ABC CHEMISTRY

Mr. Aniket Bhardwaj · 15+ Years Mentorship

Molecular Spectroscopy

Premium CSIR-NET PYQ Book

48 Previous-Year Questions · 47 with verified answers · Distractor Analysis

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

CSIR-NET · GATE · IIT-JAM — 4 Topics · 48 Real PYQs

(Mr. Aniket Bhardwaj By ABC Chemistry) · www.abcchemistry.com · 9212142427

Mr. Aniket Bhardwaj

@abcchemistry24

Instagram · YouTube · Facebook

Course Contents

4 Topics · 48 PYQs

1	**Vibrational** 6 Qs E 1 · M 4 · H 1	12%	
2	**Rotational** 6 Qs E 1 · M 5 · H 0	12%	
3	**Raman** 5 Qs E 2 · M 3 · H 0	10%	
4	**Molecular Spectroscopy – General** 31 Qs E 6 · M 25 · H 0	65%	

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

TOPIC 1

Vibrational

6 questions · Easy 1 | Medium 4 | Hard 1 · PYQ frequency: High

Q1

The vibrational frequency and anharmonicity constant of an alkali halide are 300 cm^{-1} and 0.0025 respectively. The positions (in cm^{-1}) of its fundamental mode and first overtone are respectively.

A. 300, 600

B. 298.5, 595.5

C. 301.5, 604.5

D. 290, 580

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Vibrational

PYQ FREQUENCY
High · 5 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'Stiffer and lighter = higher $\tilde{\nu}$'.

Correct Answer B 298.5, 595.5

CONCEPT

Harmonic oscillator levels $E_v = (v+½)h\nu$ equally spaced; anharmonicity (Morse) brings levels closer and allows overtones ($\Delta v = \pm 2, 3\ldots$); IR activity needs a change in dipole moment; 3N−6 (3N−5 linear) normal modes; group frequencies.

↓

LOGIC / WORKING

- Anharmonic oscillator: fundamental = $\omega_e(1 - 2x_e) = 300(1 - 0.005) = 298.5\ cm^{-1}$; first overtone = $2\omega_e(1 - 3x_e) = 600(1 - 0.0075) = 595.5\ cm^{-1}$.
- Therefore the answer is (B).

FINAL: (B) 298.5, 595.5

SHORTCUT / EXAM TRICK

Fundamental minus half the first overtone = ω_ex_e: $\omega_e x_e = \tilde{\nu}_1 - \tilde{\nu}_2/2$ … solve the two equations.

COMMON MISTAKE

Forgetting zero-point energy when relating D_0 and D_e.

EXAM TIP

$\tilde{\nu}$(C≡C) 2100 > $\tilde{\nu}$(C=C) 1650 > $\tilde{\nu}$(C–C) 1200 cm^{-1} — k dominates; C–H ≈ 3000 because μ is small.

MEMORY TRICK

'Stiffer and lighter = higher $\tilde{\nu}$'.

Why the Other Options Are Wrong

Correct answer: B

A **300, 600**

Why (B) is the key — Anharmonic oscillator: fundamental = $\omega_e(1 - 2x_e) = 300(1 - 0.005) = 298.5\ cm^{-1}$; first overtone = $2\omega_e(1 - 3x_e) = 600(1 - 0.0075) = 595.5\ cm^{-1}$.

C **301.5, 604.5**

Ruled out: Forgetting zero-point energy when relating D_0 and D_e.

D **290, 580**

Ruled out: $\tilde{\nu}$(C≡C) 2100 > $\tilde{\nu}$(C=C) 1650 > $\tilde{\nu}$(C–C) 1200 cm^{-1} — k dominates; C–H ≈ 3000 because μ is small.

Q2

Bond lengths of homonuclear diatomic molecules can be determined with the help of both

A. Rotational and vibrational spectroscopy

B. Rotational and rotational Raman spectroscopy

C. Rotational Raman and electronic spectroscopy

D. Vibrational and electronic spectroscopy

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Vibrational

PYQ FREQUENCY
High · 5 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'Stiffer and lighter = higher $\tilde{\nu}$'.

Correct Answer C Rotational Raman and electronic spectroscopy

CONCEPT

Harmonic oscillator levels $E_v = (v+½)hν$ equally spaced; anharmonicity (Morse) brings levels closer and allows overtones ($Δv = ±2, 3…$); IR activity needs a change in dipole moment; $3N−6$ ($3N−5$ linear) normal modes; group frequencies.

↓

LOGIC / WORKING

- Homonuclear diatomics have no dipole moment — no microwave or IR spectrum. Bond lengths come from rotational Raman spectra (B from line spacing) and from the rotational fine structure of electronic (UV–vis) spectra.
- Therefore the answer is (C).

FINAL: (C) Rotational Raman and electronic spectroscopy

SHORTCUT / EXAM TRICK

Fundamental minus half the first overtone = $ω_ex_e$: $ω_ex_e = \tilde{ν}_1 − \tilde{ν}_2/2$ … solve the two equations.

COMMON MISTAKE

Forgetting zero-point energy when relating D_0 and D_e.

EXAM TIP

$\tilde{ν}$(C≡C) 2100 > $\tilde{ν}$(C=C) 1650 > $\tilde{ν}$(C–C) 1200 cm^{-1} — k dominates; C–H ≈ 3000 because μ is small.

MEMORY TRICK

'Stiffer and lighter = higher $\tilde{ν}$'.

Why the Other Options Are Wrong

Correct answer: C

A — **Rotational and vibrational spectroscopy**

Why (C) is the key — Homonuclear diatomics have no dipole moment — no microwave or IR spectrum. Bond lengths come from rotational Raman spectra (B from line spacing) and from the rotational fine structure of electronic (UV–vis) spectra.

B — **Rotational and rotational Raman spectroscopy**

Ruled out: Forgetting zero-point energy when relating D_0 and D_e.

D — **Vibrational and electronic spectroscopy**

Ruled out: ν̃(C≡C) 2100 > ν̃(C=C) 1650 > ν̃(C–C) 1200 cm^{-1} — k dominates; C–H ≈ 3000 because μ is small.

Q3

If the component of the orbital angular momentum along the molecular axis of a heteronuclear diatomic molecule is non-zero, the rotational-vibrational spectrum will show

A. P and R branches only

B. P and Q branches only

C. Q and R branches only

D. All the P, Q and R branches

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Vibrational

PYQ FREQUENCY
High · 5 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'Stiffer and lighter = higher $\tilde{\nu}$'.

Correct Answer D All the P, Q and R branches

CONCEPT

Harmonic oscillator levels $E_v = (v+½)h\nu$ equally spaced; anharmonicity (Morse) brings levels closer and allows overtones ($\Delta v = \pm 2, 3\ldots$); IR activity needs a change in dipole moment; 3N−6 (3N−5 linear) normal modes; group frequencies.

↓

LOGIC / WORKING

- When $\Lambda \neq 0$ (e.g. NO, $^2\Pi$) the electronic angular momentum along the axis allows $\Delta J = 0$ transitions, so a Q branch appears in addition to P and R.
- Therefore the answer is (D).

FINAL: (D) All the P, Q and R branches

SHORTCUT / EXAM TRICK

Fundamental minus half the first overtone = ω_e: $\omega_e = \tilde{\nu}_1 - \tilde{\nu}_2/2$ … solve the two equations.

COMMON MISTAKE

Forgetting zero-point energy when relating D_0 and D_e.

EXAM TIP

$\tilde{\nu}$(C≡C) 2100 > $\tilde{\nu}$(C=C) 1650 > $\tilde{\nu}$(C–C) 1200 cm^{-1} — k dominates; C–H ≈ 3000 because μ is small.

MEMORY TRICK

'Stiffer and lighter = higher $\tilde{\nu}$'.

Why the Other Options Are Wrong

Correct answer: D

A **P and R branches only**

Why (D) is the key — When $\Lambda \neq 0$ (e.g. NO, $^2\Pi$) the electronic angular momentum along the axis allows $\Delta J = 0$ transitions, so a Q branch appears in addition to P and R.

B **P and Q branches only**

Ruled out: Forgetting zero-point energy when relating D_0 and D_e.

C **Q and R branches only**

Ruled out: $\tilde{\nu}$(C≡C) 2100 > $\tilde{\nu}$(C=C) 1650 > $\tilde{\nu}$(C–C) 1200 cm^{-1} — k dominates; C–H ≈ 3000 because μ is small.

Q4

The vibrational transition energies of a diatomic molecule corresponding to v = 1 ← v = 0 and v = 2 ← v = 1 are 2143.1 cm^{-1} and 2116.1 cm^{-1}, respectively. The anharmonic constant ($\omega_e\chi_e$) of the molecule in cm^{-1} is

A. 27

B. 13.5

C. 10

D. 54

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Vibrational

PYQ FREQUENCY
High · 5 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'Stiffer and lighter = higher $\tilde{\nu}$'.

Correct Answer B 13.5

CONCEPT

Harmonic oscillator levels $E_v = (v+½)h\nu$ equally spaced; anharmonicity (Morse) brings levels closer and allows overtones ($\Delta v = \pm2, 3\ldots$); IR activity needs a change in dipole moment; 3N−6 (3N−5 linear) normal modes; group frequencies.

↓

LOGIC / WORKING

- Anharmonic: $\Delta G(v+½) = \omega_e - 2\omega_e x_e(v+1)$. Successive spacings differ by $2\omega_e x_e$ = 2143.1 − 2116.1 = 27 → $\omega_e x_e$ = 13.5 cm^{-1}.
- Therefore the answer is (B).

FINAL: (B) 13.5

SHORTCUT / EXAM TRICK

Fundamental minus half the first overtone = ω_ex_e: ω_ex_e = $\tilde{\nu}_1 - \tilde{\nu}_2/2$ … solve the two equations.

COMMON MISTAKE

Forgetting zero-point energy when relating D_0 and D_e.

EXAM TIP

$\tilde{\nu}$(C≡C) 2100 > $\tilde{\nu}$(C=C) 1650 > $\tilde{\nu}$(C–C) 1200 cm^{-1} — k dominates; C–H ≈ 3000 because μ is small.

MEMORY TRICK

'Stiffer and lighter = higher $\tilde{\nu}$'.

Why the Other Options Are Wrong

Correct answer: B

A — **27**

Why (B) is the key — Anharmonic: $\Delta G(v+½) = \omega_e - 2\omega_e x_e(v + 1)$. Successive spacings differ by $2\omega_e x_e = 2143.1 - 2116.1 = 27 \rightarrow \omega_e x_e = 13.5\ cm^{-1}$.

