

# Tanabe-Sugano Diagrams

This document contains expressions for Coulomb repulsion matrices (with the corresponding crystal-field energies added to the diagonal) and representative energy diagrams for the energy levels of transition metal ions with  $d^n$  configurations as split by a crystal field with cubic symmetry of varying intensity  $Dq$ . These diagrams only depend on the ratio  $C/B$  of Racah parameters, with the energy scale taken as the magnitude of the Racah  $B$  parameter.

In all of these diagrams the energy levels are always referenced against the ground state. In each figure the data in red on the leftmost margin corresponds to experimental energy values of the correlate free-ion. The left vertical axis shows the energy scaled by the Racah  $B$  parameter, and the right vertical axis shows the corresponding energy in  $eV$ . In the horizontal axis the strength of the crystal field  $Dq$  is scaled by  $B$ .

In these calculations no configuration mixing is considered, and both spin-orbit and effective operators (such as the Trees operator) are neglected.

The range of values chosen in the horizontal axis are so that the magnitude of the Coulomb repulsion is comparable to the intensity of the crystal-field. When the strength of the crystal-field becomes increasingly larger, the more each branch of the energy spectrum turns into a linear function of  $Dq/B$ .

Each of the branches in the energy spectra is labeled according to the irreducible representations of the cubic group.

In the figures shown below the title shows the parameters used for an example ion for the corresponding configuration. These diagrams resemble the diagrams and use the data provided in the book “Multiplets of Transition-Metal Ions in Crystals” by Sugano, Tanabe, and Kamimura. The group-theory data used in these calculations is the one provided in this same book.

Data used for creating this figures can be found in the binary file `./calculations/all_terms.pkl`, and the script `./tsk_diagrams.py` can be used to generate them.

The  $d^1$  and  $d^9$  configurations are omitted since they are trivial.

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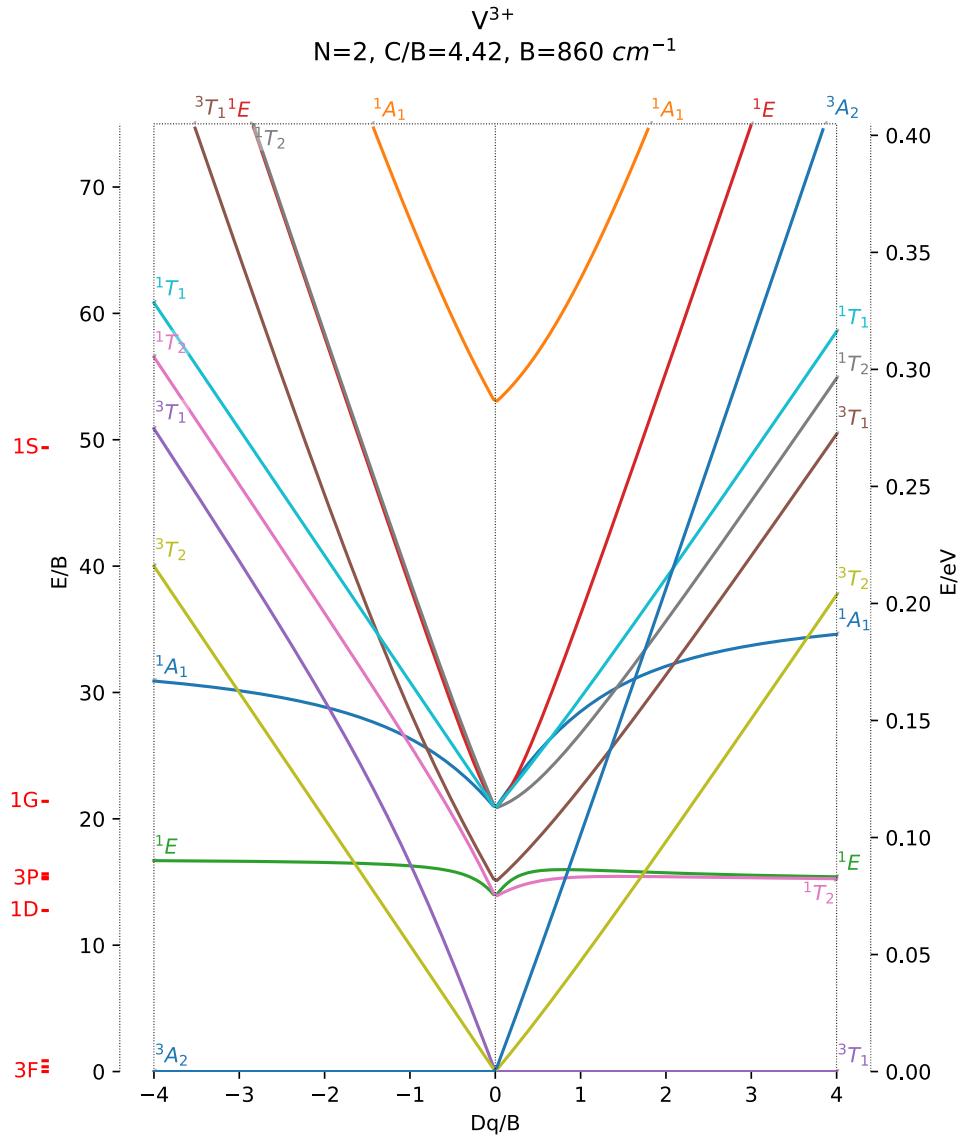
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**1**     $d^2$



$$^1A_1(^1G, ^1S)$$

$$\begin{bmatrix} t_2^2 & e^2 \\ \frac{10B+5C}{2\sqrt{6}B+\sqrt{6}C}-8Dq & \frac{2\sqrt{6}B+\sqrt{6}C}{8B+4C+12Dq} \end{bmatrix} \quad (1)$$

$$^1E(^1D, ^1G)$$

$$\begin{bmatrix} t_2^2 & -2\sqrt{3}B \\ B+2C-8Dq & \frac{-2\sqrt{3}B}{2C+12Dq} \end{bmatrix} \quad (2)$$

$$^3T_1(^3F, ^3P)$$

$$\begin{bmatrix} t_2^2 & t_2e \\ -5B-\frac{8Dq}{6B} & \frac{-6B}{4B+2Dq} \end{bmatrix} \quad (3)$$

$$^1T_2(^1D, ^1G)$$

$$\begin{bmatrix} t_2^2 & t_2e \\ B+\frac{t_2^2}{2C}-8Dq & \frac{2\sqrt{3}B}{2C+2Dq} \end{bmatrix} \quad (4)$$

$$^3T_2(^3F)$$

$$\begin{bmatrix} t_2e & \\ -8B+2Dq & \end{bmatrix} \quad (5)$$

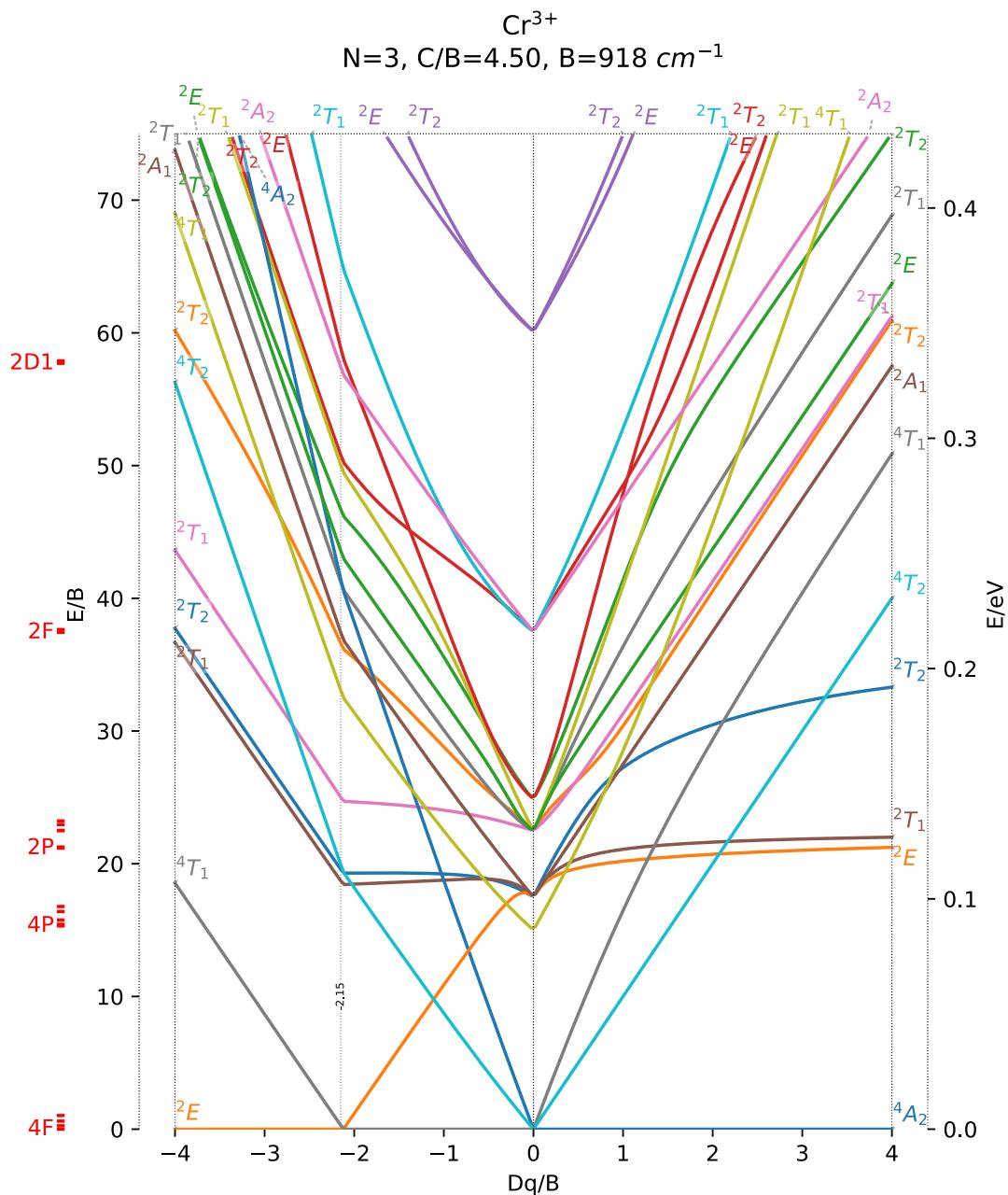
$$^1T_1(^1G)$$

$$\begin{bmatrix} t_2e & \\ 4B+\frac{t_2e}{2C}+2Dq & \end{bmatrix} \quad (6)$$

$$^3A_2(^3F)$$

$$\begin{bmatrix} e^2 & \\ -8B+12Dq & \end{bmatrix} \quad (7)$$

2  $d^3$



$$^2T_2(^2D, ^2D, ^2F, ^2G, ^2H)$$

$$\begin{bmatrix} t_2^3 & t_2^2(^3T_1)e & t_2^2(^1T_2)e & t_2e^2(^1A_1) & t_2e^2(^1E) \\ 5C - \frac{12}{12Dq} & 3\sqrt{3}B & -5\sqrt{3}B & 4B + 2C & 2B \\ 3\sqrt{3}B & -6B + 3C - 2Dq & -3B & 3\sqrt{3}B & 3\sqrt{3}B \\ -5\sqrt{3}B & -3B & 4B + 3C - 2Dq & -\sqrt{3}B & \sqrt{3}B \\ 4B + 2C & 3\sqrt{3}B & -\sqrt{3}B & 6B + 5C + 8Dq & 10B \\ 2B & 3\sqrt{3}B & \sqrt{3}B & 10B & -2B + 3C + 8Dq \end{bmatrix} \quad (8)$$

$$^2T_1(^2F, ^2G, ^2H, ^2P)$$

$$\begin{bmatrix} t_2^3 & t_2^2(^3T_1)e & t_2^2(^1T_2)e & t_2e^2(^1E) & t_2e^2(^3A_2) \\ -6B + 3C - 12Dq & 3B & 3B & -2\sqrt{3}B & 0 \\ 3B & 3C - 2Dq & 3B & -3\sqrt{3}B & 3B \\ 3B & 3B & -6B + 3C - 2Dq & -\sqrt{3}B & 3B \\ -2\sqrt{3}B & -3\sqrt{3}B & -\sqrt{3}B & -2B + 3C + 8Dq & -2\sqrt{3}B \\ 0 & 3B & 3B & -2\sqrt{3}B & -6B + 3C + 8Dq \end{bmatrix} \quad (9)$$

$$^4A_2(^4F)$$

$$\begin{bmatrix} t_2^3 \\ -15B & t_2^3 \\ 12Dq \end{bmatrix} \quad (10)$$

$$^2E(^2D, ^2D, ^2G, ^2H)$$

$$\begin{bmatrix} t_2^3 & t_2^2(^1A_1)e & t_2^2(^1E)e & e^3 \\ -6B + 3C - 12Dq & -6\sqrt{2}B & -3\sqrt{2}B & 0 \\ -6\sqrt{2}B & 8B + 6C - 2Dq & 10B & 2\sqrt{3}B + \sqrt{3}C \\ -3\sqrt{2}B & 10B & -B + 3C - 2Dq & 2\sqrt{3}B \\ 0 & 2\sqrt{3}B + \sqrt{3}C & 2\sqrt{3}B & -8B + 4C + 18Dq \end{bmatrix} \quad (11)$$

$$^2A_1(^2G)$$

$$\begin{bmatrix} t_2^2(^1E)e \\ -11B + 3C - 2Dq \end{bmatrix} \quad (12)$$

$$^2A_2(^2F)$$

$$\begin{bmatrix} t_2^2(^1E)e \\ 9B + 3C - 2Dq \end{bmatrix} \quad (13)$$

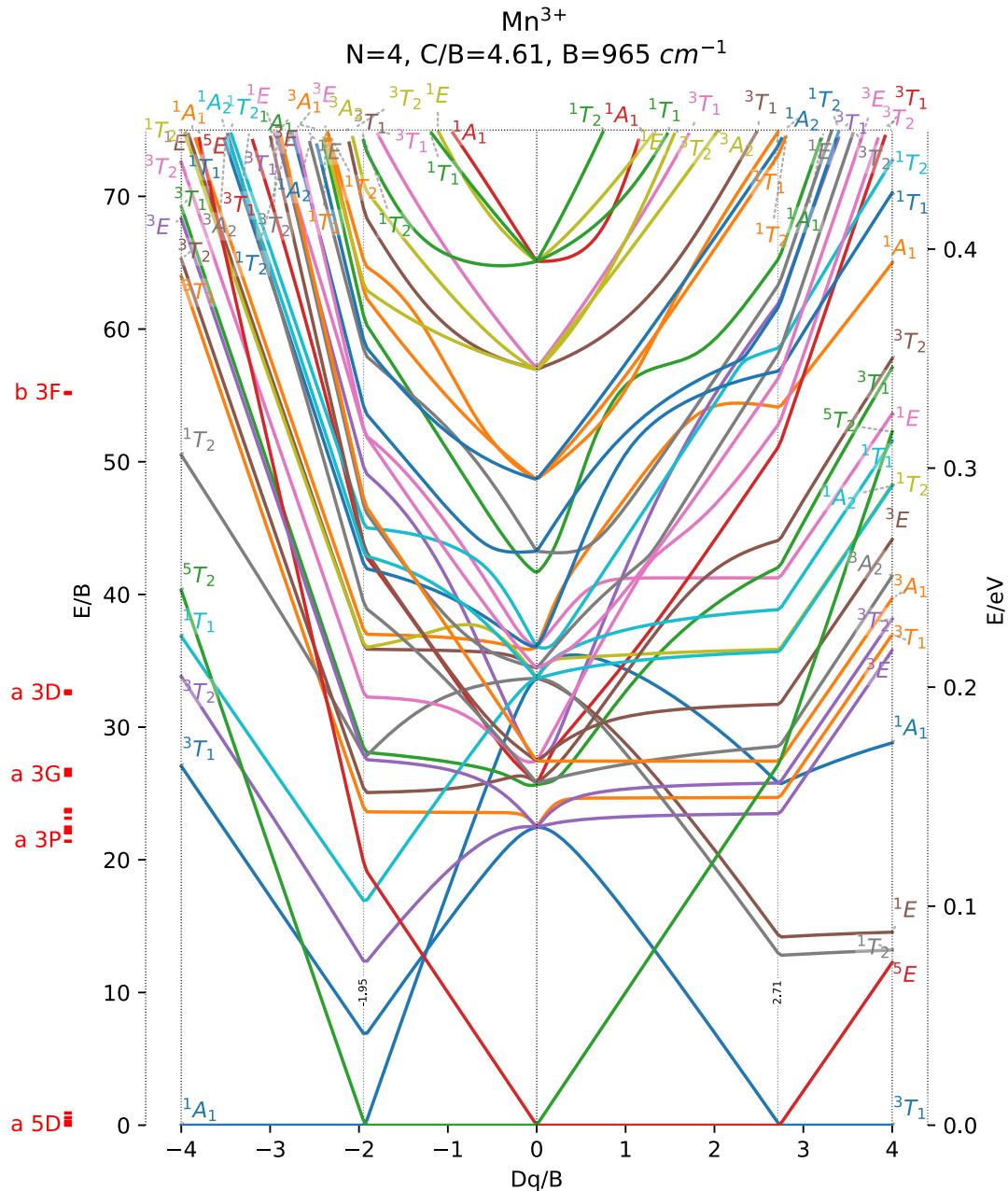
$$^4T_1(^4F, ^4P)$$

$$\begin{bmatrix} t_2^2(^3T_1)e & t_2e^2(^3A_2) \\ -\frac{3}{2}B - 2Dq & 6B \\ 6B & -12B + 8Dq \end{bmatrix} \quad (14)$$

$$^4T_2(^4F)$$

$$\begin{bmatrix} t_2^2(^3T_1)e \\ -\frac{15}{2}B - 2Dq \end{bmatrix} \quad (15)$$

3  $d^4$



$$^1A_1(^1G, ^1G, ^1I, ^1S, ^1S)$$

$$\begin{bmatrix} t_2^4 & t_2^3(2E)e & t_2^2(1A_1)e^2(1A_1) & t_2^2(1E)e^2(1E) & e^4 \\ -12\sqrt{2}B & 6C-6Dq & 4\sqrt{2}B+2\sqrt{2}C & 2\sqrt{2}B & 0 \\ -12\sqrt{2}B & -12B & 14B+11C+4Dq & -6B & 2\sqrt{6}B+\sqrt{6}C \\ 4\sqrt{2}B+2\sqrt{2}C & -6B & 20B & -3B+6C+4Dq & 2\sqrt{6}B \\ 2\sqrt{2}B & 0 & 2\sqrt{6}B+\sqrt{6}C & 2\sqrt{6}B & -16B+8C+24Dq \end{bmatrix} \quad (16)$$

$$^1E(^1D, ^1D, ^1G, ^1G, ^1I)$$

$$\begin{bmatrix} -9B+7C-16Dq & t_2^3(2E)e & t_2^2(1E)e^2(1A_1) & t_2^2(1A_1)e^2(1E) & t_2^2(1E)e^2(1E) \\ 6B & -6B+6C-6Dq & 2\sqrt{2}B+\sqrt{2}C & -2B & -4B \\ 2\sqrt{2}B+\sqrt{2}C & -3\sqrt{2}B & 5B+8C+4Dq & -12B & 0 \\ -2B & -12B & 10\sqrt{2}B & 6B+9C+4Dq & -10\sqrt{2}B \\ 0 & 0 & -10\sqrt{2}B & 0 & -3B+6C+4Dq \end{bmatrix} \quad (17)$$

$$3T_1(^3F, ^3F, ^3G, ^3H, ^3P, ^3P)$$

$$\begin{bmatrix} -15B+5C-16Dq & t_2^3(2T_2)e & t_2^2(^3T_1)e^2(^1A_1) & t_2^2(^3T_1)e^2(^1E) & t_2^2(^1T_2)e^2(^3A_2) \\ 3\sqrt{2}B & -3B+6C-6Dq & 5\sqrt{3}B & -2\sqrt{2}B+\sqrt{2}C & 0 \\ \sqrt{6}B & 5\sqrt{3}B & -11B-\sqrt{3}B & 3B & -5\sqrt{3}B \\ 2\sqrt{2}B+\sqrt{2}C & -2\sqrt{2}B & -B+6C-6Dq & -\sqrt{3}B & -3B \\ -2\sqrt{2}B & 0 & -10B & -9B+10B & 0 \\ 0 & 0 & 0 & -9B+2\sqrt{3}B+4Dq & -2\sqrt{3}B \\ 0 & \sqrt{2}B+\sqrt{2}C & \sqrt{6}B & -3\sqrt{2}B & 3\sqrt{2}B \end{bmatrix} \quad (18)$$

$$^1T_2(^1D, ^1D, ^1F, ^1G, ^1G, ^1I)$$

$$\begin{bmatrix} -9B+7C-16Dq & t_2^3(2T_2)e & t_2^3(^2T_1)e & t_2^2(^1T_2)e^2(^1A_1) & t_2^2(^1T_2)e^2(^1E) & t_2(^3T_1)e^2(^3A_2) & t_2e^{3(2E)} \\ 3\sqrt{2}B & 3B+8C-6Dq & -5\sqrt{3}B & 2\sqrt{2}B+\sqrt{2}C & -2\sqrt{2}B & 0 & 0 \\ 3\sqrt{6}B & -5\sqrt{3}B & -9B+6C-6Dq & -5\sqrt{3}B & -5\sqrt{3}B & -5\sqrt{3}B & \sqrt{2}B+\sqrt{2}C \\ 2\sqrt{2}B+\sqrt{2}C & -2\sqrt{2}B & -3B & -5\sqrt{3}B & -3B & 0 & -3\sqrt{6}B \\ -2\sqrt{2}B & 0 & 3\sqrt{3}B & 3B & 0 & 0 & \sqrt{6}B \\ 0 & 3\sqrt{2}B+\sqrt{2}C & -\sqrt{6}B & \sqrt{6}B & -6B & -9B+6C+4Dq & -3\sqrt{6}B \\ 0 & \sqrt{2}B+\sqrt{2}C & 3\sqrt{2}B & -3\sqrt{2}B & \sqrt{6}B & -11B+4C+4Dq & -16B+5C+14Dq \end{bmatrix} \quad (19)$$

$$3T_2(^3D, ^3F, ^3F, ^3G, ^3H)$$

$$\begin{bmatrix} -5B+6C-6Dq & t_2^3(2T_2)e & t_2^3(^2T_1)e & t_2^2(^3T_1)e^2(^1E) & t_2^2(^3T_1)e^2(^3A_2) & t_2(^3T_1)e^2(^3A_2) & t_2e^{3(2E)} \\ -5\sqrt{2}B & -9B+4C-6Dq & -9B+4C-6Dq & -3B & -3\sqrt{2}B & 0 & 0 \\ -5\sqrt{6}B & -3B & -\sqrt{3}B & -\sqrt{3}B & \sqrt{6}B & -3B & \sqrt{6}B \\ 3\sqrt{2}B & -3\sqrt{2}B & -3B & -5\sqrt{3}B & -3B & 0 & -3\sqrt{6}B \\ 2\sqrt{2}B+\sqrt{2}C & -2\sqrt{2}B & 0 & -10B & -13B+4C+4Dq & -13B+4C+4Dq & -8B+5C+14Dq \\ -2\sqrt{2}B & 0 & 0 & -9B+6C+4Dq & -9B+6C+4Dq & -9B+6C+4Dq & -8B+5C+14Dq \end{bmatrix} \quad (20)$$

$$^1T_1(^1F, ^1G, ^1G, ^1I)$$

$$\begin{bmatrix} -3B+8C-6Dq & t_2^3(2T_2)e & t_2^3(^2T_1)e & t_2^2(^3T_1)e^2(^1E) & t_2e^{3(2E)} \\ 5\sqrt{3}B & -3B+6C-6Dq & 3B & -5\sqrt{3}B & 3\sqrt{2}B+\sqrt{2}C \\ 5\sqrt{3}B & -3B & -3B & 3B & -3\sqrt{2}B \\ -5\sqrt{3}B & \sqrt{6}B & -3\sqrt{2}B & -6B & -6B \\ \sqrt{2}B+\sqrt{2}C & 0 & \sqrt{6}B & -\sqrt{6}B & -16B+7C+14Dq \end{bmatrix} \quad (21)$$

$$5E(^5D)$$

$$\begin{bmatrix} t_2^3(^4A_2)e & t_2^3(^4A_2)e & t_2^3(^4A_2)e \\ -2\sqrt{1}B-6Dq & -2\sqrt{1}B-6Dq & -2\sqrt{1}B-6Dq \end{bmatrix} \quad (22)$$

$$^3E(^3D, ^3G, ^3H)$$

$$\begin{bmatrix} t_2^3(2E)e & t_2^3(A_2)e \\ -10B + \frac{4C}{3\sqrt{2B}} - 6Dq & -13B + 4C - 6Dq \\ 4B & 0 \\ 3\sqrt{2B} & -11B + 4C + 4Dq \end{bmatrix} \quad (23)$$

$$^3A_2(^3F, ^3F)$$

$$\begin{bmatrix} t_2^3(2E)e & t_2^2(^1A_1)e^2(^3A_2) \\ -8B + \frac{4C}{12B} - 6Dq & -2B + 7C + 4Dq \\ -12B & -12B \\ -12B + 6C - 6Dq & -3B + 6C + 4Dq \end{bmatrix} \quad (24)$$

$$^1A_2(^1F, ^1I)$$

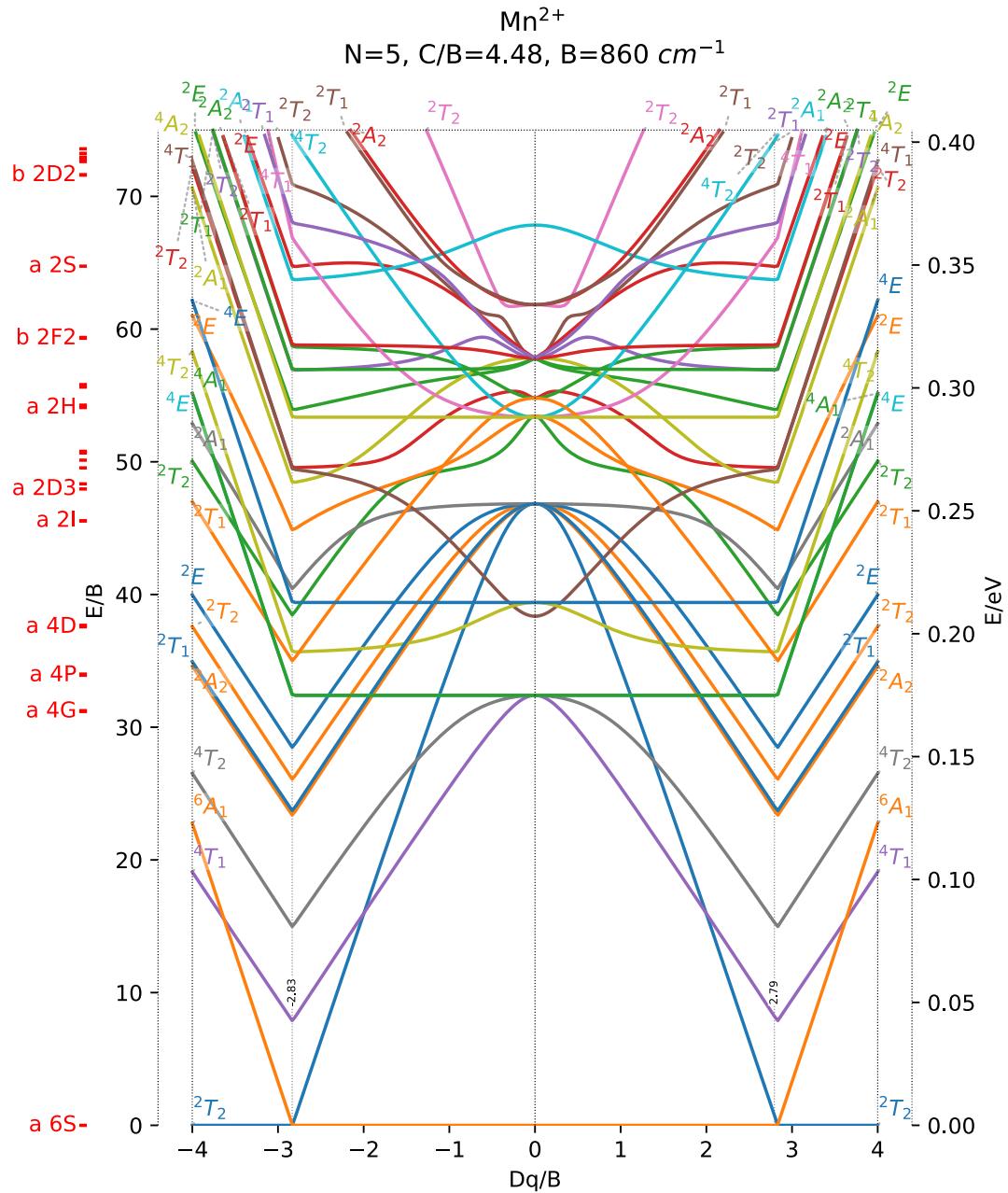
$$\begin{bmatrix} t_2^3(2E)e & t_2^2(^1E)e^2(^1E) \\ -12B + 6C - 6Dq & -3B + 6B \\ 6B & -3B + 6C + 4Dq \end{bmatrix} \quad (25)$$

$$^3A_1(^3G)$$

$$\begin{bmatrix} t_2^3(2E)e & t_2^2(^1E)e^2(^1E) \\ -12B + 4C - 6Dq & -3B + 6B \\ -12B + 4C - 6Dq & -21B + 4Dq \end{bmatrix} \quad (26)$$

$$^5T_2(^5D)$$

$$\begin{bmatrix} t_2^2(^3T_1)e^2(^3A_2) \\ -21B + 4Dq \end{bmatrix} \quad (27)$$



$$^2T_2(^2D, ^2D, ^2D, ^2F, ^2F, ^2G, ^2G, ^2H, ^2I)$$

$$\left[ \begin{array}{cccccc} t_2^5 & t_2^4(^3T_1)e & t_2^3(^2T_2)e & t_2^3(^2T_2)e^2(^1A_1) & t_2^3(^2T_2)e^2(^1E) & t_2^3(^2T_1)e^2(^1E) & t_2^2(^3T_1)e^3(^2E) \\ -20B + 10C - 20Dq & -8B + 9C - 10Dq & t_2^4(^1A_1)e & 4B + 2C & -2\sqrt{3}B & 0 & t_2^2(^1T_2)e^3(^2E) \\ -3\sqrt{6}B & \sqrt{6}B & -3B & -3\sqrt{6}B & \frac{5\sqrt{6}B}{2} & \frac{\sqrt{6}B}{2} & 0 \\ \sqrt{6}B & -3B & -18B + 9C - 10Dq & 2B + 12C' & -3\sqrt{6}B & -3\sqrt{6}B & 0 \\ 4B + 2C & -3\sqrt{6}B & \frac{5\sqrt{6}B}{2} & 0 & 0 & 0 & 4B + 2C \\ 2B & -3\sqrt{6}B & -\frac{5\sqrt{6}B}{2} & -10\sqrt{3}B & -10\sqrt{3}B & 0 & C \\ -2\sqrt{3}B & 3\sqrt{2}B & -\frac{3\sqrt{2}B}{2} & 0 & 0 & -\frac{3\sqrt{6}B}{2} & -\frac{5\sqrt{6}B}{2} \\ 0 & \frac{\sqrt{6}B}{2} & -\frac{3\sqrt{6}B}{2} & -12B + 10C' & 0 & 0 & -2B \\ 0 & 0 & 0 & -12B + 8C' & -12B + 8C' & -2\sqrt{3}B & -2\sqrt{3}B \\ 4B + C & C & 0 & 0 & -2\sqrt{3}B & -16B + 8C' & 0 \\ 0 & 0 & 0 & -2\sqrt{3}B & -3\sqrt{6}B & -8B + 9C + 10Dq & 3\sqrt{6}B \\ 0 & 0 & 0 & -2\sqrt{3}B & -3\sqrt{6}B & -3B & -\sqrt{6}B \\ 0 & 0 & 0 & -2\sqrt{3}B & 0 & -18B + 9C + 10Dq & -20B + 10C + 20Dq \end{array} \right] \quad (28)$$

$$\left[ \begin{array}{cccccc} t_2^4(^1A_1)e & t_2^4(^1A_1)e & t_2^3(^2E)e^2(^1A_1) & t_2^3(^2E)e^2(^1E) & t_2^3(^2E)e^2(^3A_2) & t_2^2(^1A_1)e^3(^2E) & t_2^2(^1E)e^3(^2E) \\ -4B + 12C - 10Dq & 10B & -13B + 9C - 10Dq & -4B + 10C & 6B & 4B + 2C & -2B \\ 6B & 6\sqrt{2}B & -3B & 0 & 0 & 2B & 2B \\ -6\sqrt{3}B & -6\sqrt{3}B & 0 & -12B + 8C' & -12B + 8C' & -6B & +C \\ 4B + 2C & -2B & 2B & -6B & -6\sqrt{3}B & 6\sqrt{2}B & -3B \\ -2B & 0 & 2B + C & -3B & 0 & 0 & 0 \end{array} \right] \quad (29)$$

$$2E(^2D, ^2D, ^2D, ^2G, ^2H, ^2I)$$

$$\left[ \begin{array}{cccccc} t_2^4(^1A_1)e & t_2^4(^1A_1)e & t_2^3(^2E)e^2(^1A_1) & t_2^3(^2E)e^2(^1E) & t_2^3(^2E)e^2(^3A_2) & t_2^2(^1A_1)e^3(^2E) & t_2^2(^1E)e^3(^2E) \\ -3B + 9C - 10Dq & -3\sqrt{2}B & -12B + 8C' & -12B + 8C' & -6\sqrt{3}B & 4B + 2C & -2B \\ 0 & 0 & -4\sqrt{3}B & -12B + 8C' & -12B + 8C' & 2B & +C \\ 6B + C & 3\sqrt{2}B & -3\sqrt{2}B & -19B + 8C & -19B + 8C & -6B & -3B \\ 0 & 0 & 0 & 0 & 3\sqrt{3}B & 3\sqrt{2}B & 0 \end{array} \right] \quad (30)$$

$$2A_1(^2G, ^2G, ^2I, ^2S)$$

$$\left[ \begin{array}{cccccc} t_2^4(^1E)e & t_2^3(^2E)e^2(^1E) & t_2^3(^4A_2)e^2(^3A_2) & t_2^2(^1E)e^3(^2E) & t_2^2(^1E)e^3(^2E) & t_2^2(^1A_1)e^3(^2E) & t_2^2(^1E)e^3(^2E) \\ -3B + 9C - 10Dq & -3\sqrt{2}B & -12B + 8C' & -4\sqrt{3}B & -4\sqrt{3}B & 6B + C & -2B \\ 0 & 0 & -4\sqrt{3}B & -19B + 8C & -19B + 8C & 2B & +C \\ 6B + C & 3\sqrt{2}B & 0 & 0 & 0 & -6B & -3B \\ 0 & 0 & 0 & 0 & -10B & -10B & 0 \end{array} \right] \quad (31)$$

$$2A_2(^2F, ^2F, ^2I)$$

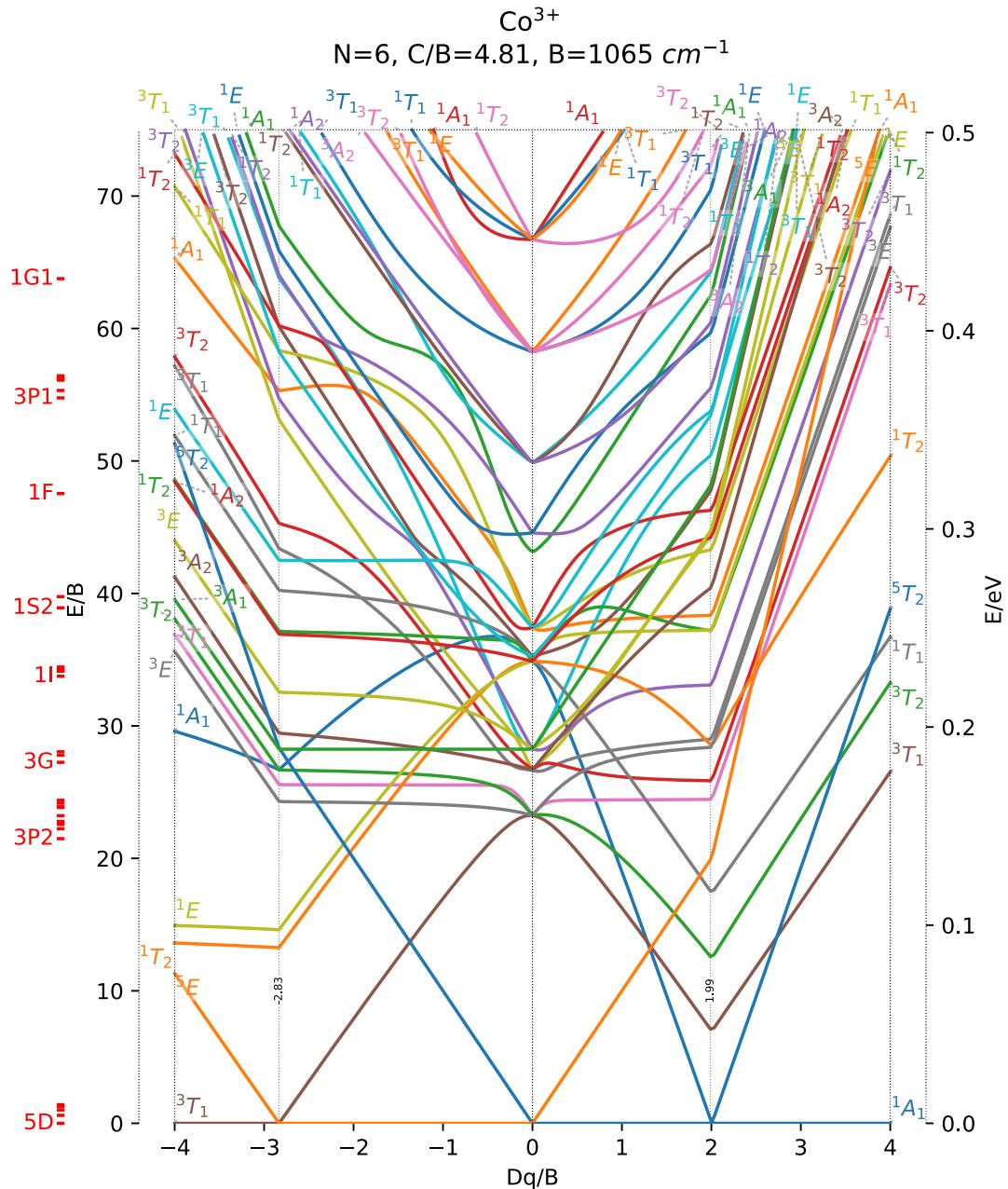
$$\left[ \begin{array}{cccccc} t_2^4(^1E)e & t_2^3(^2E)e^2(^1E) & t_2^3(^4A_2)e^2(^3A_2) & t_2^2(^1E)e^3(^2E) & t_2^2(^1E)e^3(^2E) & t_2^2(^1A_1)e^3(^2E) & t_2^2(^1E)e^3(^2E) \\ -23B + 9C - 10Dq & -3\sqrt{2}B & -12B + 8C' & -3\sqrt{2}B & -3\sqrt{2}B & 4B + C & -2B \\ 0 & 0 & -16B + 8C & -16B + 8C & -16B + 8C & -6B & +C \\ -2B + C & -3\sqrt{2}B & -3\sqrt{2}B & -23B + 9C + 10Dq & -23B + 9C + 10Dq & -17B + 8C + 10Dq & -17B + 8C + 10Dq \end{array} \right] \quad (32)$$

$$4T_1(^4F, ^4G, ^4P)$$

$$\left[ \begin{array}{cccccc} t_2^4(^3T_1)e & t_2^3(^2T_2)e^2(^3A_2) & t_2^3(^2T_2)e^2(^3A_2) & t_2^2(^3T_1)e^3(^2E) & t_2^2(^3T_1)e^3(^2E) & t_2^2(^3T_1)e^3(^2E) & t_2^2(^3T_1)e^3(^2E) \\ -17B + 6C - 10Dq & -3\sqrt{2}B & -16B + 8C & -3\sqrt{2}B & -3\sqrt{2}B & 4B + C & -2B \\ 0 & 0 & -16B + 8C & -16B + 8C & -16B + 8C & -6B & +C \\ -3\sqrt{2}B & -3\sqrt{2}B & -3\sqrt{2}B & -25B + 6C + 10Dq & -25B + 6C + 10Dq & -17B + 8C + 10Dq & -17B + 8C + 10Dq \end{array} \right] \quad (33)$$

$$2T_1(^2F, ^2F, ^2G, ^2G, ^2H, ^2I, ^2P)$$

$$\begin{aligned}
& \left[ \begin{array}{cccccc} t_2^4(3T_1)e & t_2^4(1T_2)e & t_2^3(2T_1)e^2(1A_1) & t_2^3(2T_2)e^2(1E) & t_2^3(2T_1)e^2(3A_2) & t_2^3(2T_2)e^3(2E) \\ -22B + 9C - 10Dq & 3B & \frac{3\sqrt{2}B}{2} & \frac{3\sqrt{6}B}{2} & \frac{-3\sqrt{2}B}{2} & t_2^2(1T_2)e^3(2E) \\ 3B & -8B + 9C - 10Dq & \frac{3\sqrt{2}B}{2} & \frac{5\sqrt{6}B}{2} & \frac{3\sqrt{2}B}{2} & 0 \\ \frac{3\sqrt{2}B}{2} & \frac{3\sqrt{6}B}{2} & -4B + 10C & 10\sqrt{3}B & -15\sqrt{2}B & 4B + C \\ \frac{3\sqrt{6}B}{2} & \frac{5\sqrt{6}B}{2} & 10\sqrt{3}B & 0 & 0 & \frac{3\sqrt{2}B}{2} \\ \frac{-3\sqrt{2}B}{2} & \frac{3\sqrt{2}B}{2} & 0 & -6B + 10C & 0 & \frac{5\sqrt{6}B}{2} \\ \frac{-3\sqrt{2}B}{2} & \frac{-15\sqrt{2}B}{2} & 0 & 0 & -2\sqrt{3}B & \frac{5\sqrt{2}B}{2} \\ C & 0 & 3\sqrt{2}B & -2\sqrt{3}B & 0 & -\frac{3\sqrt{2}B}{2} \\ 0 & 4B + C & \frac{3\sqrt{2}B}{2} & \frac{3\sqrt{6}B}{2} & -10B + 10C & -22B + 9C + 10Dq \\ \end{array} \right] \\
& \left[ \begin{array}{c} 4A_2(4F) \\ 4E(4D, 4G) \\ 6A_1(6S) \\ 4A_1(4G) \\ [t_2^3(4A_2)e^2(3A_2) \quad t_2^3(4A_2)e^2(1E)] \\ [-22B + 5C \quad -2\sqrt{3}B \quad -21B + 5C] \\ [-22B + 5C \quad -35B \quad -21B + 5C] \\ [t_2^3(4A_2)e^2(3A_2) \quad t_2^3(4A_2)e^2(3A_2)] \\ [-23B + 5C \quad -23B + 5C] \end{array} \right]
\end{aligned}$$



$$^1A_1( ^1G, ^1G, ^1I, ^1S, ^1S)$$

$$\left[ \begin{array}{cc} -30B + 15C & t_6^6 \\ 2\sqrt{6}B + \sqrt{6}C & 2\sqrt{6}B + \sqrt{6}C \\ 2\sqrt{6}B & 2\sqrt{6}B + 4Dq \\ 0 & -12B \\ 0 & 4\sqrt{2}B + 2\sqrt{2}C \end{array} \right]^{(39)}$$

$$^3T_1( ^3F, ^3F, ^3G, ^3H, ^3P, ^3P)$$

$$\left[ \begin{array}{cc} t_5^5( ^2T_2)e & t_4^4( ^1A_1)e^2( ^1A_1) \\ -30B + 12C - 14Dq & 18C - 4Dq \\ -3\sqrt{2}B & 10B \\ -3\sqrt{2}B & 0 \\ \sqrt{2}B + \sqrt{2}C & 3B \\ -\sqrt{6}B & 2\sqrt{2}B + \sqrt{2}C \\ 0 & 2\sqrt{2}B + \sqrt{2}C \end{array} \right]^{(40)}$$

$$^3T_2( ^3D, ^3F, ^3F, ^3G, ^3H)$$

$$\left[ \begin{array}{cc} t_2^4( ^3T_1)e^2( ^1E) & t_2^4( ^1T_2)e^2( ^1E) \\ -23B + 11C - 4Dq & -23B + 11C - 4Dq \\ 0 & 2\sqrt{3}B \\ -2\sqrt{3}B & 5\sqrt{3}B \\ -3B & -3B \\ \sqrt{3}B & 0 \\ 2\sqrt{2}B & 2\sqrt{2}B \end{array} \right]^{(41)}$$

$$^1T_1( ^1F, ^1G, ^1G, ^1I)$$

$$\left[ \begin{array}{cc} t_2^4( ^3T_1)e^2( ^1E) & t_2^4( ^3T_2)e^2( ^1E) \\ -23B + 11C - 4Dq & -27B + 11C - 4Dq \\ 3B & 3B \\ 2\sqrt{2}B & 3\sqrt{2}B \\ 3B & \sqrt{6}B \\ -\sqrt{6}B & -\sqrt{6}B \end{array} \right]^{(42)}$$

$$^1T_2( ^1D, ^1D, ^1F, ^1G, ^1G, ^1I)$$

$$\left[ \begin{array}{cc} t_2^4( ^2T_2)e & t_2^4( ^1T_2)e^2( ^1E) \\ -30B + 14C - 14Dq & -17B + 13C - 4Dq \\ \sqrt{2}B + \sqrt{2}C & 5\sqrt{3}B \\ \sqrt{6}B & 3B \\ -\sqrt{6}B & -\sqrt{6}B \end{array} \right]^{(43)}$$

$$^1E( ^1D, ^1D, ^1G, ^1G, ^1I)$$

$$\left[ \begin{array}{cc} t_2^4( ^2T_2)e^2( ^1A_1) & t_2^4( ^1A_1)e^2( ^1A_1) \\ -14B + 14C & -9B + 15C - 4Dq \\ -\sqrt{6}B & 0 \\ 3\sqrt{2}B + \sqrt{2}C & 3\sqrt{2}B \\ \sqrt{6}B & 2\sqrt{2}B + \sqrt{2}C \\ 0 & 2\sqrt{2}B + \sqrt{2}C \end{array} \right]^{(44)}$$

$$^1A_2( ^1F, ^1I)$$

$$\left[ \begin{array}{cc} t_2^4( ^1E)e^2( ^1E) & t_2^4( ^1E)e^2( ^1E) \\ -17B + 13C - 4Dq & -17B + 13C - 4Dq \\ 6B & 0 \\ 10\sqrt{2}B & 12B \\ 3\sqrt{2}B & 4B \\ 2\sqrt{2}B + \sqrt{2}C & -2B \end{array} \right]^{(45)}$$

$$^3A_2(^3F, ^3F)$$

$$\begin{bmatrix} t_2^4(^1A_1)e^2(^3A_2) & t_2^3(^2E)e^3(^2E) \\ -16B + 14C - 4Dq & 12B \\ 12B & -22B + 11C + 6Dq \end{bmatrix} \quad (46)$$

$$^3E(^3D, ^3G, ^3H)$$

$$\begin{bmatrix} t_2^4(^1E)e^2(^3A_2) & t_2^3(^2E)e^3(^2E) \\ -25B + 11C - 4Dq & 3\sqrt{2}B \\ 3\sqrt{2}B & -24B + 11C + 6Dq \\ 0 & 4B \end{bmatrix} \quad (47)$$

$$^5T_2(^5D)$$

$$\begin{bmatrix} t_2^4(^1T_1)e^2(^3A_2) \\ -35B + 7C - 4Dq \end{bmatrix} \quad (48)$$

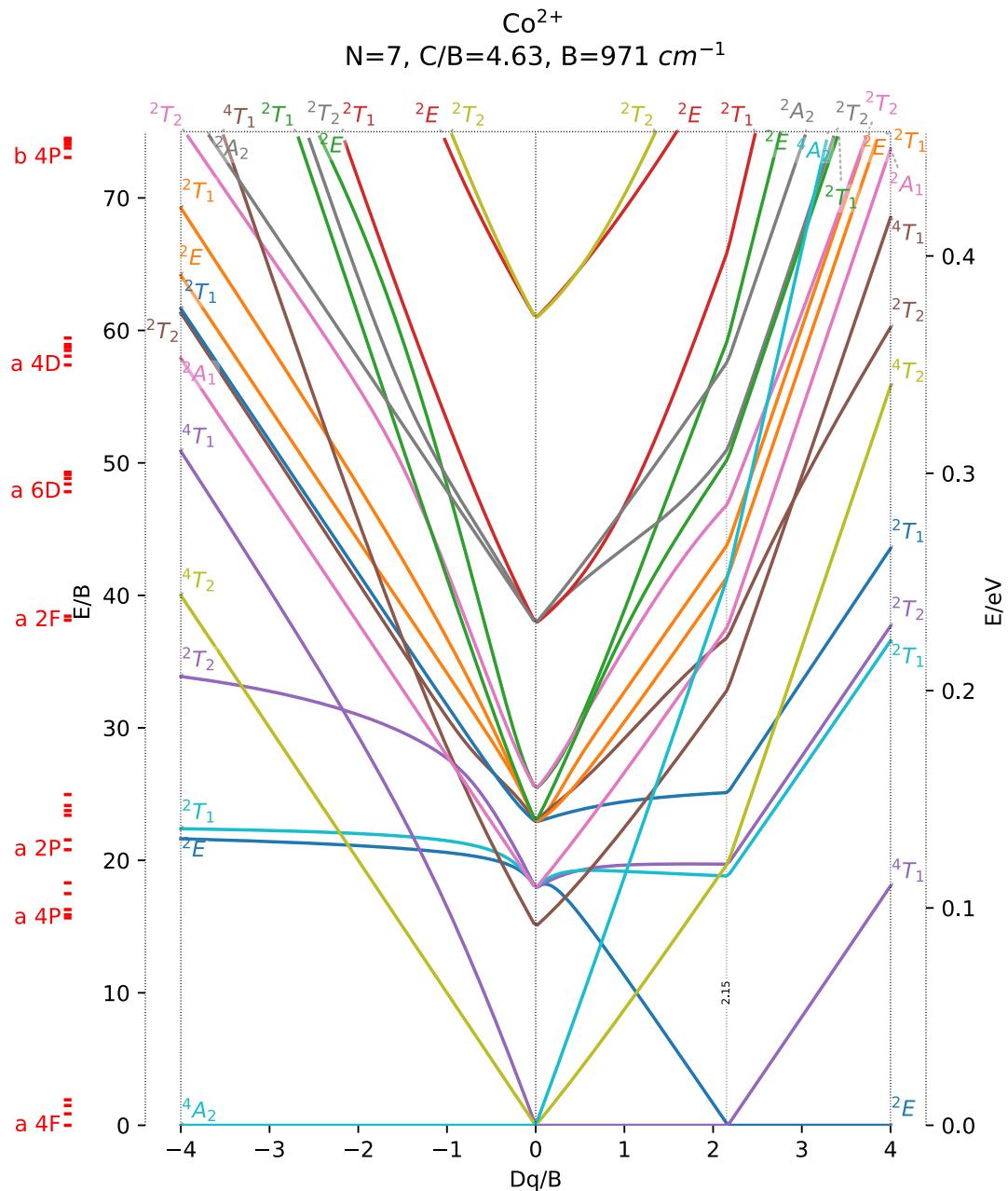
$$^5E(^5D)$$

$$\begin{bmatrix} t_2^3(^4A_2)e^3(^2E) \\ -35B + 7C + 6Dq \end{bmatrix} \quad (49)$$

$$^3A_1(^3G)$$

$$\begin{bmatrix} t_3^3(^2E)e^3(^2E) \\ -26B + 11C + 6Dq \end{bmatrix} \quad (50)$$

6  $d^7$



$$^2E(^2D, ^2D, ^2G, ^2H)$$

$$\begin{bmatrix} t_2^6(^1A_1)e & t_2^4(^1A_1)e^3(^2E) & t_2^4(^1E)e^3(^2E) & t_2^3(^2E)e^4(^1A_1) \\ -36B + 18C - 18Dq & 2\sqrt{3}B + \sqrt{3}C & -2\sqrt{3}B & 0 \\ 2\sqrt{3}B + \sqrt{3}C & -20B + 20C + 2Dq & -10B & 6\sqrt{2}B \\ -2\sqrt{3}B & -10B & -29B + 17C + 2Dq & -3\sqrt{2}B \\ 0 & 6\sqrt{2}B & -3\sqrt{2}B & -34B + 17C + 12Dq \end{bmatrix} \quad (51)$$

$$^2T_2(^2D, ^2D, ^2F, ^2G, ^2H)$$

$$\begin{bmatrix} t_2^5(^2T_2)e^2(^1A_1) & t_2^5(^2T_2)e^2(^1E) & t_2^4(^3T_1)e^3(^2E) & t_2^4(^1T_2)e^3(^2E) & t_2^3(^2T_2)e^4(^1A_1) \\ -22B + 19C - 8Dq & -10B & -3\sqrt{3}B & \sqrt{3}B & 4B + 2C \\ -10B & -30B + 17C - 8Dq & 3\sqrt{3}B & \sqrt{3}B & -2B \\ -3\sqrt{3}B & 3\sqrt{3}B & -34B + 17C + 2Dq & -3B & -3\sqrt{3}B \\ \sqrt{3}B & \sqrt{3}B & -3B & -24B + 17C + 2Dq & 5\sqrt{3}B \\ 4B + 2C & -2B & -3\sqrt{3}B & 5\sqrt{3}B & -28B + 19C + 12Dq \end{bmatrix} \quad (52)$$

$$^2T_1(^2F, ^2G, ^2H, ^2P)$$

$$\begin{bmatrix} t_2^5(^2T_2)e^2(^1E) & t_2^5(^2T_2)e^2(^3A_2) & t_2^4(^3T_1)e^3(^2E) & t_2^4(^1T_2)e^3(^2E) & t_2^3(^2T_1)e^4(^1A_1) \\ -30B + 17C - 8Dq & -2\sqrt{3}B & -3\sqrt{3}B & -\sqrt{3}B & -2\sqrt{3}B \\ -2\sqrt{3}B & -34B + 17C - 8Dq & 3B & 3B & 0 \\ -3\sqrt{3}B & 3B & -28B + 17C + 2Dq & 3B & 3B \\ -\sqrt{3}B & 3B & 3B & -34B + 17C + 2Dq & 3B \\ -2\sqrt{3}B & 0 & 3B & 3B & -34B + 17C + 12Dq \end{bmatrix} \quad (53)$$

$$^4T_1(^4F, ^4P)$$

$$\begin{bmatrix} t_2^5(^2T_2)e^2(^3A_2) & t_2^4(^3T_1)e^3(^2E) \\ -40B + 14C - 8Dq & 6B \\ 6B & -31B + 14C + 2Dq \end{bmatrix} \quad (54)$$

$$^2A_1(^2G)$$

$$\begin{bmatrix} t_2^4(^1E)e^3(^2E) \\ -39B + 17C + 2Dq \end{bmatrix} \quad (55)$$

$$^2A_2(^2F)$$

$$\begin{bmatrix} t_2^4(^1E)e^3(^2E) \\ -19B + 17C + 2Dq \end{bmatrix} \quad (56)$$

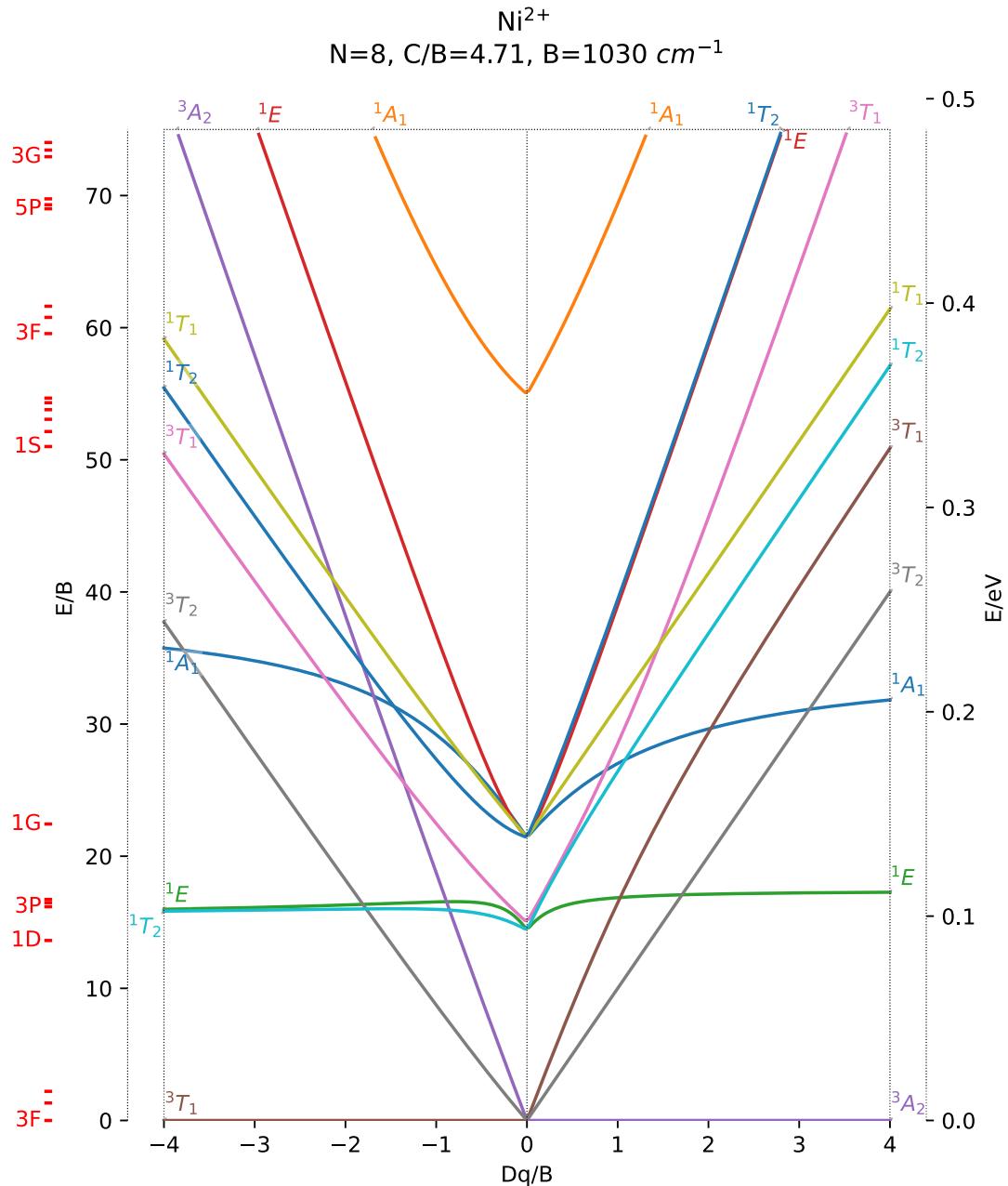
$$^4T_2(^4F)$$

$$\begin{bmatrix} t_2^4(^3T_1)e^3(^2E) \\ -43B + 14C + 2Dq \end{bmatrix} \quad (57)$$

$$^4A_2(^4F)$$

$$\begin{bmatrix} t_2^3(^4A_2)e^4(^1A_1) \\ -43B + 14C + 12Dq \end{bmatrix} \quad (58)$$

7  $d^8$



$$^1A_1(^1G, ^1S)$$

$$\begin{bmatrix} t_2^6(^1A_1)e^2(^1A_1) & t_2^4(^1A_1)e^4(^1A_1) \\ -\frac{34B+25C-12Dq}{2\sqrt{6}B+\sqrt{6}C} & \frac{-2\sqrt{6}B+\sqrt{6}C}{-32B+26C+8Dq} \end{bmatrix} \quad (59)$$

$$^1E(^1D, ^1G)$$

$$\begin{bmatrix} t_2^6(^1A_1)e^2(^1E) & t_2^4(^1E)e^4(^1A_1) \\ -\frac{42B+23C-12Dq}{-2\sqrt{3}B} & \frac{-2\sqrt{3}B}{-41B+23C+8Dq} \end{bmatrix} \quad (60)$$

$$^3A_2(^3F)$$

$$\begin{bmatrix} t_2^6(^1A_1)e^2(^3A_2) \\ -\frac{50B+21C-12Dq}{-50B+21C-12Dq} \end{bmatrix} \quad (61)$$

$$^3T_1(^3F, ^3P)$$

$$\begin{bmatrix} t_2^5(^2T_2)e^3(^2E) & t_2^4(^3T_1)e^4(^1A_1) \\ -\frac{38B+21C-2Dq}{-6B} & \frac{-6B}{-47B+21C+8Dq} \end{bmatrix} \quad (62)$$

$$^3T_2(^3F)$$

$$\begin{bmatrix} t_2^5(^2T_2)e^3(^2E) \\ -\frac{50B+21C-2Dq}{-50B+21C-2Dq} \end{bmatrix} \quad (63)$$

$$^1T_1(^1G)$$

$$\begin{bmatrix} t_2^5(^2T_2)e^3(^2E) \\ -\frac{38B+23C-2Dq}{-38B+23C-2Dq} \end{bmatrix} \quad (64)$$

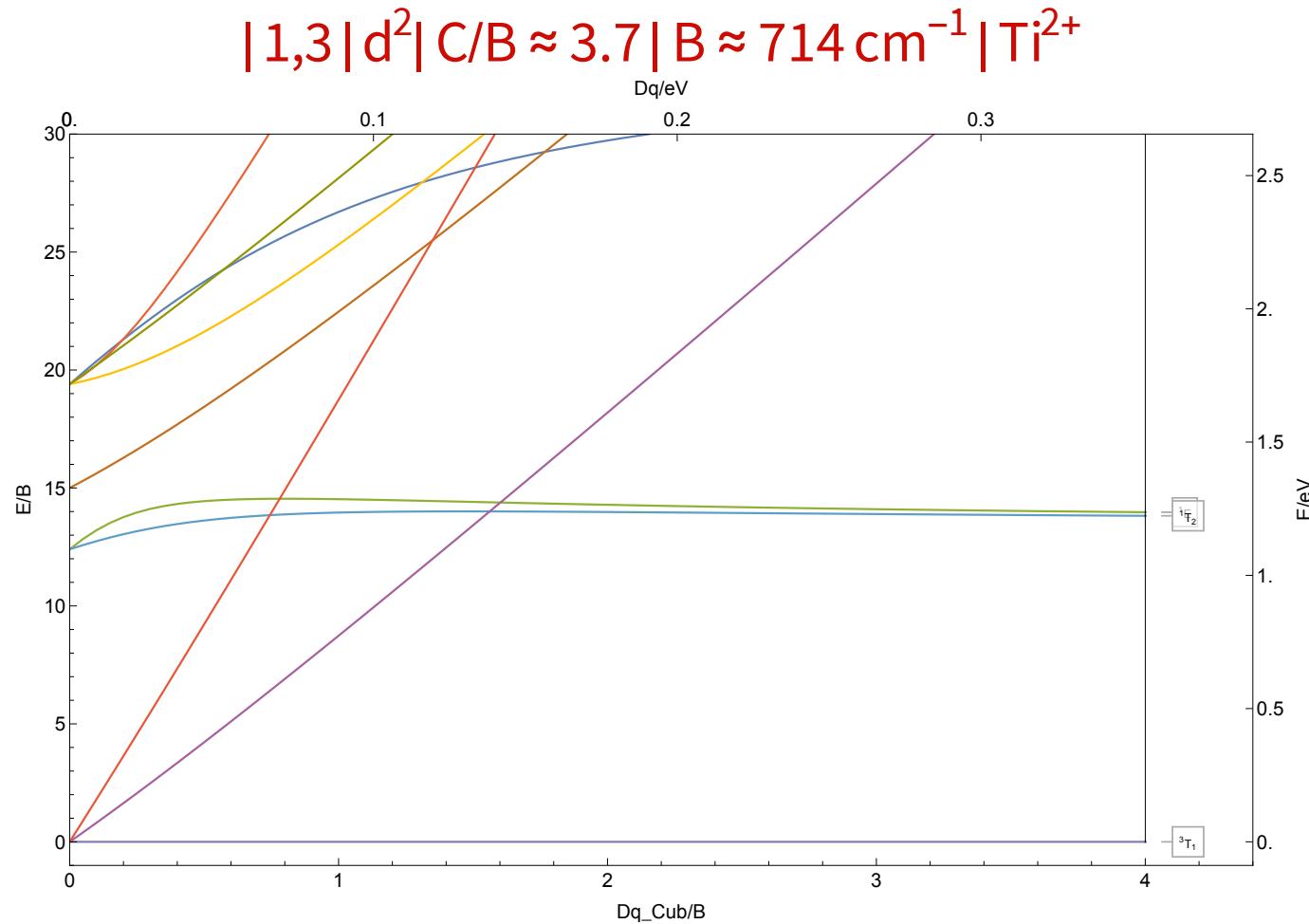
$$^1T_2(^1D, ^1G)$$

$$\begin{bmatrix} t_2^5(^2T_2)e^3(^2E) & t_2^4(^1T_2)e^4(^1A_1) \\ -\frac{42B+23C-2Dq}{2\sqrt{3}B} & \frac{-2\sqrt{3}B}{-41B+23C+8Dq} \end{bmatrix} \quad (65)$$

