Short Test Questions for Physical Chemistry and Structural Chemistry

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Possible Questions for the 1^{st} Test

1. What is the polar form of a complex number? Illustrate it using the concept of the complex plane!
2. Give the exponential form of complex numbers!
3. Define the linear momentum and the angular momentum (classical case)!
4. What is the complex conjugate of $z = a - ib$ and e^{ix} complex numbers?
5. What is kinetic energy and how it relates to linear momentum?
6. What is potential energy for a spring which obeys Hooke's law ($F = -kx$) and how can one calculate it?
7. Give the Taylor expansion for the exponential function!
8. Show that $x(t) = A\sin\omega t$ is a solution for $m\frac{d^2x}{dt^2} = -kx$! What is the connection between ω, k, and m?
9. Give the Bohr condition for the angular momentum (quantization of angular momentum)!
10. Describe the de Broglie postulate! What is the relation between the wavelength and the momentum?
11. What is the energy of a single photon?
12. Give the equation for the centripetal force in uniform circular motion!
13. Give the form of the 1D classical wave equation!
14. What is the solution of the classical wave function?
15. Give the form of the time-dependent Schrödinger equation for a single particle!
16. Write the 1D Schrödinger equation for a free particle!
17. Write the 1D Schrödinger equation for the particle in the 1D box problem!
18. Give the general form of an eigenvalue equation and also give a specific example!
19. Describe the Born/probability interpretation of the wave function!
20. Give the formula for the energy levels for the 1D particle in the box problem!

Possible Questions for the 2^{nd} Test

1. What is the definition of Hermitian operators?
2. What do you know about the eigenvalues of Hermitian operators?
3. What do you know about the eigenfunctions of Hermitian operators?
4. What are the observable values of a physical quantity in quantum mechanics?
5. How can we calculate the average of a measurable physical quantity?
6. What does the uncertainty principle state about Δp_x and Δx?
7. What is the definition of the momentum operator, $\hat{\boldsymbol{p}}$?
8. What is the definition of the position operator, $\hat{\boldsymbol{x}}$?
9. What is the definition of the kinetic energy operator, $\hat{\boldsymbol{K}}$?
10. What is the definition of the total energy operator, $\hat{\boldsymbol{H}}$?
11. What is the commutator of two operators ($\hat{\boldsymbol{A}}$ and $\hat{\boldsymbol{B}}$)?
12. What does degeneracy mean?
13. Write the Schrödinger equation for the harmonic oscillator!
14. Give the formula for the energy levels in the case of the quantum harmonic oscillator!
15. Write the Schrödinger equation for the particle on the ring problem in spherical coordinates!
16. Give the formula for the energy levels for the particle on the ring problem!
17. Give the form of the wavefunctions of the particle on the ring problem!
18. What are the eigenfunctions and the eigenvalues of the $\hat{L}^2$ operator?
19. What are the eigenfunctions and the eigenvalues of the $\hat{L}_z$ operator?
20. What is the commutator of $\hat{L}^2$ and $\hat{L}_z$?
21. What is the commutator of $\hat{L}_x$ and $\hat{L}_y$?
22. Describe the Stern-Gerlach experiment!
23. How can we explain the Stern-Gerlach experiment?
24. What is the connection between the angular momenta and the magnetic moment in quantum mechanics?

Possible Questions for the 3^{rd} Test[1]

Please, introduce the applied notations!

1. What are the fermions and bosons?
2. What does the Pauli exclusion principle say about the wavefunction of a fermionic system?
3. What are the possible values of quantum number j belonging to the total angular momentum ($\hat{J}^2$) for a system with a single electron on a d orbital? Explain your answer!
4. How is the spin-orbit interaction described in the case of the Russel-Saunders coupling? (Give the formula!)
5. What is the jj-coupling and when can it be applied?
6. Give the Hamiltonian operator for He in atomic units!
7. How does the ground state of Li atom look like in the Slater determinant approximation?
8. What do L, $2S+1$, and J denote in a term symbol, ${}^{2S+1}L_J$?
9. What is the concept of shell and subshell for an atom?
10. What are the Hund's rules?
11. Give the energetic order (starting from the lowest one) of the ${}^1S_0$, ${}^3P_2$, ${}^3P_1$, ${}^3P_0$, and ${}^1D_2$ atomic terms of the $2p^4$ configuration?
12. Give the energetic order (starting from the lowest one) of the ${}^1S_0$, ${}^3P_2$, ${}^3P_1$, ${}^3P_0$, and ${}^1D_2$ atomic terms of the $2p^2$ configuration?
13. What is the transition dipole moment? How is it related to the selection rules?
14. What are the selection rules for light atoms?
15. Write the Hamiltonian for a molecule (M atoms and N electrons) in atomic units!
16. What is the physical basis of the Born-Oppenheimer approximation?
17. What does the Born-Oppenheimer approximation say about the interaction between the nuclei?
18. What is the variational principle?
19. Describe the Hartree-Fock approximation! (How does the wavefunction look like? How is the wavefunction optimized?)
20. How does the wave function ansatz of the configuration interaction method look like?

