6: $n(A_1) = (6\cdot1 + 2\cdot0\cdot1 + 3\cdot2\cdot1)/6 = 2$; $n(A_2) = (6 + 0 - 6)/6 = 0$; $n(E) = (12 + 0 + 0)/6 = 2$ → $\Gamma = 2A_1 + 2E$ (dimension check 2 + 4 = 6).

C — **$2A_2 + 2E$**

Ruled out: Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

D — **$2A_1 + 2A_2 + E$**

Ruled out: Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

Q29

The molecule that possesses symmetry S_4 element is

A. ethylene

B. allene

C. benzene

D. 1,3-butadiene

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Group Theory – General

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'Rule of mutual exclusion lives with i'.

Correct Answer B allene

CONCEPT

Operations form a group (closure, identity, inverse, associativity); classes of operations; representations (matrices) and characters; reduction formula $n_i = (1/h)\ \Sigma\ \chi_R\ \chi_i\ g$; direct products decide selection rules and orbital overlap.

↓

LOGIC / WORKING

- Allene (D_2d) has an S_4 axis along the C=C=C line (the two CH_2 planes are perpendicular). Ethylene and benzene have S_2/S_6 but not S_4; butadiene (C_2h) has none.
- Therefore the answer is (B).

FINAL: (B) allene

SHORTCUT / EXAM TRICK

A mode is IR-active if its irrep transforms as x, y or z; Raman-active if as x^2, xy, etc.

COMMON MISTAKE

Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

EXAM TIP

Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

MEMORY TRICK

'Rule of mutual exclusion lives with i'.

Why the Other Options Are Wrong

Correct answer: B

A **ethylene**

Why (B) is the key — Allene (D_2d) has an S_4 axis along the C=C=C line (the two CH_2 planes are perpendicular). Ethylene and benzene have S_2/S_6 but not S_4; butadiene (C_2h) has none.

C **benzene**

Ruled out: Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

D **1,3-butadiene**

Ruled out: Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

Q30

For H_2O molecule, the electronic transition from the ground state to an excited state of B_1 symmetry is C_2 p E C_2 σ_v σ_v^′ A_1 1 1 1 1 z_0, z^2, x^2, y^2 A_2 1 1 -1 -1 x y B_1 1 -1 1 -1 x,xz B_2 1 -1 -1 1 y,yz

A. not allowed

B. allowed with x polarization

C. allowed with y polarization

D. allowed with z polarization

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Group Theory – General

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'Rule of mutual exclusion lives with i'.

Correct Answer B allowed with x polarization

CONCEPT

Operations form a group (closure, identity, inverse, associativity); classes of operations; representations (matrices) and characters; reduction formula $n_i = (1/h)\ \Sigma\ \chi_R\ \chi_i\ g$; direct products decide selection rules and orbital overlap.

↓

LOGIC / WORKING

- $A_1 \rightarrow B_1$ is allowed if a dipole component spans B_1: x transforms as B_1 in this table, so the transition is allowed with x polarisation.
- Therefore the answer is (B).

FINAL: (B) allowed with x polarization

SHORTCUT / EXAM TRICK

A mode is IR-active if its irrep transforms as x, y or z; Raman-active if as x^2, xy, etc.

COMMON MISTAKE

Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

EXAM TIP

Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

MEMORY TRICK

'Rule of mutual exclusion lives with i'.

Why the Other Options Are Wrong

Correct answer: B

A — **not allowed**

Why (B) is the key — $A_1 \rightarrow B_1$ is allowed if a dipole component spans B_1: x transforms as B_1 in this table, so the transition is allowed with x polarisation.

C — **allowed with y polarization**

Ruled out: Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

D — **allowed with z polarization**

Ruled out: Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

Q31

The product $C_2\hat{}x.\sigma_xy$ ($C_2\hat{}x$ is the two-fold rotation axis around the x-axis and σ_xy is the xy mirror plane) is

A. σ_xz

B. σ_yz

C. $C_2\hat{}y$

D. $C_2\hat{}z$

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Group Theory – General

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'Rule of mutual exclusion lives with i'.