## 8 Hartree-Fock Tanabe-Sugano Diagrams

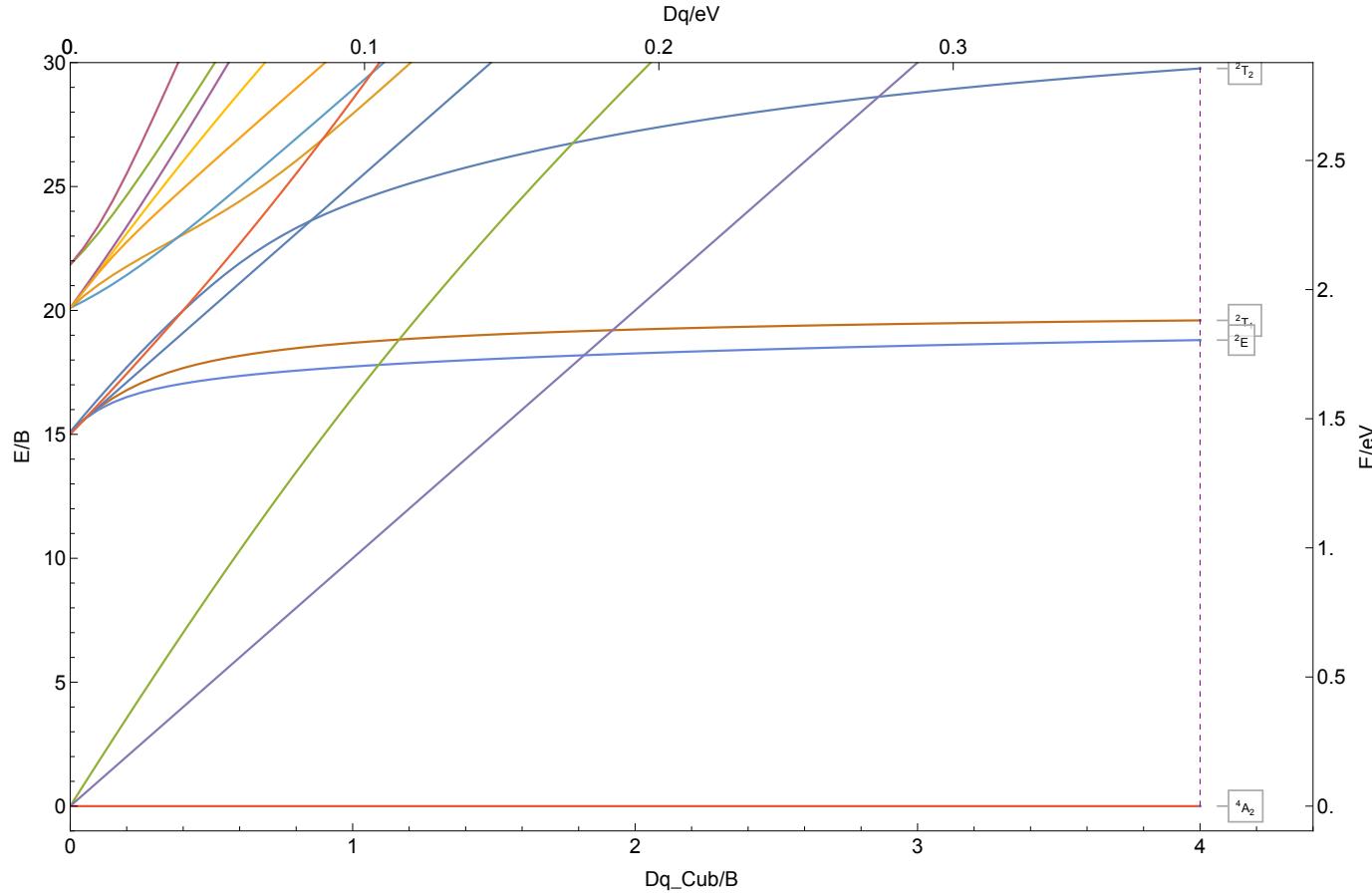
### 8.1 Cubic field

#### 8.1.1 $\text{Ti}^{2+}$



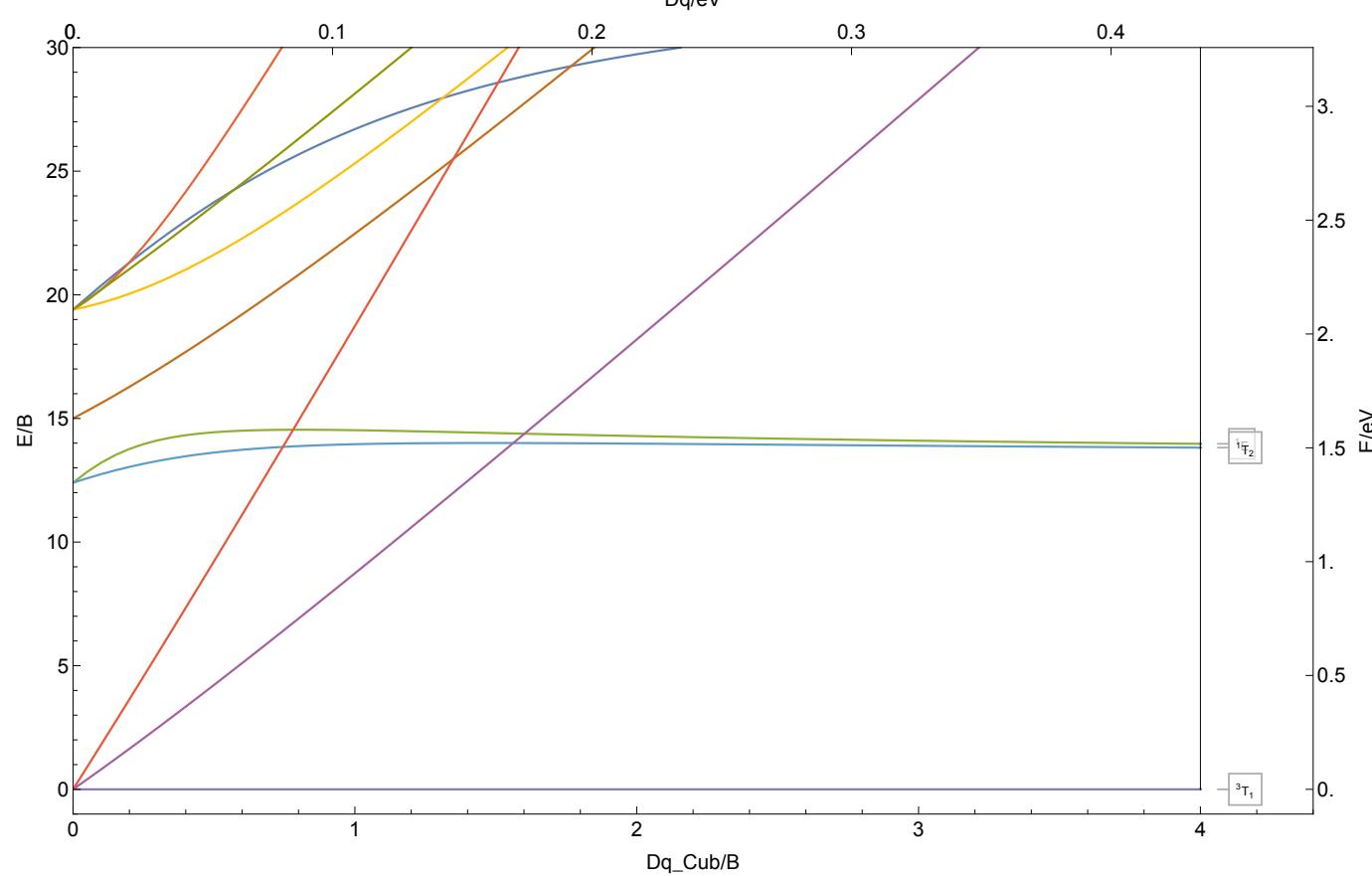
### 8.1.2 $V^{2+}$

$|2,4|d^3|C/B \approx 3.7|B \approx 774\text{ cm}^{-1}|V^{2+}$



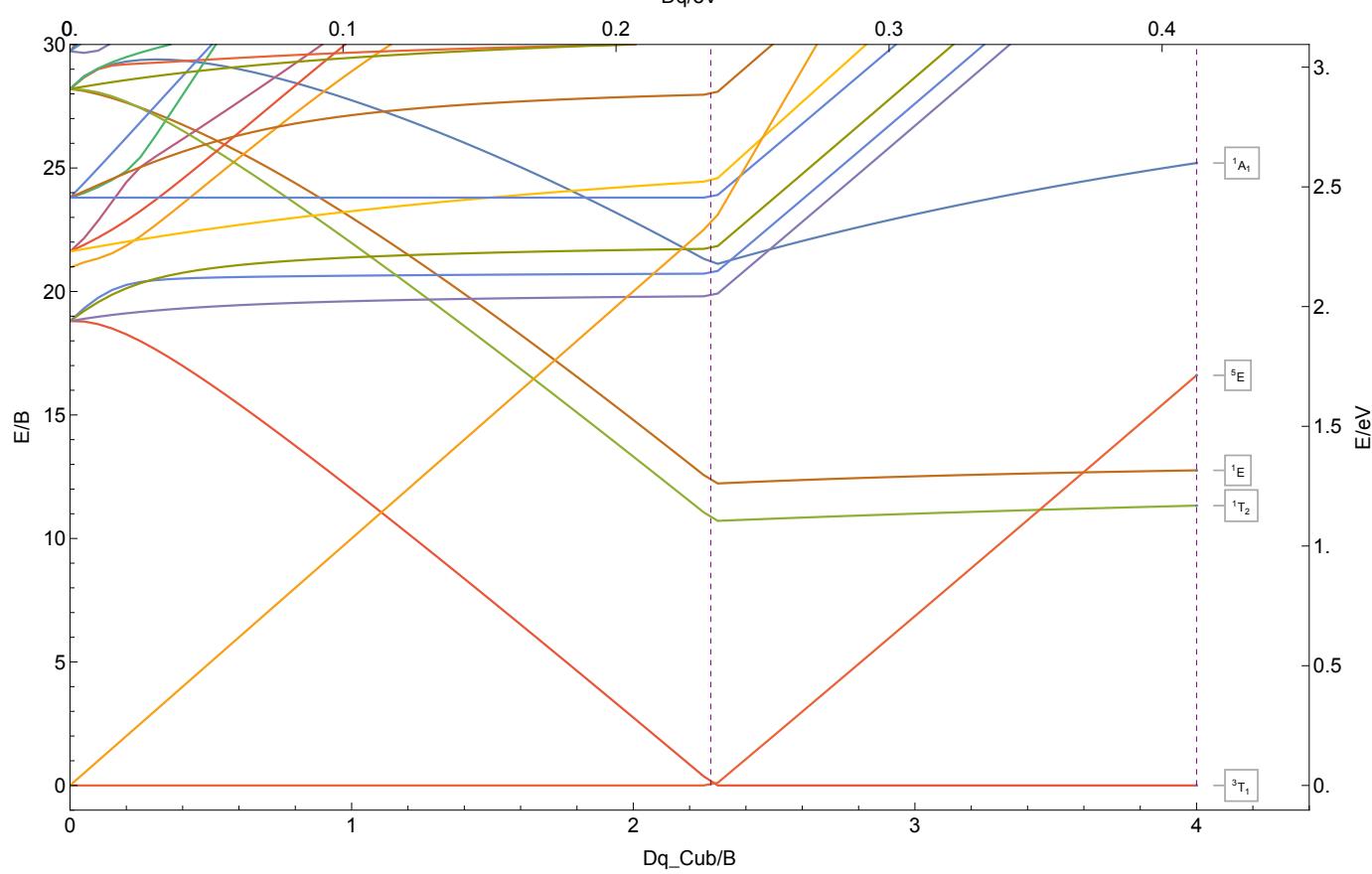
### 8.1.3 V<sup>3+</sup>

$$|1,3|d^2| C/B \approx 3.7 | B \approx 876 \text{ cm}^{-1} |V^{3+}$$



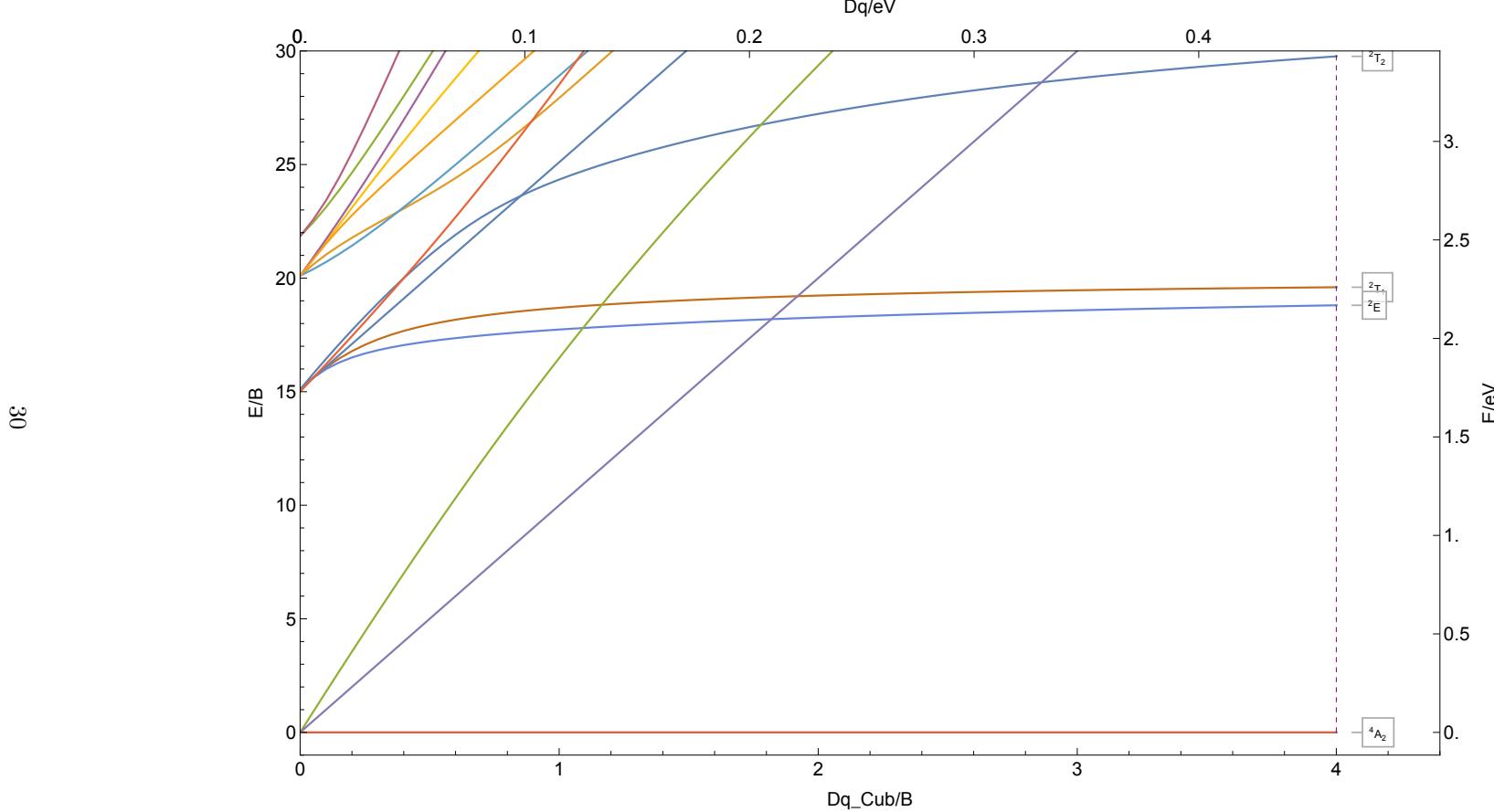
#### 8.1.4 Cr<sup>2+</sup>

$|1,3,5|d^4|C/B \approx 3.7|B \approx 832\text{ cm}^{-1}|Cr^{2+}$



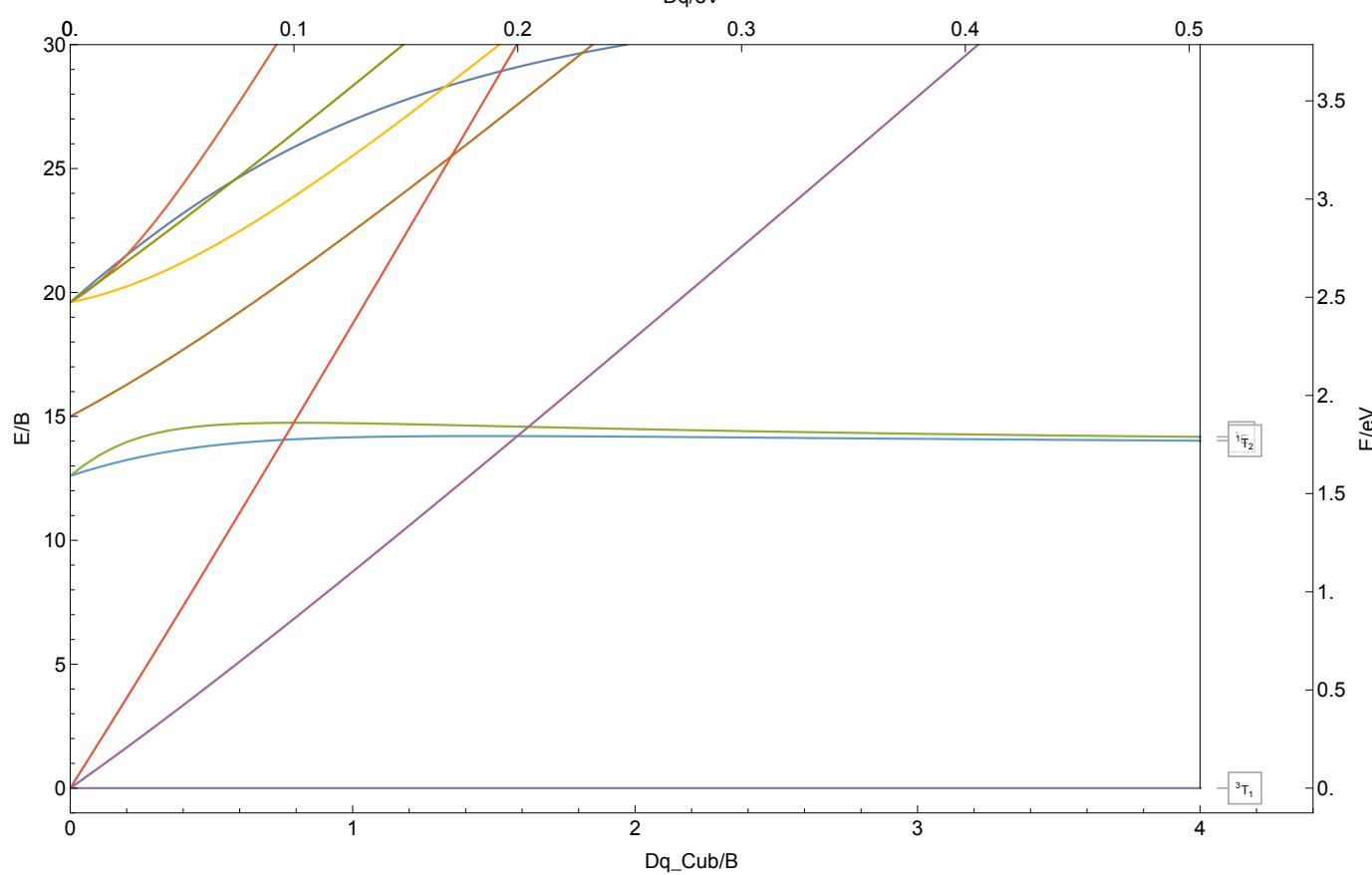
### 8.1.5 Cr<sup>3+</sup>

$|2,4|d^3|C/B \approx 3.7|B \approx 930\text{ cm}^{-1}|Cr^{3+}$



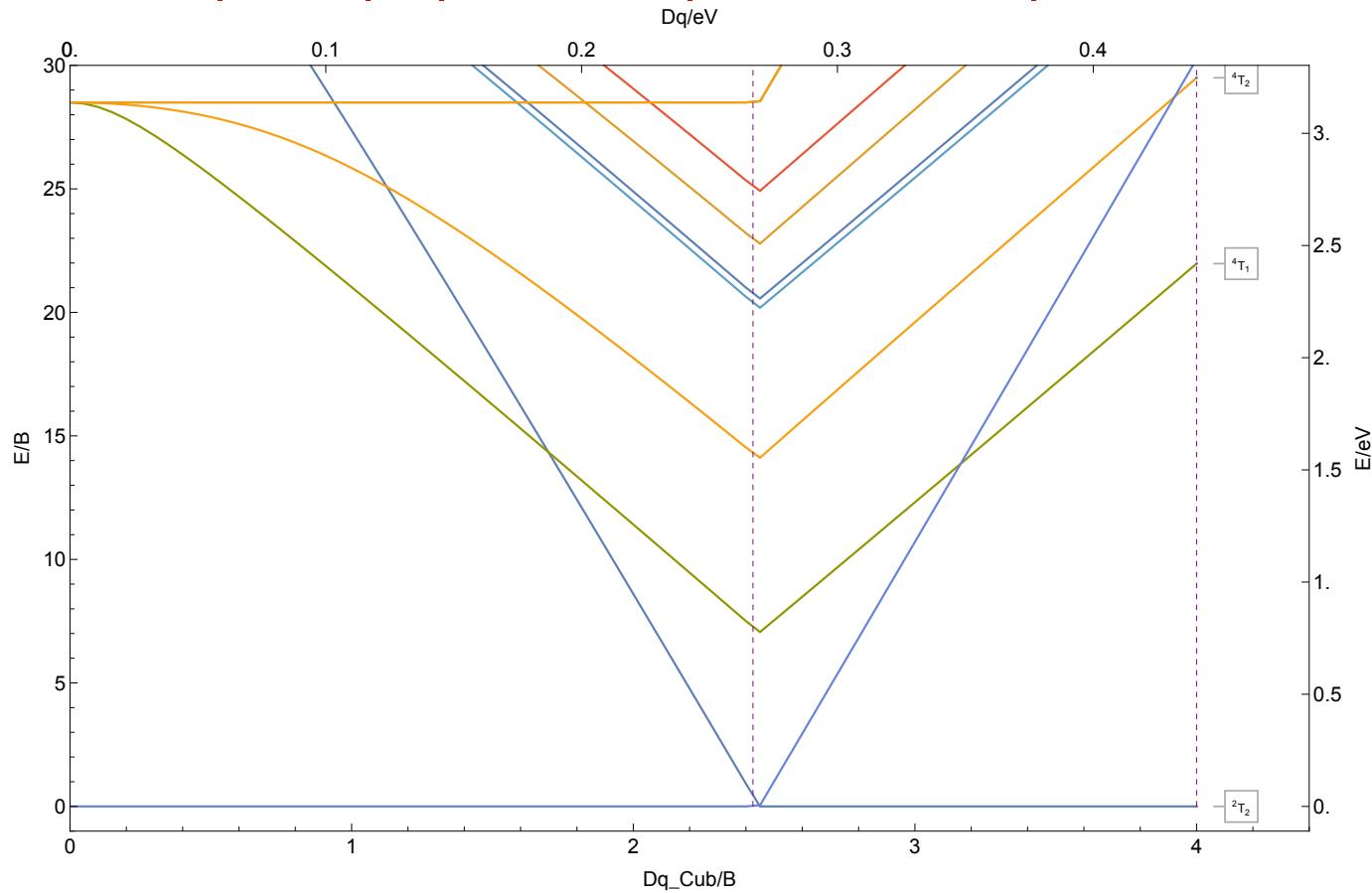
### 8.1.6 Cr<sup>4+</sup>

$|1,3|d^2|C/B \approx 3.8|B \approx 1018\text{cm}^{-1}|Cr^{4+}$



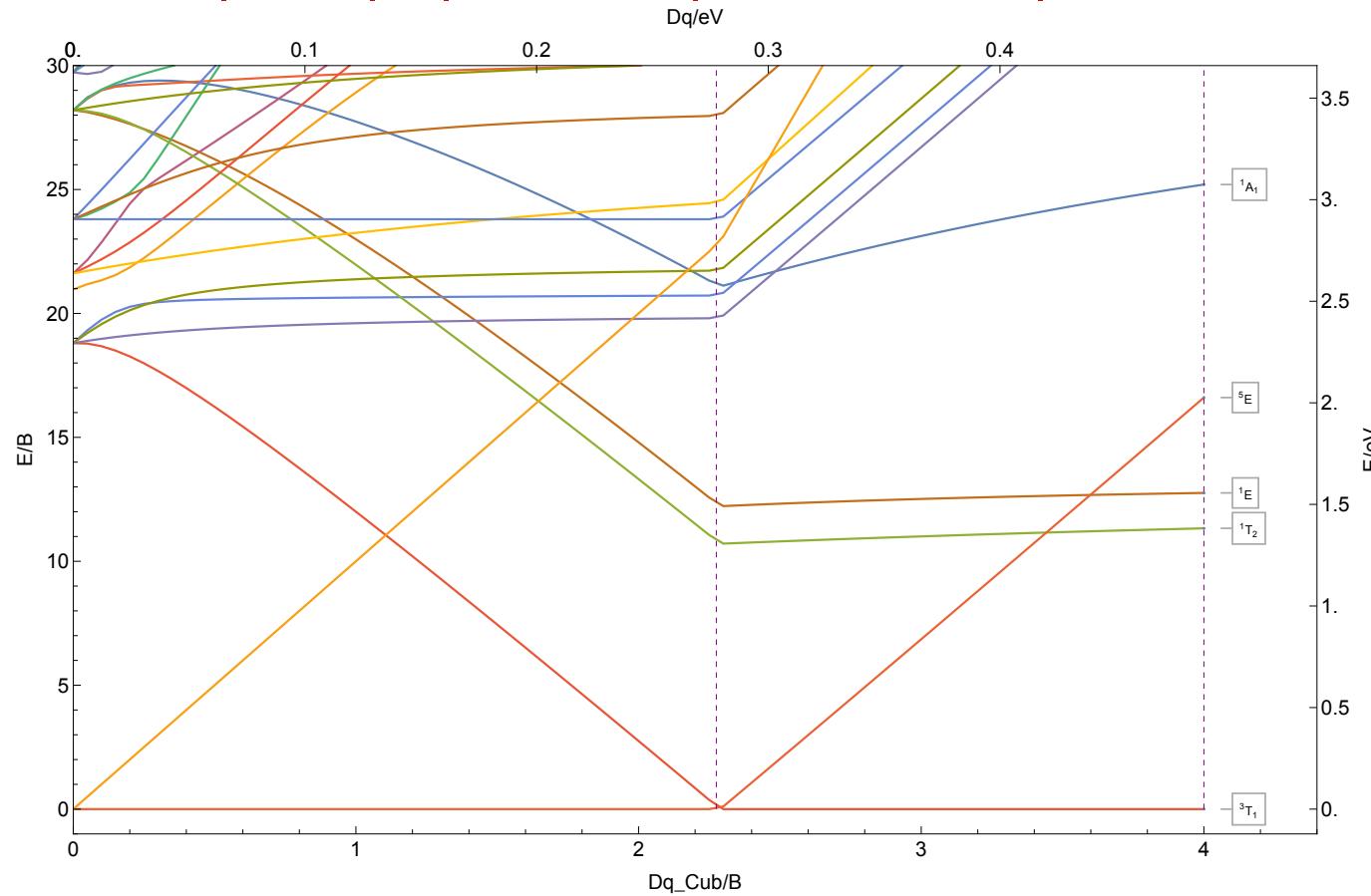
### 8.1.7 Mn<sup>2+</sup>

$|2,4,6|d^5|C/B \approx 3.7|B \approx 888\text{ cm}^{-1}|Mn^{2+}$



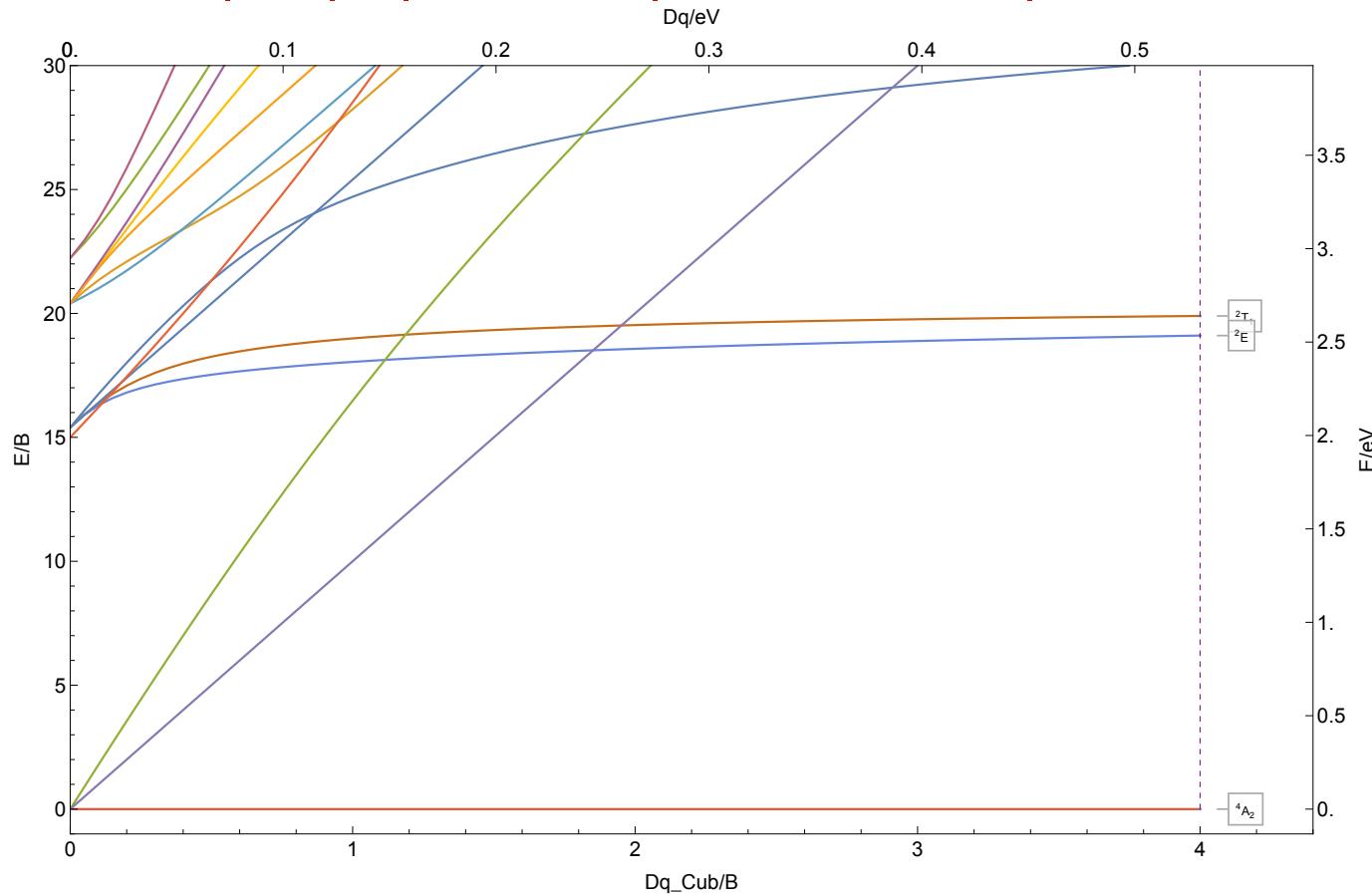
### 8.1.8 Mn<sup>3+</sup>

$|1,3,5|d^4|C/B \approx 3.7|B \approx 984\text{ cm}^{-1}|Mn^{3+}$



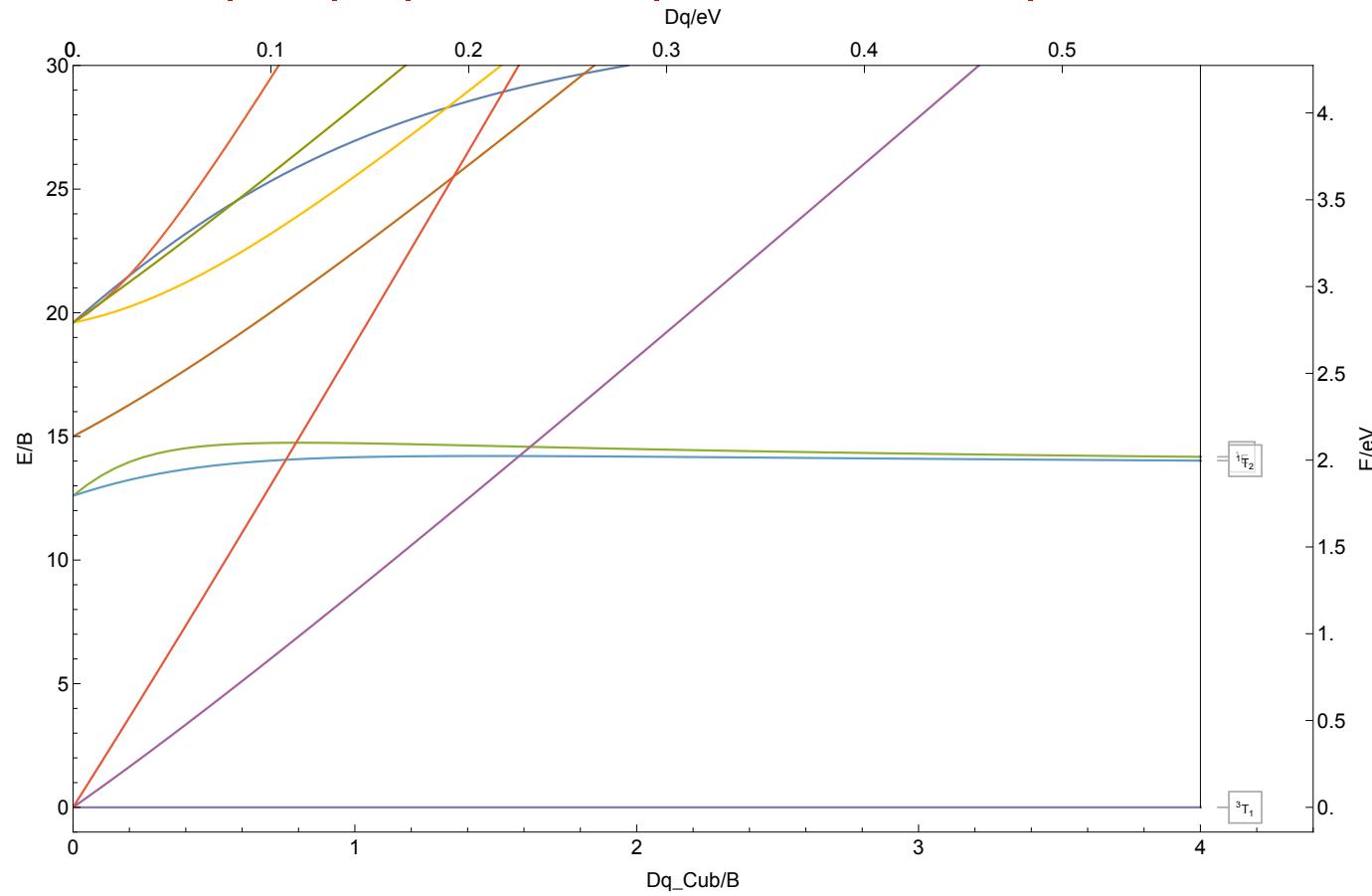
### 8.1.9 Mn<sup>4+</sup>

$|2,4|d^3|C/B \approx 3.8|B \approx 1070\text{ cm}^{-1}|Mn^{4+}$



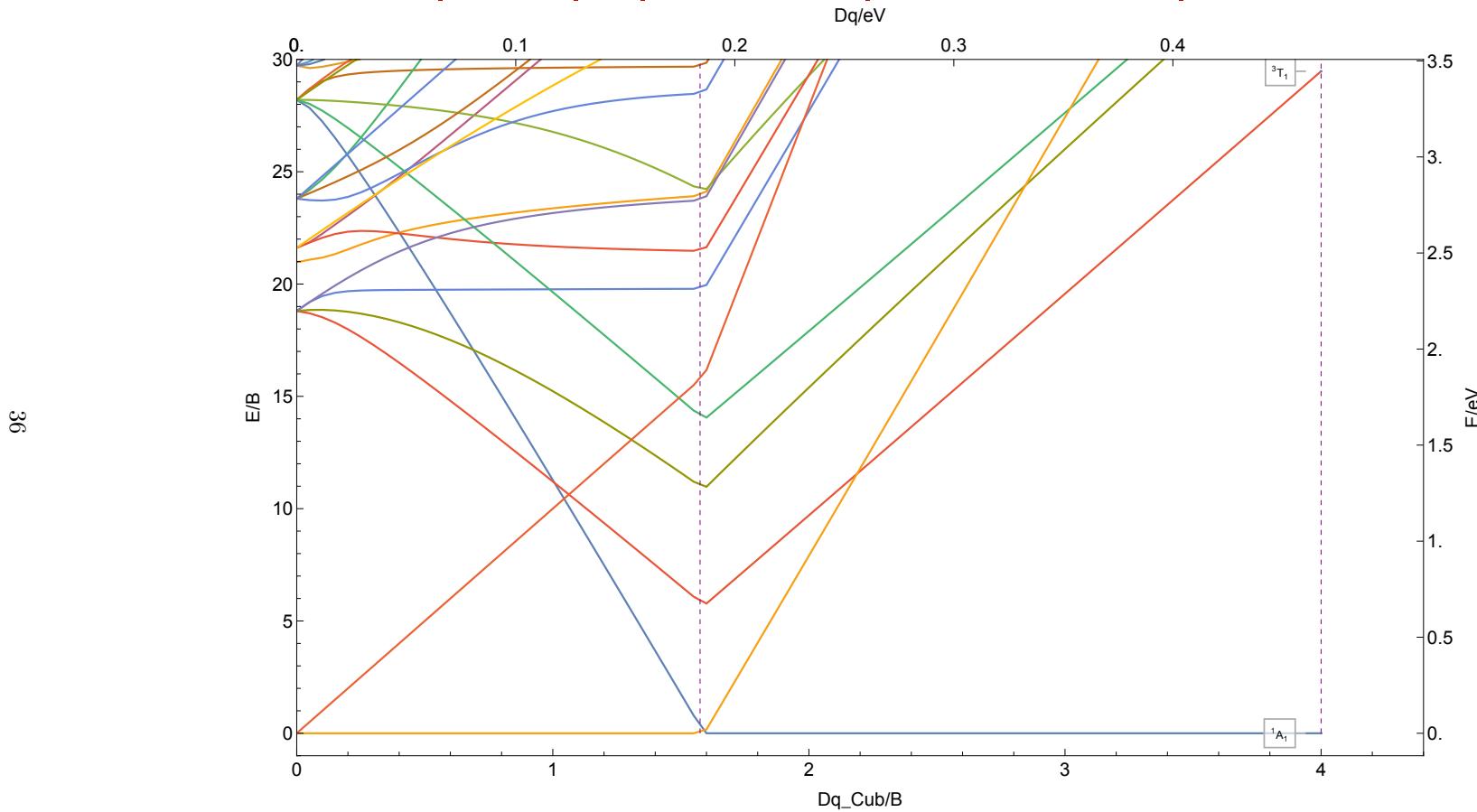
### 8.1.10 Mn<sup>5+</sup>

$|1,3|d^2|C/B \approx 3.8|B \approx 1149\text{ cm}^{-1}|Mn^{5+}$



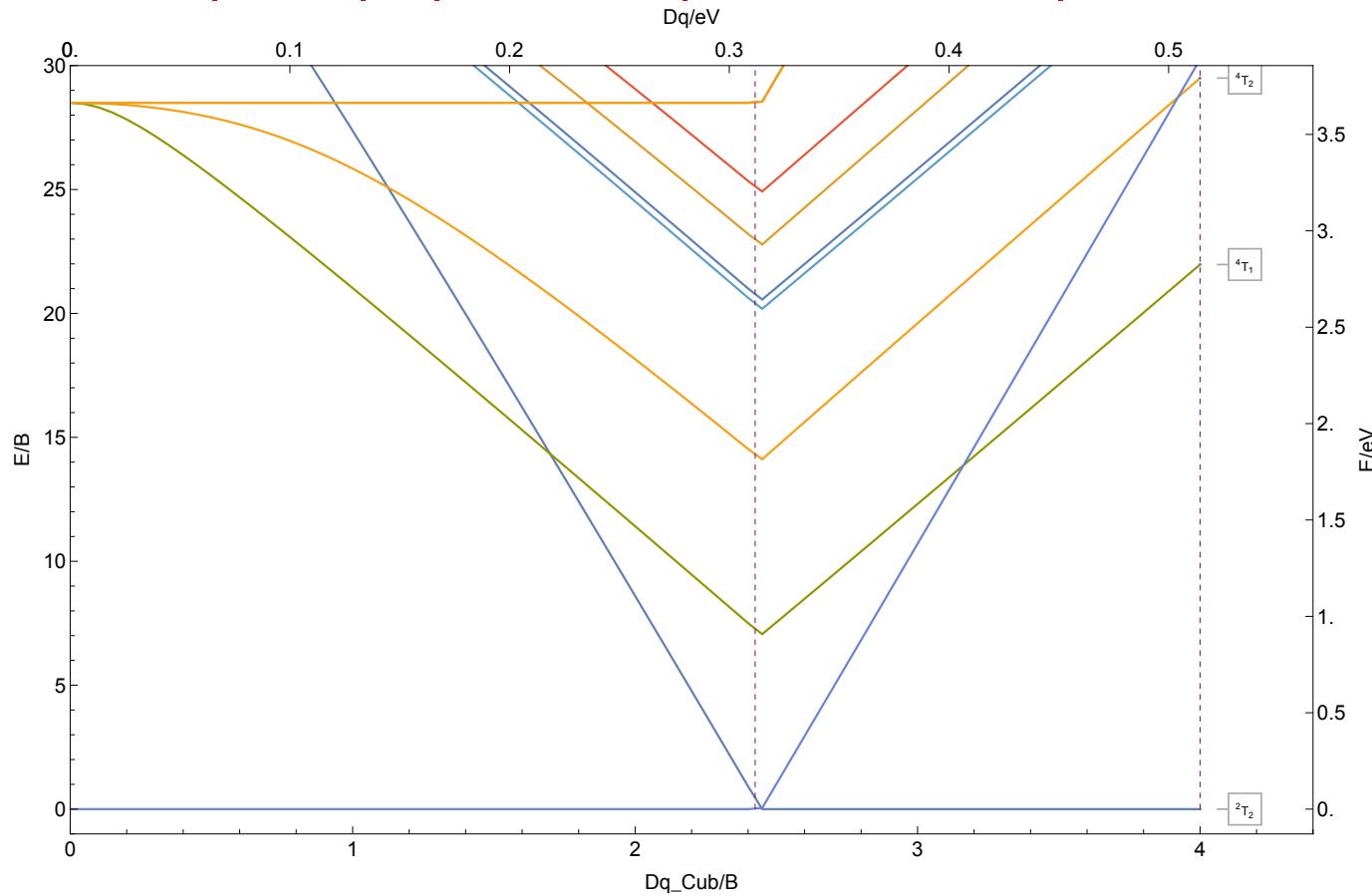
### 8.1.11 Fe<sup>2+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 3.7 | B ≈ 943 cm<sup>-1</sup> | Fe<sup>2+</sup>



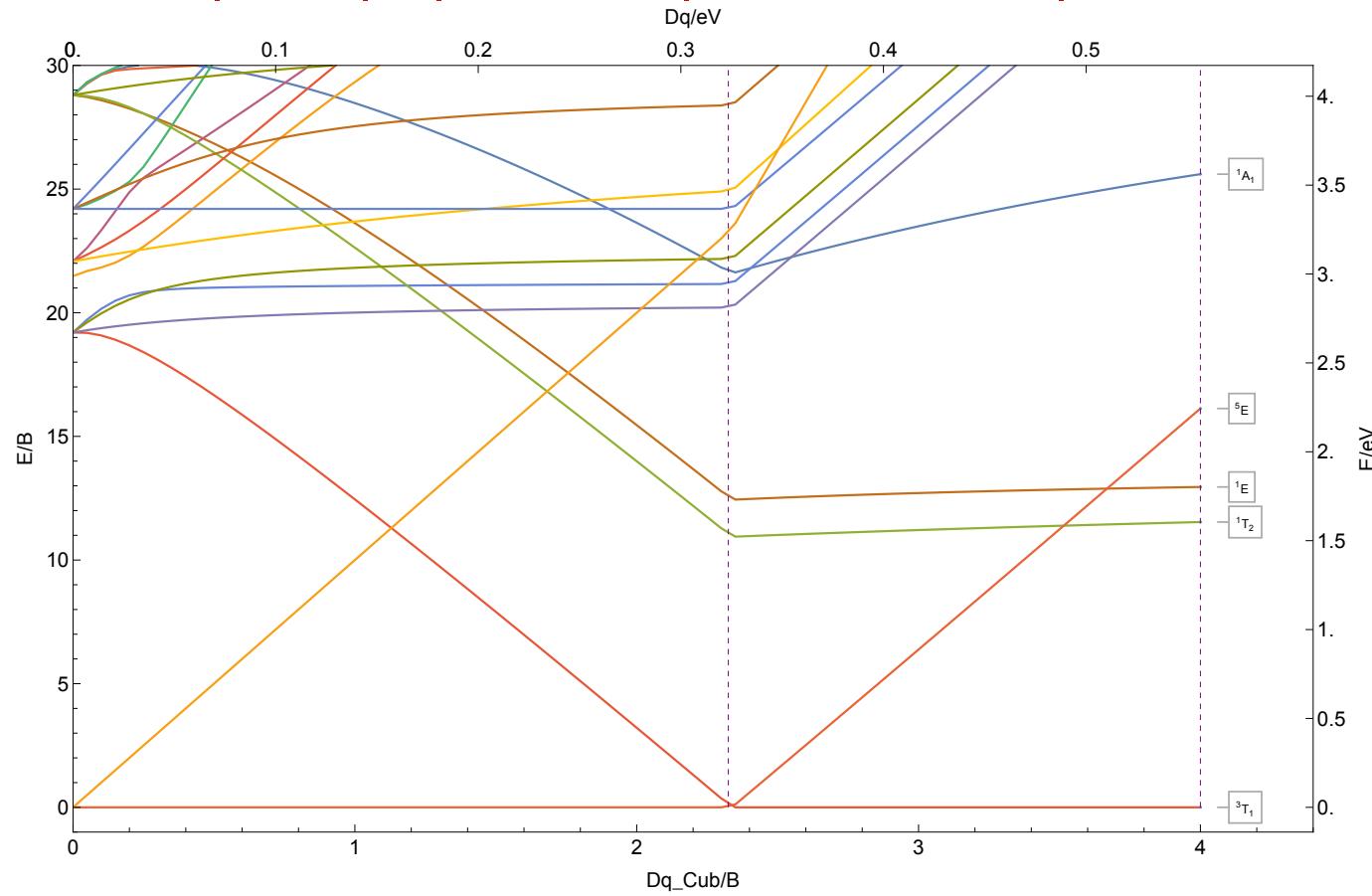
### 8.1.12 Fe<sup>3+</sup>

|2,4,6|d<sup>5</sup>|C/B ≈ 3.7|B ≈ 1037 cm<sup>-1</sup>|Fe<sup>3+</sup>



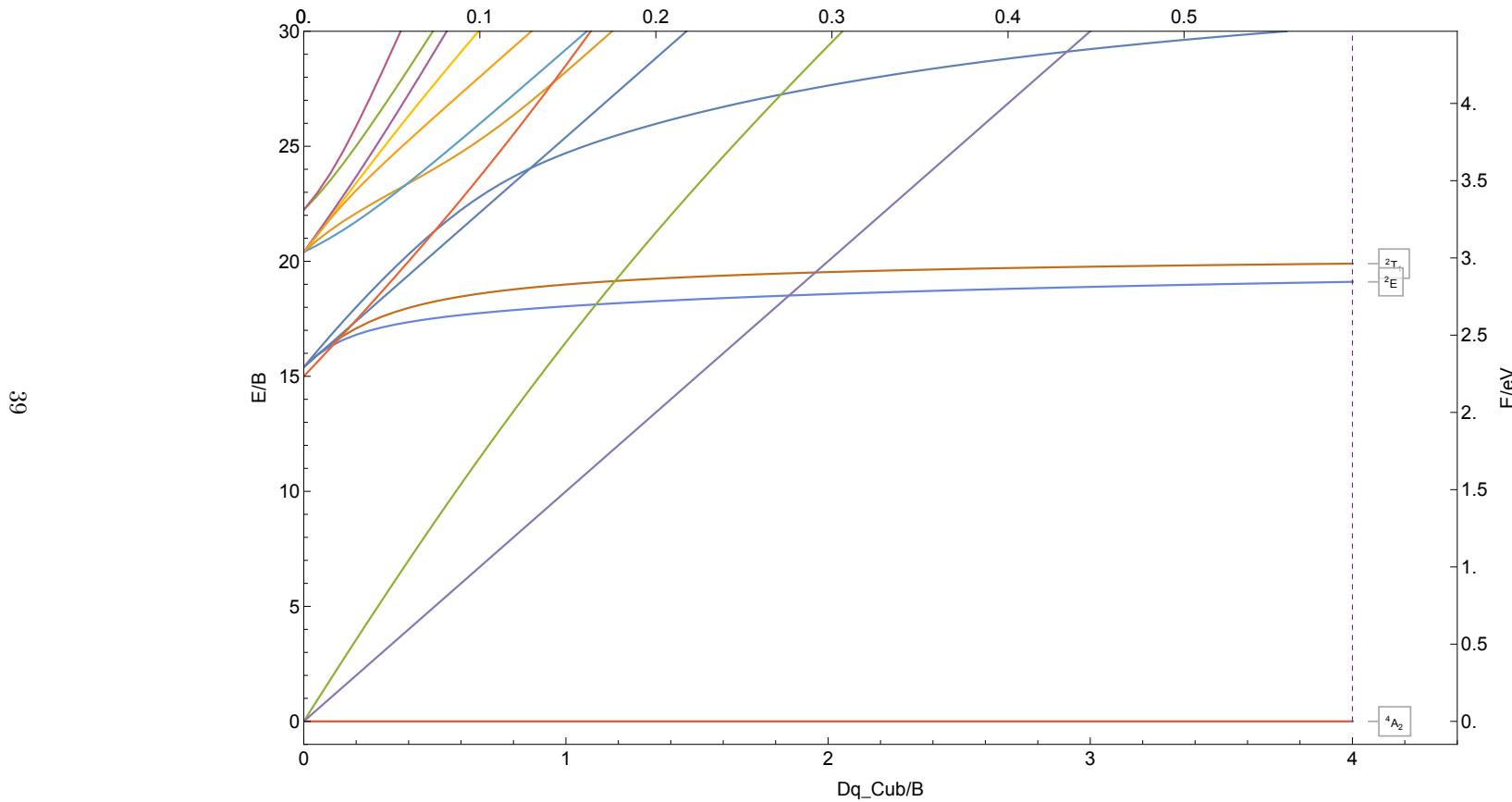
### 8.1.13 Fe<sup>4+</sup>

$|1,3,5|d^4|C/B \approx 3.8|B \approx 1122\text{ cm}^{-1}|Fe^{4+}$



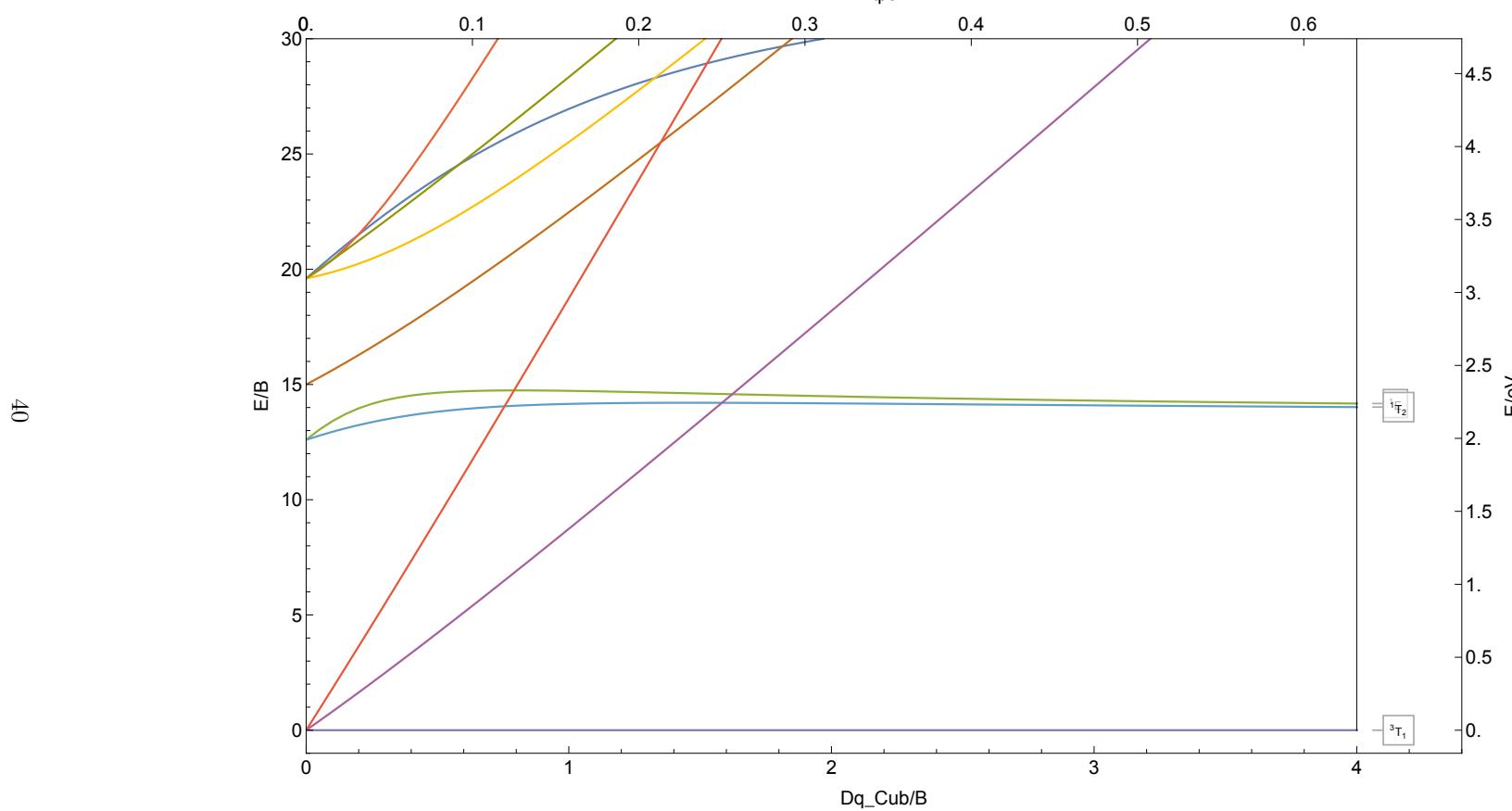
### 8.1.14 Fe<sup>5+</sup>

$$|2,4|d^3|C/B \approx 3.8|B \approx 1201\text{cm}^{-1}|Fe^{5+}$$



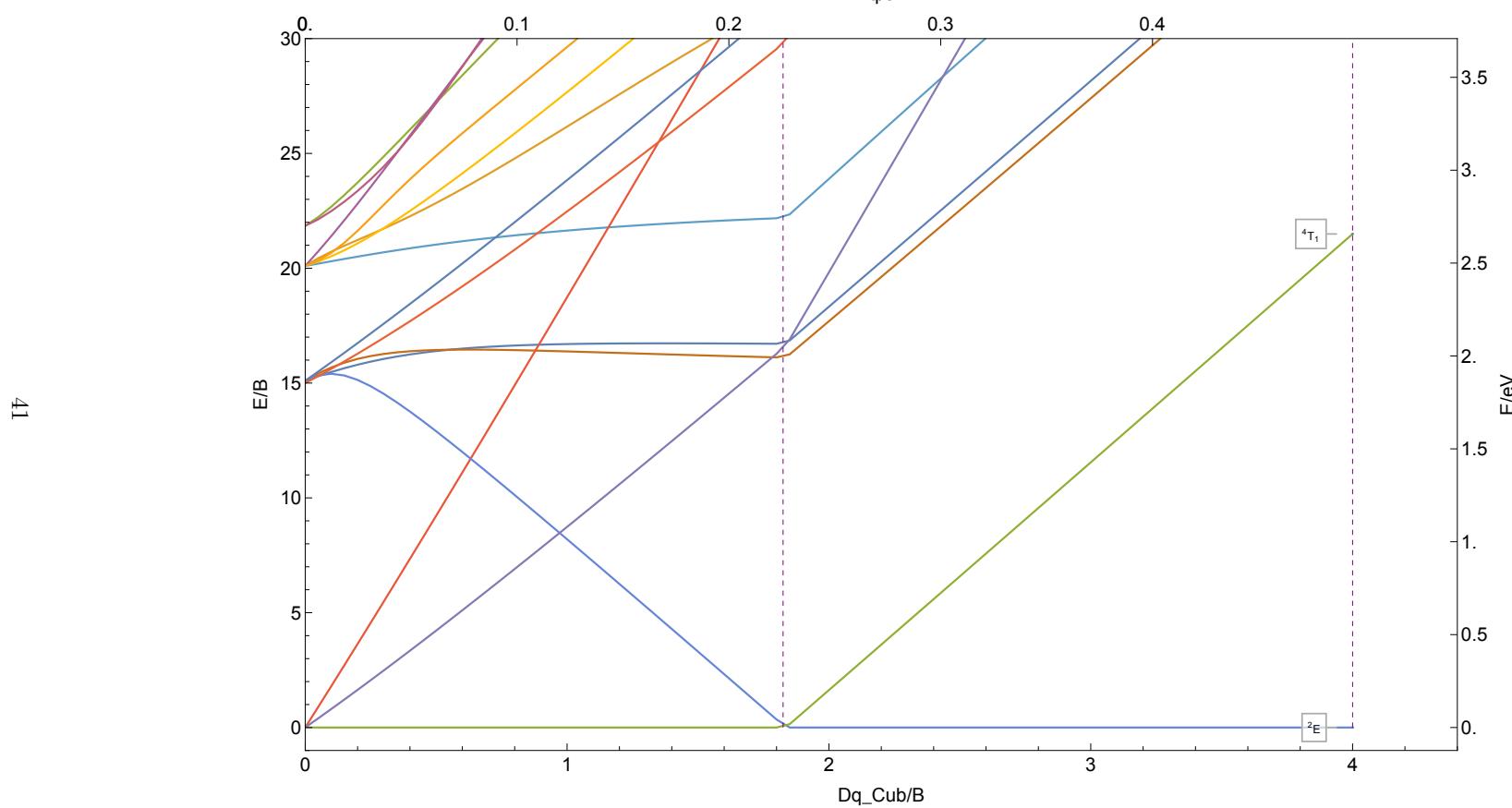
### 8.1.15 Fe<sup>6+</sup>

$|1,3|d^2|C/B \approx 3.8|B \approx 1274\text{ cm}^{-1}|Fe^{6+}$



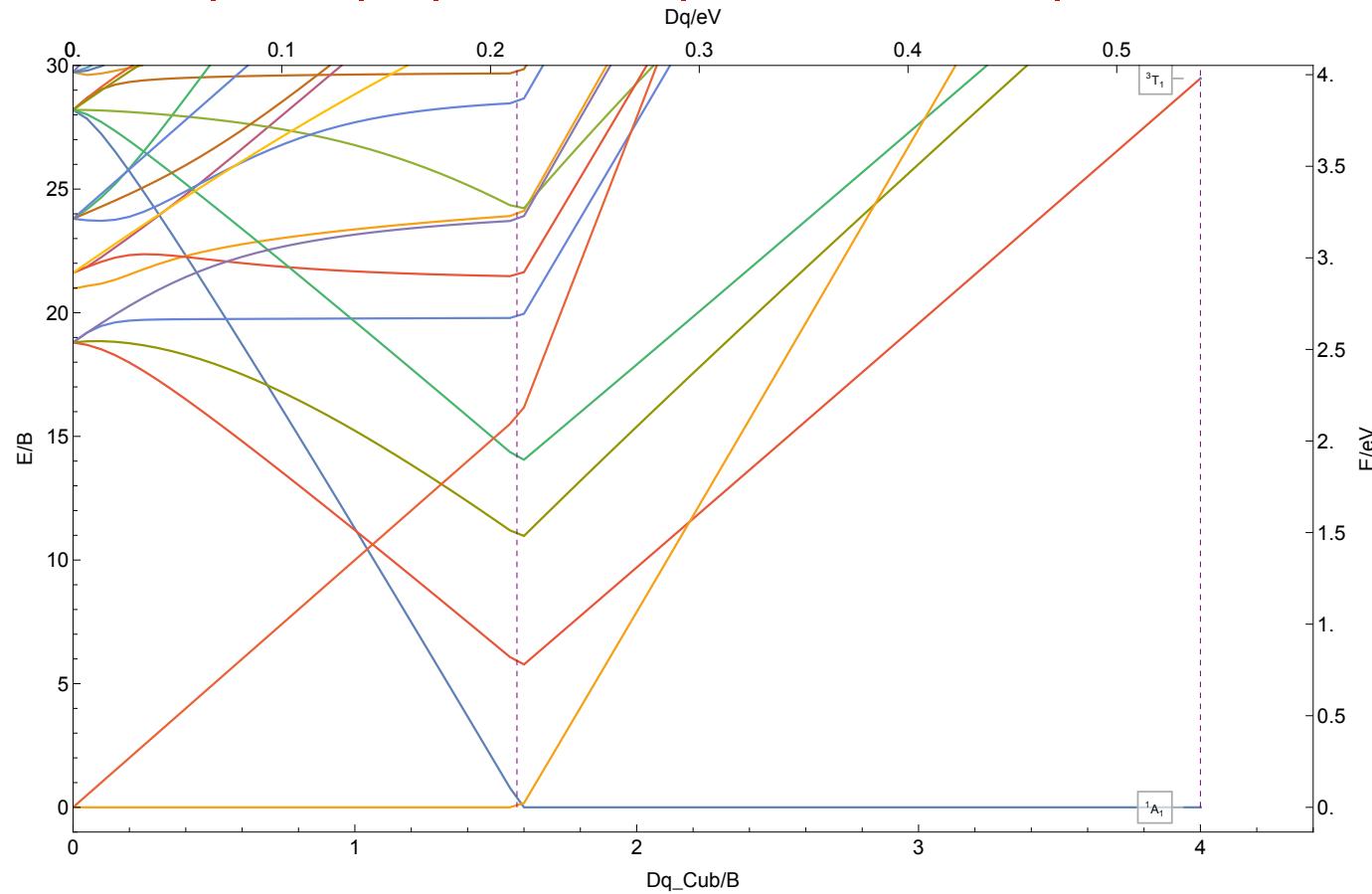
### 8.1.16 Co<sup>2+</sup>

$|2,4|d^7|C/B \approx 3.7| B \approx 997\text{ cm}^{-1}|Co^{2+}$



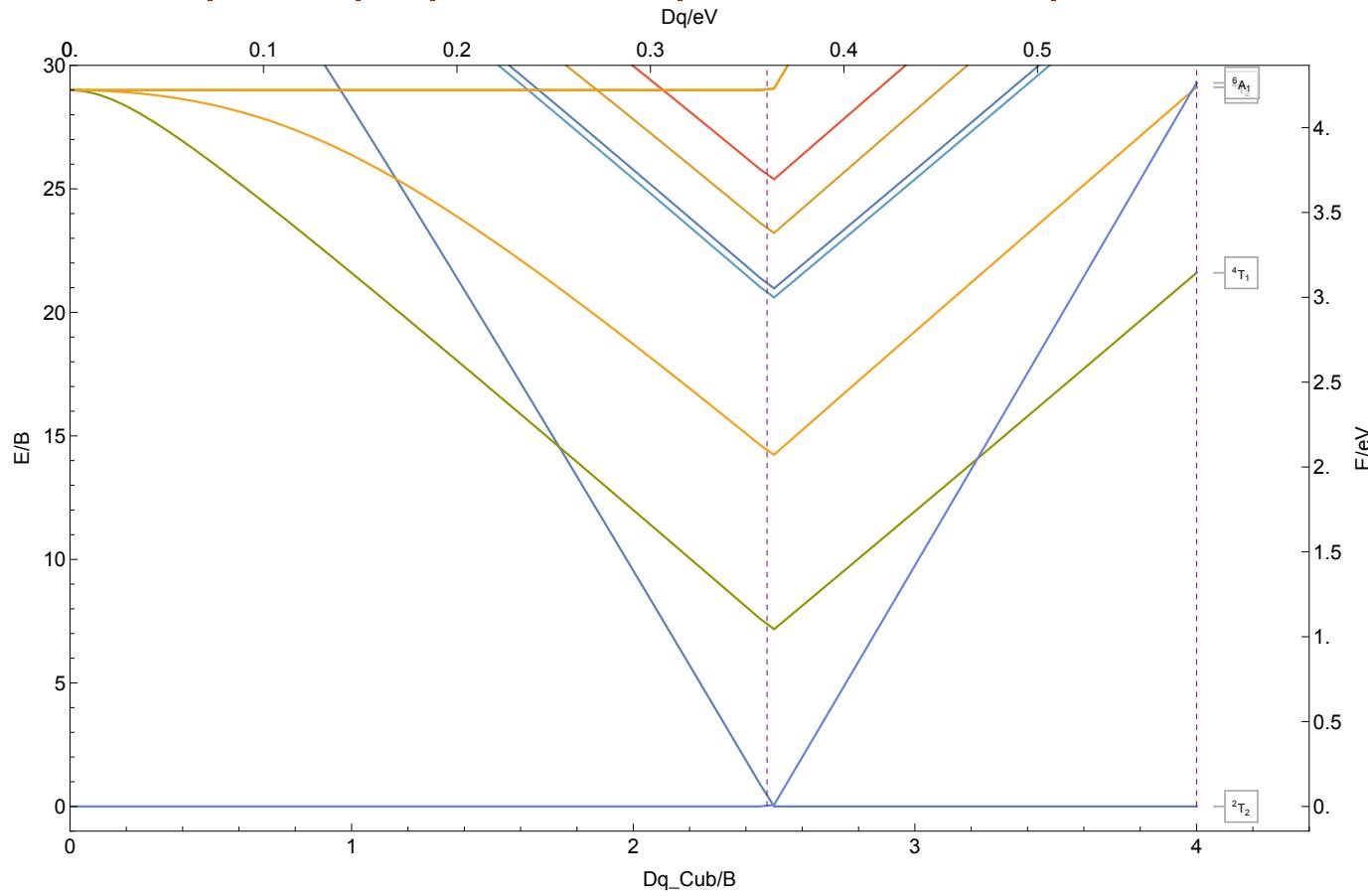
8.1.17  $\text{Co}^{3+}$

$|1,3,5| \text{d}^6 | \text{C/B} \approx 3.7 | \text{B} \approx 1089 \text{ cm}^{-1} | \text{Co}^{3+}$



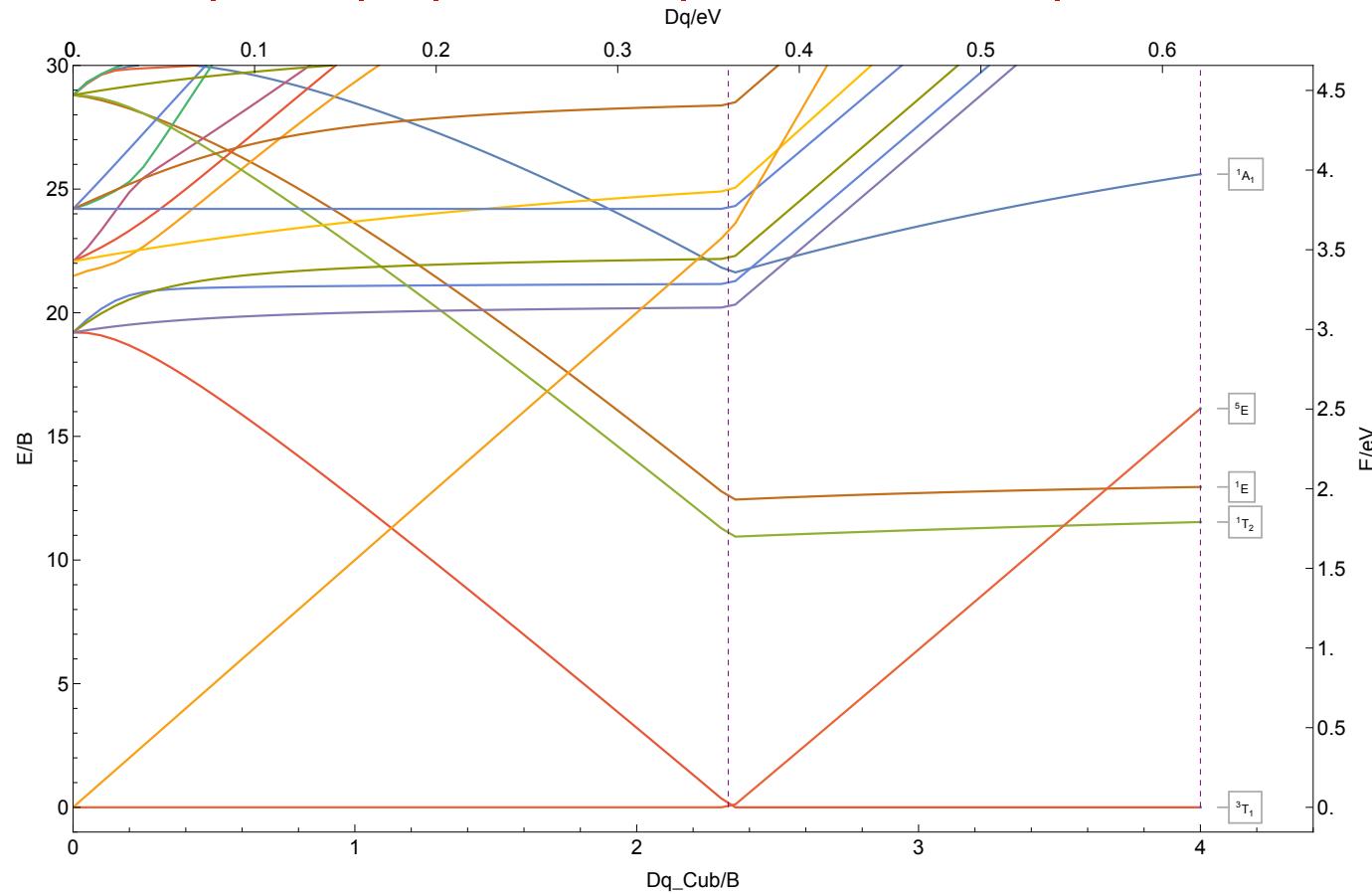
8.1.18  $\text{Co}^{4+}$

$|2,4,6| \text{d}^5 | \text{C/B} \approx 3.8 | \text{B} \approx 1174 \text{ cm}^{-1} | \text{Co}^{4+}$



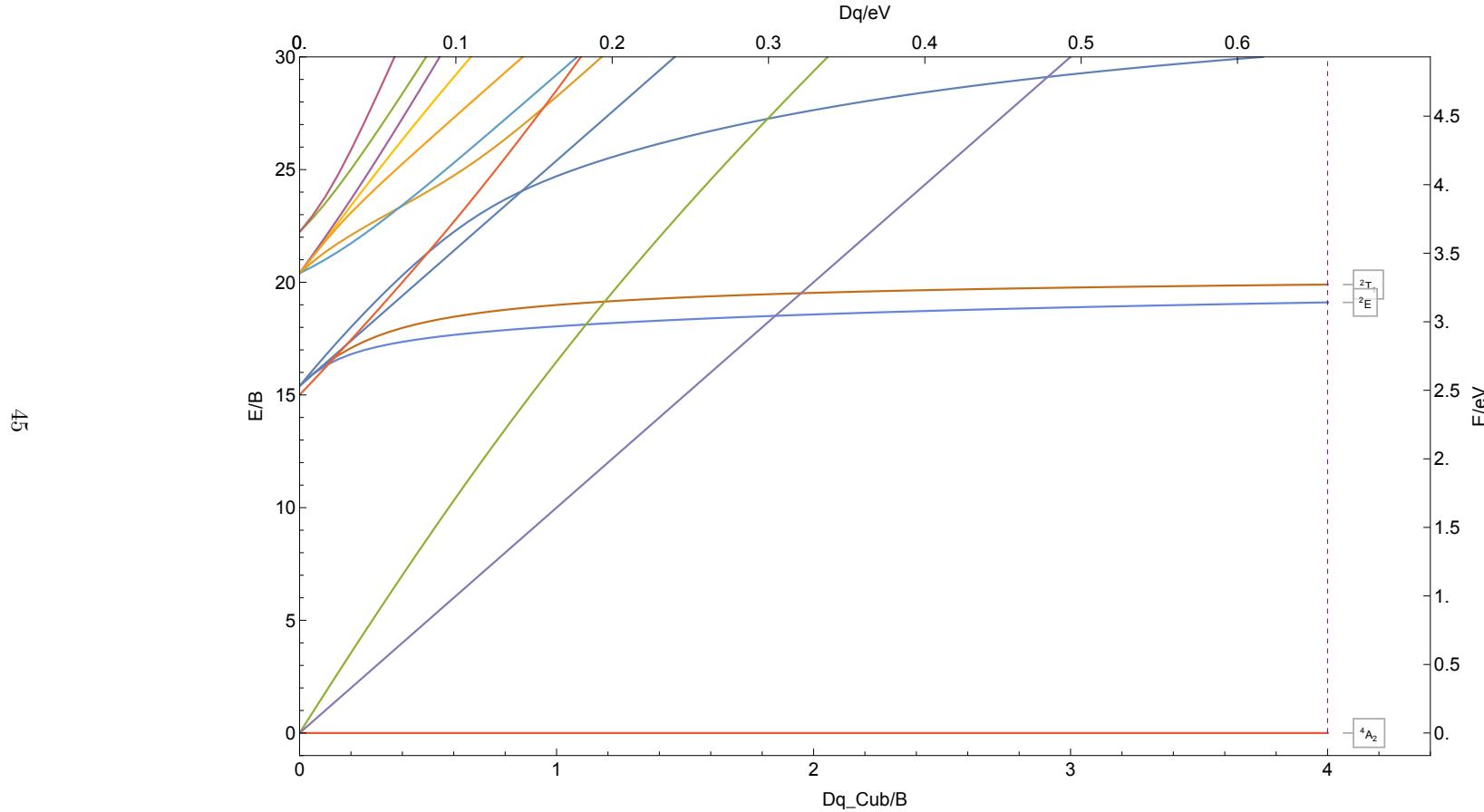
8.1.19  $\text{Co}^{5+}$

$|1,3,5|d^4|C/B \approx 3.8|B \approx 1252\text{ cm}^{-1}| \text{Co}^{5+}$



8.1.20 Co<sup>6+</sup>

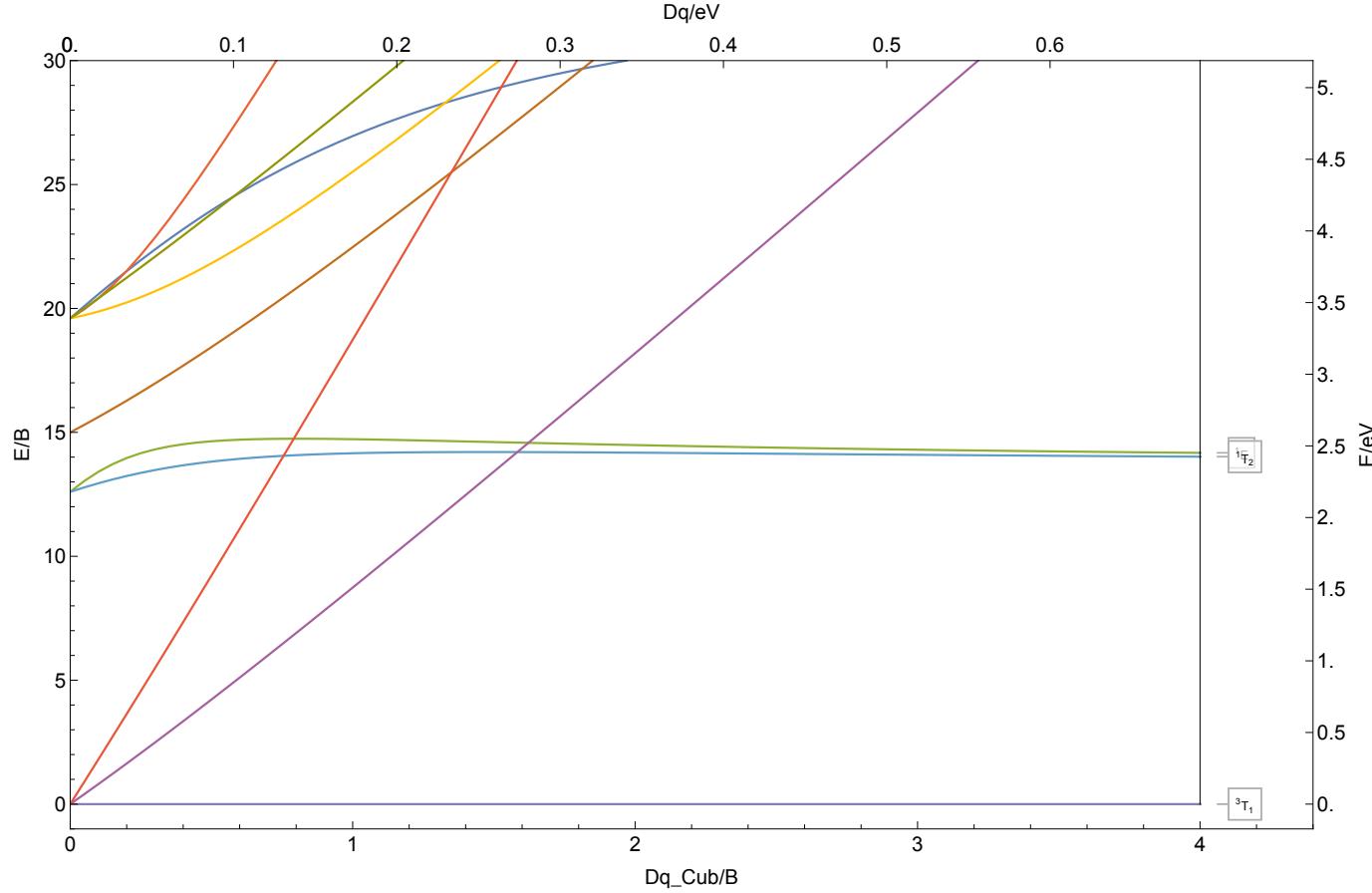
|2,4|d<sup>3</sup>|C/B ≈ 3.8|B ≈ 1326 cm<sup>-1</sup>|Co<sup>6+</sup>



8.1.21 Co<sup>7+</sup>

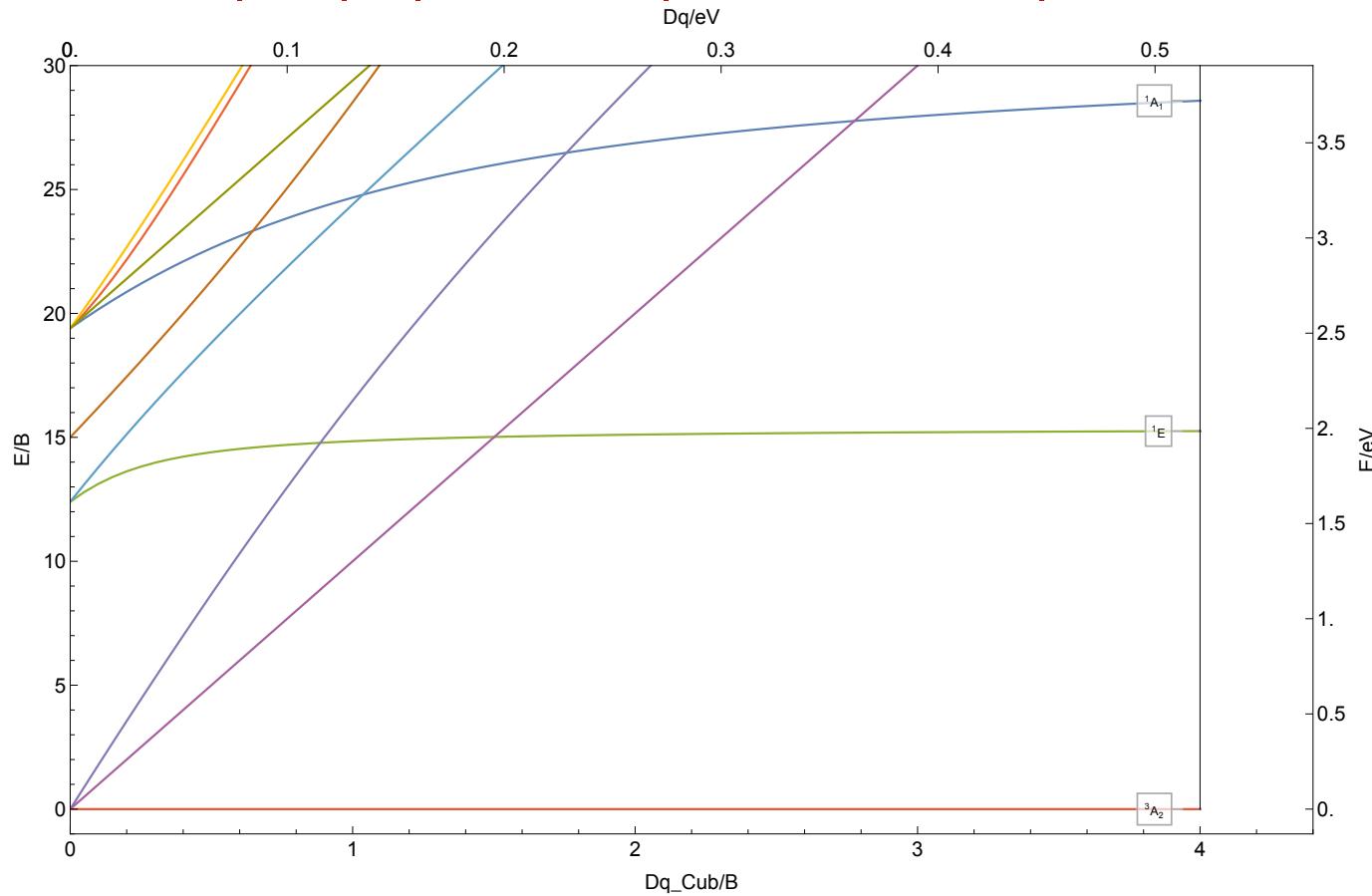
| 1,3 | d<sup>2</sup> | C/B ≈ 3.8 | B ≈ 1395 cm<sup>-1</sup> | Co<sup>7+</sup>

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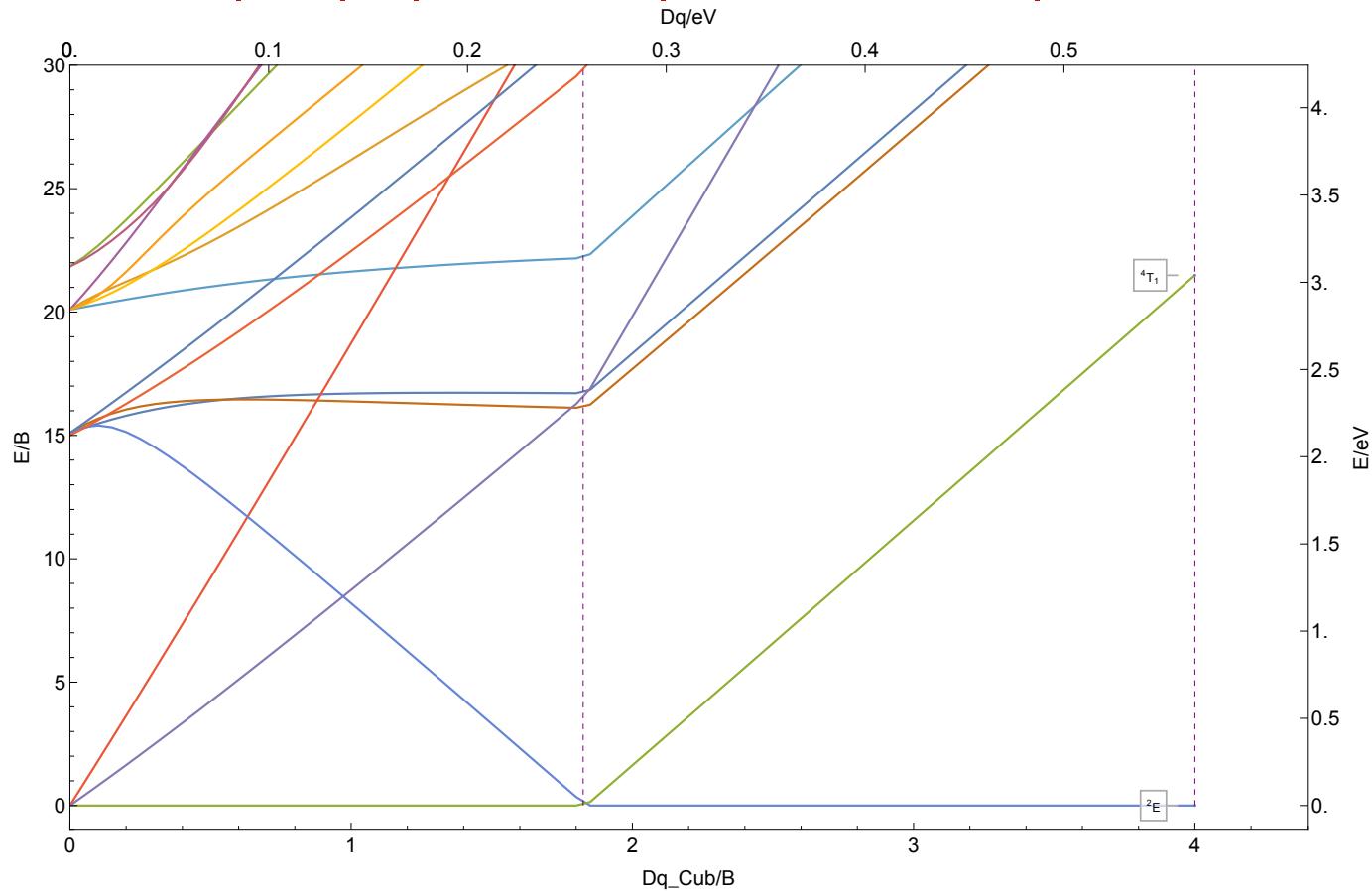
8.1.22  $\text{Ni}^{2+}$

$|1,3|d^8| \text{C/B} \approx 3.7 | \text{B} \approx 1050 \text{ cm}^{-1} | \text{Ni}^{2+}$



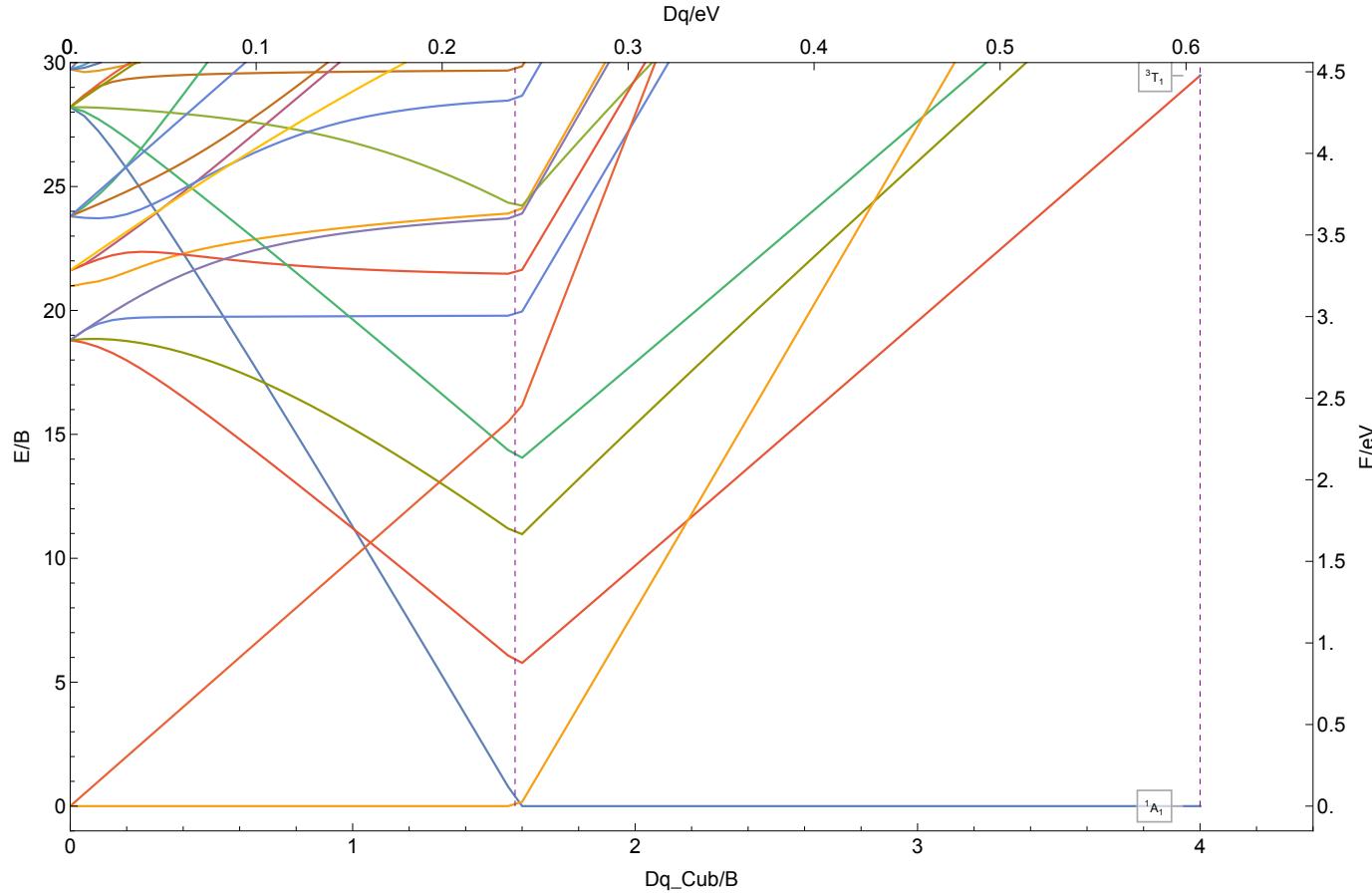
8.1.23 Ni<sup>3+</sup>

|2,4|d<sup>7</sup>| C/B ≈ 3.7| B ≈ 1141 cm<sup>-1</sup> | Ni<sup>3+</sup>



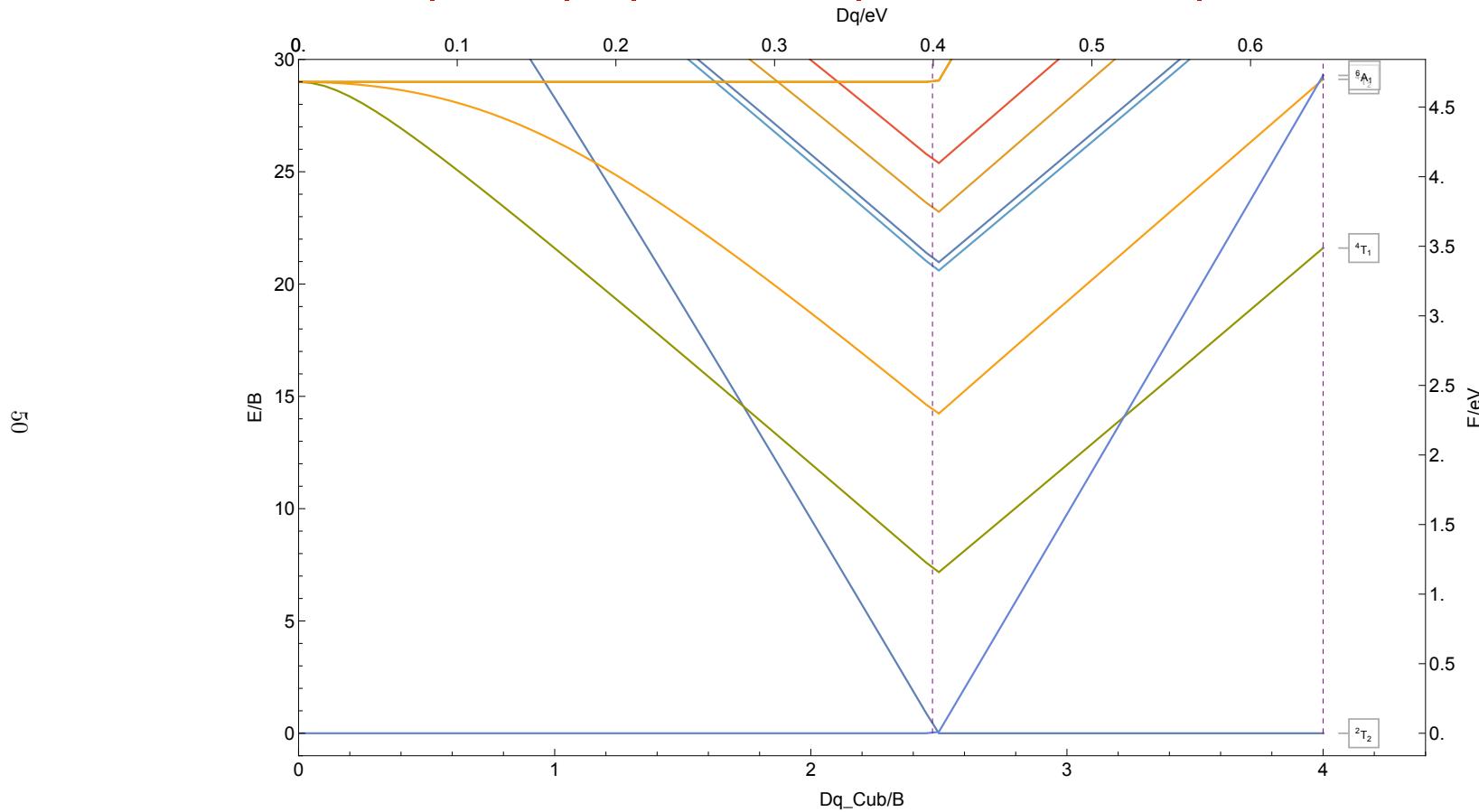
8.1.24 Ni<sup>4+</sup>

$|1,3,5|d^6|C/B \approx 3.7|B \approx 1225\text{ cm}^{-1}|Ni^{4+}$



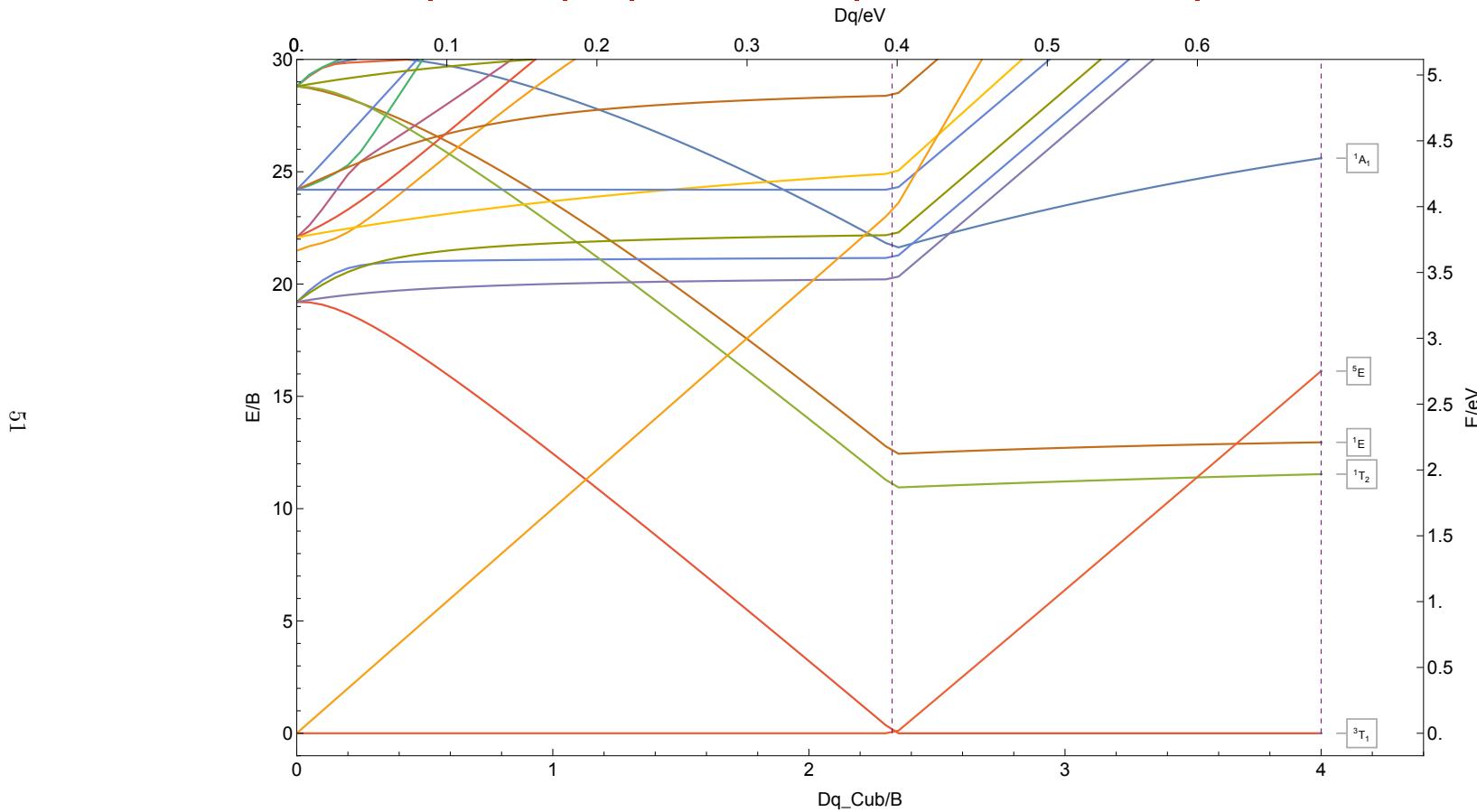
8.1.25 Ni<sup>5+</sup>

|2,4,6|d<sup>5</sup>|C/B ≈ 3.8|B ≈ 1302 cm<sup>-1</sup>|Ni<sup>5+</sup>



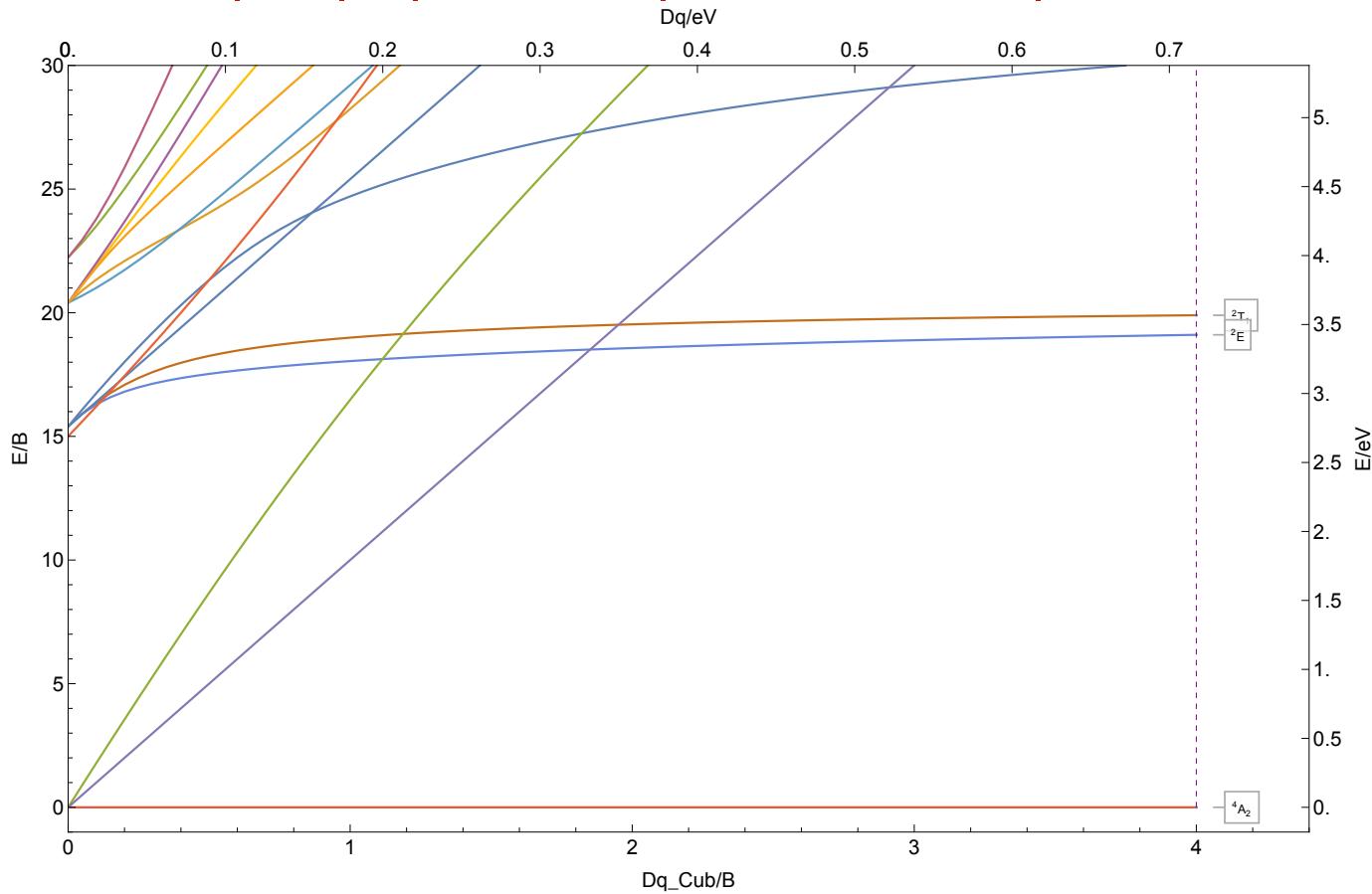
8.1.26 Ni<sup>6+</sup>

$|1,3,5|d^4|C/B \approx 3.8|B \approx 1376\text{ cm}^{-1}|Ni^{6+}$



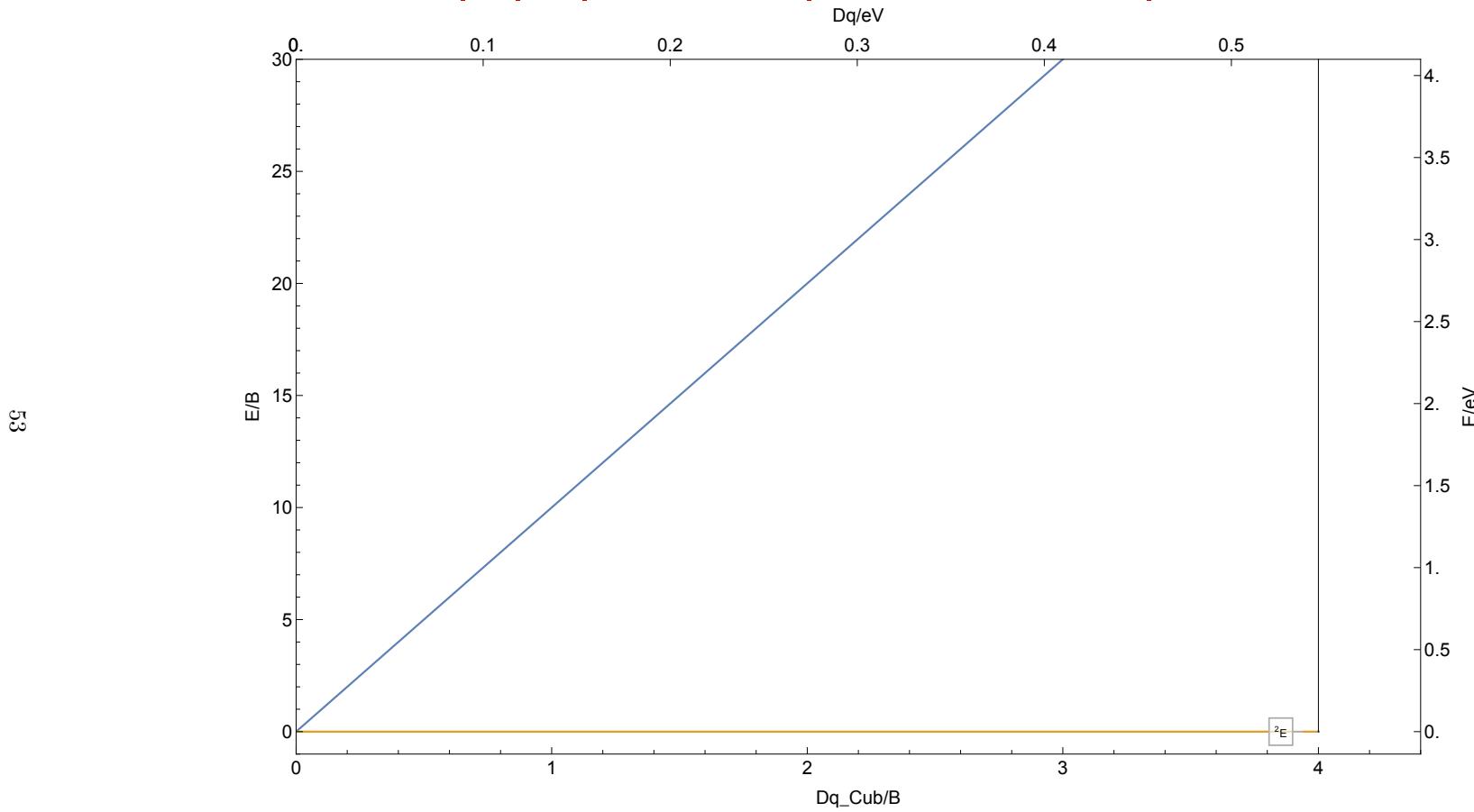
8.1.27 Ni<sup>7+</sup>

|2,4|d<sup>3</sup>| C/B ≈ 3.8 | B ≈ 1446 cm<sup>-1</sup> | Ni<sup>7+</sup>



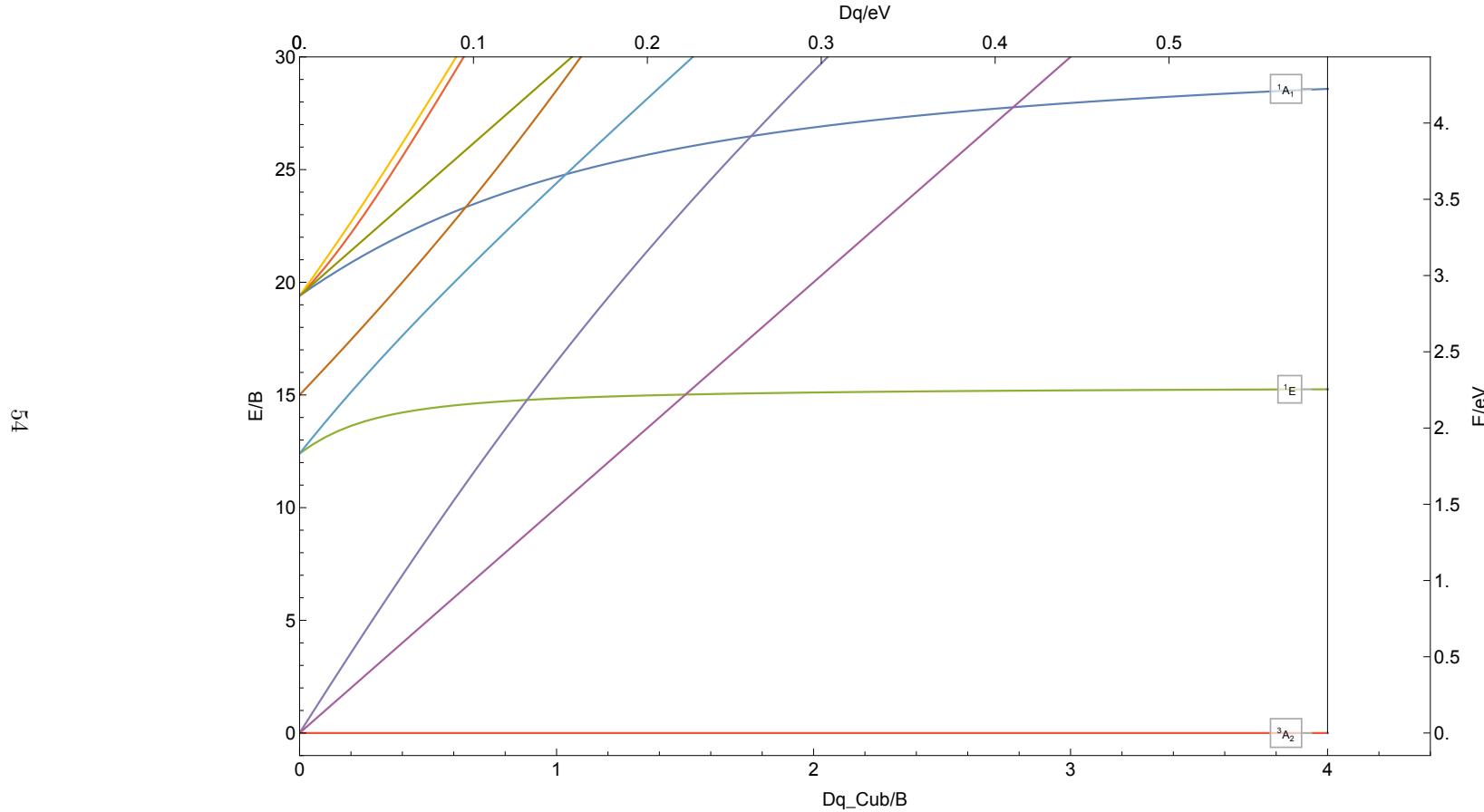
8.1.28 Cu<sup>2+</sup>

|2|d<sup>9</sup>|C/B ≈ 3.7|B ≈ 1102 cm<sup>-1</sup>|Cu<sup>2+</sup>



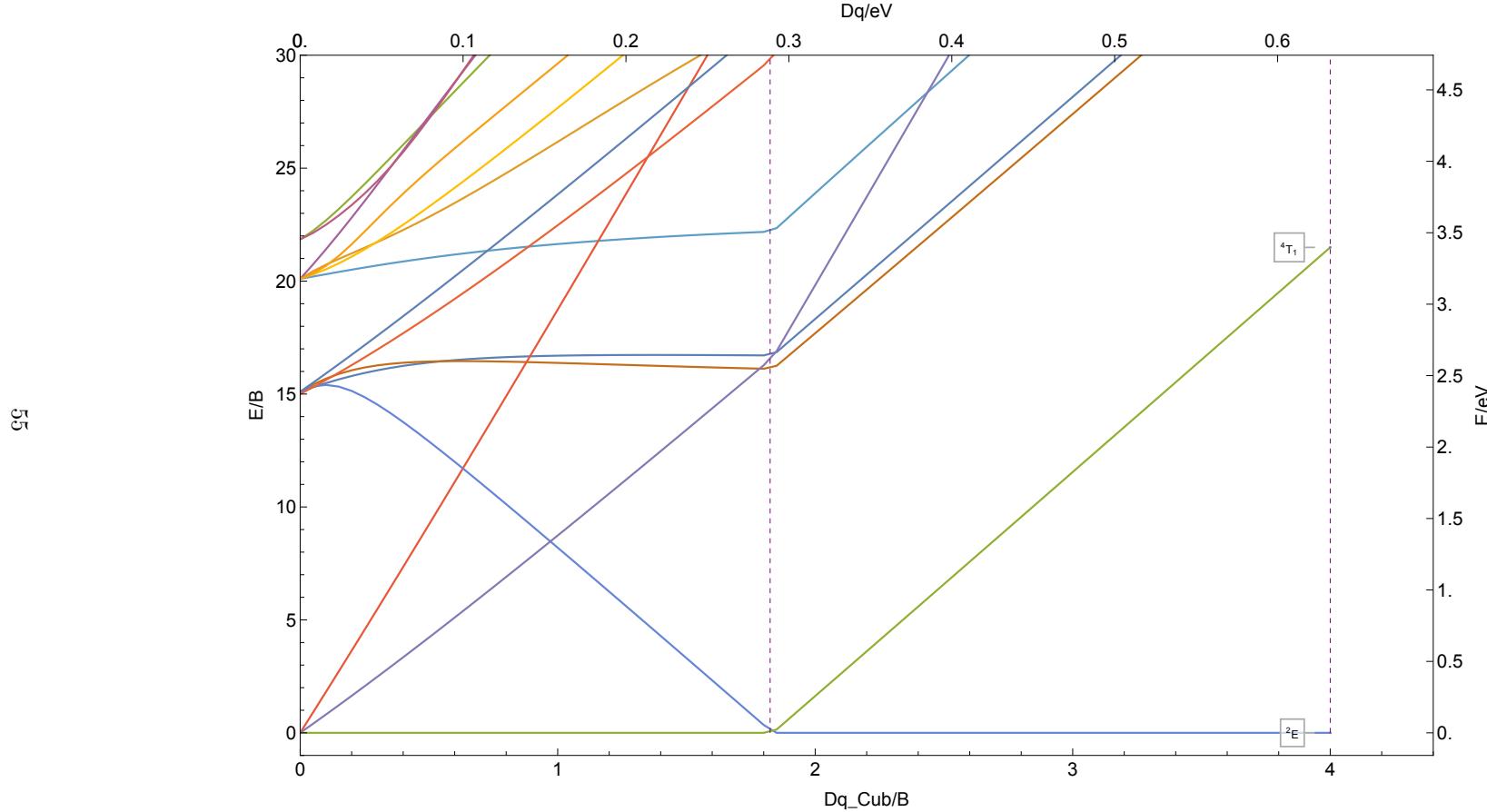
8.1.29 Cu<sup>3+</sup>

| 1,3 | d<sup>8</sup> | C/B ≈ 3.7 | B ≈ 1192 cm<sup>-1</sup> | Cu<sup>3+</sup>



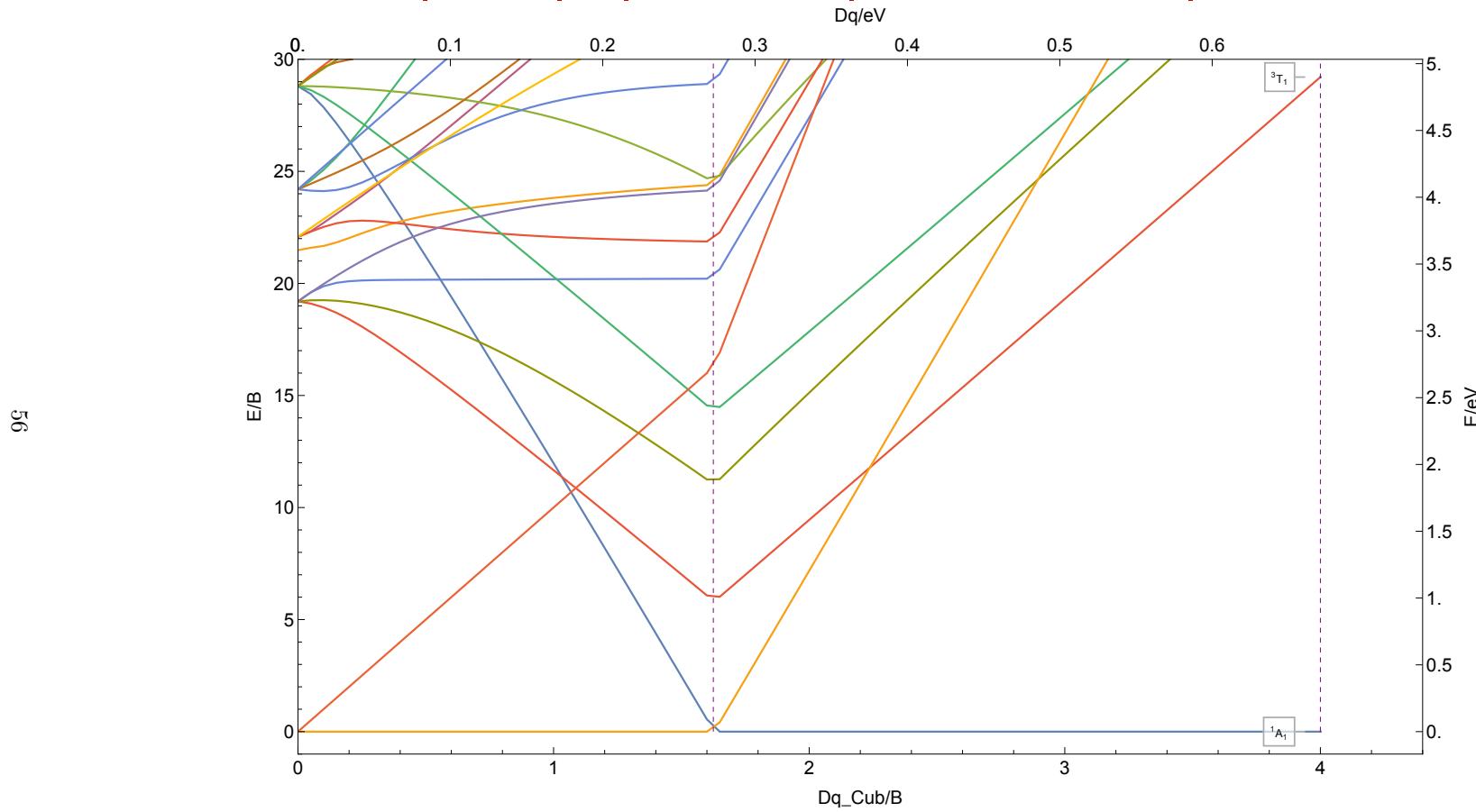
8.1.30 Cu<sup>4+</sup>

|2,4|d<sup>7</sup>|C/B ≈ 3.7|B ≈ 1275 cm<sup>-1</sup>|Cu<sup>4+</sup>



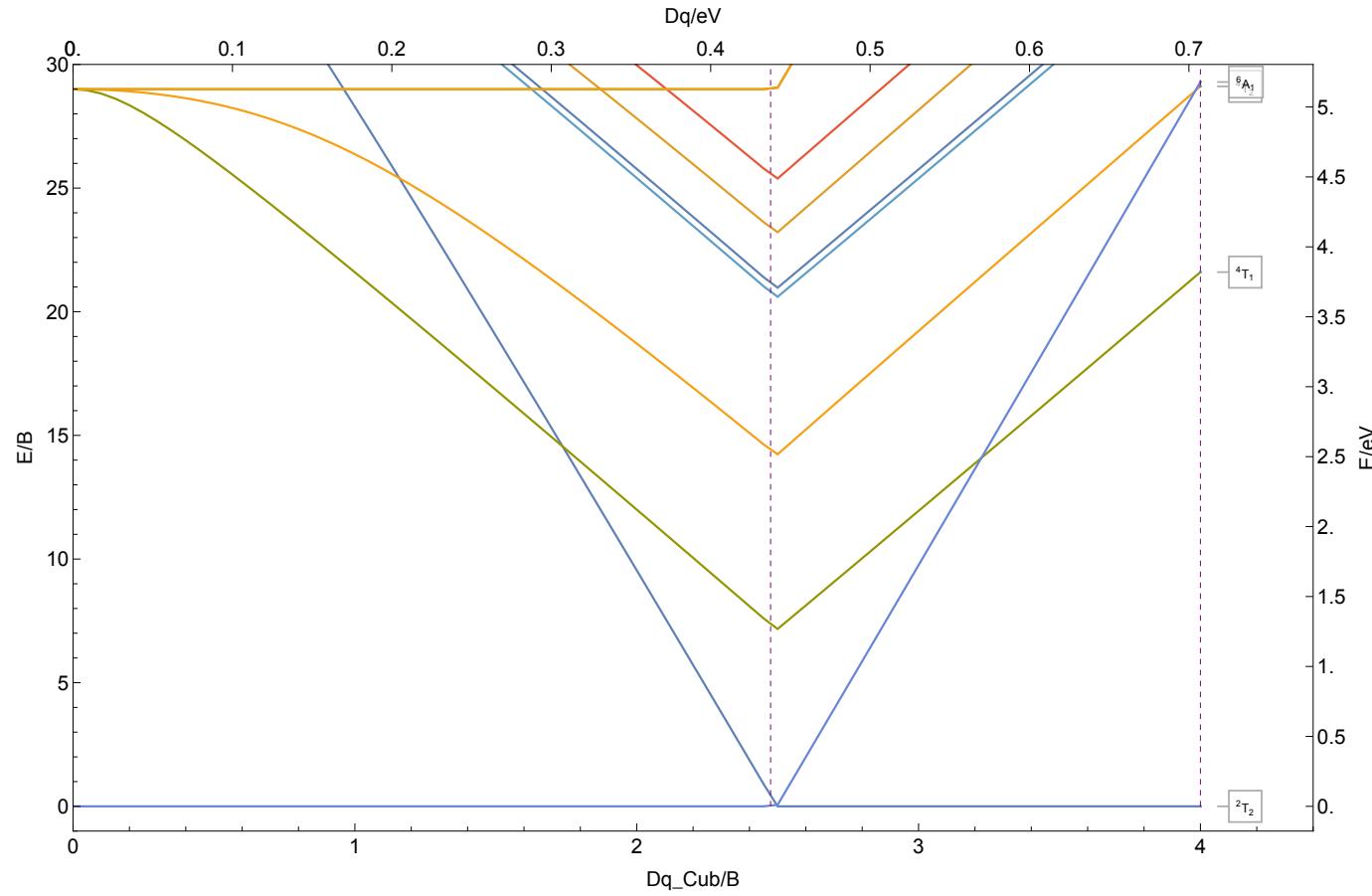
8.1.31 Cu<sup>5+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 3.8 | B ≈ 1353 cm<sup>-1</sup> | Cu<sup>5+</sup>



