Basic Physical Chemistry I

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Q21
Calculate the wave number (cm^{-1}) of 1 eV photons. Further, estimate the energy in unit of eV for 500 nm wave length.

Q22
Estimate the Coulomb repulsion energy in unit of eV when two electrons are located with the distance of 1, 2, and 3 Å cases. Use the values of e=1.6×10^{-19} C and ϵ=8.85×10^{-12} F.

Q23
Prepare the d^6 Tanabe-Sugano (TS) diagram.

1. The line around Δ/B∼20 means the change of lowest term. Answer the lowest term for Δ/B is larger and smaller cases.
2. When Δ/B =30, the energy term symbols are plotted from the low energies: $^1A_{1g}$ (ground state), $^3T_{1g}$, $^5T_{2g}$, $^3T_{2g}$, $^1T_{1g}$, and $^1T_{2g}$. By using the TS diagram, estimate the energy difference between $^1A_{1g}$ and other excited states. Assuming $B = 1 \times 10^3$ cm^{-1}, answer in the units of wave number cm^{-1}.
3. In the five cases discussed in above Q.23-2, only $^5T_{2g}$ case shows twice larger slope than other cases. From the viewpoint of electron configuration, explain the reason.

Q24
For O_h symmetry, confirm the following direct product relation using character table.

$$T_2 \times T_2 = A_1 + E + T_1 + T_2$$

Q25
For O_h symmetry, explain the following energy term splitting of free ion G states using character table.

$$G \rightarrow A_1 + E + T_1 + T_2$$

Q26
Summarize the principle of synchrotron-radiation beam generation.

Q27
Prove the Fermi's golden rule.

Q28
Summarize the principle of photoemission spectroscopy.

Q29
Explain the origin of chemical shift in XPS.

Q30
Draw the C 1s XPS line shapes in CH_3COOCH_3 and CH_3-CHCl-CHI-CH_2-CH_3.

Q31
Absorption spectra of $[Cr(H_2O)_6]^{n+}$ ions are shown in Figure. Determine crystal field splitting Δ and Coulomb interaction energy B by using Tanabe-Sugano diagram for d^3.

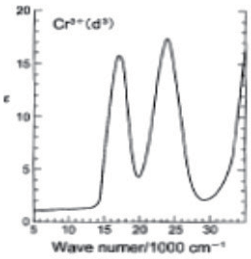

Fig: Electron absorption spectroscopy of Cr complexes.

Q32
Explain the reason why Coulomb potential in O_h symmetry is written as follows. Here, $A = \frac{6Ze^2}{a}$ and $D = \frac{35Ze^2}{4a^5}$ are defined using the distance a, electron number in center ions Z, and electron charge e.

$$U = A + D\left(x^4 + y^4 + z^4 - \frac{3}{5}r^4\right)$$

(Summation of symmetric six kinds of sites and spherical harmonic functions are necessary for the calculation.)