Correct Answer A σ_xz

CONCEPT

Operations form a group (closure, identity, inverse, associativity); classes of operations; representations (matrices) and characters; reduction formula $n_i = (1/h)\ \Sigma\ \chi_R\ \chi_i\ g$; direct products decide selection rules and orbital overlap.

↓

LOGIC / WORKING

- Track a point: C_2^x: (x, y, z) → (x, −y, −z); then σ_xy: (x, −y, z)… applied as C_2^x after σ_xy: (x, y, z) → (x, y, −z) → (x, −y, z) = reflection in the xz plane → σ_xz.
- Therefore the answer is (A).

FINAL: (A) σ_xz

SHORTCUT / EXAM TRICK

A mode is IR-active if its irrep transforms as x, y or z; Raman-active if as x^2, xy, etc.

COMMON MISTAKE

Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

EXAM TIP

Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

MEMORY TRICK

'Rule of mutual exclusion lives with i'.

Why the Other Options Are Wrong

Correct answer: A

B **σ_yz**

Why (A) is the key — Track a point: C_2^x: (x, y, z) → (x, −y, −z); then σ_xy: (x, −y, z)… applied as C_2^x after σ_xy: (x, y, z) → (x, y, −z) → (x, −y, z) = reflection in the xz plane → σ_xz.

C **C_2^y**

Ruled out: Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

D **C_2^z**

Ruled out: Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

Q32

The molecule with a C_2 axis of symmetry among the following is

A BH_2Cl

B CH_3Cl

C NH_2Cl

D HOCl

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Group Theory – General

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'Rule of mutual exclusion lives with i'.

Correct Answer A BH_2Cl

CONCEPT

Operations form a group (closure, identity, inverse, associativity); classes of operations; representations (matrices) and characters; reduction formula $n_i = (1/h)\ \Sigma\ \chi_R\ \chi_i\ g$; direct products decide selection rules and orbital overlap.

↓

LOGIC / WORKING

- BH_2Cl is trigonal planar with a C_2 axis along B–Cl (C_2v). CH_3Cl has C_3 only; NH_2Cl is pyramidal (Cs); HOCl is bent (Cs).
- Therefore the answer is (A).

FINAL: (A) BH_2Cl

SHORTCUT / EXAM TRICK

A mode is IR-active if its irrep transforms as x, y or z; Raman-active if as x^2, xy, etc.

COMMON MISTAKE

Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

EXAM TIP

Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

MEMORY TRICK

'Rule of mutual exclusion lives with i'.

Why the Other Options Are Wrong

Correct answer: A

B **CH_3Cl**

Why (A) is the key — BH_2Cl is trigonal planar with a C_2 axis along B–Cl (C_2v). CH_3Cl has C_3 only; NH_2Cl is pyramidal (Cs); HOCl is bent (Cs).

C **NH_2Cl**

Ruled out: Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

D **HOCl**

Ruled out: Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

Q33

The observed IR spectrum of BCl_3 exhibits three bands at 995, 480 and 244 cm^{-1}, while the Raman bands are observed at 995, 471 and 244 cm^{-1}. Given that for BCl_3 Gamma$_{vib}$ = A_1' + 2E' + A_2'', the frequency of A_1' mode in cm^{-1} is D_{3h} E 2 C_3 3 C_2 σ_h 2 S_3 3 σ_v A_I ^´ 1 1 1 1 1 1 x^2+y^2, z^2 A_2 ^´ 1 1 -1 1 1 -1 R_z E^´ 2 -1 0 2 -1 0 (x, y) A_1 ^´ ´ 1 1 1 -1 -1 -1 A_2 ^´ ´ 1 1 -1 -1 -1 1 z E^´ ´ 2 -1 0 -2 1 0 (R_x, R_y)

A. 244

B. 471

C. 480

D. 995

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Group Theory – General

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
'Rule of mutual exclusion lives with i'.

