

60(3) : Absorption in Atoms and Molecules

This process depends on an interaction Hamiltonian:

$$H = -\underline{\mu} \cdot \underline{E} \quad - (1)$$

where $\underline{\mu}$ is the transition dipole moment and \underline{E} is the electric component of the electromagnetic field. The electric field strength is:

$$\underline{E}^a = -\frac{\partial \underline{A}^a}{\partial t} - \underline{\nabla} \phi^a - c \omega^{a,b} \underline{A}^b + \omega^{a,b} \phi^b \quad - (2)$$

$$\underline{\nabla} \cdot \underline{E}^a = \rho^a / \epsilon_0 \quad - (3)$$

The interaction of the e/m field with the atom or molecule is therefore governed by the resonance equation:

$$-\underline{\nabla} \cdot \frac{\partial \underline{A}^a}{\partial t} - \nabla^2 \phi^a - c \underline{\nabla} \cdot (\omega^{a,b} \underline{A}^b) + \underline{\nabla} \cdot (\omega^{a,b} \phi^b) = \rho^a / \epsilon_0 \quad - (4)$$

The transition dipole moment $\underline{\mu}$ is defined by the charge density ρ^a of an electron in an orbital. For a plane wave in the standard model eqn. (4) reduces to:

$$\nabla^2 \phi^a = -\rho^a / \epsilon_0 \quad - (5)$$

and orbital angular momentum is imparted to the electron from the field (photon). Eq. (5) is a Poisson equation with no resonance.

2) In eq. (4) :

$$\underline{\nabla} \cdot (\underline{\phi}^b \underline{\omega}^a_b) = (\underline{\nabla} \cdot \underline{\omega}^a_b) \underline{\phi}^b + \underline{\omega}^a_b \cdot \underline{\nabla} \underline{\phi}^b \quad - (6)$$

and

$$\underline{\nabla} \cdot (\underline{\omega}^a_b \underline{A}^b) = (\underline{\nabla} \cdot \underline{A}^b) \underline{\omega}^a_b + \underline{A}^b \cdot \underline{\nabla} \underline{\omega}^a_b \quad - (7)$$

If the vector potential is regarded as being a plane wave in the first approximation for $\underline{\omega}^a_b$ is dual to \underline{A}^c , so in this approximation :

$$\underline{\nabla} \cdot \frac{\partial \underline{A}^c}{\partial t} \sim \underline{\nabla} \cdot \underline{A}^b \sim \underline{\nabla} \cdot \underline{\omega}^a_b \sim 0 \quad - (8)$$

and eq. (4) becomes :

$$-\nabla^2 \underline{\phi}^a - c (\underline{\nabla} \underline{\omega}^a_b) \cdot \underline{A}^b + \underline{\omega}^a_b \cdot \underline{\nabla} \underline{\phi}^b = \rho^a / \epsilon \quad - (9)$$

Now assume that $c \underline{A}^b$ is equal to $\underline{\phi}^b$, and that $\underline{\omega}^a_b$ is negative to obtain :

$$\boxed{\nabla^2 \underline{\phi}^a + (\underline{\nabla} \underline{\omega}^a_b) \cdot \underline{\phi}^b + \underline{\omega}^a_b \cdot \underline{\nabla} \underline{\phi}^b = \rho^a / \epsilon} \quad - (10)$$

This is

$$\boxed{\nabla^2 \underline{\phi}^a + g \underline{\phi}^c \cdot \underline{\nabla} \underline{\phi}^b + g \underline{\nabla} \underline{\phi}^c \cdot \underline{\phi}^b = \rho^a / \epsilon} \quad - (11)$$

where g is a constant. Eq. (11) is an wave equation. $- (11)$