[1]continued on the next page

21. How can we obtain the coefficients of the configuration interaction method?
22. What symmetry operations are generated by a C_3 axis?
23. What operations are generated by an improper S_3 rotation axis?
24. What is the inverse operation for i (inversion)?
25. Give the point groups for H_2O, NH_3, CO, and CO_2 !
26. What are the possible point groups for molecules possessing a dipole moment?

Possible Questions for the 4^{th} Test[2]

Please, introduce the applied notations!

1. Which symmetry operation is missing for a chiral molecule?
2. What do the characters represent in a character table?
3. How can we determine the irreducible representations appear in a reducible representation?
4. Which parts of the electromagnetic spectra are connected to the electronic, vibrational, and rotational transitions?
5. What is the transmittance?
6. What is the absorbance?
7. What is the Beer-Lambert law?
8. Describe the effect of intermolecular interactions to the optical spectra! (brief explanation)
9. Describe the influence of Doppler effect to the optical spectra! (brief explanation)
10. What is the natural line broadening?
11. What is the moment of inertia?
12. In terms of the principal axes how do you define the linear and spherical top molecules?
13. In terms of the principal axes how do you define the prolate and oblate molecules?
14. What are the selection rules for rotational spectroscopy?
15. Describe the quantum numbers of a symmetric top! (physical meaning, possible values)
16. What are the possible energy levels of a symmetric top?
17. Plot a typical rotational spectra! What are on the axes?
18. Why does the application of isotopomers modify the rotational spectra?
19. How does the centrifugal distortion modify the rotational energy levels? (equation)
20. What are the selection rules for the vibrational spectra of a diatomic molecule?
21. How does the Morse potential look like? Briefly compare it with the harmonic oscillator potential!

[2]continued on the next page

22. What is the Birge-Sponer extrapolation? (equation)

23. In rovibrational spectroscopy what are the differences between the P, Q, and R branches considering ΔJ?

24. Plot a typical band of a vibrational spectra (diatomic molecule, gas sample)! What are on the axes?

Possible Questions for the 5^{th} Test [3]

Please, introduce the applied notations!

1. Define the normal modes of a polyatomic molecule!
2. Give the vibrational Hamiltonian in terms of the normal coordinates!
3. Plot a typical band of a vibrational spectra (polyatomic molecule, gas sample)! What are on the axes?
4. How many vibrational frequencies can be found in the IR spectra of folmaldehyde? Explain your answer!
5. Explain why four vibrational frequencies can be seen in the IR spectrum of ammonia!
6. Sketch the components of a Fourier transform spectrometer!
7. Give the mathematical form and plot the HOMO and the LUMO orbitals of the hydrogen molecule in the LCAO approximation!
8. How do the σ and π orbitals look like?
9. The ground state of the electronic wave function of water is a totally symmetric, singlet state, 1^1A_1! The energetic order of the lowest lying excited states are the following: 1^3B_1, 1^1B_1, 1^3A_2, 1^2A_2, 1^3A_1, 2^3B_1, and 2^1A_1. Using the C_{2v} character table and the list above give the allowed radiative transitions from the ground state!
10. Describe the fluorescence using the Jablonski-diagram!
11. What is the difference between the fluorescence and the phosphorescence?
12. What is measured in the ORD spectroscopy?
13. What is measured in the CD spectroscopy?
14. What is the inverse population?
15. What are the possible frequencies of standing waves in an optical resonator?
16. Explain the radiation mechanism of the CO_2 laser!
17. List the possible options for the tuning the frequency of a laser!
18. What is the Rayleigh-, Raman-, Stoks-, and anti-Stoks-scattering?
19. What are the selection rules in the vibrational Raman spectroscopy?
20. Why are lasers applied as light sources in the two-photon spectroscopy?
21. Describe how the Doppler broadening can be eliminated using the two-photon spectroscopy!

[3] continued on the next page

Table 12.2* The C_{2v} character table

C_{2v}, $2mm$	E	C_2	σ_v	σ_v'	$h=4$	
A_1	1	1	1	1	z	z^2, y^2, x^2
A_2	1	1	−1	−1		xy
B_1	1	−1	1	−1	x	zx
B_2	1	−1	−1	1	y	yz