Correct Answer B 471

CONCEPT

Operations form a group (closure, identity, inverse, associativity); classes of operations; representations (matrices) and characters; reduction formula $n_i = (1/h)\ \Sigma\ \chi_R\ \chi_i\ g$; direct products decide selection rules and orbital overlap.

↓

LOGIC / WORKING

- A_1' ($x^2 + y^2, z^2$) is Raman-active but IR-inactive (no x, y, z); E' is both; A_2'' (z) is IR-only. The band seen only in Raman, 471 cm^{-1}, is the A_1' symmetric stretch; 480 (IR only) is A_2''.
- Therefore the answer is (B).

FINAL: (B) 471

SHORTCUT / EXAM TRICK

A mode is IR-active if its irrep transforms as x, y or z; Raman-active if as x^2, xy, etc.

COMMON MISTAKE

Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

EXAM TIP

Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

MEMORY TRICK

'Rule of mutual exclusion lives with i'.

Why the Other Options Are Wrong

Correct answer: B

A — **244**

Why (B) is the key — A_1' ($x^2 + y^2$, z^2) is Raman-active but IR-inactive (no x, y, z); E′ is both; A_2'' (z) is IR-only. The band seen only in Raman, 471 cm^{-1}, is the A_1' symmetric stretch; 480 (IR only) is A_2''.

C — **480**

Ruled out: Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

D — **995**

Ruled out: Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

Q34

Given the matrices for C_3 and σ_h below C_3 = -1/2 & -√(3/2) & 0 √(3/2) & -1/2 & 0 0 & 0 & 1 σ_h = 1 & 0 & 0 0 & 1 & 0 0 & 0 & 1 the trace of the matrix representing for S_3^2 is

A. 0

B. -2

C. 1

D. -1

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Group Theory – General

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'Rule of mutual exclusion lives with i'.

Correct Answer A 0

CONCEPT

Operations form a group (closure, identity, inverse, associativity); classes of operations; representations (matrices) and characters; reduction formula $n_i = (1/h)\ \Sigma\ \chi_R\ \chi_i\ g$; direct products decide selection rules and orbital overlap.

↓

LOGIC / WORKING

- $S_3^2 = C_3^2\sigma_h^2 = C_3^2$: a rotation by 240° has trace $1 + 2\cos 240° = 1 - 1 = 0$.
- Therefore the answer is (A).

FINAL: (A) 0

SHORTCUT / EXAM TRICK

A mode is IR-active if its irrep transforms as x, y or z; Raman-active if as x^2, xy, etc.

COMMON MISTAKE

Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

EXAM TIP

Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

MEMORY TRICK

'Rule of mutual exclusion lives with i'.

Why the Other Options Are Wrong

Correct answer: A

B **-2**

Why (A) is the key — $S_3^2 = C_3^2\sigma_h^2 = C_3^2$: a rotation by 240° has trace $1 + 2\cos 240° = 1 - 1 = 0$.

C **1**

Ruled out: Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

D **-1**

Ruled out: Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

Q35

The number of IR active vibrational modes of pyridine is: $C_{2\ v}$ E $2C_2$ σ_v σ_v A_1 1 1 1 1 Z A_2 1 1 -1 -1 R_2 B_1 1 -1 1 -1 x, R_y B_2 1 -1 -1 1 y, R_x

A 12

B 20

C 24

D 33

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Group Theory – General

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'Rule of mutual exclusion lives with i'.

Correct Answer C 24

CONCEPT

Operations form a group (closure, identity, inverse, associativity); classes of operations; representations (matrices) and characters; reduction formula $n_i = (1/h)\ \Sigma\ \chi_R\ \chi_i\ g$; direct products decide selection rules and orbital overlap.

↓

LOGIC / WORKING

- Pyridine C_2v, 11 atoms → $3N - 6 = 27$ modes = $10A_1 + 3A_2 + 9B_1 + 5B_2$. A_1 (z), B_1 (x), B_2 (y) are IR-active; A_2 is not → $27 - 3 = 24$.
- Therefore the answer is (C).

FINAL: (C) 24

SHORTCUT / EXAM TRICK

A mode is IR-active if its irrep transforms as x, y or z; Raman-active if as x^2, xy, etc.