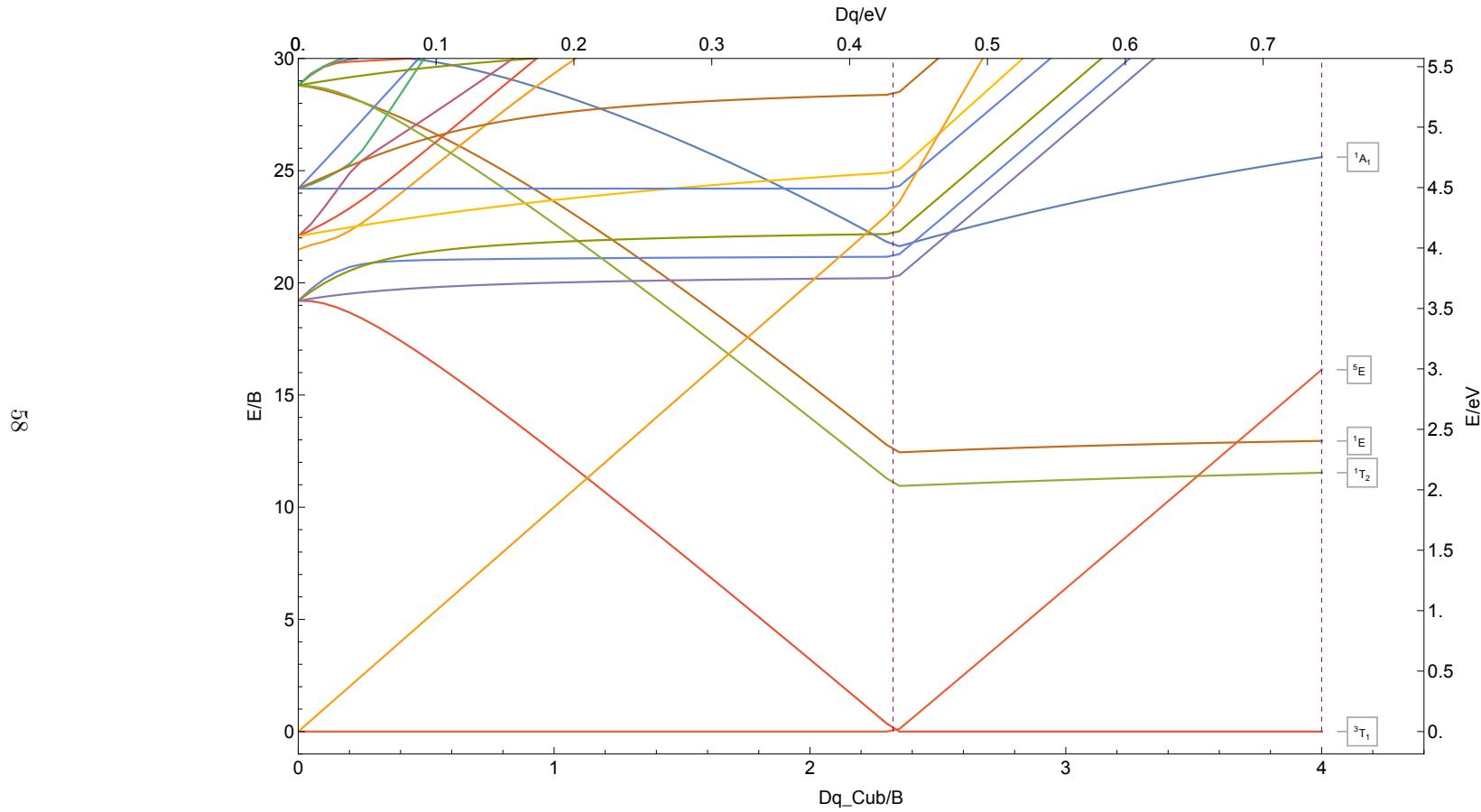
8.1.32 Cu<sup>6+</sup>

|2,4,6|d<sup>5</sup>|C/B ≈ 3.8|B ≈ 1426 cm<sup>-1</sup>|Cu<sup>6+</sup>



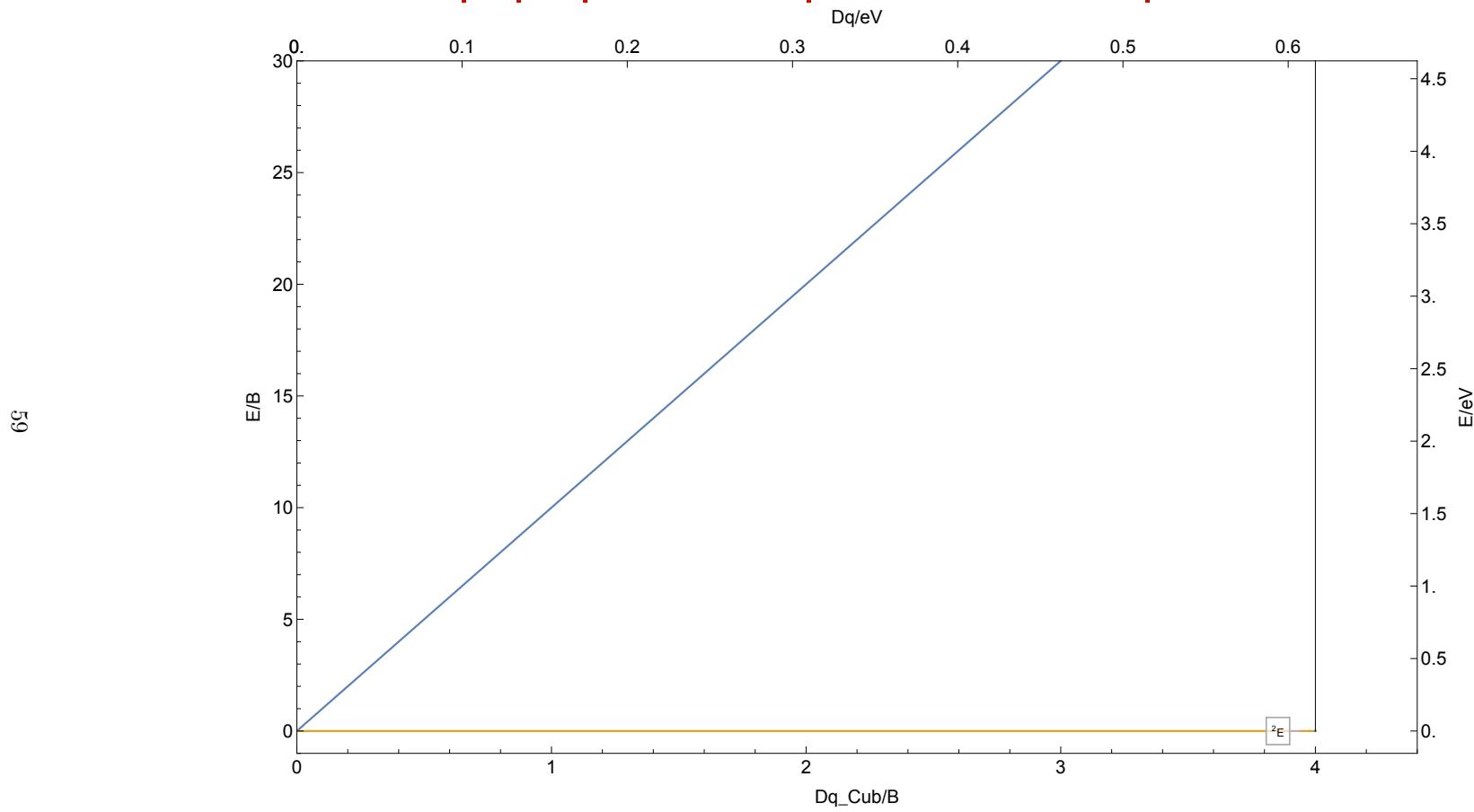
### 8.1.33 Cu<sup>7+</sup>

$|1,3,5|d^4|C/B \approx 3.8|B \approx 1497\text{ cm}^{-1}|Cu^{7+}$



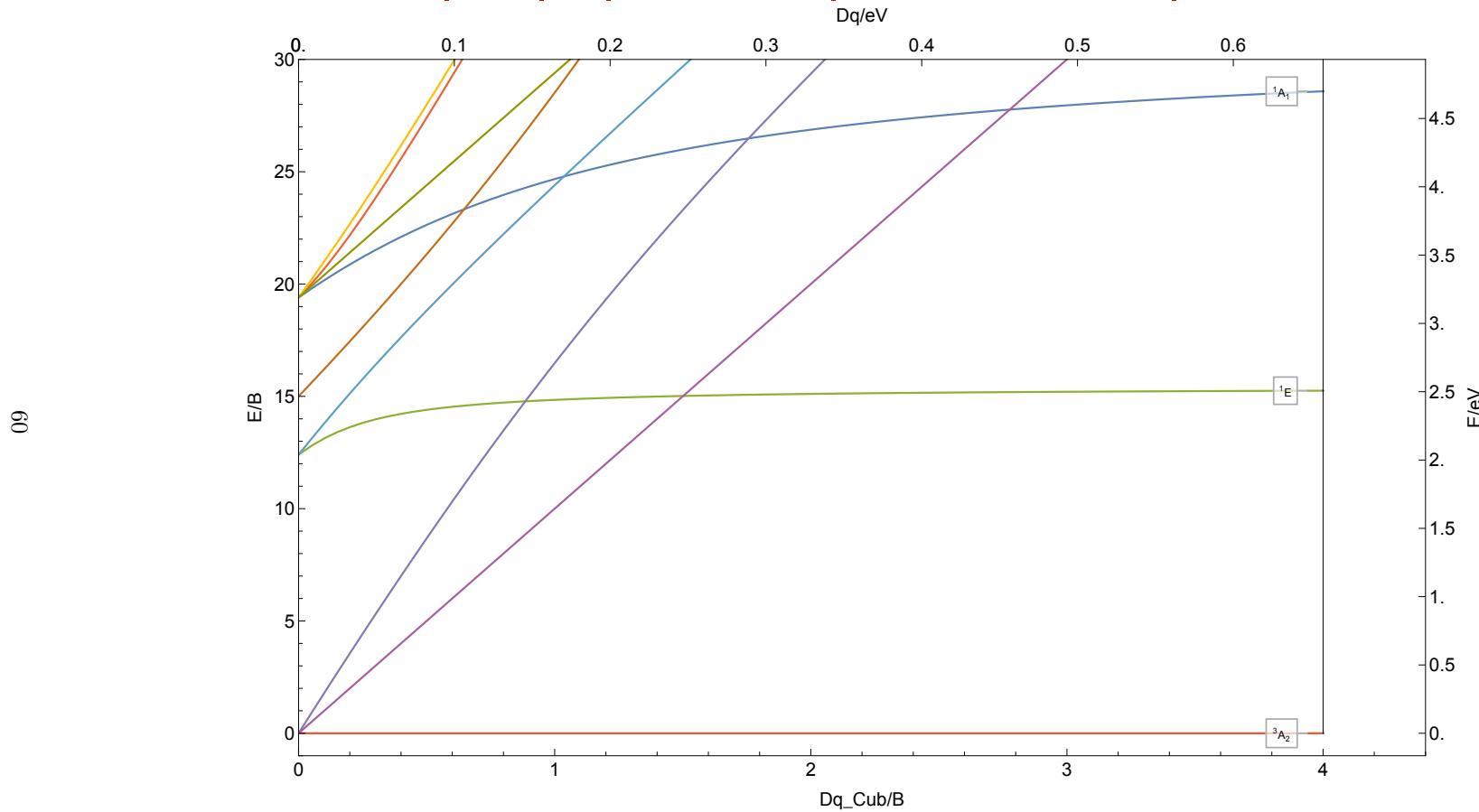
8.1.34 Zn<sup>3+</sup>

$$|2|d^9|C/B \approx 3.7|B \approx 1243\text{ cm}^{-1}|Zn^{3+}$$



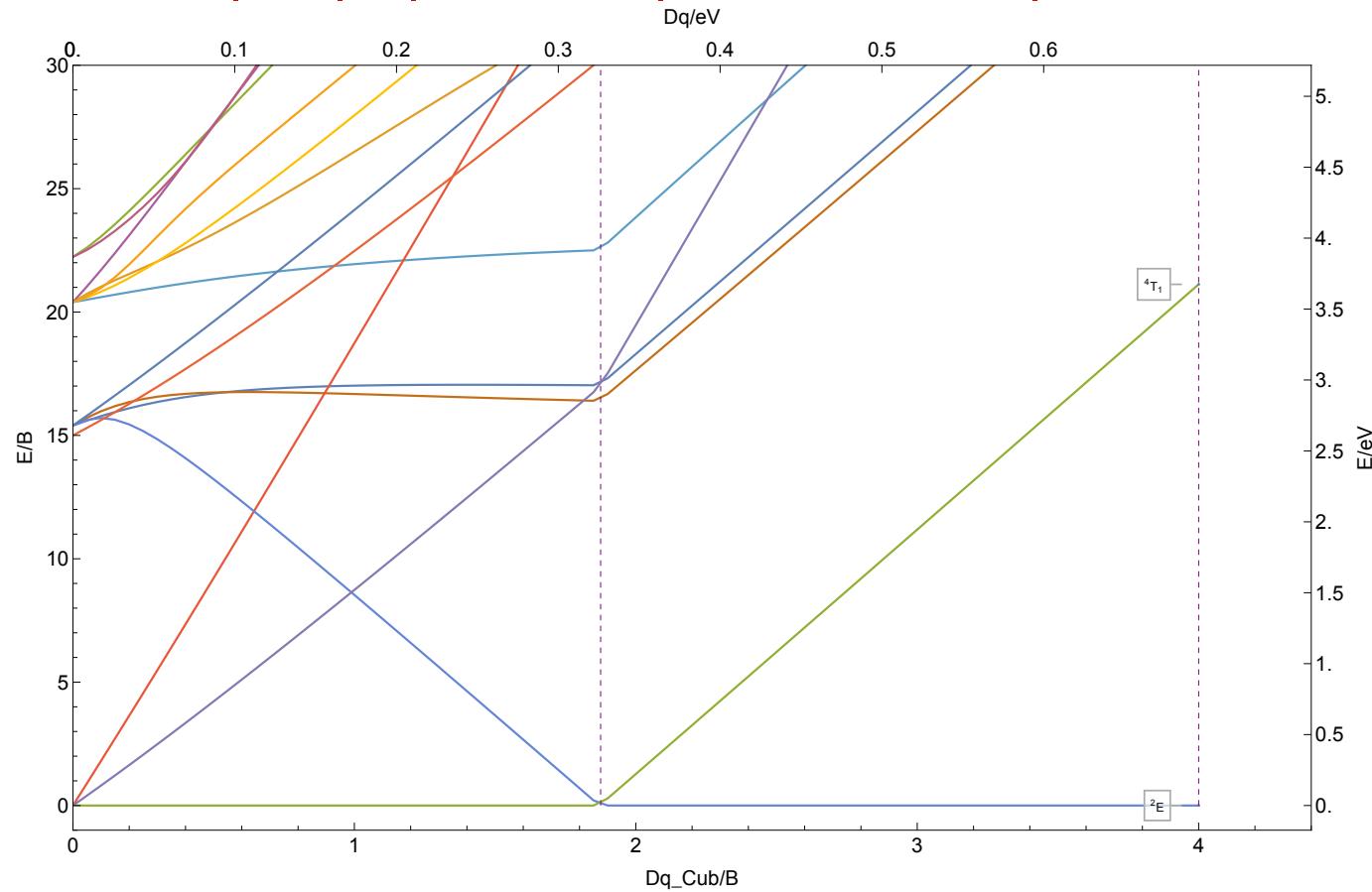
8.1.35 Zn<sup>4+</sup>

| 1,3 | d<sup>8</sup> | C/B ≈ 3.7 | B ≈ 1326 cm<sup>-1</sup> | Zn<sup>4+</sup>



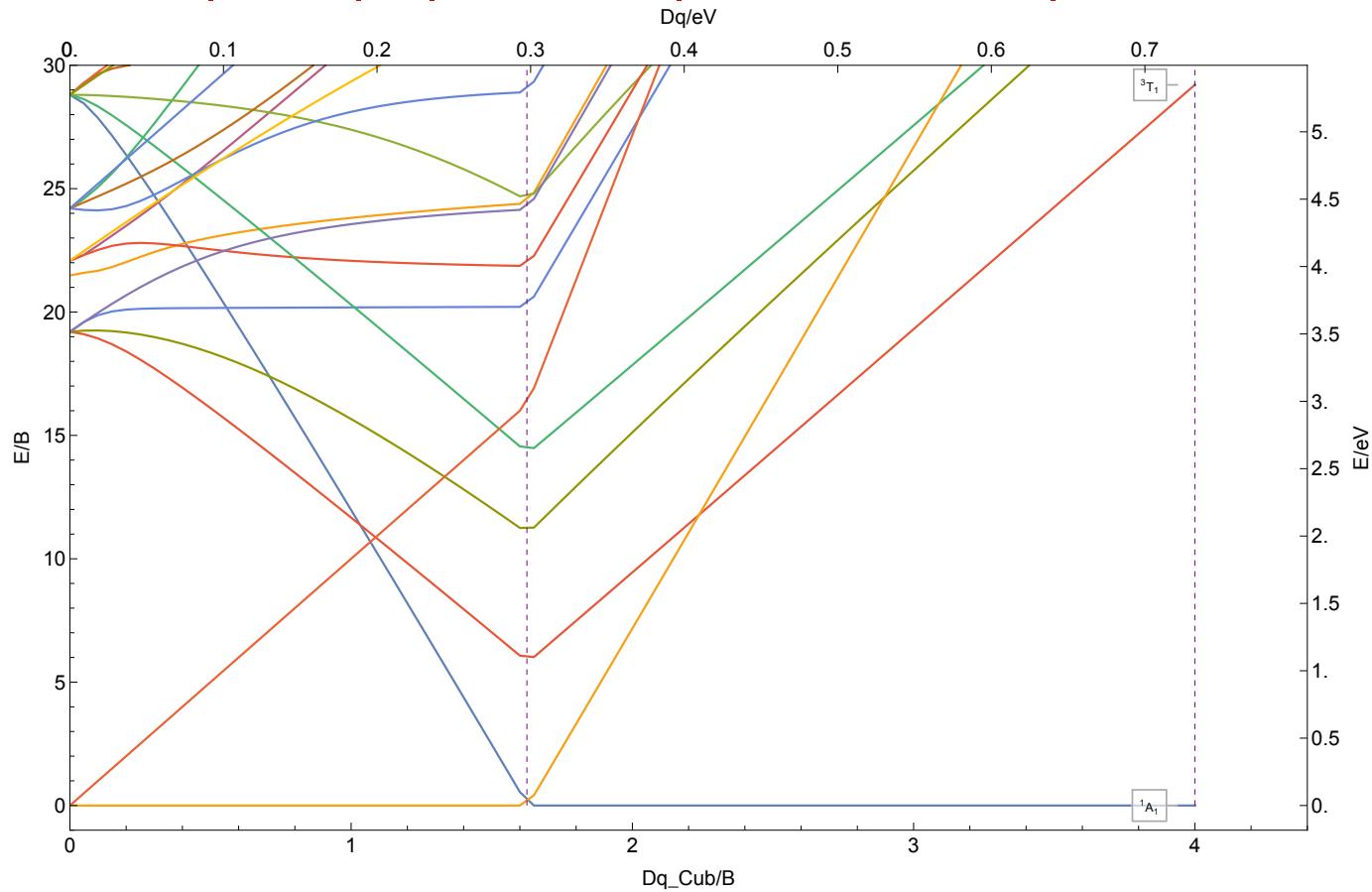
### 8.1.36 Zn<sup>5+</sup>

$|2,4|d^7|C/B \approx 3.8| B \approx 1403\text{ cm}^{-1}|Zn^{5+}$



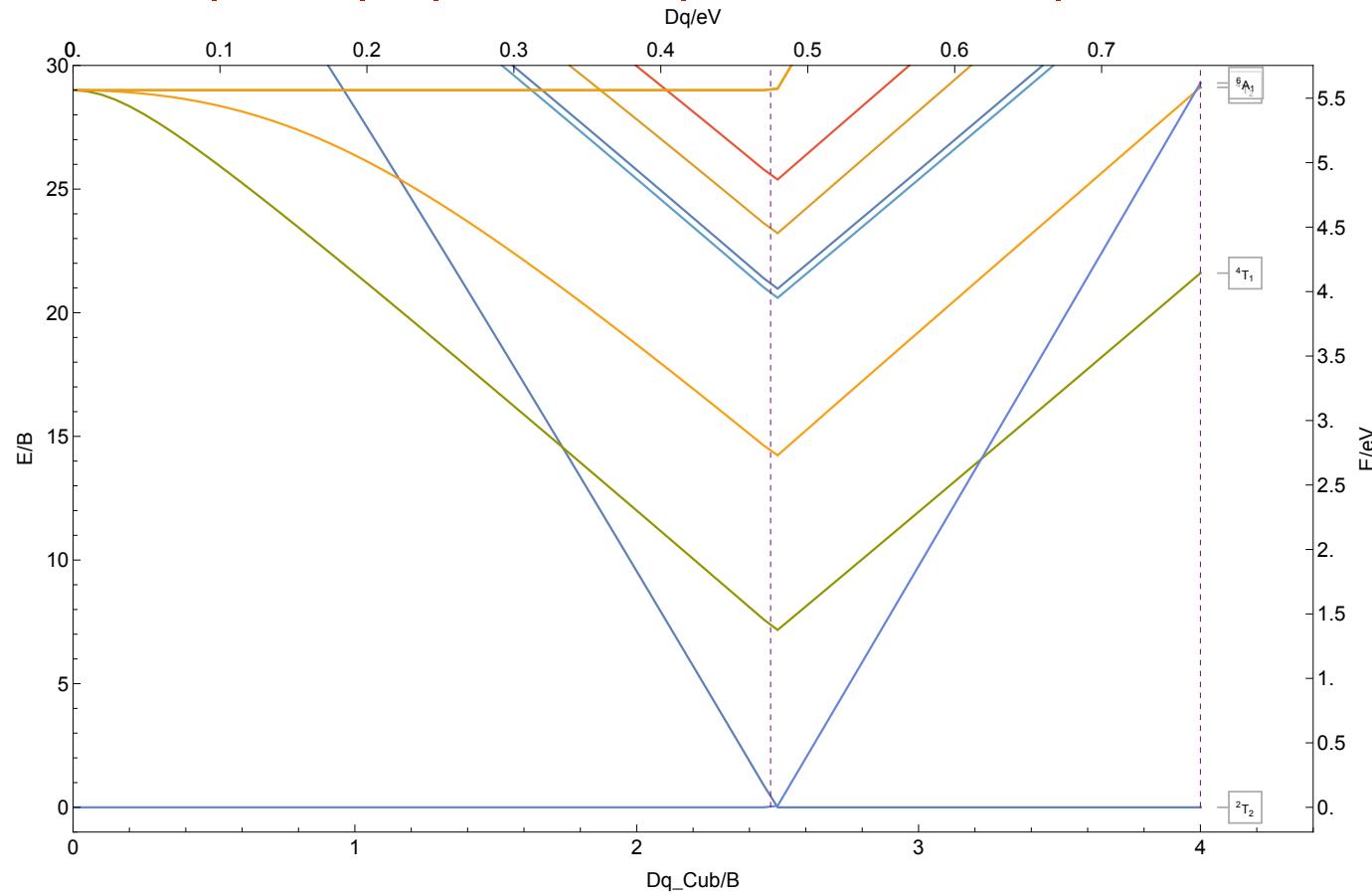
8.1.37 Zn<sup>6+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 3.8 | B ≈ 1477 cm<sup>-1</sup> | Zn<sup>6+</sup>



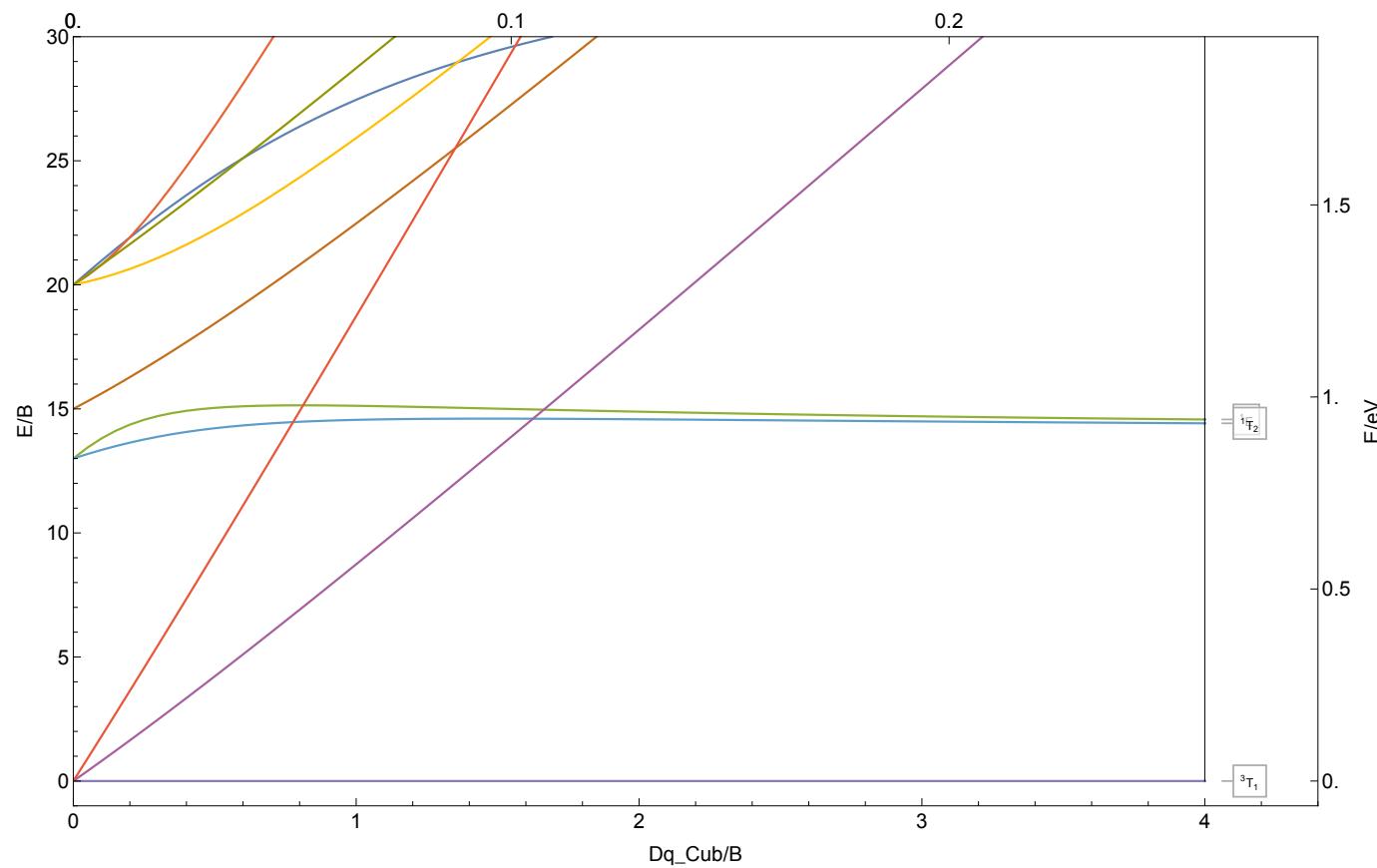
8.1.38 Zn<sup>7+</sup>

|2,4,6| d<sup>5</sup>| C/B ≈ 3.8| B ≈ 1547 cm<sup>-1</sup> | Zn<sup>7+</sup>



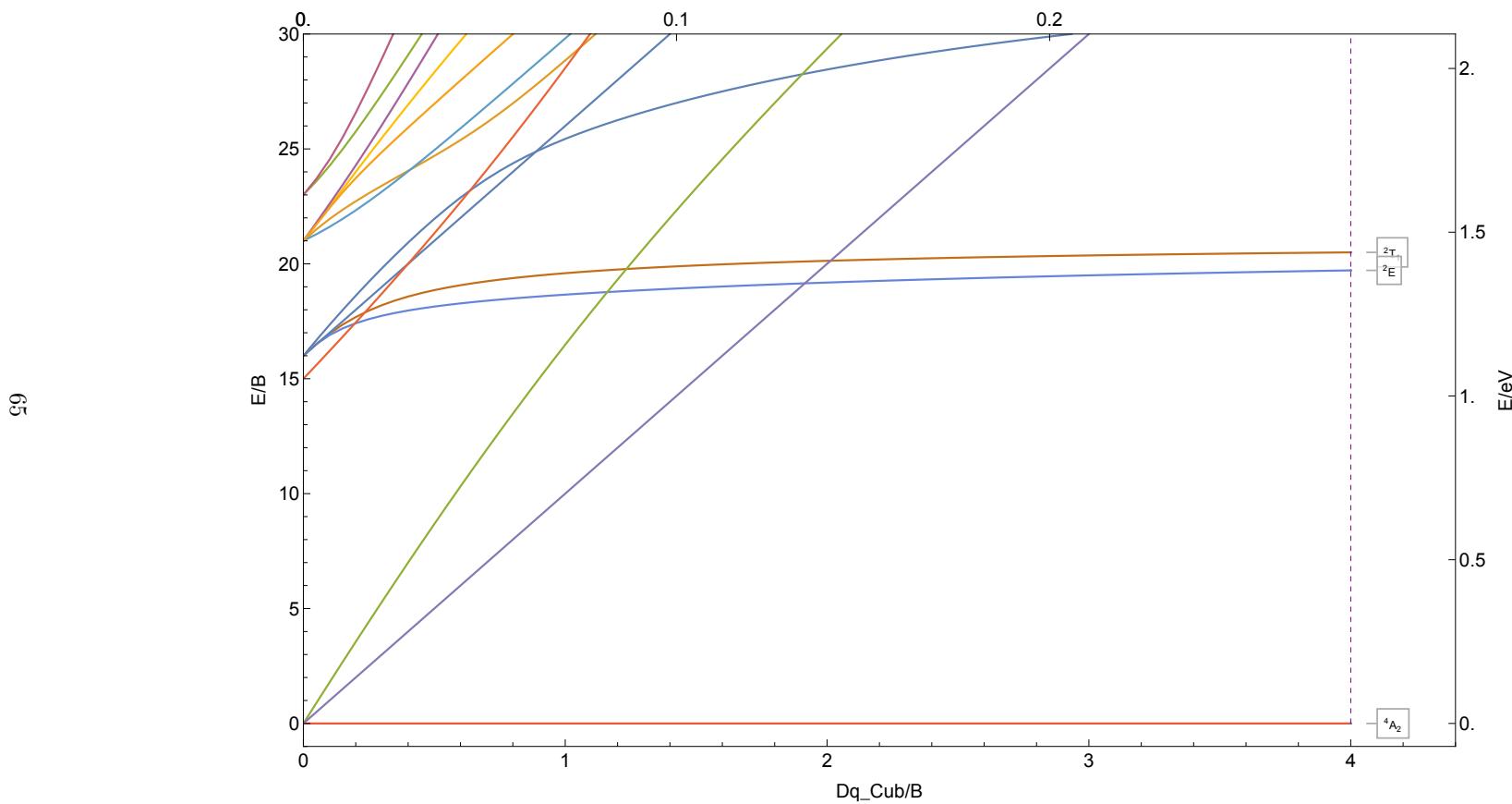
8.1.39 Zr<sup>2+</sup>

$|1,3|d^2|C/B \approx 4.|B \approx 521\text{ cm}^{-1}|Zr^{2+}$



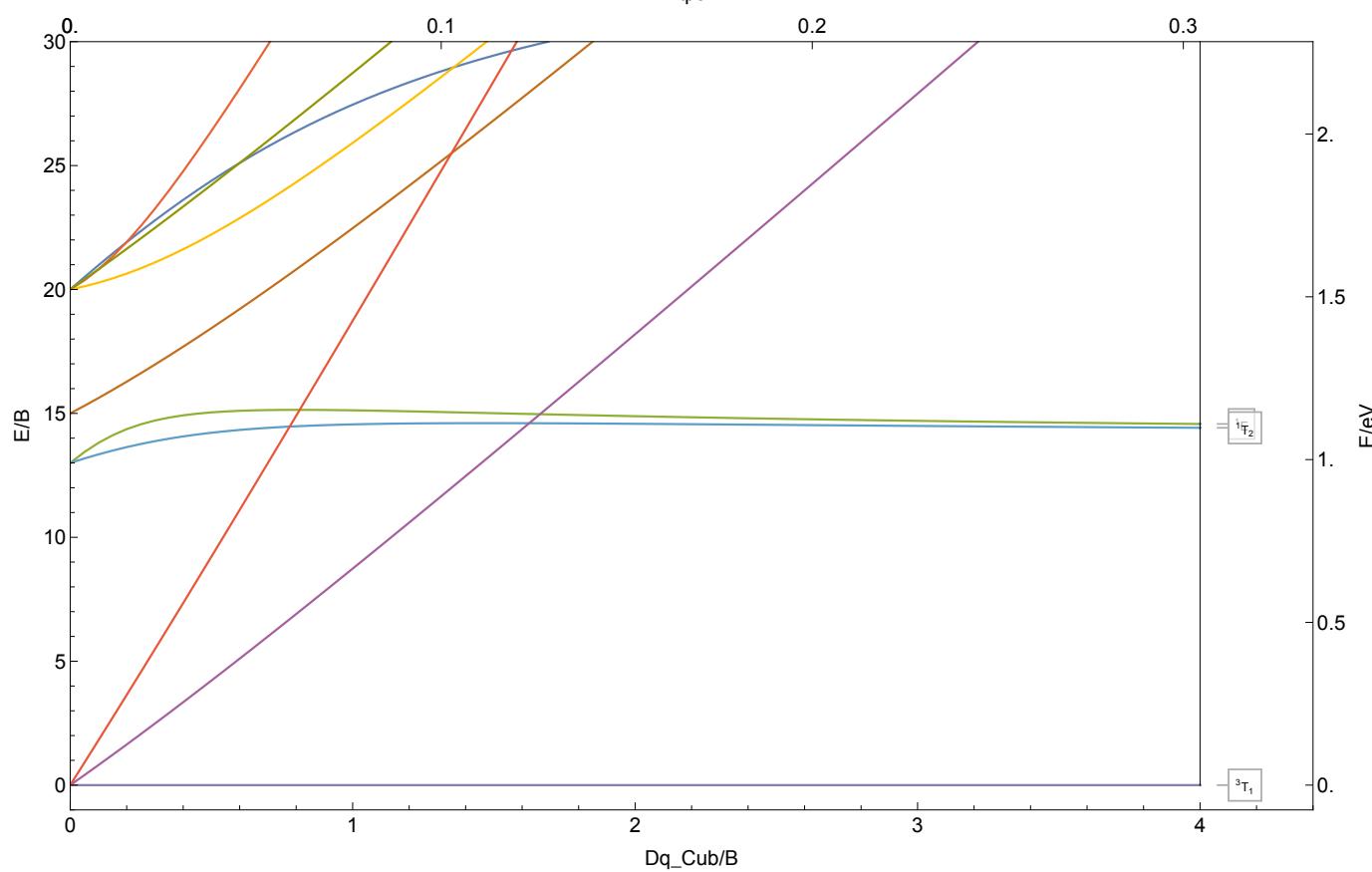
8.1.40  $\text{Nb}^{2+}$

$|2,4|d^3|C/B \approx 4. |B \approx 566 \text{ cm}^{-1}| \text{Nb}^{2+}$



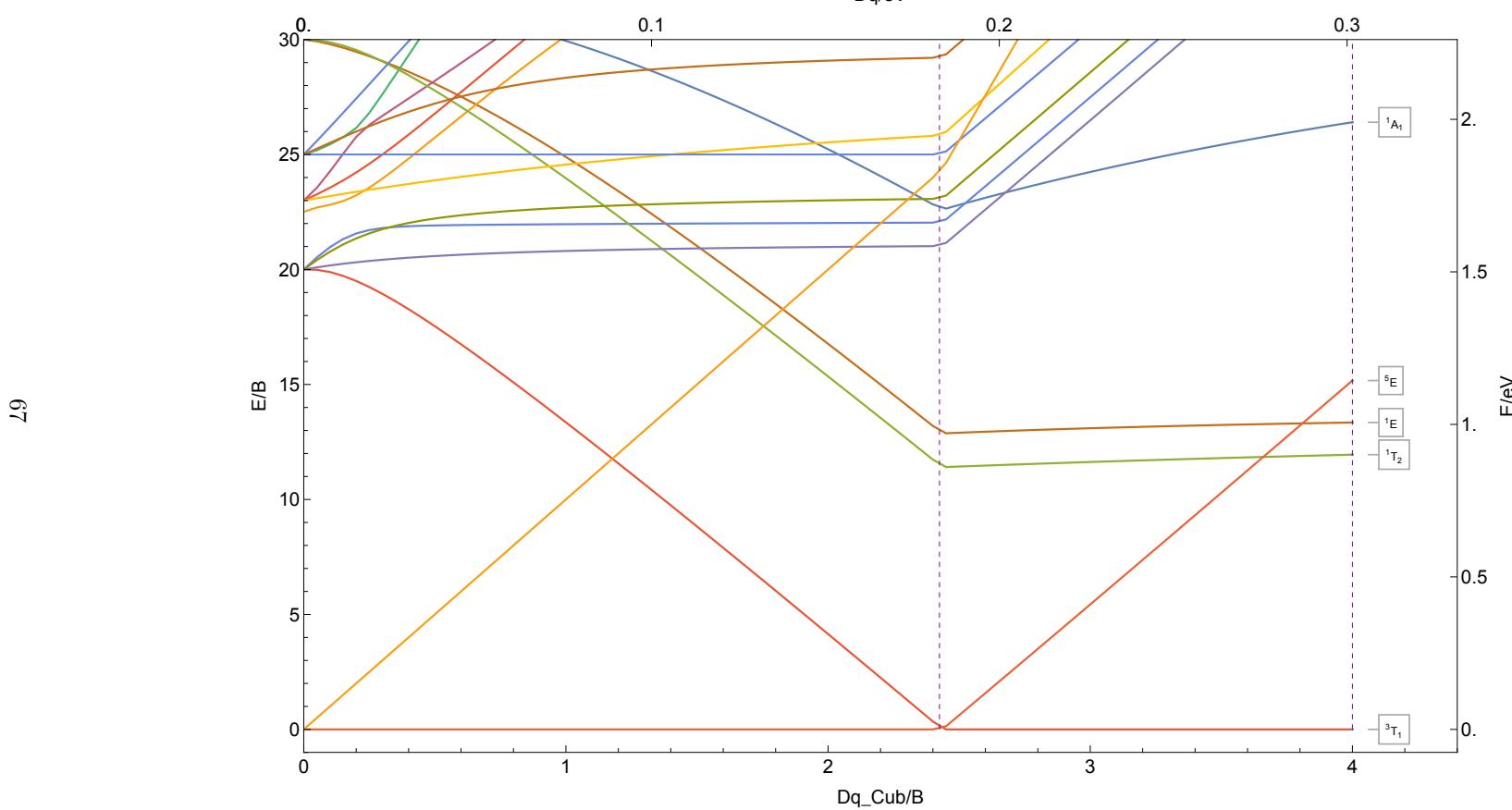
### 8.1.41 Nb<sup>3+</sup>

$|1,3|d^2|C/B \approx 4. | B \approx 614 \text{ cm}^{-1}|Nb^{3+}$



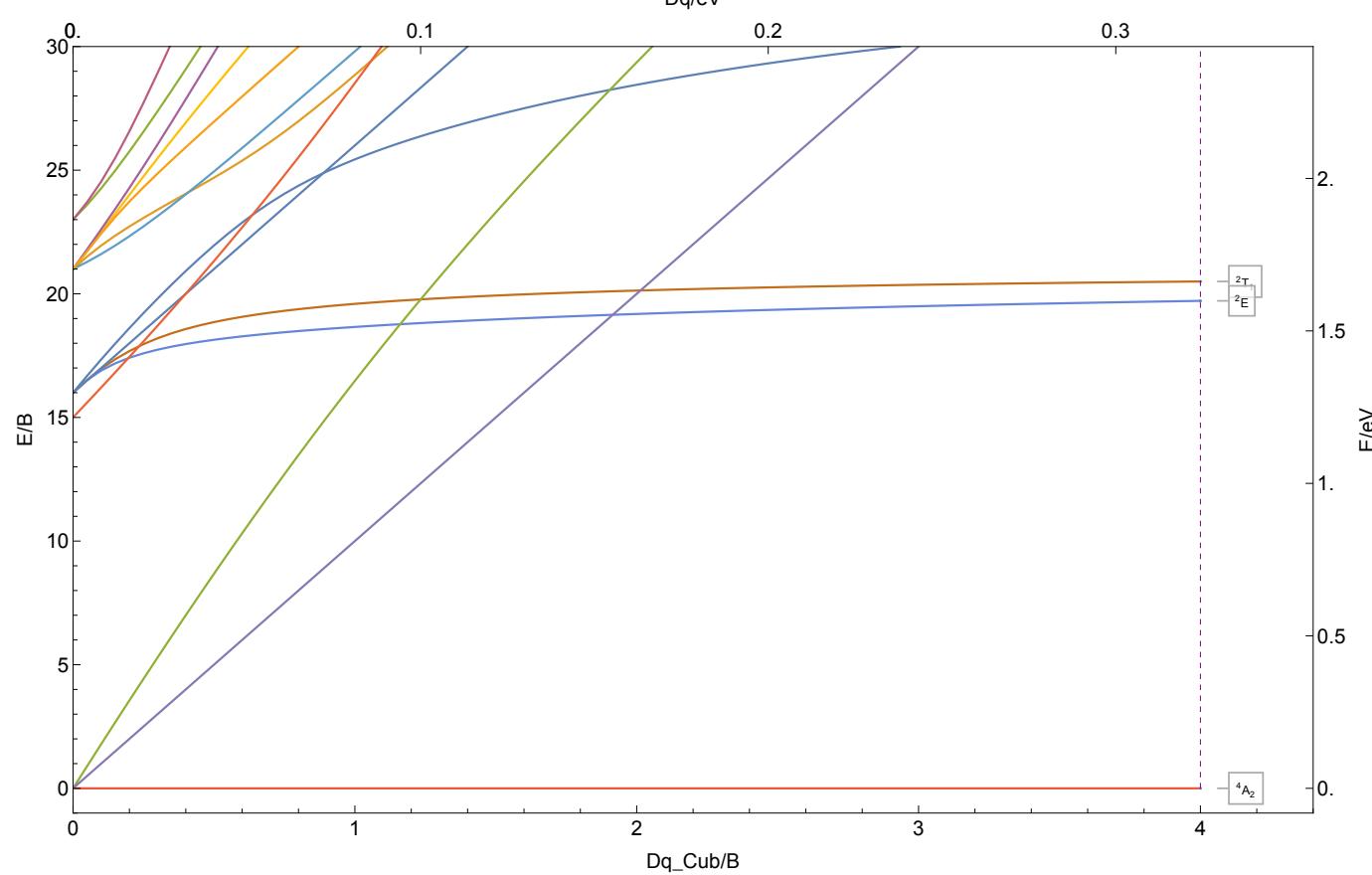
8.1.42 Mo<sup>2+</sup>

$|1,3,5|d^4|C/B \approx 4.|B \approx 608\text{ cm}^{-1}|Mo^{2+}$



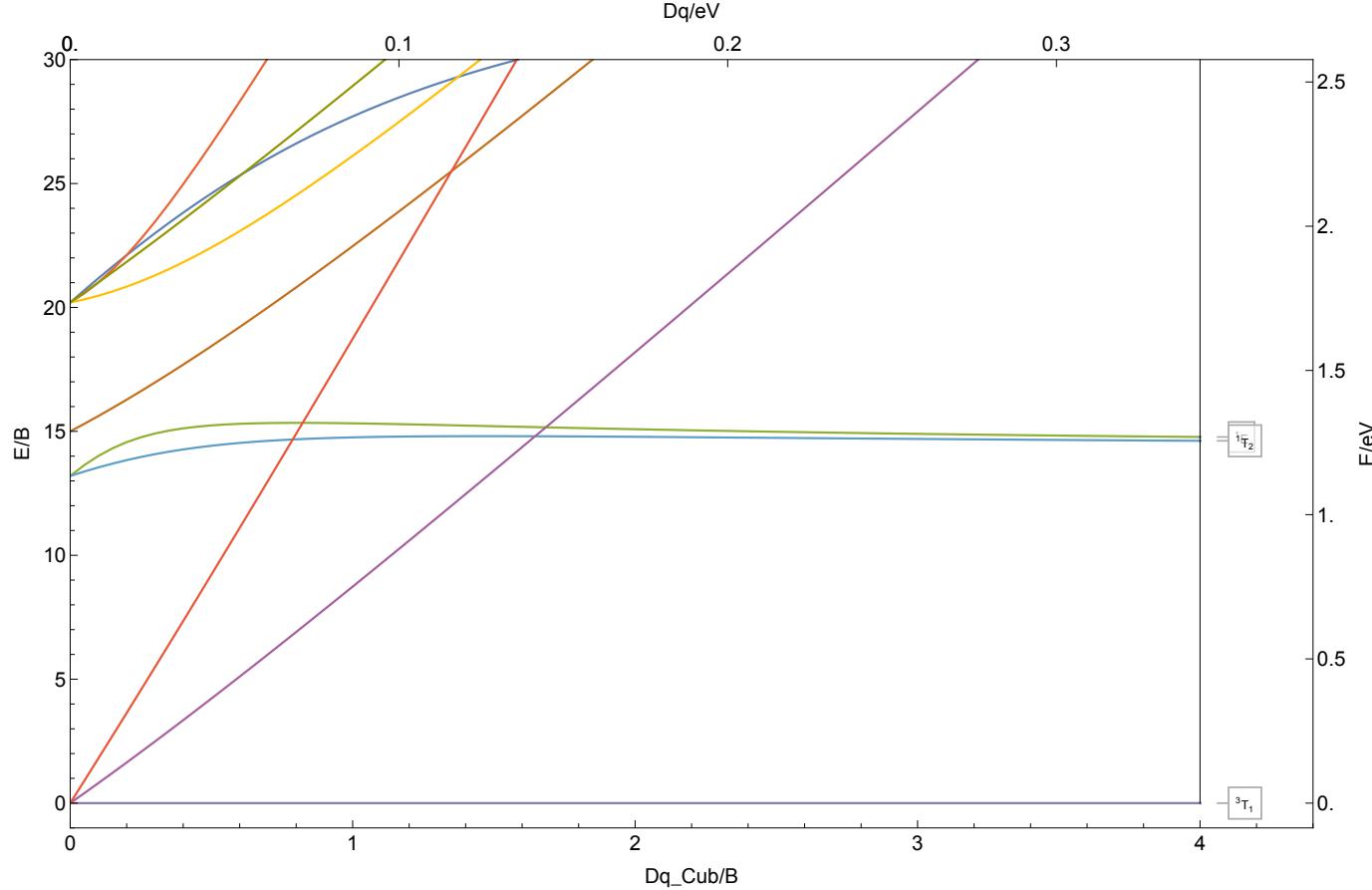
8.1.43 Mo<sup>3+</sup>

|2,4|d<sup>3</sup>|C/B ≈ 4.|B ≈ 654 cm<sup>-1</sup>|Mo<sup>3+</sup>



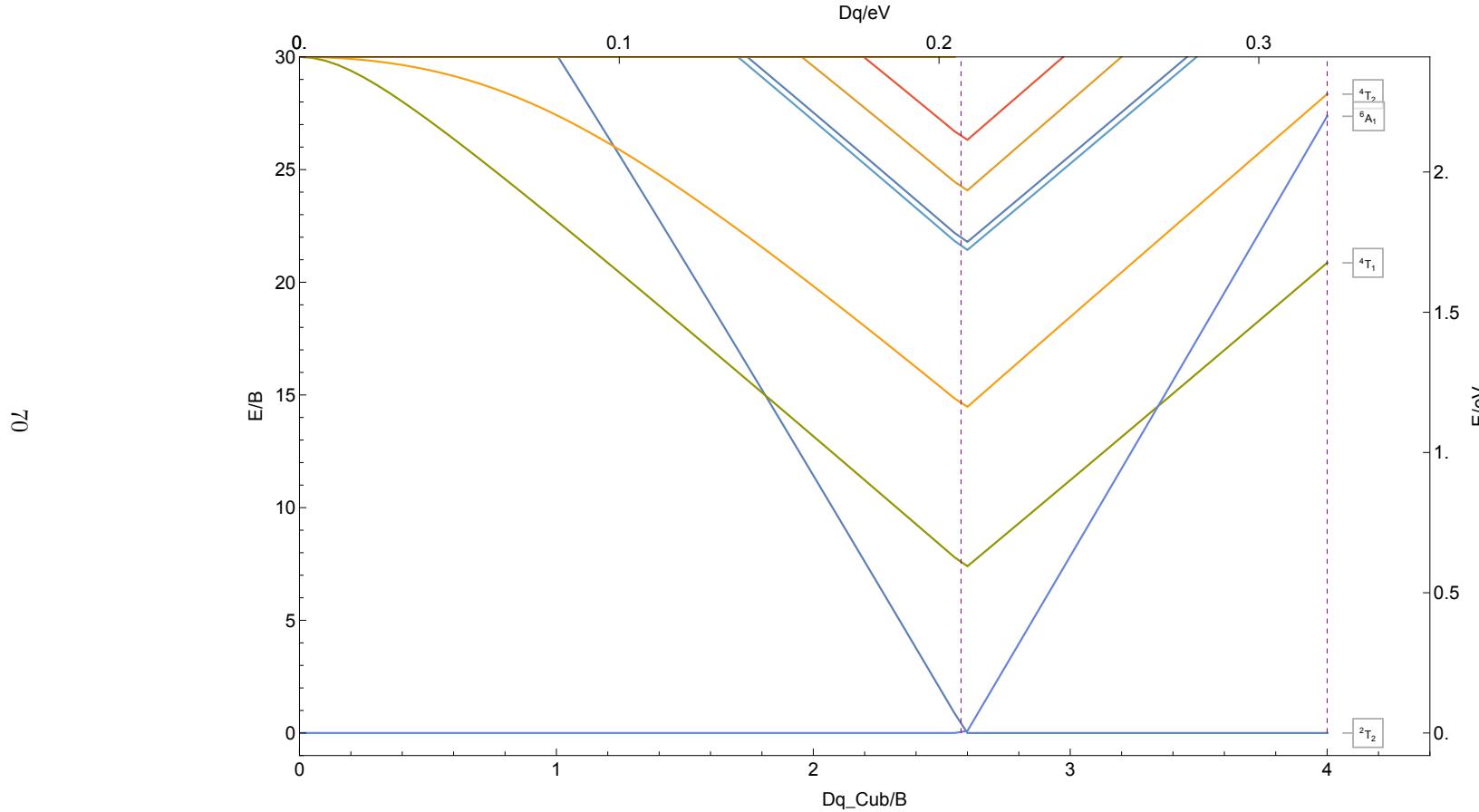
8.1.44 Mo<sup>4+</sup>

$|1,3|d^2|C/B \approx 4.1|B \approx 693\text{ cm}^{-1}|Mo^{4+}$



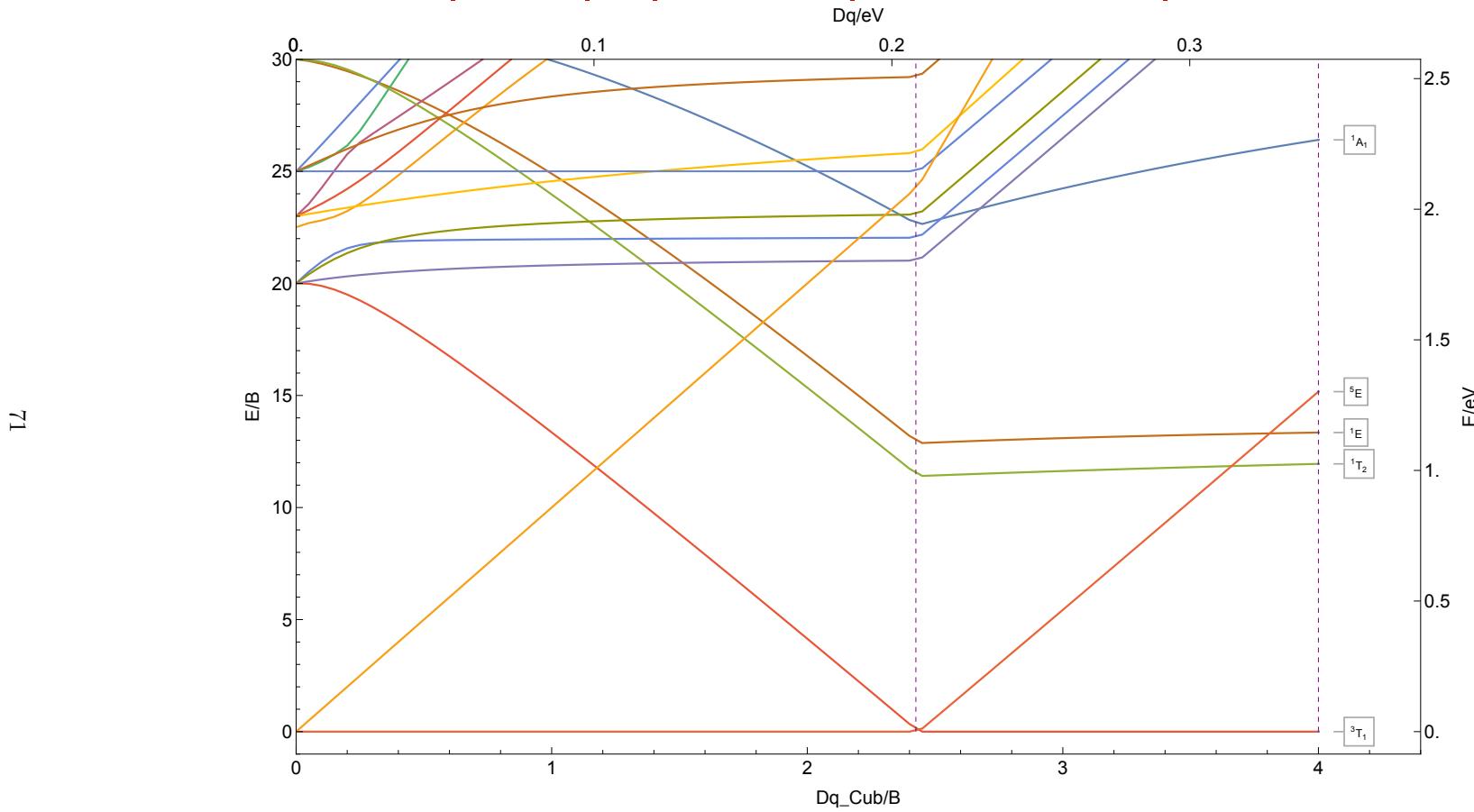
8.1.45 Tc<sup>2+</sup>

|2,4,6|d<sup>5</sup>|C/B≈4.|B≈648 cm<sup>-1</sup>|Tc<sup>2+</sup>



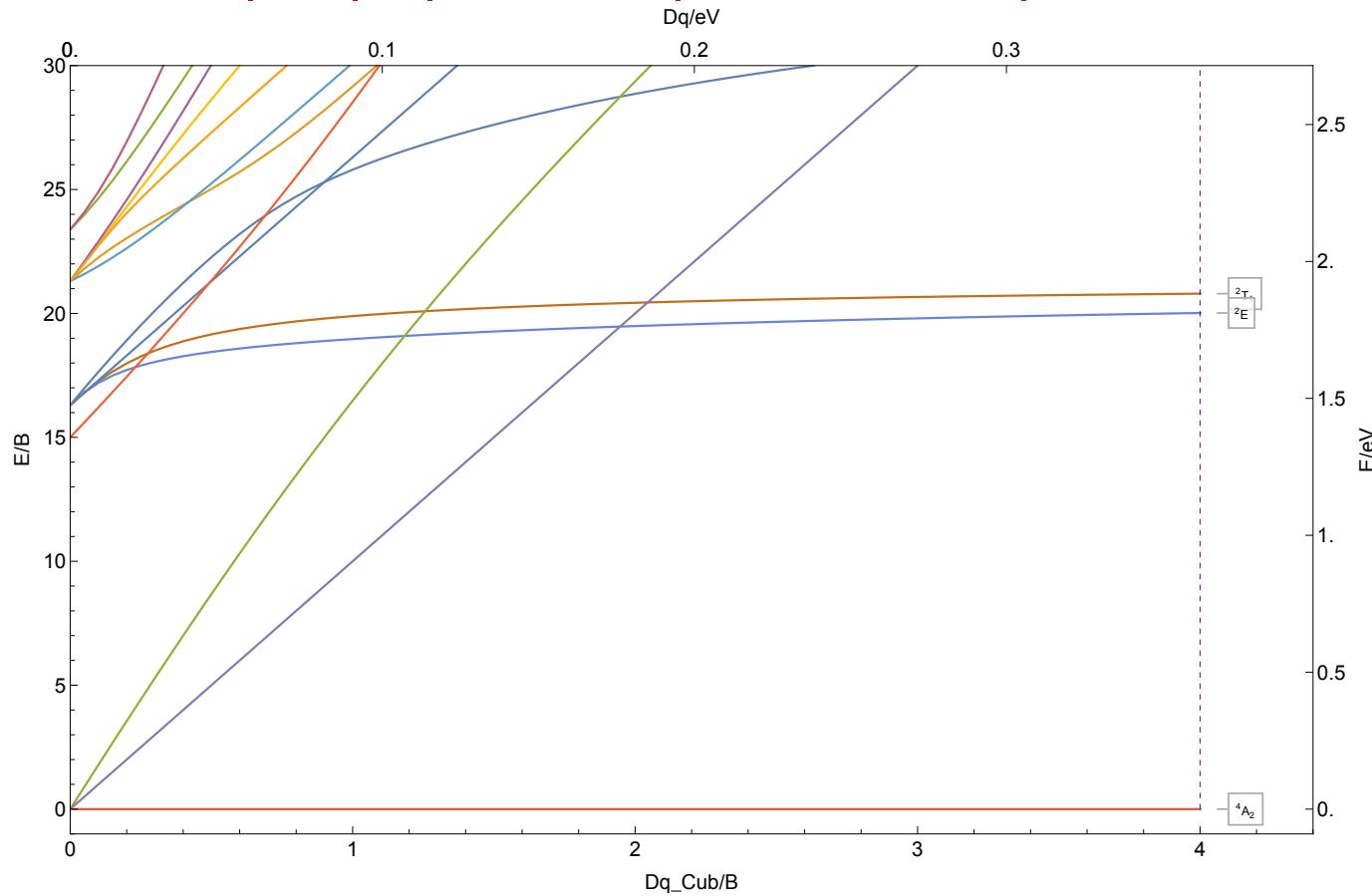
8.1.46 Tc<sup>3+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 4. | B ≈ 692 cm<sup>-1</sup> | Tc<sup>3+</sup>



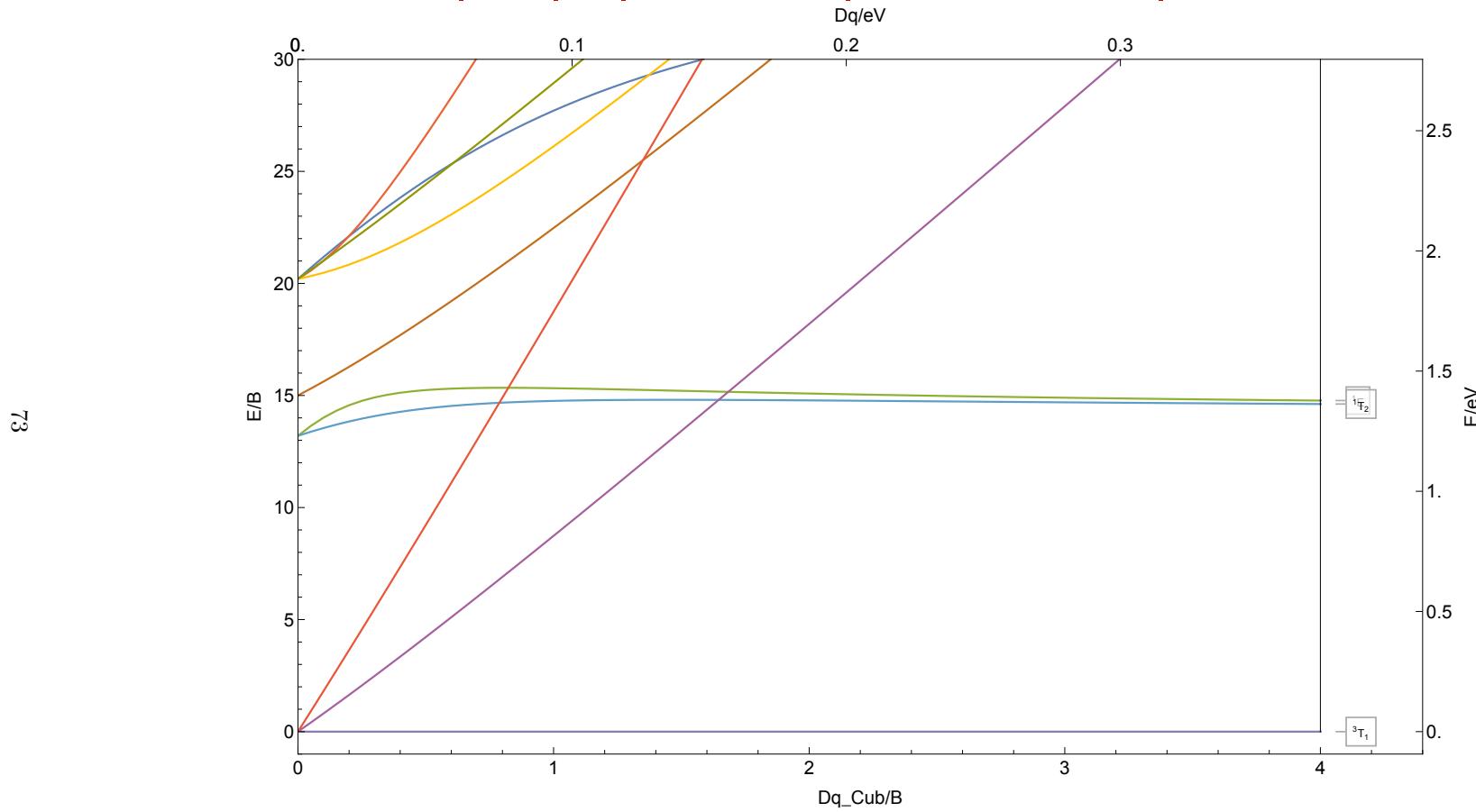
8.1.47 Tc<sup>4+</sup>

$$|2,4|d^3|C/B \approx 4.1|B \approx 730\text{ cm}^{-1}|Tc^{4+}$$



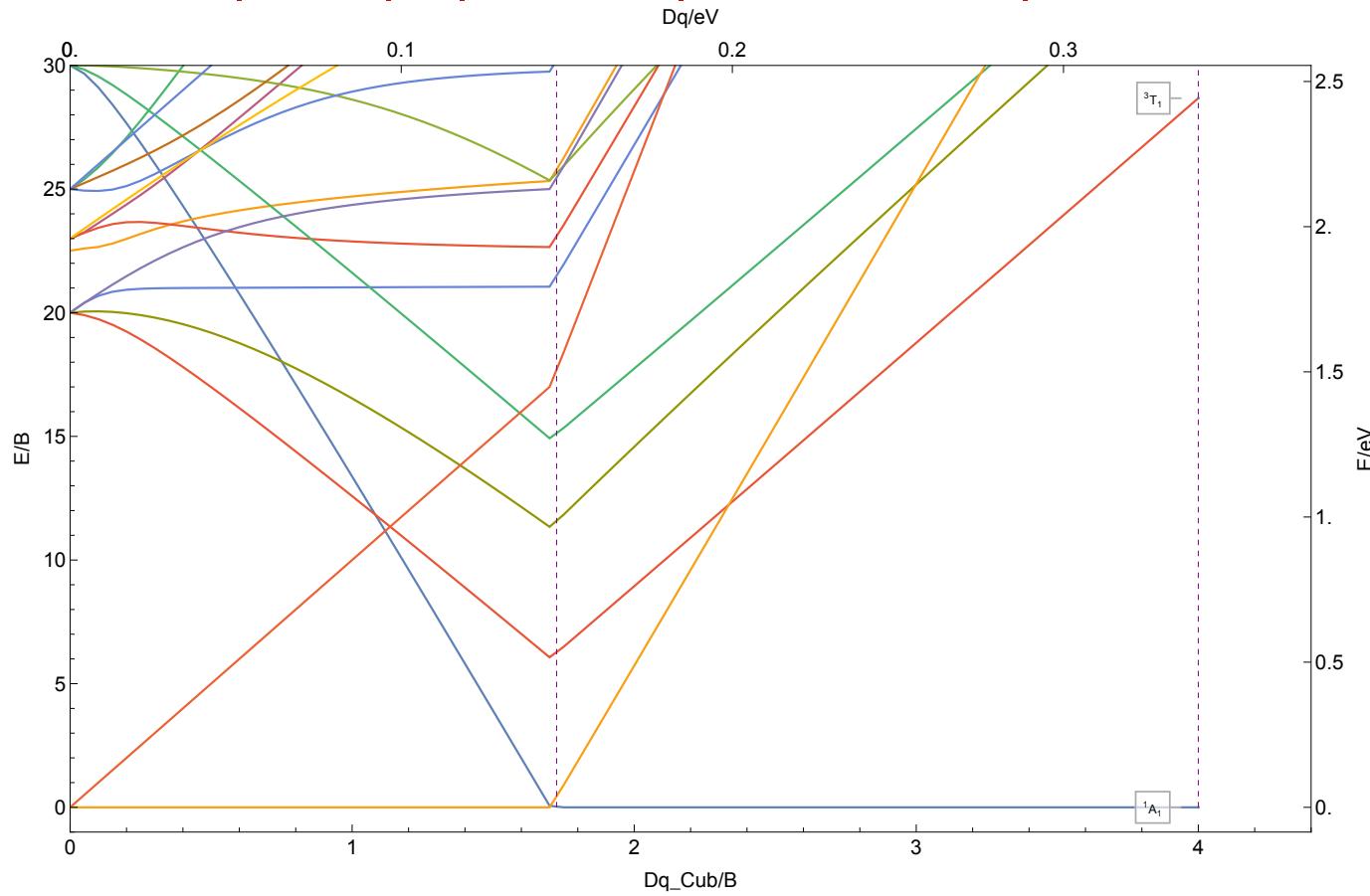
8.1.48 Tc<sup>5+</sup>

| 1,3 | d<sup>2</sup> | C/B ≈ 4.1 | B ≈ 752 cm<sup>-1</sup> | Tc<sup>5+</sup>



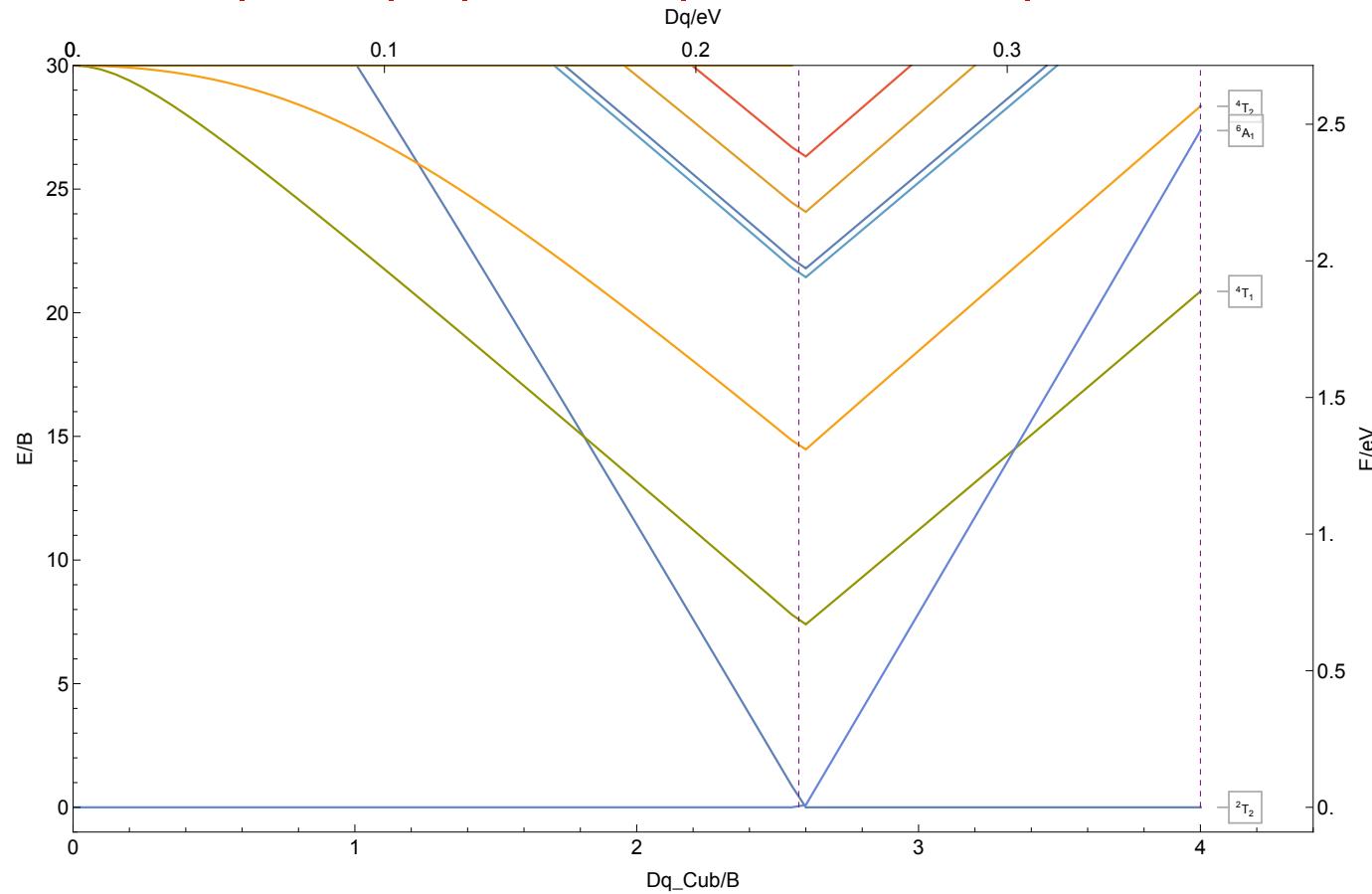
8.1.49 Ru<sup>2+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4. | B ≈ 687 cm<sup>-1</sup> | Ru<sup>2+</sup>



