

# Quiz 6

## Chemistry 3BB3; Winter 2005

1. The operator for  $x$ -component of the dipole moment for a  $P$ -atom  $N$ -electron molecule is defined as

$$\hat{\mu}_x =$$

2. Write down Fermi's golden rule for dipole transitions. You can leave out constants of proportionality (just in case you do not know them yet).

3. The sinc function is defined as

- |  |  |  |
|--|--|--|
| (a) $\text{sinc}(x) \equiv x \cdot \sin(x)$      | (e) $\text{sinc}(x) \equiv \sin^2(x) \cos(x)$      | (i) $\text{sinc}(x) \equiv x \arcsin(x)$   |
| (b) $\text{sinc}(x) \equiv \sin(x) e^x$          | (f) $\text{sinc}(x) \equiv x^2 \sin^2(x)$          | (j) $\text{sinc}(x) \equiv x^2 \arcsin(x)$ |
| (c) $\text{sinc}(x) \equiv x^{-1} \cdot \sin(x)$ | (g) $\text{sinc}(x) \equiv \sin^2(x) e^x$          | (k) $\text{sinc}(x) = x (\sin(x))^{-1}$    |
| (d) $\text{sinc}(x) \equiv \sin(x) \cos(x)$      | (h) $\text{sinc}(x) \equiv x^{-1} \cdot \sin^2(x)$ | (l) $\text{sinc}(x) = (x \sin(x))^{-1}$    |

4. What is the relationship between the frequency of absorbed radiation and the difference in energy between the initial and final states?

5. Write down the time-dependent Schrödinger Equation.

6. The long-time approximation led to the conclusion that:

- (a) In the absence of broadening, the absorption spectrum of a molecule is a collection of delta-function peaks.
- (b) Electric quadrupole-allowed and magnetic dipole allowed transitions have low intensity.
- (c) Using time-dependent perturbation theory to model the interaction between light and the molecule is justified.
- (d) Transitions which change the multiplicity of the electronic state (that is, transitions which change the spin of one or more electrons) are forbidden.
- (e) Transitions that correspond to double-excitations in the orbital picture are forbidden in the orbital picture and (usually) low in intensity.

7. You put a molecule in the presence of light. The electric field oscillates in the  $z$ -direction, and the magnetic field oscillates in the  $x$ -direction. Which axis is associated with the direction of propagation of the light?

- (a)  $x$ -axis                      (b)  $y$ -axis                      (c)  $z$ -axis

Name:

8. The momentum of a photon can be expressed in terms of the wave number,  $k$ . What is this relationship?
9. The energy of a photon can be expressed in terms of the wave number,  $k$ . What is this relationship?
10. The period of light can be expressed in terms of its wave number,  $k$ . What is this relationship?

# Quiz 6 (Key)

## Chemistry 3BB3; Winter 2005

1. The operator for  $x$ -component of the dipole moment for a  $P$ -atom  $N$ -electron molecule is defined as

$$\hat{\mu}_x = \sum_{i=1}^N -ex_i + \sum_{\alpha=1}^P Z_{\alpha} e X_{\alpha}$$

2. Write down Fermi's golden rule for dipole transitions. You can leave out constants of proportionality (just in case you do not know them yet).

$$W_{fi} = \frac{2\pi V^2 \left( g(\hbar\omega_{fi}) + g(-\hbar\omega_{fi}) \right)}{\hbar} \left| \langle \Phi_f | \hat{\mu} | \Phi_i \rangle \right|^2$$

3. The sinc function is defined as

- |   |  |  |
|---|--|--|
| (a) $\text{sinc}(x) \equiv x \cdot \sin(x)$             | (e) $\text{sinc}(x) \equiv \sin^2(x) \cos(x)$      | (i) $\text{sinc}(x) \equiv x \arcsin(x)$     |
| (b) $\text{sinc}(x) \equiv \sin(x) e^x$                 | (f) $\text{sinc}(x) \equiv x^2 \sin^2(x)$          | (j) $\text{sinc}(x) \equiv x^2 \arcsin(x)$   |
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| (d) $\text{sinc}(x) \equiv \sin(x) \cos(x)$             | (h) $\text{sinc}(x) \equiv x^{-1} \cdot \sin^2(x)$ | (l) $\text{sinc}(x) \equiv (x \sin(x))^{-1}$ |

4. What is the relationship between the frequency of absorbed radiation and the difference in energy between the initial and final states?

$$\nu_{fi} = \frac{E_f - E_i}{h}$$

5. Write down the time-dependent Schrödinger Equation.

$$\hat{H}\Psi = i\hbar \frac{\partial \Psi}{\partial t}$$

6. The long-time approximation led to the conclusion that:

- (a) In the absence of broadening, the absorption spectrum of a molecule is a collection of delta-function peaks.
- (b) Electric quadrupole-allowed and magnetic dipole allowed transitions have low intensity.
- (c) Using time-dependent perturbation theory to model the interaction between light and the molecule is justified.
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- (a)  $x$ -axis                      (b)  $y$ -axis                      (c)  $z$ -axis

Name:

8. The momentum of a photon can be expressed in terms of the wave number,  $k$ . What is this relationship?

$$p = \hbar k$$

9. The energy of a photon can be expressed in terms of the wave number,  $k$ . What is this relationship?

$$E = \hbar k c$$

10. The period of light can be expressed in terms of its wave number,  $k$ . What is this relationship?

$$T = \frac{2\pi}{kc}$$