C — **10**

Ruled out: Forgetting zero-point energy when relating D_0 and D_e.

D — **54**

Ruled out: $\tilde{\nu}$(C≡C) 2100 > $\tilde{\nu}$(C=C) 1650 > $\tilde{\nu}$(C–C) 1200 cm^{-1} — k dominates; C–H ≈ 3000 because μ is small.

Q5

The following data were obtained from the vibrational fine structure in the vibronic spectrum of a diatomic molecule: ω_e = 512 cm^{-1}, $\omega_e x_e$ = 8 cm^{-1} where ω_e is the energy associated with the natural frequency of vibration and x_e is the anharmonicity constant. The dissociation energy (D_e) of the molecule is:

A. 4096 cm^{-1}

B. 6144 cm^{-1}

C. 8192 cm^{-1}

D. 16384 cm^{-1}

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Vibrational

PYQ FREQUENCY
High · 5 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'Stiffer and lighter = higher $\tilde{\nu}$'.

Correct Answer C 8192 cm^{-1}

CONCEPT

Harmonic oscillator levels $E_v = (v+½)hν$ equally spaced; anharmonicity (Morse) brings levels closer and allows overtones ($Δv = ±2, 3…$); IR activity needs a change in dipole moment; 3N−6 (3N−5 linear) normal modes; group frequencies.

↓

LOGIC / WORKING

- Morse/Birge–Sponer: $D_e = ω_e^2/(4ω_e x_e) = 512^2/(4 × 8) = 262\ 144/32 = 8192\ cm^{-1}$.
- Therefore the answer is (C).

FINAL: (C) 8192 cm^{-1}

SHORTCUT / EXAM TRICK

Fundamental minus half the first overtone = ω_ex_e: $ω_ex_e = \tilde{ν}_1 − \tilde{ν}_2/2$ … solve the two equations.

COMMON MISTAKE

Forgetting zero-point energy when relating D_0 and D_e.

EXAM TIP

$\tilde{ν}(C≡C)$ 2100 > $\tilde{ν}(C=C)$ 1650 > $\tilde{ν}(C–C)$ 1200 cm^{-1} — k dominates; C–H ≈ 3000 because μ is small.

MEMORY TRICK

'Stiffer and lighter = higher $\tilde{ν}$'.

Why the Other Options Are Wrong

Correct answer: C

A **4096 cm⁻¹**

Why (C) is the key — Morse/Birge–Sponer: $D_e = \omega_e^2/(4\omega_e x_e) = 512^2/(4 \times 8) = 262\,144/32 = 8192$ cm⁻¹.

B **6144 cm⁻¹**

Ruled out: Forgetting zero-point energy when relating D_0 and D_e.

D **16384 cm⁻¹**

Ruled out: ν̃(C≡C) 2100 > ν̃(C=C) 1650 > ν̃(C–C) 1200 cm⁻¹ — k dominates; C–H ≈ 3000 because μ is small.

Q6

The correct statement from the following set (i) to (iv) is (i) if q is the displacement from equilibrium for harmonic motion, the potential energy is proportional to q (ii) if the vibrational frequency (ν) of HCl is 2990 cm^{-1}, its zero point energy will be 1495 cm^{-1} (iii) the correct order of vibrational frequency of mathrmO-^{1}H (X_1), mathrmO-^{2}H (X_2) and mathrmO-^{3}H (X_3) is $X_1 > X_2 > X_3$ (iv) the fundamental vibrational transition of a diatomic molecule appears at 1880 cm^{-1}. Its first overtone will be at 940 cm^{-1} (assuming anharmonicity constant as zero)

A. i, ii, iii only

B. i, ii, iii, iv

C. ii, iii only

D. i, ii, iv only

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Vibrational

PYQ FREQUENCY
High · 5 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
'Stiffer and lighter = higher $\tilde{\nu}$'.

Correct Answer C ii, iii only

CONCEPT

Harmonic oscillator levels E_v = (v+½)hν equally spaced; anharmonicity (Morse) brings levels closer and allows overtones (Δv = ±2, 3…); IR activity needs a change in dipole moment; 3N−6 (3N−5 linear) normal modes; group frequencies.

↓

LOGIC / WORKING

- (i) false: V ∝ q². (ii) true: ZPE = ½ν = 1495 cm⁻¹. (iii) true: ν ∝ 1/√μ, heavier isotope lower. (iv) false: harmonic first overtone = 2 × 1880 = 3760 cm⁻¹. So (ii) and (iii) only.
- Therefore the answer is (C).

FINAL: (C) ii, iii only

SHORTCUT / EXAM TRICK

Fundamental minus half the first overtone = ω_ex_e: ω_ex_e = $\tilde{\nu}_1 - \tilde{\nu}_2/2$ … solve the two equations.

COMMON MISTAKE

Forgetting zero-point energy when relating D_0 and D_e.

EXAM TIP

$\tilde{\nu}$(C≡C) 2100 > $\tilde{\nu}$(C=C) 1650 > $\tilde{\nu}$(C–C) 1200 cm⁻¹ — k dominates; C–H ≈ 3000 because μ is small.

MEMORY TRICK

'Stiffer and lighter = higher $\tilde{\nu}$'.

Why the Other Options Are Wrong

Correct answer: C

A **i, ii, iii only**

Why (C) is the key — (i) false: V ∝ q². (ii) true: ZPE = ½ν = 1495 cm⁻¹. (iii) true: ν ∝ 1/√μ, heavier isotope lower. (iv) false: harmonic first overtone = 2 × 1880 = 3760 cm⁻¹. So (ii) and (iii) only.

B **i, ii, iii, iv**

Ruled out: Forgetting zero-point energy when relating D_0 and D_e.

D **i, ii, iv only**

Ruled out: ν̃(C≡C) 2100 > ν̃(C=C) 1650 > ν̃(C–C) 1200 cm⁻¹ — k dominates; C–H ≈ 3000 because μ is small.

TOPIC REVISION

Vibrational

6 PYQs · Last-minute revision

TOPIC SUMMARY

Harmonic oscillator levels E_v = (v+½)hν equally spaced; anharmonicity (Morse) brings levels closer and allows overtones (Δv = ±2, 3…); IR activity needs a change in dipole moment; 3N−6 (3N−5 linear) normal modes; group frequencies.

IMPORTANT FORMULA SHEET

- $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$
- $G(v) = \omega_e(v+½) - \omega_e x_e(v+½)^2$
- Fundamental = $\omega_e - 2\omega_e x_e$; first overtone = $2\omega_e - 6\omega_e x_e$
- $D_0 = D_e - ½h\nu$; $v_{max} \approx \omega_e/2\omega_e x_e - ½$

FREQUENTLY ASKED CONCEPTS

- Force constant from $\tilde{\nu}$
- Overtone positions and anharmonicity constant
- Zero-point energy
- Isotope effect on $\tilde{\nu}$

COMMON MISTAKES & QUICK NOTES

Watch out:
Forgetting zero-point energy when relating D_0 and D_e.
$\tilde{\nu}$(C≡C) 2100 > $\tilde{\nu}$(C=C) 1650 > $\tilde{\nu}$(C–C) 1200 cm^{-1} — k dominates; C–H ≈ 3000 because μ is small.

MOST-REPEATED PYQs & EXPECTED IN EXAM

PYQs in this topic: Q1 Q2 Q3 Q4 Q5 Q6

Expect 1 question(s) next session on Vibrational.

TOPIC 2

Rotational

6 questions · Easy 1 | Medium 5 | Hard 0 · PYQ frequency: High

Q7

The molecule with the smallest rotational constant (in the microwave spectrum) among the following is

A mathrmN≡CH

B mathrmHC≡CCl

C mathrmCCl≡CF

D mathrmB≡CCl

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Rotational

PYQ FREQUENCY
High · 5 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'Lines every 2B'.

Correct Answer C mathrmCCl≡CF

CONCEPT

Rigid rotor E_J = BJ(J+1) with degeneracy 2J+1; selection ΔJ = ±1 and a permanent dipole; line spacing 2B; centrifugal distortion lowers spacing at high J; most populated level from the Boltzmann–degeneracy balance; linear vs symmetric-top molecules.

↓

LOGIC / WORKING

- B = h/(8π²cI): the heaviest, longest linear molecule has the largest I and smallest B. Cl–C≡C–F (two heavy halogens, four heavy atoms) has the largest moment of inertia.
- Therefore the answer is (C).

FINAL: (C) mathrmCCl≡CF

SHORTCUT / EXAM TRICK

B ∝ 1/μ: B(DCl)/B(HCl) ≈ μ(HCl)/μ(DCl) ≈ 0.51.

COMMON MISTAKE

Taking the spacing as B instead of 2B; using the molecular mass instead of the reduced mass.

EXAM TIP

Symmetric tops need two constants (A or C and B); spherical tops (CH_4) have no pure rotational spectrum.

MEMORY TRICK

'Lines every 2B'.

Why the Other Options Are Wrong

Correct answer: C

A **mathrmN≡CH**

Why (C) is the key — B = h/(8π²cI): the heaviest, longest linear molecule has the largest I and smallest B. Cl–C≡C–F (two heavy halogens, four heavy atoms) has the largest moment of inertia.

B **mathrmHC≡CCl**

Ruled out: Taking the spacing as B instead of 2B; using the molecular mass instead of the reduced mass.

D **mathrmB≡CCl**

Ruled out: Symmetric tops need two constants (A or C and B); spherical tops (CH_4) have no pure rotational spectrum.

Q8

The spectroscopic technique that can distinguish unambiguously between trans-1,2-dichloroethylene and cis-1,2-dichloroethylene without any numerical calculation is

A. microwave spectroscopy

B. UV-visible spectroscopy

C. X-ray photoelectron spectroscopy

D. γ-ray spectroscopy

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Rotational

PYQ FREQUENCY
High · 5 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'Lines every 2B'.

Correct Answer A microwave spectroscopy

CONCEPT

Rigid rotor $E_J = BJ(J+1)$ with degeneracy $2J+1$; selection $\Delta J = \pm 1$ and a permanent dipole; line spacing $2B$; centrifugal distortion lowers spacing at high J; most populated level from the Boltzmann–degeneracy balance; linear vs symmetric-top molecules.

↓

LOGIC / WORKING

- trans-1,2-dichloroethylene has a centre of symmetry and zero dipole moment → no microwave (rotational) spectrum; the cis isomer is polar and shows one. No calculation is needed.
- Therefore the answer is (A).