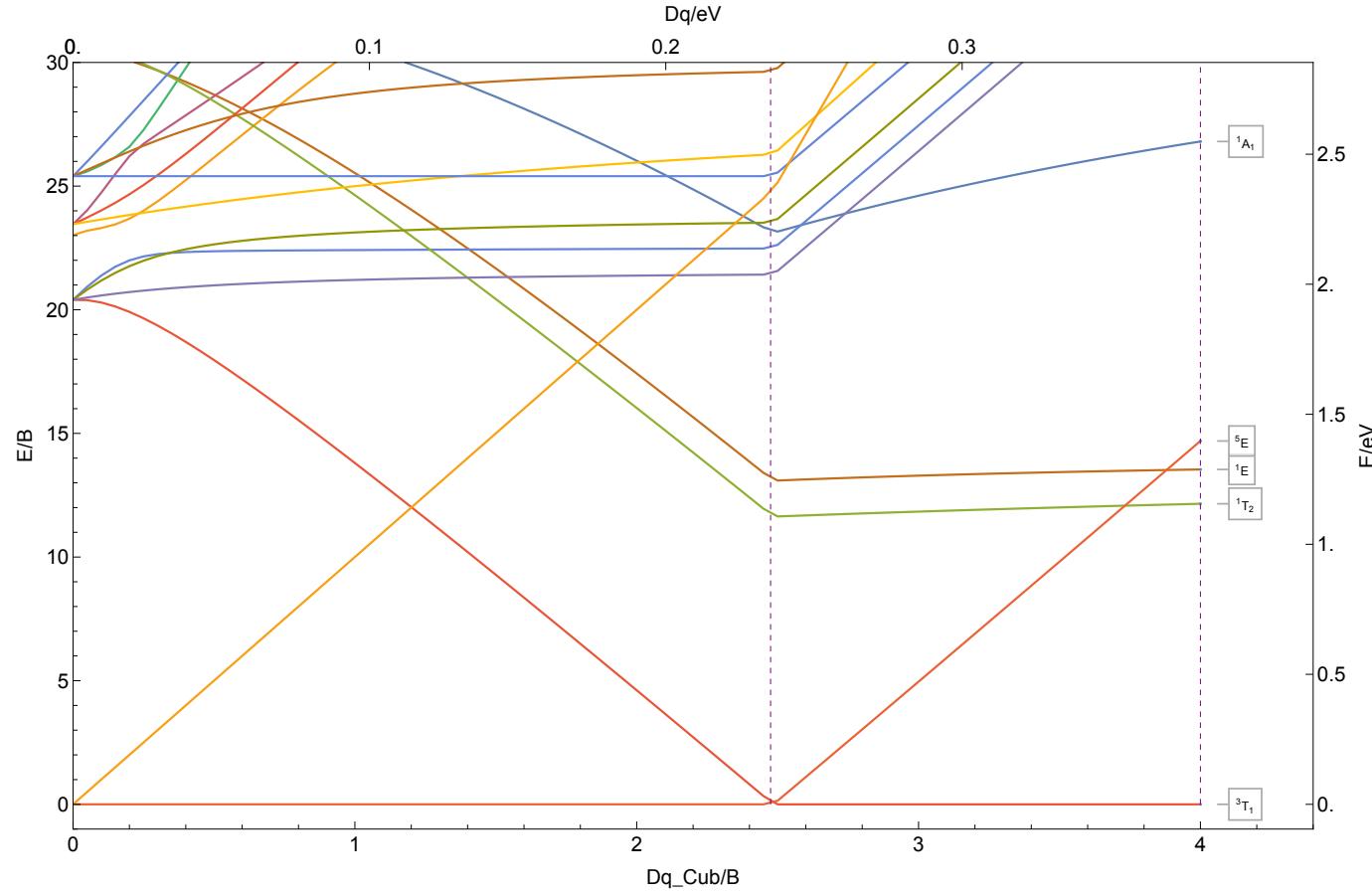
8.1.50 Ru<sup>3+</sup>

|2,4,6|d<sup>5</sup>|C/B ≈ 4.|B ≈ 730 cm<sup>-1</sup>|Ru<sup>3+</sup>



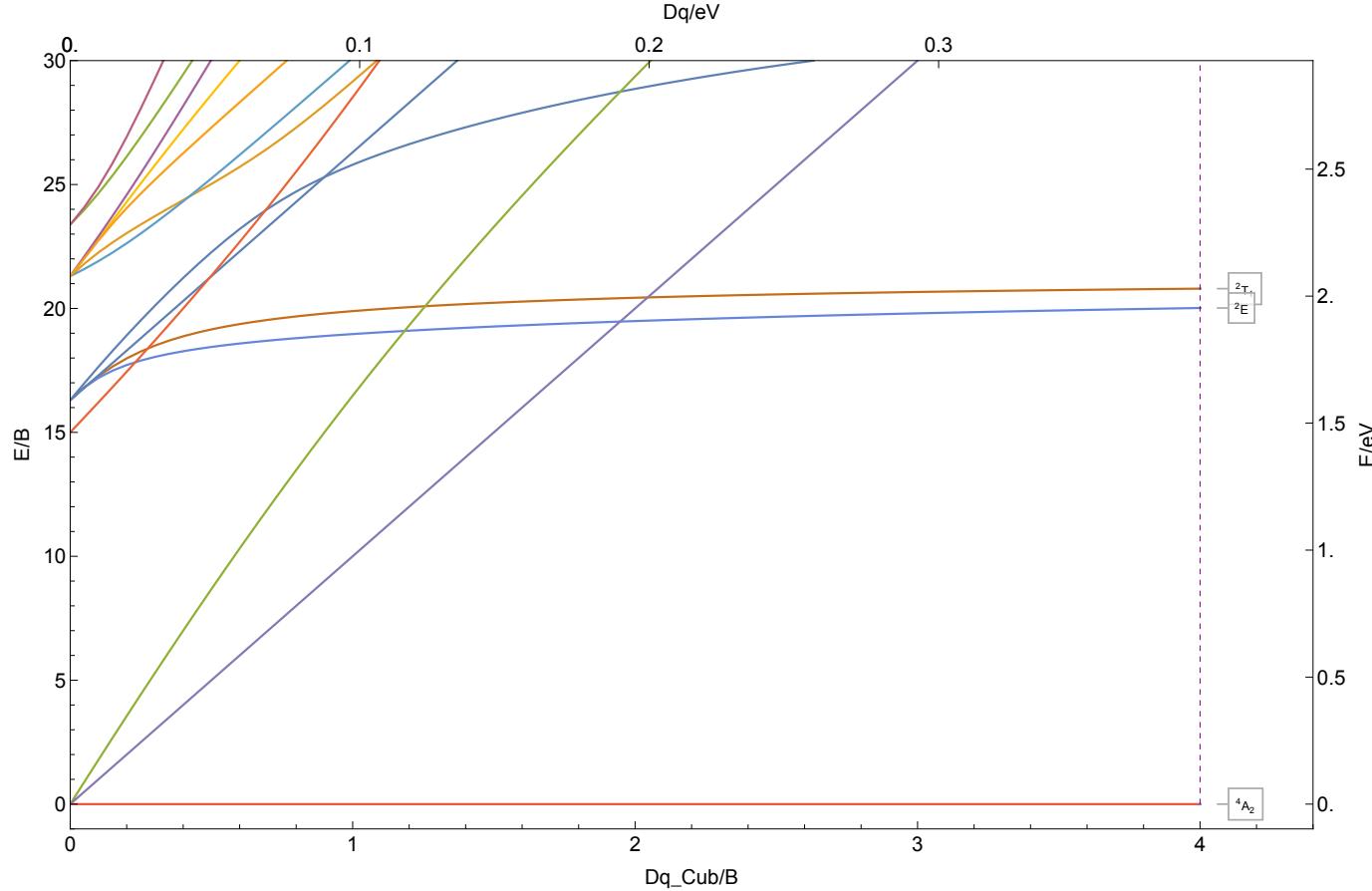
### 8.1.51 Ru<sup>4+</sup>

$|1,3,5|d^4|C/B \approx 4.1|B \approx 767\text{ cm}^{-1}|Ru^{4+}$



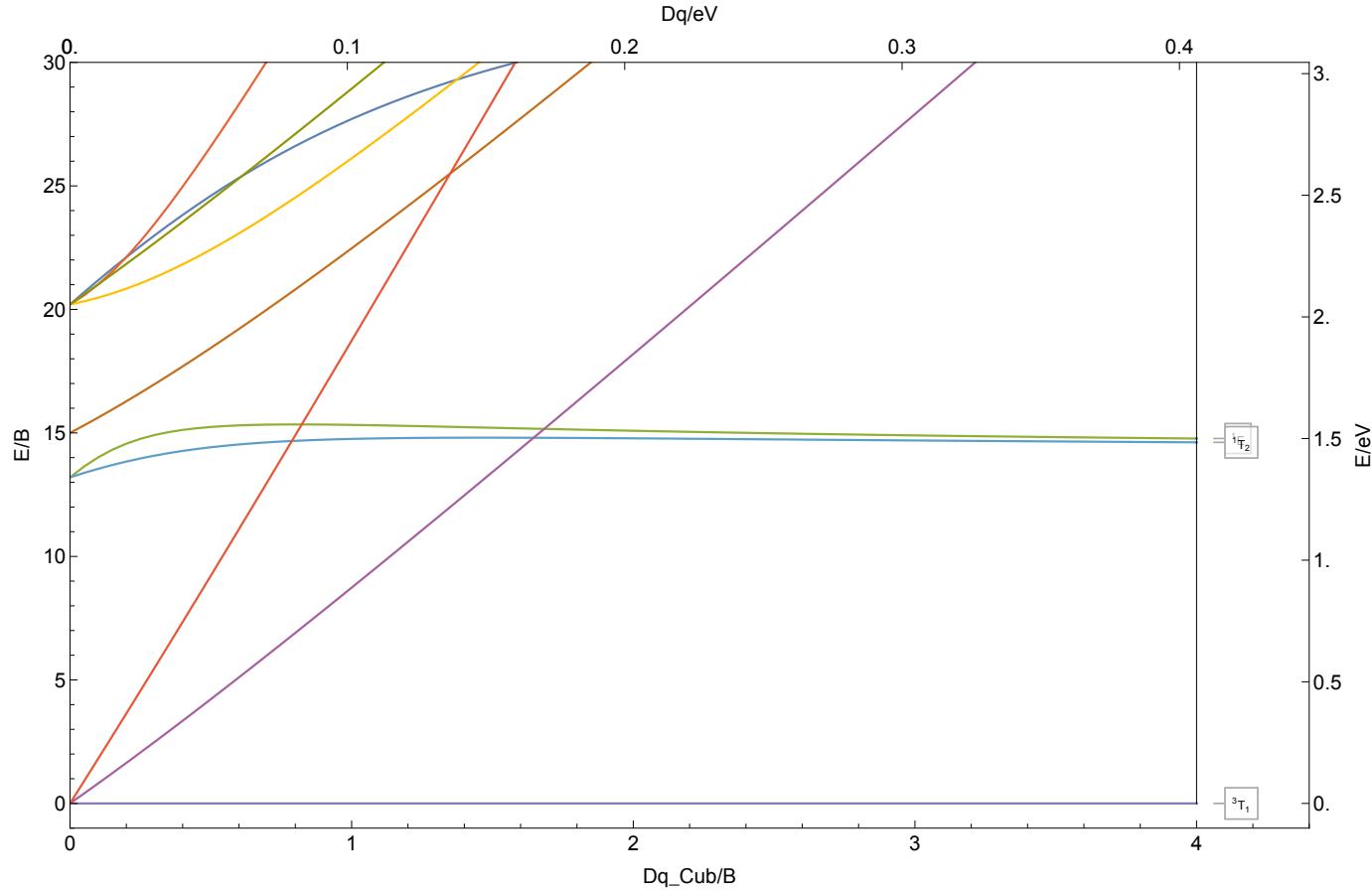
8.1.52 Ru<sup>5+</sup>

|2,4|d<sup>3</sup>| C/B ≈ 4.1| B ≈ 787 cm<sup>-1</sup> |Ru<sup>5+</sup>



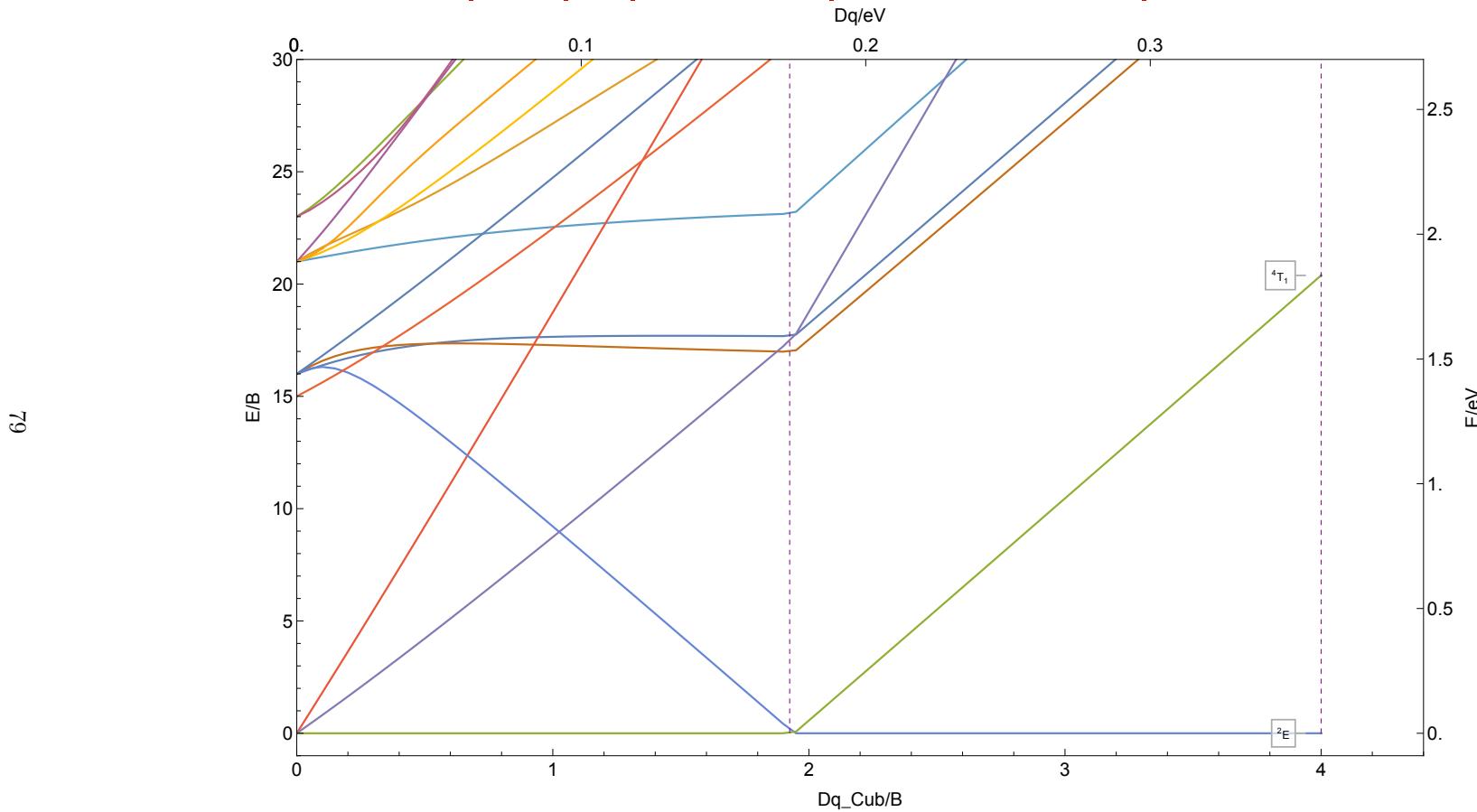
### 8.1.53 Ru<sup>6+</sup>

$|1,3|d^2|C/B \approx 4.1|B \approx 819\text{ cm}^{-1}|Ru^{6+}$



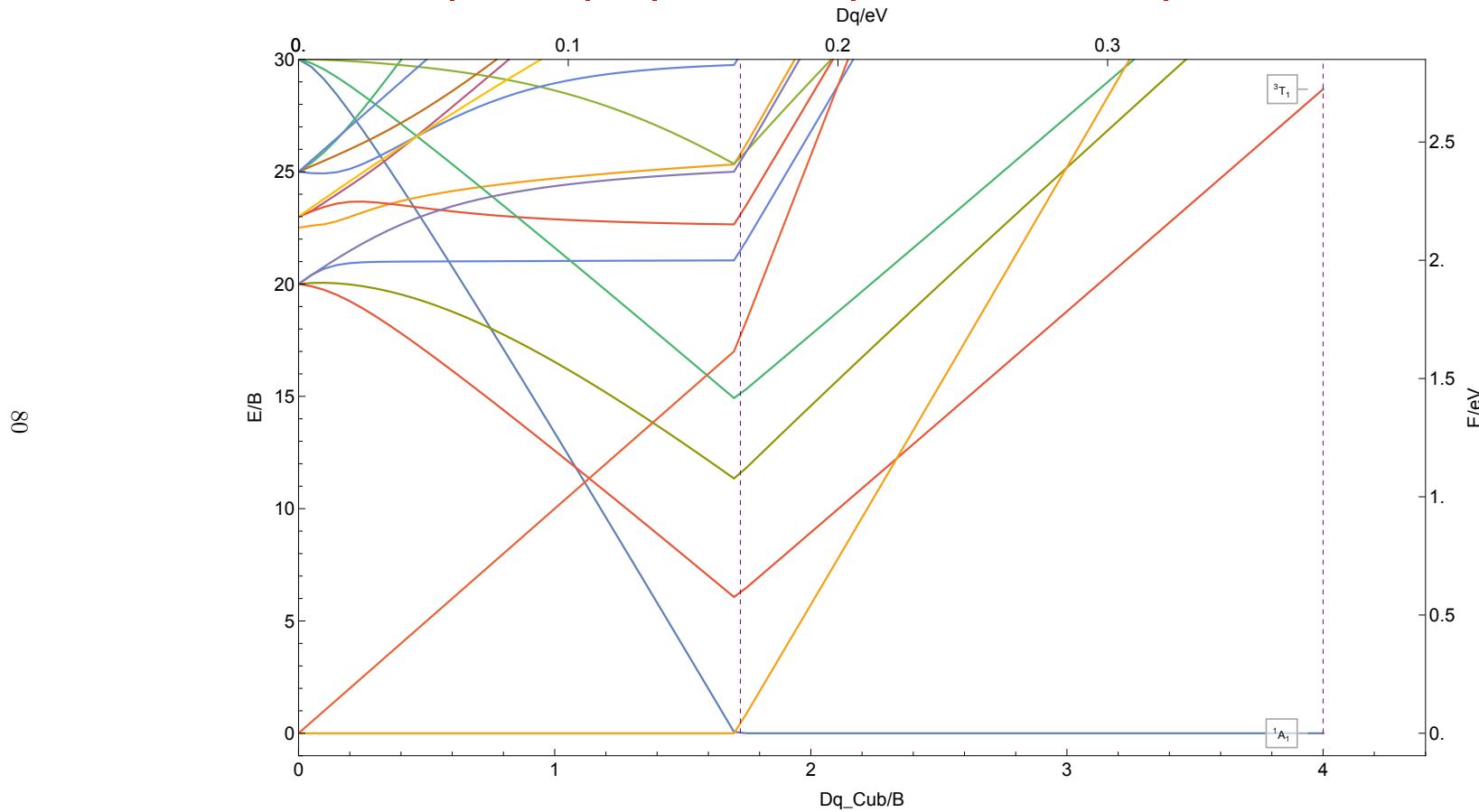
8.1.54 Rh<sup>2+</sup>

|2,4|d<sup>7</sup>| C/B ≈ 4. | B ≈ 726 cm<sup>-1</sup> | Rh<sup>2+</sup>



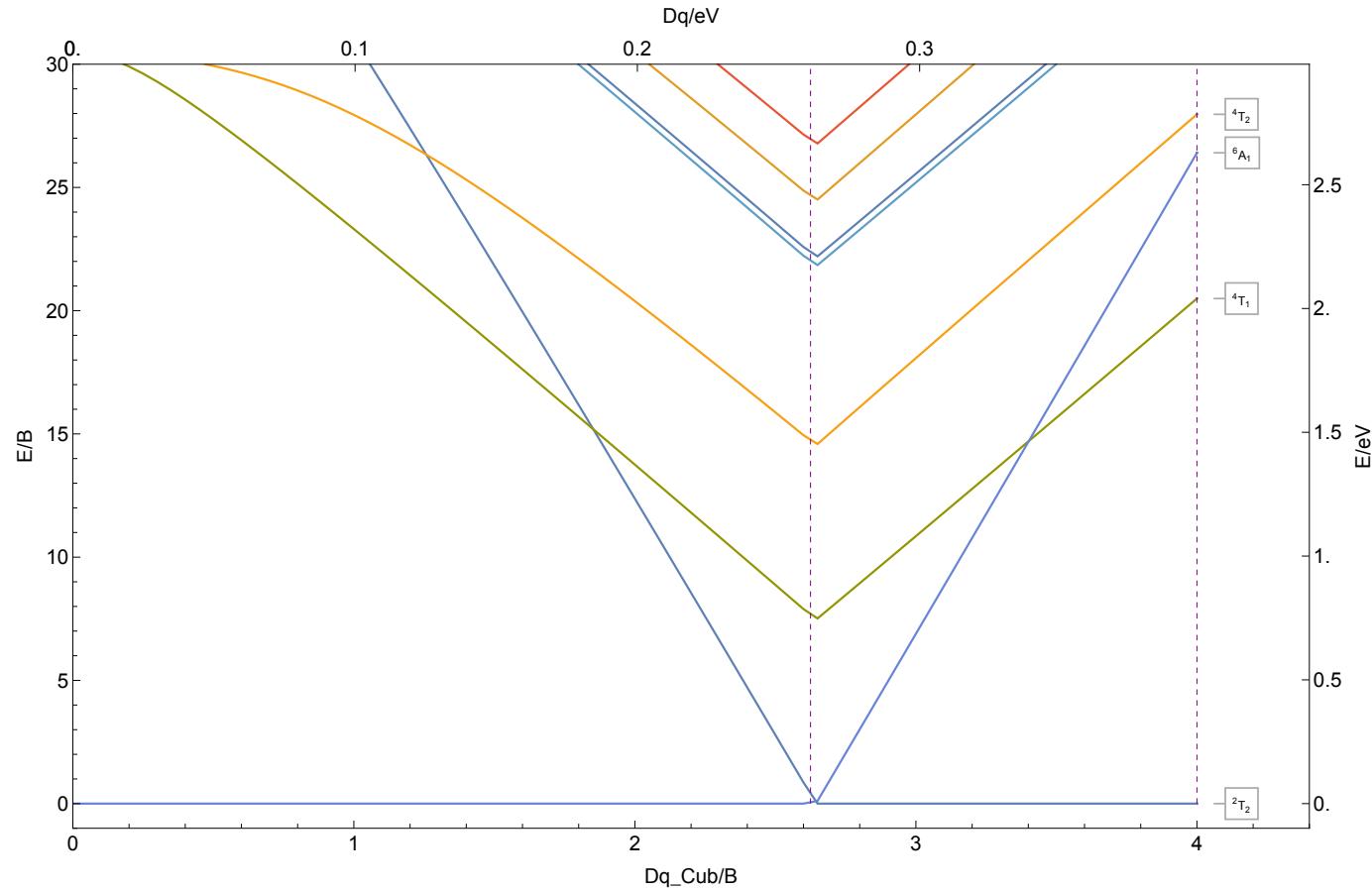
8.1.55 Rh<sup>3+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4. | B ≈ 766 cm<sup>-1</sup> | Rh<sup>3+</sup>



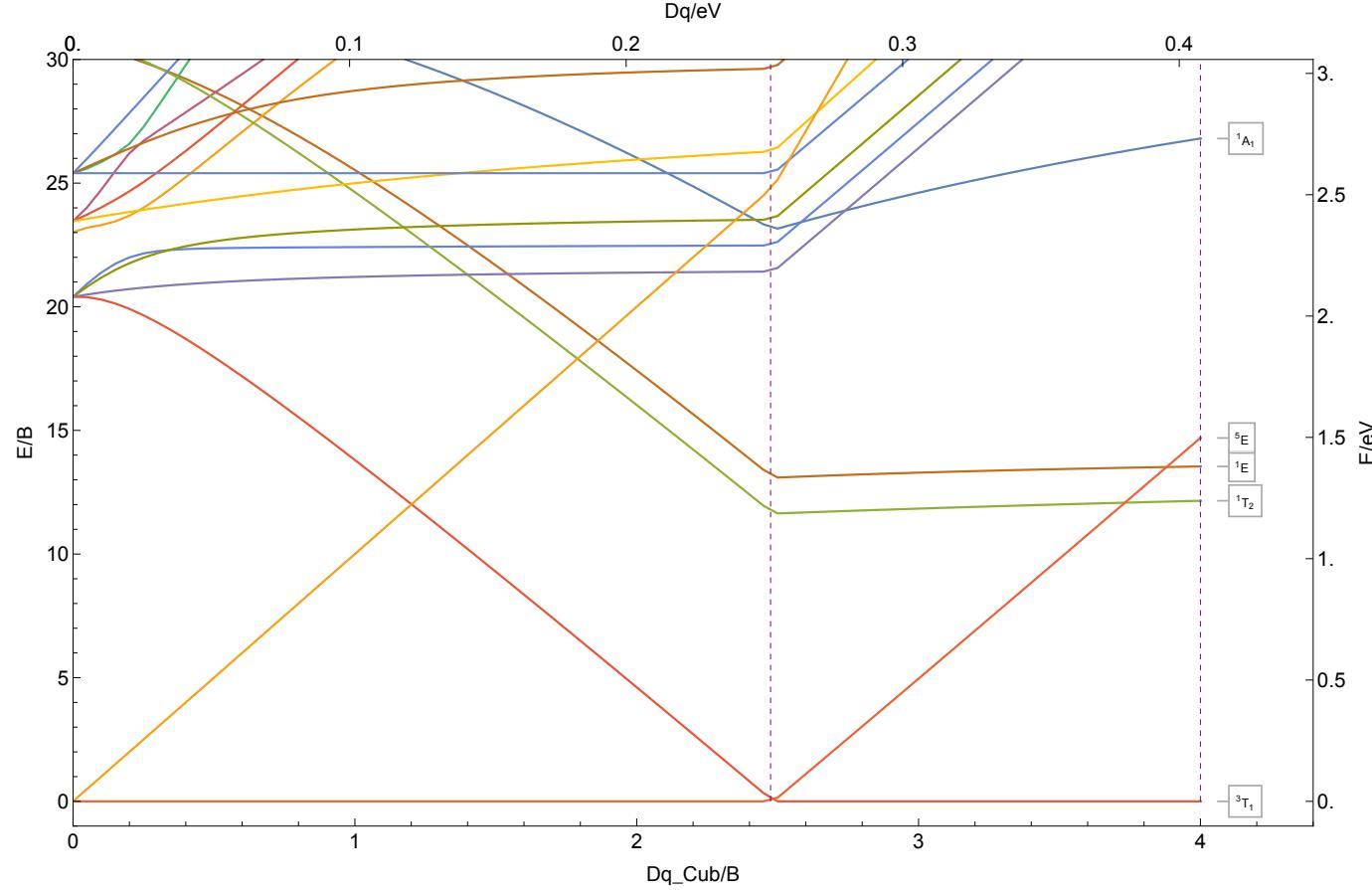
8.1.56 Rh<sup>4+</sup>

|2,4,6| d<sup>5</sup>| C/B ≈ 4.1| B ≈ 803 cm<sup>-1</sup> | Rh<sup>4+</sup>



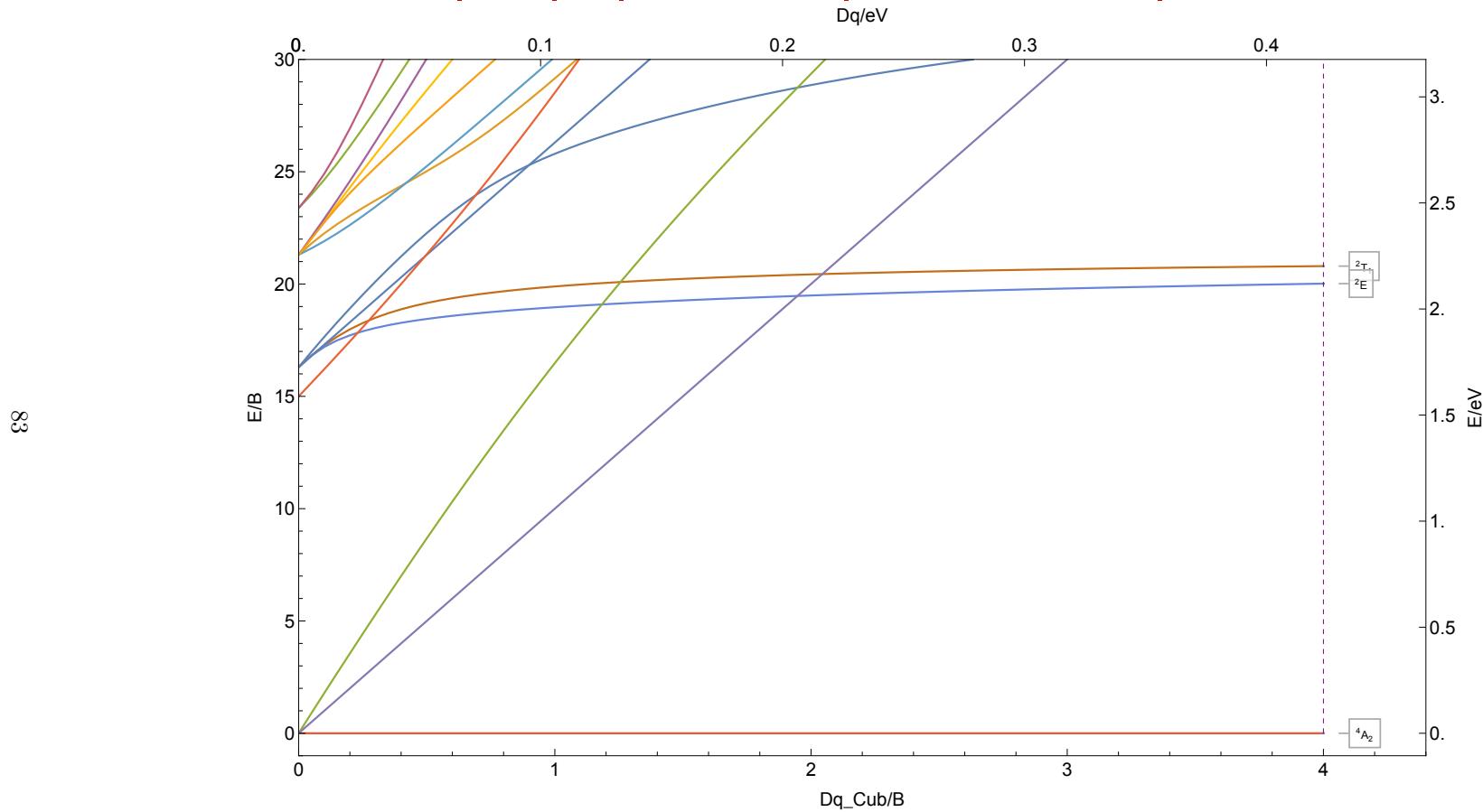
8.1.57 Rh<sup>5+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 4.1 | B ≈ 822 cm<sup>-1</sup> | Rh<sup>5+</sup>



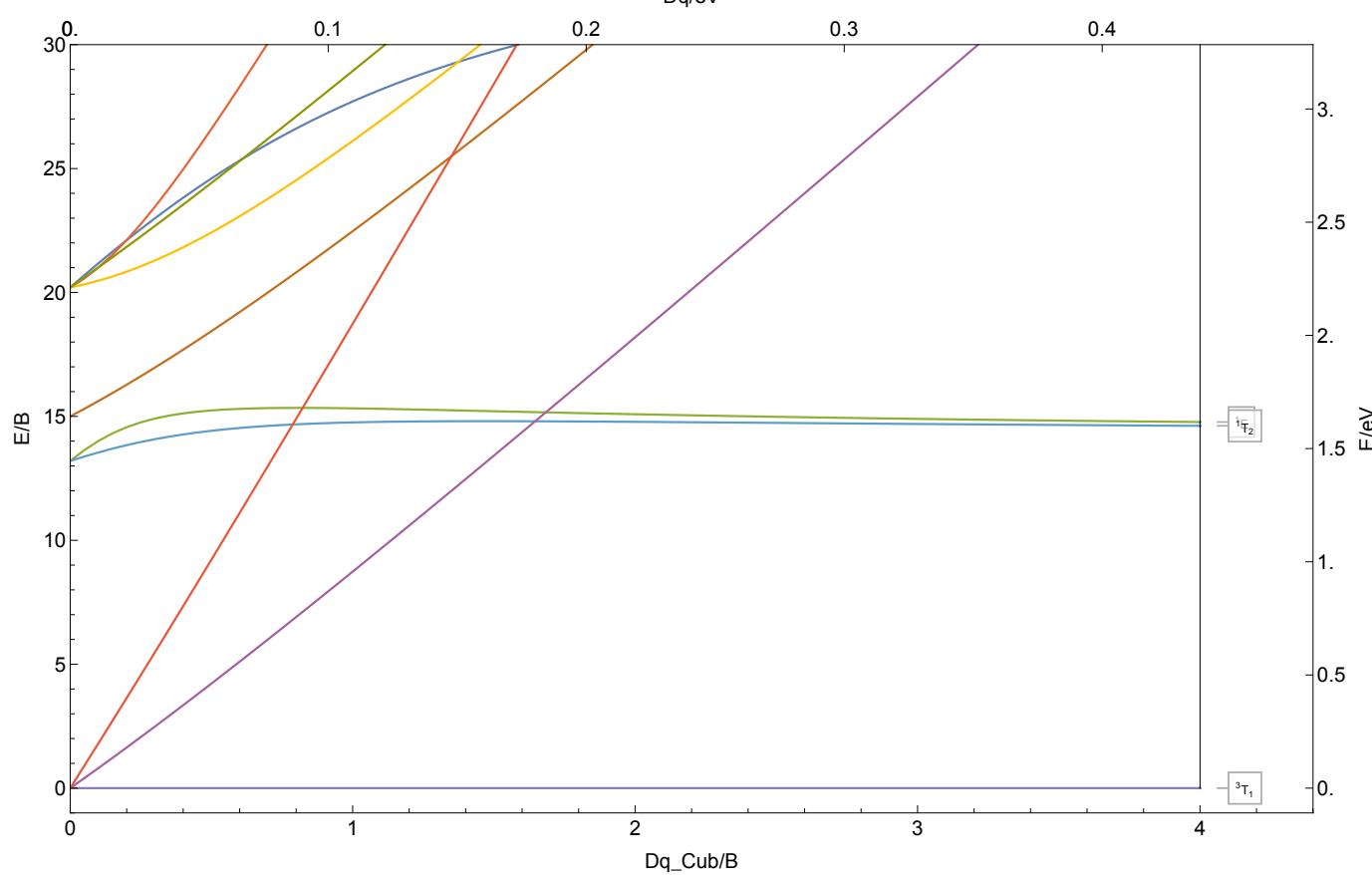
8.1.58 Rh<sup>6+</sup>

|2,4|d<sup>3</sup>| C/B ≈ 4.1| B ≈ 854 cm<sup>-1</sup> | Rh<sup>6+</sup>



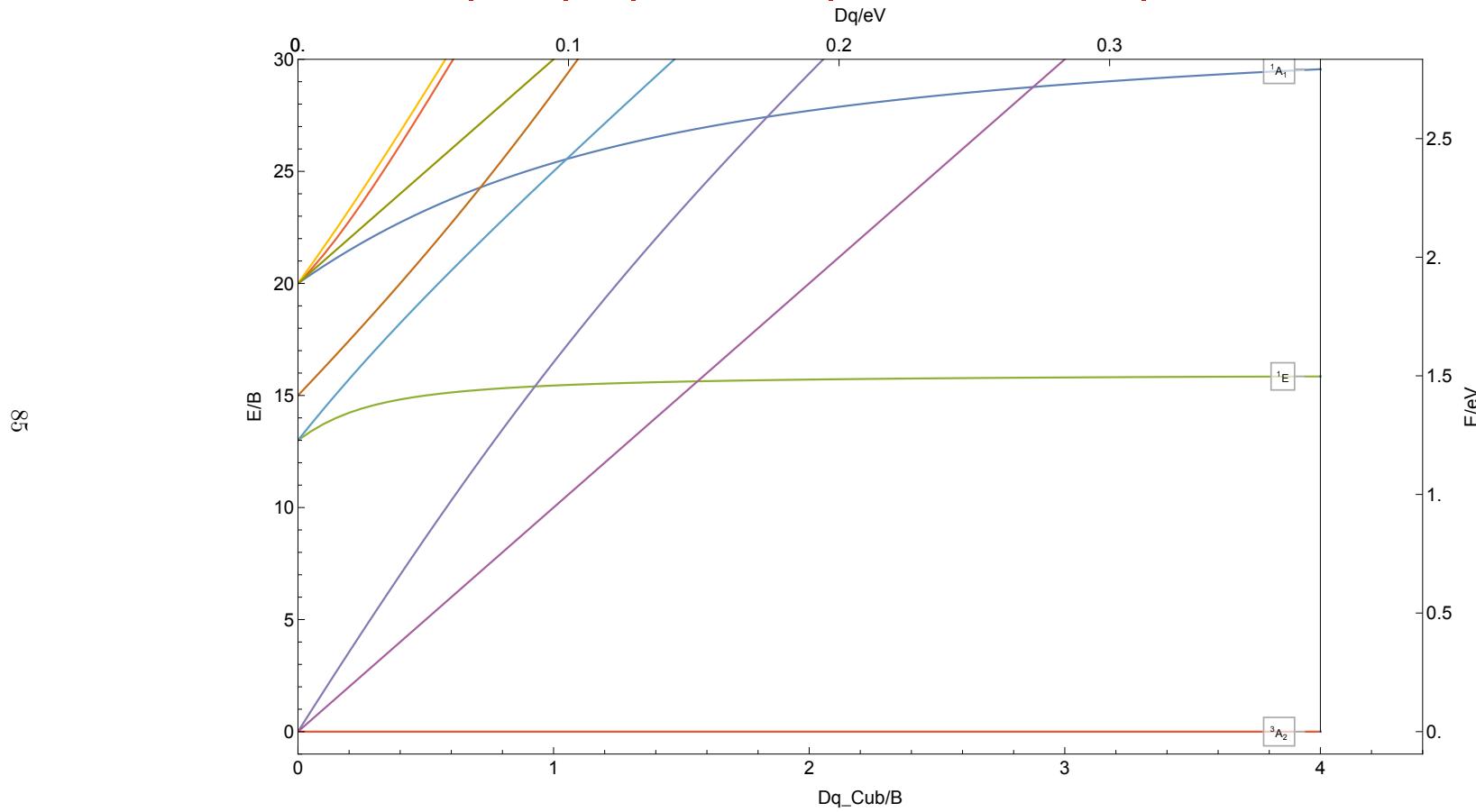
### 8.1.59 Rh<sup>7+</sup>

$|1,3|d^2|C/B \approx 4.1| B \approx 883\text{ cm}^{-1}|Rh^{7+}$



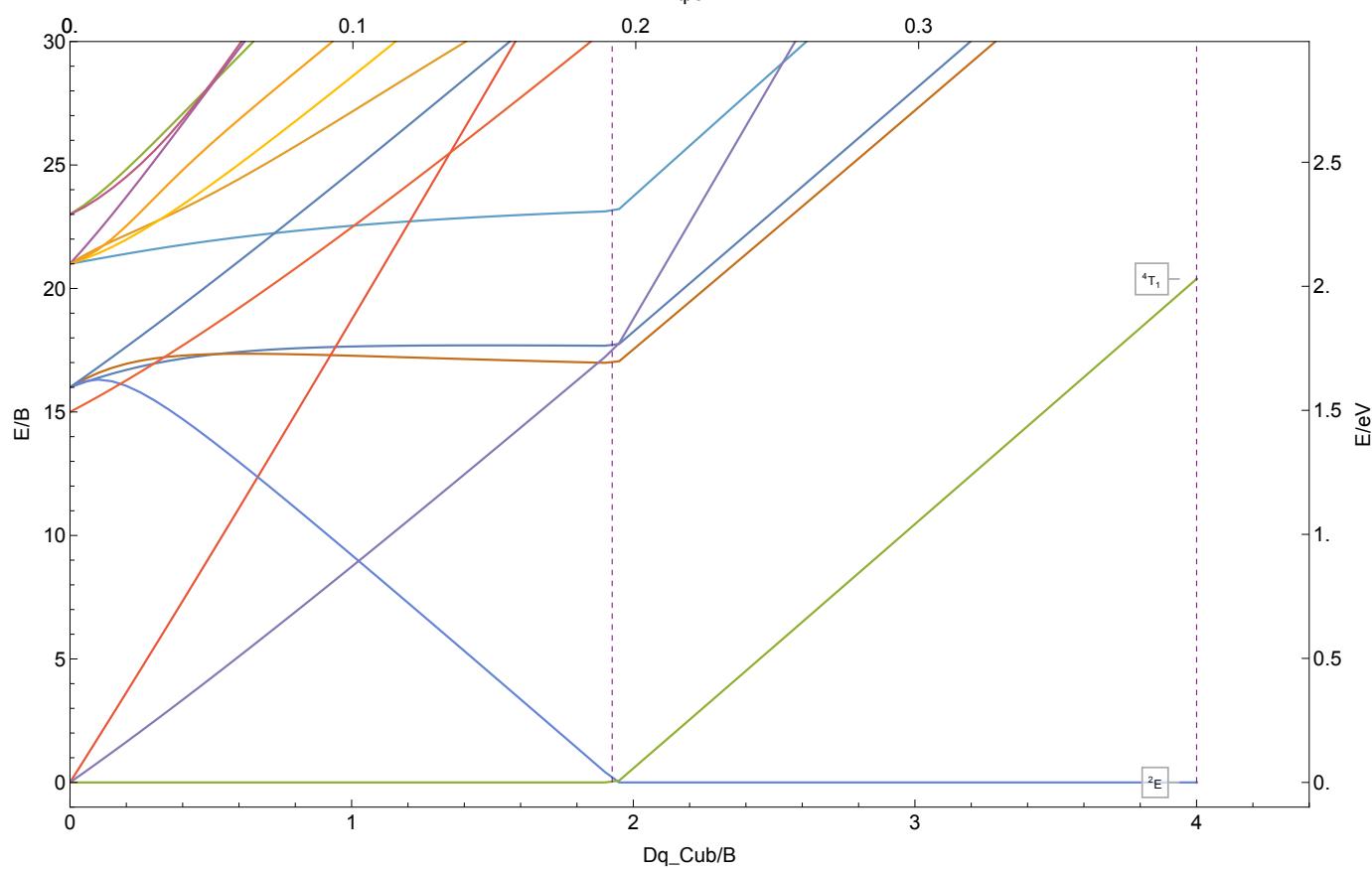
8.1.60 Pd<sup>2+</sup>

| 1,3 | d<sup>8</sup> | C/B ≈ 4. | B ≈ 762 cm<sup>-1</sup> | Pd<sup>2+</sup>



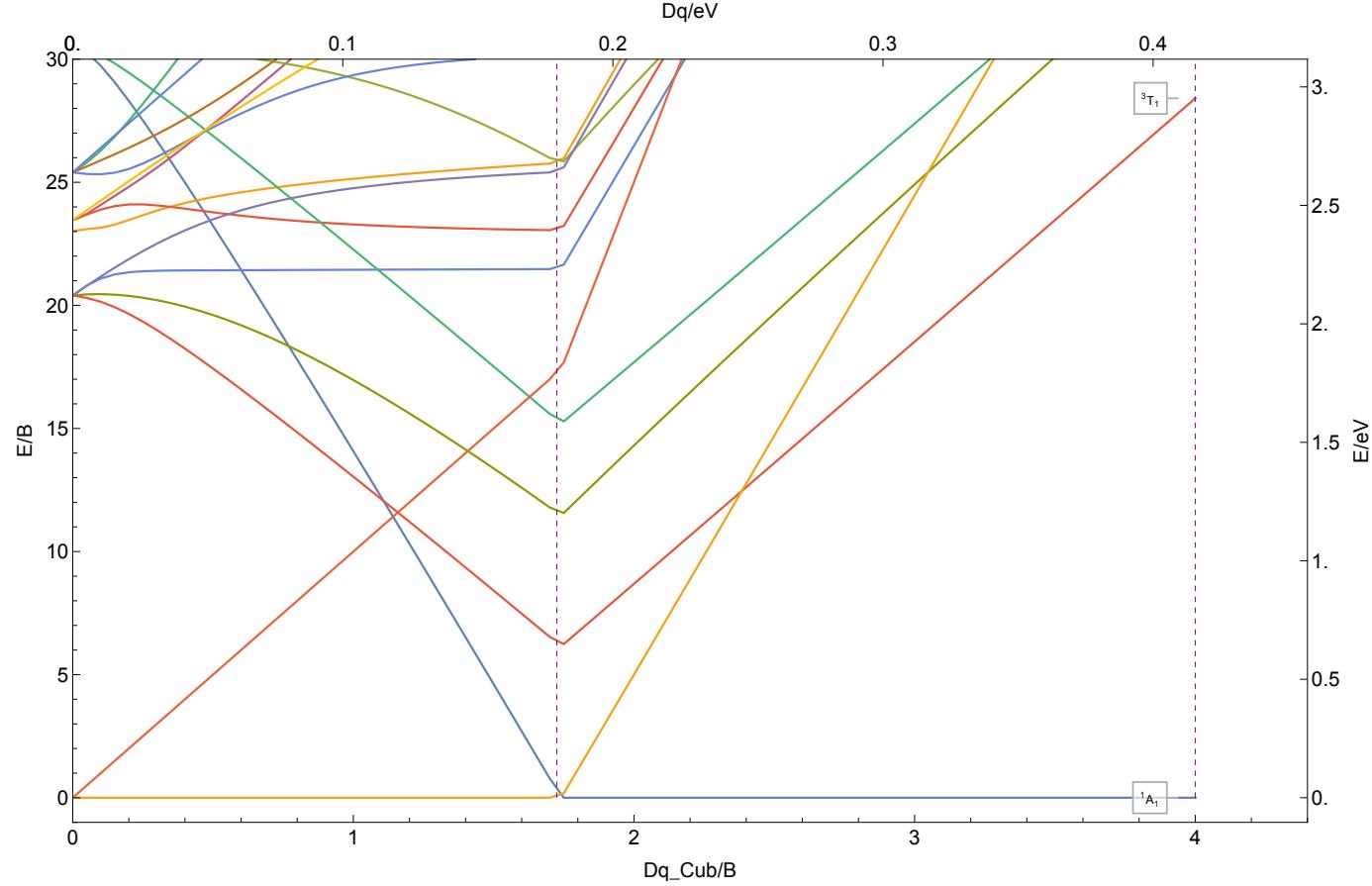
8.1.61 Pd<sup>3+</sup>

|2,4|d<sup>7</sup>|C/B ≈ 4.|B ≈ 803 cm<sup>-1</sup>|Pd<sup>3+</sup>



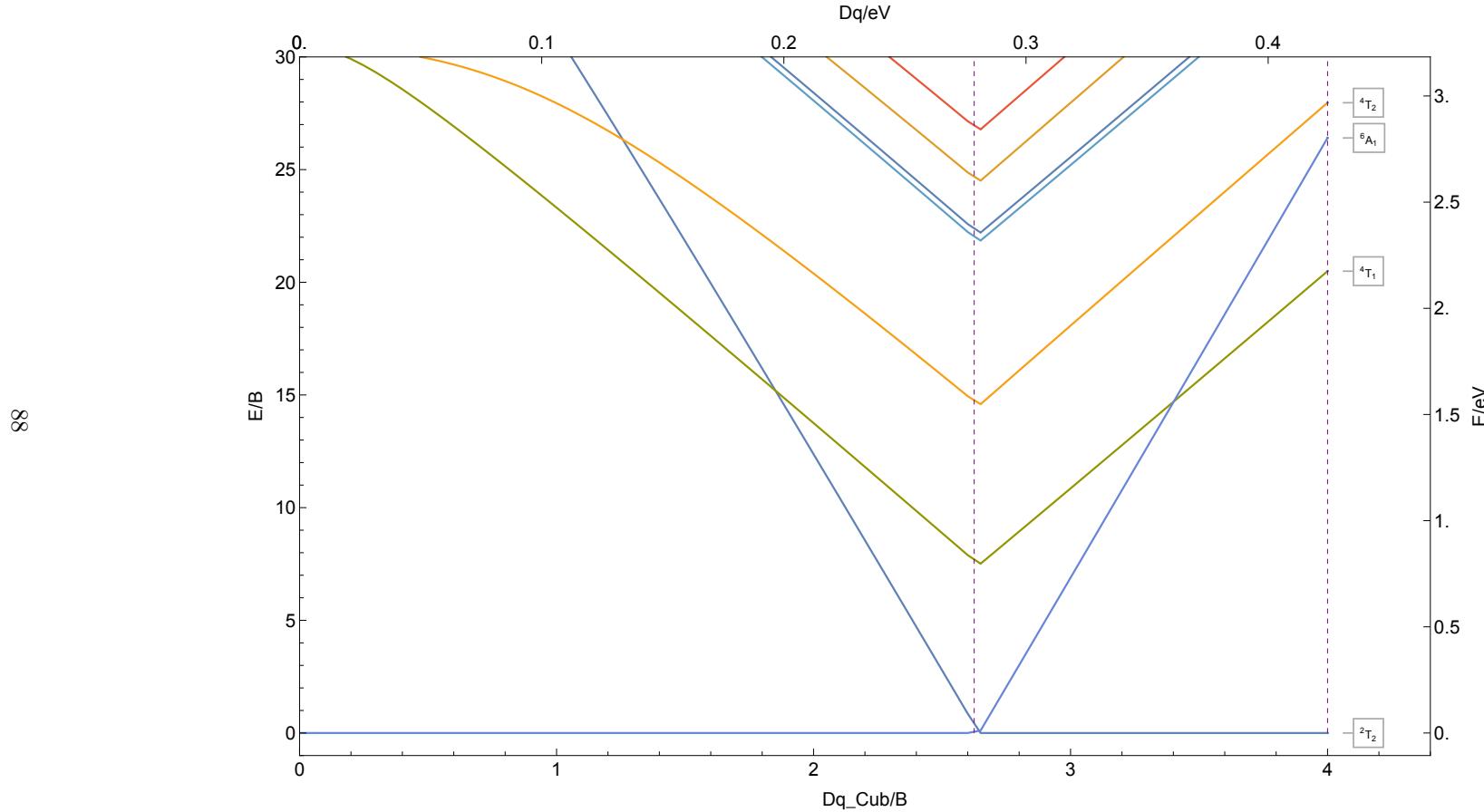
8.1.62 Pd<sup>4+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4.1 | B ≈ 838 cm<sup>-1</sup> | Pd<sup>4+</sup>



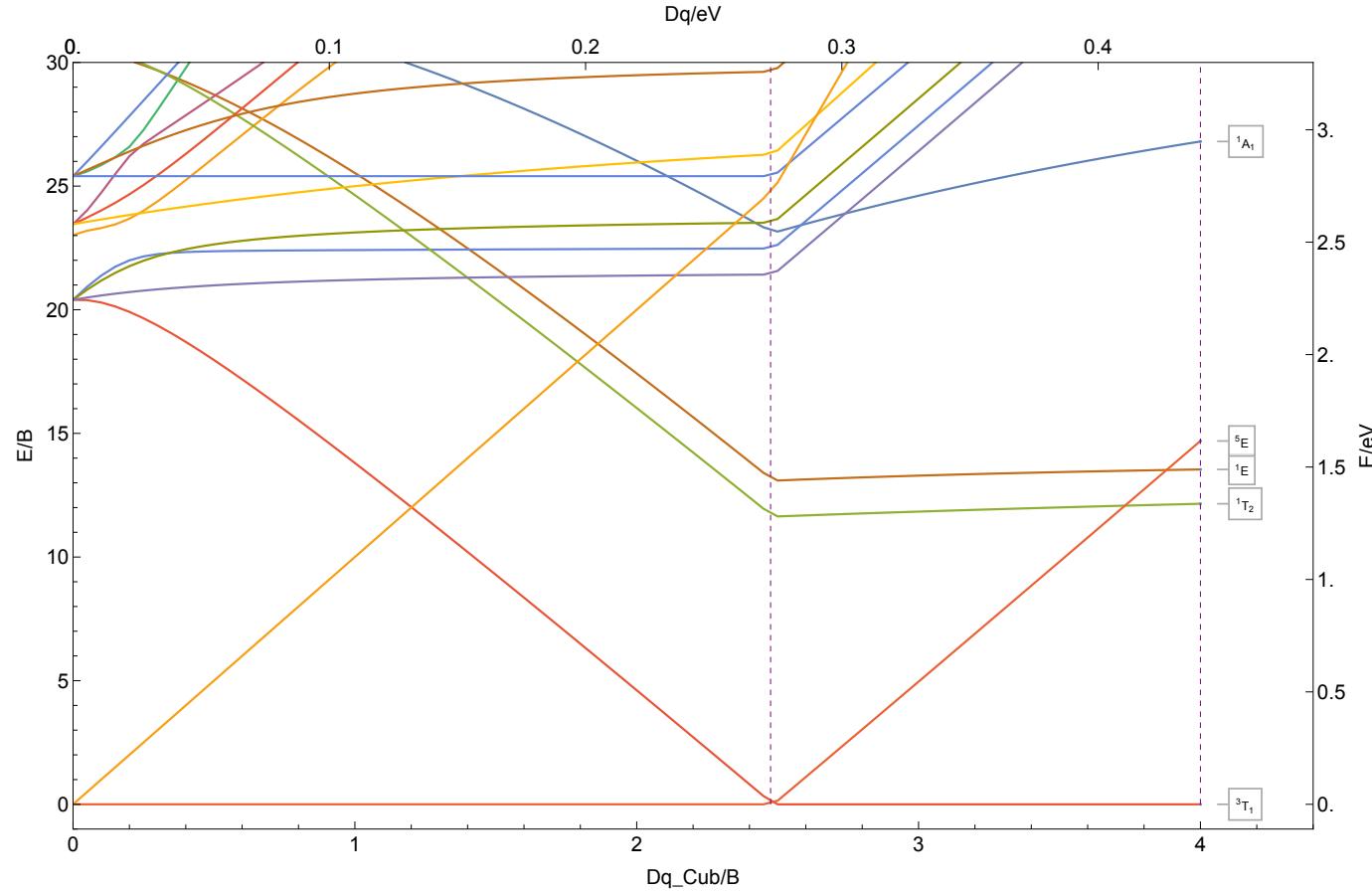
8.1.63 Pd<sup>5+</sup>

|2,4,6| d<sup>5</sup>| C/B ≈ 4.1| B ≈ 856 cm<sup>-1</sup> | Pd<sup>5+</sup>



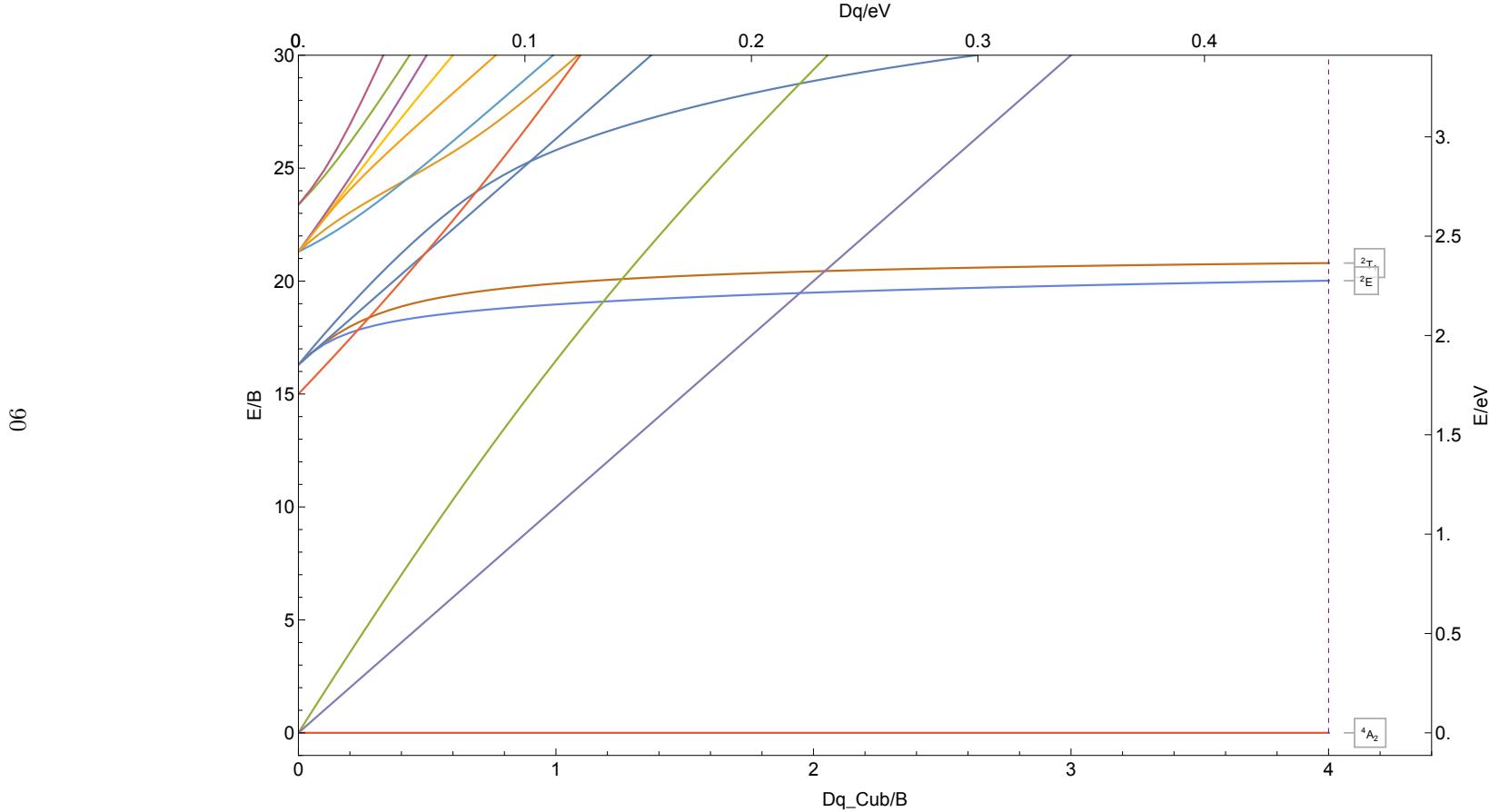
8.1.64 Pd<sup>6+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 4.1 | B ≈ 887 cm<sup>-1</sup> | Pd<sup>6+</sup>



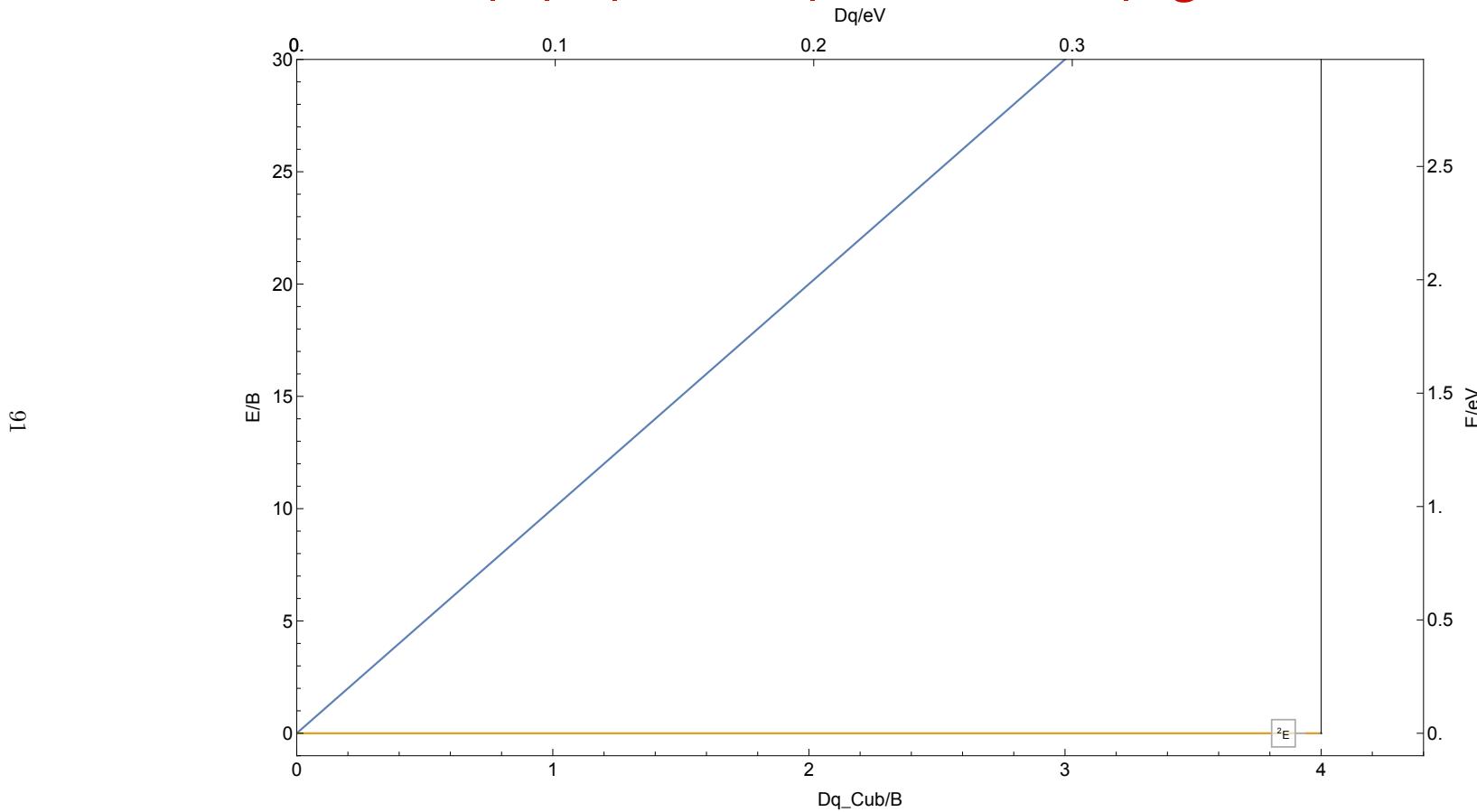
8.1.65 Pd<sup>7+</sup>

$|2,4|d^3|C/B \approx 4.1|B \approx 917\text{ cm}^{-1}|Pd^{7+}$



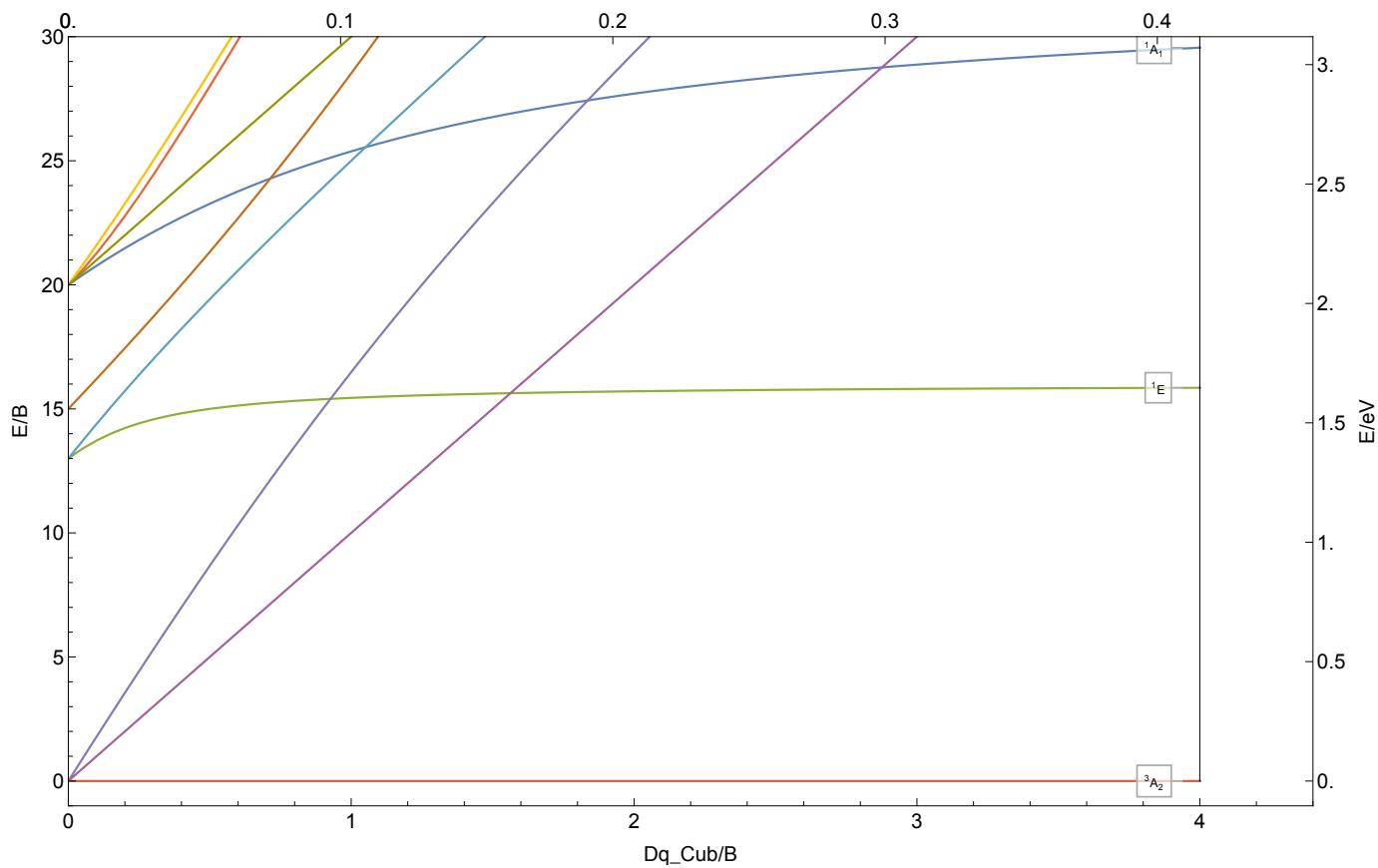
8.1.66 Ag<sup>2+</sup>

|2|d<sup>9</sup>| C/B ≈ 4. | B ≈ 799 cm<sup>-1</sup> |Ag<sup>2+</sup>



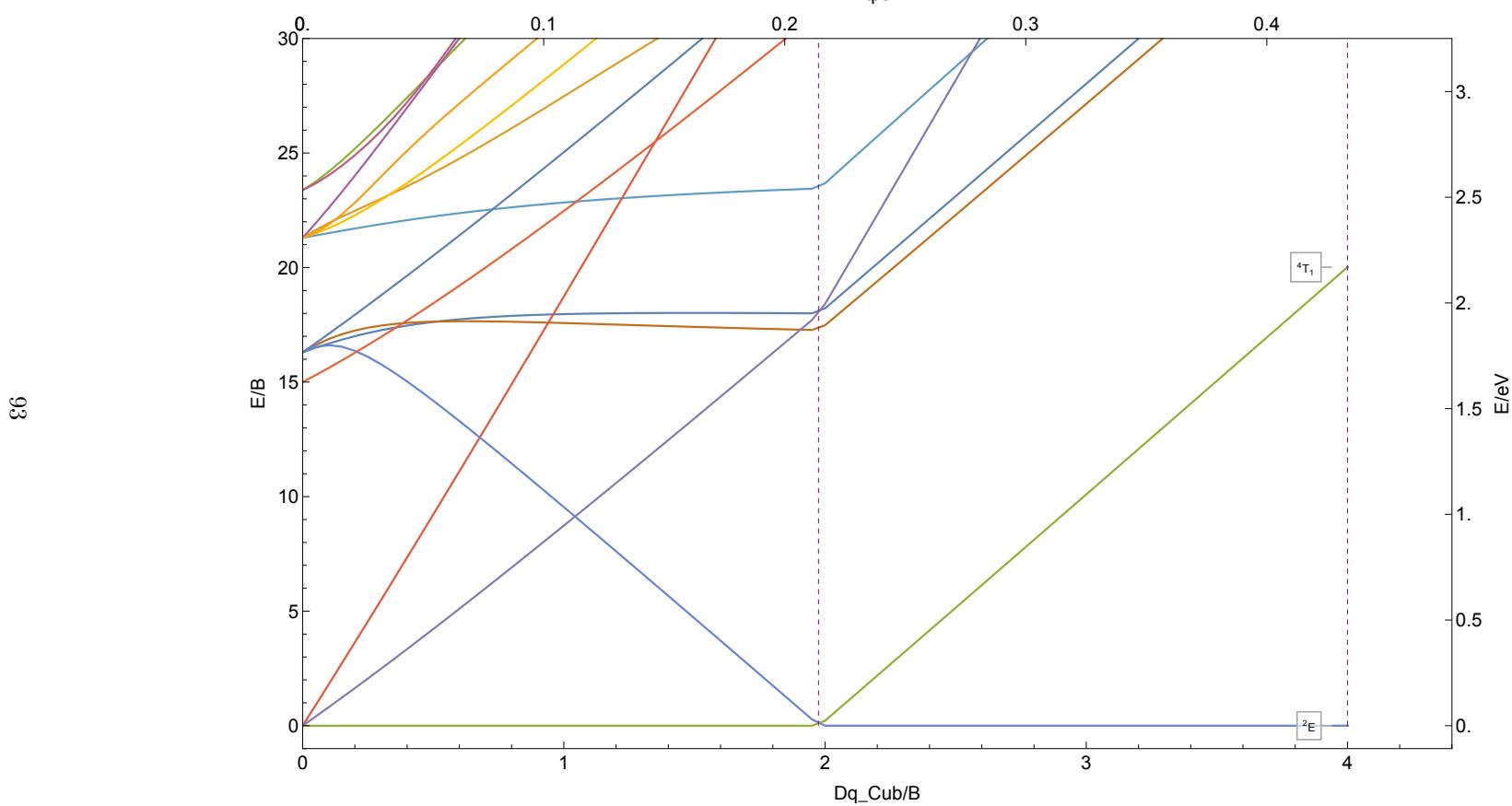
8.1.67  $\text{Ag}^{3+}$

$|1,3|d^8|C/B \approx 4.|B \approx 838 \text{ cm}^{-1}|Ag^{3+}$



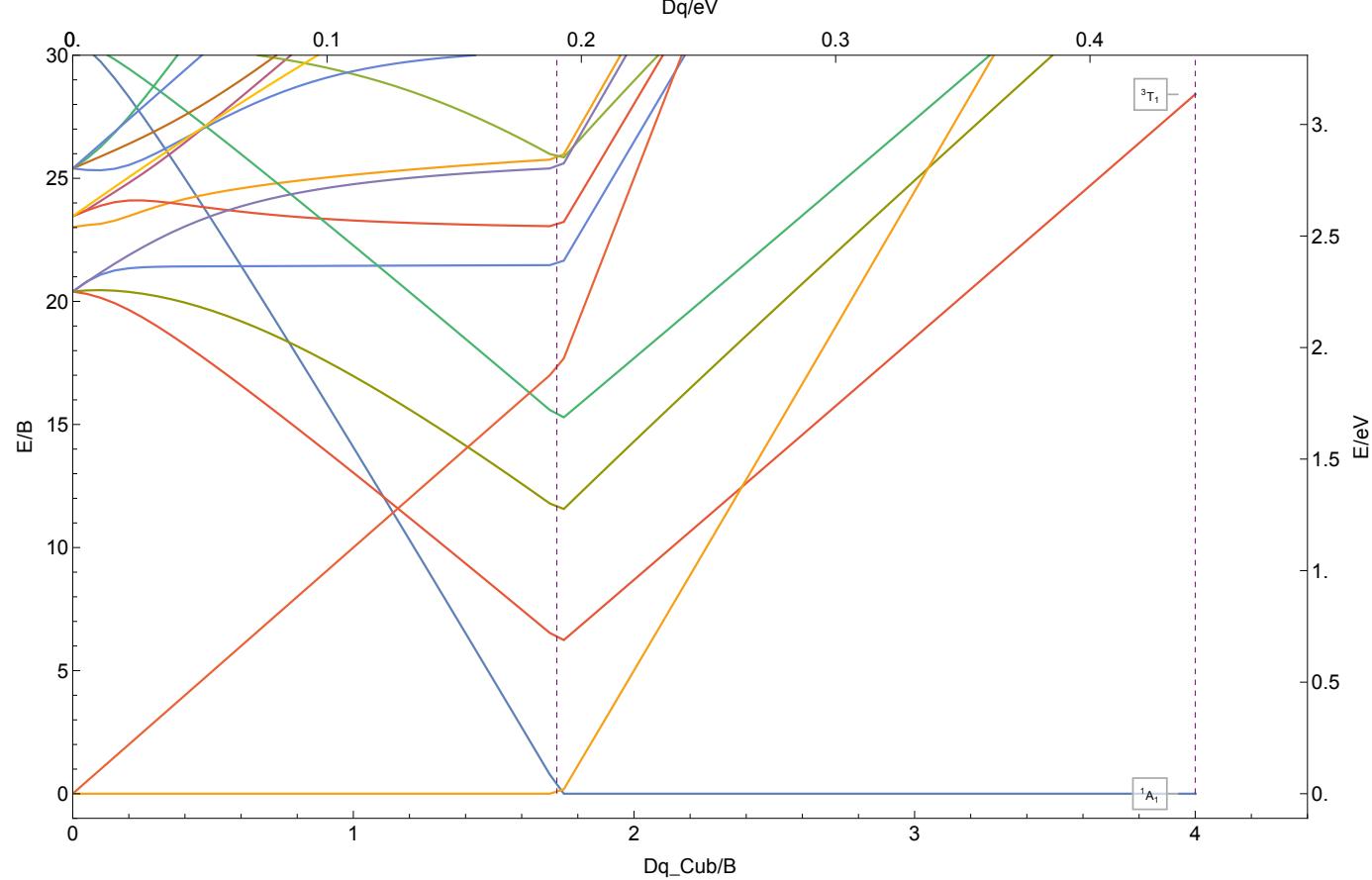
8.1.68 Ag<sup>4+</sup>

|2,4|d<sup>7</sup>| C/B ≈ 4.1| B ≈ 874 cm<sup>-1</sup> |Ag<sup>4+</sup>



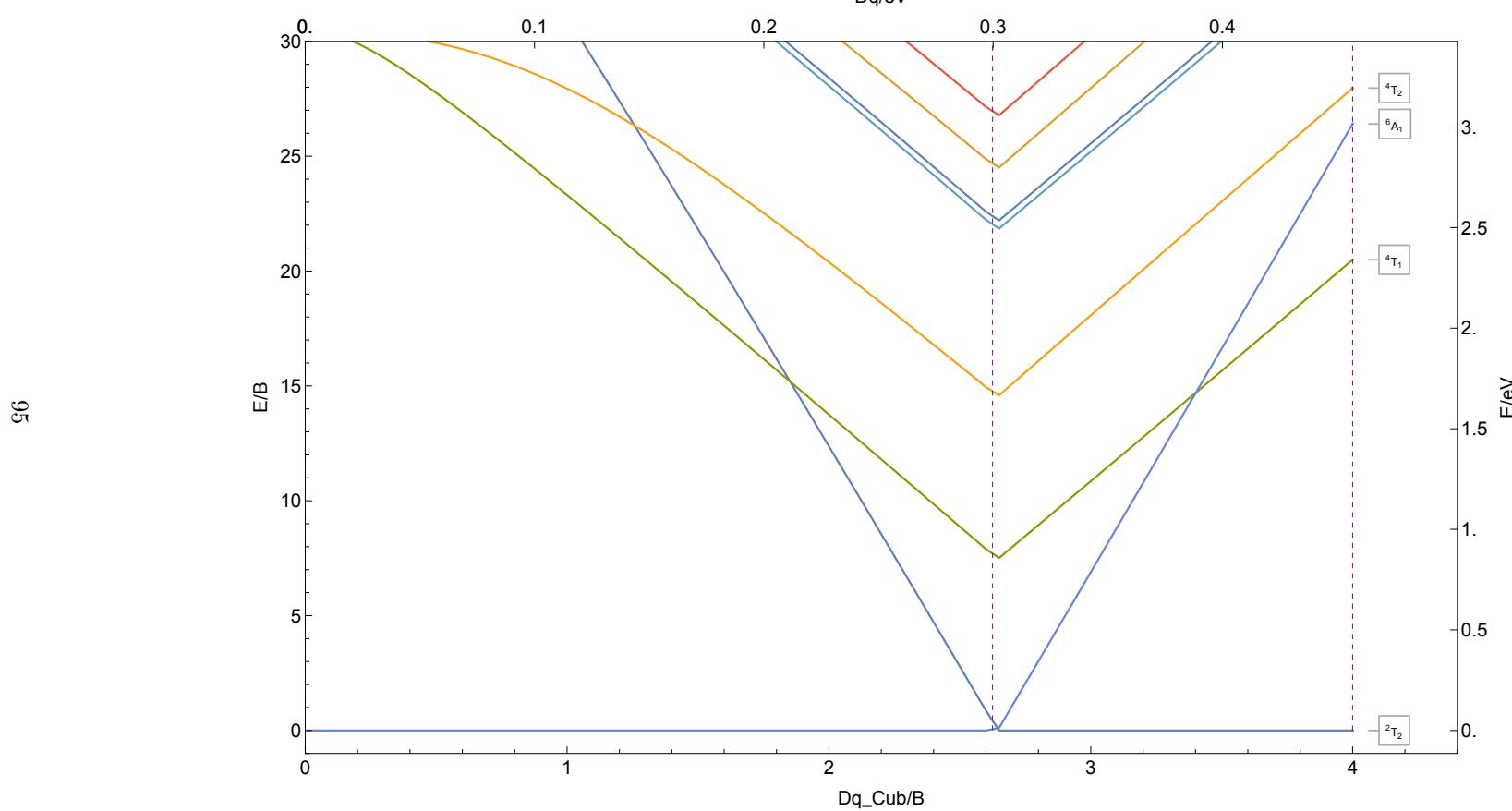
8.1.69 Ag<sup>5+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4.1 | B ≈ 890 cm<sup>-1</sup> | Ag<sup>5+</sup>



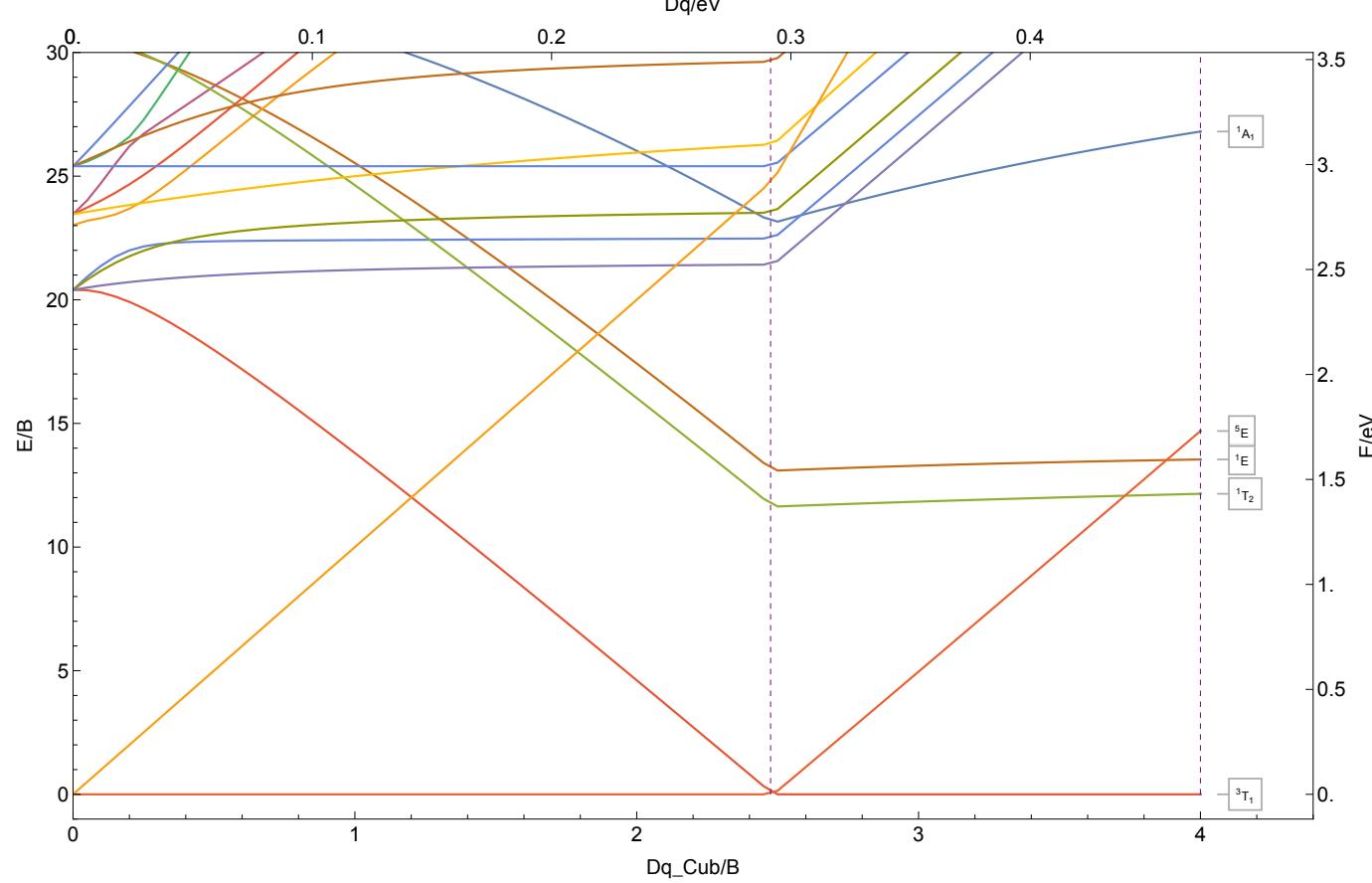
8.1.70 Ag<sup>6+</sup>

|2,4,6|d<sup>5</sup>|C/B ≈ 4.1|B ≈ 921 cm<sup>-1</sup>|Ag<sup>6+</sup>



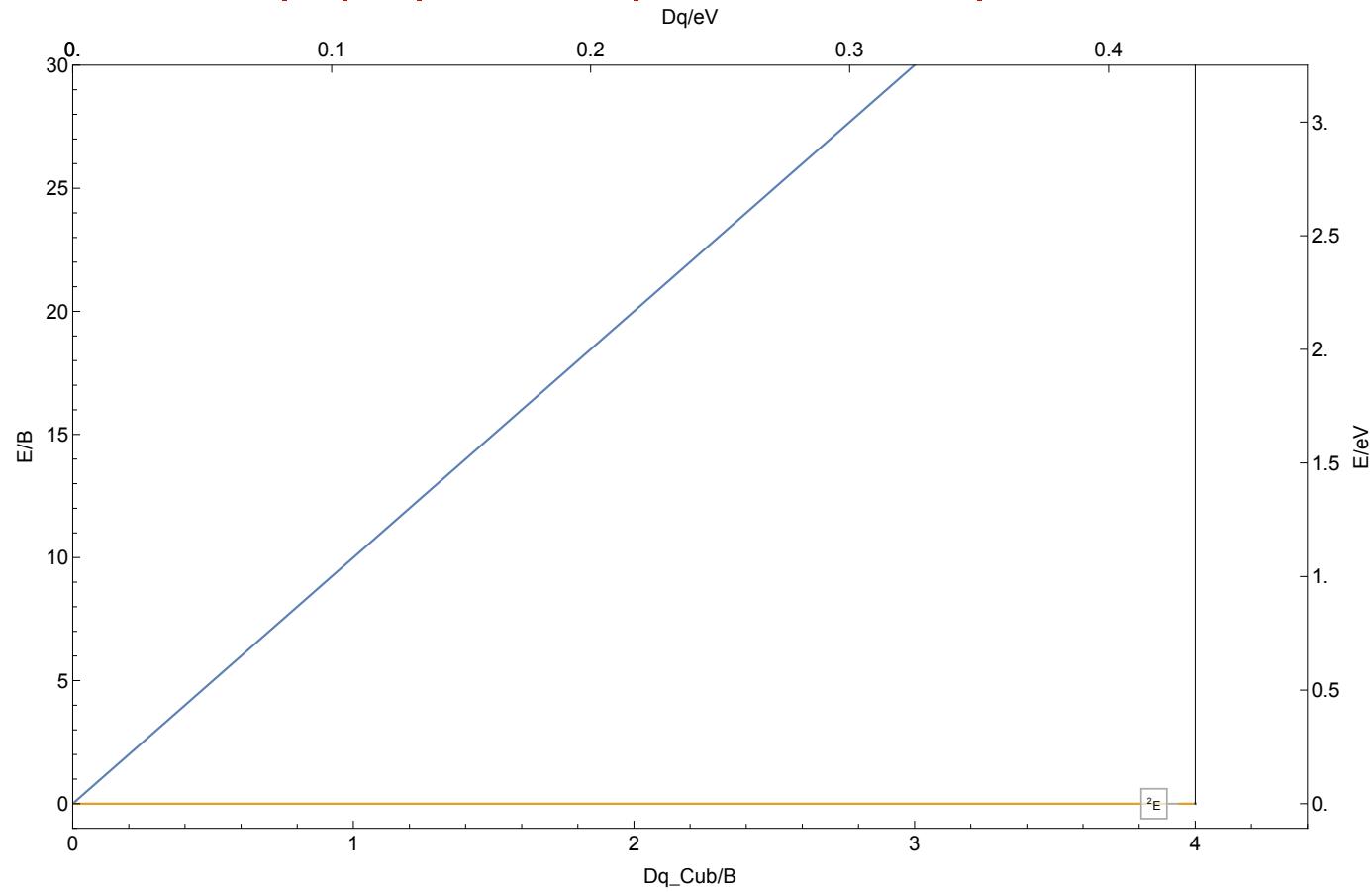
8.1.71 Ag<sup>7+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 4.1 | B ≈ 950 cm<sup>-1</sup> | Ag<sup>7+</sup>



