

Quantum Chemistry
Levine, 5th Edition

Chapter 1

1. a) The energy of one photon of infrared radiation whose wavelength is 1064 nm is given by:

$$E = h\nu = hc/\lambda = 6.626 \times 10^{-34} \text{ J s} (2.9989 \times 10^8 \text{ m s}^{-1}) / (1064 \text{ nm}) = 1.8669 \times 10^{-19} \text{ J}$$

- b) An Nd:YAG laser emitting a pulse of 1064 nm radiation of average power $5 \times 10^{-6} \text{ W}$ lasting for $2 \times 10^{-6} \text{ s}$ emits $(5 \times 10^{-6} \text{ J s}^{-1})(2 \times 10^{-6} \text{ s})/(1.8669 \times 10^{-19} \text{ J}) = 5.36 \times 10^{17}$ photons.

3. The work function of very pure Na is $\phi = 2.75 \text{ eV}$.

- a) The maximum kinetic energy of photoelectrons emitted from Na exposed to 200 nm UV radiation is given by:

$$E = hc/\lambda = (6.63 \times 10^{-34} \text{ J s})(3 \times 10^8 \text{ m s}^{-1}) / 200 \text{ nm} = 9.945 \times 10^{-19} \text{ J}$$

$$E_{\text{kin, max}} = (9.945 \times 10^{-19} \text{ J})/(1.602 \times 10^{-19} \text{ eV}) - 2.75 \text{ eV} = 3.46 \text{ eV}$$

- b) The longest wave length that will cause the photoelectric effect in pure Na is given by:

$$\lambda = hc/(2.75 \text{ eV} \times 1.602 \times 10^{-19} \text{ J/eV}) = 4.5 \times 10^{-7} = 451 \text{ nm}$$

- c) The work function of impure Na is substantially less than 2.75 eV, and when this is exposed to the same 200 nm radiation the maximum photoelectron kinetic energy will be greater than that for pure Na.

6. For a one particle, one dimensional, system with $\psi = a \exp(-ibt) \exp(-bmx^2/\hbar)$ where a and b are constants, and m is the particle's mass, the potential energy function V can be found by using the time-dependent Schrödinger equation:

$$-\frac{\hbar}{i} \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x,t) \psi(x,t)$$

Substituting the wave function and its partial derivatives gives:

$$-\frac{\hbar}{i} a \exp(-ibt) \exp(-bmx^2/\hbar)(-ib) = -\frac{\hbar^2}{2m} [a \exp(-ibt)][\exp(-bmx^2/\hbar)][\frac{-2bm}{\hbar} + \frac{4b^2m^2x^2}{\hbar^2}] + V a \exp(-ibt) \exp(-bmx^2/\hbar)$$

Cancel $[a \exp(-ibt) \exp(-bmx^2/\hbar)]$ from each term: $-\frac{\hbar}{i}(-ib) = -\frac{\hbar^2}{2m} [\frac{-2bm}{\hbar} + \frac{4b^2m^2x^2}{\hbar^2}] + V$

Finally $V = 2mb^2x^2$.

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