FINAL: (A) microwave spectroscopy

SHORTCUT / EXAM TRICK

$B \propto 1/\mu$: $B(DCl)/B(HCl) \approx \mu(HCl)/\mu(DCl) \approx 0.51$.

COMMON MISTAKE

Taking the spacing as B instead of 2B; using the molecular mass instead of the reduced mass.

EXAM TIP

Symmetric tops need two constants (A or C and B); spherical tops (CH_4) have no pure rotational spectrum.

MEMORY TRICK

'Lines every 2B'.

Why the Other Options Are Wrong

Correct answer: A

B **UV-visible spectroscopy**

Why (A) is the key — trans-1,2-dichloroethylene has a centre of symmetry and zero dipole moment → no microwave (rotational) spectrum; the cis isomer is polar and shows one. No calculation is needed.

C **X-ray photoelectron spectroscopy**

Ruled out: Taking the spacing as B instead of 2B; using the molecular mass instead of the reduced mass.

D **y-ray spectroscopy**

Ruled out: Symmetric tops need two constants (A or C and B); spherical tops (CH_4) have no pure rotational spectrum.

Q9

In the pure rotational microwave spectrum of a XY molecule, the adjacent lines are separated by 4 cm^{-1}. If the molecule is irradiated by a radiation of 30,000 cm^{-1}, the first Stokes line(in cm^{-1}) appears at

A 29988

B 30012

C 30004

D 29996

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Rotational

PYQ FREQUENCY
High · 5 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'Lines every 2B'.

Correct Answer A 29988

CONCEPT

Rigid rotor $E_J = BJ(J+1)$ with degeneracy $2J+1$; selection $\Delta J = \pm 1$ and a permanent dipole; line spacing $2B$; centrifugal distortion lowers spacing at high J; most populated level from the Boltzmann–degeneracy balance; linear vs symmetric-top molecules.

↓

LOGIC / WORKING

- Pure rotational Raman: lines at $\nu_0 \pm 2B(2J+3)$; first Stokes line ($J = 0$) at $\nu_0 - 6B$. Microwave spacing $2B = 4 \rightarrow B = 2\ cm^{-1} \rightarrow 30\,000 - 12 = 29\,988\ cm^{-1}$.
- Therefore the answer is (A).

FINAL: (A) 29988

SHORTCUT / EXAM TRICK

$B \propto 1/\mu$: $B(DCl)/B(HCl) \approx \mu(HCl)/\mu(DCl) \approx 0.51$.

COMMON MISTAKE

Taking the spacing as B instead of 2B; using the molecular mass instead of the reduced mass.

EXAM TIP

Symmetric tops need two constants (A or C and B); spherical tops (CH_4) have no pure rotational spectrum.

MEMORY TRICK

'Lines every 2B'.

Why the Other Options Are Wrong

Correct answer: A

B **30012**

Why (A) is the key — Pure rotational Raman: lines at $\nu_0 \pm 2B(2J+3)$; first Stokes line (J = 0) at $\nu_0 - 6B$. Microwave spacing $2B = 4 \rightarrow B = 2\ cm^{-1} \rightarrow 30\,000 - 12 = 29\,988\ cm^{-1}$.

C **30004**

Ruled out: Taking the spacing as B instead of 2B; using the molecular mass instead of the reduced mass.

D **29996**

Ruled out: Symmetric tops need two constants (A or C and B); spherical tops (CH_4) have no pure rotational spectrum.

Q10

The microwave spectrum of a molecule yields three rotational constants. The molecule is

A. Prolate symmetric top

B. Spherical top

C. Asymmetric top

D. Oblate symmetric top

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Rotational

PYQ FREQUENCY
High · 5 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'Lines every 2B'.

Correct Answer C Asymmetric top

CONCEPT

Rigid rotor $E_J = BJ(J+1)$ with degeneracy $2J+1$; selection $\Delta J = \pm 1$ and a permanent dipole; line spacing $2B$; centrifugal distortion lowers spacing at high J; most populated level from the Boltzmann–degeneracy balance; linear vs symmetric-top molecules.

↓

LOGIC / WORKING

- Three distinct rotational constants $A \neq B \neq C \rightarrow$ asymmetric top. Symmetric tops have two (A, B = C), spherical tops one.
- Therefore the answer is (C).

FINAL: (C) Asymmetric top

SHORTCUT / EXAM TRICK

$B \propto 1/\mu$: $B(DCl)/B(HCl) \approx \mu(HCl)/\mu(DCl) \approx 0.51$.

COMMON MISTAKE

Taking the spacing as B instead of 2B; using the molecular mass instead of the reduced mass.

EXAM TIP

Symmetric tops need two constants (A or C and B); spherical tops (CH_4) have no pure rotational spectrum.

MEMORY TRICK

'Lines every 2B'.

Why the Other Options Are Wrong

Correct answer: C

A **Prolate symmetric top**

Why (C) is the key — Three distinct rotational constants A ≠ B ≠ C → asymmetric top. Symmetric tops have two (A, B = C), spherical tops one.

B **Spherical top**

Ruled out: Taking the spacing as B instead of 2B; using the molecular mass instead of the reduced mass.

D **Oblate symmetric top**

Ruled out: Symmetric tops need two constants (A or C and B); spherical tops (CH_4) have no pure rotational spectrum.

Q11

For a diatomic molecule AB, the energy for the rotational transition from J = 0 to J = 1 state is 3.9 cm^{-1}. The energy for the rotational transition from J = 3 to J = 4 state would be

A. 3.9 cm^{-1}

B. 7.8 cm^{-1}

C. 11.7 cm^{-1}

D. 15.6 cm^{-1}

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Rotational

PYQ FREQUENCY
High · 5 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'Lines every 2B'.

Correct Answer D 15.6 cm^{-1}

CONCEPT

Rigid rotor $E_J = BJ(J+1)$ with degeneracy $2J+1$; selection $\Delta J = \pm 1$ and a permanent dipole; line spacing $2B$; centrifugal distortion lowers spacing at high J; most populated level from the Boltzmann–degeneracy balance; linear vs symmetric-top molecules.

↓

LOGIC / WORKING

- $\Delta E(J \rightarrow J+1) = 2B(J+1)$. $J = 0 \rightarrow 1$: $2B = 3.9\ cm^{-1}$. $J = 3 \rightarrow 4$: $8B = 4 \times 3.9 = 15.6\ cm^{-1}$.
- Therefore the answer is (D).

FINAL: (D) 15.6 cm^{-1}

SHORTCUT / EXAM TRICK

$B \propto 1/\mu$: $B(DCl)/B(HCl) \approx \mu(HCl)/\mu(DCl) \approx 0.51$.

COMMON MISTAKE

Taking the spacing as B instead of 2B; using the molecular mass instead of the reduced mass.

EXAM TIP

Symmetric tops need two constants (A or C and B); spherical tops (CH_4) have no pure rotational spectrum.

MEMORY TRICK

'Lines every 2B'.

Why the Other Options Are Wrong

Correct answer: D

A **3.9 cm^{-1}**

Why (D) is the key — $\Delta E(J \rightarrow J+1) = 2B(J+1)$. $J = 0 \rightarrow 1$: $2B = 3.9\ cm^{-1}$. $J = 3 \rightarrow 4$: $8B = 4 \times 3.9 = 15.6\ cm^{-1}$.

B **7.8 cm^{-1}**

Ruled out: Taking the spacing as B instead of 2B; using the molecular mass instead of the reduced mass.

C **11.7 cm^{-1}**

Ruled out: Symmetric tops need two constants (A or C and B); spherical tops (CH_4) have no pure rotational spectrum.

Q12

The spectroscopic technique, by which the ground state dissociation energies of diatomic molecules can be estimated, is

A. Microwave spectroscopy

B. Infrared spectroscopy

C. UV-visible absorption spectroscopy

D. X-ray spectroscopy

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Rotational

PYQ FREQUENCY
High · 5 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'Lines every 2B'.

Correct Answer B Infrared spectroscopy

CONCEPT

Rigid rotor $E_J = BJ(J+1)$ with degeneracy $2J+1$; selection $\Delta J = \pm 1$ and a permanent dipole; line spacing $2B$; centrifugal distortion lowers spacing at high J; most populated level from the Boltzmann–degeneracy balance; linear vs symmetric-top molecules.

↓

LOGIC / WORKING

- The anharmonic vibrational level spacings (fundamental + overtones from IR, or a vibrational progression) are extrapolated by the Birge–Sponer method to estimate D_0 of the ground electronic state.
- Therefore the answer is (B).

FINAL: (B) Infrared spectroscopy

SHORTCUT / EXAM TRICK

$B \propto 1/\mu$: $B(DCl)/B(HCl) \approx \mu(HCl)/\mu(DCl) \approx 0.51$.

COMMON MISTAKE

Taking the spacing as B instead of 2B; using the molecular mass instead of the reduced mass.

EXAM TIP

Symmetric tops need two constants (A or C and B); spherical tops (CH_4) have no pure rotational spectrum.

MEMORY TRICK

'Lines every 2B'.

Why the Other Options Are Wrong

Correct answer: B

A — **Microwave spectroscopy**

Why (B) is the key — The anharmonic vibrational level spacings (fundamental + overtones from IR, or a vibrational progression) are extrapolated by the Birge–Sponer method to estimate D_0 of the ground electronic state.

C — **UV-visible absorption spectroscopy**

Ruled out: Taking the spacing as B instead of 2B; using the molecular mass instead of the reduced mass.

D — **X-ray spectroscopy**

Ruled out: Symmetric tops need two constants (A or C and B); spherical tops (CH_4) have no pure rotational spectrum.

TOPIC REVISION

Rotational

6 PYQs · Last-minute revision

TOPIC SUMMARY

Rigid rotor $E_J = BJ(J+1)$ with degeneracy $2J+1$; selection $\Delta J = \pm 1$ and a permanent dipole; line spacing $2B$; centrifugal distortion lowers spacing at high J; most populated level from the Boltzmann–degeneracy balance; linear vs symmetric-top molecules.

IMPORTANT FORMULA SHEET

- $E_J = hcBJ(J+1)$; $B = h/(8\pi^2 cI)$
- $\tilde{\nu}(J \rightarrow J+1) = 2B(J+1)$
- $J_{max} = \sqrt{(kT/2hcB)} - ½$
- With distortion: $\tilde{\nu} = 2B(J+1) - 4D(J+1)^3$

FREQUENTLY ASKED CONCEPTS

- Bond length of CO/HCl from B
- Isotopic substitution and B ratio
- Which molecules are microwave active (CO_2 no, OCS yes)
- Population of levels

COMMON MISTAKES & QUICK NOTES

Watch out:
Taking the spacing as B instead of 2B; using the molecular mass instead of the reduced mass.
Symmetric tops need two constants (A or C and B); spherical tops (CH_4) have no pure rotational spectrum.