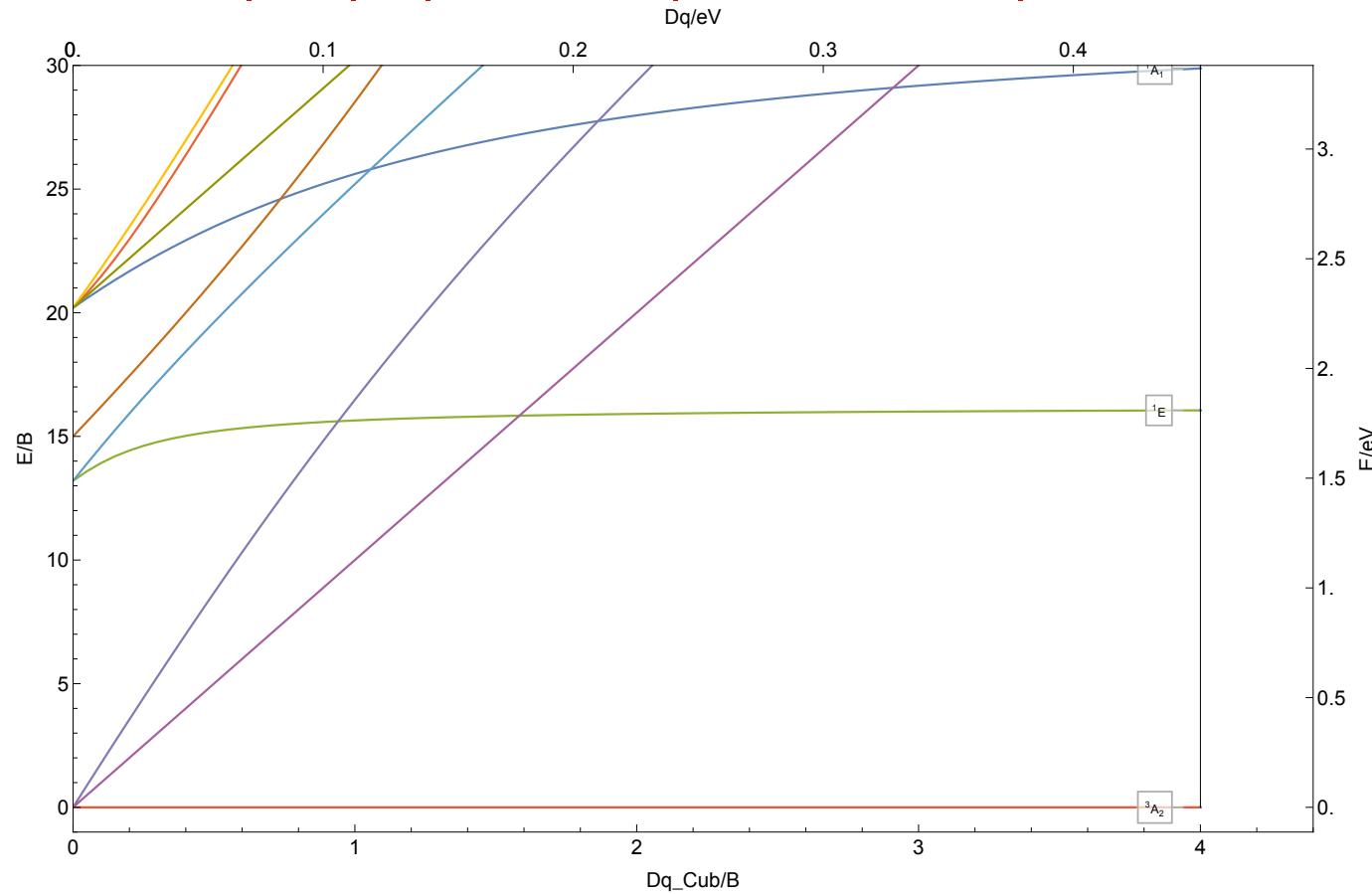
8.1.72 Cd<sup>3+</sup>

|2|d<sup>9</sup>| C/B ≈ 4. |B ≈ 874 cm<sup>-1</sup> |Cd<sup>3+</sup>



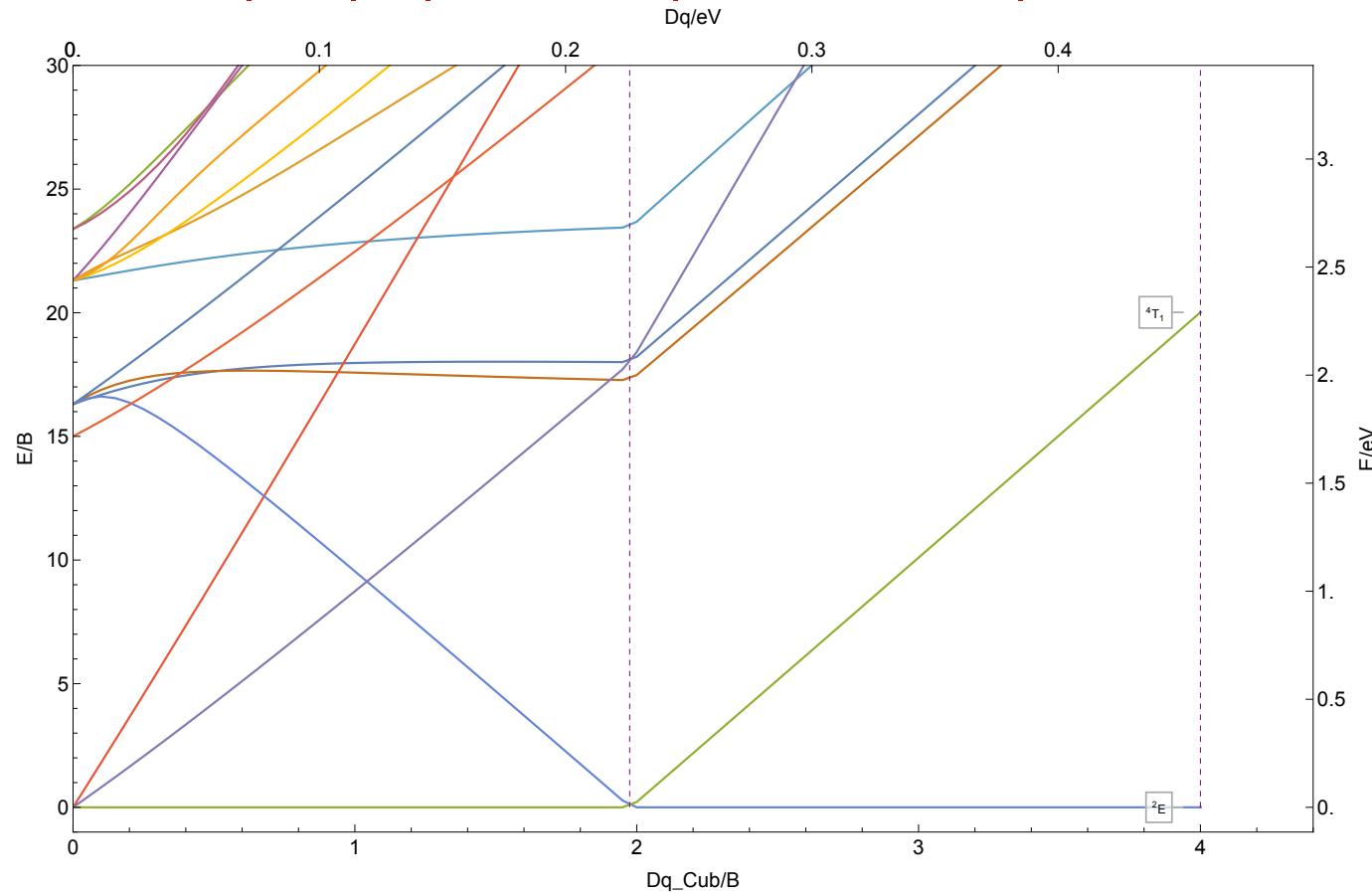
8.1.73 Cd<sup>4+</sup>

|1,3|d<sup>8</sup>| C/B ≈ 4.1| B ≈ 909 cm<sup>-1</sup> |Cd<sup>4+</sup>



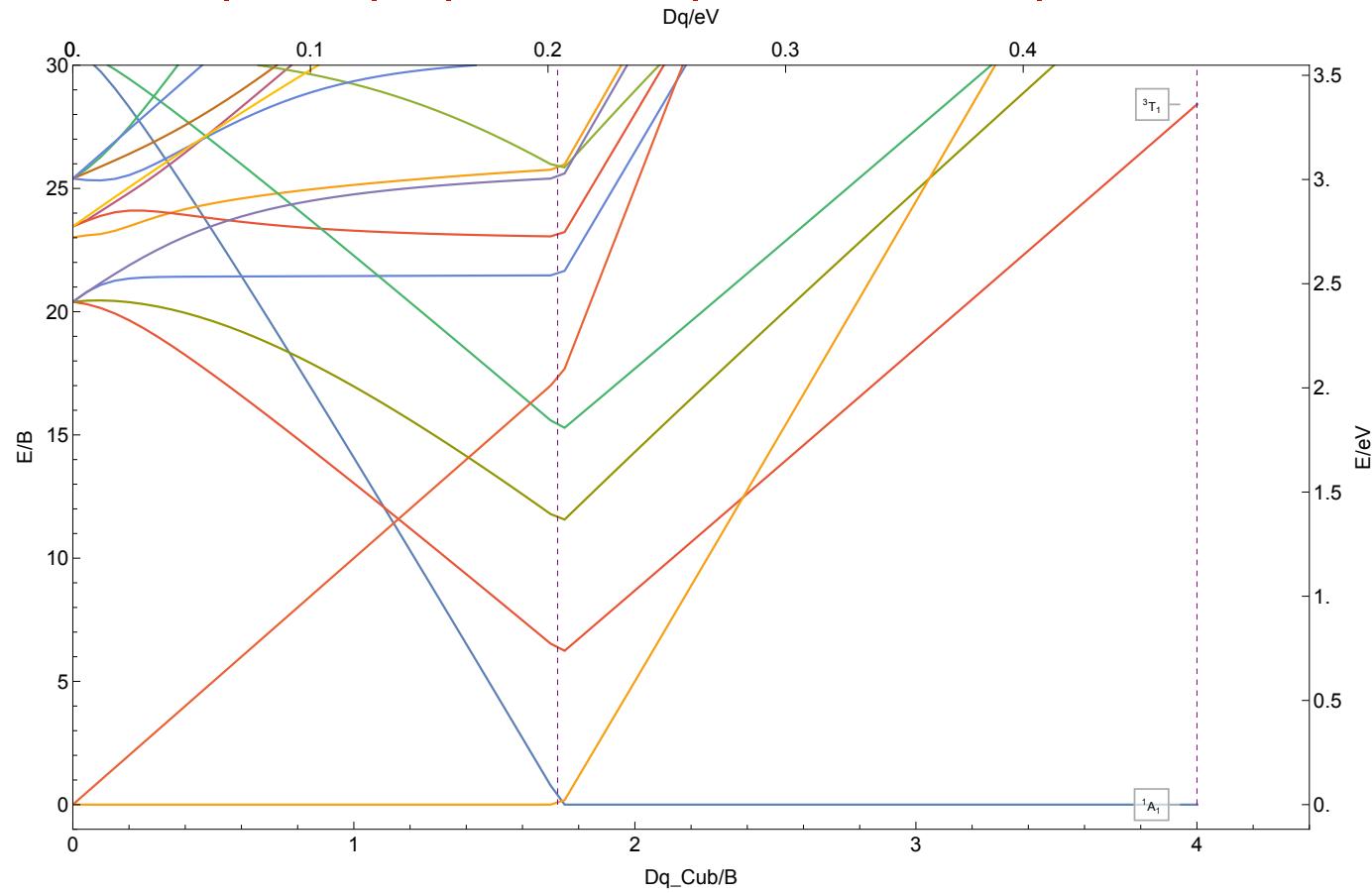
8.1.74 Cd<sup>5+</sup>

|2,4|d<sup>7</sup>| C/B ≈ 4.1| B ≈ 923 cm<sup>-1</sup> |Cd<sup>5+</sup>



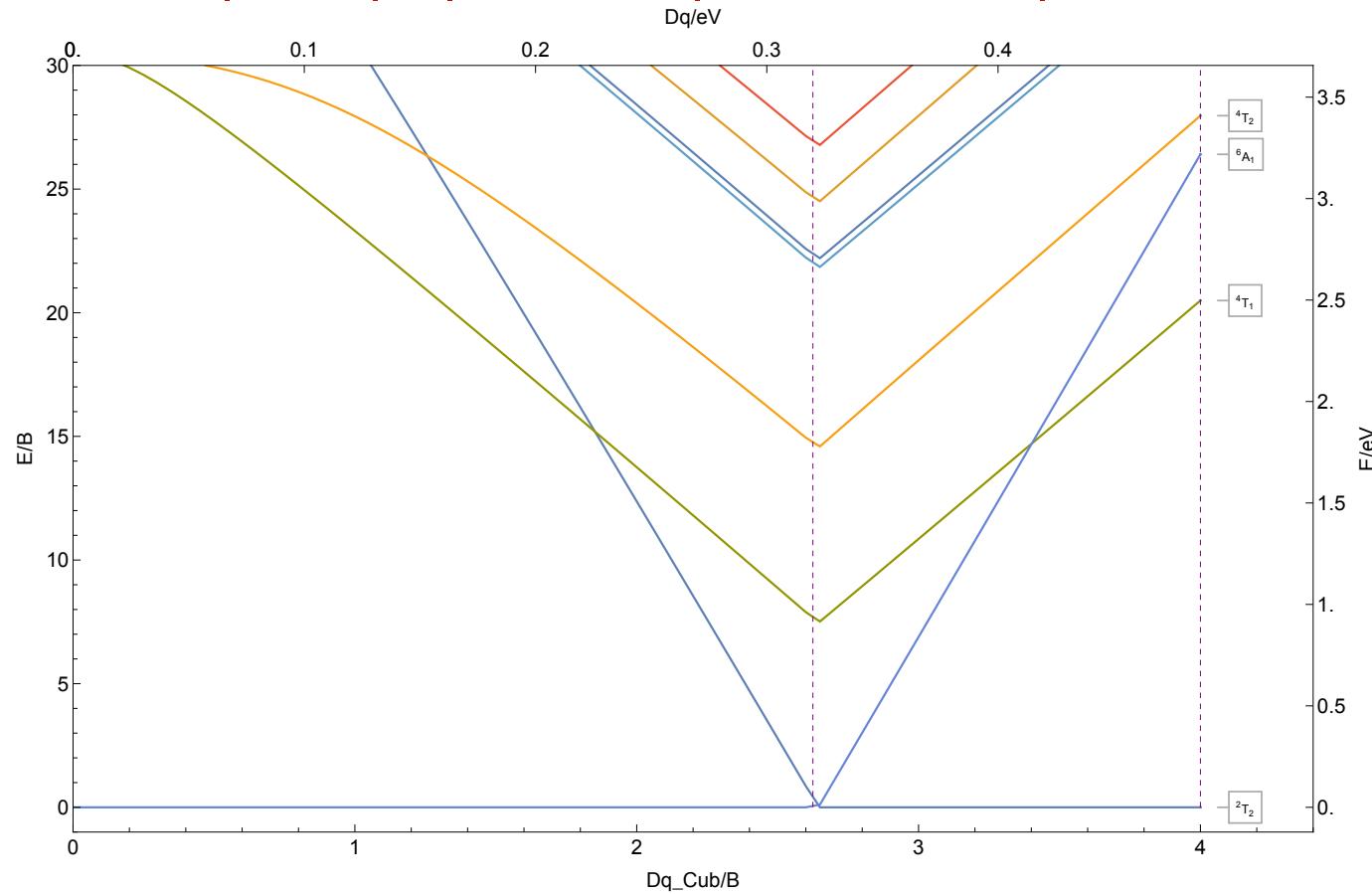
8.1.75 Cd<sup>6+</sup>

$|1,3,5|d^6|C/B \approx 4.1|B \approx 954\text{ cm}^{-1}|Cd^{6+}$



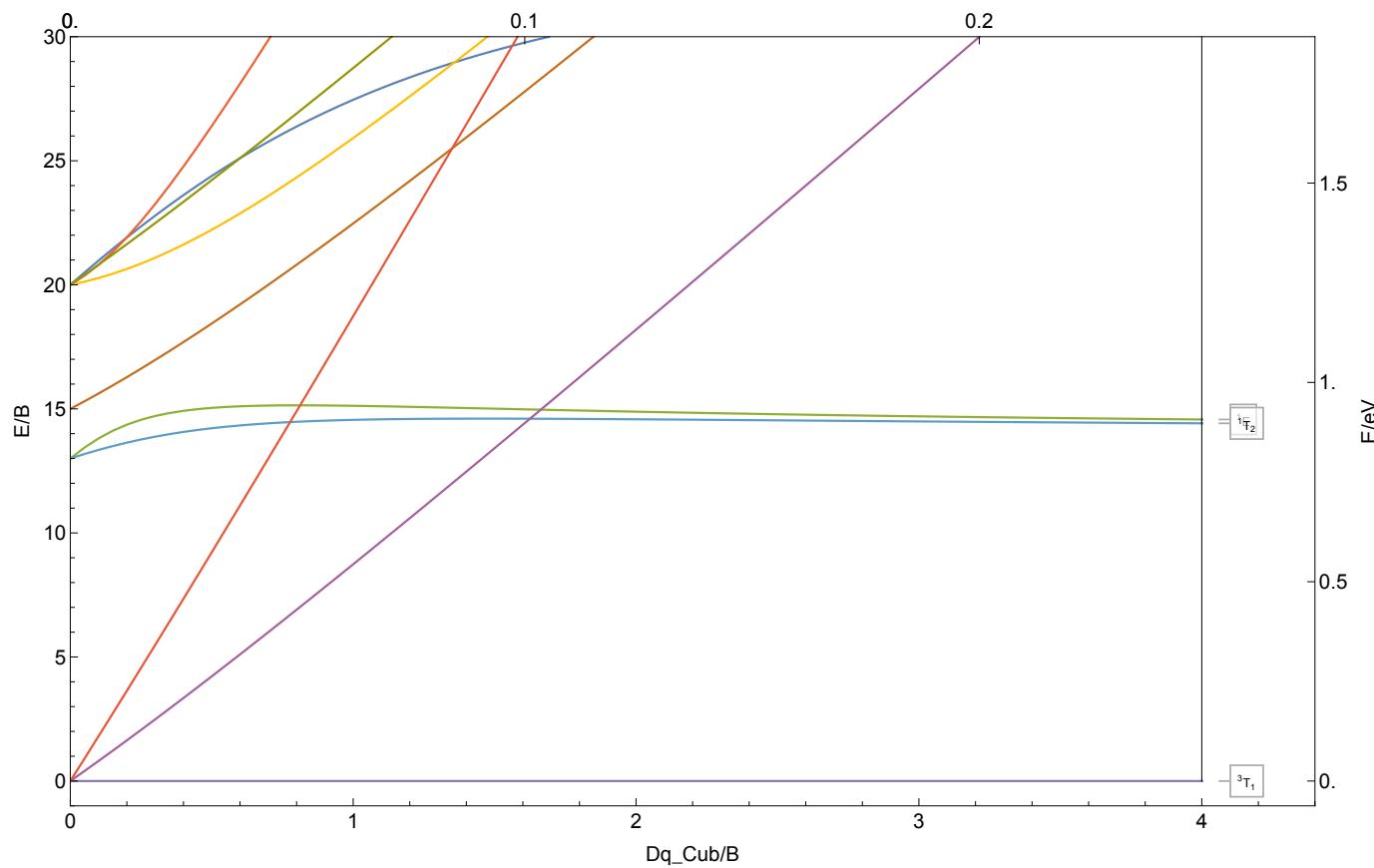
8.1.76 Cd<sup>7+</sup>

|2,4,6| d<sup>5</sup>| C/B ≈ 4.1| B ≈ 983 cm<sup>-1</sup> |Cd<sup>7+</sup>



8.1.77  $\text{Hf}^{2+}$

$|1,3|d^2| C/B \approx 4. | B \approx 502 \text{ cm}^{-1}| \text{Hf}^{2+}$

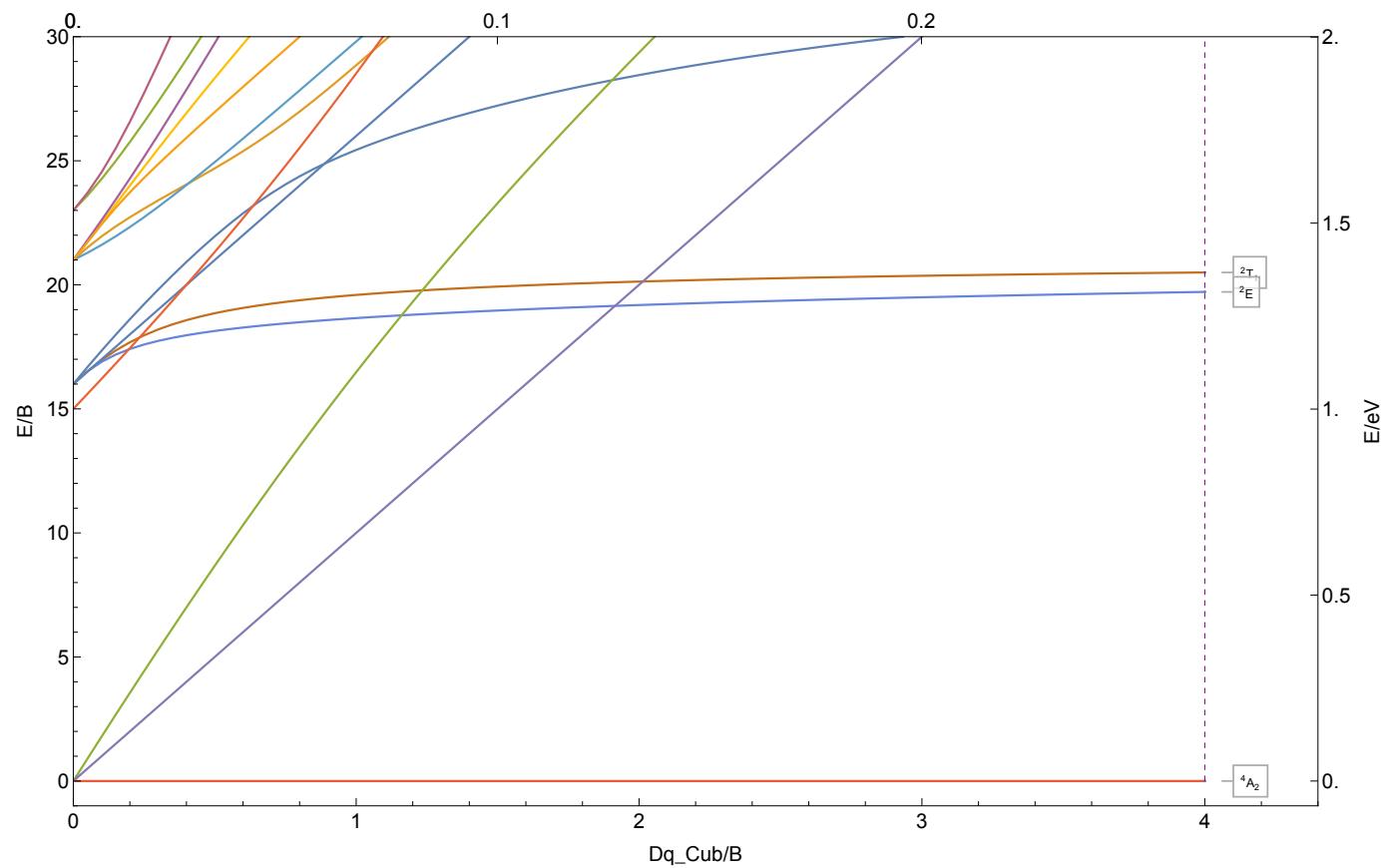


8.1.78  $Ta^{2+}$

$|2,4|d^3|C/B \approx 4. |B \approx 538\text{ cm}^{-1}|Ta^{2+}$

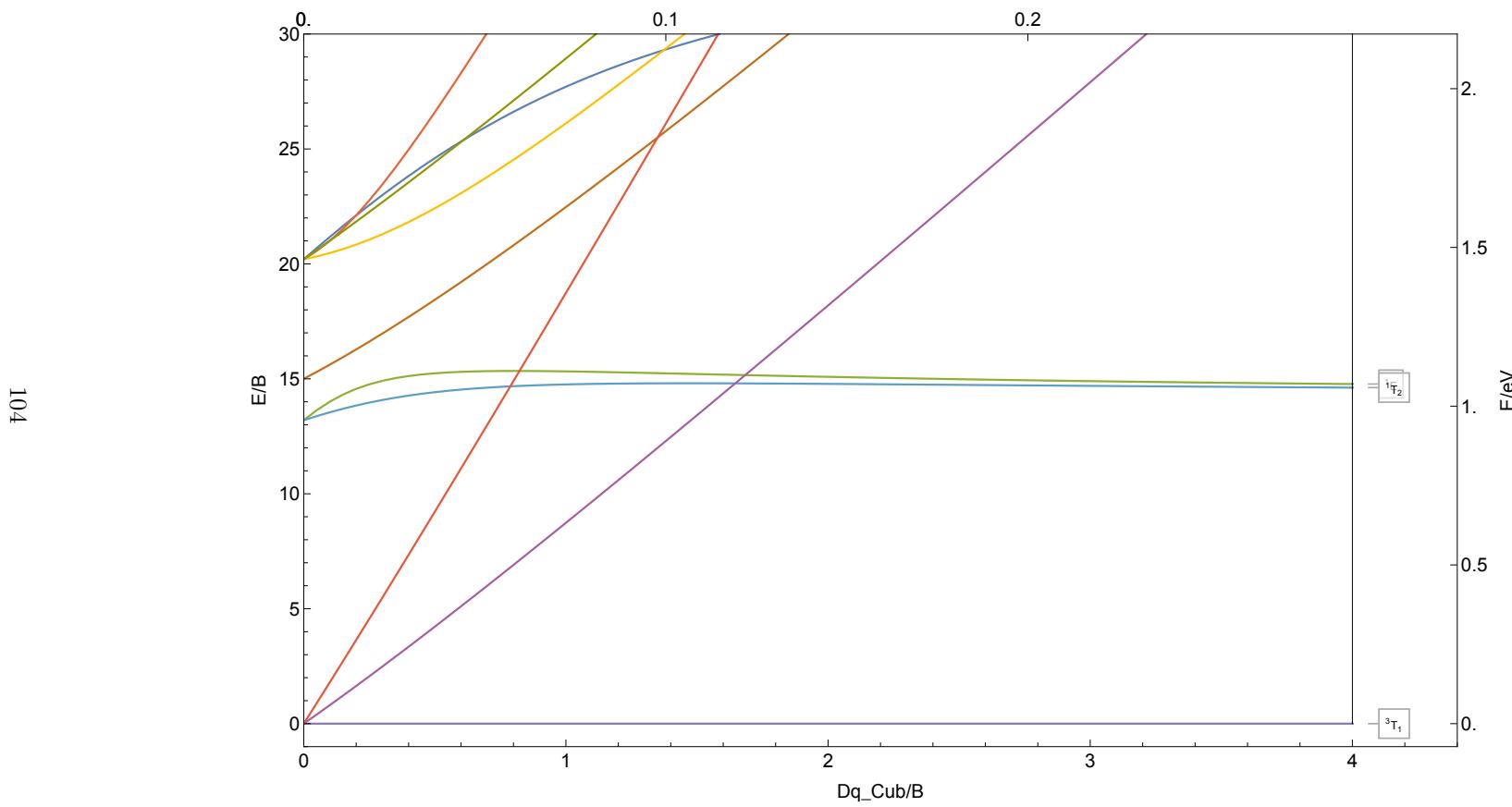
Dq/eV

10<sup>3</sup>



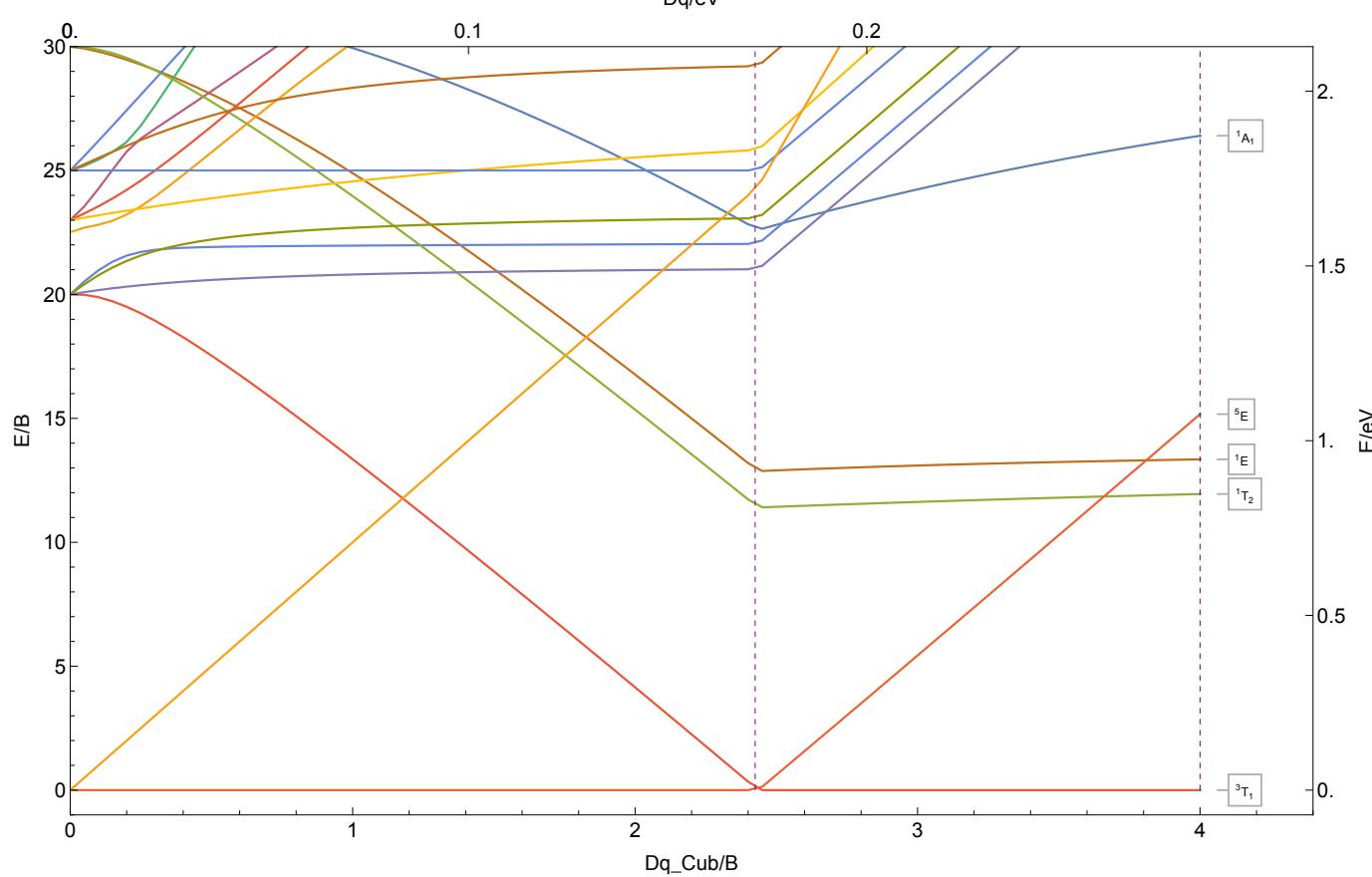
8.1.79 Ta<sup>3+</sup>

$$|1,3|d^2|C/B \approx 4.1|B \approx 584\text{ cm}^{-1}|Ta^{3+}$$



8.1.80  $W^{2+}$

$|1,3,5|d^4|C/B \approx 4. |B \approx 572\text{ cm}^{-1}|W^{2+}$

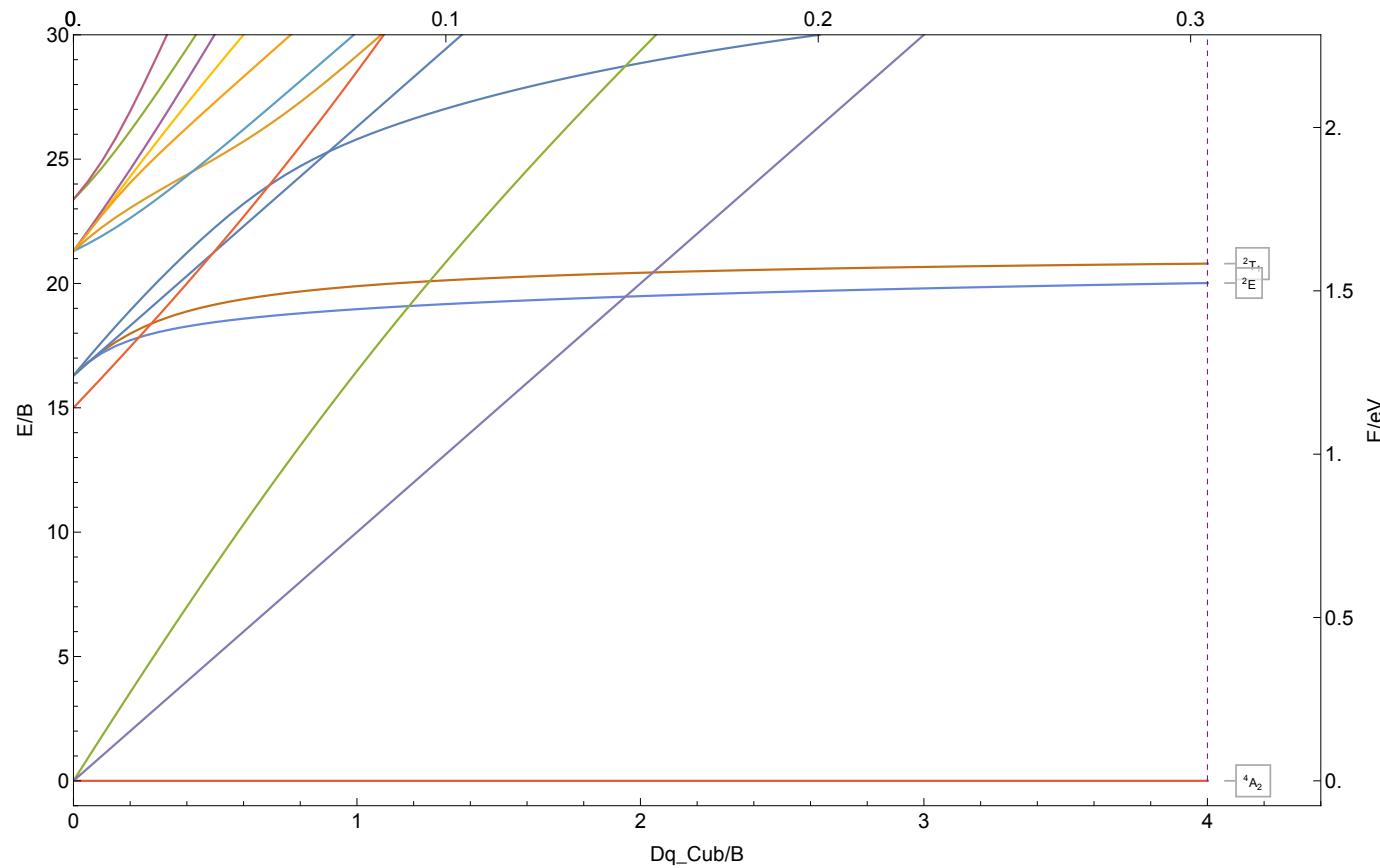


8.1.81  $\text{W}^{3+}$

$$|2,4|d^3|C/B \approx 4.1|B \approx 614\text{ cm}^{-1}|W^{3+}$$

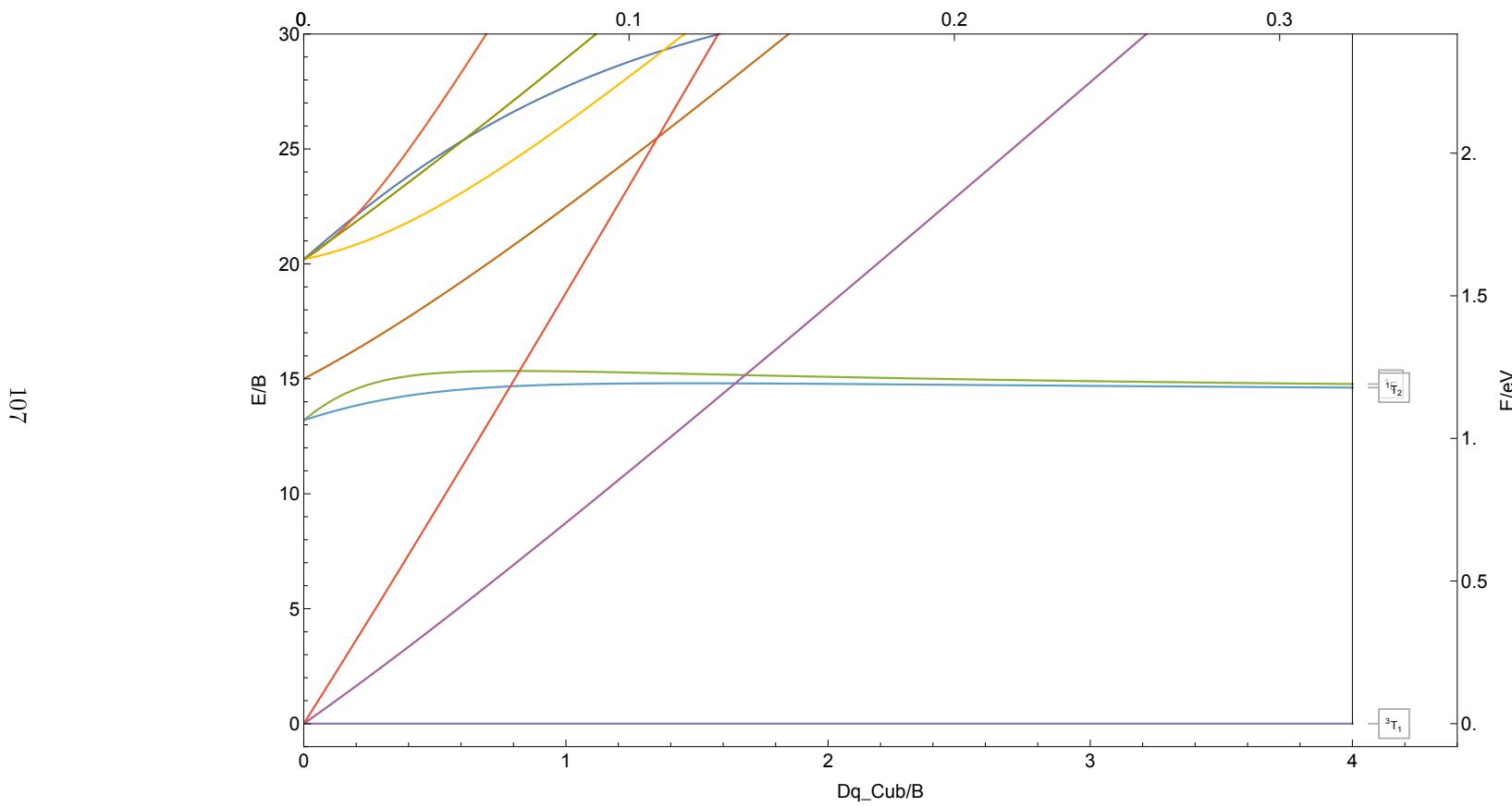
Dq/eV

10<sup>6</sup>



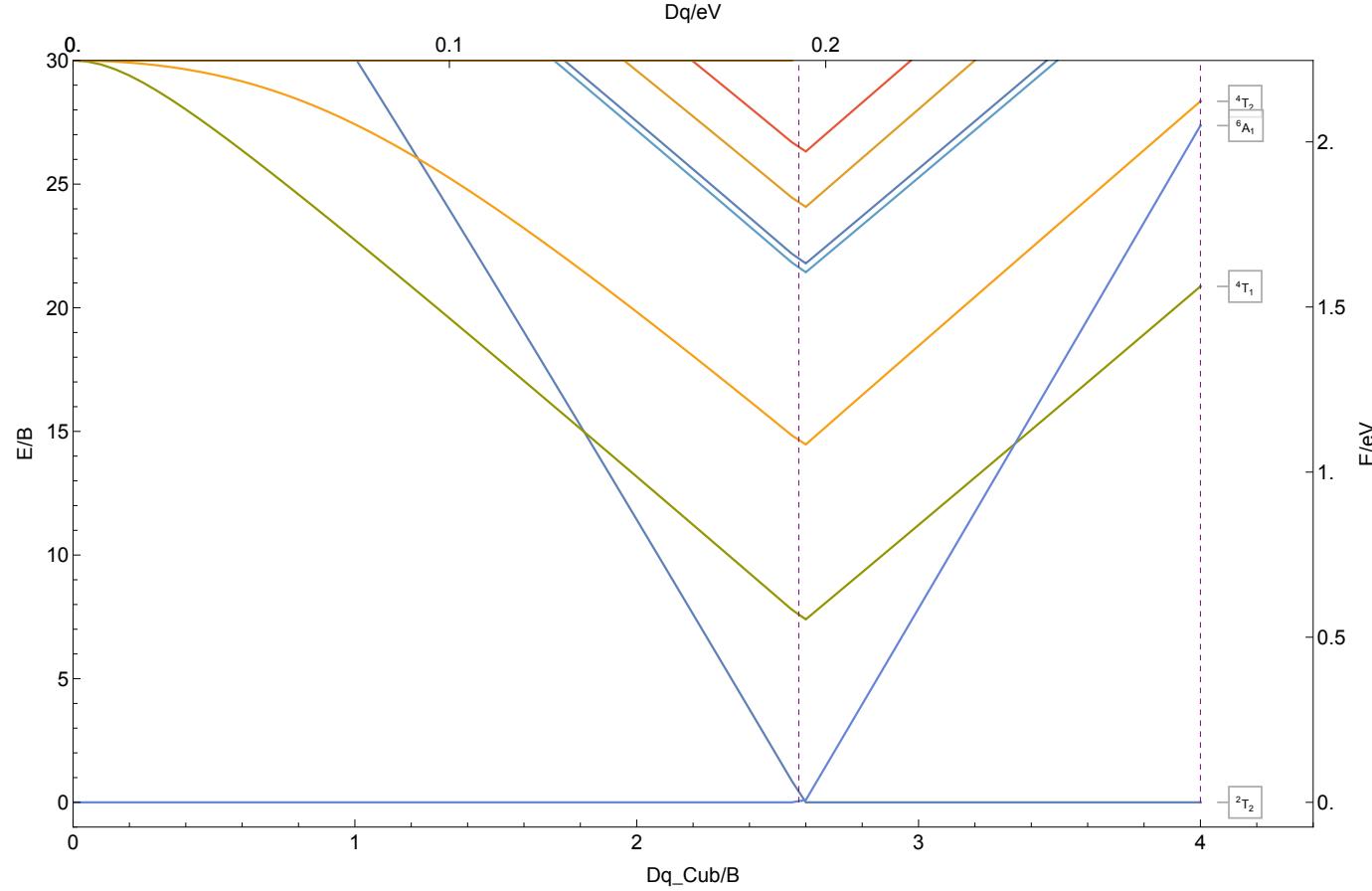
8.1.82  $\text{W}^{4+}$

$$|1,3|d^2|C/B \approx 4.1|B \approx 650 \text{ cm}^{-1}|W^{4+}$$



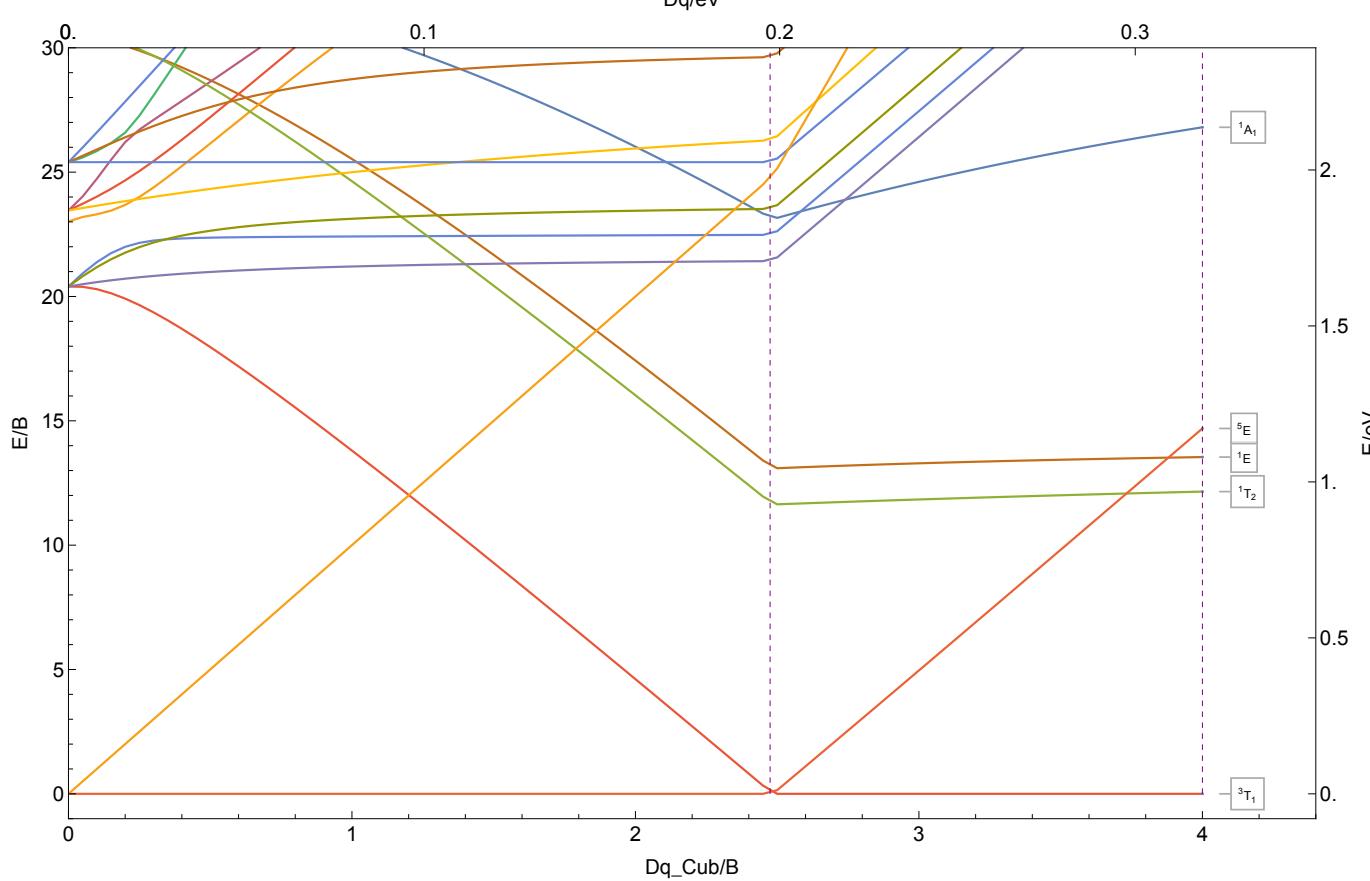
8.1.83  $\text{Re}^{2+}$

$|2,4,6| \text{d}^5 | \text{C/B} \approx 4. | \text{B} \approx 604 \text{ cm}^{-1} | \text{Re}^{2+}$



8.1.84  $\text{Re}^{3+}$

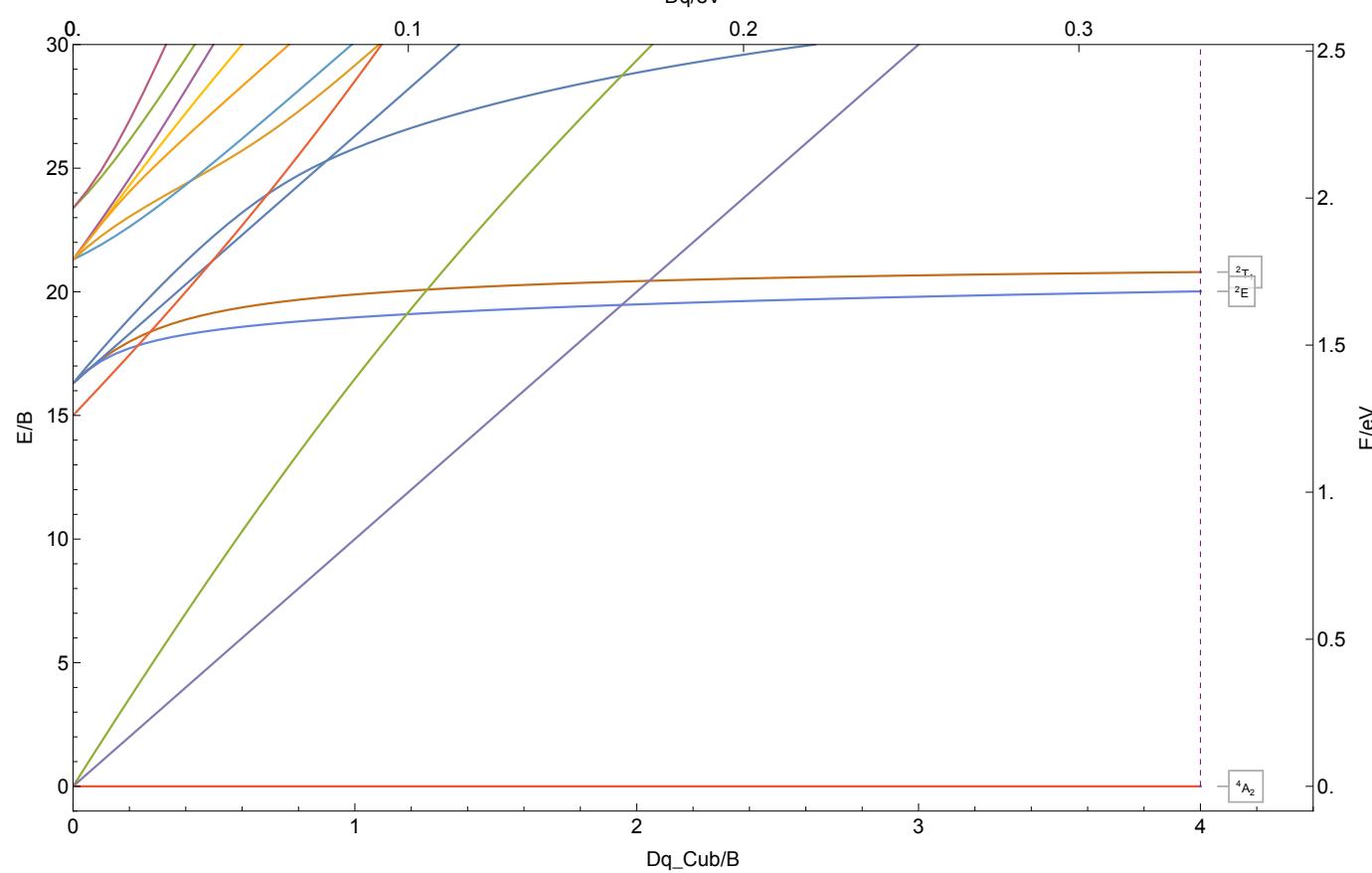
$|1,3,5|d^4|C/B \approx 4.1|B \approx 643\text{ cm}^{-1}| \text{Re}^{3+}$



8.1.85 Re<sup>4+</sup>

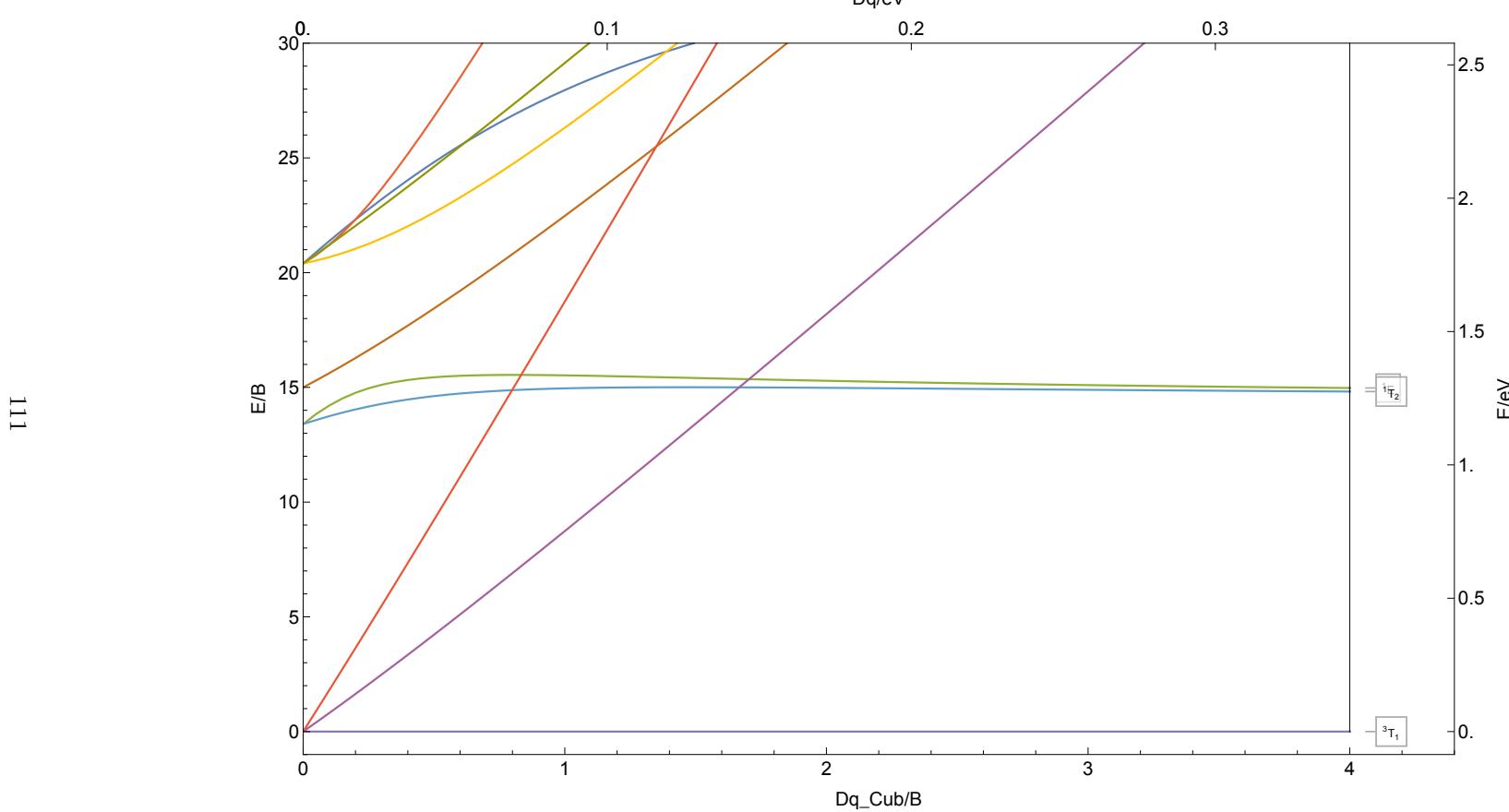
$$|2,4|d^3|C/B \approx 4.1|B \approx 678 \text{ cm}^{-1}|Re^{4+}$$

110



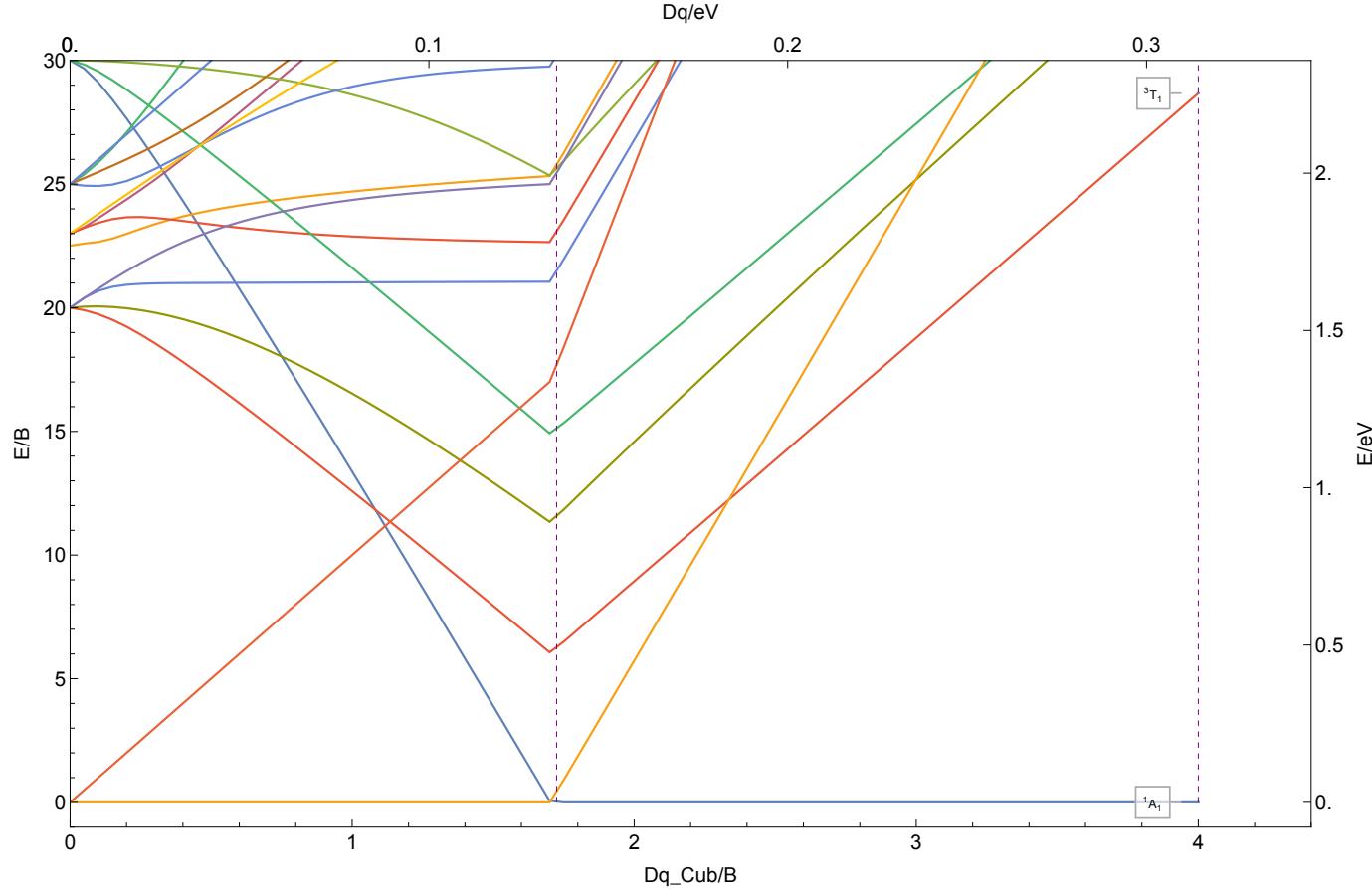
8.1.86 Re<sup>5+</sup>

$$|1,3|d^2|C/B \approx 4.2|B \approx 694\text{ cm}^{-1}|Re^{5+}$$



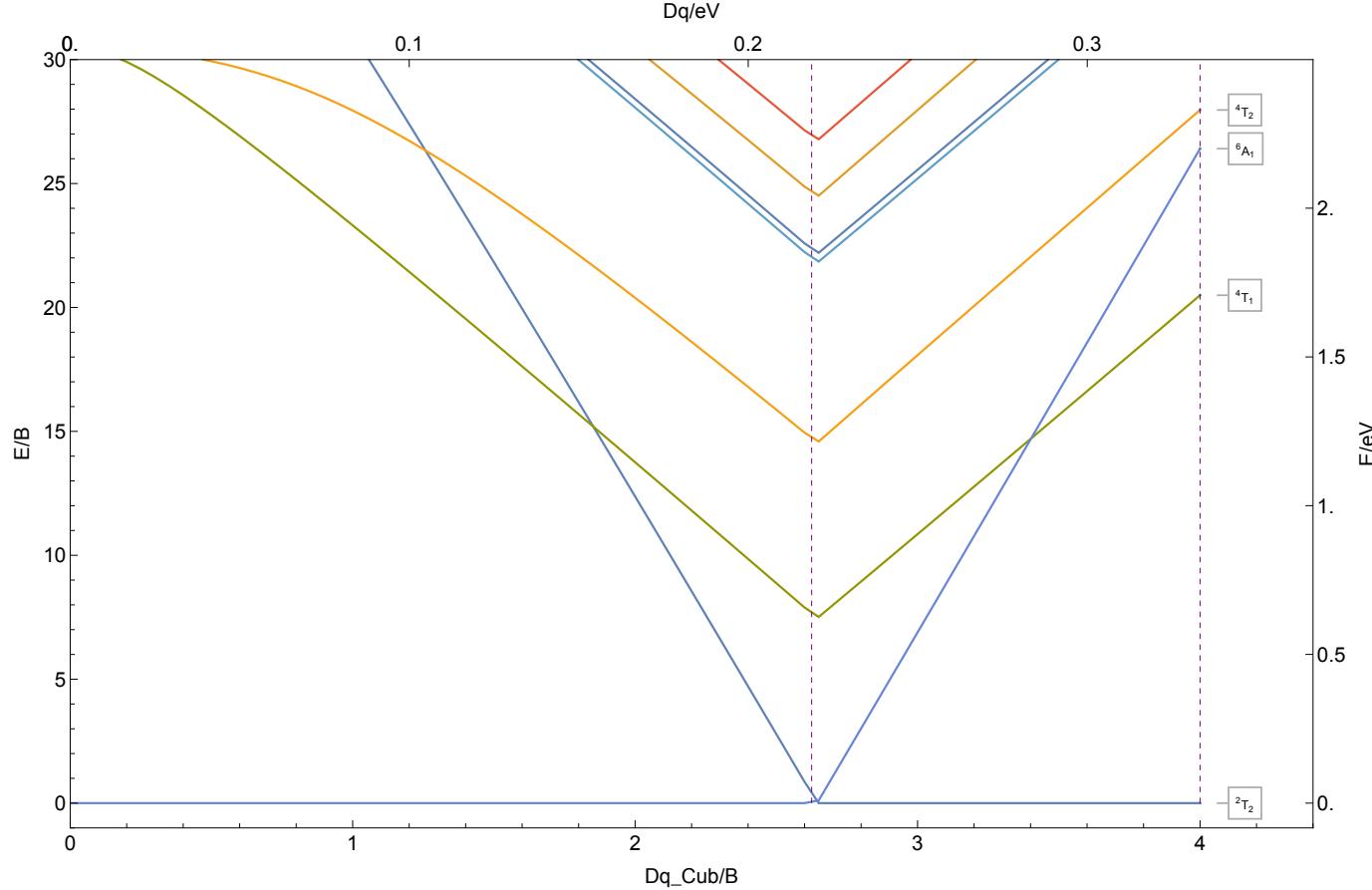
8.1.87 Os<sup>2+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4. | B ≈ 634 cm<sup>-1</sup> | Os<sup>2+</sup>



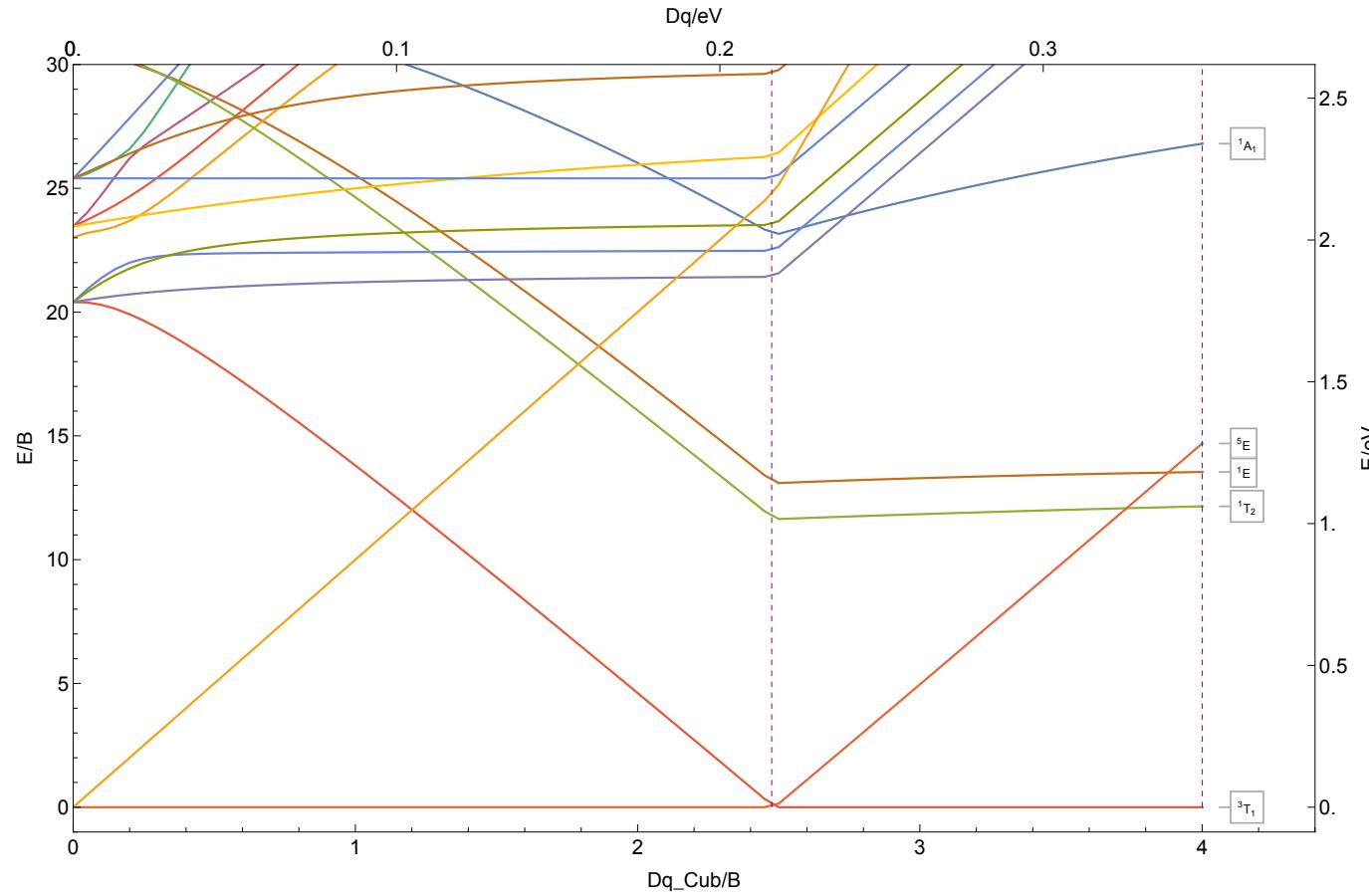
8.1.88 Os<sup>3+</sup>

|2,4,6| d<sup>5</sup>| C/B ≈ 4.1| B ≈ 672 cm<sup>-1</sup> | Os<sup>3+</sup>



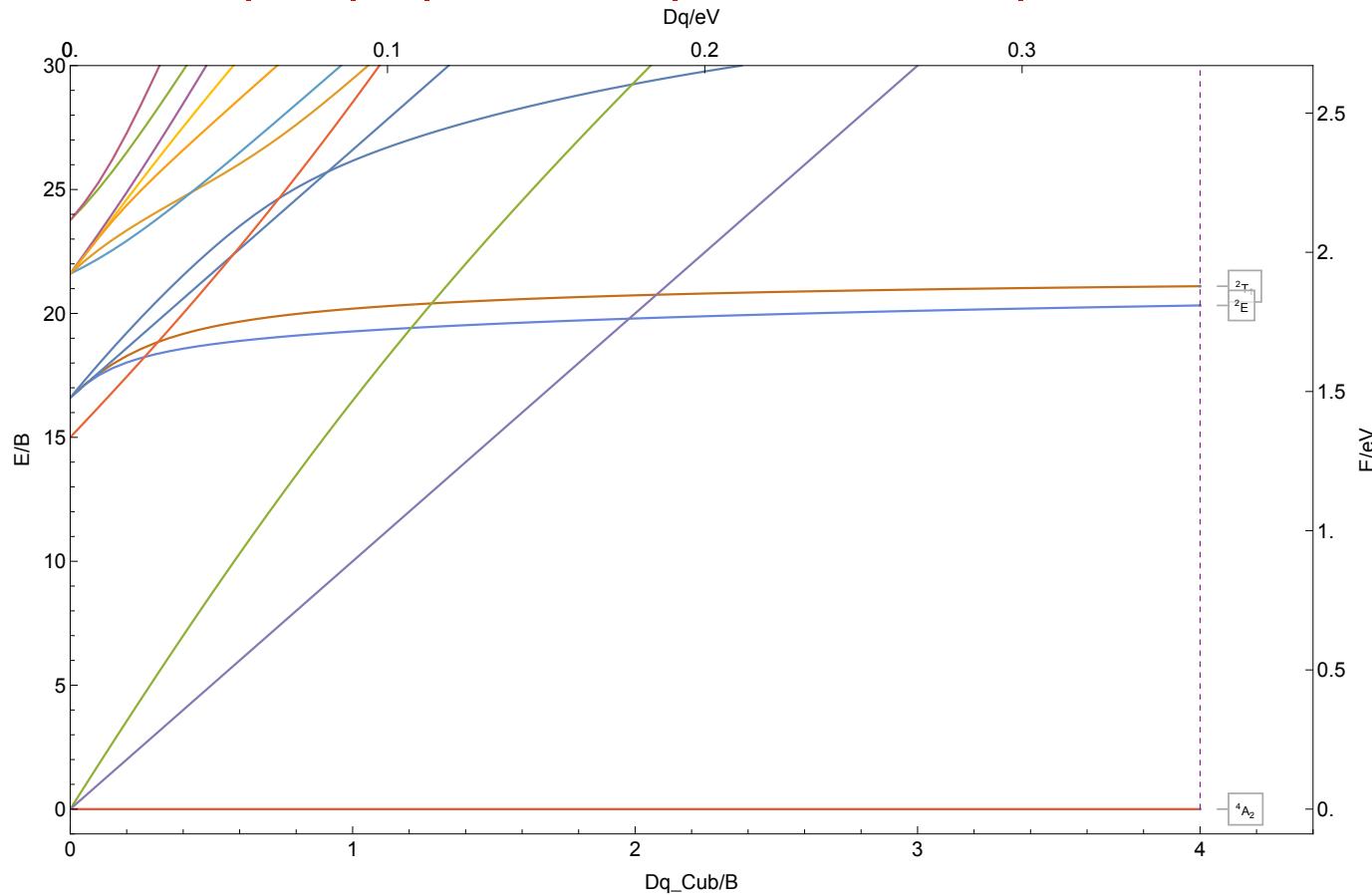
8.1.89 Os<sup>4+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 4.1 | B ≈ 704 cm<sup>-1</sup> | Os<sup>4+</sup>



8.1.90 Os<sup>5+</sup>

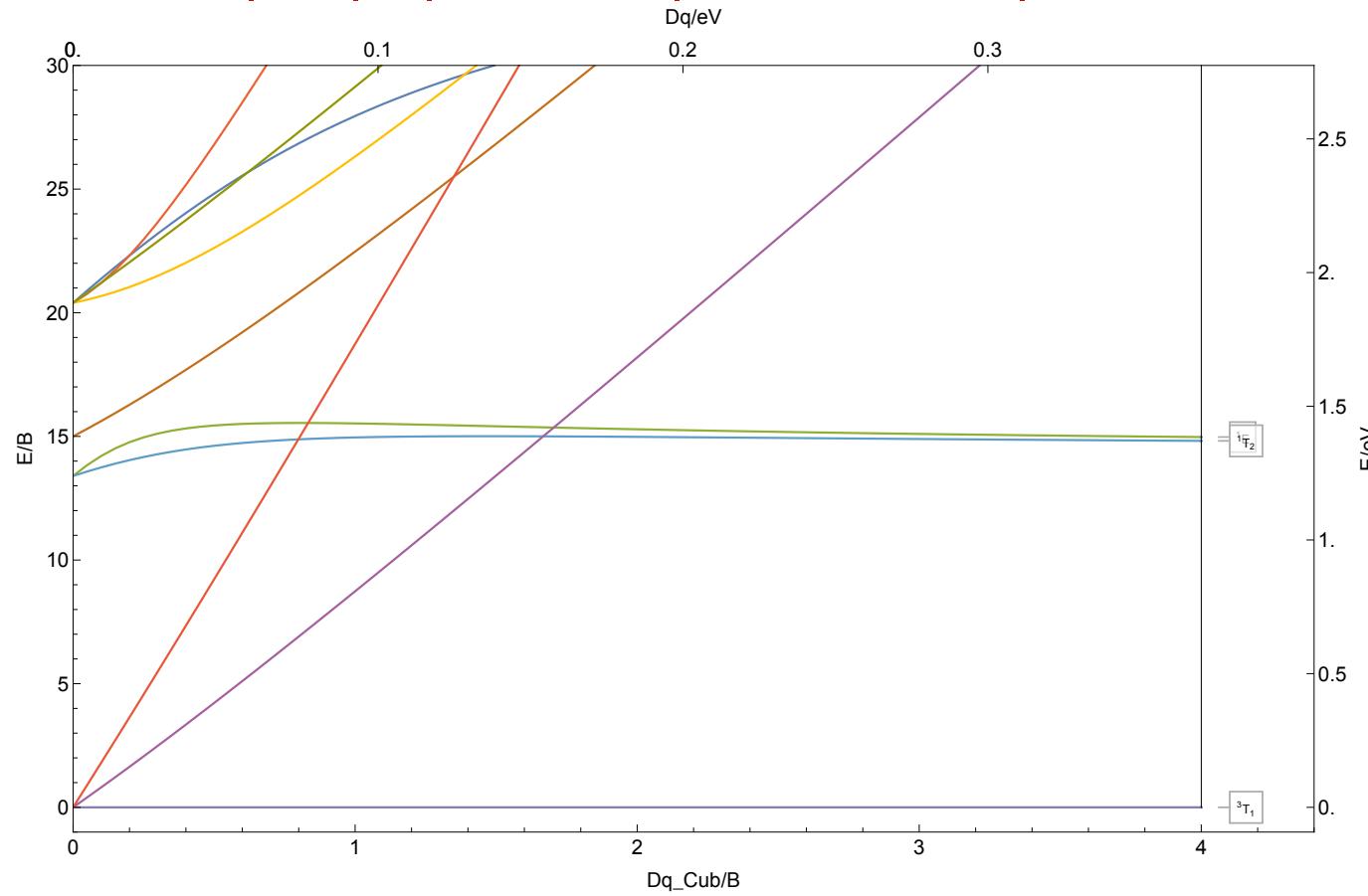
|2,4|d<sup>3</sup>| C/B ≈ 4.2| B ≈ 718 cm<sup>-1</sup> |Os<sup>5+</sup>



8.1.91 Os<sup>6+</sup>

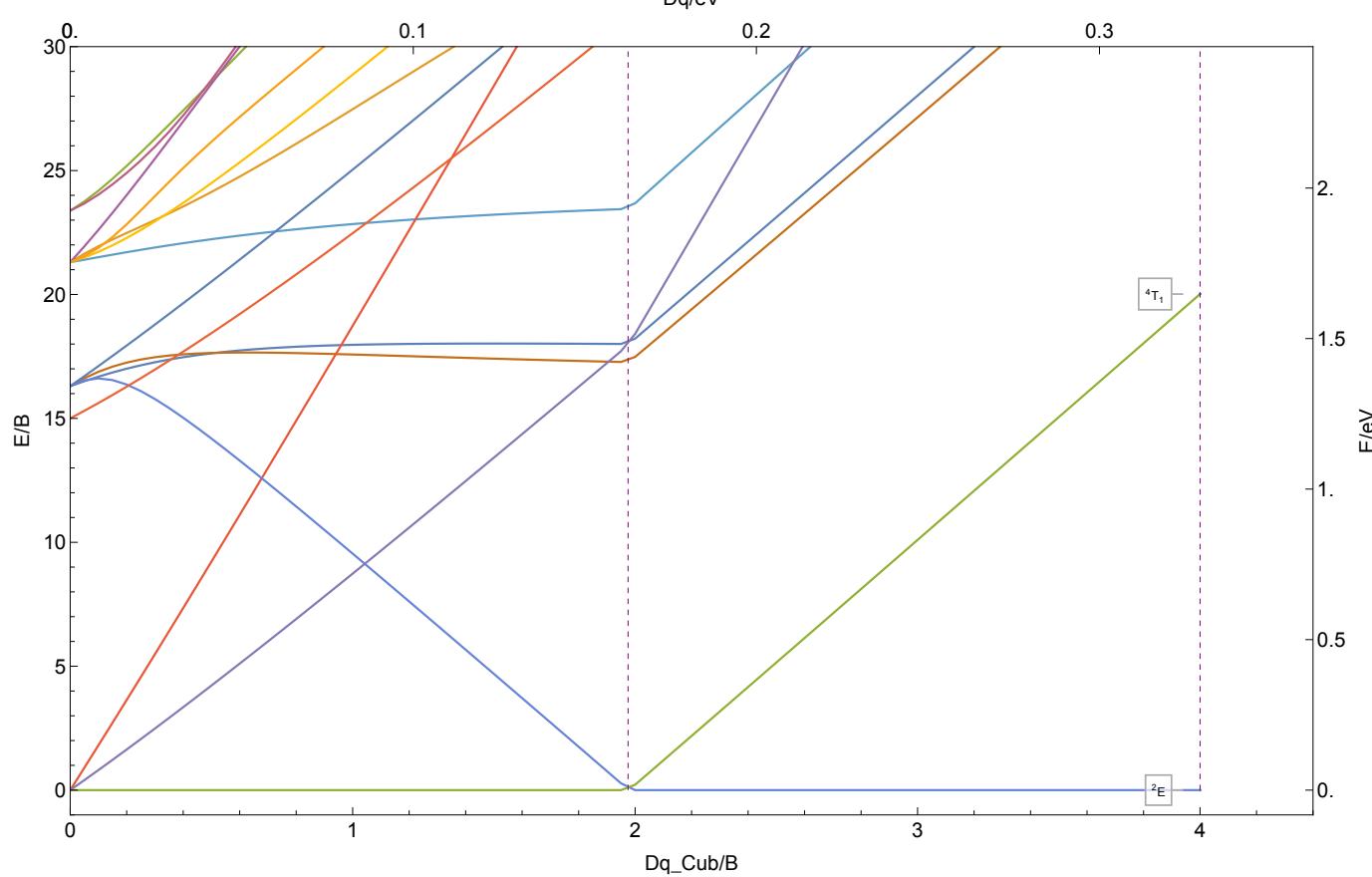
| 1,3 | d<sup>2</sup> | C/B ≈ 4.2 | B ≈ 746 cm<sup>-1</sup> | Os<sup>6+</sup>

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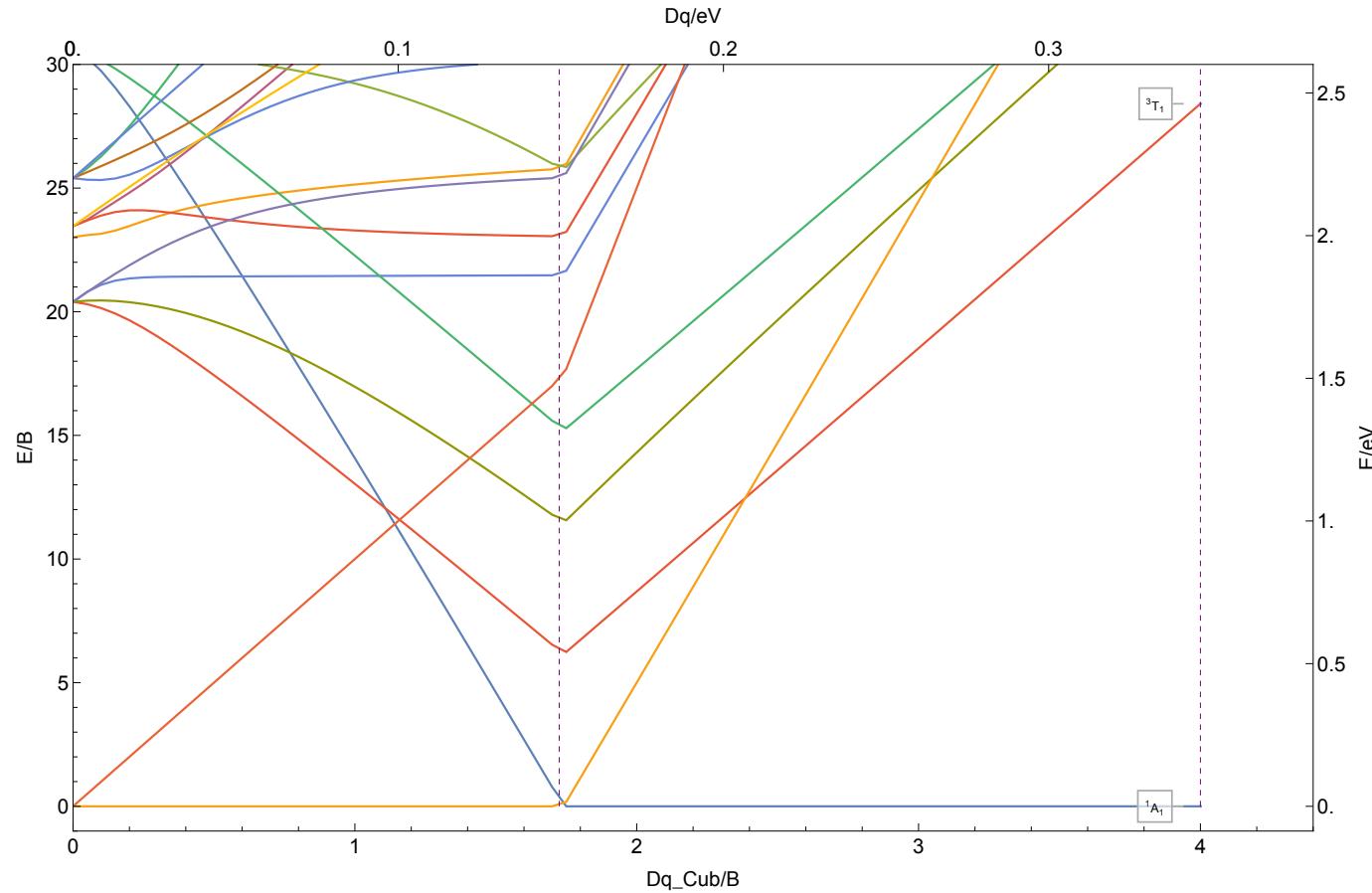
8.1.92 Ir<sup>2+</sup>

|2,4|d<sup>7</sup>| C/B ≈ 4.1| B ≈ 664 cm<sup>-1</sup> |Ir<sup>2+</sup>



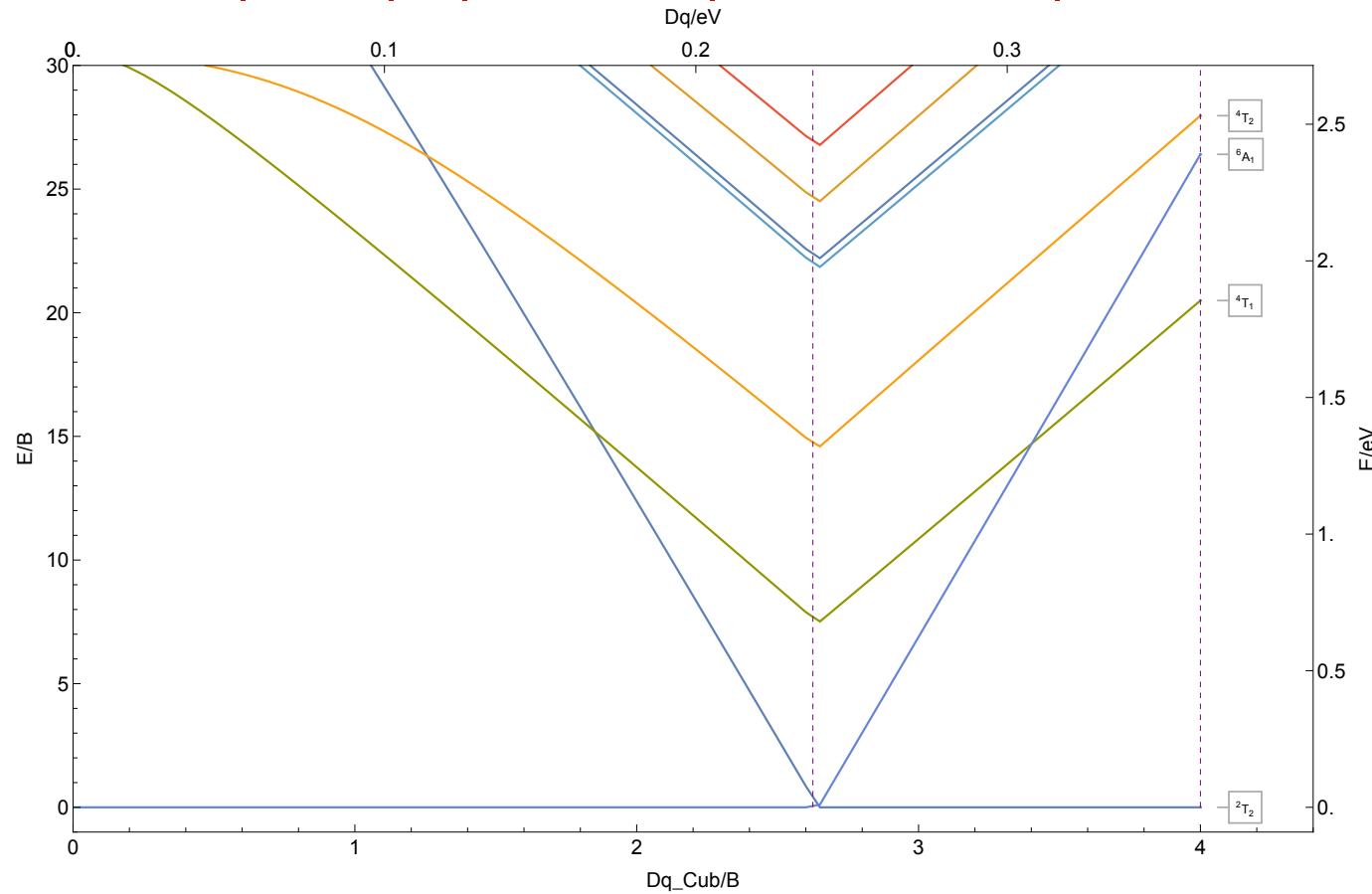
8.1.93  $\text{Ir}^{3+}$

$|1,3,5|d^6|C/B \approx 4.1|B \approx 699 \text{ cm}^{-1}| \text{Ir}^{3+}$



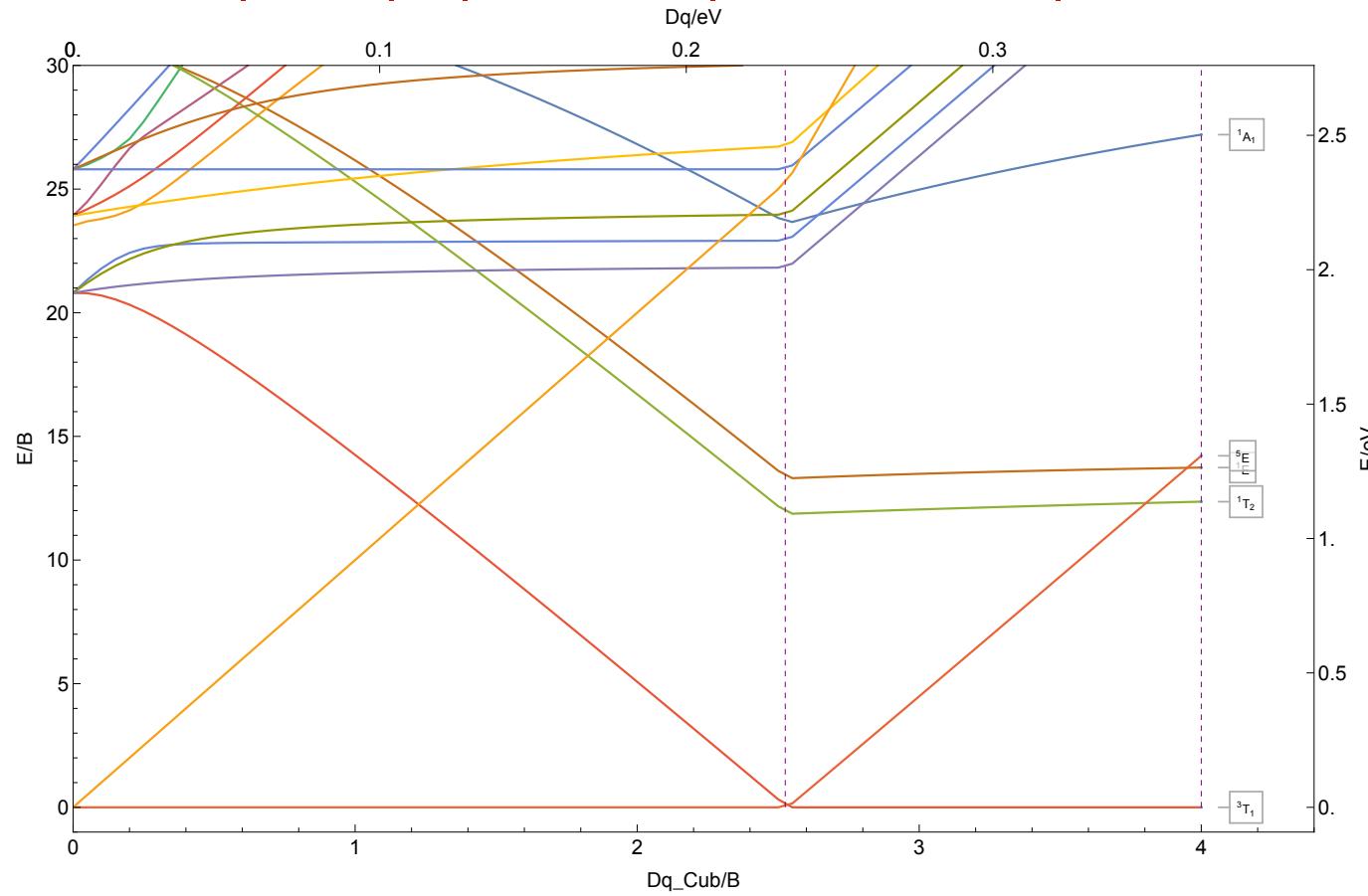
8.1.94 Ir<sup>4+</sup>

|2,4,6|d<sup>5</sup>| C/B ≈ 4.1| B ≈ 730 cm<sup>-1</sup> |Ir<sup>4+</sup>



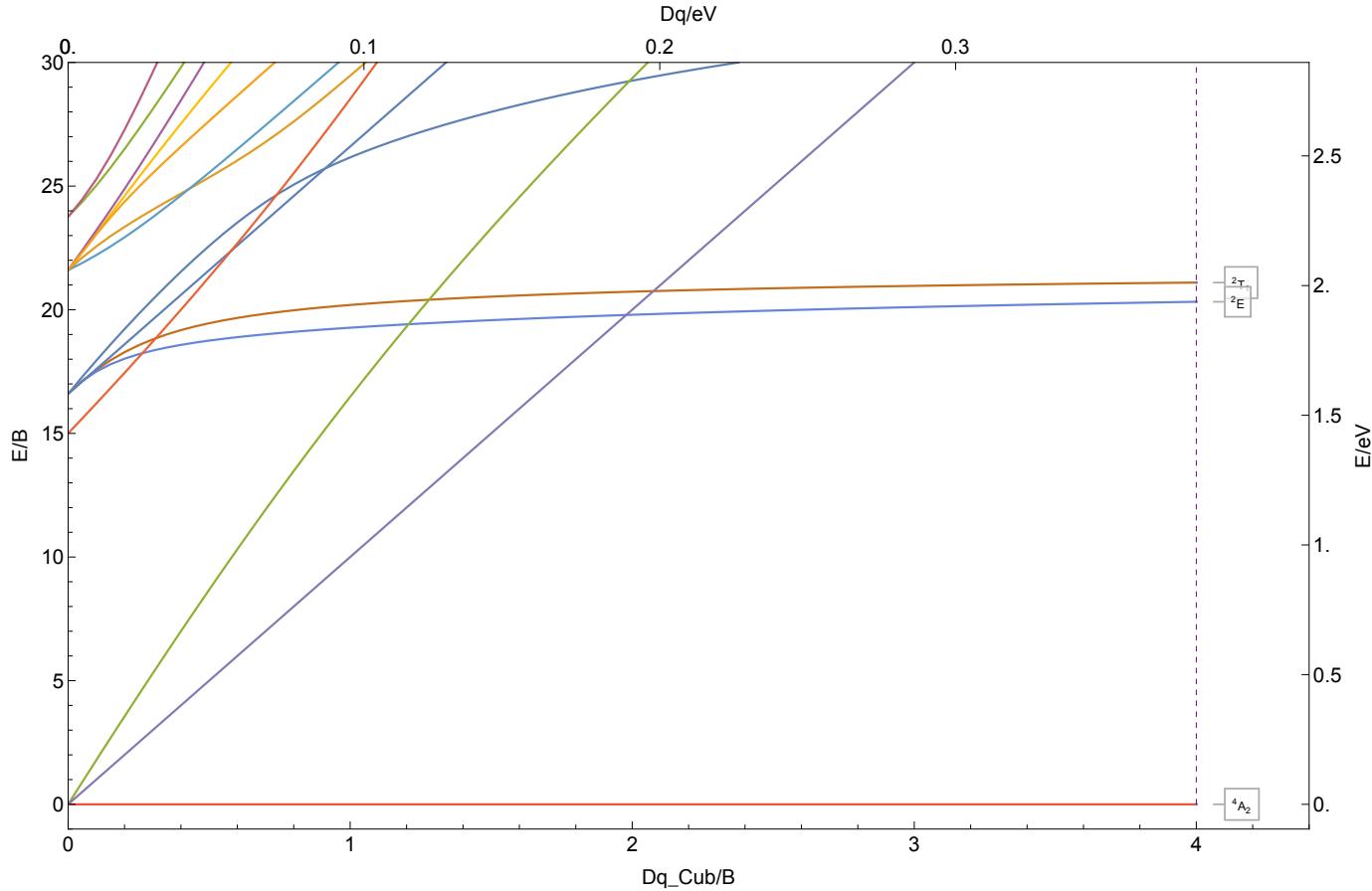
8.1.95  $\text{Ir}^{5+}$

$|1,3,5|d^4|C/B \approx 4.2|B \approx 742 \text{ cm}^{-1}| \text{Ir}^{5+}$



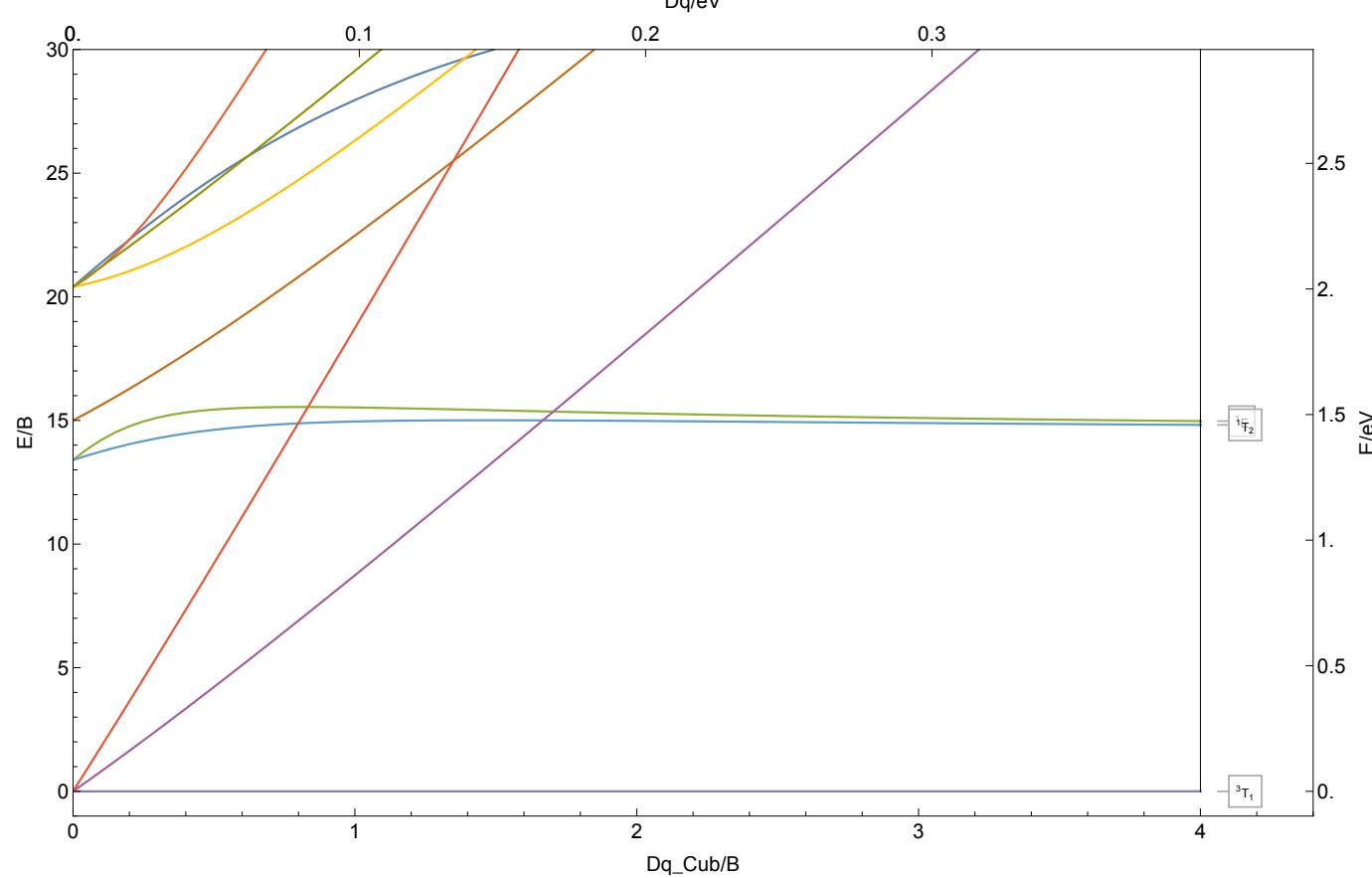
8.1.96  $\text{Ir}^{6+}$

$|2,4|d^3|C/B \approx 4.2|B \approx 769 \text{ cm}^{-1}| \text{Ir}^{6+}$



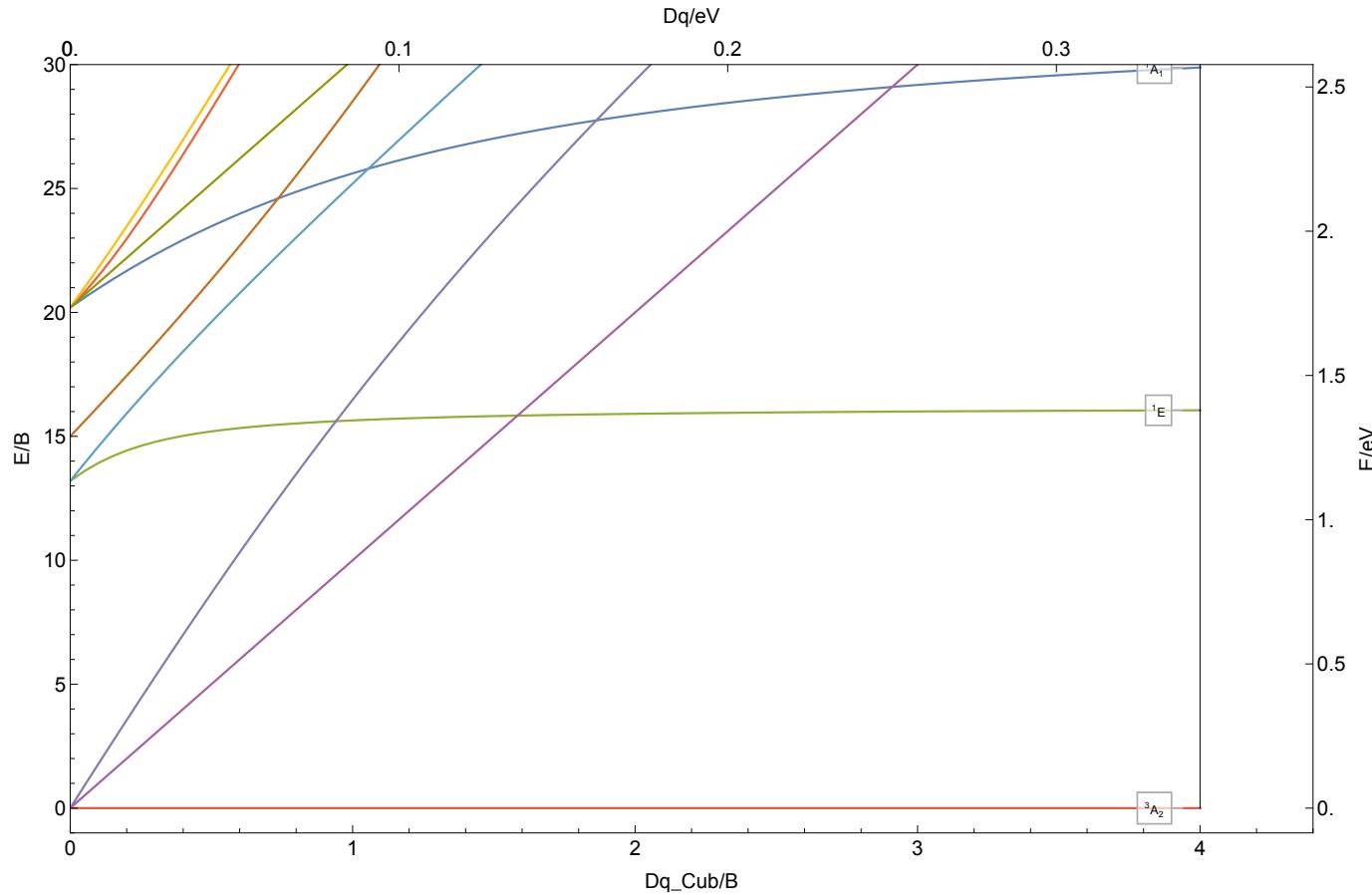
8.1.97 Ir<sup>7+</sup>

| 1,3 | d<sup>2</sup> | C/B ≈ 4.2 | B ≈ 794 cm<sup>-1</sup> | Ir<sup>7+</sup>



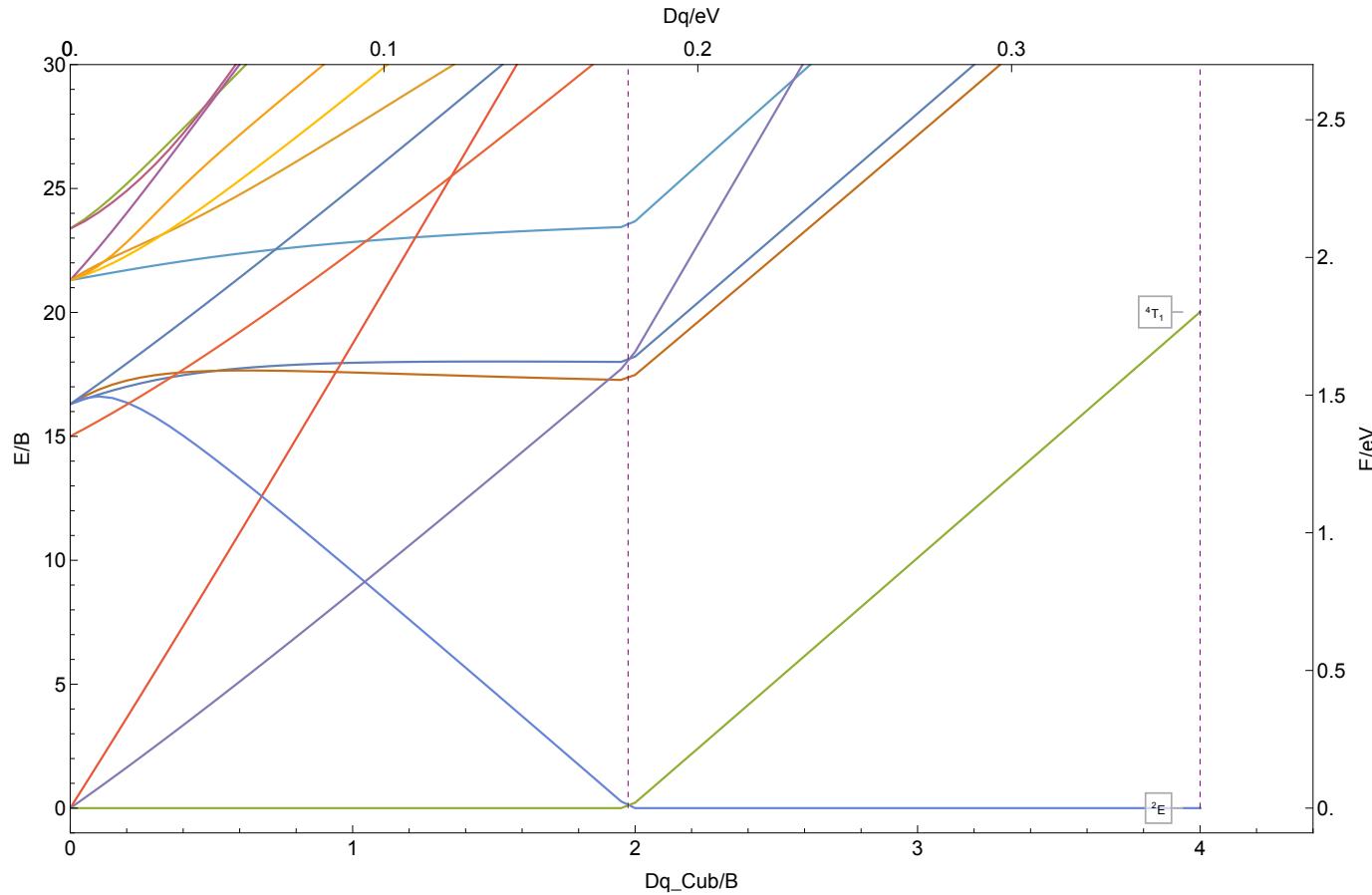
8.1.98 Pt<sup>2+</sup>

| 1,3 | d<sup>8</sup> | C/B ≈ 4.1 | B ≈ 693 cm<sup>-1</sup> | Pt<sup>2+</sup>



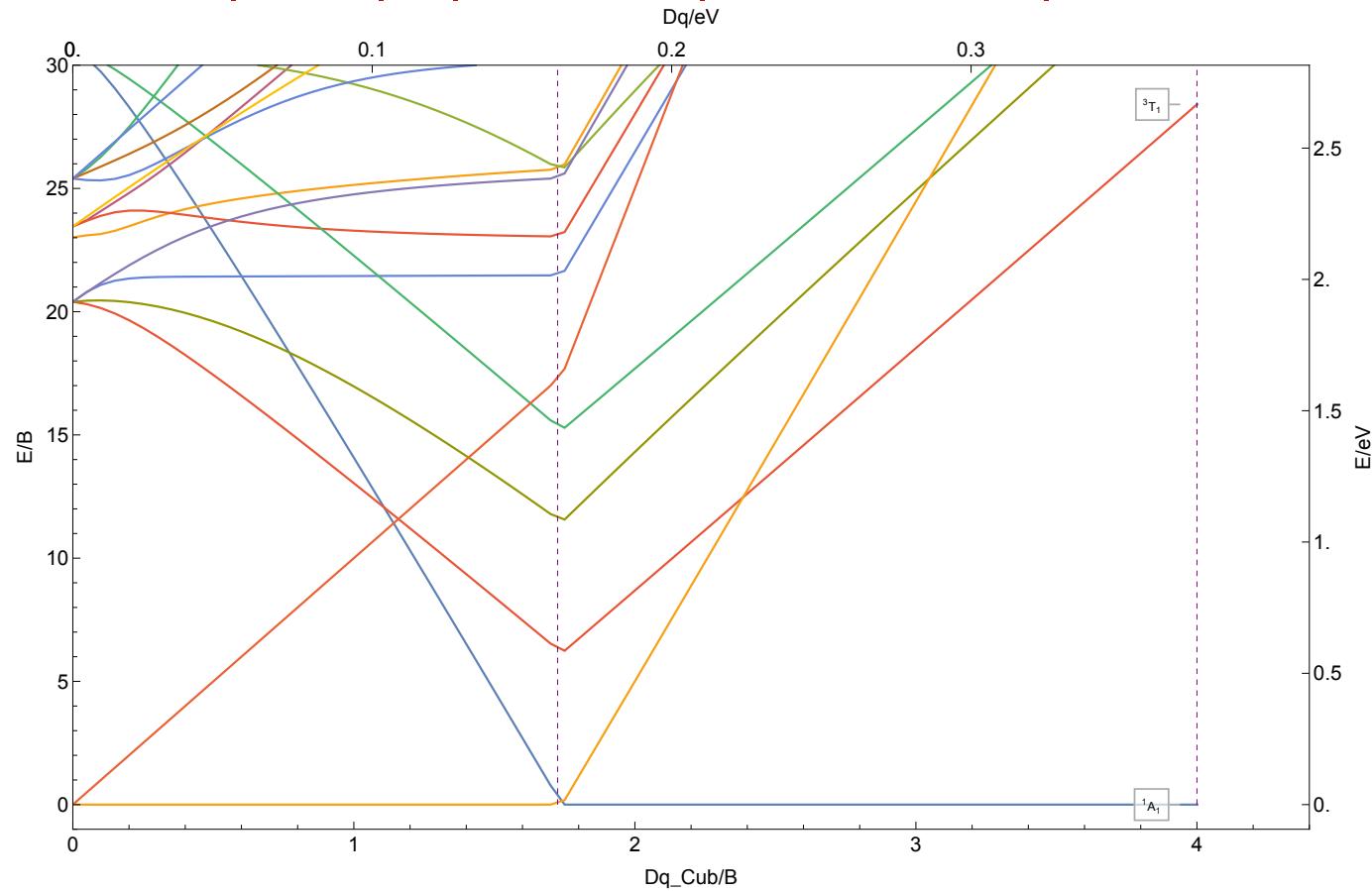
8.1.99 Pt<sup>3+</sup>

|2,4|d<sup>7</sup>|C/B ≈ 4.1|B ≈ 726 cm<sup>-1</sup>|Pt<sup>3+</sup>



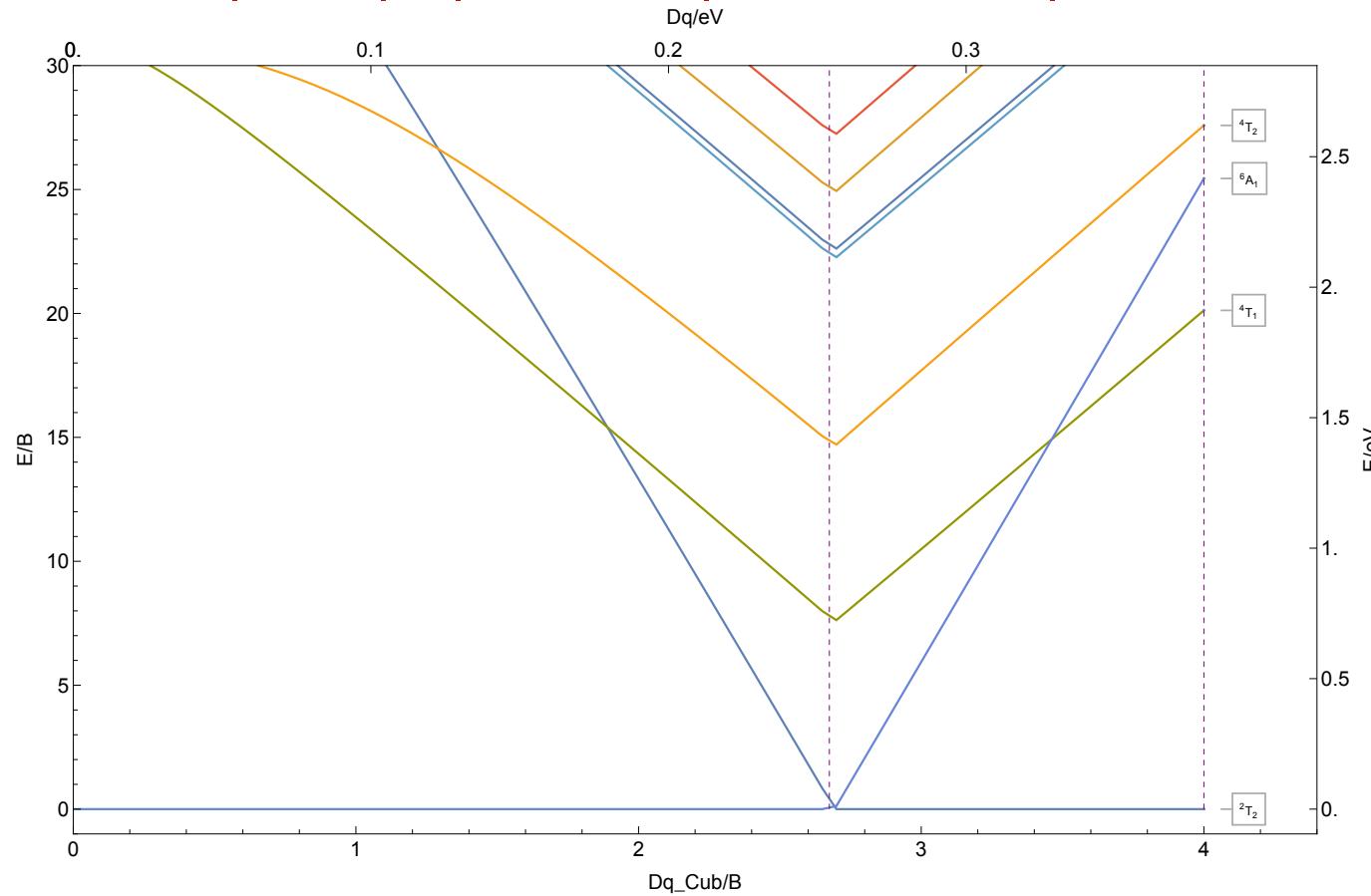
8.1.100 Pt<sup>4+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4.1 | B ≈ 757 cm<sup>-1</sup> | Pt<sup>4+</sup>