COMMON MISTAKE

Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

EXAM TIP

Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

MEMORY TRICK

'Rule of mutual exclusion lives with i'.

Why the Other Options Are Wrong

Correct answer: C

A — **12**

Why (C) is the key — Pyridine C_2v, 11 atoms → 3N − 6 = 27 modes = $10A_1 + 3A_2 + 9B_1 + 5B_2$. A_1 (z), B_1 (x), B_2 (y) are IR-active; A_2 is not → 27 − 3 = 24.

B — **20**

Ruled out: Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

D — **33**

Ruled out: Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

Q36

Number of rotational symmetry axes for triclinic crystal system is

A. 4

B. 3

C. 1

D. 0

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Group Theory – General

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'Rule of mutual exclusion lives with i'.

Correct Answer D 0

CONCEPT

Operations form a group (closure, identity, inverse, associativity); classes of operations; representations (matrices) and characters; reduction formula $n_i = (1/h)\ \Sigma\ \chi_R\ \chi_i\ g$; direct products decide selection rules and orbital overlap.

↓

LOGIC / WORKING

- The triclinic system has only the identity (and possibly inversion): no rotational symmetry axes.
- Therefore the answer is (D).

FINAL: (D) 0

SHORTCUT / EXAM TRICK

A mode is IR-active if its irrep transforms as x, y or z; Raman-active if as x^2, xy, etc.

COMMON MISTAKE

Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

EXAM TIP

Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

MEMORY TRICK

'Rule of mutual exclusion lives with i'.

Why the Other Options Are Wrong

Correct answer: D

A **4**

Why (D) is the key — The triclinic system has only the identity (and possibly inversion): no rotational symmetry axes.

B **3**

Ruled out: Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

C **1**

Ruled out: Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

Q37

The result of the product $C_2(x)C_2(y)$ is

A. E

B. $\sigma_x y$

C. $C_2(z)$

D. i

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Group Theory – General

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'Rule of mutual exclusion lives with i'.

Correct Answer C $C_2(z)$

CONCEPT

Operations form a group (closure, identity, inverse, associativity); classes of operations; representations (matrices) and characters; reduction formula $n_i = (1/h)\ \Sigma\ \chi_R\ \chi_i\ g$; direct products decide selection rules and orbital overlap.

↓

LOGIC / WORKING

- Two perpendicular C_2 rotations combine to a C_2 about the third axis: $C_2(x)C_2(y) = C_2(z)$.
- Therefore the answer is (C).

FINAL: (C) $C_2(z)$

SHORTCUT / EXAM TRICK

A mode is IR-active if its irrep transforms as x, y or z; Raman-active if as x^2, xy, etc.

COMMON MISTAKE

Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

EXAM TIP

Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

MEMORY TRICK

'Rule of mutual exclusion lives with i'.

Why the Other Options Are Wrong

Correct answer: C

A — **E**

Why (C) is the key — Two perpendicular C_2 rotations combine to a C_2 about the third axis: $C_2(x)C_2(y) = C_2(z)$.

B — **$\sigma_x y$**

Ruled out: Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

D — **i**

Ruled out: Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

Q38

A molecular orbital of a diatomic molecule changes sign when it is rotated by 180^° around the molecular axis. This orbital is

A σ

B π

C δ

D varphi

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Group Theory – General

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
'Rule of mutual exclusion lives with i'.

Correct Answer B π

CONCEPT

Operations form a group (closure, identity, inverse, associativity); classes of operations; representations (matrices) and characters; reduction formula $n_i = (1/h)\ \Sigma\ \chi_R\ \chi_i\ g$; direct products decide selection rules and orbital overlap.

↓

LOGIC / WORKING

- Rotation by 180° about the bond axis changes the sign of a π orbital (one nodal plane containing the axis); σ is unchanged, δ (two nodal planes) is unchanged by 180°.
- Therefore the answer is (B).

FINAL: (B) π

SHORTCUT / EXAM TRICK

A mode is IR-active if its irrep transforms as x, y or z; Raman-active if as x^2, xy, etc.