MOST-REPEATED PYQs & EXPECTED IN EXAM

PYQs in this topic: Q7 Q8 Q9 Q10 Q11 Q12

Expect 1 question(s) next session on Rotational.

TOPIC 3

Raman

5 questions · Easy 2 | Medium 3 | Hard 0 · PYQ frequency: High

Q13

Among the following, both microwave and rotational Raman active molecule is

A CH_4

B N_2O

C C_2H_4

D CO_2

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Raman

PYQ FREQUENCY
High · 5 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'Polarisability changes → Raman; dipole changes → IR'.

Correct Answer B N_2O

CONCEPT

Raman scattering requires a change in polarisability during the motion; Stokes (lower energy) and anti-Stokes (higher energy, weaker) lines; rotational Raman $\Delta J = \pm 2$ giving spacing 4B; rule of mutual exclusion for centrosymmetric molecules; depolarisation ratio identifies totally symmetric modes.

↓

LOGIC / WORKING

- Microwave needs a permanent dipole; rotational Raman needs anisotropic polarizability (all except spherical tops). N_2O (N–N–O, linear, polar) satisfies both. CO_2 and C_2H_4 are non-polar; CH_4 is a spherical top (Raman-inactive rotation).
- Therefore the answer is (B).

FINAL: (B) N_2O

SHORTCUT / EXAM TRICK

Homonuclear diatomics (N_2, O_2, H_2) — Raman active, IR and microwave inactive.

COMMON MISTAKE

Confusing 4B rotational Raman spacing with the 2B microwave spacing.

EXAM TIP

CO_2: symmetric stretch Raman-only, asymmetric stretch and bend IR-only (centre of symmetry).

MEMORY TRICK

'Polarisability changes → Raman; dipole changes → IR'.

Why the Other Options Are Wrong

Correct answer: B

A **CH_4**

Why (B) is the key — Microwave needs a permanent dipole; rotational Raman needs anisotropic polarizability (all except spherical tops). N_2O (N–N–O, linear, polar) satisfies both. CO_2 and C_2H_4 are non-polar; CH_4 is a spherical top (Raman-inactive rotation).

C **C_2H_4**

Ruled out: Confusing 4B rotational Raman spacing with the 2B microwave spacing.

D **CO_2**

Ruled out: CO_2: symmetric stretch Raman-only, asymmetric stretch and bend IR-only (centre of symmetry).

Q14

The molecule that will show Raman spectrum, but not IR spectrum, among the following is

A H_2

B HCl

C BrCl

D CS_2

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Raman

PYQ FREQUENCY
High · 5 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'Polarisability changes → Raman; dipole changes → IR'.

Correct Answer A H_2

CONCEPT

Raman scattering requires a change in polarisability during the motion; Stokes (lower energy) and anti-Stokes (higher energy, weaker) lines; rotational Raman $\Delta J = \pm 2$ giving spacing 4B; rule of mutual exclusion for centrosymmetric molecules; depolarisation ratio identifies totally symmetric modes.

↓

LOGIC / WORKING

- H_2 has no dipole (IR-inactive) but its polarizability changes on stretching (Raman-active). HCl and BrCl are polar; CS_2 has IR-active asymmetric stretch and bend.
- Therefore the answer is (A).

FINAL: (A) H_2

SHORTCUT / EXAM TRICK

Homonuclear diatomics (N_2, O_2, H_2) — Raman active, IR and microwave inactive.

COMMON MISTAKE

Confusing 4B rotational Raman spacing with the 2B microwave spacing.

EXAM TIP

CO_2: symmetric stretch Raman-only, asymmetric stretch and bend IR-only (centre of symmetry).

MEMORY TRICK

'Polarisability changes → Raman; dipole changes → IR'.

Why the Other Options Are Wrong

Correct answer: A

B **HCl**

Why (A) is the key — H_2 has no dipole (IR-inactive) but its polarizability changes on stretching (Raman-active). HCl and BrCl are polar; CS_2 has IR-active asymmetric stretch and bend.

C **BrCl**

Ruled out: Confusing 4B rotational Raman spacing with the 2B microwave spacing.

D **CS_2**

Ruled out: CO_2: symmetric stretch Raman-only, asymmetric stretch and bend IR-only (centre of symmetry).

Q15

For the vibrational Raman spectrum of a homonuclear diatomic molecule, the selection rule under harmonic approximation is

A. $\Delta v = 0$ only

B. $\Delta v = \pm 1$ only

C. $\Delta v = \pm 2$ only

D. $\Delta v = 0, \pm 1$

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Raman

PYQ FREQUENCY
High · 5 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'Polarisability changes → Raman; dipole changes → IR'.

Correct Answer B Δ v = ± 1 only

CONCEPT

Raman scattering requires a change in polarisability during the motion; Stokes (lower energy) and anti-Stokes (higher energy, weaker) lines; rotational Raman ΔJ = ±2 giving spacing 4B; rule of mutual exclusion for centrosymmetric molecules; depolarisation ratio identifies totally symmetric modes.

↓

LOGIC / WORKING

- Vibrational Raman (harmonic approximation): Δv = ±1 (gross selection rule: polarizability changes during the vibration — true for all diatomics, including homonuclear).
- Therefore the answer is (B).

FINAL: (B) Δ v = ± 1 only

SHORTCUT / EXAM TRICK

Homonuclear diatomics (N_2, O_2, H_2) — Raman active, IR and microwave inactive.

COMMON MISTAKE

Confusing 4B rotational Raman spacing with the 2B microwave spacing.

EXAM TIP

CO_2: symmetric stretch Raman-only, asymmetric stretch and bend IR-only (centre of symmetry).

MEMORY TRICK

'Polarisability changes → Raman; dipole changes → IR'.

Why the Other Options Are Wrong

Correct answer: B

A **Δ v = 0 only**

Why (B) is the key — Vibrational Raman (harmonic approximation): Δv = ±1 (gross selection rule: polarizability changes during the vibration — true for all diatomics, including homonuclear).

C **Δ v = ± 2 only**

Ruled out: Confusing 4B rotational Raman spacing with the 2B microwave spacing.

D **Δ v = 0, ± 1**

Ruled out: CO_2: symmetric stretch Raman-only, asymmetric stretch and bend IR-only (centre of symmetry).

Q16

The first electronic absorption band maximum of a polar and relatively rigid aromatic molecule appears at 310 nm but its fluorescence maximum in acetonitrile solution appears with a large Stokes shift at 450 nm. The most likely reason for the Stokes shift is (a) Large change in molecular geometry in the excited state (b) Increase in dipole moment of the molecule in the excited state (c) Decrease in polarizability of the molecule in the excited state

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

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Raman

PYQ FREQUENCY
High · 5 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'Polarisability changes → Raman; dipole changes → IR'.

Q17

The rotational constant of $^{14}N_2$ is 2 cm^{-1}. The wave number of incident radiation in a Raman spectrometer is 20487 cm^{-1}. What is the wave number of first scattered Stokes line (in cm^{-1}) of $^{14}N_2$?

A. 20479

B. 20475

C. 20499

D. 20495

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Raman

PYQ FREQUENCY
High · 5 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'Polarisability changes → Raman; dipole changes → IR'.

Correct Answer B 20475

CONCEPT

Raman scattering requires a change in polarisability during the motion; Stokes (lower energy) and anti-Stokes (higher energy, weaker) lines; rotational Raman $\Delta J = \pm 2$ giving spacing 4B; rule of mutual exclusion for centrosymmetric molecules; depolarisation ratio identifies totally symmetric modes.

↓

LOGIC / WORKING

- Rotational Raman first Stokes line at $\nu_0 - 6B = 20\,487 - 6 \times 2 = 20\,475\ cm^{-1}$.
- Therefore the answer is (B).

FINAL: (B) 20475

SHORTCUT / EXAM TRICK

Homonuclear diatomics (N_2, O_2, H_2) — Raman active, IR and microwave inactive.

COMMON MISTAKE

Confusing 4B rotational Raman spacing with the 2B microwave spacing.

EXAM TIP

CO_2: symmetric stretch Raman-only, asymmetric stretch and bend IR-only (centre of symmetry).

MEMORY TRICK

'Polarisability changes → Raman; dipole changes → IR'.

Why the Other Options Are Wrong

Correct answer: B

A **20479**

Why (B) is the key — Rotational Raman first Stokes line at $\nu_0 - 6B = 20\,487 - 6 \times 2 = 20\,475\ cm^{-1}$.

C **20499**

Ruled out: Confusing 4B rotational Raman spacing with the 2B microwave spacing.

D **20495**

Ruled out: CO_2: symmetric stretch Raman-only, asymmetric stretch and bend IR-only (centre of symmetry).

TOPIC REVISION

Raman

5 PYQs · Last-minute revision

TOPIC SUMMARY

Raman scattering requires a change in polarisability during the motion; Stokes (lower energy) and anti-Stokes (higher energy, weaker) lines; rotational Raman ΔJ = ±2 giving spacing 4B; rule of mutual exclusion for centrosymmetric molecules; depolarisation ratio identifies totally symmetric modes.

IMPORTANT FORMULA SHEET

- $\Delta\tilde{\nu}_{rot} = 4B(J + 3/2)$; first line 6B from the Rayleigh line, spacing 4B
- $I(\text{anti-Stokes})/I(\text{Stokes}) \propto \exp(-\Delta E/kT)$
- $\rho = I_{\perp}/I_{\parallel} < 3/4$ polarised (totally symmetric)

FREQUENTLY ASKED CONCEPTS

- Which modes are Raman vs IR active
- Rotational Raman spacing
- Stokes vs anti-Stokes intensity
- Mutual exclusion

COMMON MISTAKES & QUICK NOTES

Watch out:
Confusing 4B rotational Raman spacing with the 2B microwave spacing.
CO_2: symmetric stretch Raman-only, asymmetric stretch and bend IR-only (centre of symmetry).

MOST-REPEATED PYQs & EXPECTED IN EXAM

PYQs in this topic: Q13 Q14 Q15 Q16 Q17

Expect 1 question(s) next session on Raman.