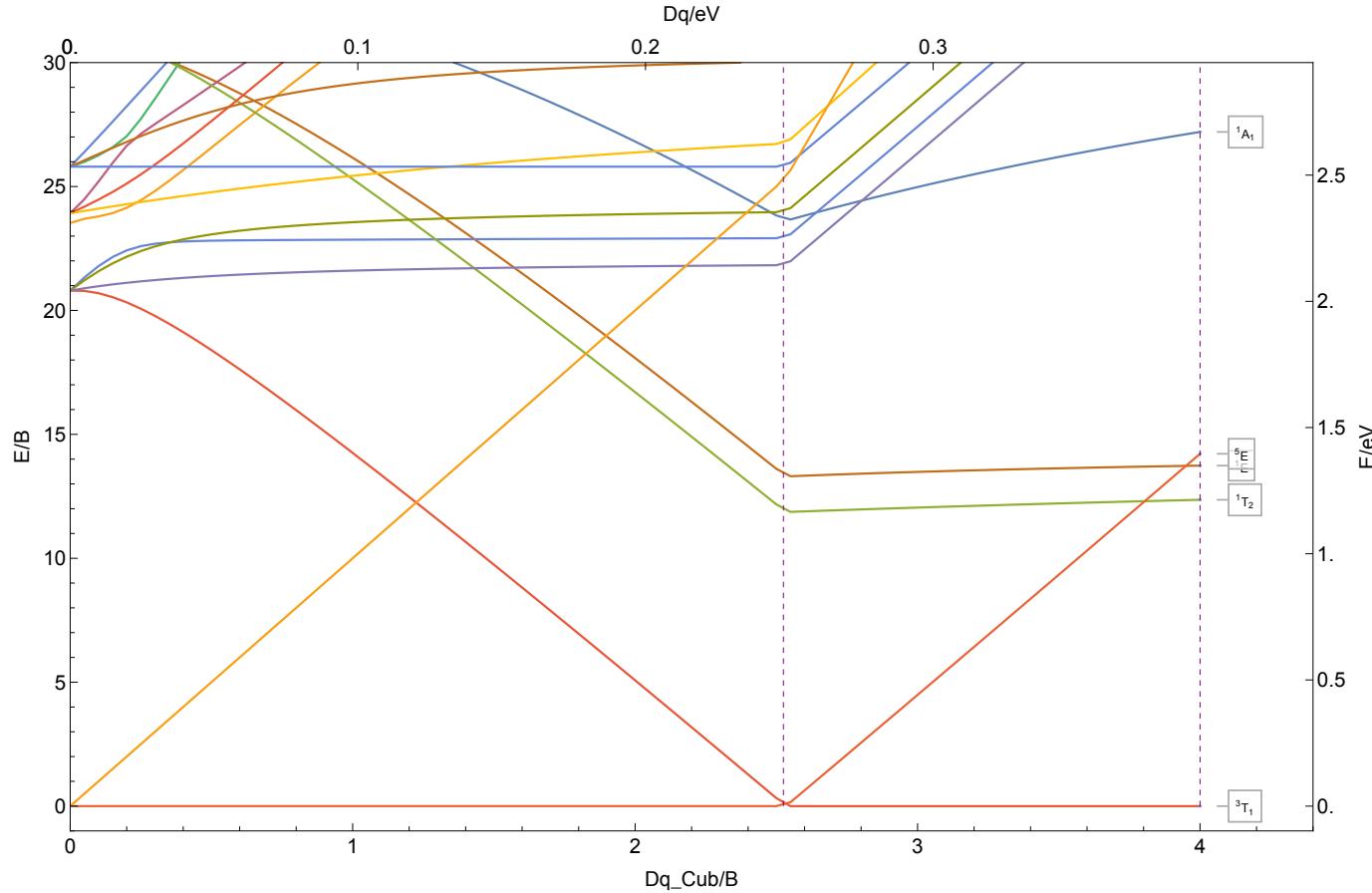
8.1.101 Pt<sup>5+</sup>

|2,4,6|d<sup>5</sup>|C/B ≈ 4.2|B ≈ 766 cm<sup>-1</sup>|Pt<sup>5+</sup>



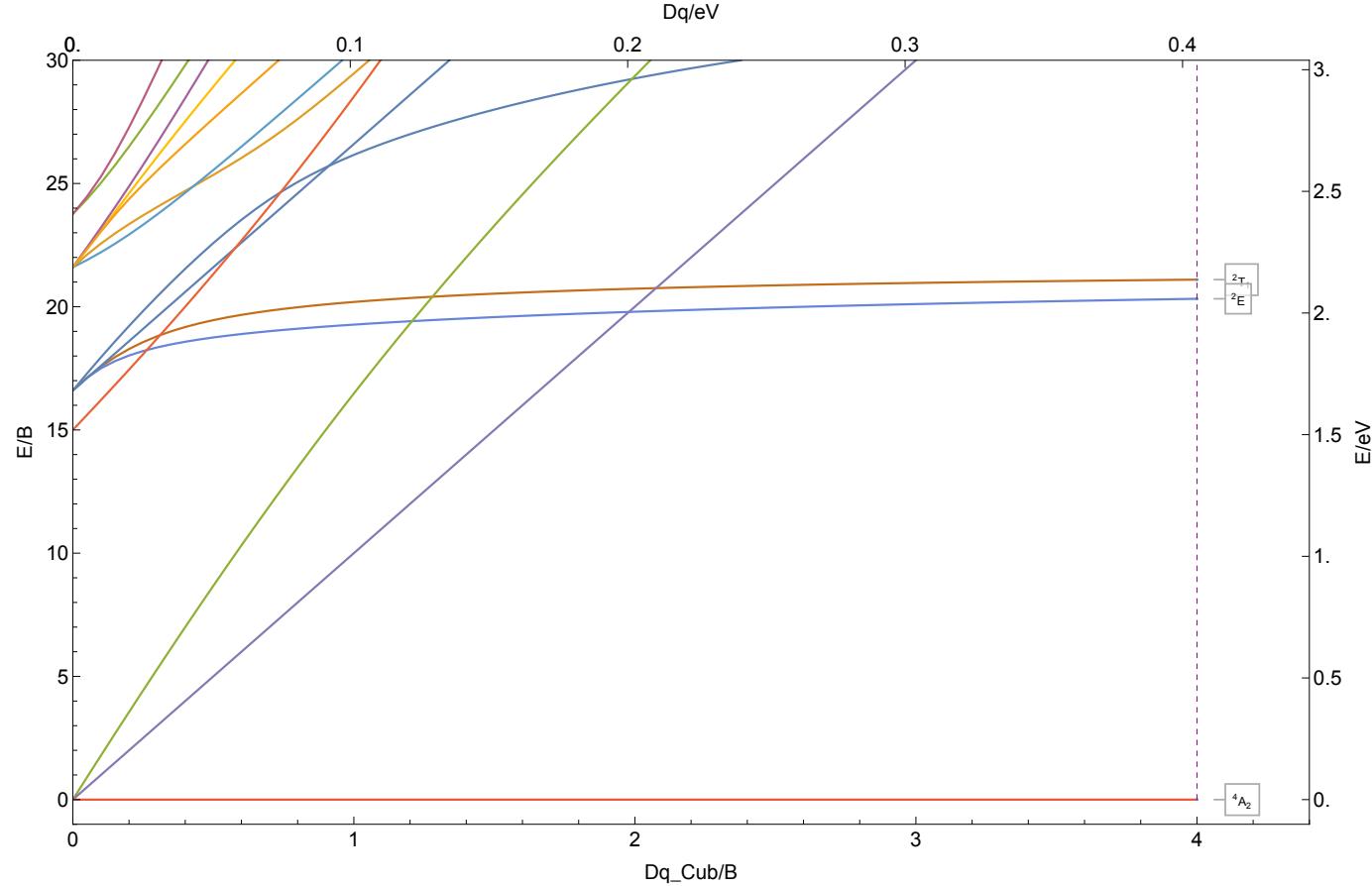
8.1.102 Pt<sup>6+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 4.2 | B ≈ 792 cm<sup>-1</sup> | Pt<sup>6+</sup>



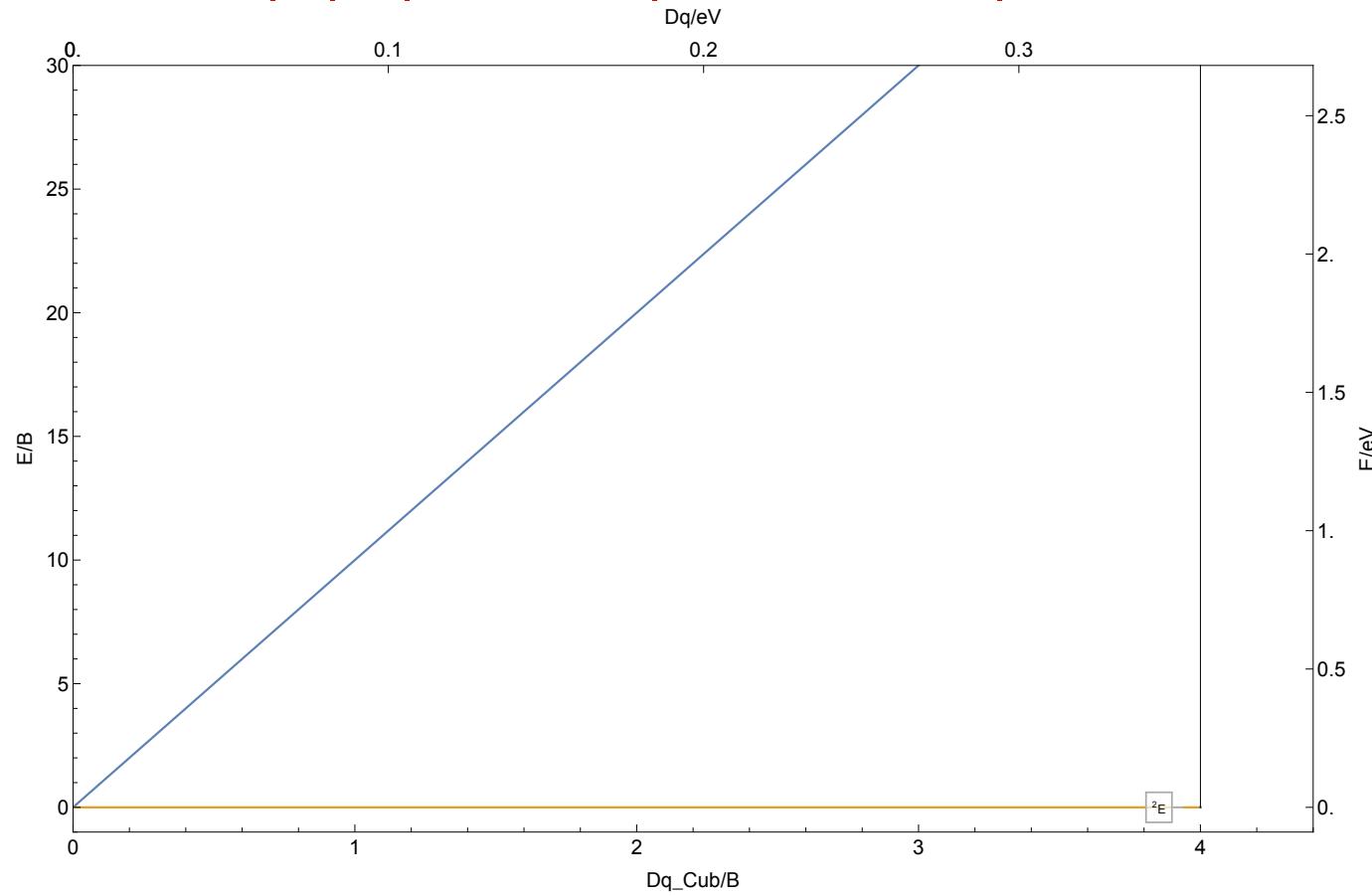
8.1.103 Pt<sup>7+</sup>

|2,4|d<sup>3</sup>|C/B ≈ 4.2|B ≈ 817 cm<sup>-1</sup>|Pt<sup>7+</sup>



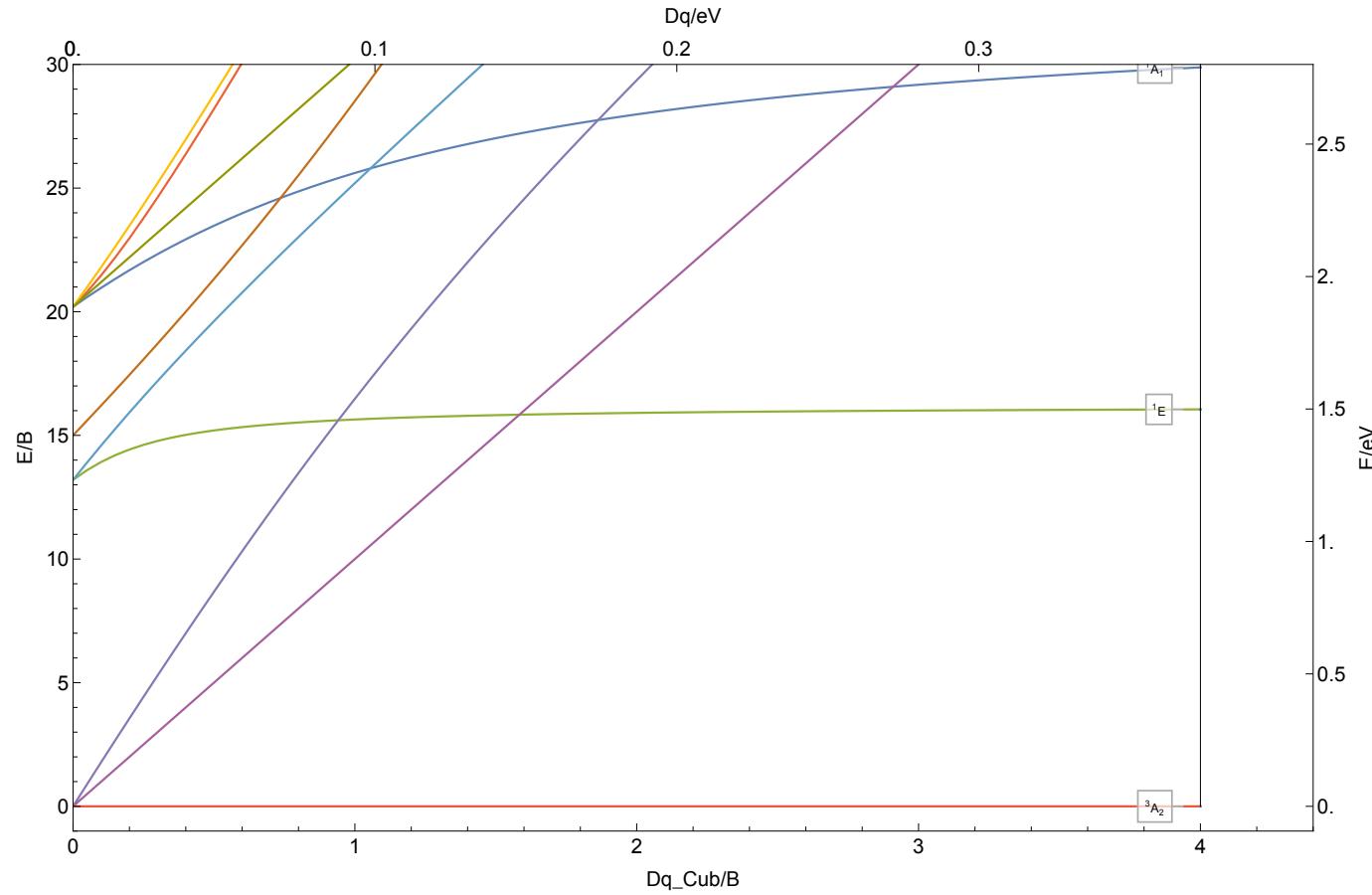
8.1.104 Au<sup>2+</sup>

|2|d<sup>9</sup>|C/B ≈ 4.1|B ≈ 721 cm<sup>-1</sup>|Au<sup>2+</sup>



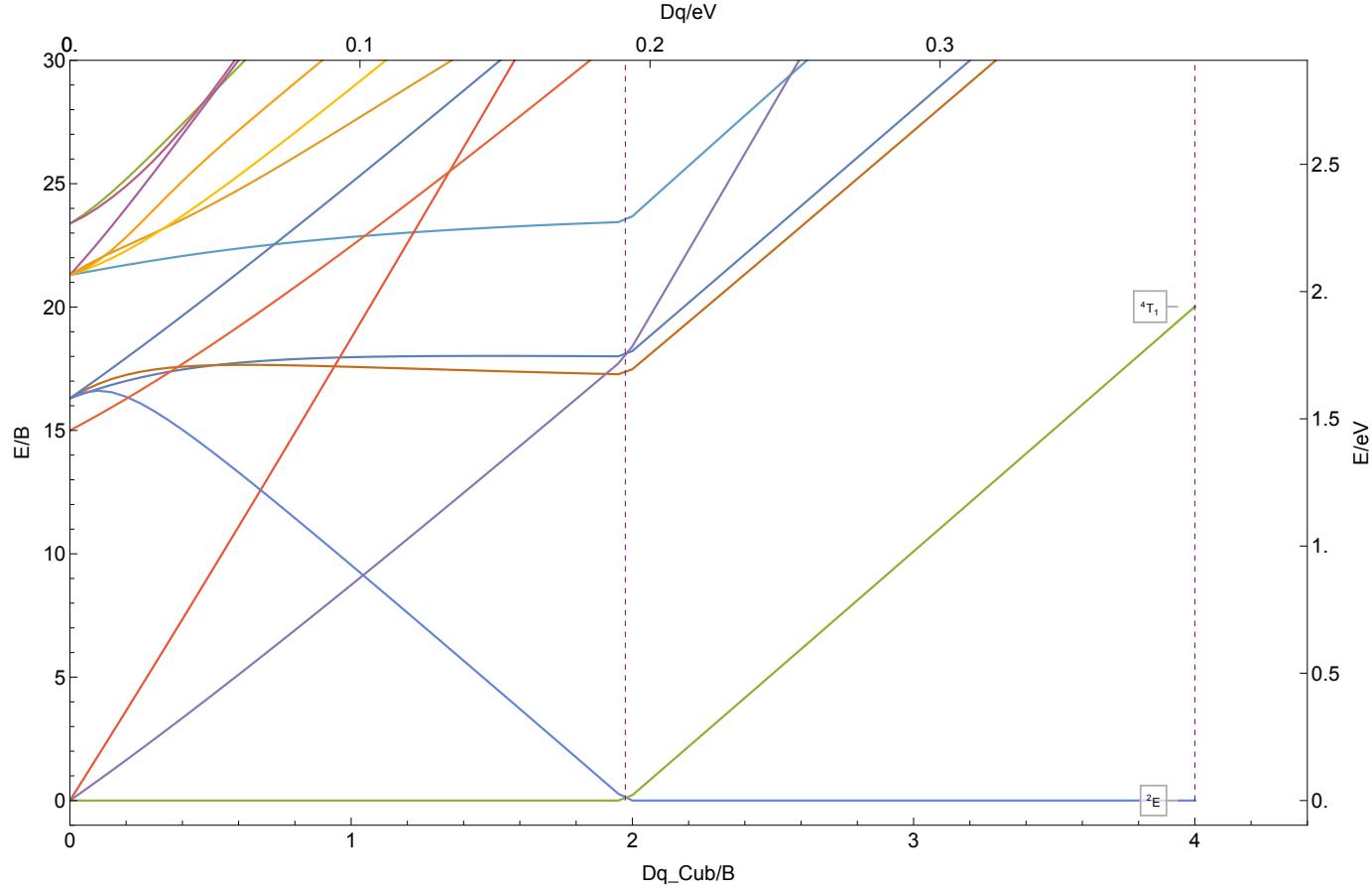
8.1.105 Au<sup>3+</sup>

| 1,3 | d<sup>8</sup> | C/B ≈ 4.1 | B ≈ 753 cm<sup>-1</sup> | Au<sup>3+</sup>



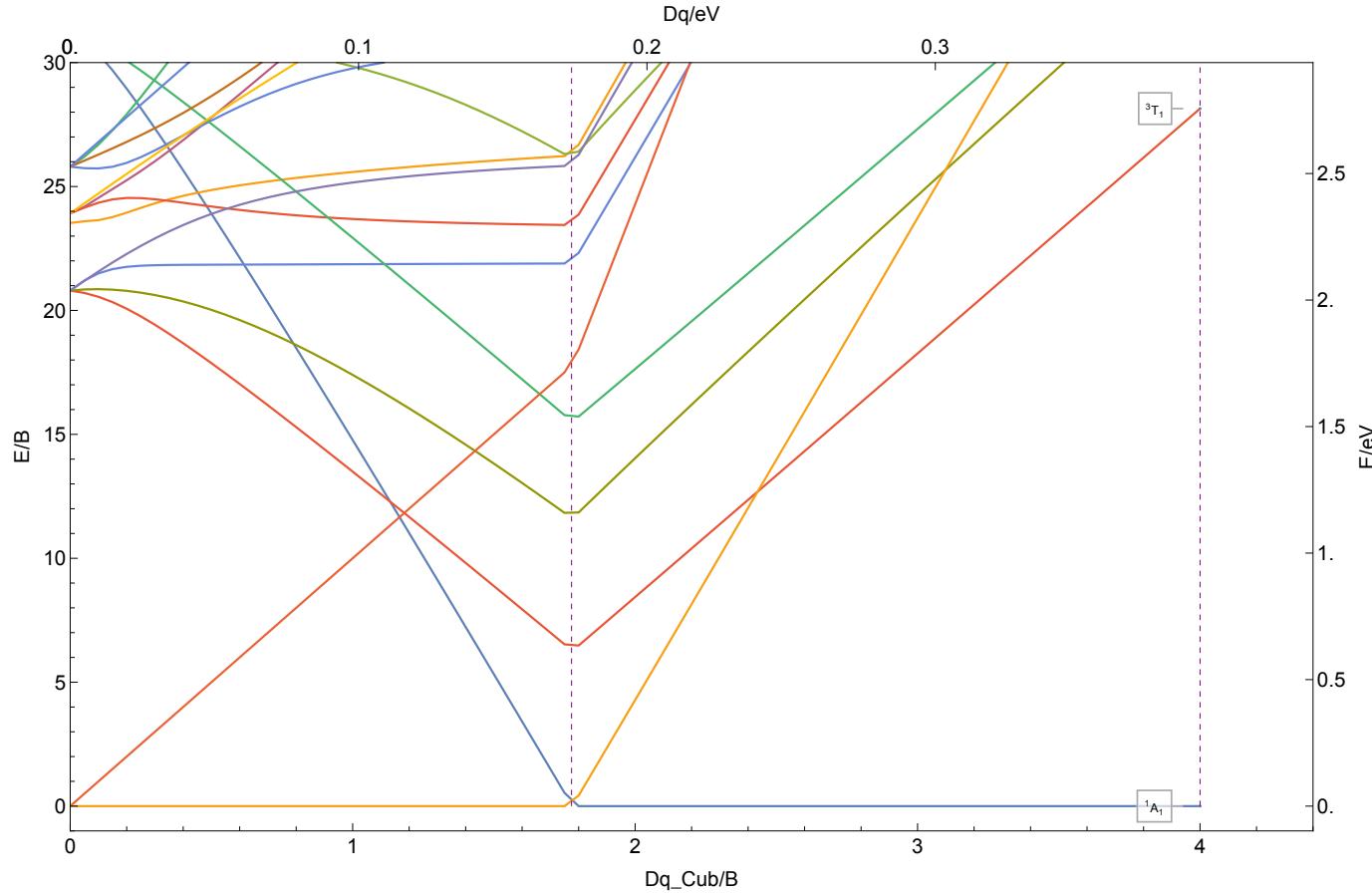
8.1.106 Au<sup>4+</sup>

|2,4|d<sup>7</sup>| C/B ≈ 4.1| B ≈ 782 cm<sup>-1</sup> |Au<sup>4+</sup>



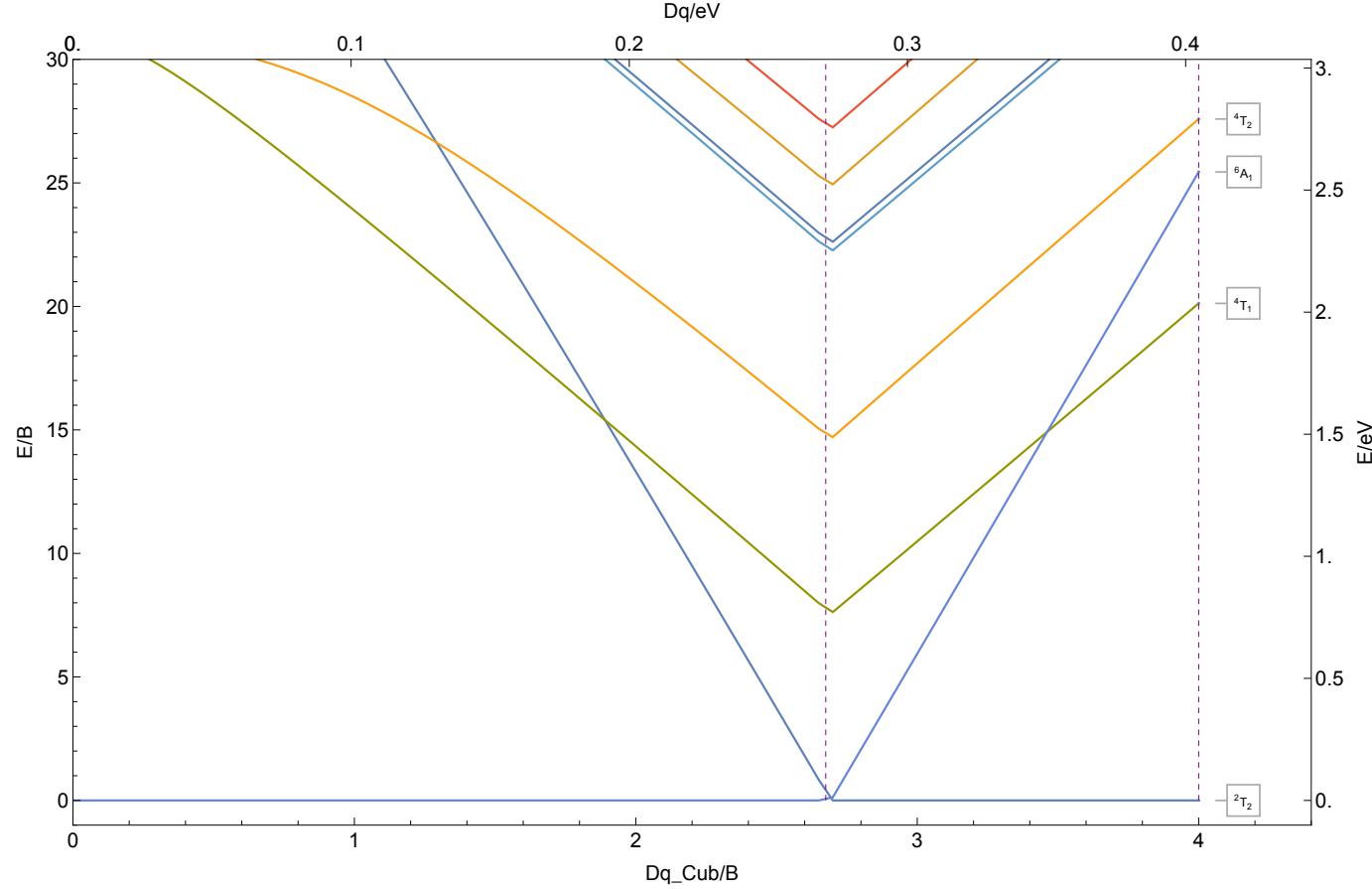
8.1.107 Au<sup>5+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4.2 | B ≈ 790 cm<sup>-1</sup> | Au<sup>5+</sup>



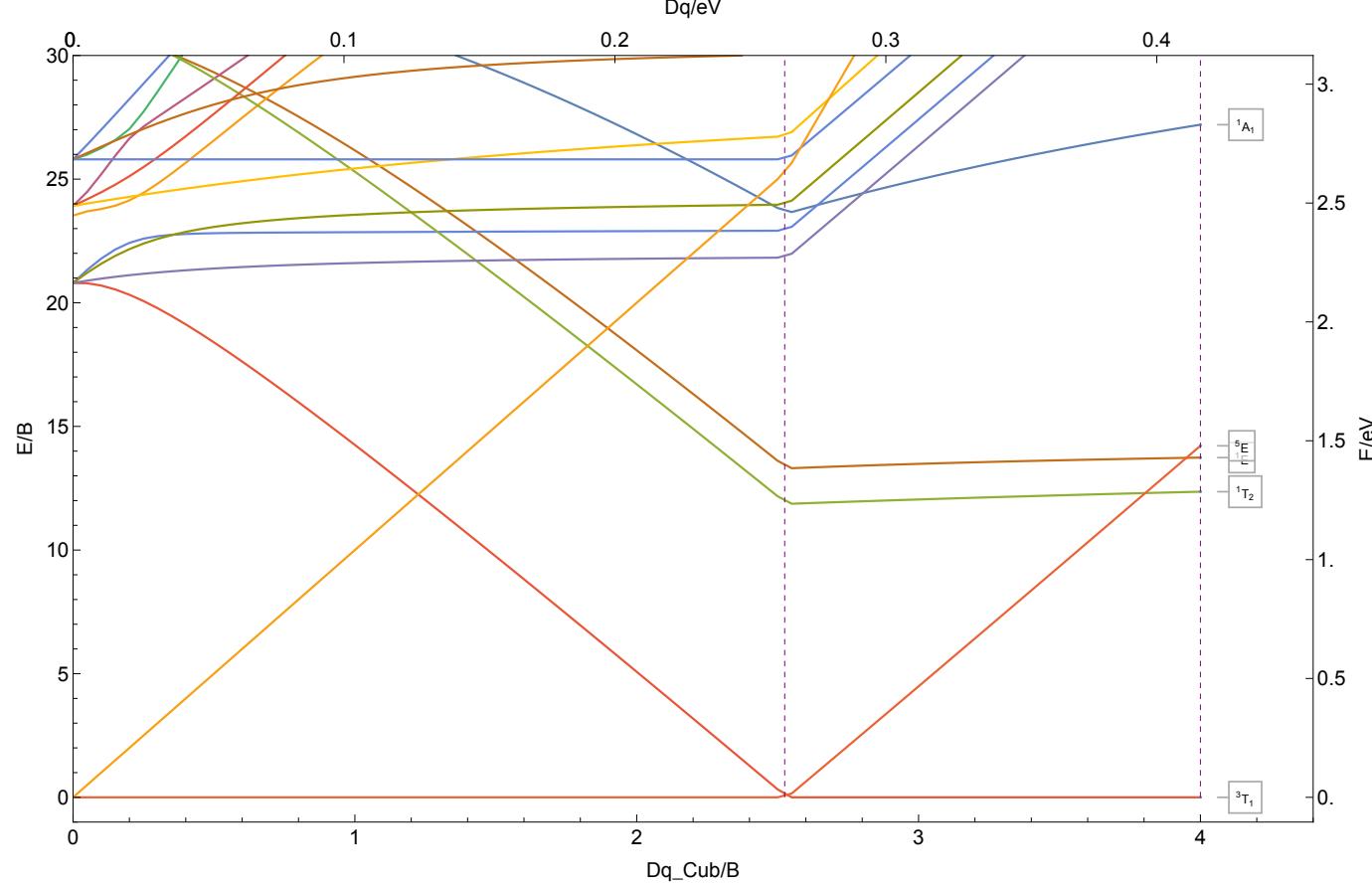
8.1.108 Au<sup>6+</sup>

|2,4,6| d<sup>5</sup>| C/B ≈ 4.2| B ≈ 816 cm<sup>-1</sup> |Au<sup>6+</sup>



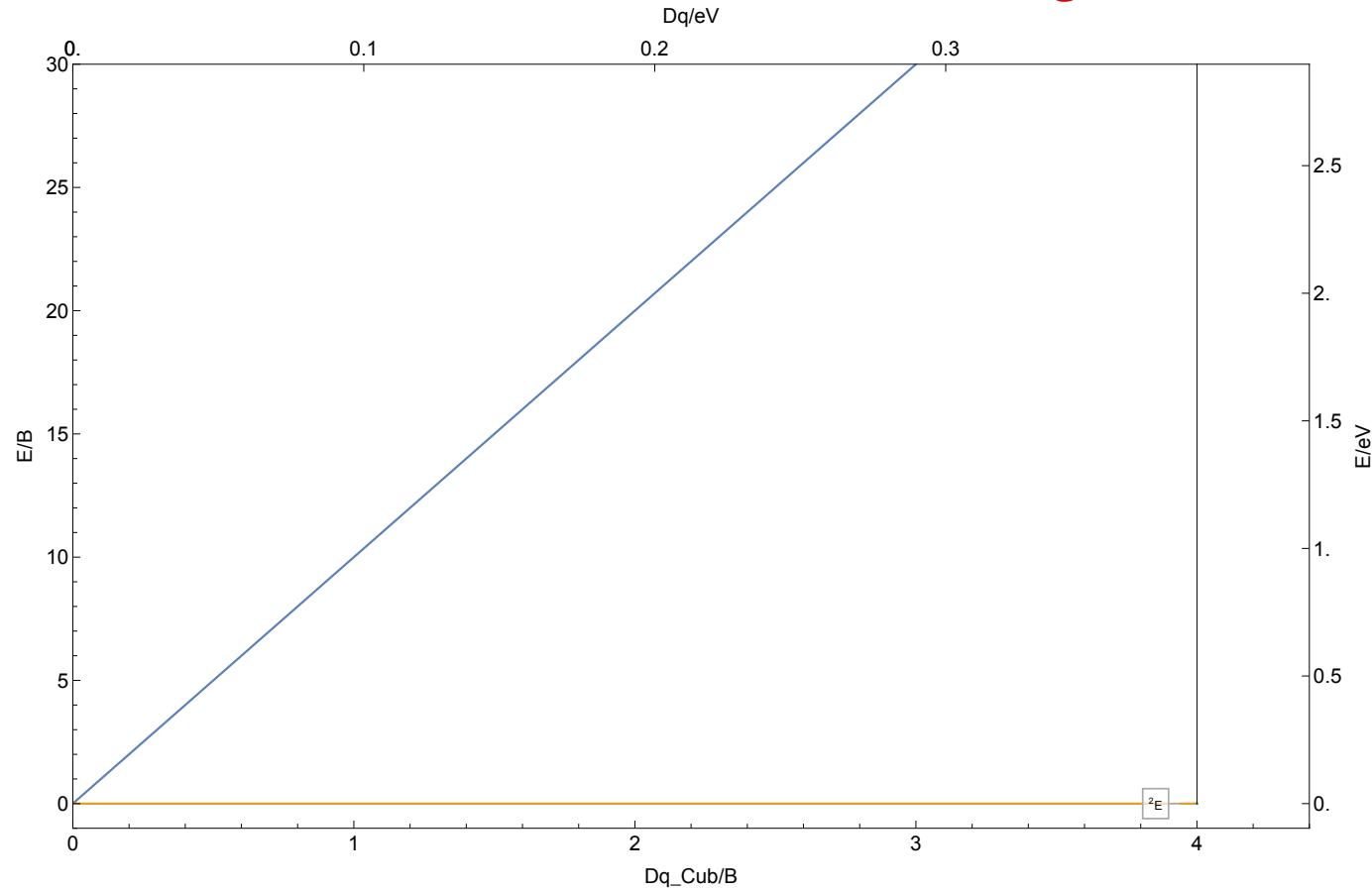
8.1.109 Au<sup>7+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 4.2 | B ≈ 839 cm<sup>-1</sup> | Au<sup>7+</sup>



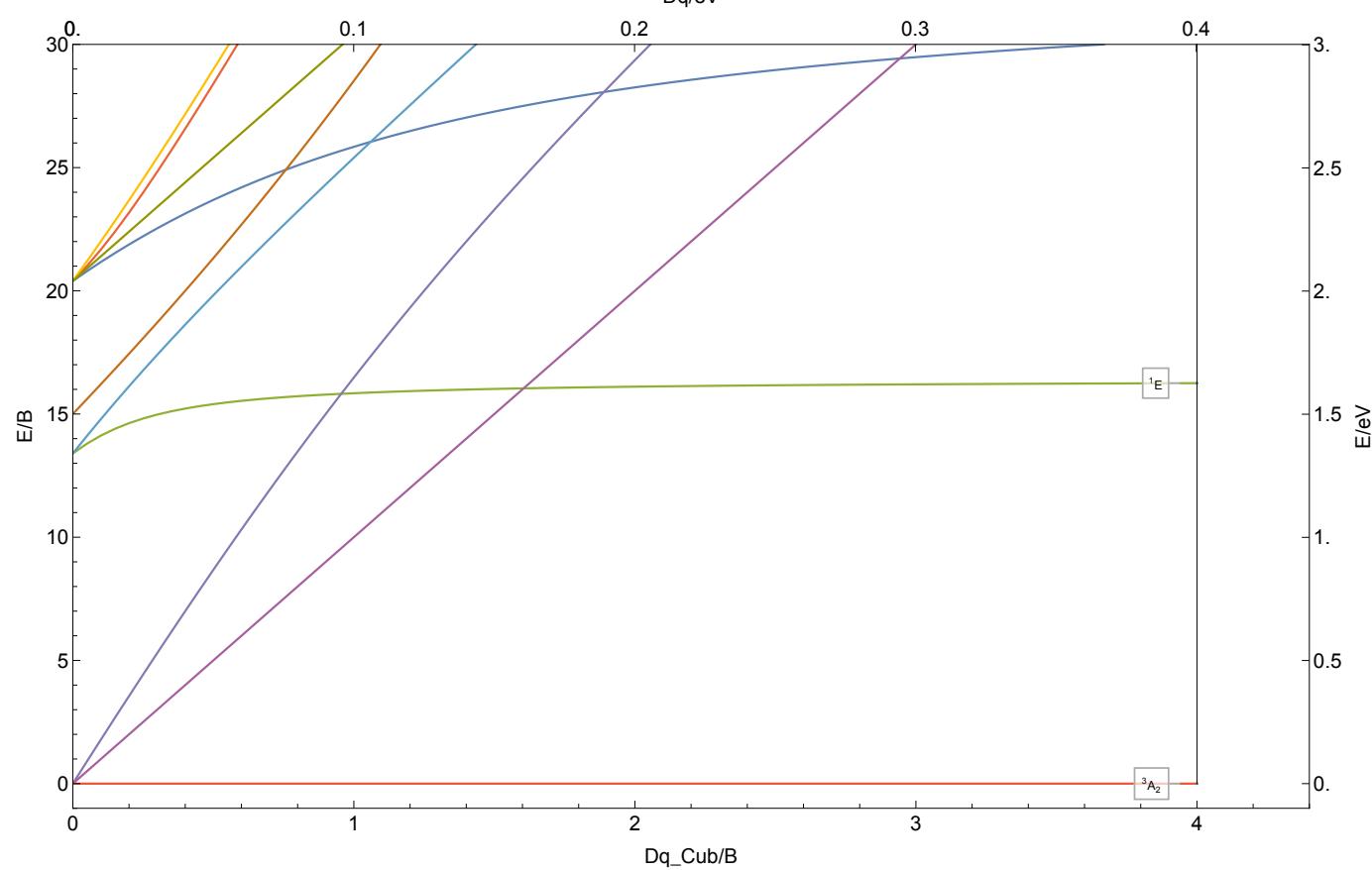
8.1.110 Hg<sup>3+</sup>

|2|d<sup>9</sup>|C/B ≈ 4.1|B ≈ 779 cm<sup>-1</sup>|Hg<sup>3+</sup>



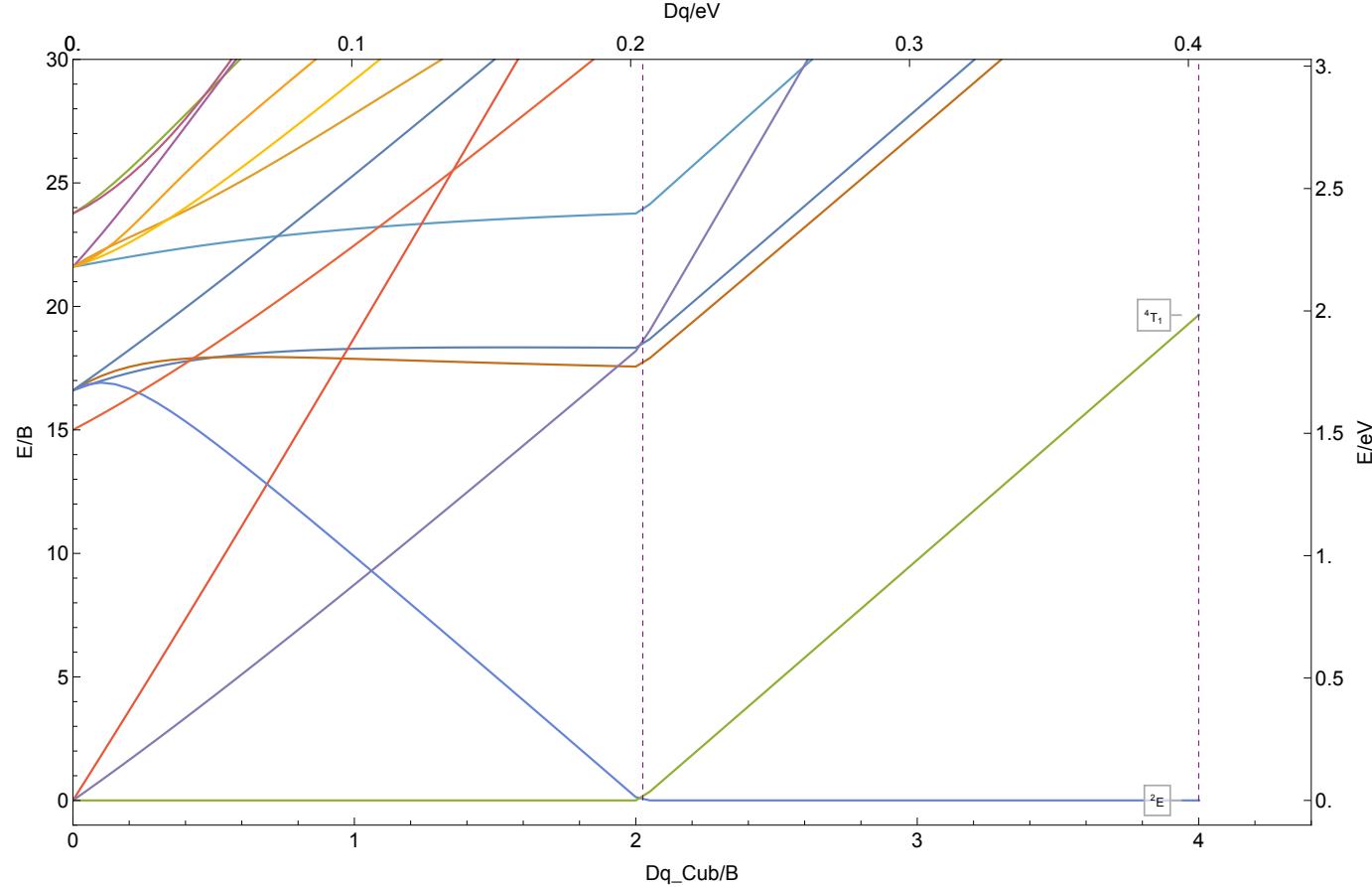
8.1.111 Hg<sup>4+</sup>

$|1,3|d^8|C/B \approx 4.2|B \approx 807\text{ cm}^{-1}|Hg^{4+}$



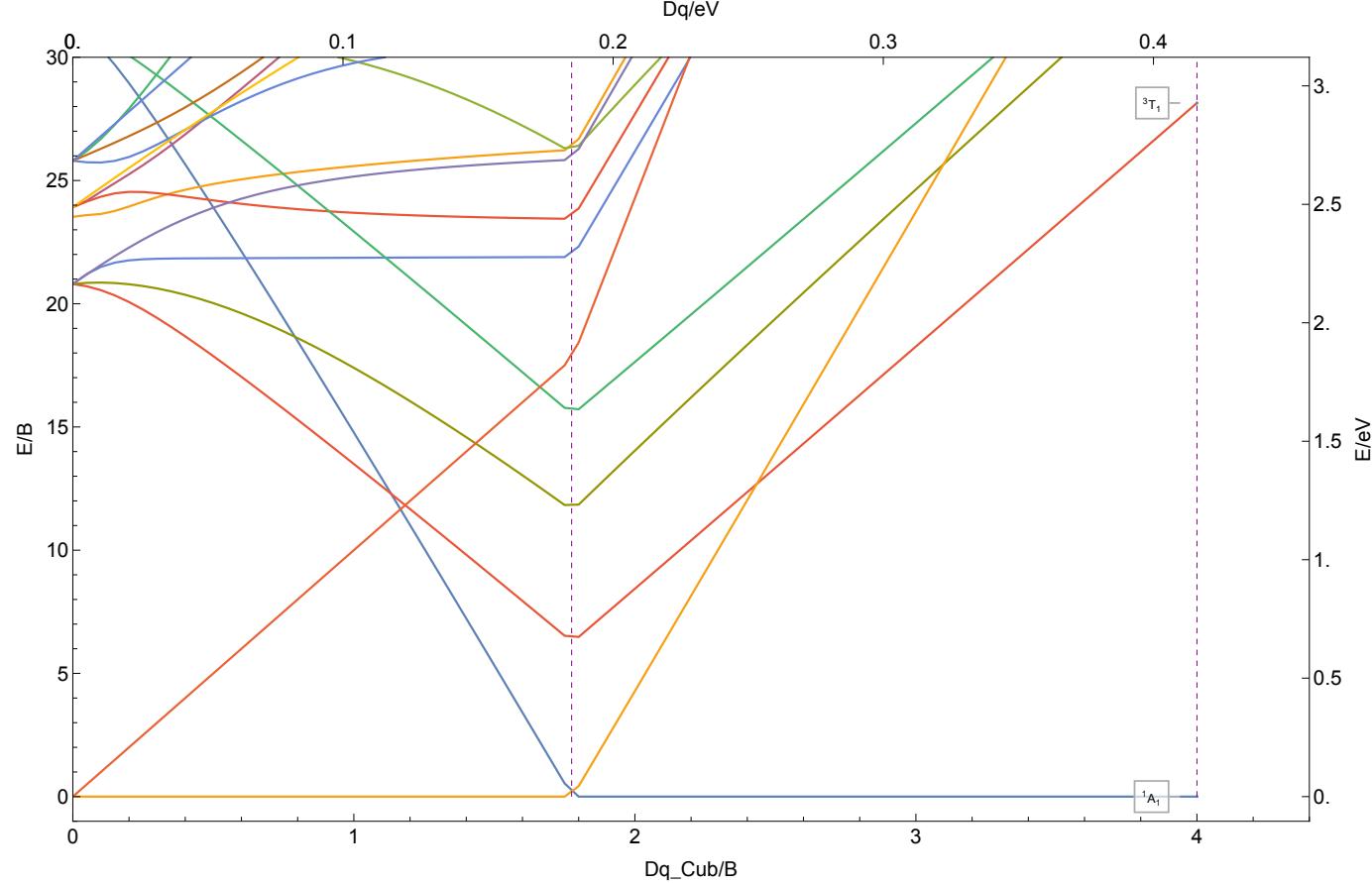
8.1.112 Hg<sup>5+</sup>

$|2,4|d^7|C/B \approx 4.2|B \approx 814\text{ cm}^{-1}|Hg^{5+}$



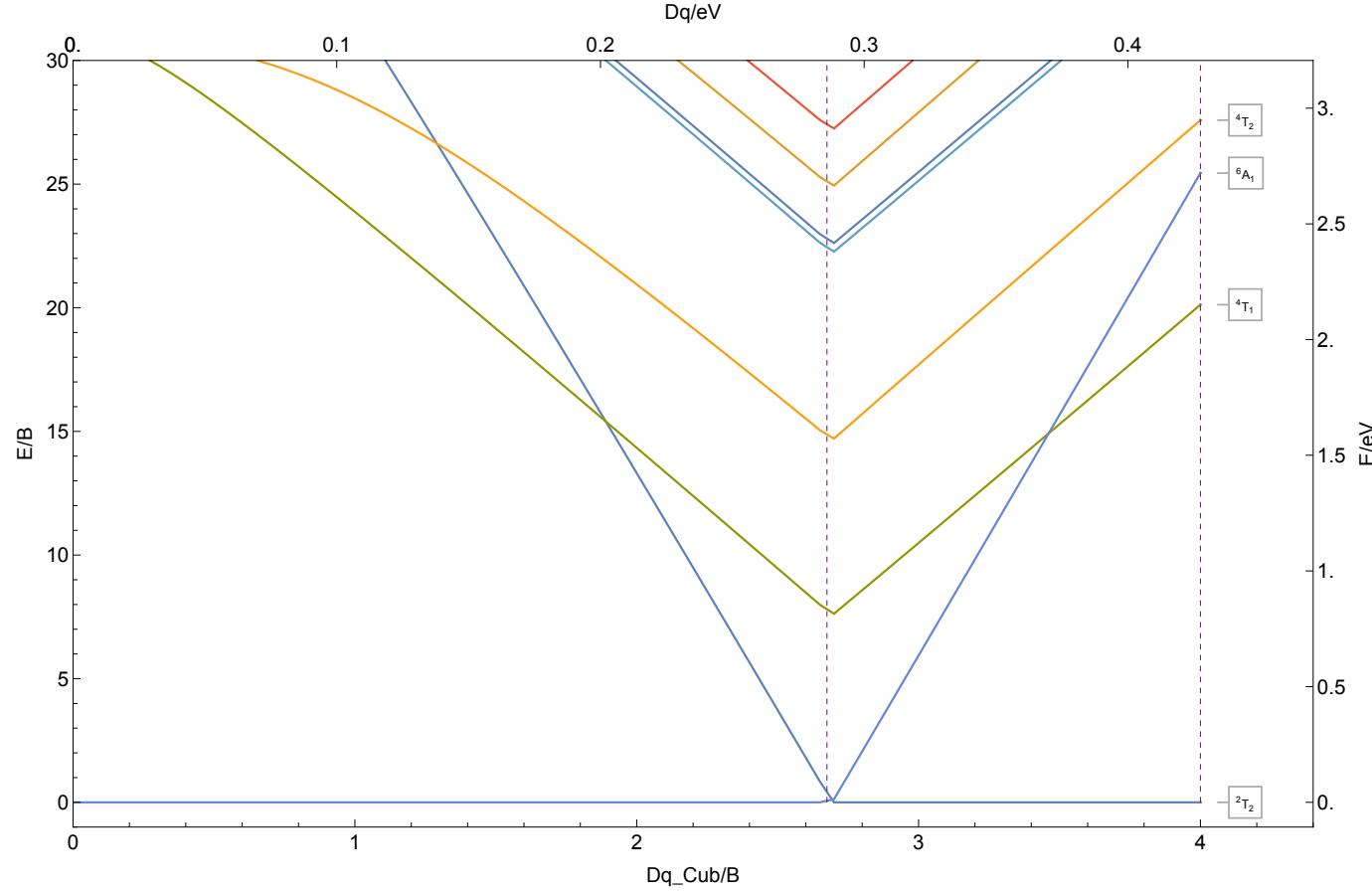
8.1.113 Hg<sup>6+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4.2 | B ≈ 839 cm<sup>-1</sup> | Hg<sup>6+</sup>



8.1.114 Hg<sup>7+</sup>

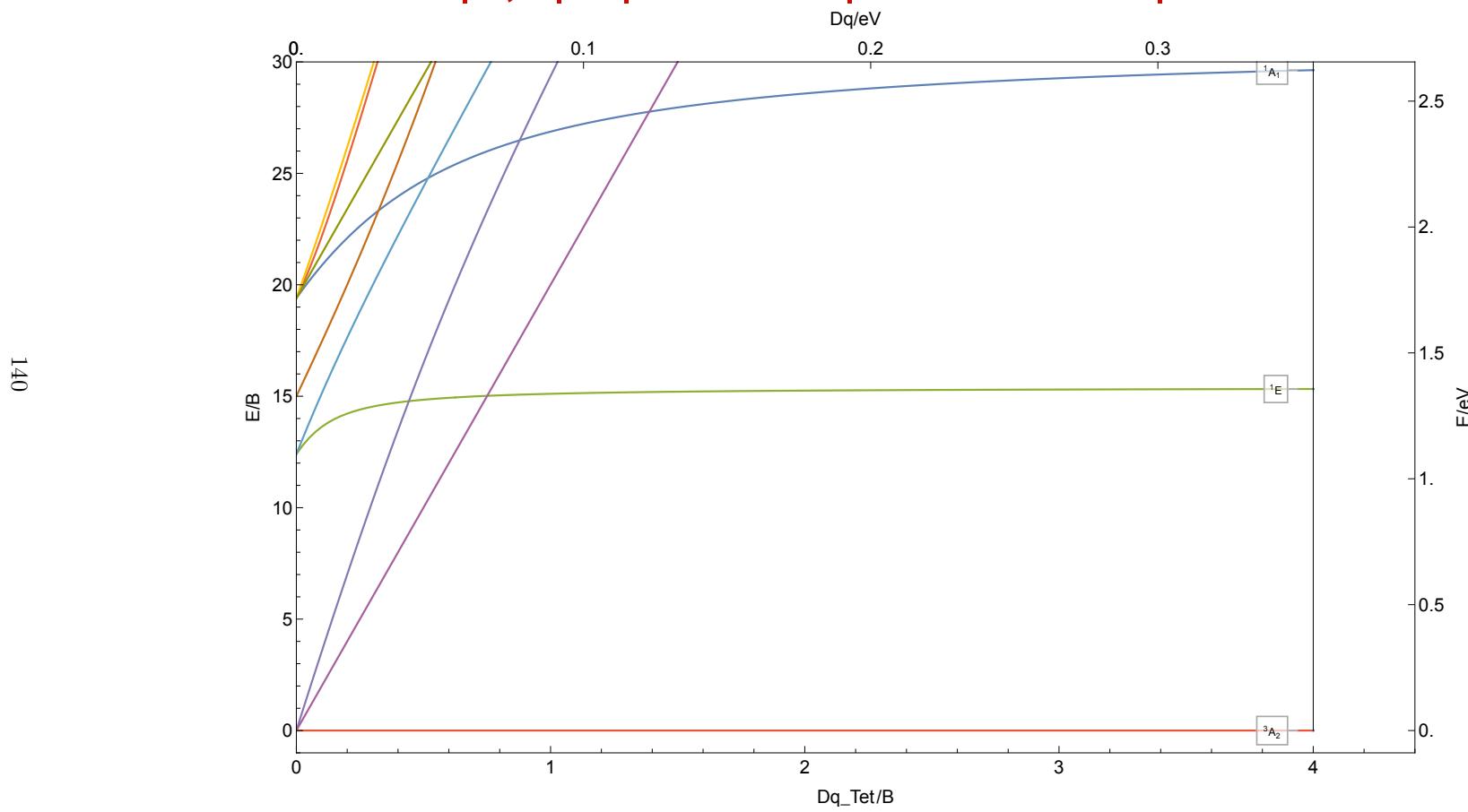
|2,4,6|d<sup>5</sup>| C/B ≈ 4.2 | B ≈ 862 cm<sup>-1</sup> | Hg<sup>7+</sup>



## 8.2 Tetrahedral field

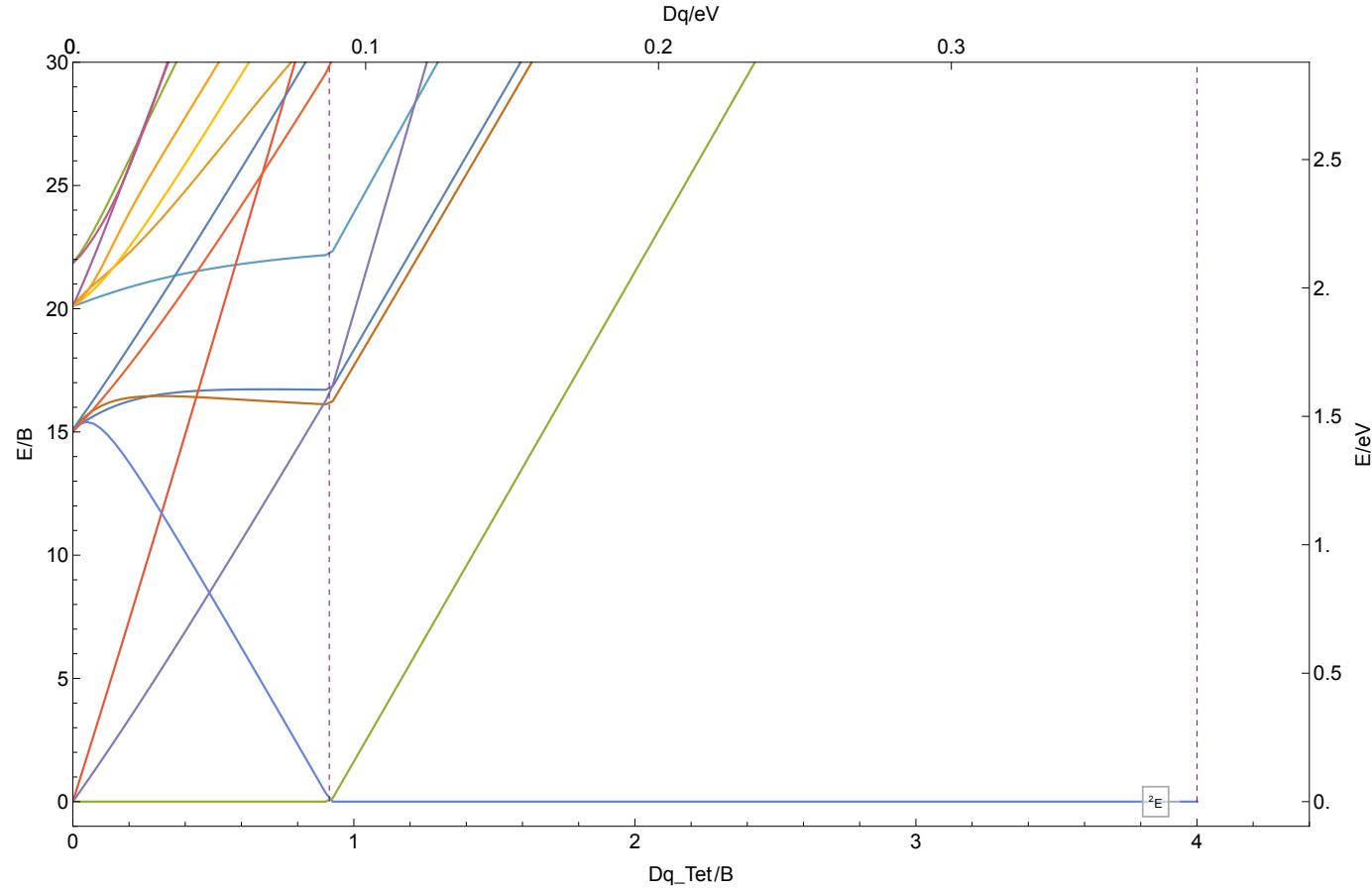
### 8.2.1 $\text{Ti}^{2+}$

$|1,3|d^2|C/B \approx 3.7|B \approx 714\text{ cm}^{-1}| \text{Ti}^{2+}$



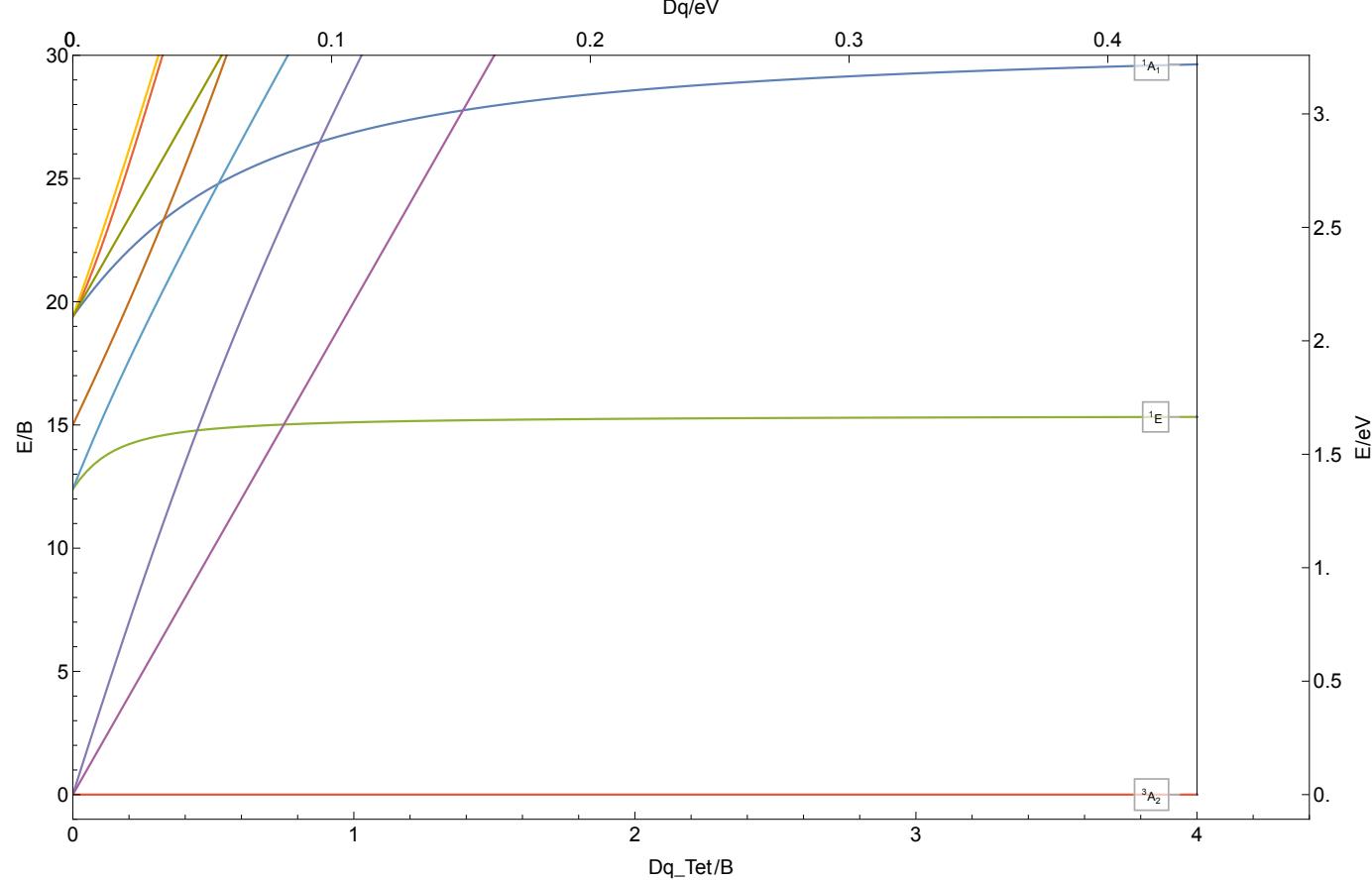
### 8.2.2 V<sup>2+</sup>

|2,4|d<sup>3</sup>| C/B ≈ 3.7 | B ≈ 774 cm<sup>-1</sup> |V<sup>2+</sup>



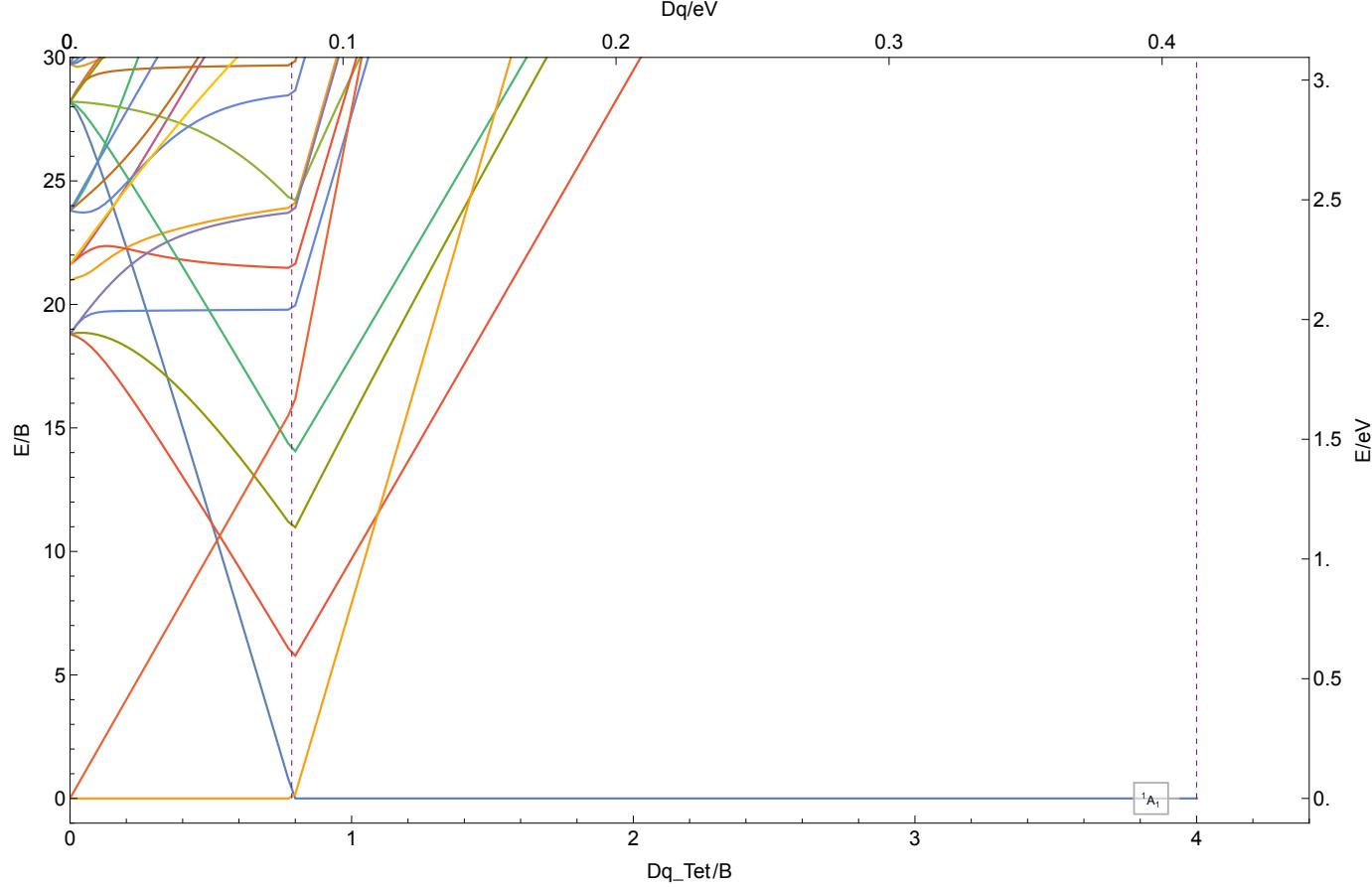
### 8.2.3 V<sup>3+</sup>

| 1,3 | d<sup>2</sup> | C/B ≈ 3.7 | B ≈ 876 cm<sup>-1</sup> | V<sup>3+</sup>



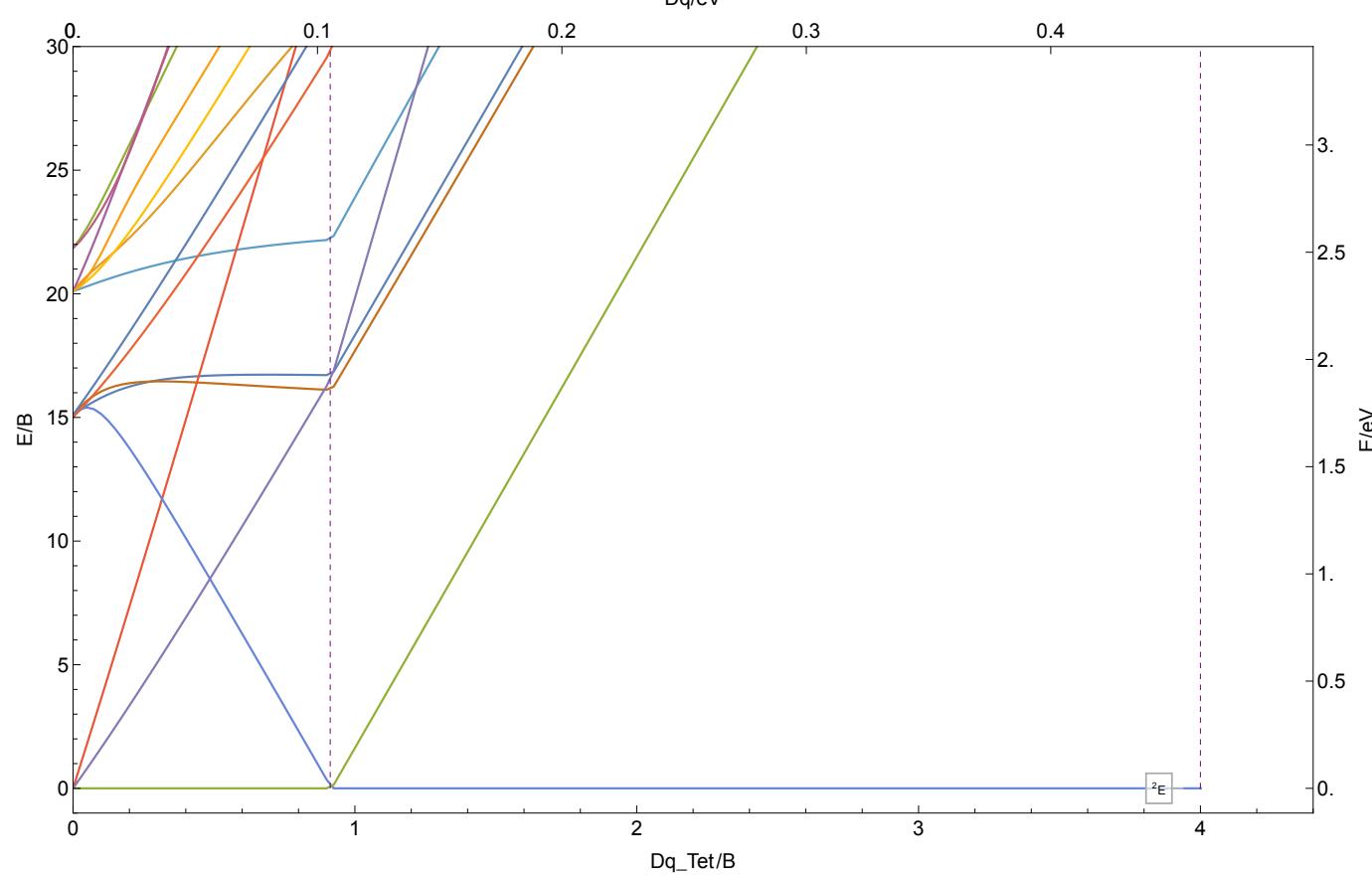
#### 8.2.4 Cr<sup>2+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 3.7 | B ≈ 832 cm<sup>-1</sup> | Cr<sup>2+</sup>



### 8.2.5 Cr<sup>3+</sup>

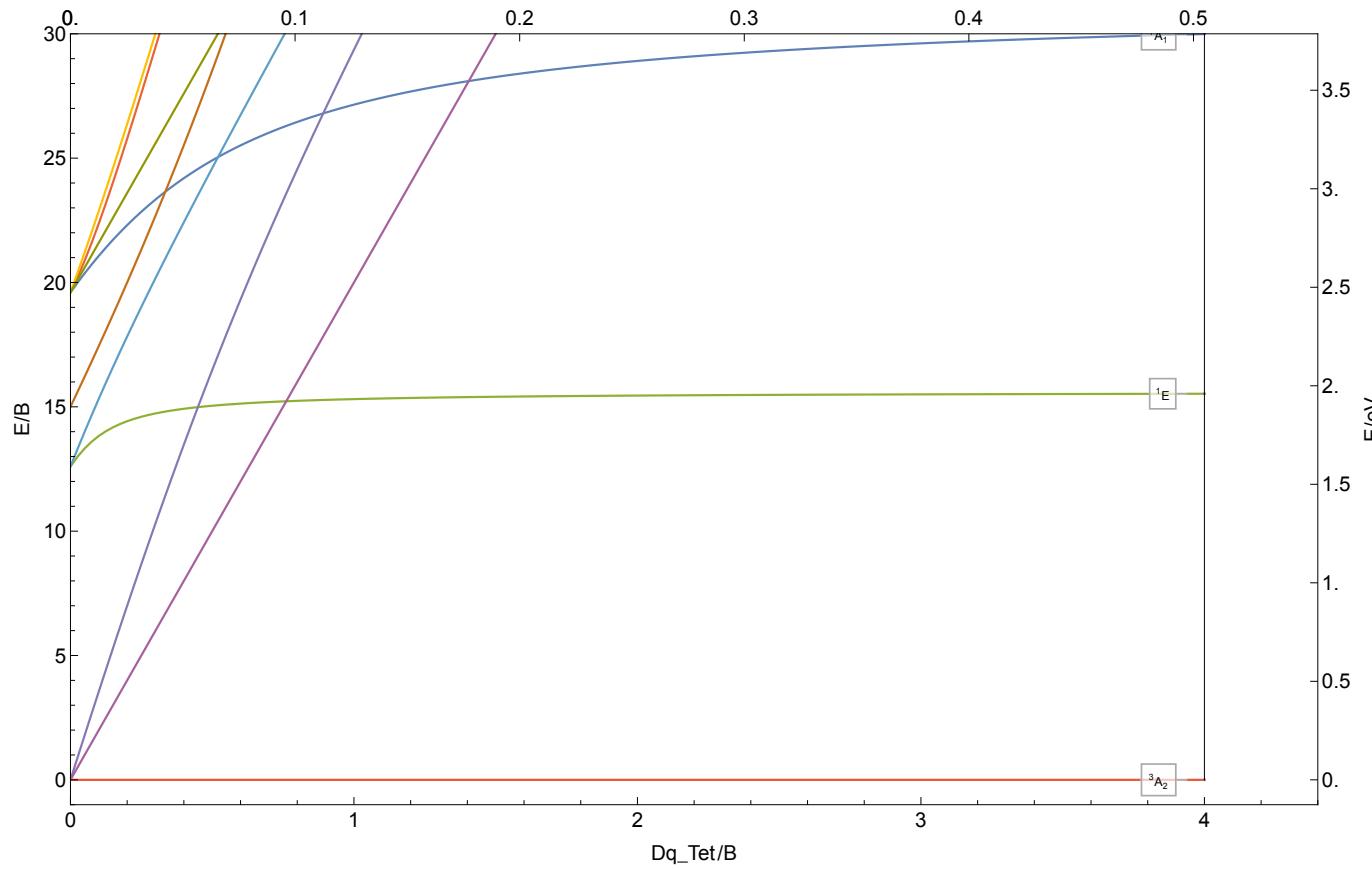
$|2,4|d^3|C/B \approx 3.7|B \approx 930\text{ cm}^{-1}|Cr^{3+}$



### 8.2.6 Cr<sup>4+</sup>

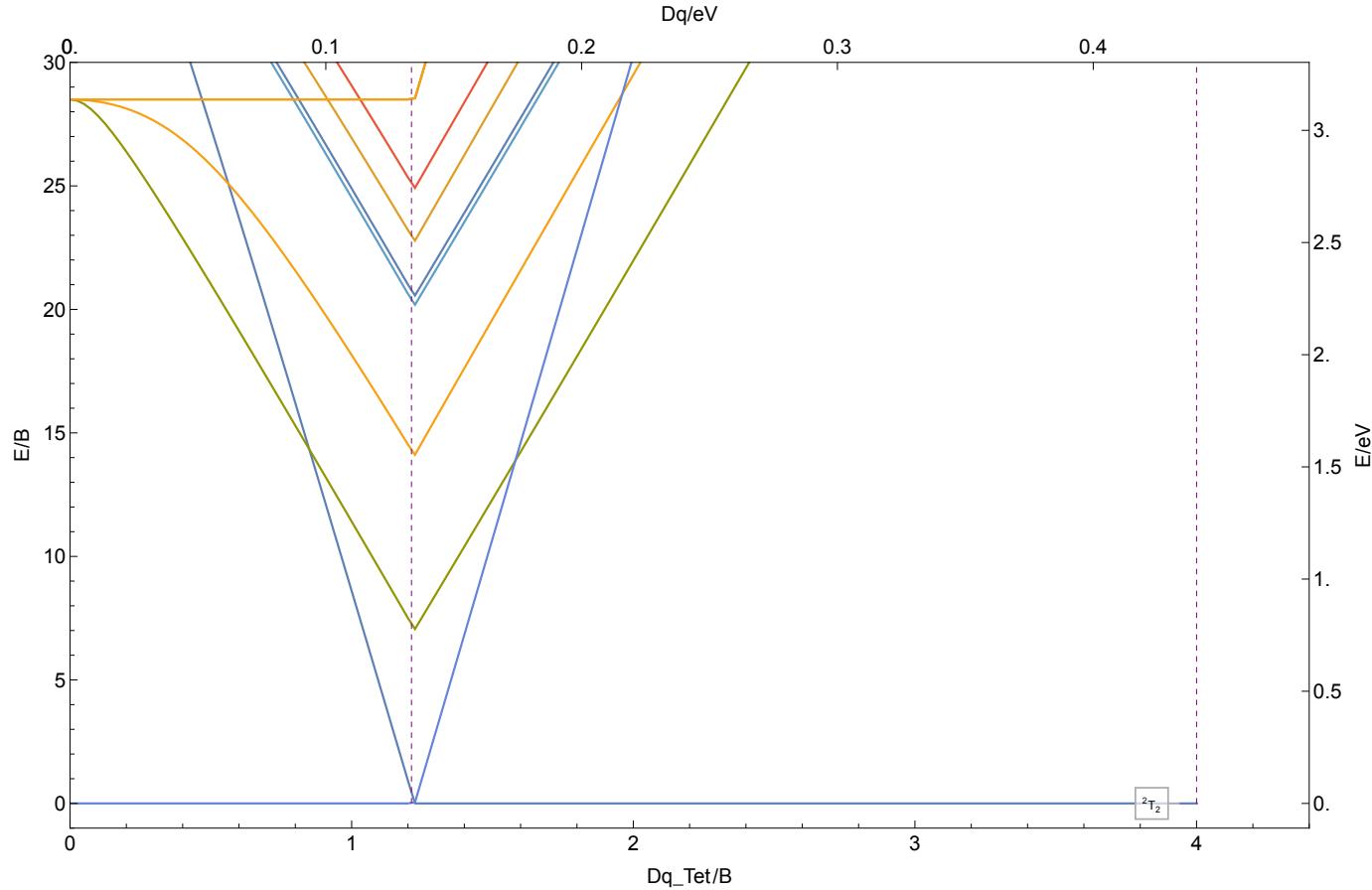
$|1,3|d^2| C/B \approx 3.8 | B \approx 1018\text{cm}^{-1}| \text{Cr}^{4+}$