COMMON MISTAKE

Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

EXAM TIP

Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

MEMORY TRICK

'Rule of mutual exclusion lives with i'.

Why the Other Options Are Wrong

Correct answer: B

A **σ**

Why (B) is the key — Rotation by 180° about the bond axis changes the sign of a π orbital (one nodal plane containing the axis); σ is unchanged, δ (two nodal planes) is unchanged by 180°.

C **δ**

Ruled out: Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

D **varphi**

Ruled out: Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

Q39

The S_2 operation on a molecule with the axis of rotation as the z axis, moves a nucleus at (x, y, z) to

A (-x, -y, x)

B (x, -y, -z)

C (-x, y, -z)

D (-x, -y, -z)

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Group Theory – General

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'Rule of mutual exclusion lives with i'.

Correct Answer D (-x, -y, -z)

CONCEPT

Operations form a group (closure, identity, inverse, associativity); classes of operations; representations (matrices) and characters; reduction formula $n_i = (1/h)\ \Sigma\ \chi_R\ \chi_i\ g$; direct products decide selection rules and orbital overlap.

↓

LOGIC / WORKING

- $S_2 = C_2(z)$ followed by σ_xy: (x, y, z) → (−x, −y, z) → (−x, −y, −z) — identical to inversion.
- Therefore the answer is (D).

FINAL: (D) (-x, -y, -z)

SHORTCUT / EXAM TRICK

A mode is IR-active if its irrep transforms as x, y or z; Raman-active if as x^2, xy, etc.

COMMON MISTAKE

Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

EXAM TIP

Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

MEMORY TRICK

'Rule of mutual exclusion lives with i'.

Why the Other Options Are Wrong

Correct answer: D

A **(-x, -y, x)**

Why (D) is the key — $S_2 = C_2(z)$ followed by σ_{xy}: (x, y, z) → (−x, −y, z) → (−x, −y, −z) — identical to inversion.

B **(x, -y, -z)**

Ruled out: Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

C **(-x, y, -z)**

Ruled out: Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

Q40

Conversion of boron trifluoride to tetrafluoroborate accompanies

A. Increase in symmetry and bond elongation

B. Increase in symmetry and bond contraction

C. Decrease in symmetry and bond contraction

D. Decrease in symmetry and bond elongation

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Group Theory – General

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'Rule of mutual exclusion lives with i'.

Correct Answer A Increase in symmetry and bond elongation

CONCEPT

Operations form a group (closure, identity, inverse, associativity); classes of operations; representations (matrices) and characters; reduction formula $n_i = (1/h)\ \Sigma\ \chi_R\ \chi_i\ g$; direct products decide selection rules and orbital overlap.

↓

LOGIC / WORKING

- BF_3 (D_3h, sp^2, B–F 130 pm with π back-bonding) → BF_4^- (T_d, higher symmetry, sp^3, B–F 140 pm): symmetry increases and the bond lengthens.
- Therefore the answer is (A).

FINAL: (A) Increase in symmetry and bond elongation

SHORTCUT / EXAM TRICK

A mode is IR-active if its irrep transforms as x, y or z; Raman-active if as x^2, xy, etc.

COMMON MISTAKE

Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

EXAM TIP

Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

MEMORY TRICK

'Rule of mutual exclusion lives with i'.

Why the Other Options Are Wrong

Correct answer: A

B **Increase in symmetry and bond contraction**

Why (A) is the key — BF_3 (D_3h, sp^2, B–F 130 pm with π back-bonding) → BF_4^- (T_d, higher symmetry, sp^3, B–F 140 pm): symmetry increases and the bond lengthens.

C **Decrease in symmetry and bond contraction**

Ruled out: Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.

D **Decrease in symmetry and bond elongation**

Ruled out: Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

Q41

The number of C_2 axes in CCl_4 is _____
GATE 2020
(Numerical answer type — write the value.)

