

# Problems

1. For a  $d^7$  metal ion determine the energy ratios for allowed transitions at  $\Delta_{\text{oct}}/B$  of 20.
2. For a  $d^6$  metal ion of  $\Delta_{\text{oct}}/B = 30$  and  $B=530 \text{ cm}^{-1}$  what would the energies of the 5 allowed transitions be? How many are in the UV-Vis range? How many are in the IR range?
3. Write out the allowed transitions for a  $d^5$  metal ion in a  $E/B > 28$  ligand field.
4. A  $d^4$  complex exhibits absorptions at  $5500 \text{ cm}^{-1}$  (strong) and  $31350 \text{ cm}^{-1}$  (weak). What are the transitions that are being exhibited in the complex? What is the corresponding  $\Delta_{\text{oct}}$  for the complex?
5. A spectrum of  $d^7$  metal complex seemingly exhibits only two intense transitions. What is the  $\Delta_{\text{oct}}/B$  that this situation occurs? Please use reference to specific transitions and energy splitting.

# Answers



1.  $\Delta_{\text{oct}}/B$  of 20 yields  $E/B$  values of 38, 32, 18. Ratios then are 2.11 and 1.78
2.  $\Delta_{\text{oct}}/B = 30$  yields  $E/B$  heights of 27, 40, 57, 65, 85. Energies are then 14310, 21200, 30210, 34450 and 45050  $\text{cm}^{-1}$ . All are in the UV-Vis range. \*note you need to infer the  $E/B$  value for the last transition as the diagram does not extend that far up.
3.  ${}^2A_{2g} < {}^2T_{2g}$ ,  ${}^2T_{1g} < {}^2T_{2g}$ ,  ${}^2E_g < {}^2T_{2g}$ , and  ${}^2A_{1g} < {}^2T_{2g}$ .
4.  $31,350/5,500$  gives a ratio of 5.7/1. The only  $\Delta_{\text{oct}}/B$  value that matches is at 10.  $B$  value is then  $550 \text{ cm}^{-1}$ .  $\Delta_{\text{oct}}$  equals  $5500 \text{ cm}^{-1}$ .
5. Three transitions are generated at low  $\Delta_{\text{oct}}/B$ . However, at about a value of  $\Delta_{\text{oct}}/B = 13$  the transitions  ${}^4A_{2g} < {}^4T_{1g}$ , and  ${}^4T_{1g} < {}^4T_{1g}$  have the same energies which results in the appearance of only two absorptions.