Dq/eV



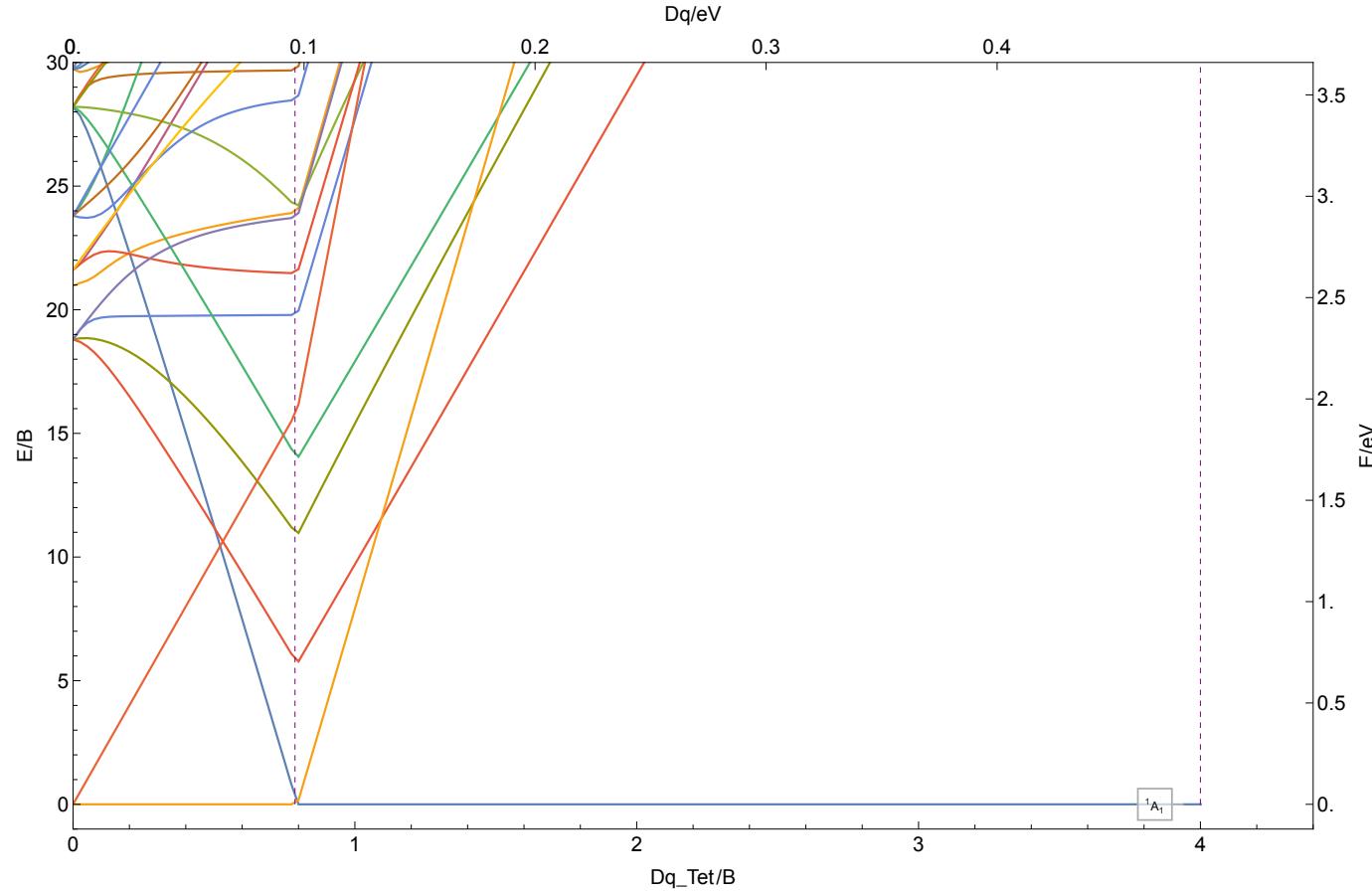
### 8.2.7 Mn<sup>2+</sup>

$|2,4,6|d^5|C/B \approx 3.7|B \approx 888\text{ cm}^{-1}|Mn^{2+}$



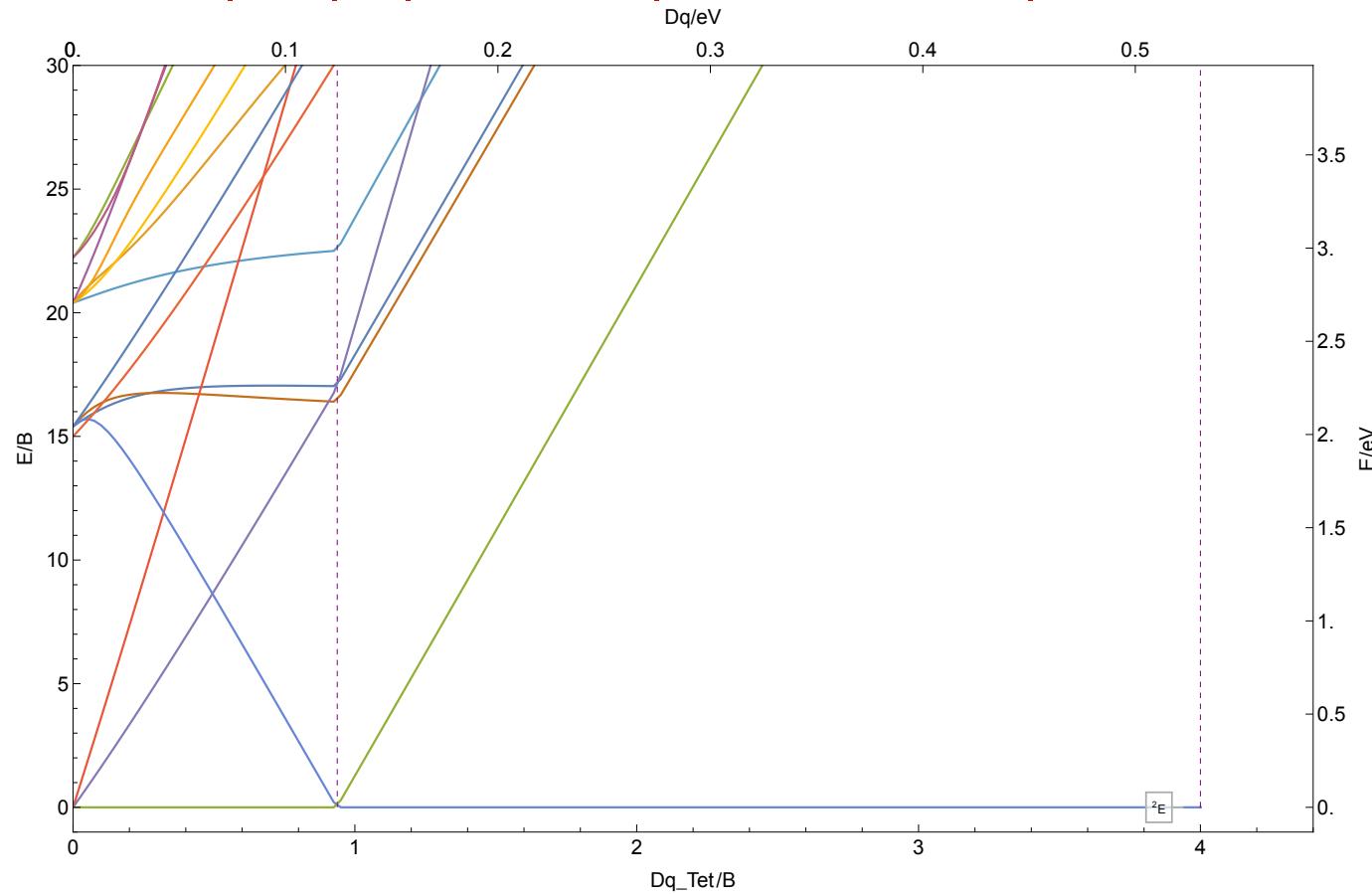
### 8.2.8 Mn<sup>3+</sup>

$|1,3,5|d^4|C/B \approx 3.7|B \approx 984\text{ cm}^{-1}|Mn^{3+}$



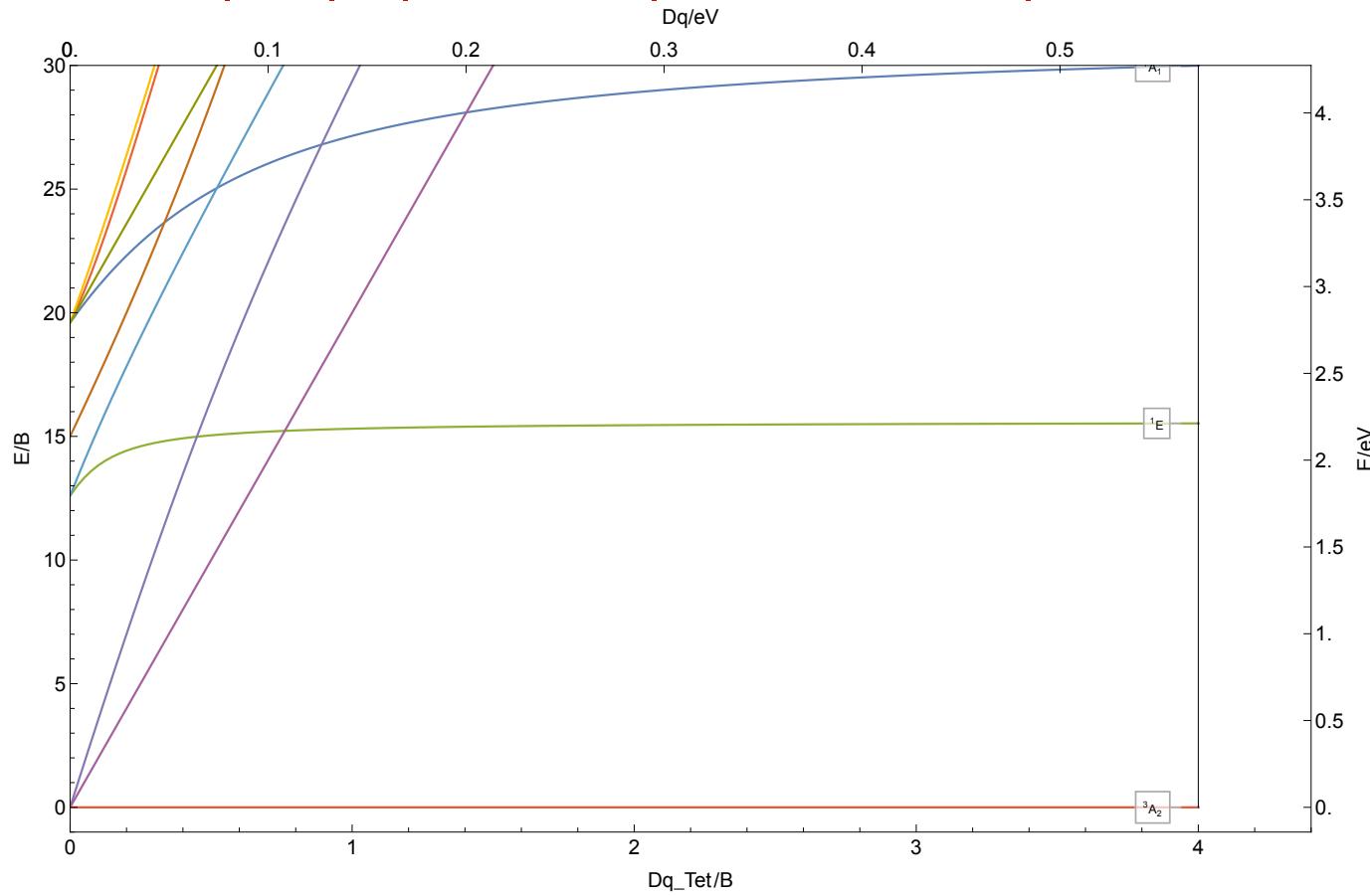
### 8.2.9 Mn<sup>4+</sup>

$|2,4|d^3|C/B \approx 3.8|B \approx 1070\text{ cm}^{-1}|Mn^{4+}$



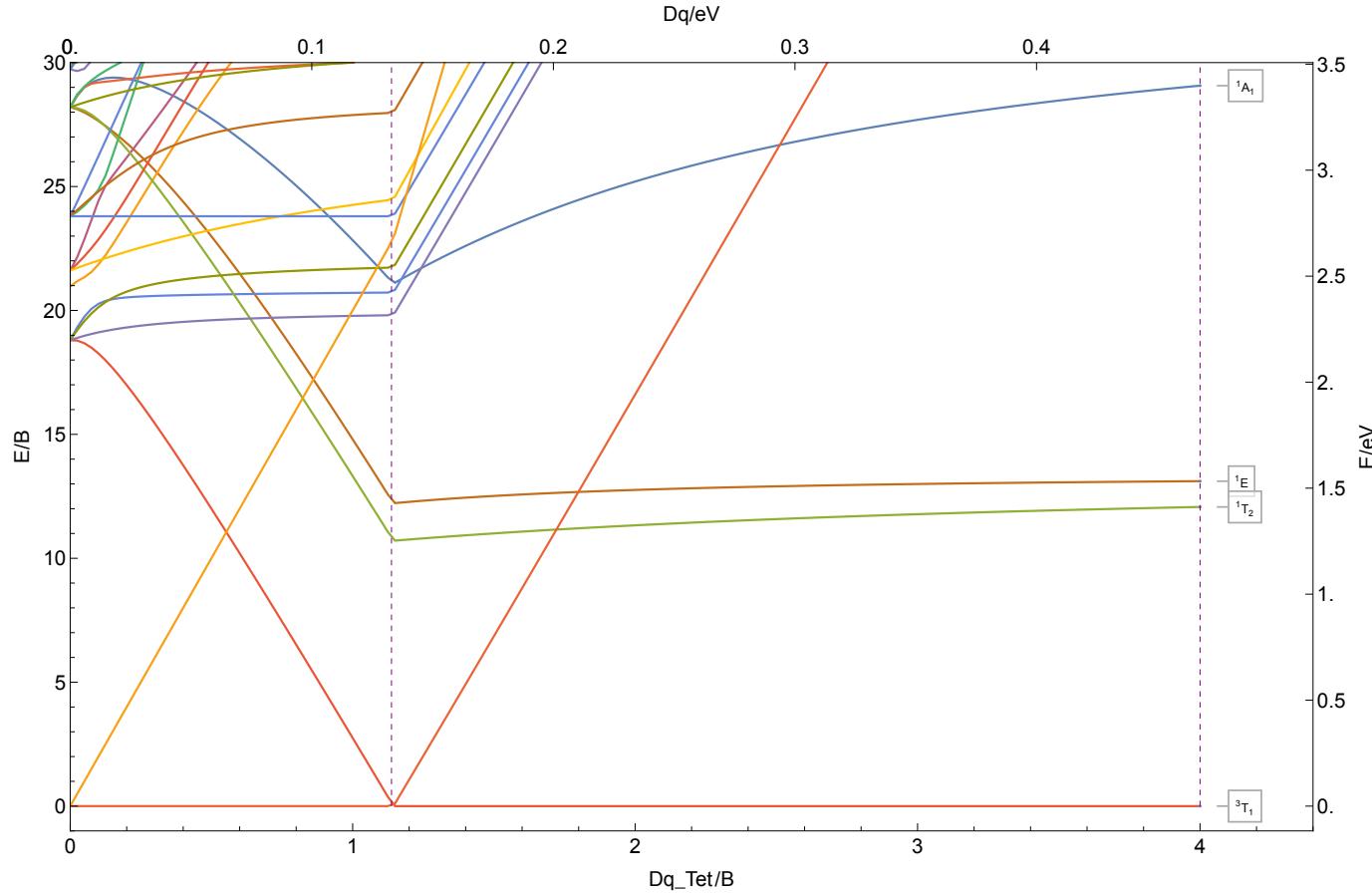
8.2.10 Mn<sup>5+</sup>

| 1,3 | d<sup>2</sup> | C/B ≈ 3.8 | B ≈ 1149 cm<sup>-1</sup> | Mn<sup>5+</sup>



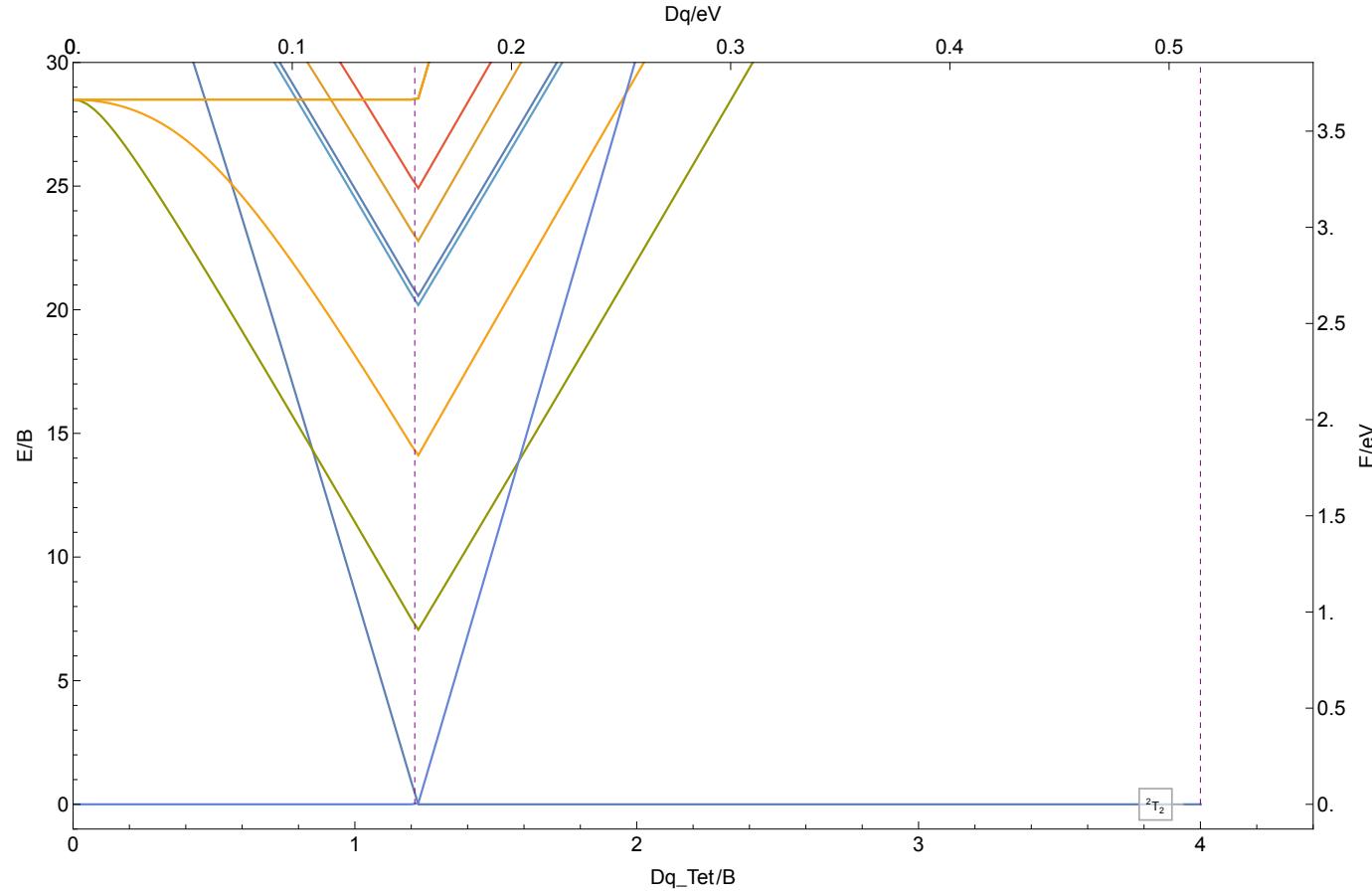
### 8.2.11 Fe<sup>2+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 3.7 | B ≈ 943 cm<sup>-1</sup> | Fe<sup>2+</sup>



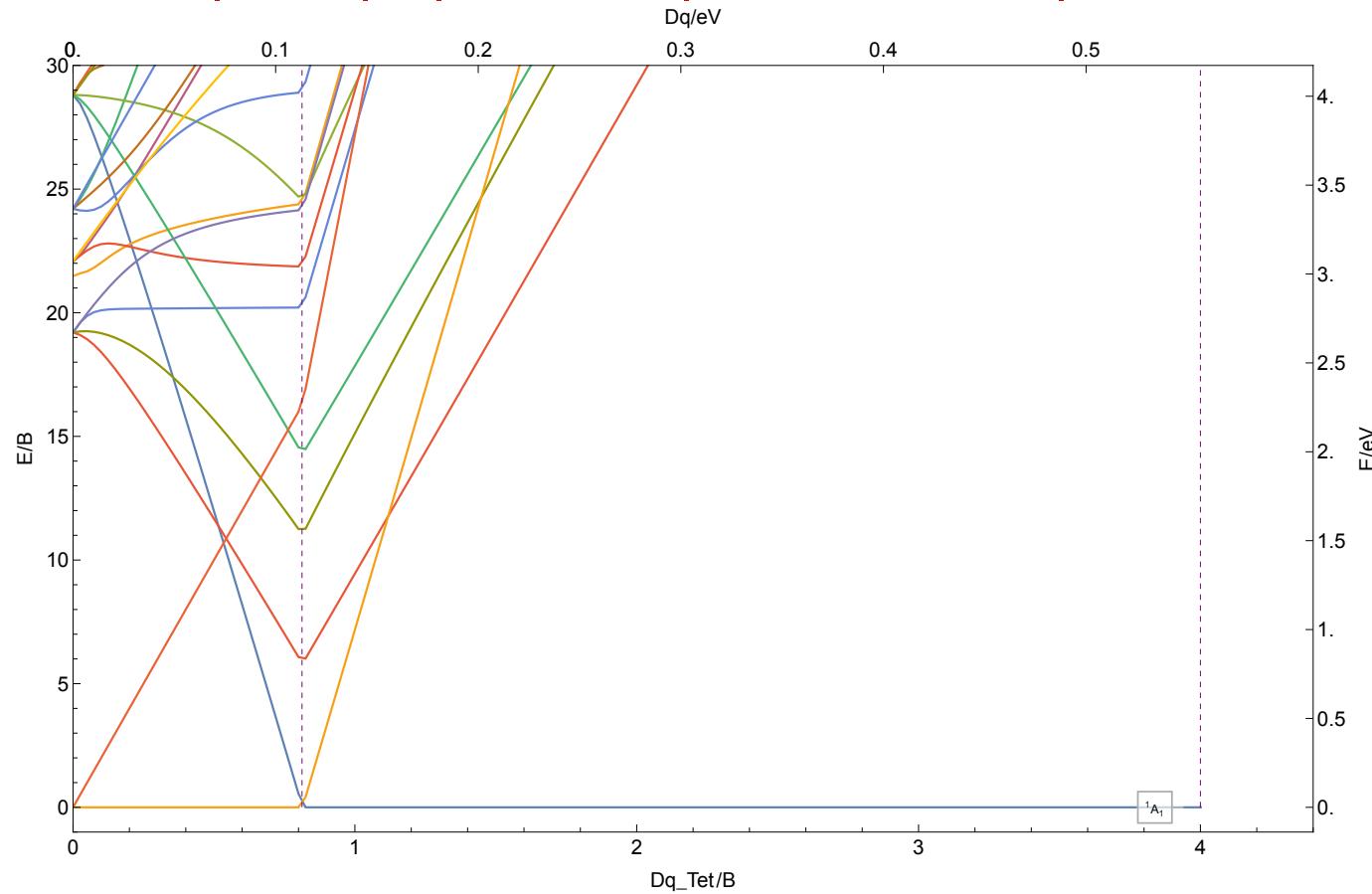
### 8.2.12 Fe<sup>3+</sup>

|2,4,6|d<sup>5</sup>|C/B ≈ 3.7|B ≈ 1037 cm<sup>-1</sup>|Fe<sup>3+</sup>



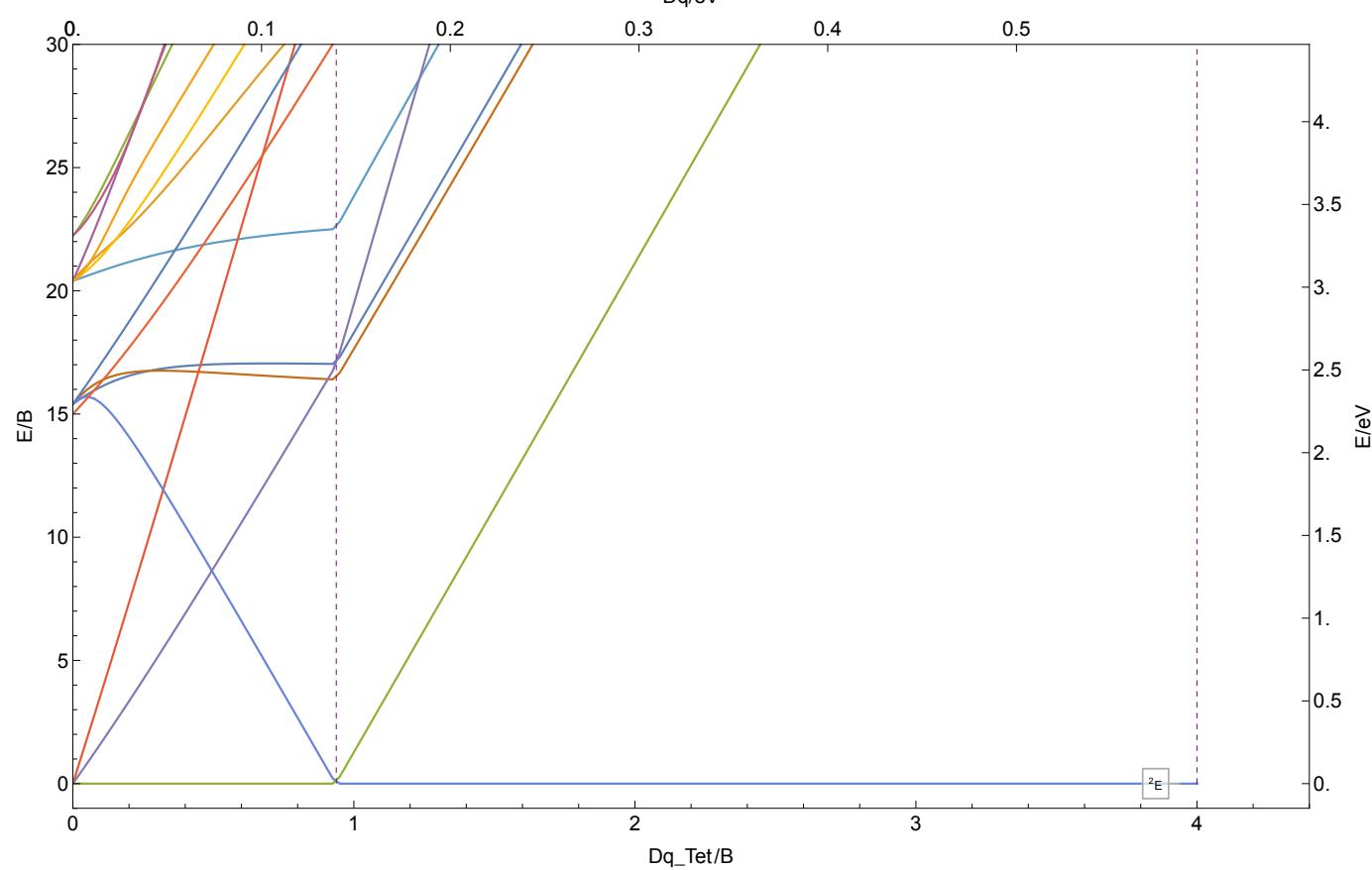
8.2.13 Fe<sup>4+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 3.8 | B ≈ 1122 cm<sup>-1</sup> | Fe<sup>4+</sup>



8.2.14 Fe<sup>5+</sup>

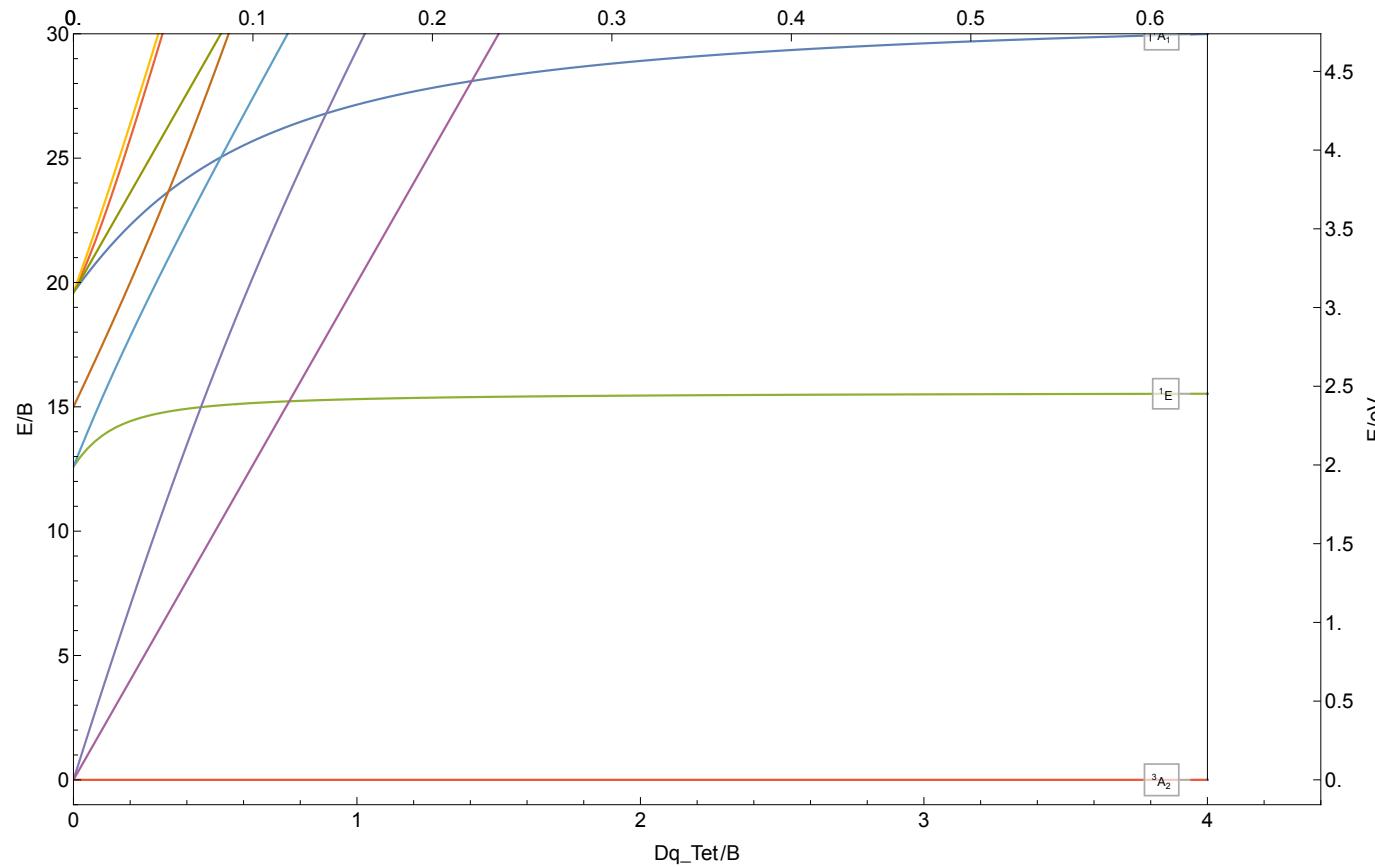
|2,4|d<sup>3</sup>| C/B ≈ 3.8 | B ≈ 1201 cm<sup>-1</sup> | Fe<sup>5+</sup>



8.2.15 Fe<sup>6+</sup>

$|1,3|d^2|C/B \approx 3.8|B \approx 1274\text{ cm}^{-1}|Fe^{6+}$

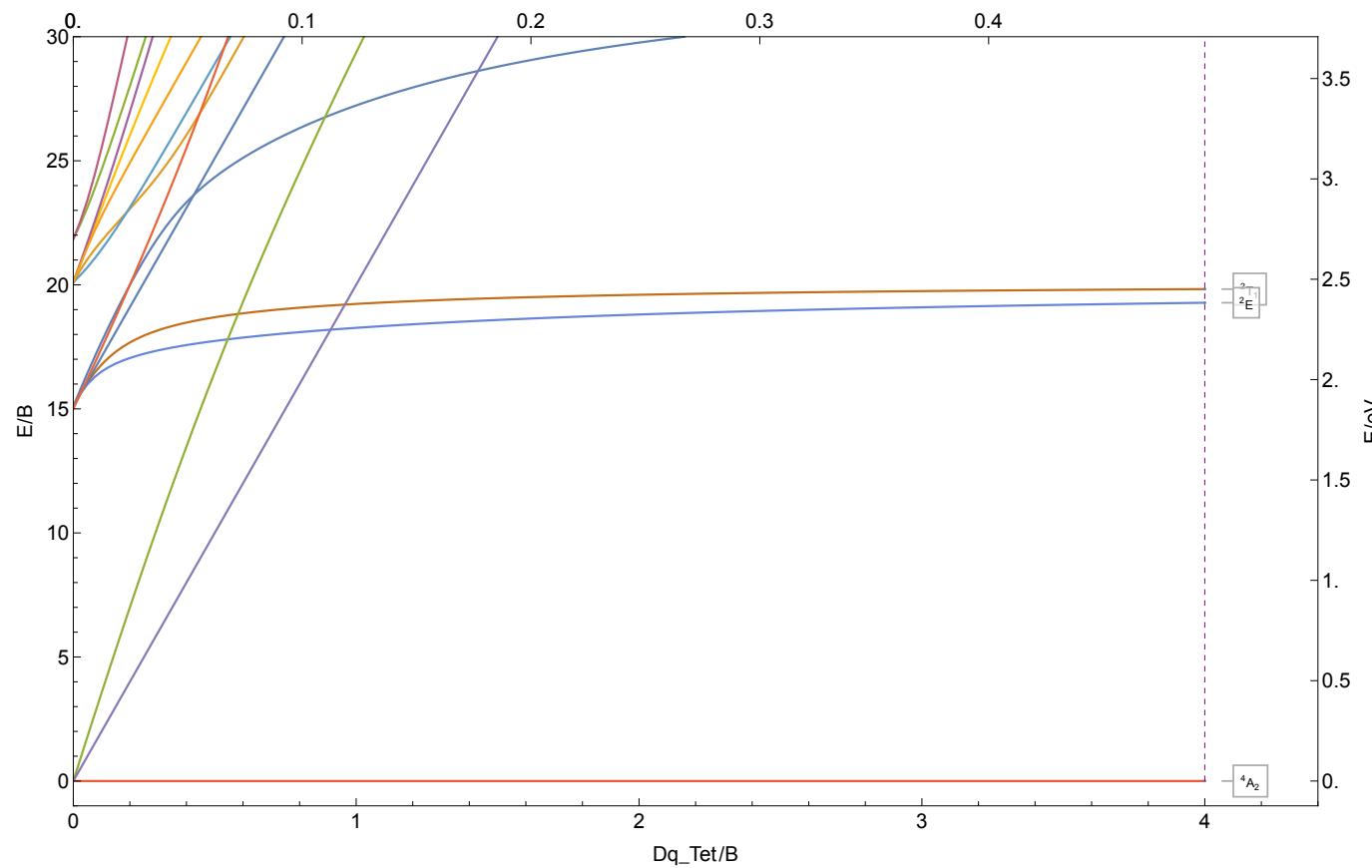
Dq/eV



8.2.16  $\text{Co}^{2+}$

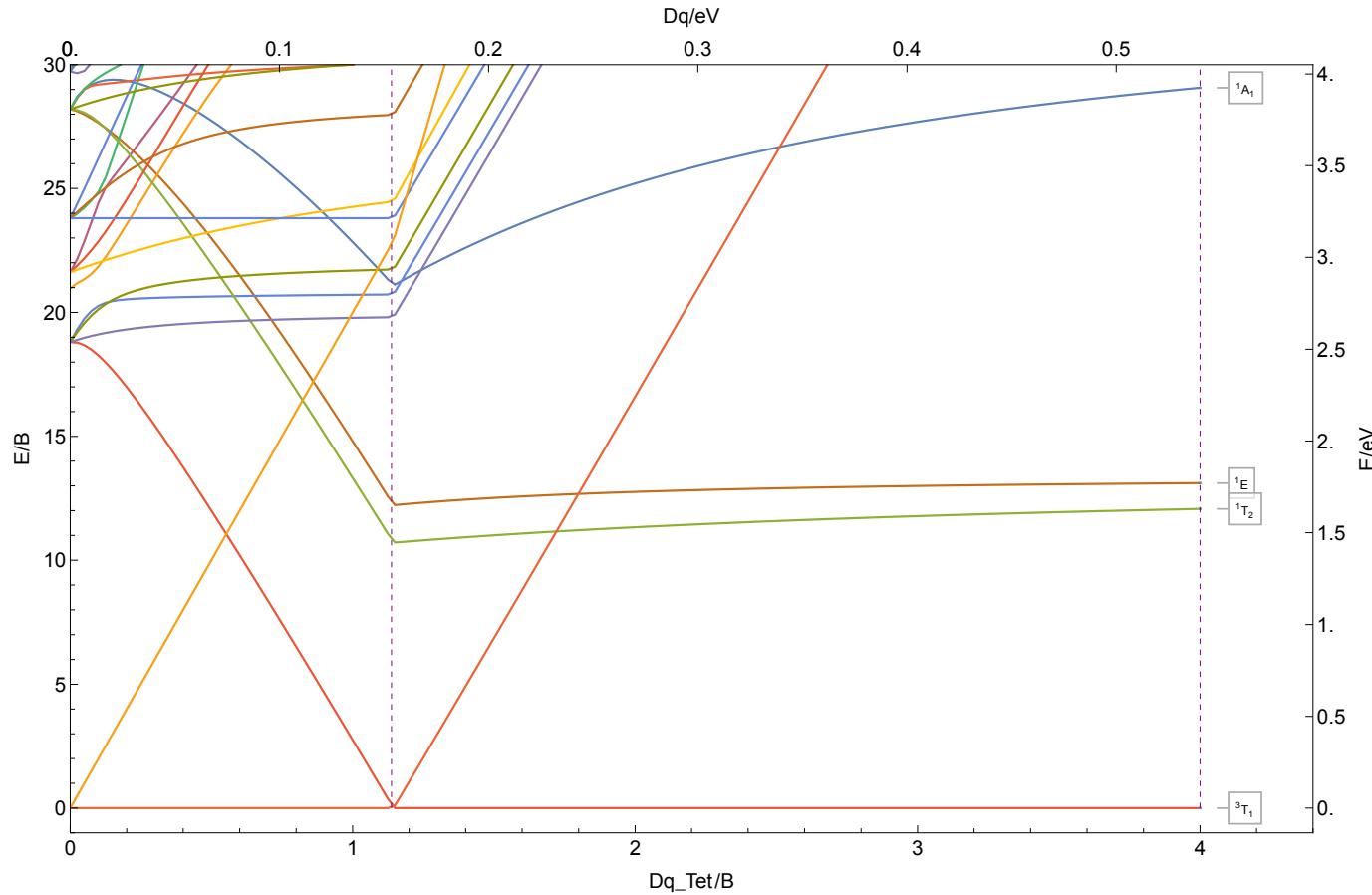
$|2,4|d^7| \text{C/B} \approx 3.7 | \text{B} \approx 997 \text{ cm}^{-1} | \text{Co}^{2+}$

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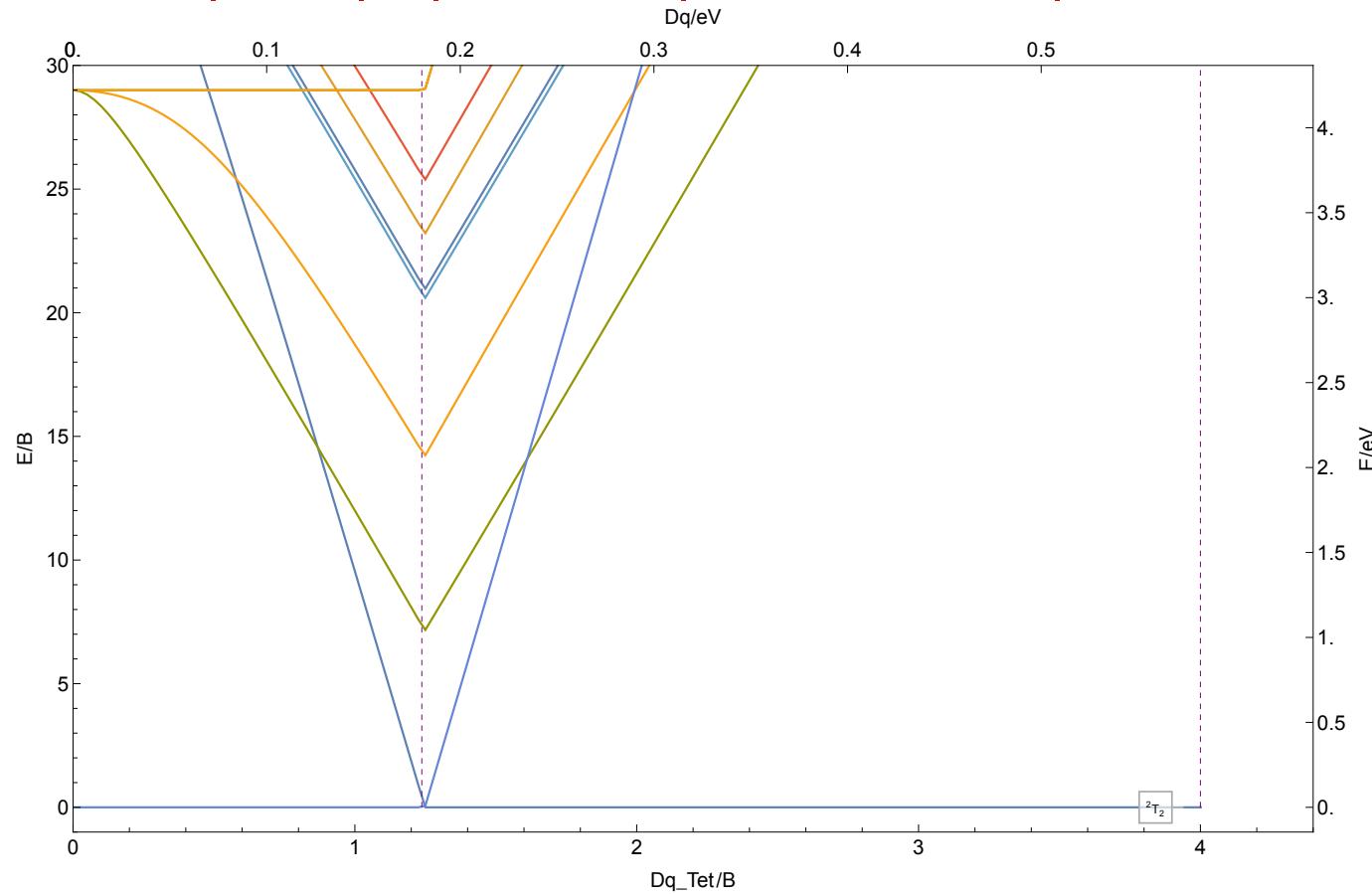
8.2.17  $\text{Co}^{3+}$

$|1,3,5| \text{d}^6 | \text{C/B} \approx 3.7 | \text{B} \approx 1089 \text{ cm}^{-1} | \text{Co}^{3+}$



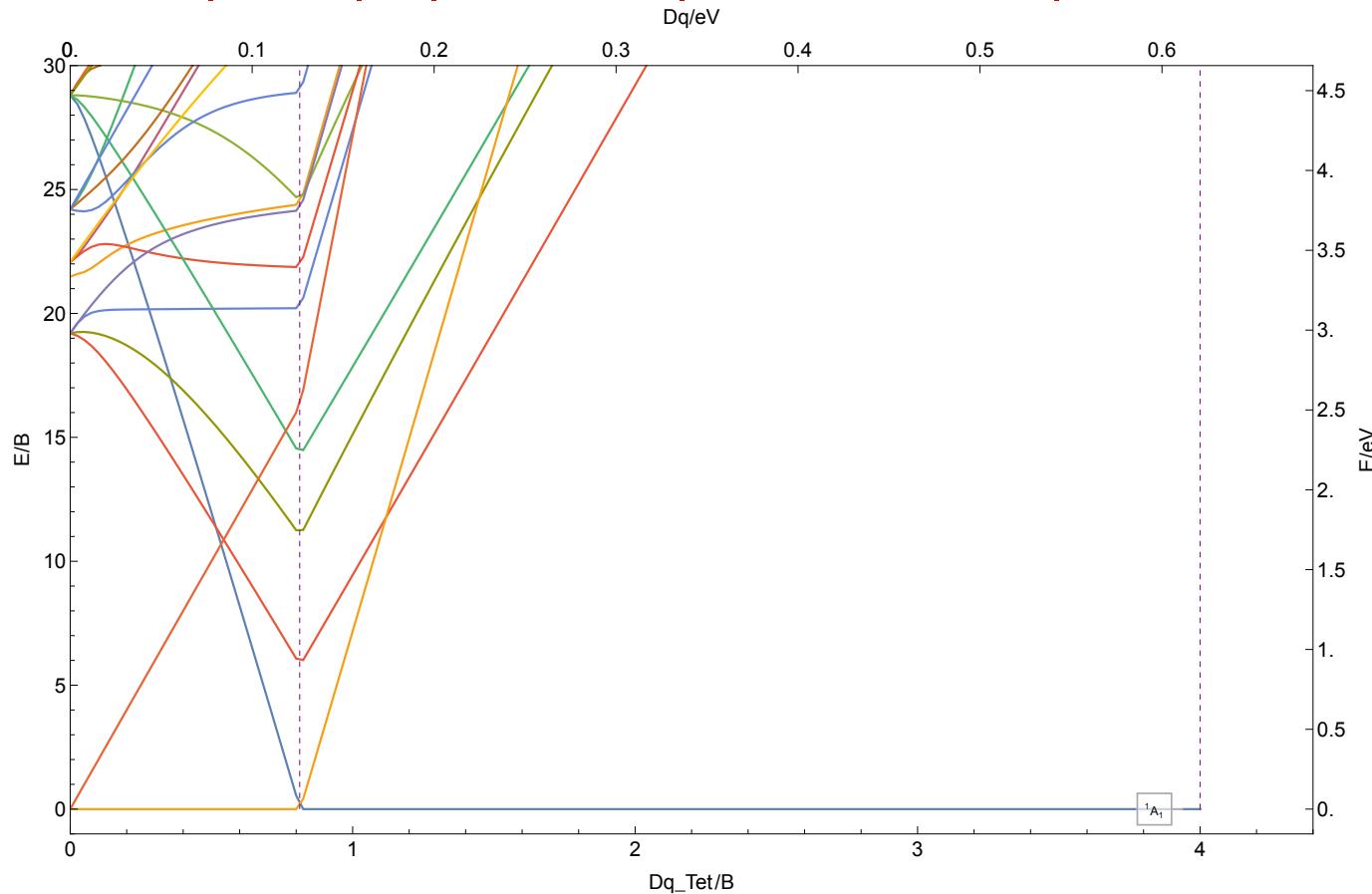
8.2.18  $\text{Co}^{4+}$

$|2,4,6| \text{d}^5 | \text{C/B} \approx 3.8 | \text{B} \approx 1174 \text{ cm}^{-1} | \text{Co}^{4+}$



8.2.19  $\text{Co}^{5+}$

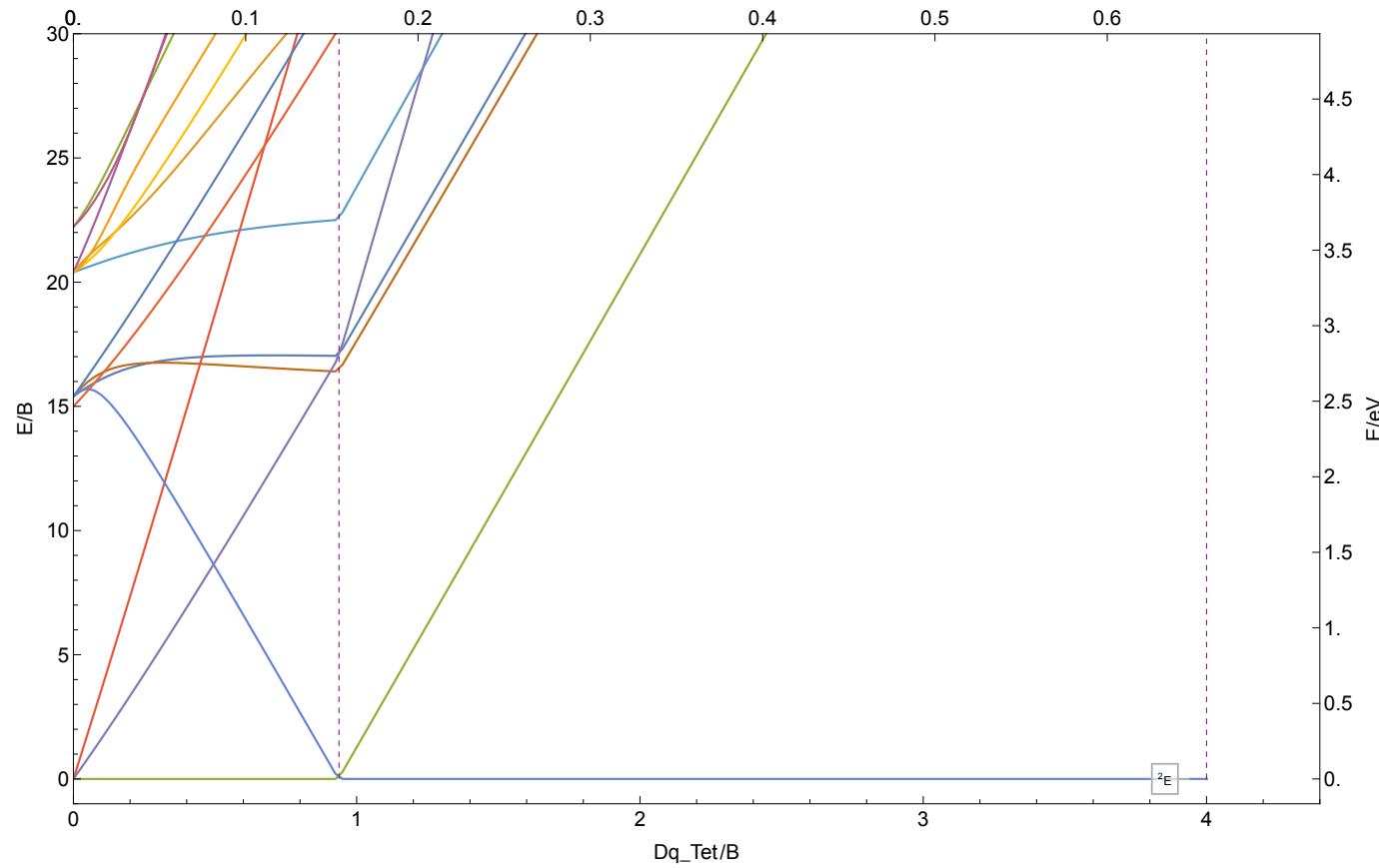
$|1,3,5|d^4|C/B \approx 3.8|B \approx 1252\text{ cm}^{-1}|Co^{5+}$



8.2.20  $\text{Co}^{6+}$

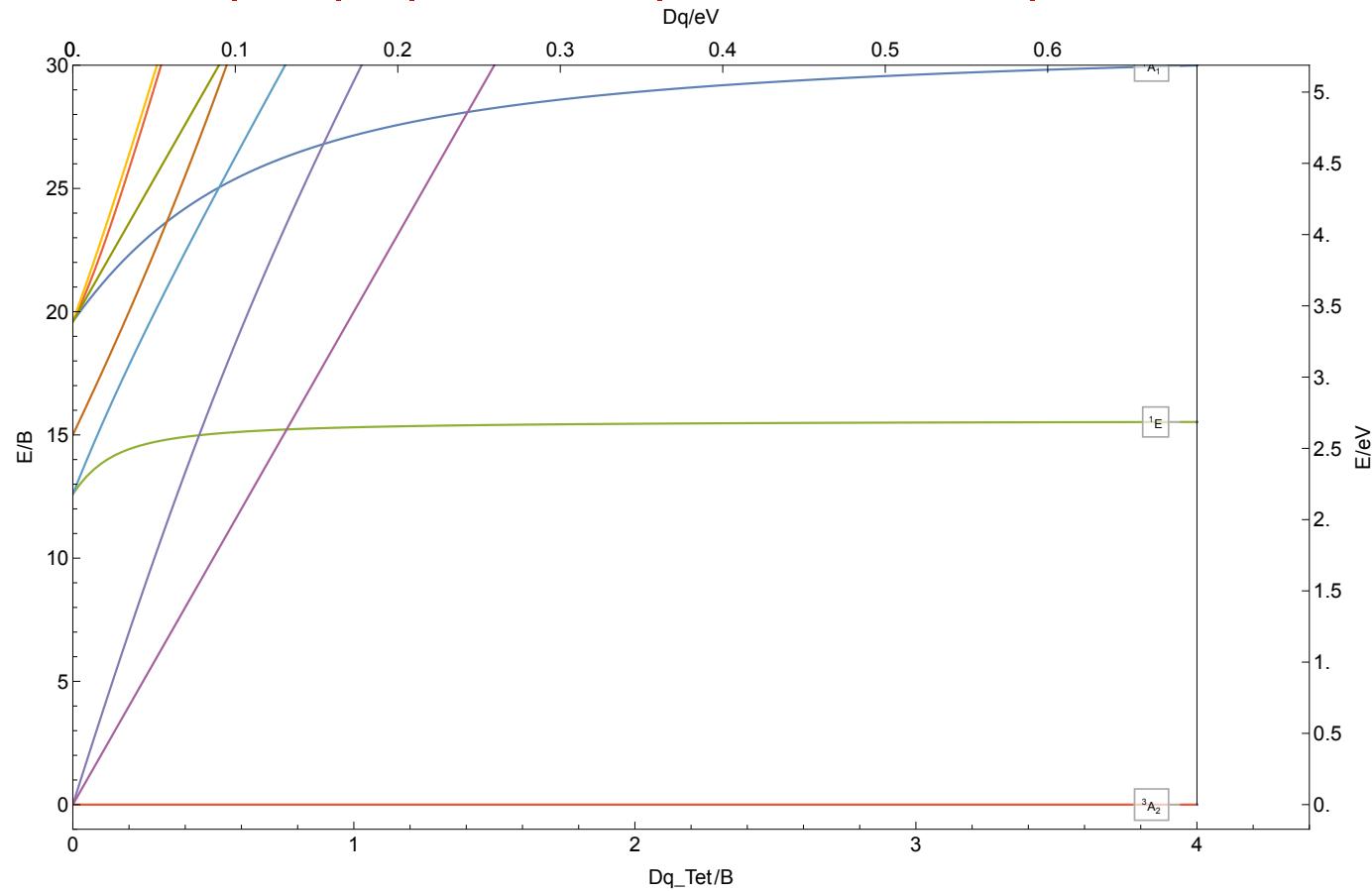
$|2,4|d^3|C/B \approx 3.8|B \approx 1326\text{ cm}^{-1}|Co^{6+}$

Dq/eV



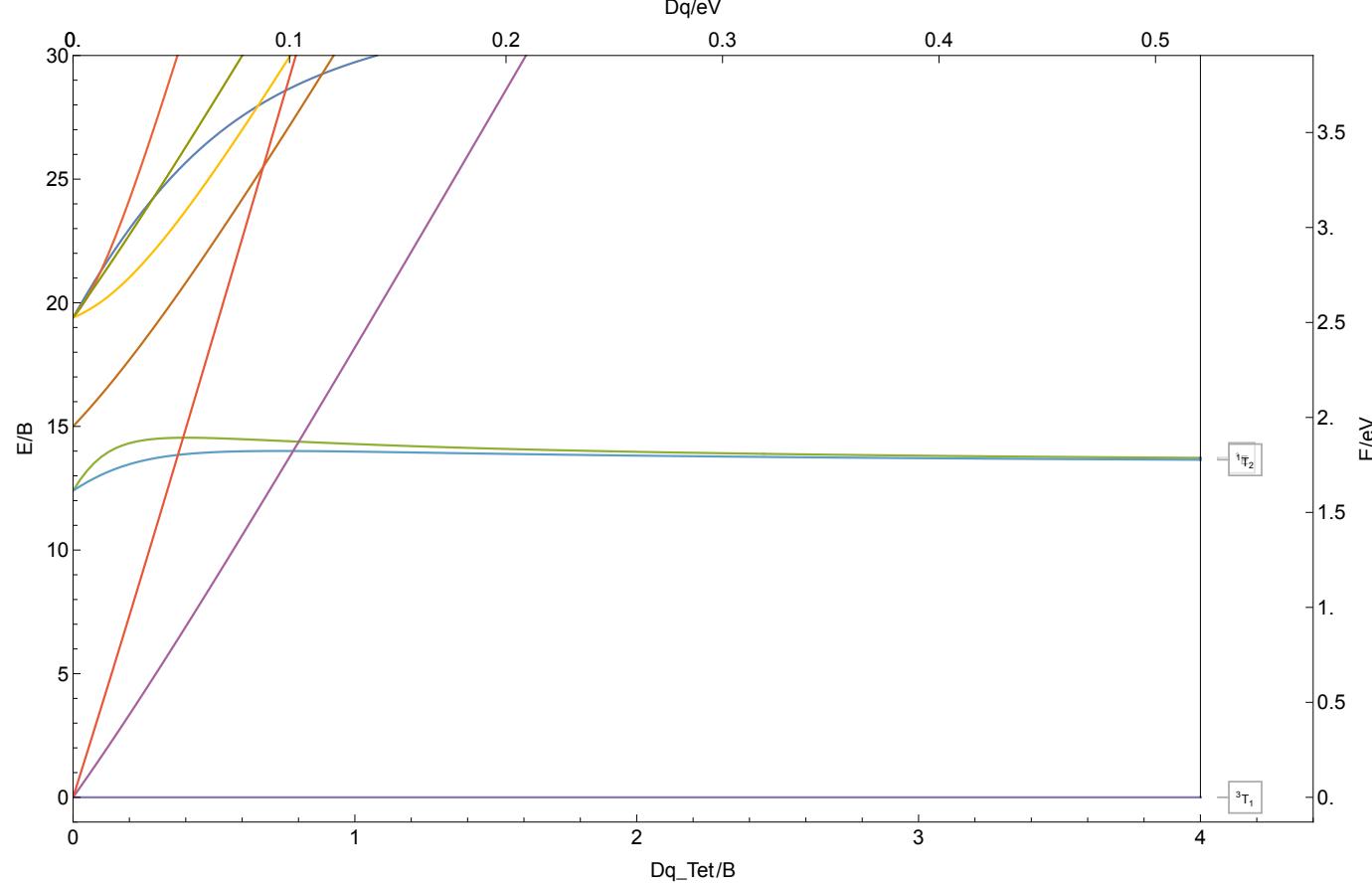
8.2.21 Co<sup>7+</sup>

| 1,3 | d<sup>2</sup> | C/B ≈ 3.8 | B ≈ 1395 cm<sup>-1</sup> | Co<sup>7+</sup>



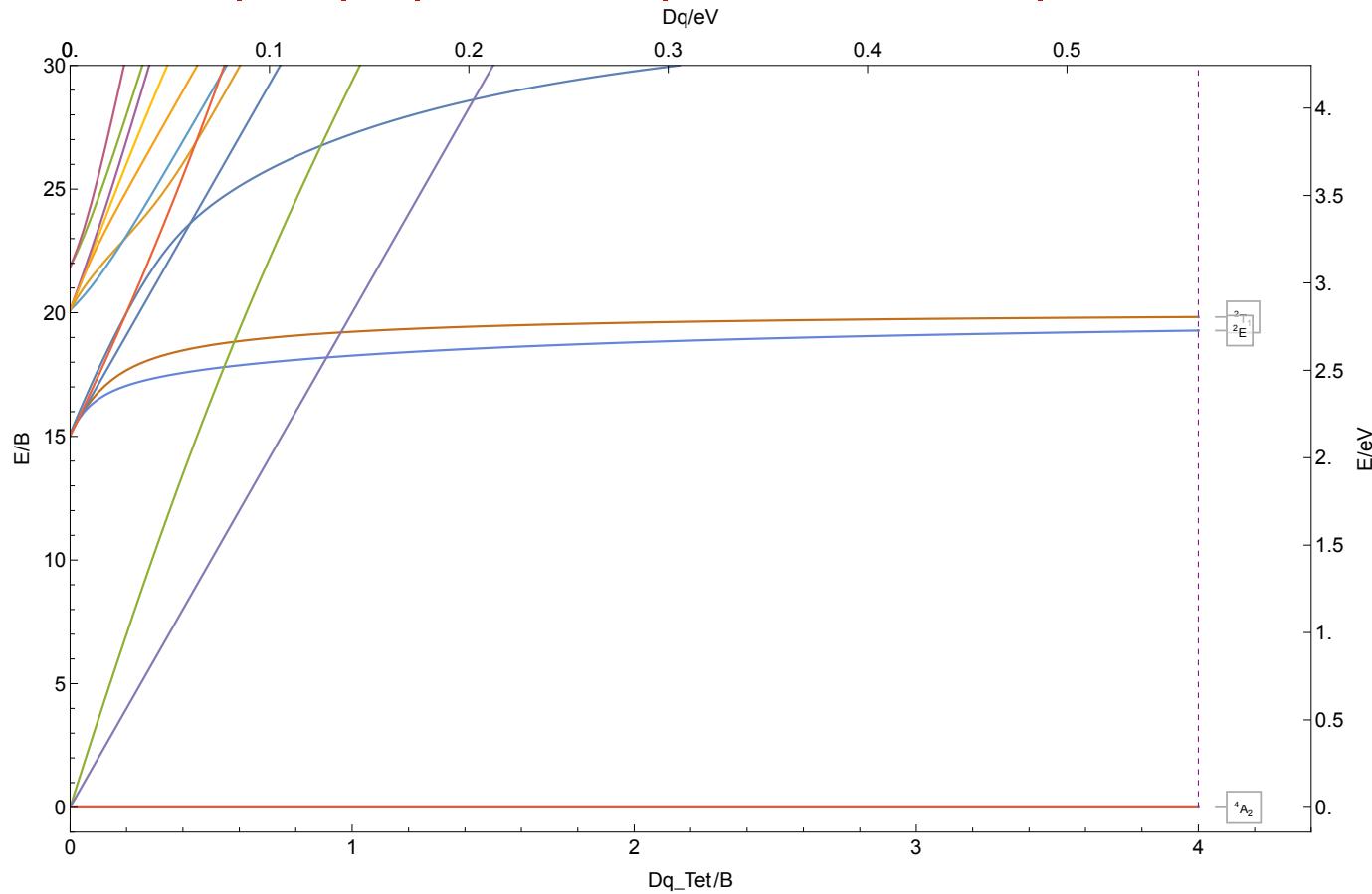
8.2.22 Ni<sup>2+</sup>

$|1,3|d^8|C/B \approx 3.7|B \approx 1050\text{ cm}^{-1}|Ni^{2+}$



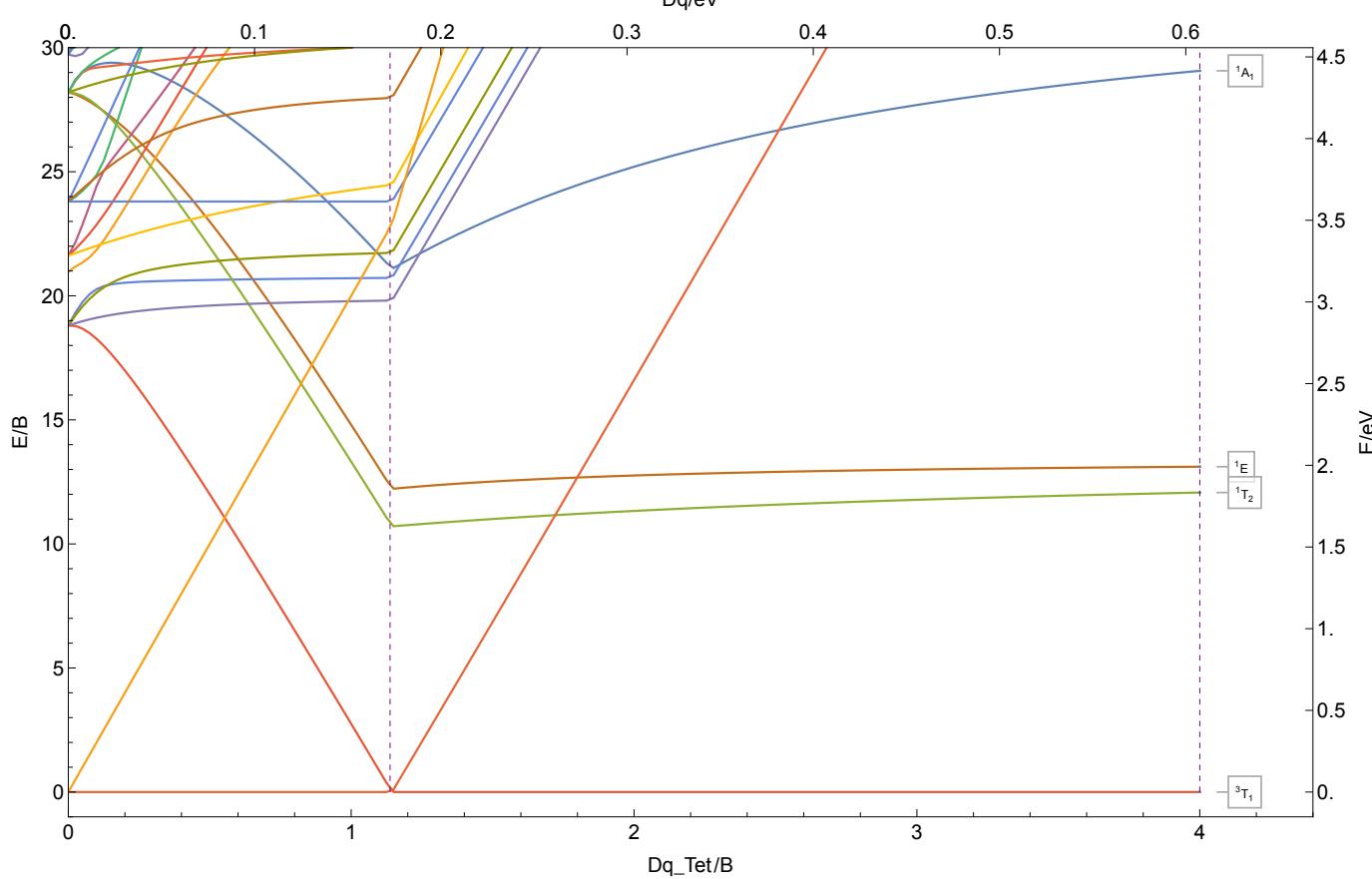
8.2.23 Ni<sup>3+</sup>

|2,4|d<sup>7</sup>| C/B ≈ 3.7 | B ≈ 1141 cm<sup>-1</sup> | Ni<sup>3+</sup>



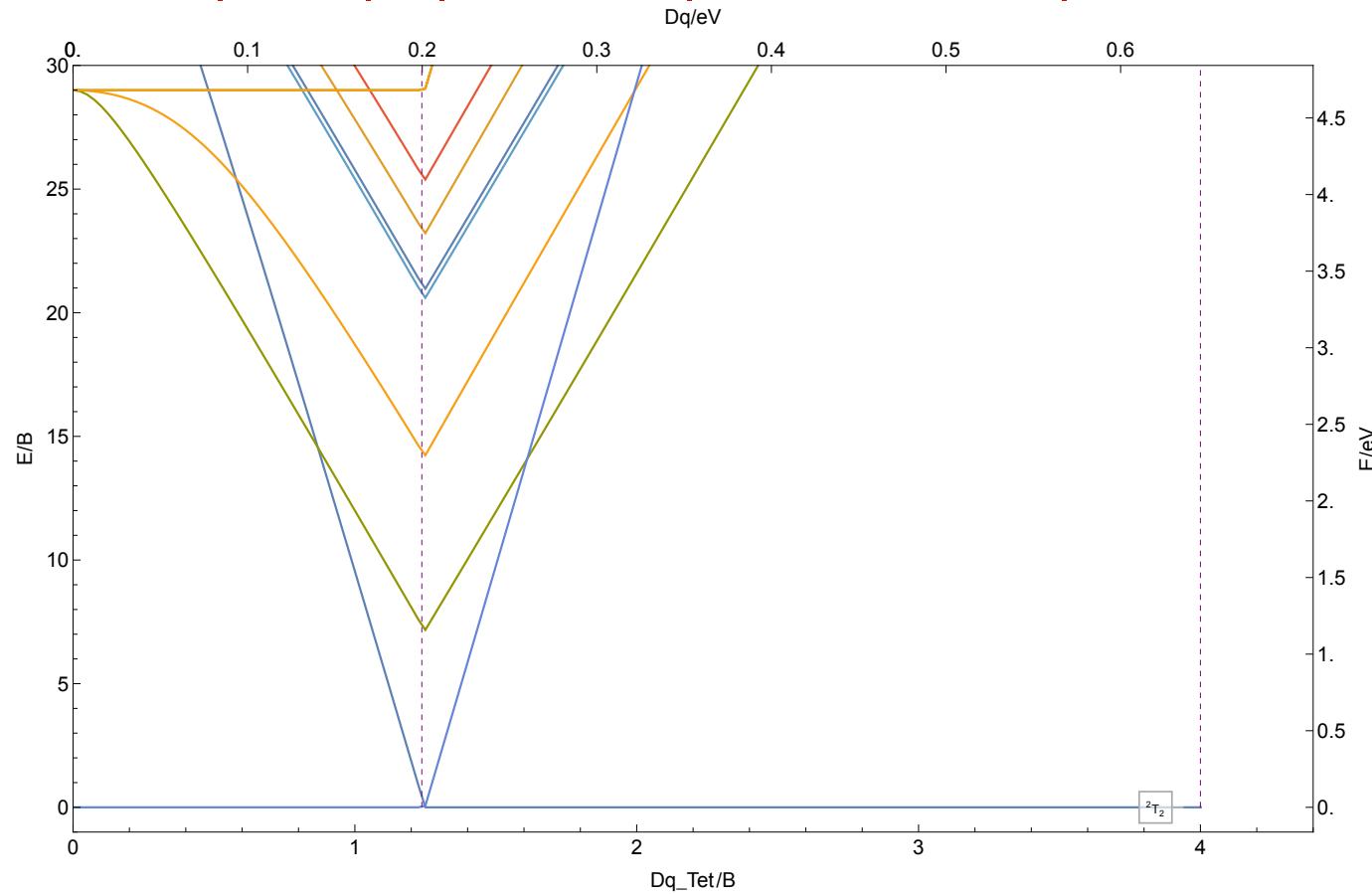
8.2.24 Ni<sup>4+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 3.7 | B ≈ 1225 cm<sup>-1</sup> | Ni<sup>4+</sup>



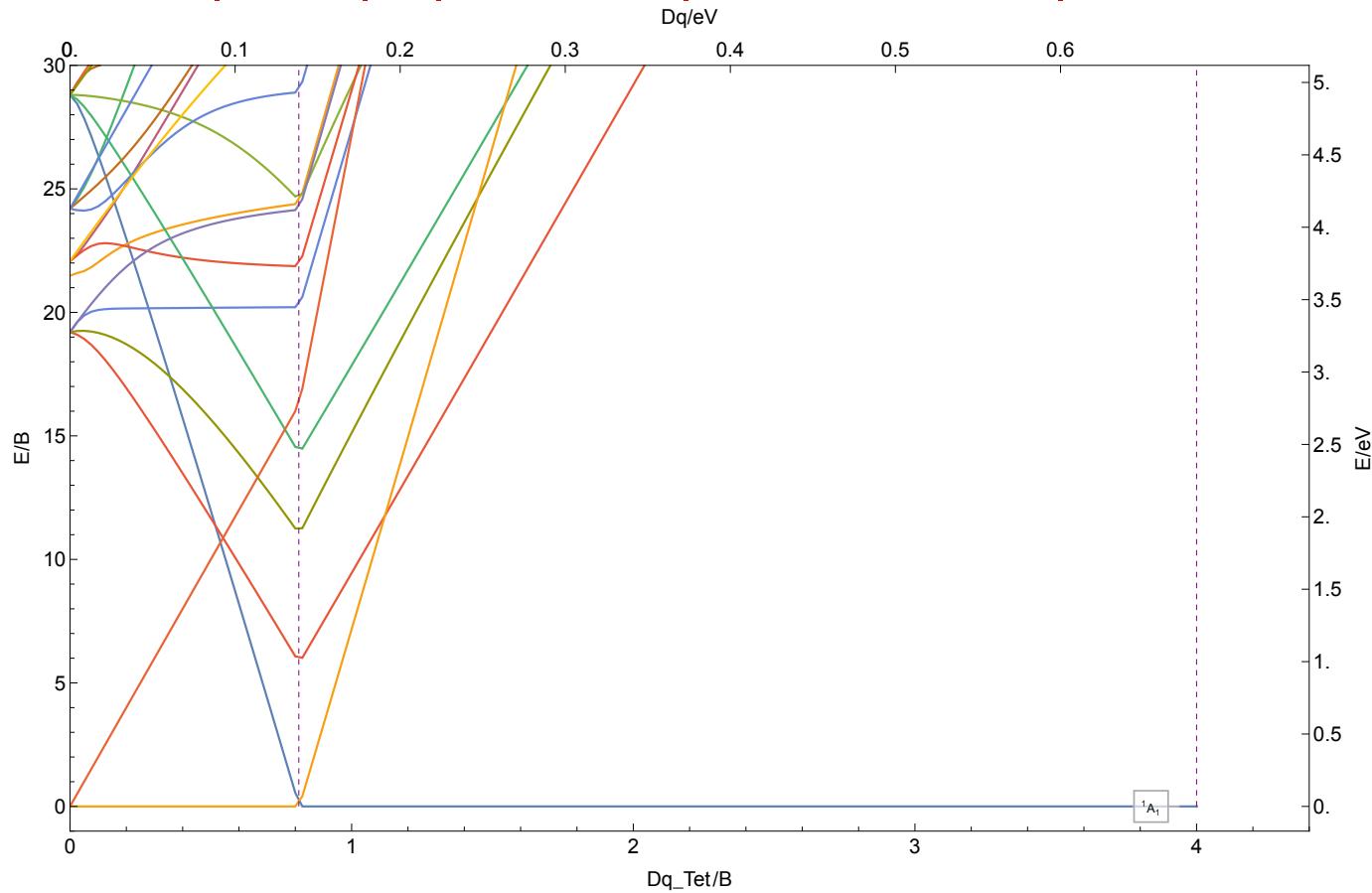
8.2.25 Ni<sup>5+</sup>

|2,4,6|d<sup>5</sup>|C/B ≈ 3.8|B ≈ 1302 cm<sup>-1</sup>|Ni<sup>5+</sup>



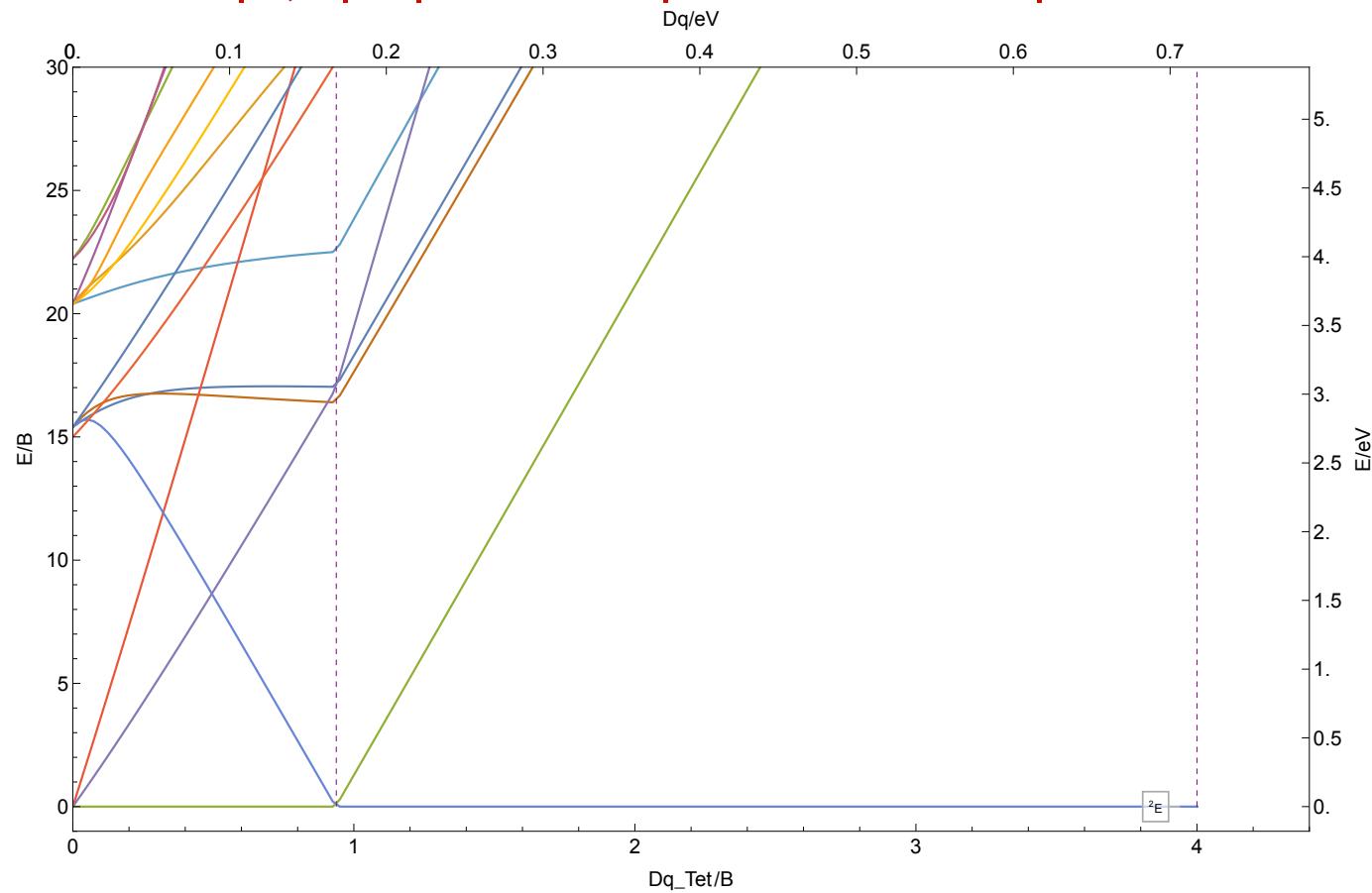
8.2.26 Ni<sup>6+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 3.8 | B ≈ 1376 cm<sup>-1</sup> | Ni<sup>6+</sup>