ANSWER: 3

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Group Theory – General

PYQ FREQUENCY
High · 7 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
T_d has three C_2 axes (coincident with the S_4 axes, bisecting Cl–C–Cl angles), four C_3 and six σ_d.

TOPIC REVISION

Group Theory – General

14 PYQs · Last-minute revision

TOPIC SUMMARY

Operations form a group (closure, identity, inverse, associativity); classes of operations; representations (matrices) and characters; reduction formula $n_i = (1/h)\ \Sigma\ \chi_R\ \chi_i\ g$; direct products decide selection rules and orbital overlap.

IMPORTANT FORMULA SHEET

- $n_i = (1/h)\ \Sigma_\text{classes}\ g_c\ \chi_\text{red}(c)\ \chi_i(c)$
- $\Sigma\ (\text{dimension})^2 = h$
- Number of irreps = number of classes
- $\Gamma_\text{vib} = \Gamma_3N - \Gamma_\text{trans} - \Gamma_\text{rot}$

FREQUENTLY ASKED CONCEPTS

- Reducing a representation
- IR/Raman active modes from the character table
- SALCs and orbital symmetry
- Number of classes = irreps

COMMON MISTAKES & QUICK NOTES

Watch out:
Using the order of the group as the number of classes; forgetting to multiply by the class size g in the reduction formula.
Centrosymmetric molecules: IR and Raman modes are mutually exclusive.

MOST-REPEATED PYQs & EXPECTED IN EXAM

PYQs in this topic: Q28 Q29 Q30 Q31 Q32 Q33 Q34 Q35 Q36 Q37 Q38 Q39 Q40 Q41

Expect 2 question(s) next session on Group Theory – General.

FOR STUDENTS AND EDUCATORS

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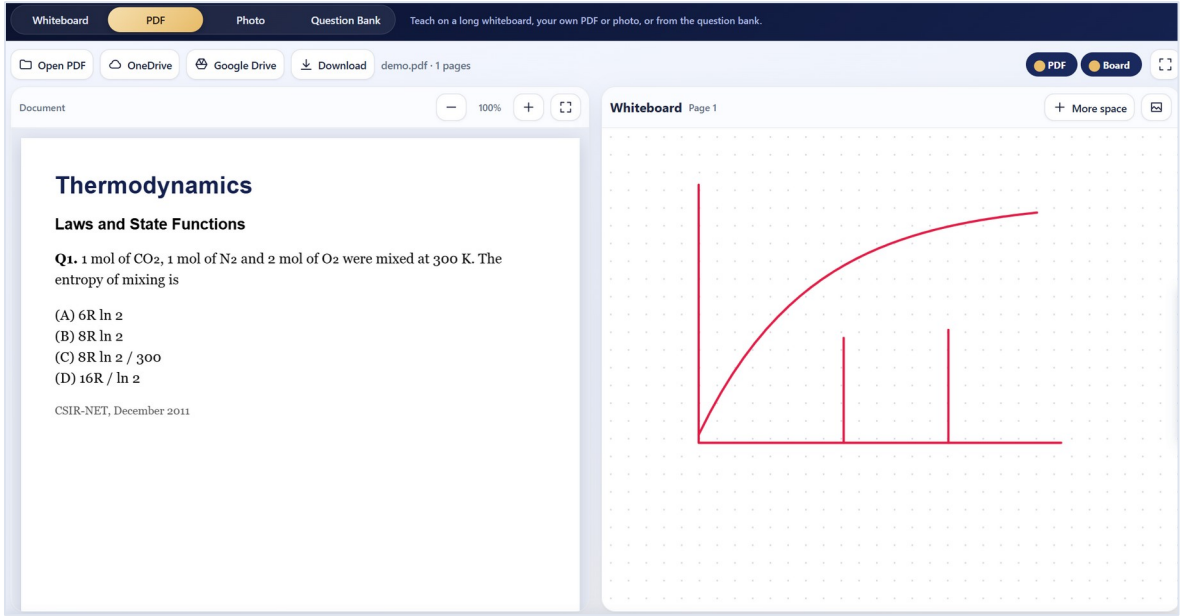
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