1) **For a d^2 complex three spin allowed ligand field excitations were located at:**
ν_1 = 17500 cm^{-1} ν_2 = 26000 cm^{-1} ν_3 = 35890 cm^{-1}
Interpret these bands and calculate the Dq, Q, ans B parameters
Knowing that $B_{free\ ion}$ for M^{3+} is equal to 862 cm^{-1}, evaluate the β?

Energy of ν_1 = 8Dq + Q
Energy of ν_2 = 18Dq + Q
Energy of ν_3 = 6Dq + 15B + 2Q

$^4T_{2g} \leftarrow {}^4T_{1g}$ 8Dq + Q
$E\nu_1$= 18Dq + Q = **17500** cm^{-1}
$^4A_{2g} \leftarrow {}^4T_{1g}$ 18Dq + Q
$E\nu_2$= 18Dq + Q = **26000** cm^{-1}

$E\nu_2 - E\nu_1$ = 18Dq + Q – (8Dq + Q) = 10Dq
26000 – 17500 = 10Dq
Dq = 850 cm^{-1}
$E\nu_1$= 8(850) + Q = **17500** cm^{-1}
Q= 10700 cm^{-1}
$^4T_{1g}(^4P) \leftarrow {}^4T_{1g}$ 6Dq + 15B + Q
$E\nu_3$= 6Dq + 15B + 2Q = **35890** cm^{-1}, **B= 626 cm^{-1}**

$$\beta = \frac{\beta_{Complex}}{\beta_{Free\ ion}} = \frac{626}{862} = 0.726\ cm^{-1}$$

2) **For a d^3 complex three spin allowed ligand field excitations were located at:**
ν_1 = 15300 cm^{-1} ν_2 = 23500 cm^{-1} ν_3 = 34790 cm^{-1}
Interpret these bands and calculate the Dq, Q, ans B parameters
Knowing that $B_{free\ ion}$ for M^{3+} is equal to 918 cm^{-1}, evaluate the β?

Energy of ν_1 = 10Dq
Energy of ν_2 = 18Dq - Q
Energy of ν_3 = = 12Dq + 15B + Q

$^4T_{2g} \leftarrow {}^4A_{2g}$ 10 Dq
$E\nu_1$= 10Dq= 15300 cm^{-1}, **Dq = 1530 cm^{-1}**

$^4T_{1g} \leftarrow {}^4A_{2g}$ 18Dq – Q
$E\nu_2$= 18Dq – Q= 23500 cm^{-1}, **Q= 4040 cm^{-1}**

$^4T_{1g} \leftarrow {}^4A_{2g}$ 15B + 12Dq + Q
$E\nu_3$= 15B + 12Dq + Q= 34790 cm^{-1}, **B= 826 cm^{-1}**

$$\beta = \frac{\beta_{Complex}}{\beta_{Free\ ion}} = \frac{826}{918} = 0.9\ cm^{-1}$$