TOPIC 4

Molecular Spectroscopy – General

31 questions · Easy 6 | Medium 25 | Hard 0 · PYQ frequency: Very High

Q18

The Q band in the vibrational spectrum of acetylene is observed in the

A. C–C stretching mode

B. C-H symmetric stretching mode

C. Bending mode

D. C-H antisymmetric stretching mode

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer C Bending mode

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced 2B; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- The Q branch ($\Delta J = 0$) is allowed only for vibrations with a transition dipole perpendicular to the molecular axis. For linear acetylene that is the (doubly degenerate) bending mode; the stretches are parallel bands with P and R branches only.
- Therefore the answer is (C).

FINAL: (C) Bending mode

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced 4B (first Stokes line 6B from the exciting line); microwave lines spaced 2B.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \to {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: C

A **C–C stretching mode**

Why (C) is the key — The Q branch (ΔJ = 0) is allowed only for vibrations with a transition dipole perpendicular to the molecular axis. For linear acetylene that is the (doubly degenerate) bending mode; the stretches are parallel bands with P and R branches only.

B **C-H symmetric stretching mode**

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D **C-H antisymmetric stretching mode**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^{1}H \rightarrow {}^{2}D$ shifts $\tilde{\nu}$ by ≈ 1/√2.

Q19 The absorption spectrum of O_2 shows a vibrational structure that becomes continuum at 56875 cm^{-1}. At the continuum, it dissociates into one ground state atom (O_g) and one excited state atom (O_e). The energy difference between O_e and O_g is 15125 cm^{-1}. The dissociation energy (in cm^{-1}) of ground state of O_2 is:

A. 56875/15125

B. 15125/56875

C. 7200

D. 41750

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer D 41750

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced 2B; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- The convergence limit (56 875 cm^{-1}) = D_0(ground state) + excitation energy of the excited atom. $D_0 = 56\,875 - 15\,125 = 41\,750\ cm^{-1}$ (≈ 5.2 eV for O_2).
- Therefore the answer is (D).

FINAL: (D) 41750

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced 4B (first Stokes line 6B from the exciting line); microwave lines spaced 2B.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by ≈ $1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: D

A **56875/15125**

Why (D) is the key — The convergence limit (56 875 cm^{-1}) = D_0(ground state) + excitation energy of the excited atom. D_0 = 56 875 − 15 125 = 41 750 cm^{-1} (≈ 5.2 eV for O_2).

B **15125/56875**

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

C **7200**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by ≈ 1/√2.

Q20

The C=O bond length is 120 pm in CO_2. The moment of inertia of CO_2 would be close to (masses of C and O are 1.9×10^{-27} kg and 2.5×10^{-27} kg, respectively)

A. 1.8×10^{-45} kg m²

B. 3.6×10^{-45} kg m²

C. 5.4×10^{-45} kg m²

D. 7.2×10^{-45} kg m²

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer D 7.2×10^{-45} kg m²

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced 2B; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- Linear CO_2 with C at the centre of mass: $I = 2m_O r^2 = 2 \times 2.5\times10^{-27} \times (1.2\times10^{-10})^2 = 7.2\times10^{-47}$ kg m². Matches the numeral of option (d) (the exponent printed in the options is a typo).
- Therefore the answer is (D).

FINAL: (D) 7.2×10^{-45} kg m²

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced 4B (first Stokes line 6B from the exciting line); microwave lines spaced 2B.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: D

A **1.8×10^{-45} kg m²**

Why (D) is the key — Linear CO_2 with C at the centre of mass: $I = 2m_O\, r^2 = 2 \times 2.5\times10^{-27} \times (1.2\times10^{-10})^2 = 7.2\times10^{-47}$ kg m². Matches the numeral of option (d) (the exponent printed in the options is a typo).

B **3.6×10^{-45} kg m²**

Ruled out: Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

C **5.4×10^{-45} kg m²**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \to {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

Q21

The molecule with the smallest rotation partition function at any temperature among the following is:

A mathrmCH_3-C≡C-H

B mathrmH-C≡C-H

C mathrmH-C≡C-D

D mathrmD-C≡C-D

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer B mathrmH-C≡C-H

CONCEPT

Rotational (microwave): E_J = BJ(J+1), lines spaced 2B; vibrational (IR): harmonic ν̃ = (1/2πc)√(k/μ), anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- q_rot = kT/(σhcB) ∝ I/σ. Among the acetylenes H–C≡C–H has the smallest moment of inertia and the highest symmetry number (σ = 2, like D–C≡C–D which is heavier) → smallest q_rot.
- Therefore the answer is (B).

FINAL: (B) mathrmH-C≡C-H

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced 4B (first Stokes line 6B from the exciting line); microwave lines spaced 2B.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller ν̃; $^{1}H \rightarrow {}^{2}D$ shifts ν̃ by ≈ 1/√2.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: B

A **mathrmCH₃-C≡C-H**

Why (B) is the key — q_rot = kT/(σhcB) ∝ I/σ. Among the acetylenes H–C≡C–H has the smallest moment of inertia and the highest symmetry number (σ = 2, like D–C≡C–D which is heavier) → smallest q_rot.

C **mathrmH-C≡C-D**

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D **mathrmD-C≡C-D**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^{1}H \rightarrow {}^{2}D$ shifts $\tilde{\nu}$ by ≈ 1/√2.

Q22

If the reduced mass of a diatomic molecule is doubled without changing its force constant, the vibrational frequency of the molecule will be

A. √(2) times the original frequency

B. 1/√(2) times the vibrational frequency

C. twice the original frequency

D. unchanged

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer B 1/√(2) times the vibrational frequency

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced 2B; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- $\nu = (1/2\pi)\sqrt{(k/\mu)}$; doubling μ with k fixed → ν → ν/√2.
- Therefore the answer is (B).

FINAL: (B) 1/√(2) times the vibrational frequency

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced 4B (first Stokes line 6B from the exciting line); microwave lines spaced 2B.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by ≈ 1/√2.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: B

A — **√(2) times the original frequency**

Why (B) is the key — ν = (1/2π)√(k/μ); doubling μ with k fixed → ν → ν/√2.

C — **twice the original frequency**

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D — **unchanged**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^{1}H \rightarrow {}^{2}D$ shifts $\tilde{\nu}$ by ≈ 1/√2.

Q23 The vibrational frequency of a homo-nuclear diatomic molecule is ν. The temperature at which the population of the first excited state will be half that of the ground state is given by

A. hν · ln 2/k_B

B. hν/(ln 2 · k_B)

C. ln 2/(hν · k_B)

D. hν · log 2/k_B

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer B hν/(ln 2 · k_B)

CONCEPT

Rotational (microwave): E_J = BJ(J+1), lines spaced 2B; vibrational (IR): harmonic ν̃ = (1/2πc)√(k/μ), anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- Boltzmann: $N_1/N_0 = e^{-h\nu/k_BT} = ½ \rightarrow h\nu/k_BT = \ln 2 \rightarrow T = h\nu/(k_B \ln 2)$.
- Therefore the answer is (B).

FINAL: (B) hν/(ln 2 · k_B)

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced 4B (first Stokes line 6B from the exciting line); microwave lines spaced 2B.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller ν̃; $^1H \rightarrow {}^2D$ shifts ν̃ by ≈ 1/√2.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: B

A **hν · ln 2/k_B**

Why (B) is the key — Boltzmann: $N_1/N_0 = e^{-h\nu/k_BT} = ½ \rightarrow h\nu/k_BT = \ln 2 \rightarrow T = h\nu/(k_B \ln 2)$.

C **ln 2/(hν · k_B)**

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D **hν · log 2/k_B**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow ^2D$ shifts $\tilde{\nu}$ by ≈ 1/√2.

Q24

The ^{1}H NMR frequency at 1.0T is 42.4 MHz. If the gyromagnetic ratios of ^{1}H and ^{13}C are 27×10^{7} and $6.75 \times 10^{7} T^{-1} S^{-1}$ respectively, what will be the ^{13}C frequency at 1.0 T ?

A. 10.6 MHz

B. 169.6 MHz

C. 42.6 MHz

D. 21.3 MHz

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer A 10.6 MHz

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced $2B$; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- Larmor frequency $\nu = \gamma B/2\pi \propto \gamma$. $\nu(^{13}C) = 42.4 \times (6.75/27) = 42.4/4 = 10.6$ MHz.
- Therefore the answer is (A).

FINAL: (A) 10.6 MHz

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced $4B$ (first Stokes line $6B$ from the exciting line); microwave lines spaced $2B$.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \to {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: A

B **169.6 MHz**

Why (A) is the key — Larmor frequency $\nu = \gamma B/2\pi \propto \gamma$. $\nu(^{13}C) = 42.4 \times (6.75/27) = 42.4/4 = 10.6$ MHz.

C **42.6 MHz**

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D **21.3 MHz**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^{1}H \rightarrow {}^{2}D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

Q25

In a 200 MHz NMR spectrometer, a molecule shows two doublets separated by 2 ppm. The observed coupling constant is 10 Hz. The separation between these two signals and the coupling constant in a 600 MHz spectrometer will be, respectively

A. 600 Hz and 30 Hz

B. 1200 Hz and 30 Hz

C. 600 Hz and 10 Hz

D. 1200 Hz and 10 Hz

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer D 1200 Hz and 10 Hz

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced 2B; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- Chemical shift in ppm is field-independent, so the separation in Hz scales with the spectrometer frequency: 2 ppm × 600 MHz = 1200 Hz. The coupling constant J (10 Hz) is a molecular property, independent of B_0.
- Therefore the answer is (D).

FINAL: (D) 1200 Hz and 10 Hz

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced 4B (first Stokes line 6B from the exciting line); microwave lines spaced 2B.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: D

A **600 Hz and 30 Hz**

Why (D) is the key — Chemical shift in ppm is field-independent, so the separation in Hz scales with the spectrometer frequency: 2 ppm × 600 MHz = 1200 Hz. The coupling constant J (10 Hz) is a molecular property, independent of B_0.

B **1200 Hz and 30 Hz**

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

C **600 Hz and 10 Hz**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by ≈ 1/√2.

Q26

^{1}H NMR spectrum of an organic compound recorded on a 500 MHz spectrometer showed a quartet with line positions at 1759, 1753, 1747, 1741 Hz. Chemical shift and coupling constant (Hz) of the quartet are

A. 3.5 ppm, 6 Hz

B. 3.5 ppm, 12 Hz

C. 3.6 ppm, 6 Hz

D. 3.6 ppm, 12 Hz

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer A 3.5 ppm, 6 Hz

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced $2B$; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- Centre of the quartet = (1759 + 1741)/2 = 1750 Hz; at 500 MHz that is 1750/500 = 3.5 ppm. Line spacing = 6 Hz = J.
- Therefore the answer is (A).

FINAL: (A) 3.5 ppm, 6 Hz

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced $4B$ (first Stokes line $6B$ from the exciting line); microwave lines spaced $2B$.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: A

B **3.5 ppm, 12 Hz**

Why (A) is the key — Centre of the quartet = (1759 + 1741)/2 = 1750 Hz; at 500 MHz that is 1750/500 = 3.5 ppm. Line spacing = 6 Hz = J.

C **3.6 ppm, 6 Hz**

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D **3.6 ppm, 12 Hz**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^{1}H \rightarrow {}^{2}D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

Q27

Vibrations of diatomic molecules are usually modelled by a harmonic potential. If the potential is given by x^2, the correct statement is

A. force is 2 x and force constant is 2

B. force is -2 x and force constant is 2

C. force is 2 x and force constant is -1

D. force is -2 x and force constant is -1

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer B force is -2 x and force constant is 2

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced 2B; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- For $V = x^2$, $F = -dV/dx = -2x$ and the force constant $k = d^2V/dx^2 = 2$.
- Therefore the answer is (B).

FINAL: (B) force is -2 x and force constant is 2

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced 4B (first Stokes line 6B from the exciting line); microwave lines spaced 2B.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: B

A **force is 2 x and force constant is 2**

Why (B) is the key — For $V = x^2$, $F = -dV/dx = -2x$ and the force constant $k = d^2V/dx^2 = 2$.

C **force is 2 x and force constant is -1**

Ruled out: Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D **force is -2 x and force constant is -1**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

Q28

The rotational constant and the fundamental vibrational frequency of HBr are, respectively, 10 cm^{-1} and 2000 cm^{-1}. The corresponding values for DBr approximately are

A. 20 cm^{-1} and 2000 cm^{-1}

B. 10 cm^{-1} and 1410 cm^{-1}

C. 5 cm^{-1} and 2000 cm^{-1}

D. 5 cm^{-1} and 1410 cm^{-1}

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer D 5 cm^{-1} and 1410 cm^{-1}

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced 2B; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- $B \propto 1/\mu$ and $\nu \propto 1/\sqrt{\mu}$. Since Br is heavy, $\mu(DBr) \approx 2\mu(HBr)$: $B \rightarrow 10/2 = 5\ cm^{-1}$; $\nu \rightarrow 2000/\sqrt{2} = 1414 \approx 1410\ cm^{-1}$.
- Therefore the answer is (D).

FINAL: (D) 5 cm^{-1} and 1410 cm^{-1}

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced 4B (first Stokes line 6B from the exciting line); microwave lines spaced 2B.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: D

A **20 cm⁻¹ and 2000 cm⁻¹**

Why (D) is the key — B ∝ 1/μ and ν ∝ 1/√μ. Since Br is heavy, μ(DBr) ≈ 2μ(HBr): B → 10/2 = 5 cm⁻¹; ν → 2000/√2 = 1414 ≈ 1410 cm⁻¹.

B **10 cm⁻¹ and 1410 cm⁻¹**

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

C **5 cm⁻¹ and 2000 cm⁻¹**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^{1}H \rightarrow {}^{2}D$ shifts $\tilde{\nu}$by ≈ 1/√2.

Q29 **Vibrations of diatomic molecules are usually modelled by a harmonic potential. If the potential is given by x^2, the correct statement is**

A. Force is 2x and force constant is 2

B. Force is -2x and force constant is 2

C. Force is 2x and force constant is -1

D. Force is -2x and force constant is -1

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer B Force is -2x and force constant is 2

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced 2B; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- $V = x^2 \rightarrow$ force $F = -dV/dx = -2x$ (restoring); force constant $k = d^2V/dx^2 = 2$.
- Therefore the answer is (B).

FINAL: (B) Force is -2x and force constant is 2

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced 4B (first Stokes line 6B from the exciting line); microwave lines spaced 2B.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: B

A **Force is 2x and force constant is 2**

Why (B) is the key — $V = x^2$ → force $F = -dV/dx = -2x$ (restoring); force constant $k = d^2V/dx^2 = 2$.

C **Force is 2x and force constant is -1**

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D **Force is -2x and force constant is -1**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow ^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

Q30

The transition that belongs to the Lyman series in the hydrogen-atom spectrum is

A. 1s ← 4s

B. 1s ← 4p

C. 2s ← 4s

D. 2s ← 4p

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer B 1s ← 4p

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced 2B; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- Lyman series ends on n = 1 (1s). Electric-dipole selection rule $\Delta l = \pm 1$ → only 1s ← np transitions: 1s ← 4p.
- Therefore the answer is (B).

FINAL: (B) 1s ← 4p

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced 4B (first Stokes line 6B from the exciting line); microwave lines spaced 2B.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: B

A **1s ← 4s**

Why (B) is the key — Lyman series ends on n = 1 (1s). Electric-dipole selection rule Δl = ±1 → only 1s ← np transitions: 1s ← 4p.

C **2s ← 4s**

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D **2s ← 4p**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^{1}H \rightarrow {}^{2}D$ shifts $\tilde{\nu}$by ≈ 1/√2.

Q31

The pair that contains a spherical top and a symmetric top, among the following, is

A. CH_4, CH_2Cl_2

B. CH_2Cl_2, CH_3Cl

C. CH_3Cl, CH_4

D. CH_4, $C(CH_3)_4$

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer C CH_3Cl, CH_4

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced 2B; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- CH_4 (T_d): $I_A = I_B = I_C$ → spherical top. CH_3Cl (C_{3v}): $I_A \neq I_B = I_C$ → symmetric top. CH_2Cl_2 is an asymmetric top; $C(CH_3)_4$ is spherical.
- Therefore the answer is (C).

FINAL: (C) CH_3Cl, CH_4

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced 4B (first Stokes line 6B from the exciting line); microwave lines spaced 2B.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: C

A **CH_4, CH_2Cl_2**

Why (C) is the key — CH_4 (T_d): $I_A = I_B = I_C$ → spherical top. CH_3Cl (C_{3v}): $I_A \neq I_B = I_C$ → symmetric top. CH_2Cl_2 is an asymmetric top; $C(CH_3)_4$ is spherical.

B **CH_2Cl_2, CH_3Cl**

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D **CH_4, $C(CH_3)_4$**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

Q32

The g-factors of ^{1}H and ^{13}C are 5.6 and 1.4 respectively. For the same value of the magnetic field strength, if the ^{1}H resonates at 600 MHz, the ^{13}C would resonate at

A. 2400 MHz

B. 600 MHz

C. 150 MHz

D. 38 MHz

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer C 150 MHz

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced $2B$; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- $\nu \propto g$ at fixed B: $\nu(^{13}C) = 600 \times 1.4/5.6 = 150$ MHz.
- Therefore the answer is (C).

FINAL: (C) 150 MHz

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced $4B$ (first Stokes line $6B$ from the exciting line); microwave lines spaced $2B$.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: C

A **2400 MHz**

Why (C) is the key — ν ∝ g at fixed B: ν(¹³C) = 600 × 1.4/5.6 = 150 MHz.

B **600 MHz**

Ruled out: Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D **38 MHz**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^{1}H \rightarrow {}^{2}D$ shifts $\tilde{\nu}$ by ≈ 1/√2.

Q33

The frequency of O – H stretch occurs at sim 3600 cm^{-1}. The O – D stretch frequency (in cm^{-1}) would be closest to

A 3000

B 2600

C 1800

D 900

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer B 2600

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced $2B$; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- $\nu \propto 1/\sqrt{\mu}$. $\mu(OH) = 16/17 = 0.94$, $\mu(OD) = 32/18 = 1.78 \rightarrow \nu(OD) = 3600 \times \sqrt{(0.94/1.78)} = 3600/1.37 \approx 2620\ cm^{-1}$.
- Therefore the answer is (B).

FINAL: (B) 2600

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced $4B$ (first Stokes line $6B$ from the exciting line); microwave lines spaced $2B$.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: B

A — **3000**

Why (B) is the key — $\nu \propto 1/\sqrt{\mu}$. $\mu(OH) = 16/17 = 0.94$, $\mu(OD) = 32/18 = 1.78 \rightarrow \nu(OD) = 3600 \times \sqrt{(0.94/1.78)} = 3600/1.37 \approx 2620$ cm^{-1}.

C — **1800**

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D — **900**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^{1}H \rightarrow {}^{2}D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

Q34

The equilibrium dissociation energy of a diatomic molecule is 4.75 eV and its stretching frequency corresponds to 0.5 eV. The minimum energy required to dissociate the molecule in eV is

A. 4.75

B. 4.25

C. 4.50

D. 5.00

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer C 4.50

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced 2B; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- $D_0 = D_e$ − zero-point energy = 4.75 − ½(0.5) = 4.75 − 0.25 = 4.50 eV.
- Therefore the answer is (C).

FINAL: (C) 4.50

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced 4B (first Stokes line 6B from the exciting line); microwave lines spaced 2B.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: C

A **4.75**

Why (C) is the key — $D_0 = D_e$ − zero-point energy = 4.75 − ½(0.5) = 4.75 − 0.25 = 4.50 eV.

B **4.25**

Ruled out: Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D **5.00**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by ≈ 1/√2.

Q35

The atomic masses of fluorine and hydrogen are 19.0 and 1.0 amu, respectively (1 amu = 1.67×10^{-27} kg). The bond length of HF is 2.0 . The moment of inertia of HF is

A. 3.2×10^{-47} kg m²

B. 6-4 $\times 10^{-47}$ kg m²

C. 9-6 $\times 10^{-47}$ kg m²

D. 4.8×10^{-47} kg m²

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer B 6-4 × 10⁻⁴⁷ kg m²

CONCEPT

Rotational (microwave): E_J = BJ(J+1), lines spaced 2B; vibrational (IR): harmonic ν˜= (1/2πc)√(k/μ), anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- F atomic mass = 19.0amu . H atomic mass = 1 amu H – F bond length =2 . 0 / - I = *μr* 0 , I = *r*0 / .- 8Ä×8 Æ - 8Ä I= ×2.0 ×2.0 = *amu* ×2.0×2.0× 0 0“ Æ 0 19×1.67×10107 *kg*×4 = ×1018“ × 1018“ *m*0 20 76×1.67×101P7 *kgm*0 = 6.4×101P7 *kgm*0 20 Explanation as extracted from the printed page; notation may be imperfect.
- Therefore the answer is (B).

FINAL: (B) 6-4 × 10⁻⁴⁷ kg m²

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced 4B (first Stokes line 6B from the exciting line); microwave lines spaced 2B.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller ν˜; ¹H→²D shifts ν˜ by ≈ 1/√2.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: B

A

3.2 × 10⁻⁴⁷ kg m²

Why (B) is the key — F atomic mass = 19.0amu . H atomic mass = 1 amu H – F bond length =2 . 0 / - I = *μr* 0 , I = *r*0 / .- 8Ä×8 Æ - 8Ä I= ×2.0 ×2.0 = *amu* ×2.0×2.0× 0 0“ Æ 0 19×1.67×10107 *kg*×4 = ×1018“ × 1018“ *m*0 20 76×1.67×101P7 *kgm*0 = 6.4×101P7 *kgm*0 20 Explanation as extracted from the printed page; notation may be imperfect.

C

9-6 × 10⁻⁴⁷ kg m²

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D

4.8 × 10⁻⁴⁷ kg m²

Ruled out: Heavier isotope → smaller B and smaller ν̃; ¹H→²D shifts ν̃by ≈ 1/√2.

Q36

A molecule, AX, has a vibrational energy of 1000 cm^{-1} and rotational energy of 10 cm^{-1}. Another molecule, BX, has a vibrational energy of 400 cm^{-1} and rotational energy of 40 cm^{-1}. Which one of the following statements about the coupling of vibrational and rotational motion is true?

A. The coupling is stronger in BX

B. The coupling is stronger in AX

C. Magnitude of coupling is same in both AX and BX

D. There is no coupling in both AX and BX

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer A The coupling is stronger in BX

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced 2B; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- Vibration–rotation coupling ($\alpha_e \approx 6B^2/\omega_e$) grows with the rotational constant and falls with the vibrational frequency. BX has larger B (40) and smaller ω (400) → much stronger coupling than AX.
- Therefore the answer is (A).

FINAL: (A) The coupling is stronger in BX

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced 4B (first Stokes line 6B from the exciting line); microwave lines spaced 2B.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: A

B **The coupling is stronger in AX**

Why (A) is the key — Vibration–rotation coupling ($\alpha_e \approx 6B^2/\omega_e$) grows with the rotational constant and falls with the vibrational frequency. BX has larger B (40) and smaller ω (400) → much stronger coupling than AX.

C **Magnitude of coupling is same in both AX and BX**

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D **There is no coupling in both AX and BX**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by ≈ $1/\sqrt{2}$.

Q37

At room temperature, which molecule has the maximum rotational entropy?

A. H_2

B. O_2

C. D_2

D. N_2

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer B O_2

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced 2B; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- $S_{rot} \propto R \ln q_{rot}$, $q_{rot} = kT/(\sigma hcB) \propto I$. O_2 has the largest moment of inertia ($I \approx 1.9\times10^{-46}$ kg m² vs 1.4×10^{-46} for N_2, 0.9×10^{-47} for D_2, 0.46×10^{-47} for H_2) → largest rotational entropy.
- Therefore the answer is (B).

FINAL: (B) O_2

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced 4B (first Stokes line 6B from the exciting line); microwave lines spaced 2B.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \to {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: B

A — **H_2**

Why (B) is the key — S_rot ∝ R ln q_rot, q_rot = kT/(σhcB) ∝ I. O_2 has the largest moment of inertia (I ≈ 1.9×10^{-46} kg m² vs 1.4×10^{-46} for N_2, 0.9×10^{-47} for D_2, 0.46×10^{-47} for H_2) → largest rotational entropy.

C — **D_2**

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D — **N_2**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by ≈ 1/√2.

Q38

In IR spectrum of $[Co(CN)_5H]^{3-}$ the Co–H stretch is observed at 1840 cm^{-1}. The (Co–D) stretch in $[Co(CN)_5D]^{3-}$ will appear at nearly

A. 1300 cm^{-1}

B. 1400 cm^{-1}

C. 1500 cm^{-1}

D. 1600 cm^{-1}

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer A 1300 cm^{-1}

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced 2B; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- $\nu \propto 1/\sqrt{\mu}$; Co is heavy so $\mu \approx$ mass of H or D: $\nu(Co–D) \approx 1840/\sqrt{2} \approx 1300\ cm^{-1}$.
- Therefore the answer is (A).

FINAL: (A) 1300 cm^{-1}

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced 4B (first Stokes line 6B from the exciting line); microwave lines spaced 2B.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: A

B **1400 cm⁻¹**

Why (A) is the key — ν ∝ 1/√μ; Co is heavy so μ ≈ mass of H or D: ν(Co–D) ≈ 1840/√2 ≈ 1300 cm⁻¹.

C **1500 cm⁻¹**

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D **1600 cm⁻¹**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^{1}H \rightarrow {}^{2}D$ shifts $\tilde{\nu}$ by ≈ 1/√2.

Q39

The uncertainty in the NMR frequency of a compound in liquid state (relaxation time = 1 s) is 0.1 Hz. The uncertainty in the frequency (in Hz) of same compound in solid state (relaxation time = 10^{-4} s) is

A. 10

B. 100

C. 1000

D. 10^{-3}

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer C 1000

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced $2B$; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- Lifetime broadening $\Delta\nu \propto 1/T_2$. Relaxation time drops by 10^4 → linewidth rises by 10^4: 0.1 Hz × 10^4 = 1000 Hz (solids give broad lines).
- Therefore the answer is (C).

FINAL: (C) 1000

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced 4B (first Stokes line 6B from the exciting line); microwave lines spaced 2B.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: C

A **10**

Why (C) is the key — Lifetime broadening $\Delta\nu \propto 1/T_2$. Relaxation time drops by 10^4 → linewidth rises by 10^4: 0.1 Hz × 10^4 = 1000 Hz (solids give broad lines).

B **100**

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D **10^{-3}**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by ≈ $1/\sqrt{2}$.

Q40 **In NMR spectroscopy, the product of the nuclear 'g' factor (g_N), the nuclear magneton (β_N) and the magnetic field strength (B_0) gives the**

A. energy of transition from α to β state

B. chemical shift

C. spin-spin coupling constant

D. gyromagnetic ratio

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer A energy of transition from α to β state

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced 2B; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- Nuclear Zeeman splitting: $\Delta E = g_N \beta_N B_0 = h\nu$ — the energy of the α → β transition (resonance condition). Chemical shift and J are small corrections to it. (Bank key (b) was wrong — corrected.)
- Therefore the answer is (A).

FINAL: (A) energy of transition from α to β state

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced 4B (first Stokes line 6B from the exciting line); microwave lines spaced 2B.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \to {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: A

B — **chemical shift**

Why (A) is the key — Nuclear Zeeman splitting: $\Delta E = g_N \beta_N B_0 = h\nu$ — the energy of the $\alpha \rightarrow \beta$ transition (resonance condition). Chemical shift and J are small corrections to it. (Bank key (b) was wrong — corrected.)

C — **spin-spin coupling constant**

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D — **gyromagnetic ratio**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

Q41

The symmetric rotor among the following is

A CH_4

B CH_3Cl

C CH_2Cl_2

D CCl_4

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer B CH_3Cl

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced 2B; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- CH_3Cl (C_3 axis, $I_A \neq I_B = I_C$) is a prolate symmetric top. CH_4 and CCl_4 are spherical tops; CH_2Cl_2 is an asymmetric top.
- Therefore the answer is (B).

FINAL: (B) CH_3Cl

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced 4B (first Stokes line 6B from the exciting line); microwave lines spaced 2B.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: B

A — **CH_4**

Why (B) is the key — CH_3Cl (C_3 axis, $I_A \neq I_B = I_C$) is a prolate symmetric top. CH_4 and CCl_4 are spherical tops; CH_2Cl_2 is an asymmetric top.

C — **CH_2Cl_2**

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D — **CCl_4**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

Q42

The nuclear g-factors of $_{1}H$ and $_{14}N$ are 5.6 and 0.40 respectively. If the magnetic field in an NMR spectrometer is set such that the proton resonates at 700 MHz, the $_{14}N$ nucleus would resonate at

A. 1750 MHz

B. 700 MHz

C. 125 MHz

D. 50 MHz

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer D 50 MHz

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced $2B$; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- $\nu \propto g_N$ (or γ) at fixed B_0: $\nu(^{14}N) = 700 \times 0.40/5.6 = 50$ MHz.
- Therefore the answer is (D).

FINAL: (D) 50 MHz

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced $4B$ (first Stokes line $6B$ from the exciting line); microwave lines spaced $2B$.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: D

A **1750 MHz**

Why (D) is the key — ν ∝ g_N (or γ) at fixed B_0: $\nu(^{14}N) = 700 \times 0.40/5.6 = 50$ MHz.

B **700 MHz**

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

C **125 MHz**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by ≈ $1/\sqrt{2}$.

Q43

In an NMR spectrometer containing a 2.5 T magnet, Larmor precession frequency of ^1H is 100 MHz. The radiofrequency used in this spectrometer has an associated magnetic field strength of 2.5×10^{-4} T. The duration of a 90Â° pulse in this instrument is

A. 25×10^{-6} s

B. 50×10^{-6} s

C. 25×10^{-5} s

D. 50×10^{-5} s

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer A 25 × 10⁻⁶ s

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced 2B; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- $\gamma/2\pi$ = 100 MHz/2.5 T = 40 MHz T^{-1}. Nutation frequency $\nu_1 = (\gamma/2\pi)B_1 = 40\times10^6 \times 2.5\times10^{-4} = 10^4$ Hz. A 90° pulse = ¼ period = $1/(4\nu_1)$ = 25 μs.
- Therefore the answer is (A).

FINAL: (A) 25 × 10⁻⁶ s

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced 4B (first Stokes line 6B from the exciting line); microwave lines spaced 2B.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: A

B **50×10^{-6} s**

Why (A) is the key — $\gamma/2\pi$ = 100 MHz/2.5 T = 40 MHz T^{-1}. Nutation frequency $\nu_1 = (\gamma/2\pi)B_1 = 40\times10^6 \times 2.5\times10^{-4} = 10^4$ Hz. A 90° pulse = ¼ period = $1/(4\nu_1)$ = 25 μs.

C **25×10^{-5} s**

Ruled out: Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D **50×10^{-5} s**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by ≈ $1/\sqrt{2}$.

Q44

Upon application of a weak magnetic field, a line in the microwave absorption spectrum of rigid rotor splits into 3 lines. The quantum number (J) of the rotational energy level from which the transition originates is

A. 0

B. 1

C. 2

D. 3

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer A 0

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced $2B$; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- A weak field lifts the M_J degeneracy. The transition $J = 0 \rightarrow 1$ (upper level $M = -1, 0, +1$; selection $\Delta M = 0, \pm 1$ from $M = 0$) splits into exactly 3 lines, so the transition originates from $J = 0$.
- Therefore the answer is (A).

FINAL: (A) 0

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced $4B$ (first Stokes line $6B$ from the exciting line); microwave lines spaced $2B$.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: A

B

1

Why (A) is the key — A weak field lifts the M_J degeneracy. The transition J = 0 → 1 (upper level M = −1, 0, +1; selection ΔM = 0, ±1 from M = 0) splits into exactly 3 lines, so the transition originates from J = 0.

C

2

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D

3

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^{1}H \rightarrow {}^{2}D$ shifts $\tilde{\nu}$ by ≈ 1/√2.

Q45

For a certain magnetic field strength, a free proton spin transition occurs at 700 MHz. Keeping the magnetic field strength constant the ^{14}N nucleus will resonate at (g(p) = 5.6 and g(^{14}N) = 0.4)

A. 700 MHz

B. 400 MHz

C. 200 MHz

D. 50 MHz

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer D 50 MHz

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced $2B$; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- $\nu \propto g_N$ (or γ) at fixed B_0: $\nu(^{14}N) = 700 \times 0.40/5.6 = 50$ MHz.
- Therefore the answer is (D).

FINAL: (D) 50 MHz

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced $4B$ (first Stokes line $6B$ from the exciting line); microwave lines spaced $2B$.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: D

A **700 MHz**

Why (D) is the key — ν ∝ g_N (or γ) at fixed B_0: $\nu(^{14}N) = 700 \times 0.40/5.6 = 50$ MHz.

B **400 MHz**

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

C **200 MHz**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by ≈ $1/\sqrt{2}$.

Q46

A symmetric top molecule, among the following, is

A. Ethylene

B. Allene

C. butatriene

D. Hexatriene

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer B Allene

CONCEPT

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced 2B; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- Allene $H_2C{=}C{=}CH_2$ (D_2d) has an S_4 axis and two equal moments of inertia perpendicular to the C=C=C axis → symmetric top. Ethylene, butatriene and hexatriene are planar asymmetric tops.
- Therefore the answer is (B).

FINAL: (B) Allene

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced 4B (first Stokes line 6B from the exciting line); microwave lines spaced 2B.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \to {}^2D$ shifts $\tilde{\nu}$ by $\approx 1/\sqrt{2}$.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: B

A **Ethylene**

Why (B) is the key — Allene $H_2C=C=CH_2$ (D_2d) has an S_4 axis and two equal moments of inertia perpendicular to the C=C=C axis → symmetric top. Ethylene, butatriene and hexatriene are planar asymmetric tops.

C **butatriene**

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D **Hexatriene**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$by ≈ 1/√2.

Q47

The correct statements about HCl and DCl , among the following is

A. DCl has smaller Zero Point Energy than HCl

B. HCl has smaller vibrational frequency than DCl

C. The force constant k for HCl bond is half that of DCl

D. The reduced mass of DCl is smaller than that of HCl

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer A DCl has smaller Zero Point Energy than HCl

CONCEPT

Rotational (microwave): E_J = BJ(J+1), lines spaced 2B; vibrational (IR): harmonic ν˜= (1/2πc)√(k/μ), anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- Same force constant, larger reduced mass: DCl vibrates more slowly and has the smaller zero-point energy (Â½hÎ½).
- Therefore the answer is (A).

FINAL: (A) DCl has smaller Zero Point Energy than HCl

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced 4B (first Stokes line 6B from the exciting line); microwave lines spaced 2B.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller ν˜; $^{1}H \rightarrow {}^{2}D$ shifts ν˜ by ≈ 1/√2.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: A

B **HCl has smaller vibrational frequency than DCl**

Why (A) is the key — Same force constant, larger reduced mass: DCl vibrates more slowly and has the smaller zero-point energy (Â½hÎ½).

C **The force constant k for HCl bond is half that of DCl**

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D **The reduced mass of DCl is smaller than that of HCl**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^{1}H \rightarrow {}^{2}D$ shifts $\tilde{\nu}$ by ≈ 1/√2.

Q48

The molecule that will not absorb in the microwave region, but will absorb in the infra-red region

A. N_2

B. C_2H_2

C. HCl

D. H_2O

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Molecular Spectroscopy – General

PYQ FREQUENCY
Very High · 15 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
'2B micro, 4B Raman'.

Correct Answer B C_2H_2

CONCEPT

Rotational (microwave): E_J = BJ(J+1), lines spaced 2B; vibrational (IR): harmonic ν̃ = (1/2πc)√(k/μ), anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

↓

LOGIC / WORKING

- C_2H_2 is linear and non-polar (no microwave spectrum) but its asymmetric C–H stretch and bending modes change the dipole → IR-active. N_2 is inactive in both; HCl and H_2O are active in both.
- Therefore the answer is (B).

FINAL: (B) C_2H_2

SHORTCUT / EXAM TRICK

Rotational Raman lines are spaced 4B (first Stokes line 6B from the exciting line); microwave lines spaced 2B.

COMMON MISTAKE

Using atomic masses in g instead of kg (or u → kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

EXAM TIP

Heavier isotope → smaller B and smaller ν̃; $^1H \rightarrow {}^2D$ shifts ν̃ by ≈ 1/√2.

MEMORY TRICK

'2B micro, 4B Raman'.

Why the Other Options Are Wrong

Correct answer: B

A — **N_2**

Why (B) is the key — C_2H_2 is linear and non-polar (no microwave spectrum) but its asymmetric C–H stretch and bending modes change the dipole → IR-active. N_2 is inactive in both; HCl and H_2O are active in both.

C — **HCl**

Ruled out: Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.

D — **H_2O**

Ruled out: Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by ≈ $1/\sqrt{2}$.

TOPIC REVISION

Molecular Spectroscopy – General

31 PYQs · Last-minute revision

TOPIC SUMMARY

Rotational (microwave): $E_J = BJ(J+1)$, lines spaced $2B$; vibrational (IR): harmonic $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$, anharmonic overtones; rotation–vibration P/R branches; Raman (polarisability change, Stokes/anti-Stokes); electronic (Franck–Condon); NMR/ESR basics.

IMPORTANT FORMULA SHEET

- $B = h/(8\pi^2 cI)$; $I = \mu r^2$; $\Delta E = 2B(J+1)$
- $\tilde{\nu} = (1/2\pi c)\sqrt{(k/\mu)}$; $\mu = m_1 m_2/(m_1+m_2)$
- $G(v) = \omega_e(v+½) - \omega_{ex}e(v+½)^2$
- Raman: $\Delta\tilde{\nu} = 4B(J+3/2)$; first line at $6B$
- $J_{max} = \sqrt{(kT/2hcB)} - ½$

FREQUENTLY ASKED CONCEPTS

- Bond length from rotational spacing
- Isotope shifts
- Selection rules per spectroscopy
- Number of normal modes and their activity
- P, Q, R branches

COMMON MISTAKES & QUICK NOTES

Watch out:
Using atomic masses in g instead of kg (or u→kg) in μ; forgetting that homonuclear diatomics have no IR or microwave spectrum but do have Raman.
Heavier isotope → smaller B and smaller $\tilde{\nu}$; $^1H \rightarrow {}^2D$ shifts $\tilde{\nu}$ by ≈ $1/\sqrt{2}$.

MOST-REPEATED PYQs & EXPECTED IN EXAM

PYQs in this topic: Q18 Q19 Q20 Q21 Q22 Q23 Q24 Q25 Q26 Q27 Q28 Q29 Q30 Q31 …

Expect 2 question(s) next session on Molecular Spectroscopy – General.

FOR STUDENTS AND EDUCATORS

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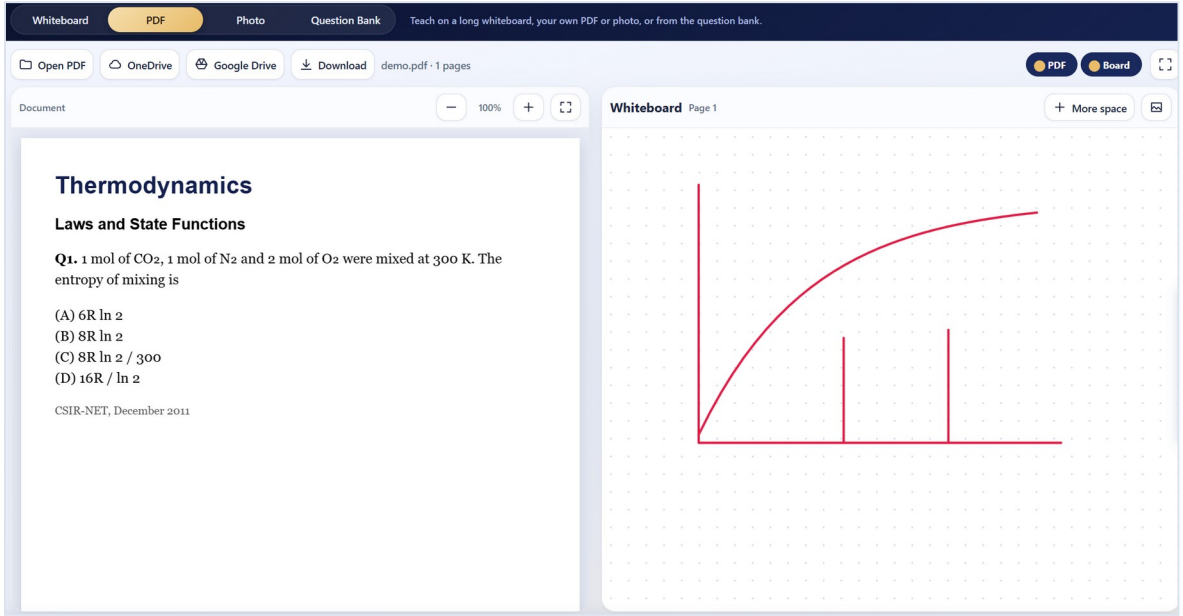
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