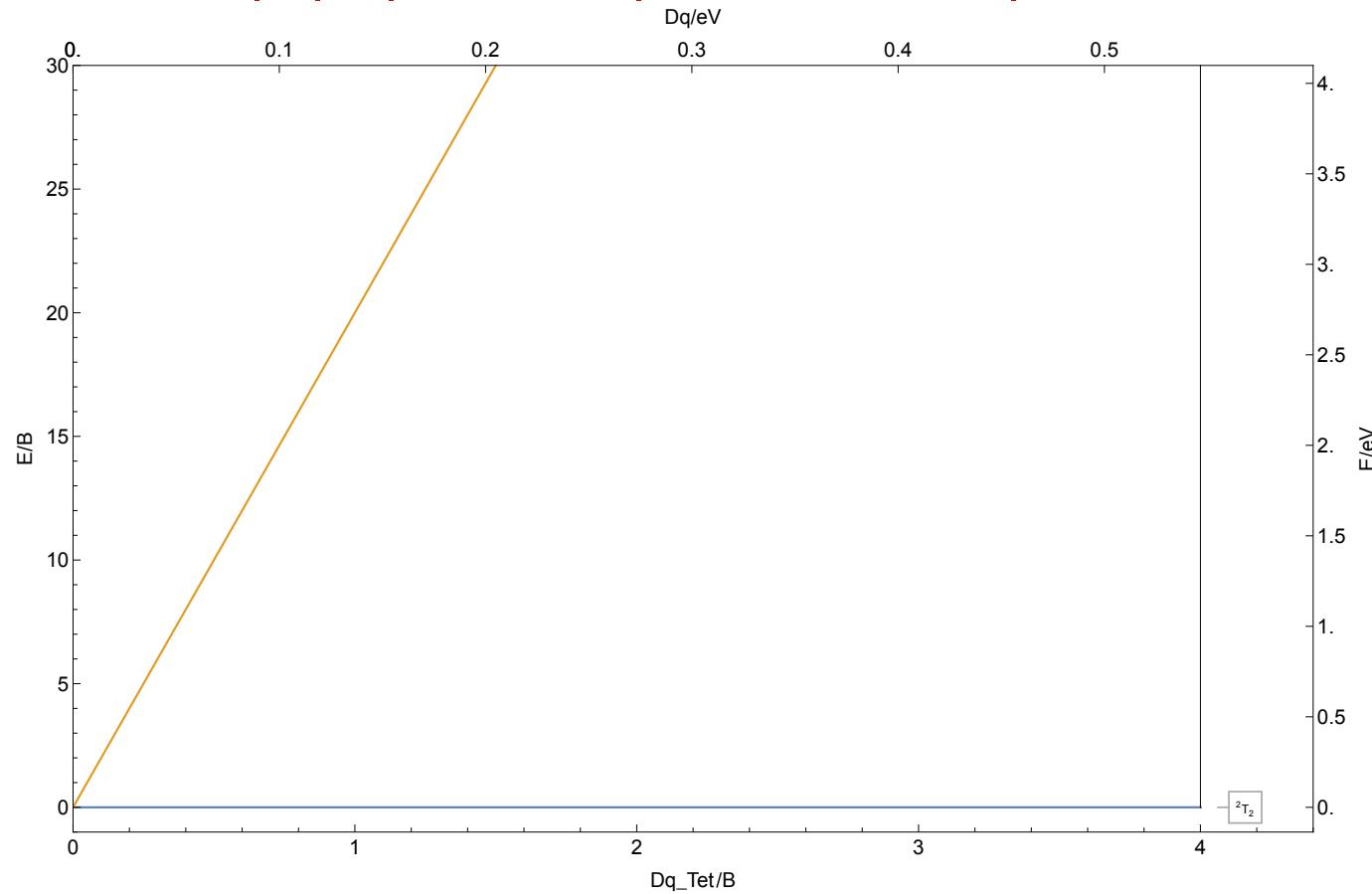
8.2.27 Ni<sup>7+</sup>

|2,4|d<sup>3</sup>| C/B ≈ 3.8 | B ≈ 1446 cm<sup>-1</sup> | Ni<sup>7+</sup>



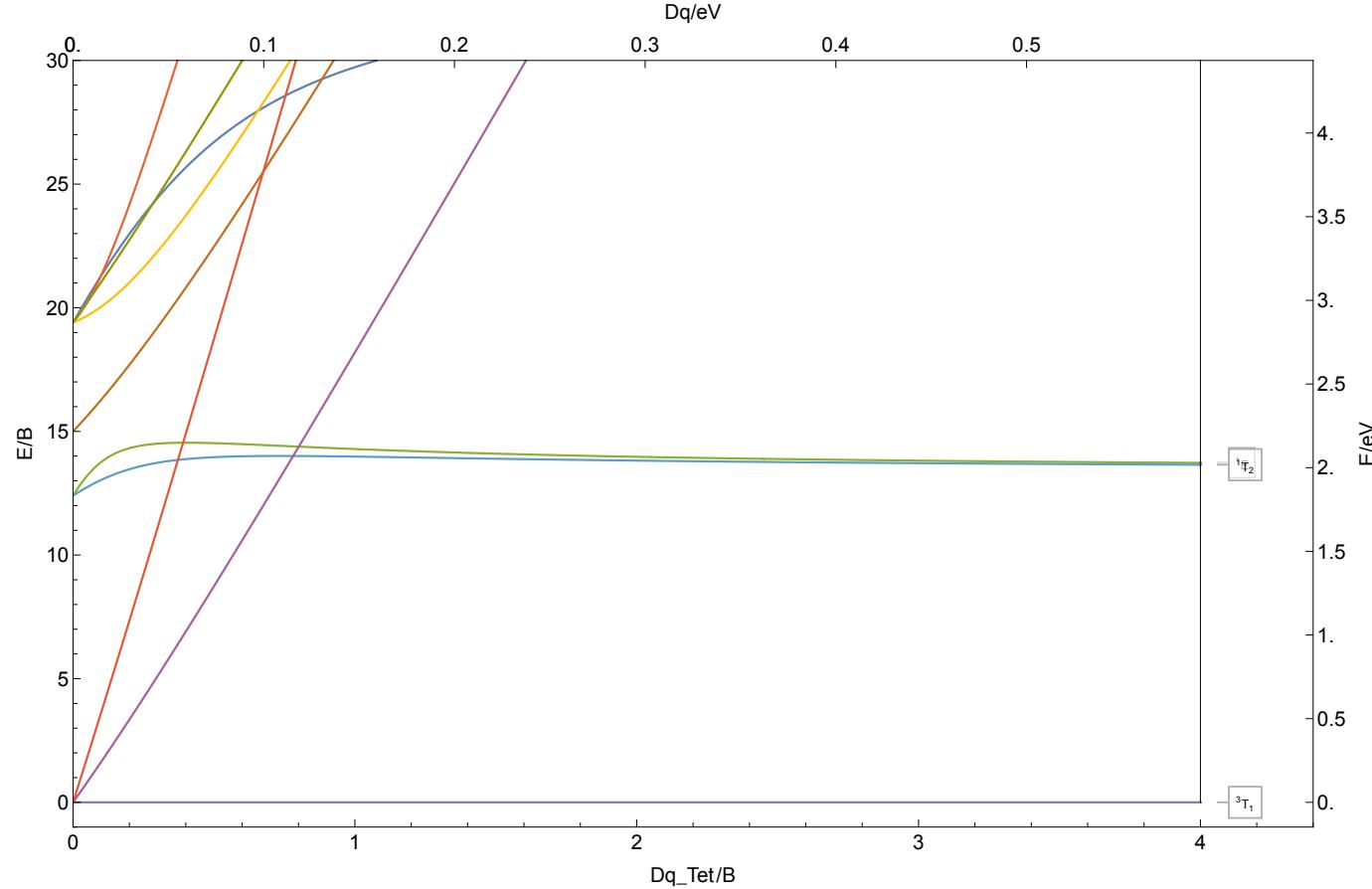
8.2.28 Cu<sup>2+</sup>

|2|d<sup>9</sup>| C/B ≈ 3.7 | B ≈ 1102 cm<sup>-1</sup> | Cu<sup>2+</sup>



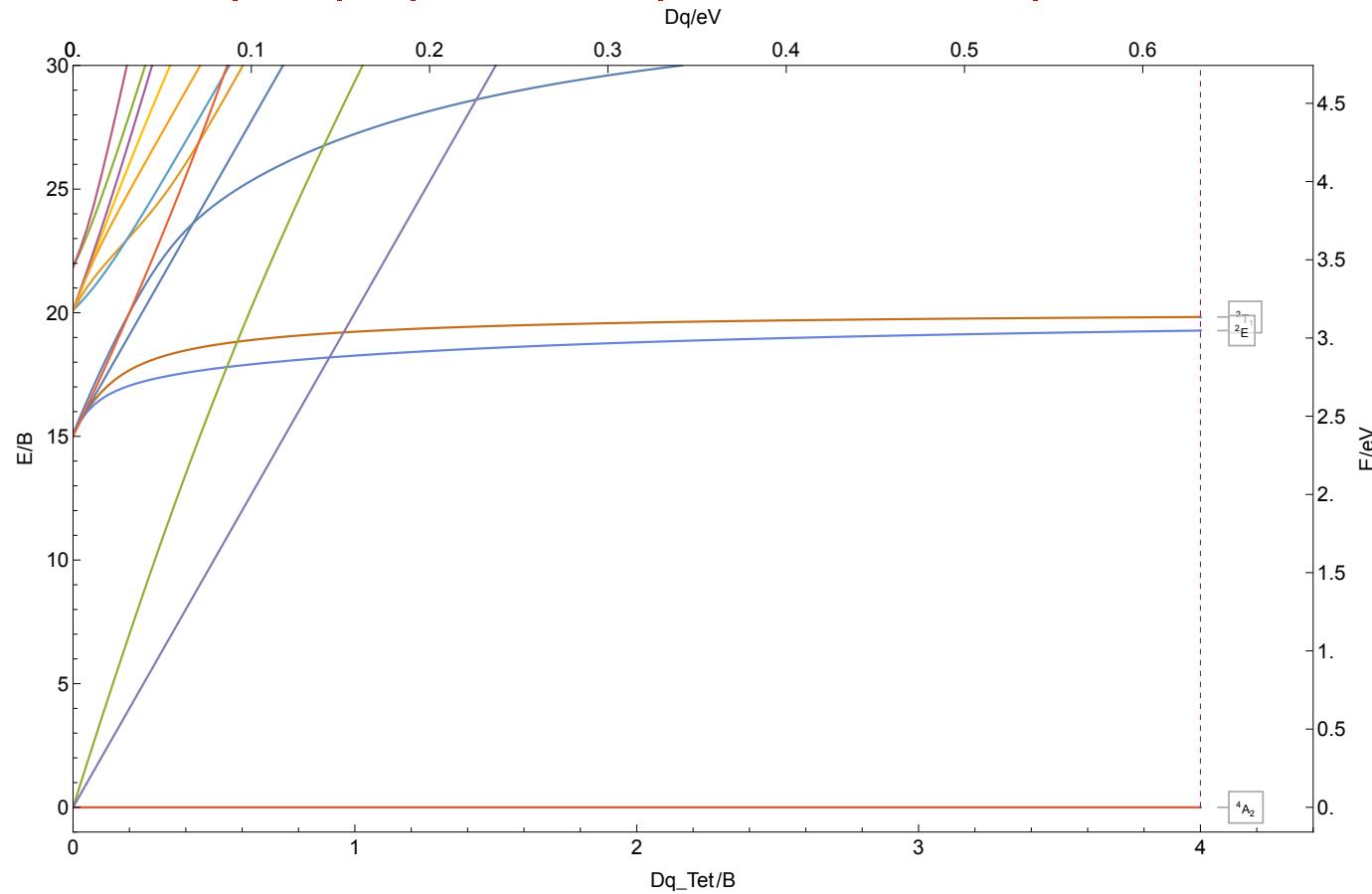
8.2.29 Cu<sup>3+</sup>

| 1,3 | d<sup>8</sup> | C/B ≈ 3.7 | B ≈ 1192 cm<sup>-1</sup> | Cu<sup>3+</sup>



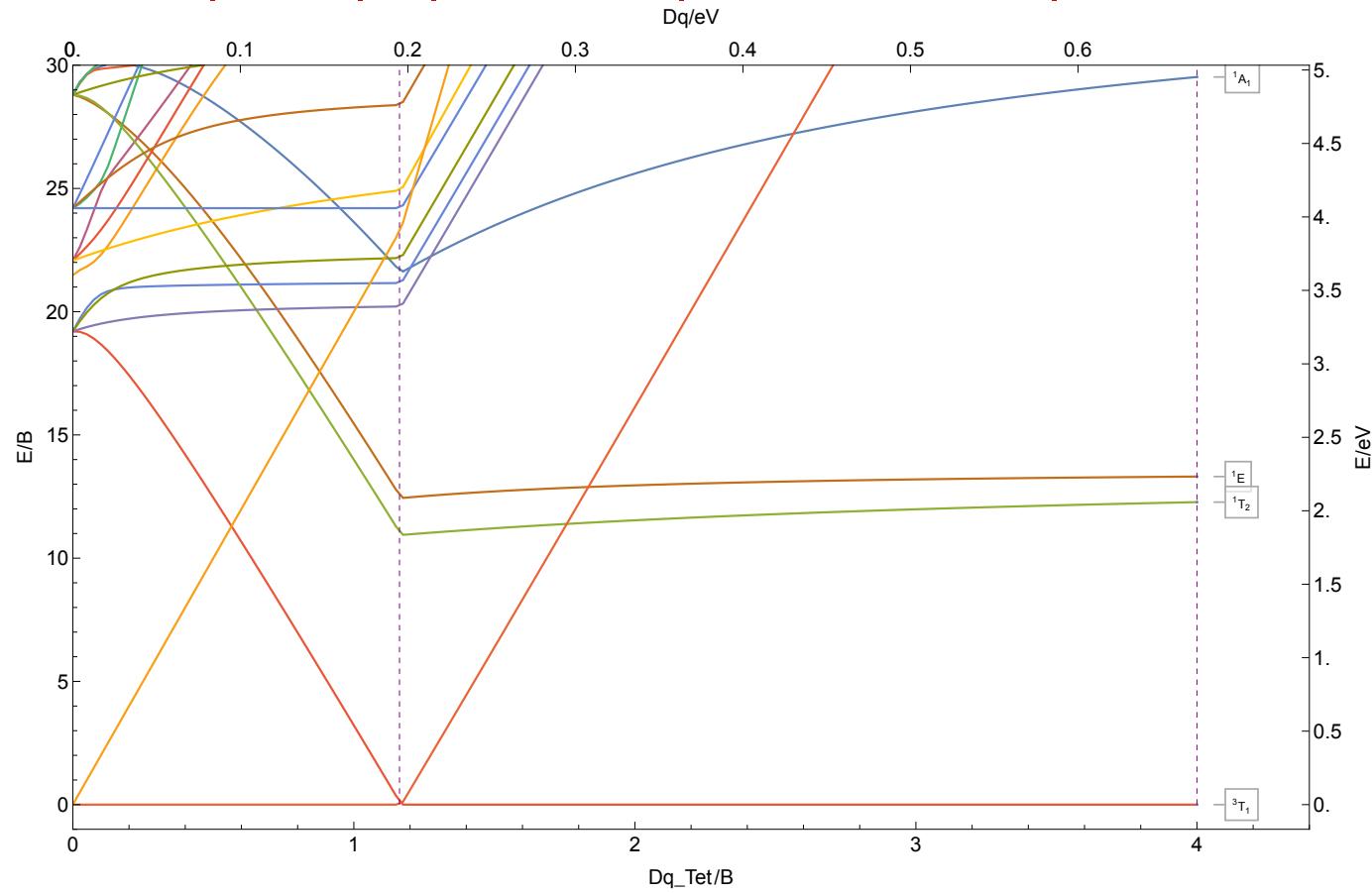
8.2.30 Cu<sup>4+</sup>

|2,4|d<sup>7</sup>|C/B ≈ 3.7|B ≈ 1275 cm<sup>-1</sup>|Cu<sup>4+</sup>



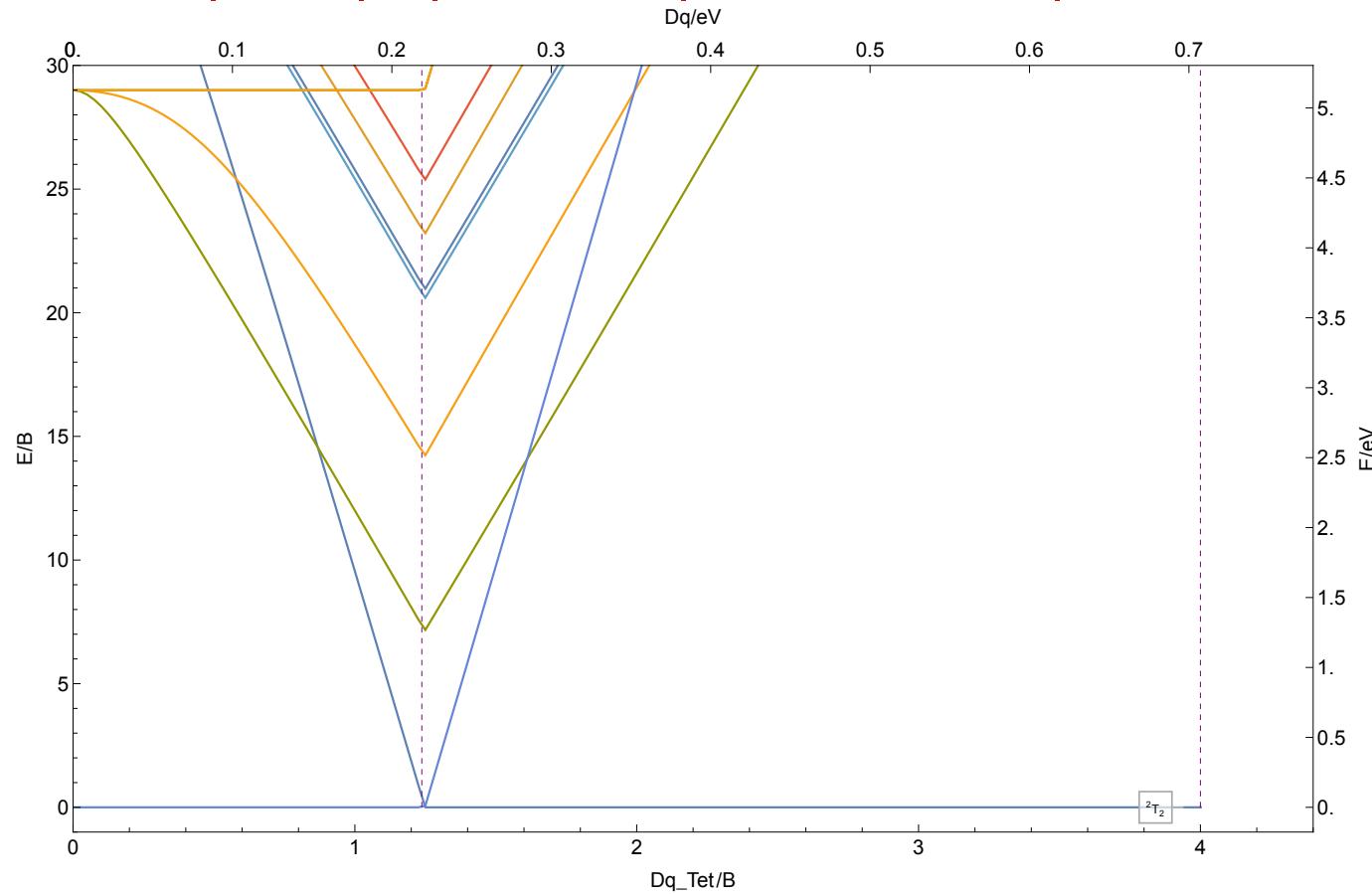
### 8.2.31 Cu<sup>5+</sup>

$|1,3,5|d^6|C/B \approx 3.8|B \approx 1353\text{ cm}^{-1}|Cu^{5+}$



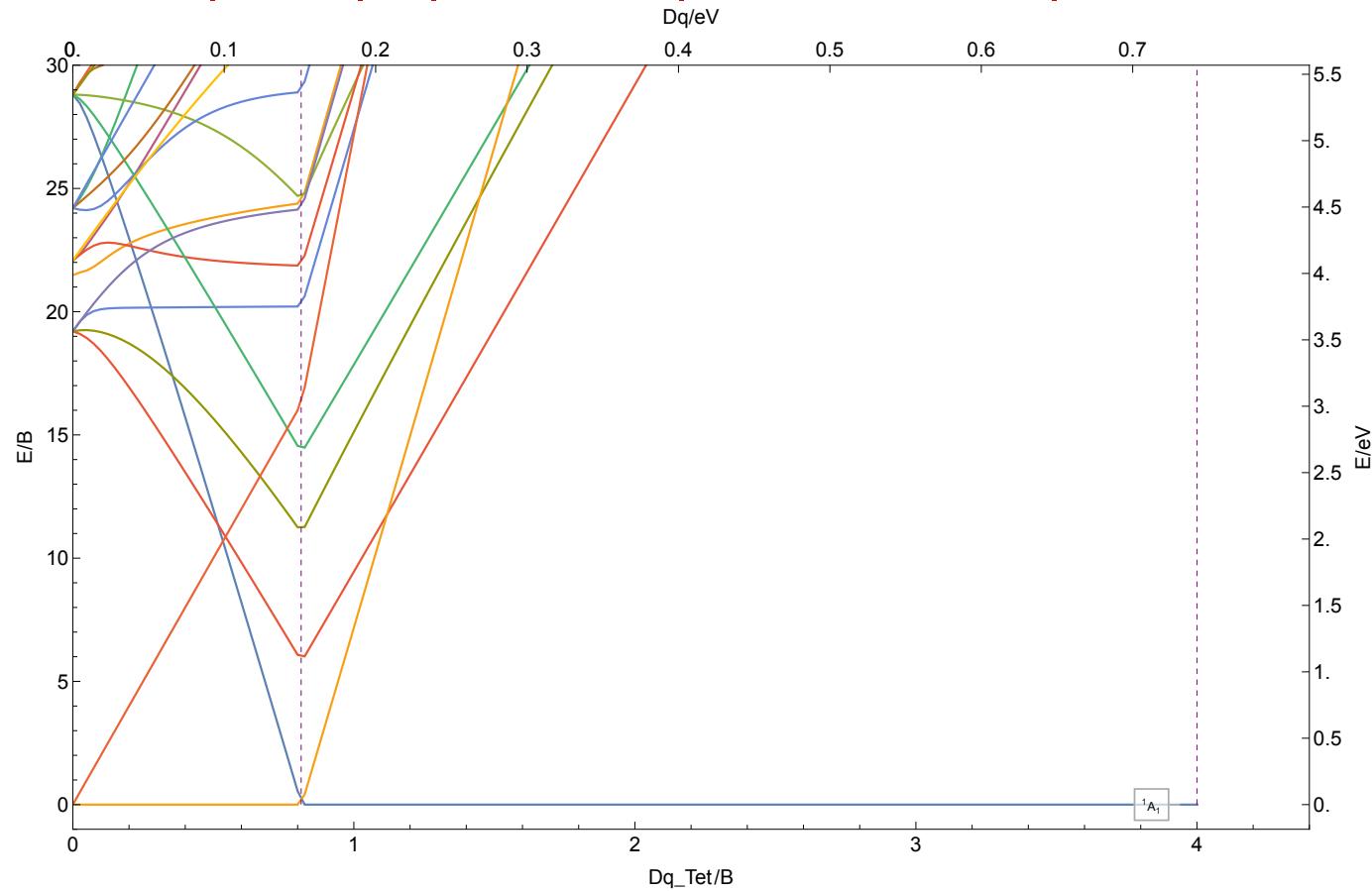
8.2.32 Cu<sup>6+</sup>

|2,4,6| d<sup>5</sup>| C/B ≈ 3.8 | B ≈ 1426 cm<sup>-1</sup> | Cu<sup>6+</sup>



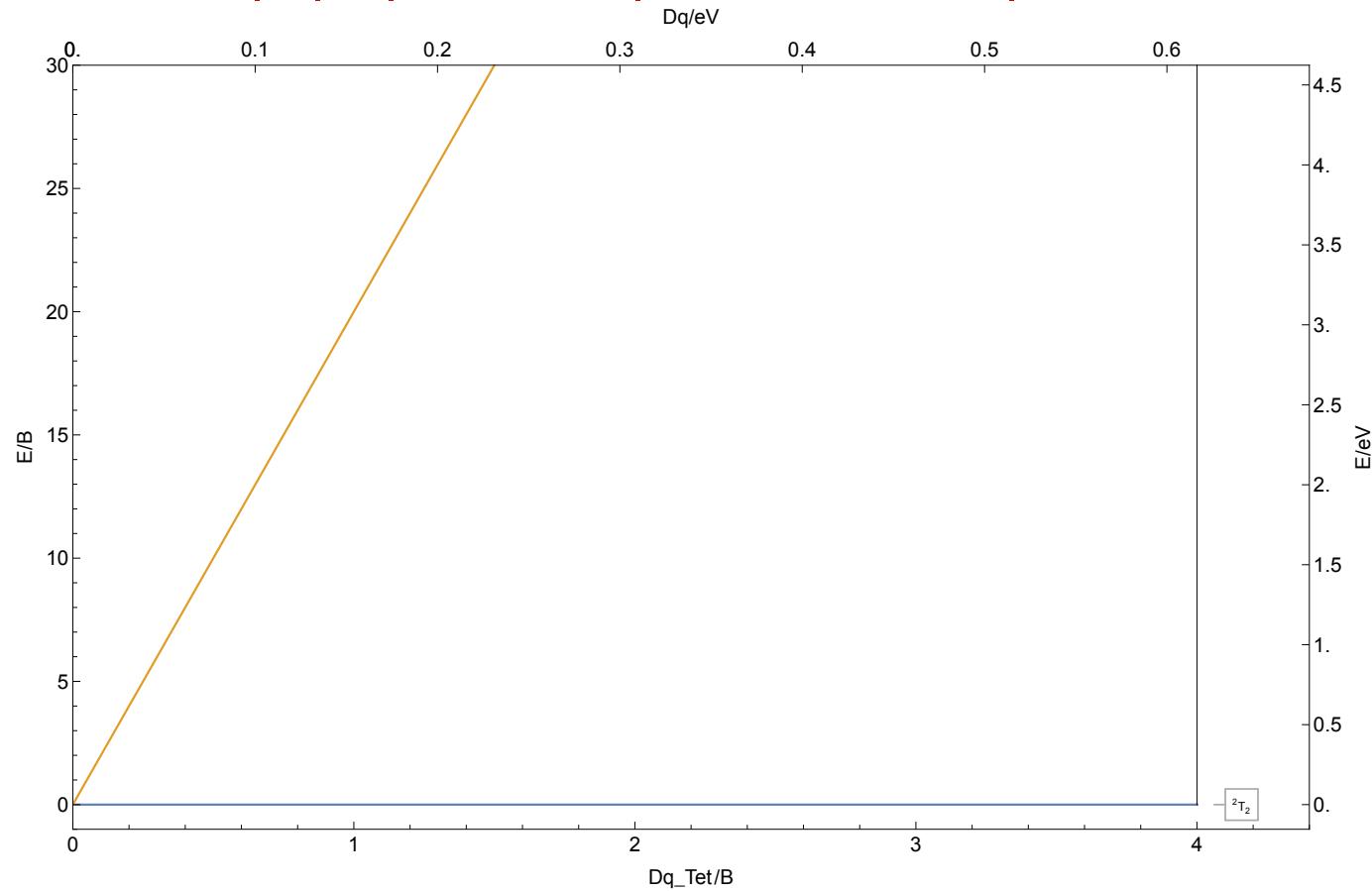
8.2.33 Cu<sup>7+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 3.8 | B ≈ 1497 cm<sup>-1</sup> | Cu<sup>7+</sup>



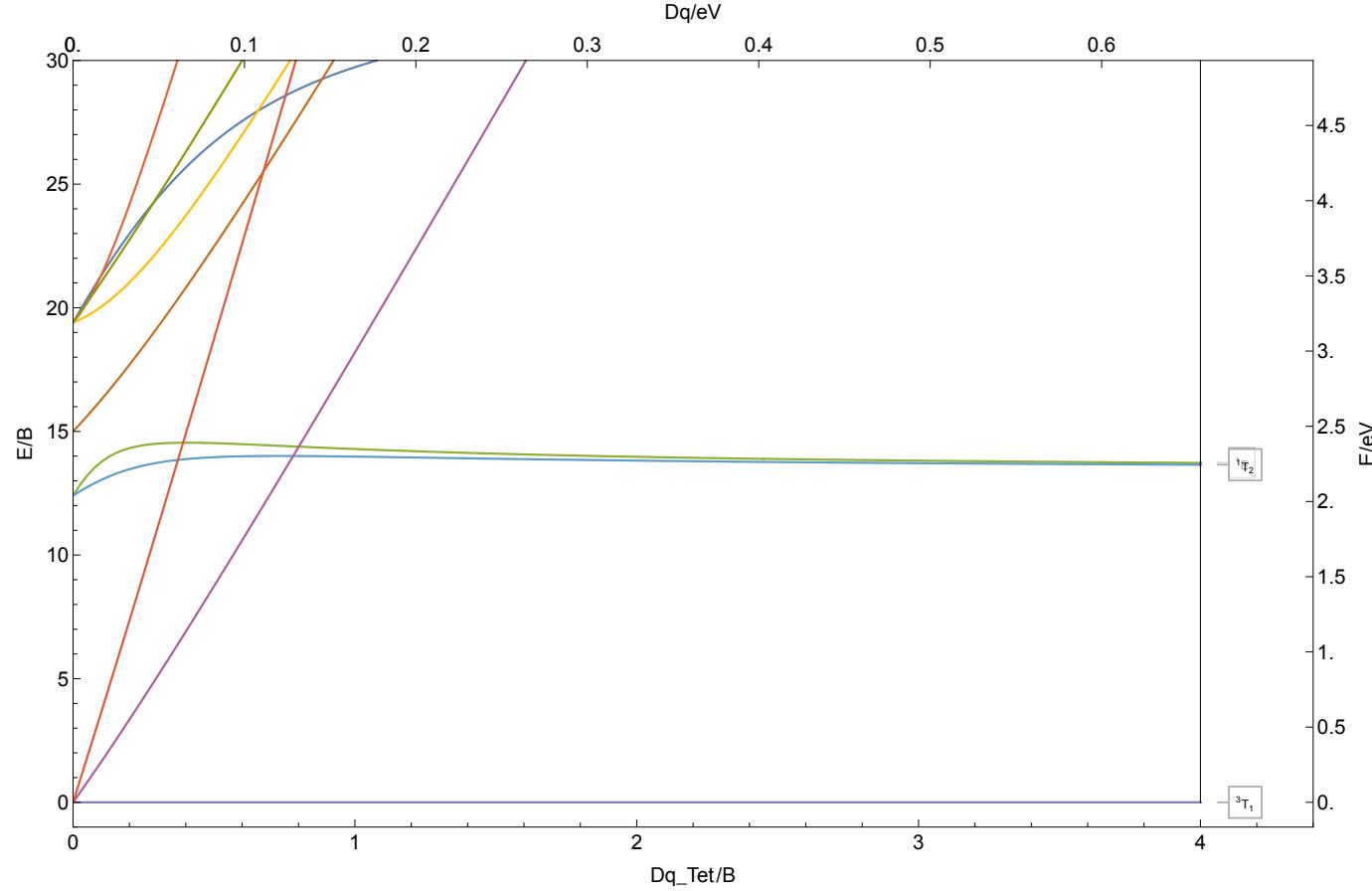
8.2.34 Zn<sup>3+</sup>

|2|d<sup>9</sup>| C/B ≈ 3.7 | B ≈ 1243 cm<sup>-1</sup> | Zn<sup>3+</sup>



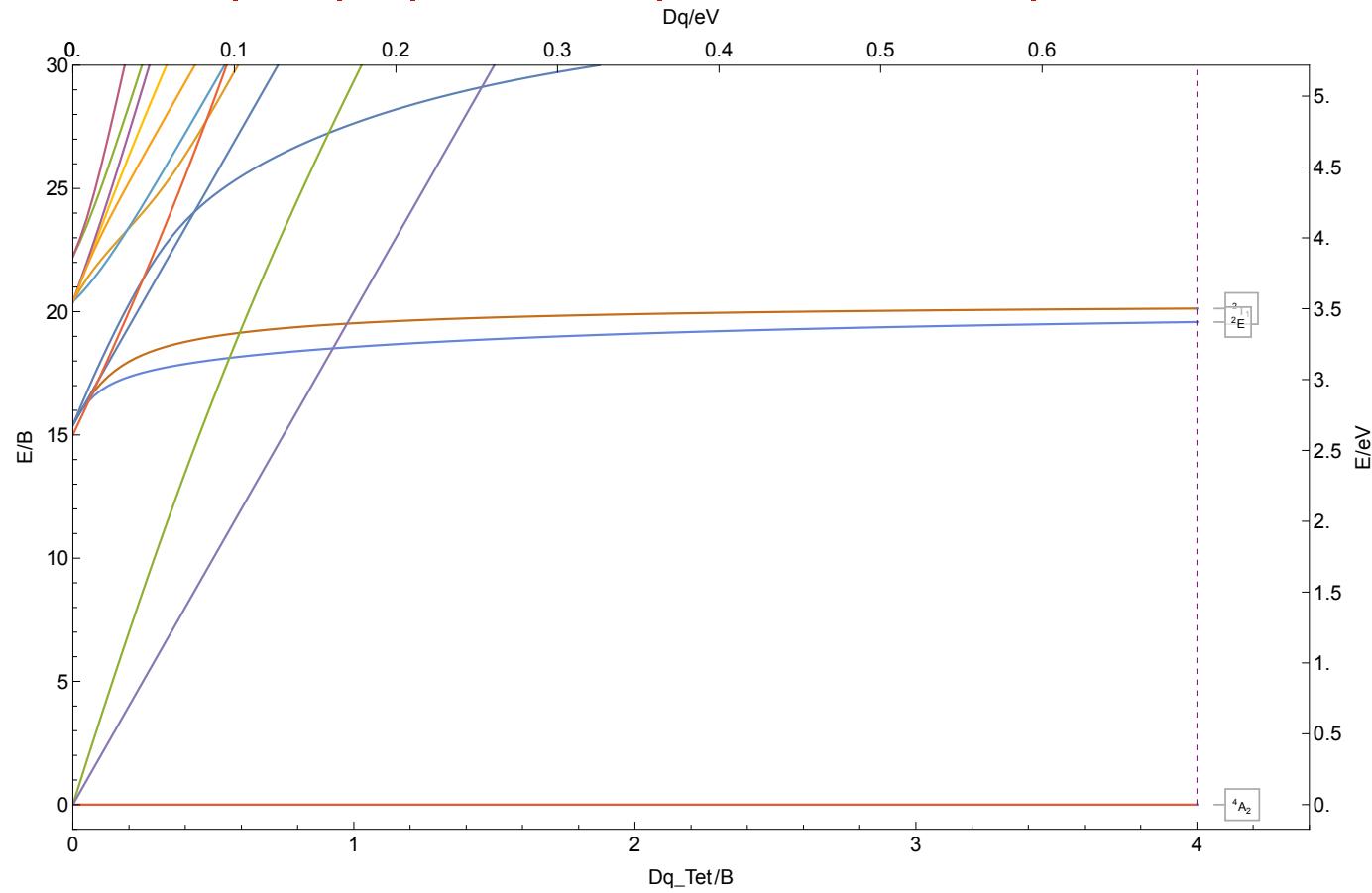
8.2.35 Zn<sup>4+</sup>

| 1,3 | d<sup>8</sup> | C/B ≈ 3.7 | B ≈ 1326 cm<sup>-1</sup> | Zn<sup>4+</sup>



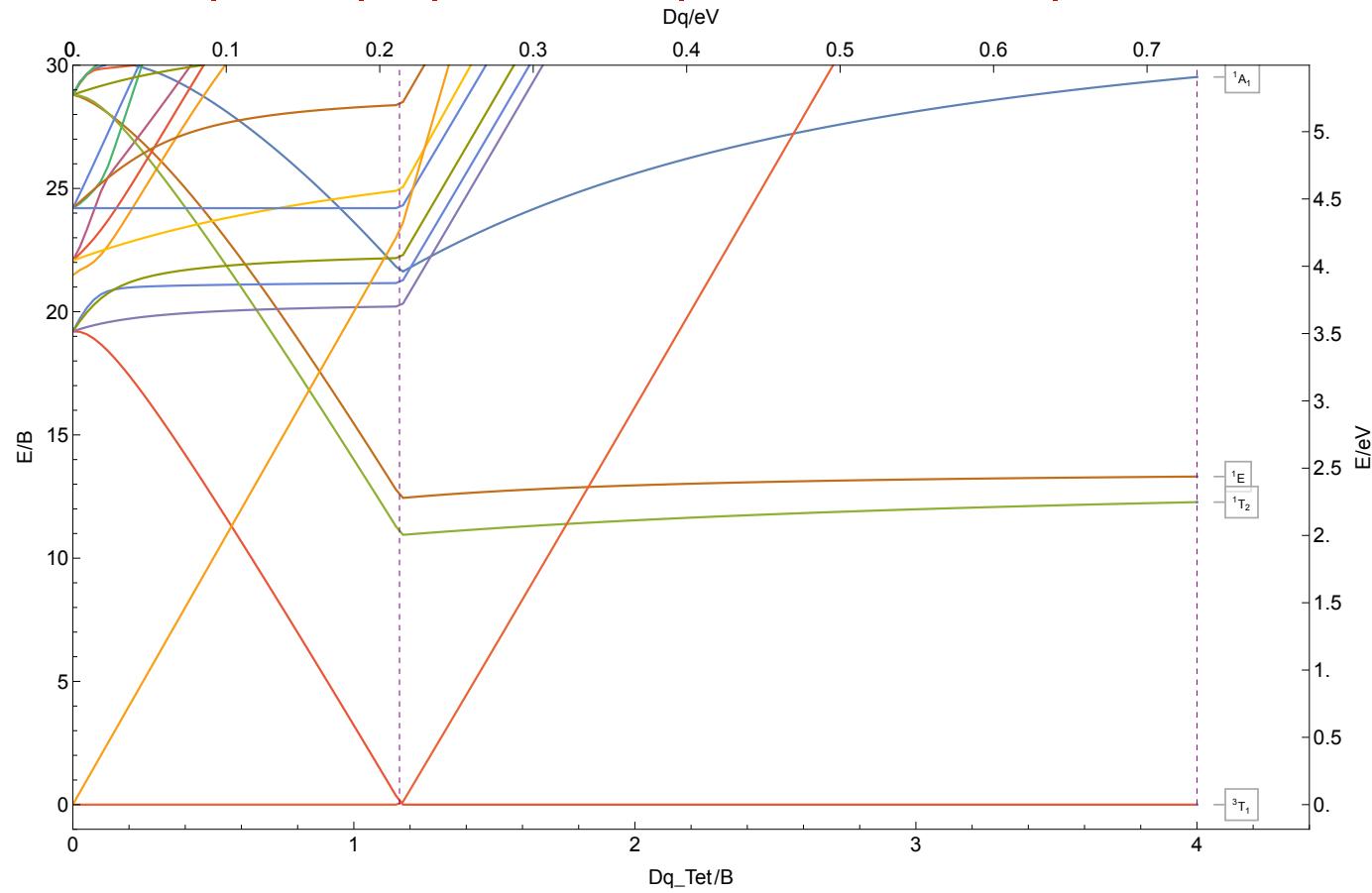
8.2.36 Zn<sup>5+</sup>

|2,4|d<sup>7</sup>|C/B ≈ 3.8|B ≈ 1403 cm<sup>-1</sup>|Zn<sup>5+</sup>



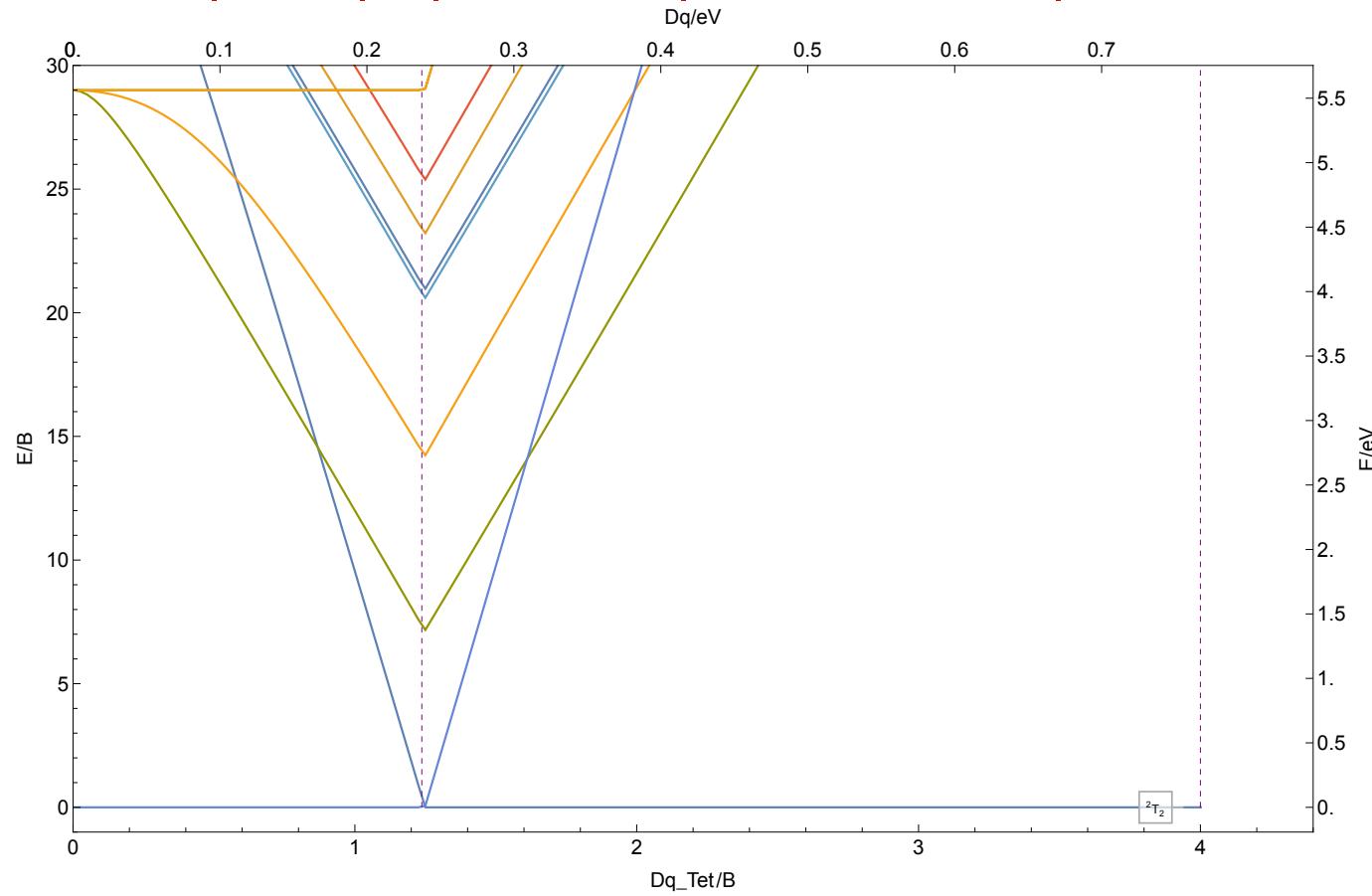
8.2.37  $\text{Zn}^{6+}$

$|1,3,5|d^6|C/B \approx 3.8|B \approx 1477\text{ cm}^{-1}|Zn^{6+}$



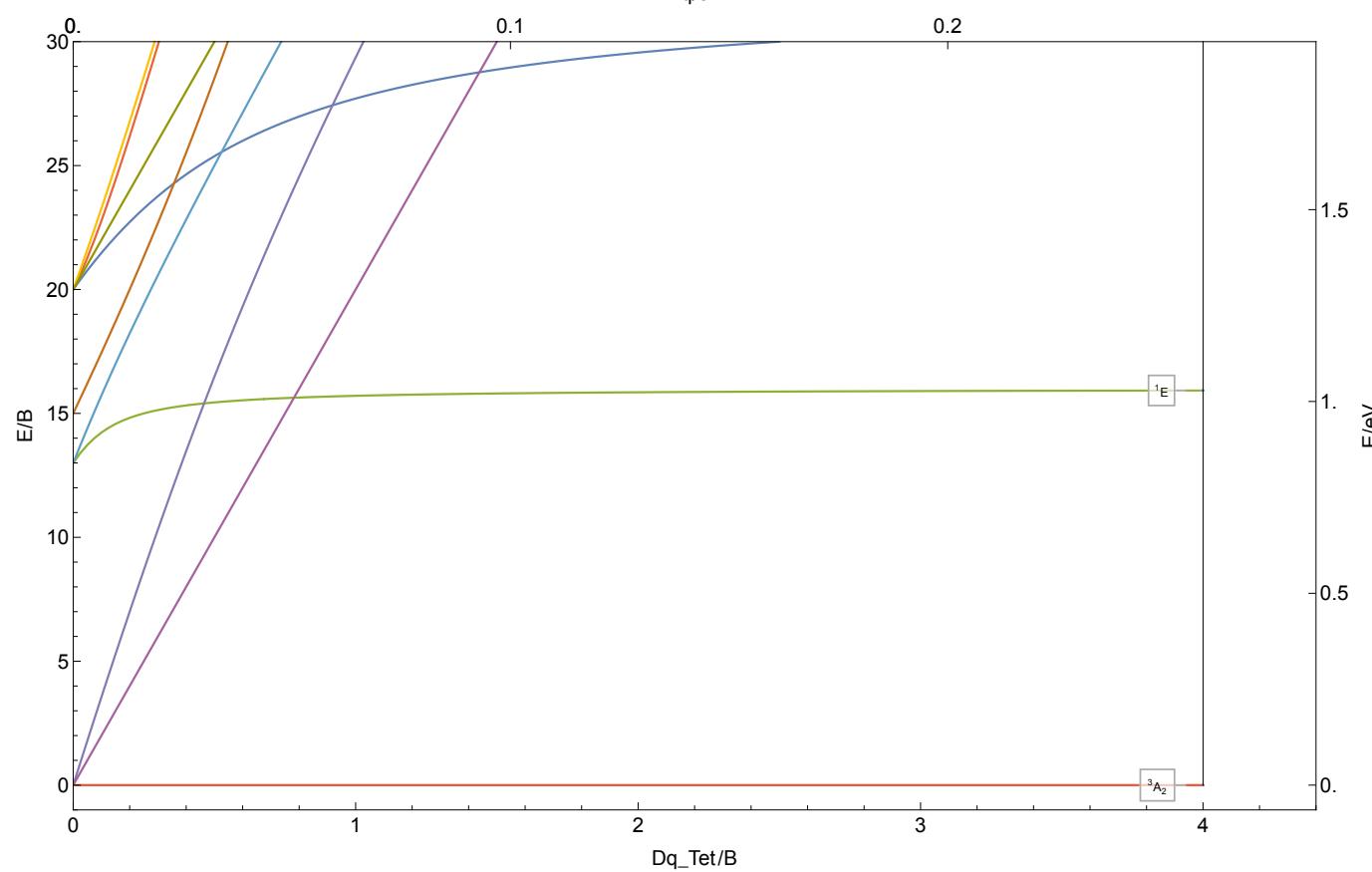
8.2.38 Zn<sup>7+</sup>

|2,4,6| d<sup>5</sup>| C/B ≈ 3.8| B ≈ 1547 cm<sup>-1</sup> | Zn<sup>7+</sup>



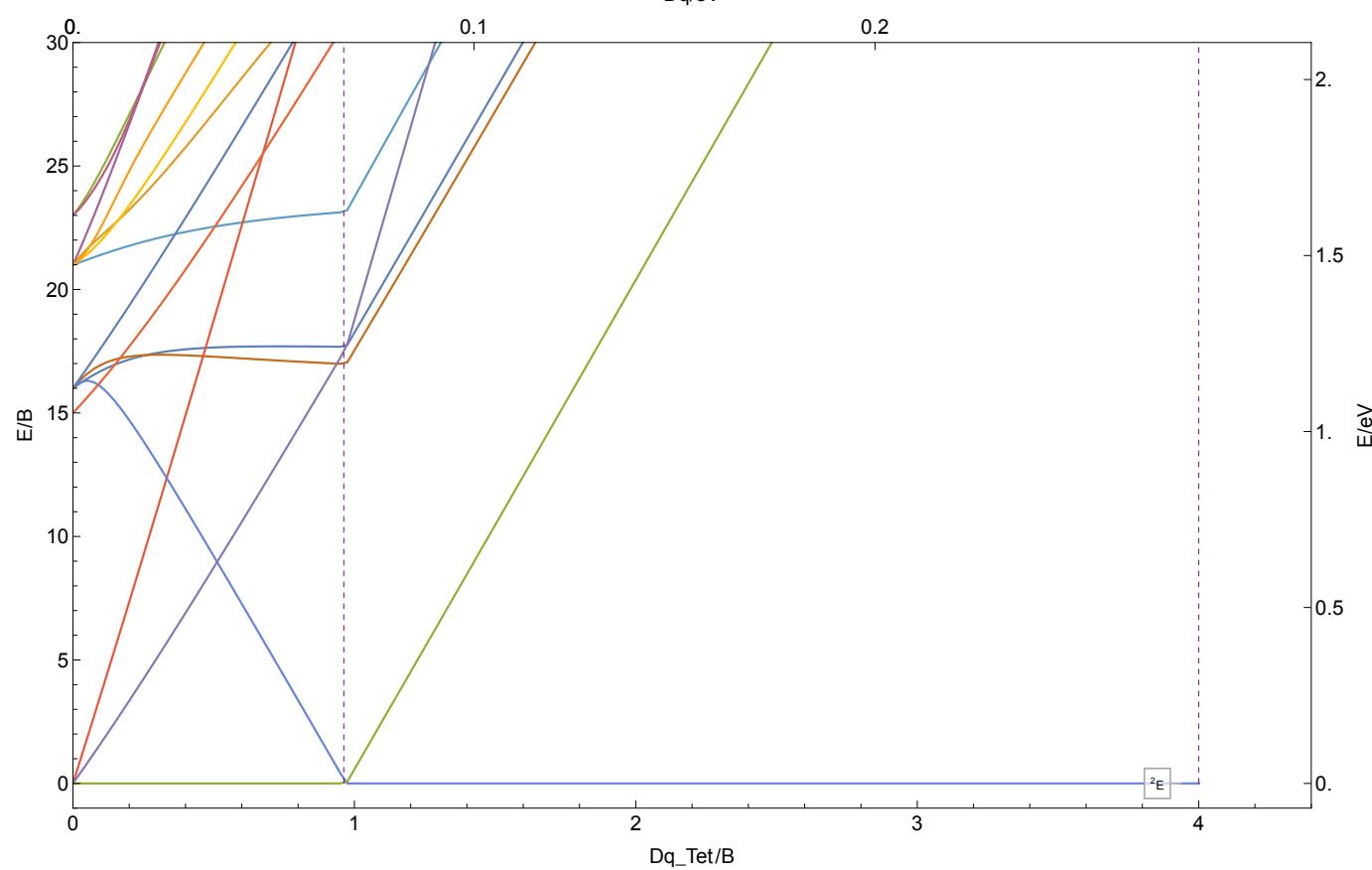
8.2.39 Zr<sup>2+</sup>

| 1,3 | d<sup>2</sup> | C/B ≈ 4. | B ≈ 521 cm<sup>-1</sup> | Zr<sup>2+</sup>



8.2.40  $\text{Nb}^{2+}$

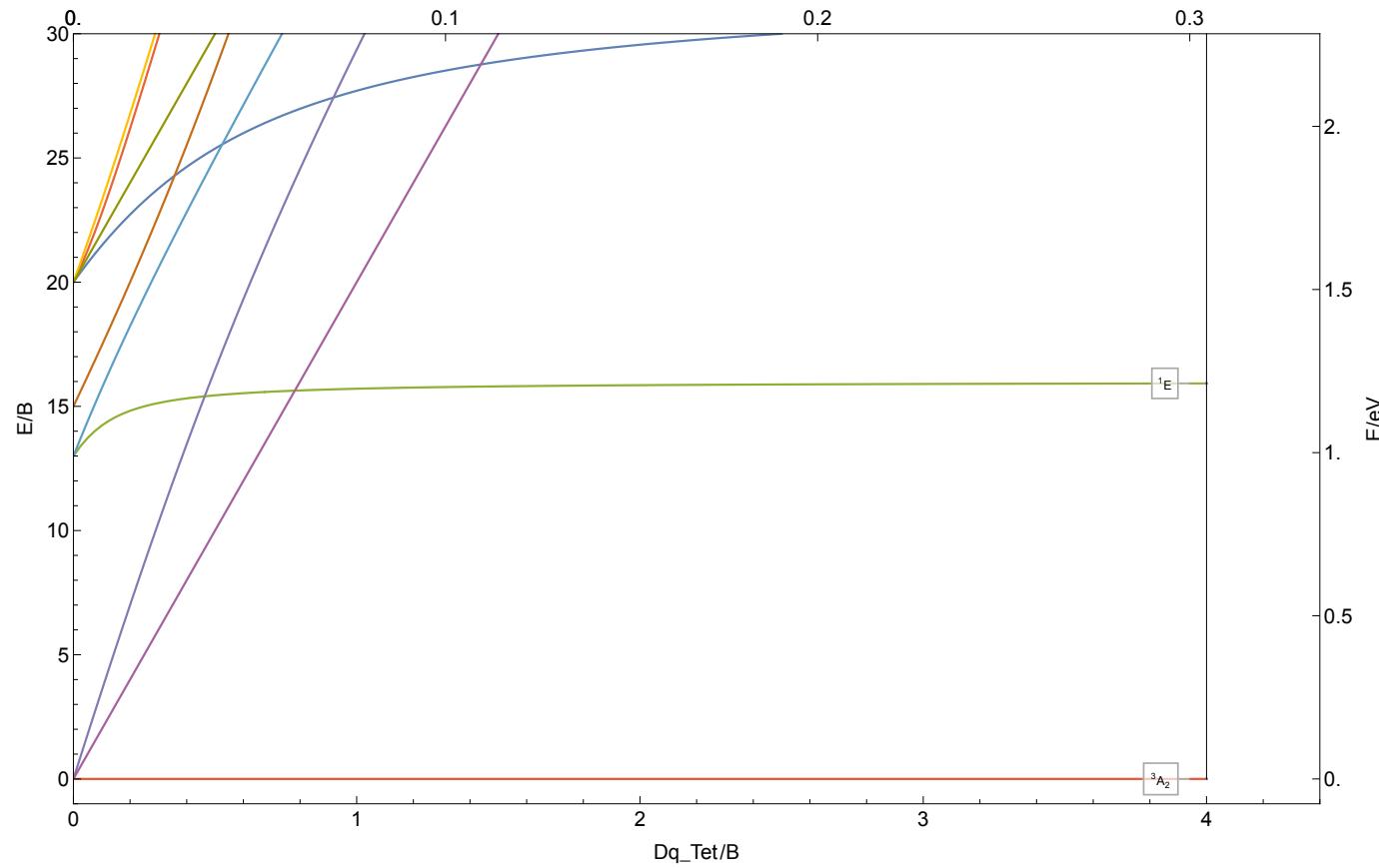
$|2,4|d^3|C/B \approx 4.|B \approx 566 \text{ cm}^{-1}|Nb^{2+}$



8.2.41 Nb<sup>3+</sup>

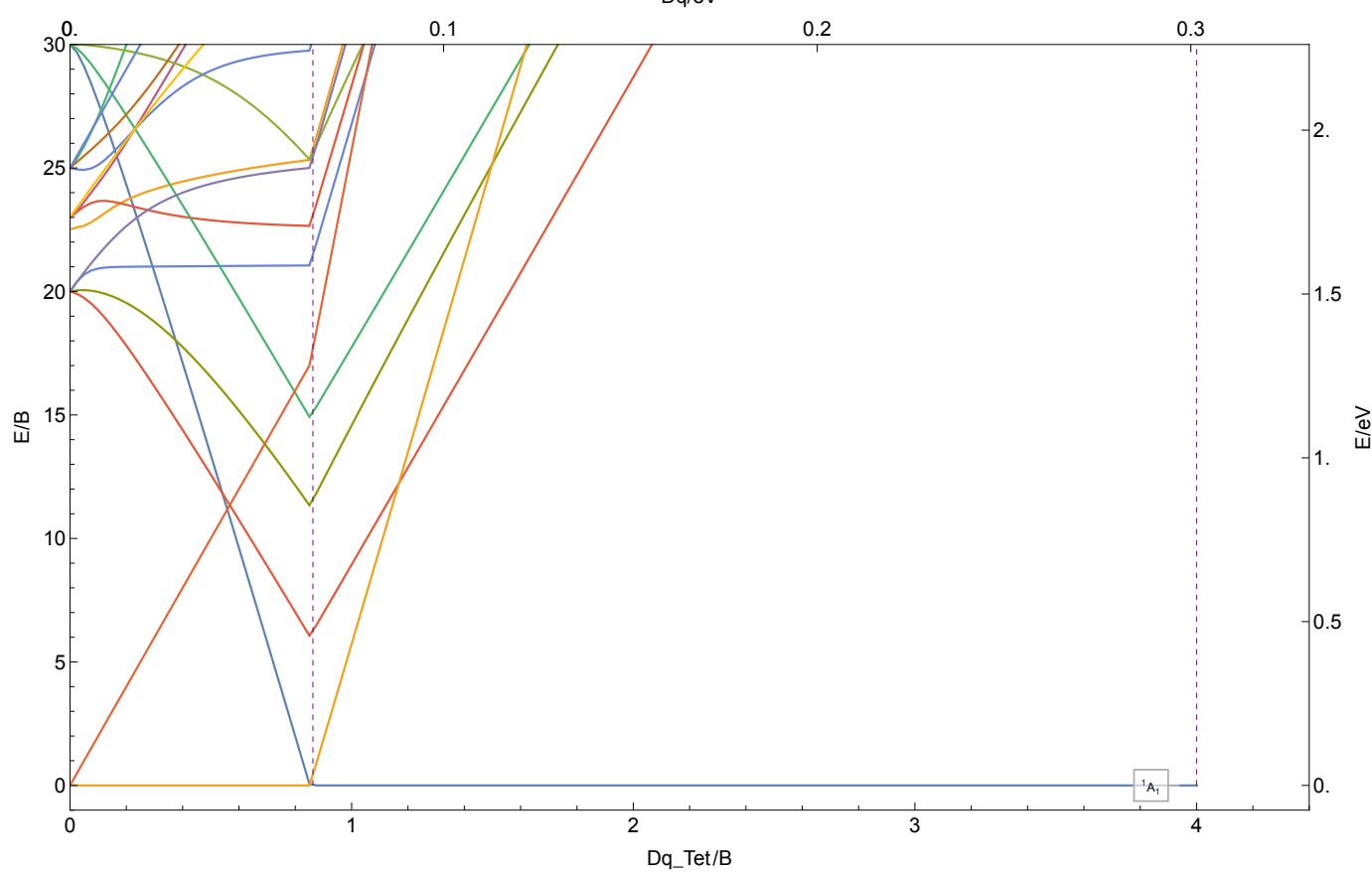
| 1,3 | d<sup>2</sup> | C/B ≈ 4. | B ≈ 614 cm<sup>-1</sup> | Nb<sup>3+</sup>

Dq/eV



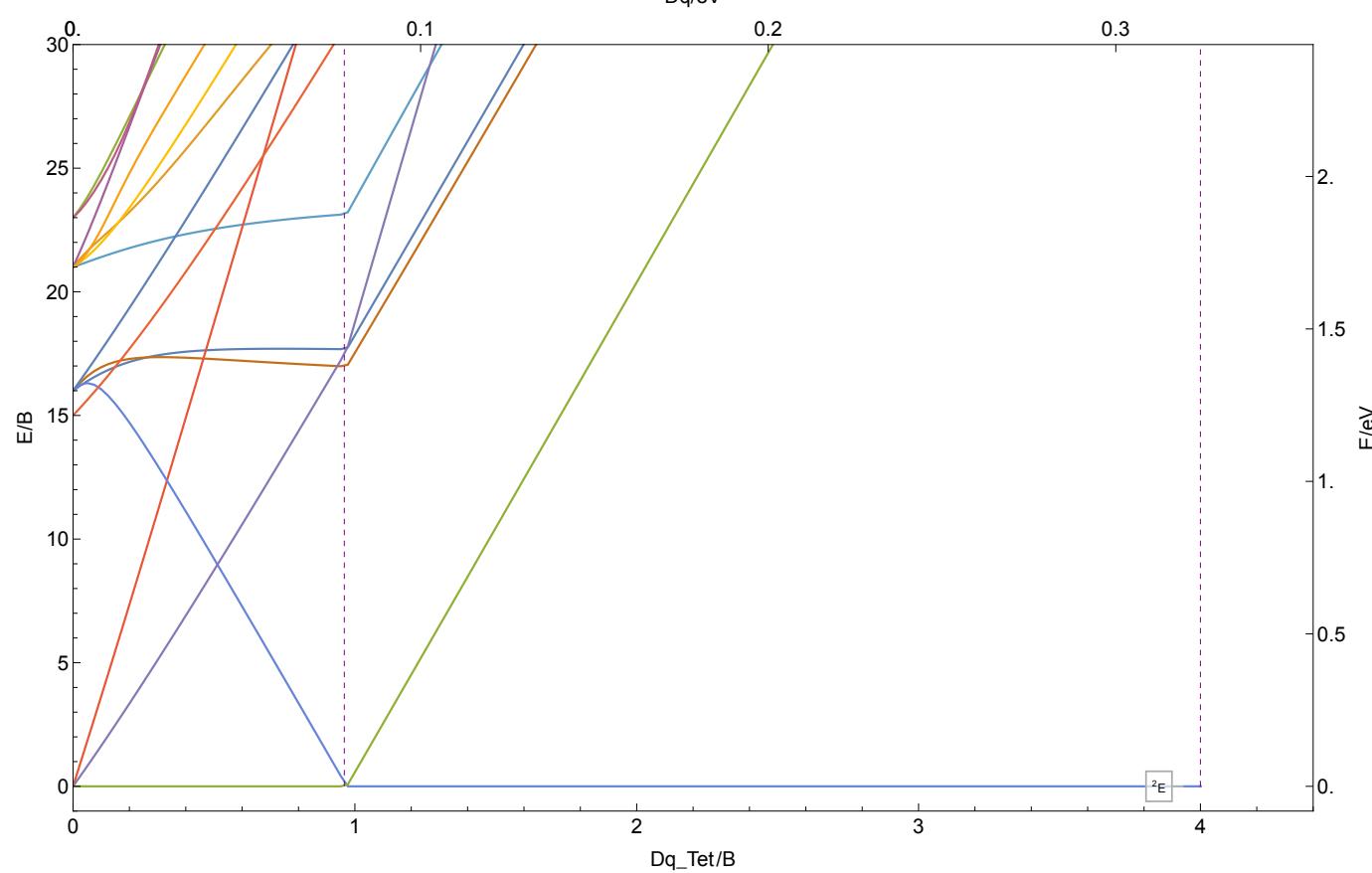
8.2.42 Mo<sup>2+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 4. | B ≈ 608 cm<sup>-1</sup> | Mo<sup>2+</sup>



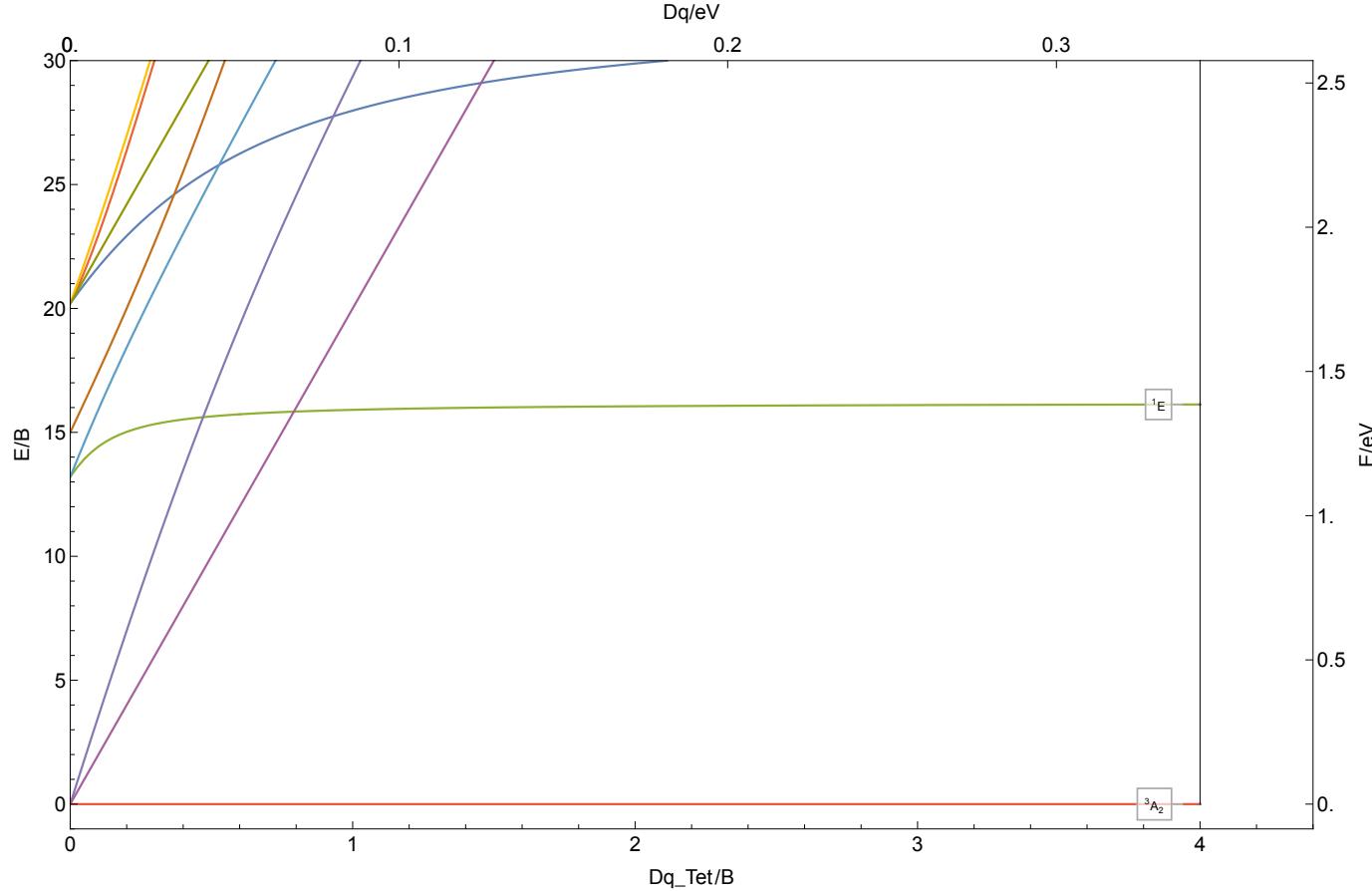
8.2.43 Mo<sup>3+</sup>

|2,4|d<sup>3</sup>|C/B ≈ 4.|B ≈ 654 cm<sup>-1</sup>|Mo<sup>3+</sup>



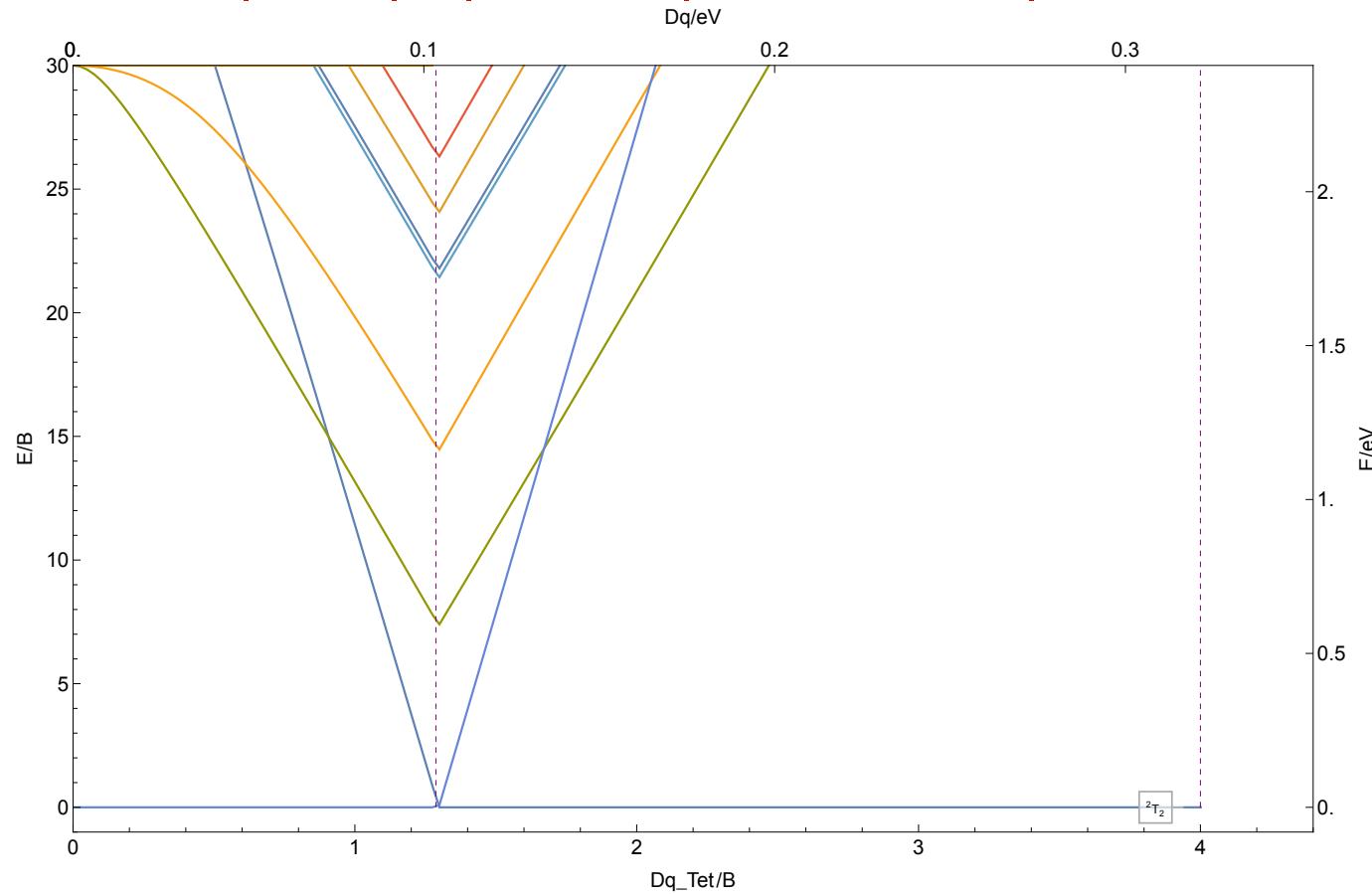
8.2.44 Mo<sup>4+</sup>

|1,3|d<sup>2</sup>| C/B ≈ 4.1| B ≈ 693 cm<sup>-1</sup>| Mo<sup>4+</sup>



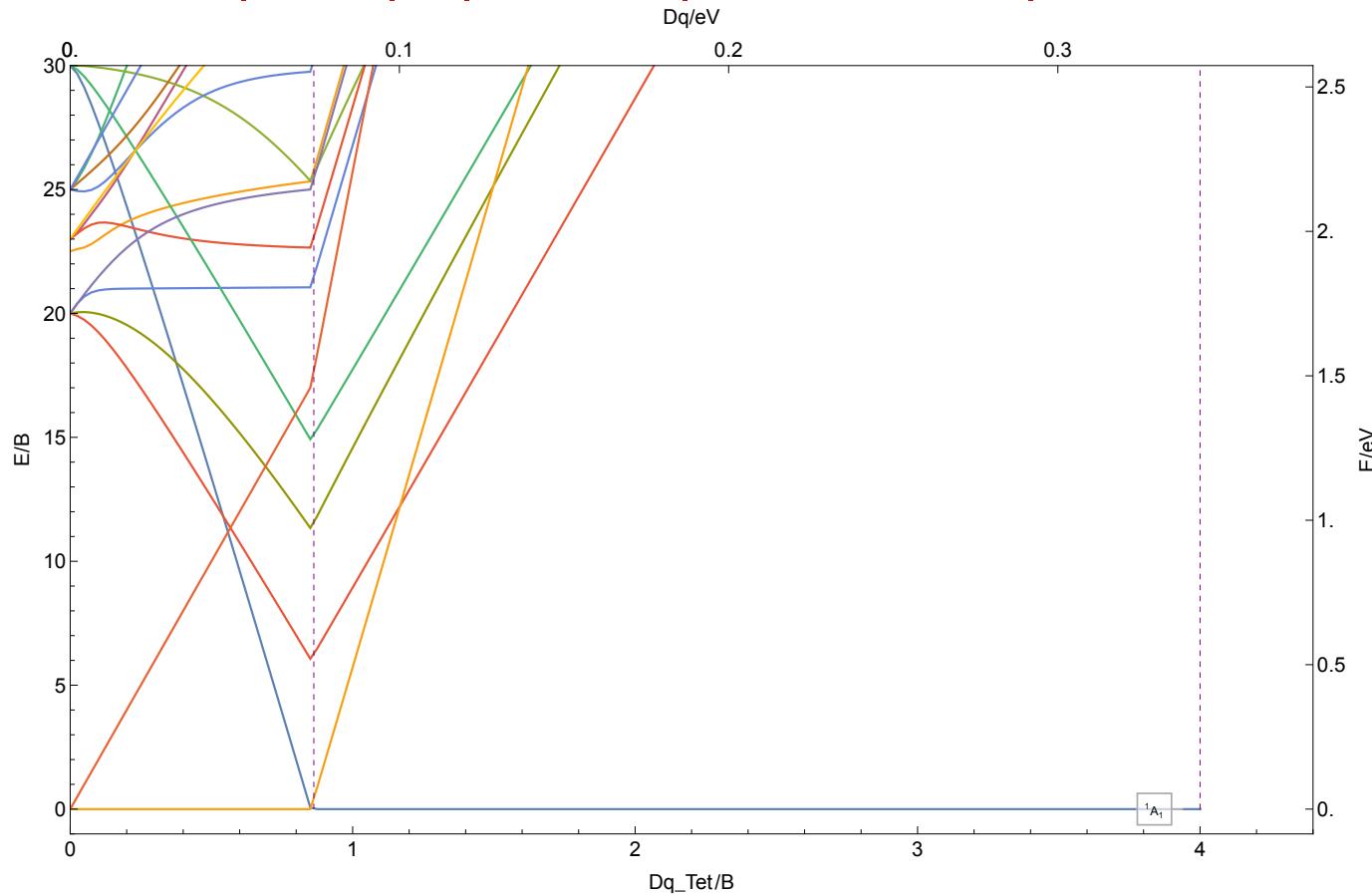
8.2.45 Tc<sup>2+</sup>

|2,4,6|d<sup>5</sup>|C/B ≈ 4.|B ≈ 648 cm<sup>-1</sup>|Tc<sup>2+</sup>



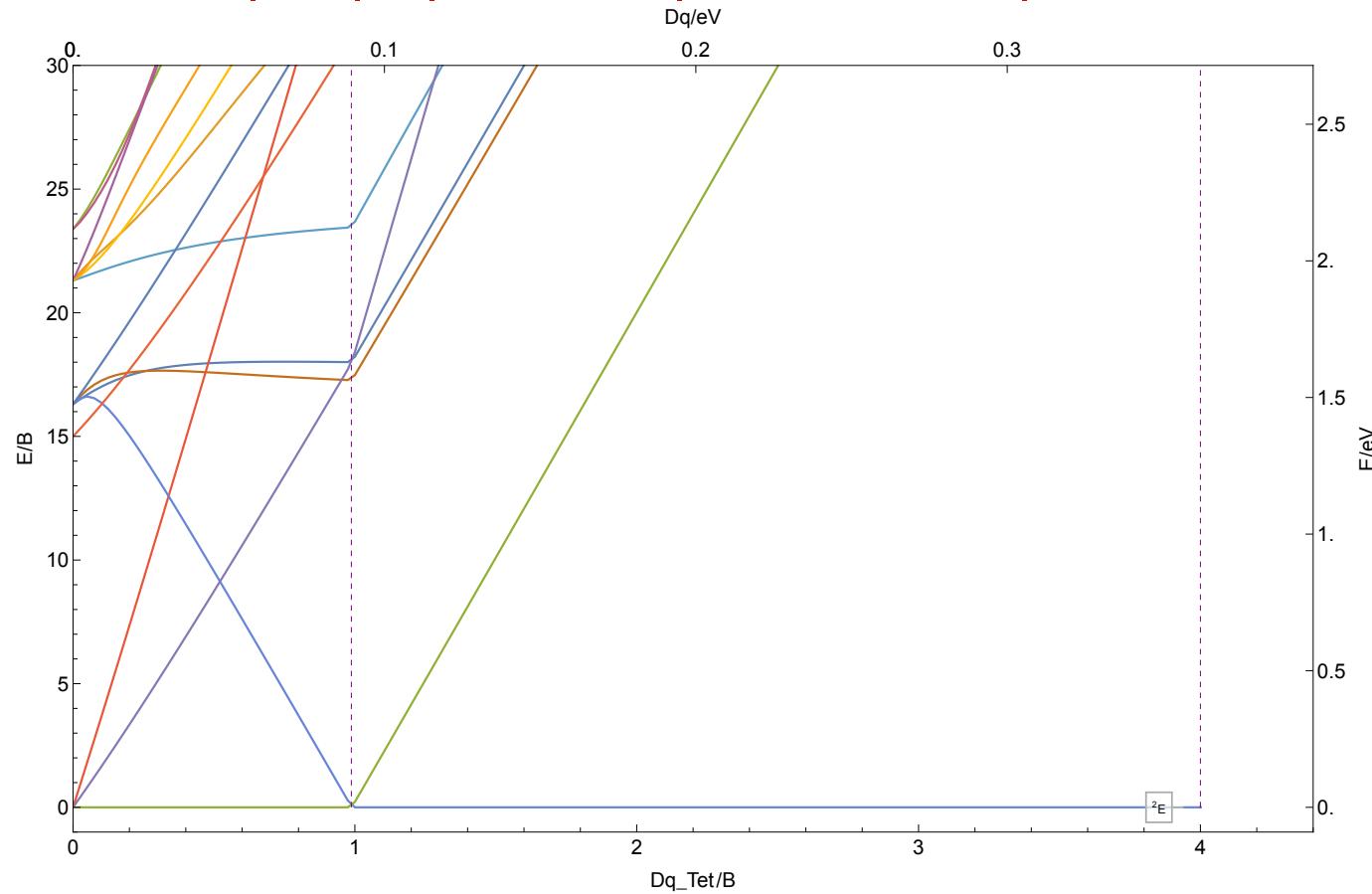
8.2.46 Tc<sup>3+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 4. | B ≈ 692 cm<sup>-1</sup> | Tc<sup>3+</sup>



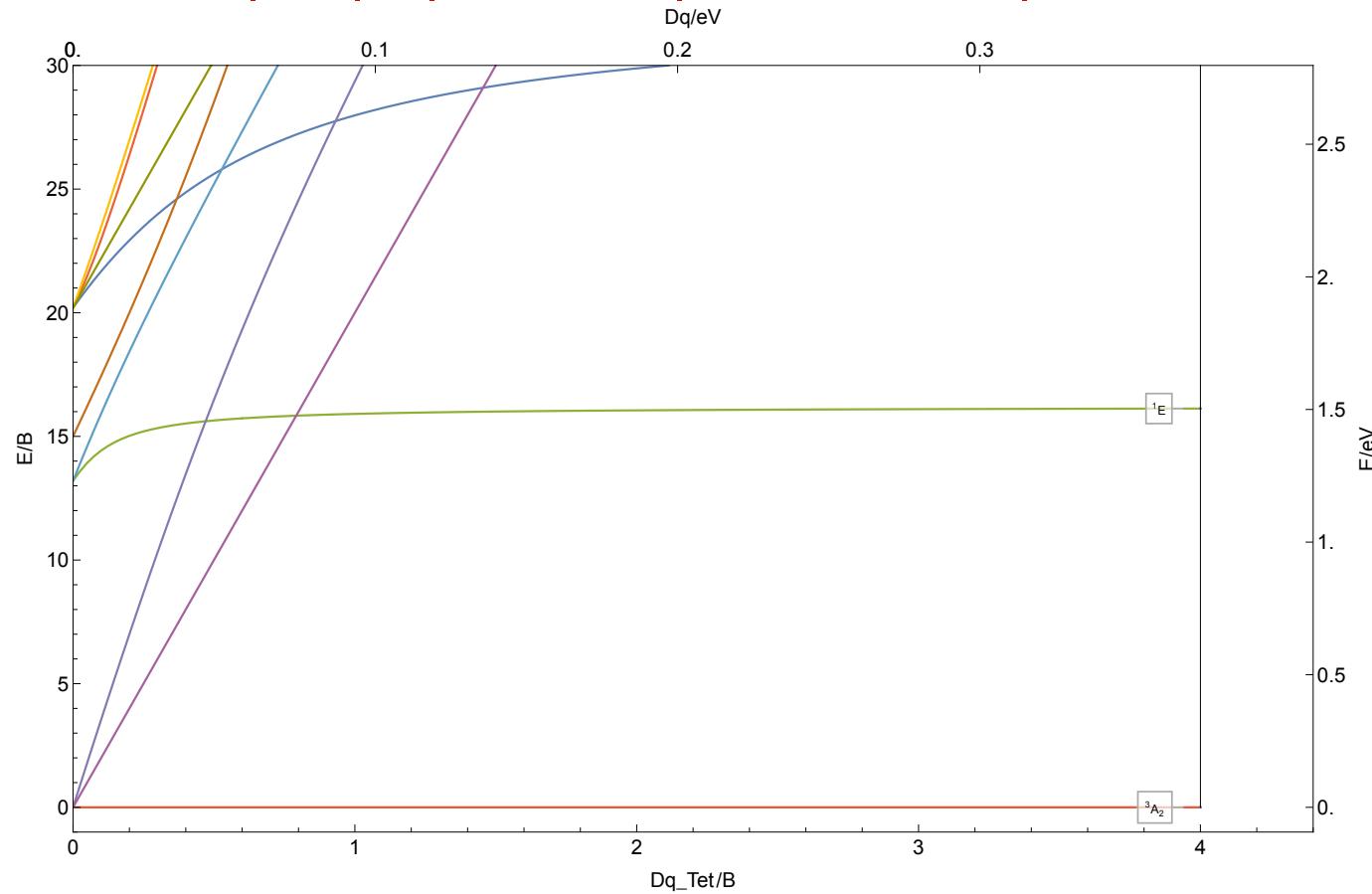
8.2.47 Tc<sup>4+</sup>

|2,4| d<sup>3</sup> C/B ≈ 4.1 | B ≈ 730 cm<sup>-1</sup> | Tc<sup>4+</sup>



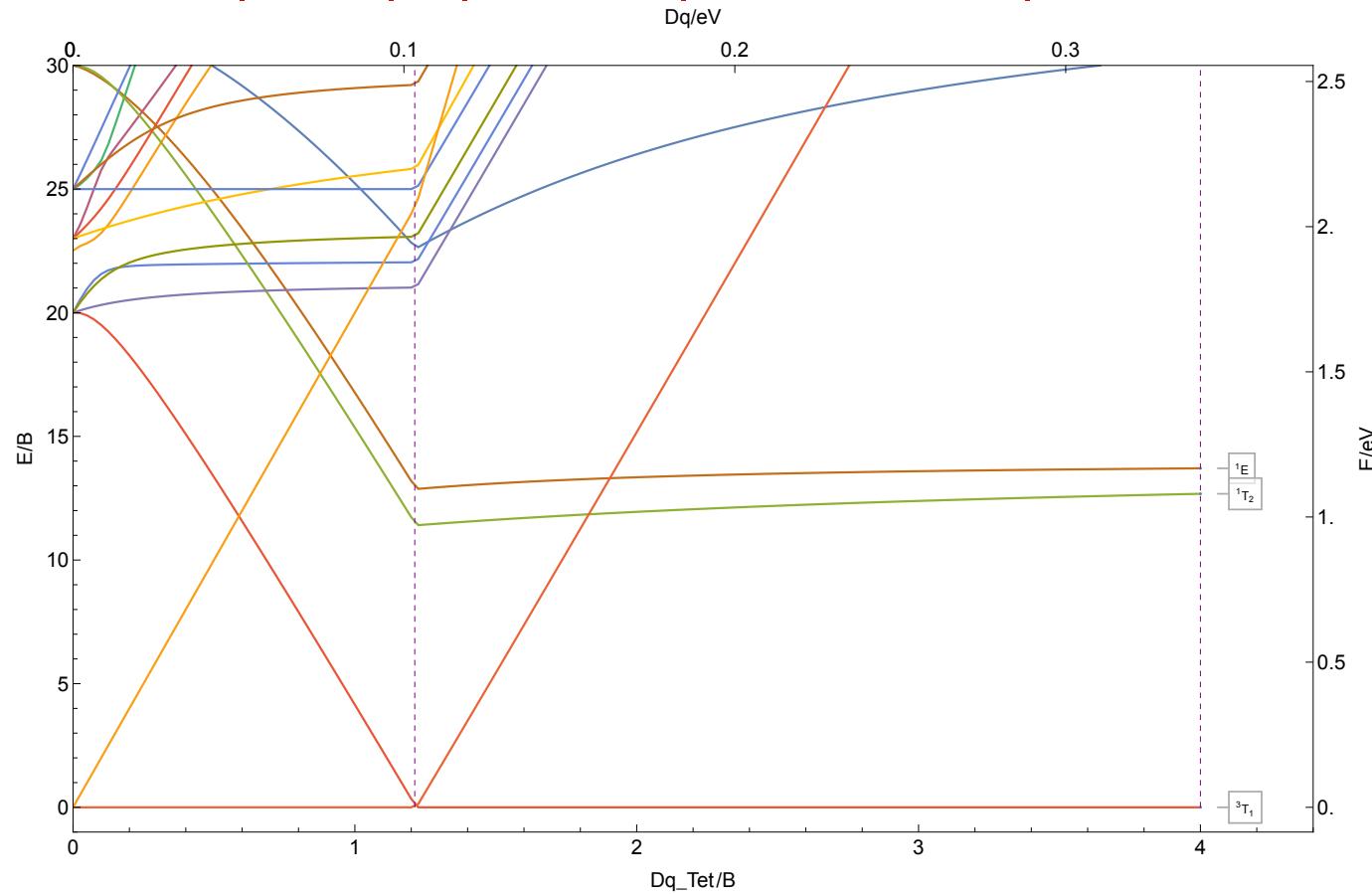
8.2.48 Tc<sup>5+</sup>

| 1,3 | d<sup>2</sup> | C/B ≈ 4.1 | B ≈ 752 cm<sup>-1</sup> | Tc<sup>5+</sup>



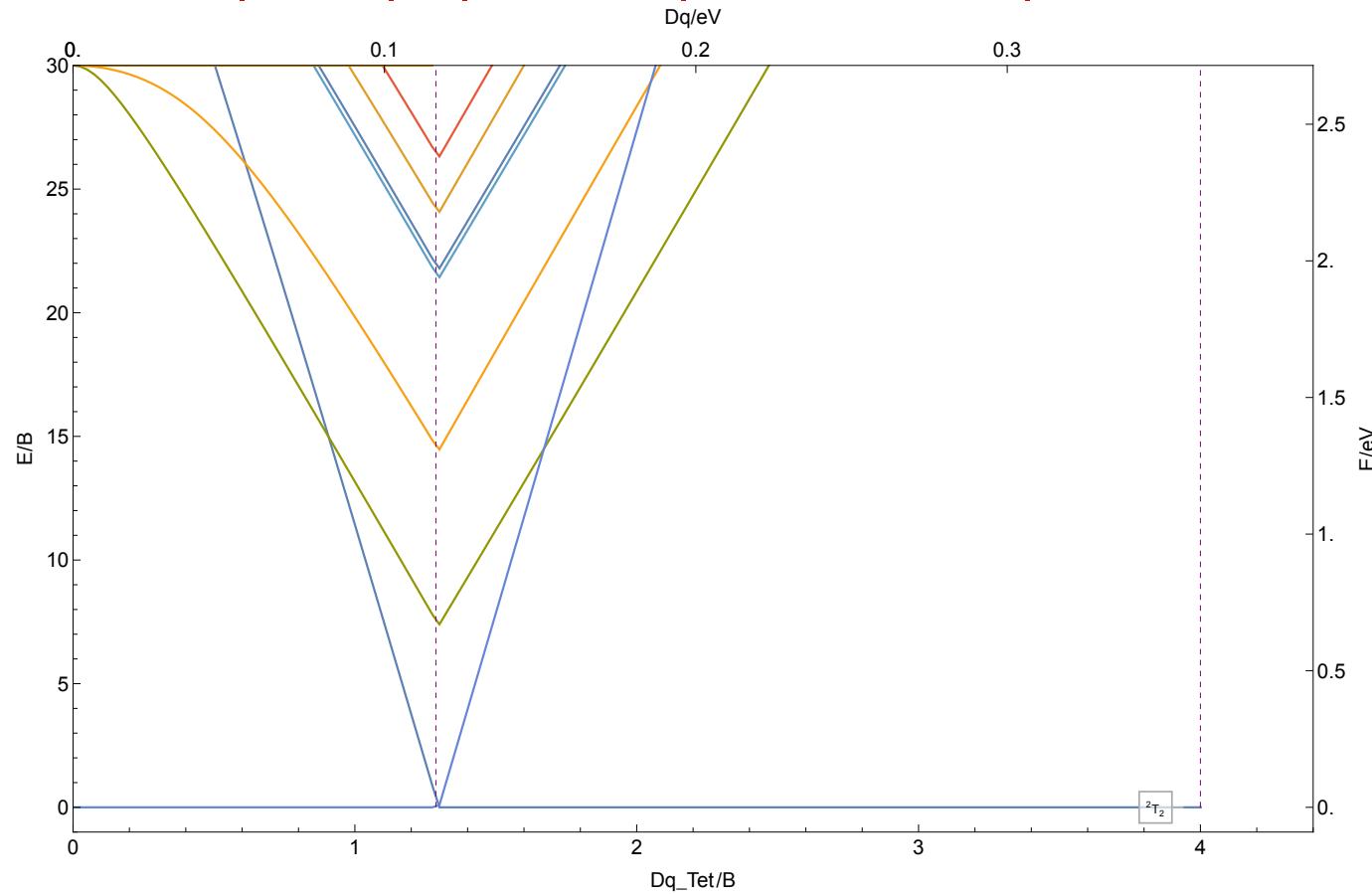
8.2.49 Ru<sup>2+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4. | B ≈ 687 cm<sup>-1</sup> | Ru<sup>2+</sup>



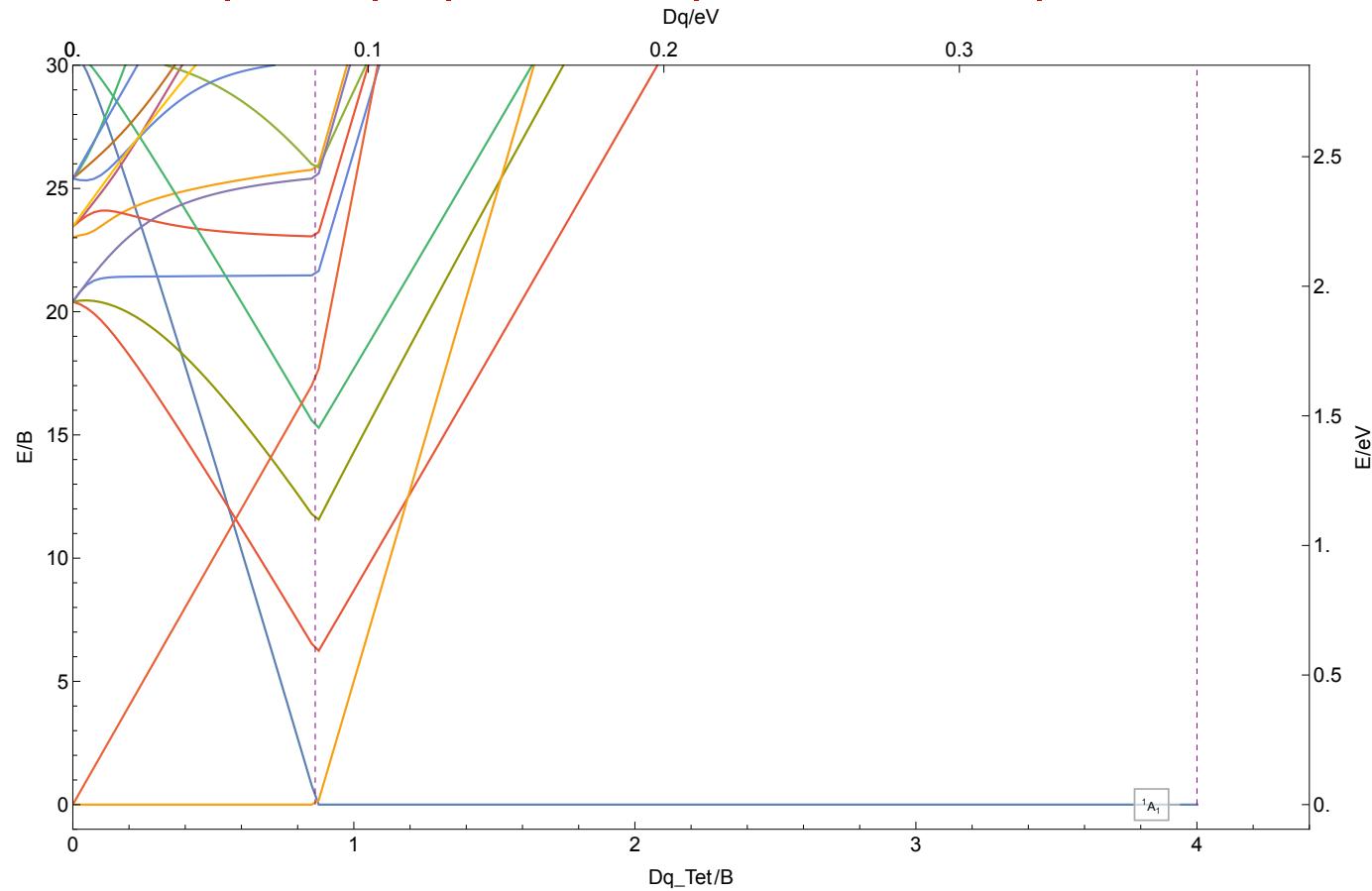
8.2.50 Ru<sup>3+</sup>

|2,4,6|d<sup>5</sup>|C/B ≈ 4.|B ≈ 730 cm<sup>-1</sup>|Ru<sup>3+</sup>



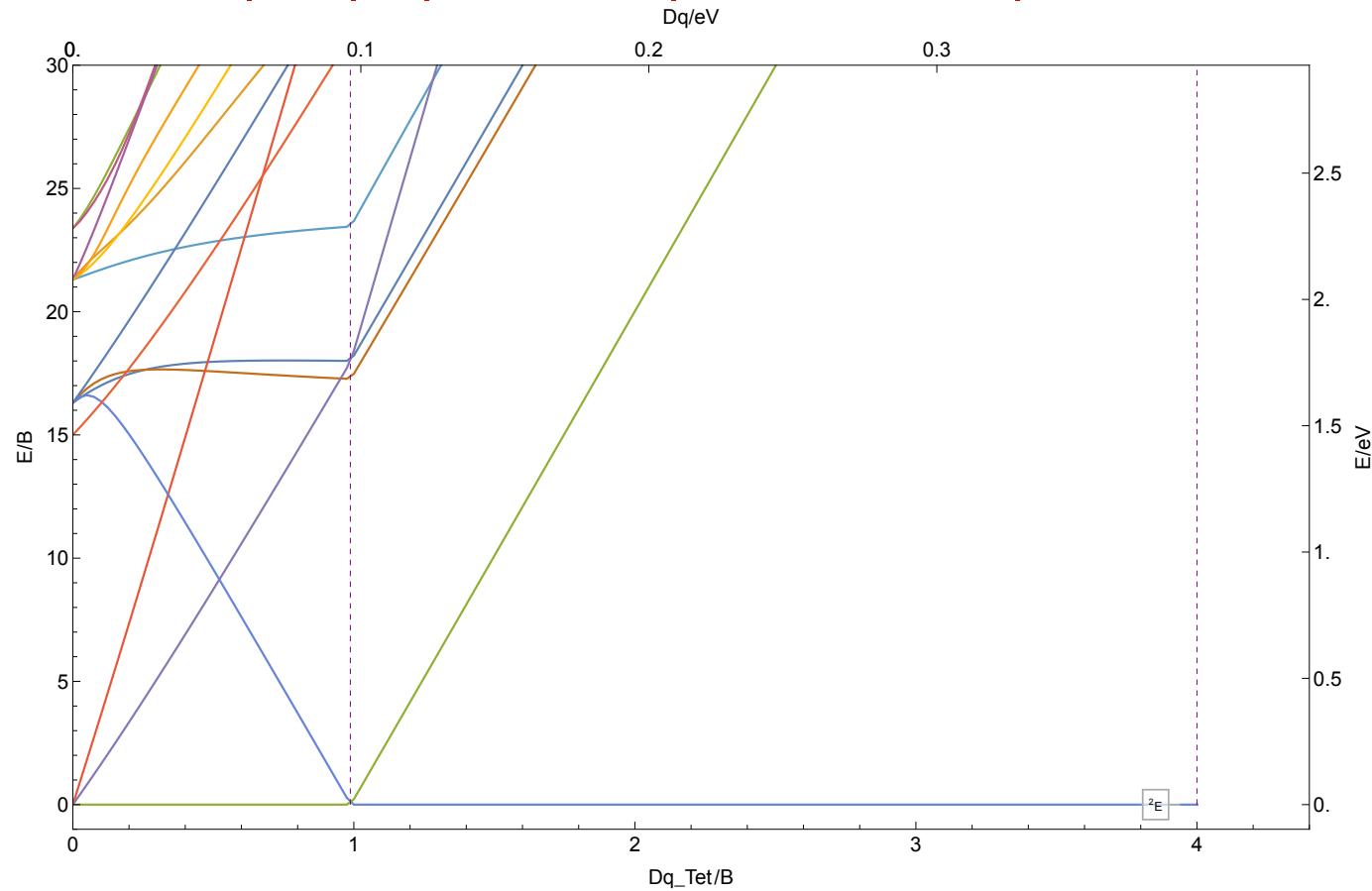
8.2.51 Ru<sup>4+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 4.1 | B ≈ 767 cm<sup>-1</sup> | Ru<sup>4+</sup>



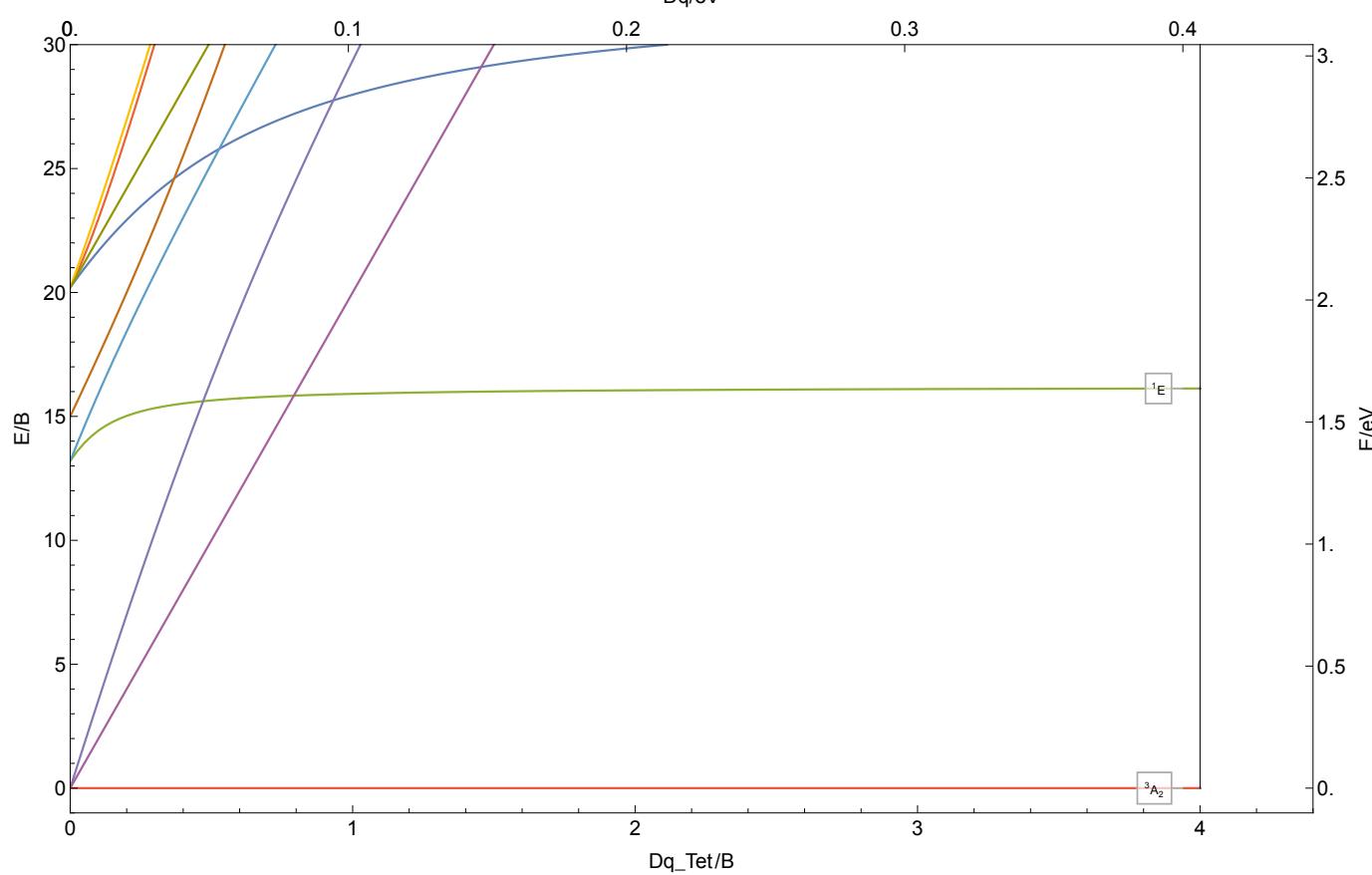
8.2.52 Ru<sup>5+</sup>

|2,4|d<sup>3</sup>| C/B ≈ 4.1| B ≈ 787 cm<sup>-1</sup> |Ru<sup>5+</sup>



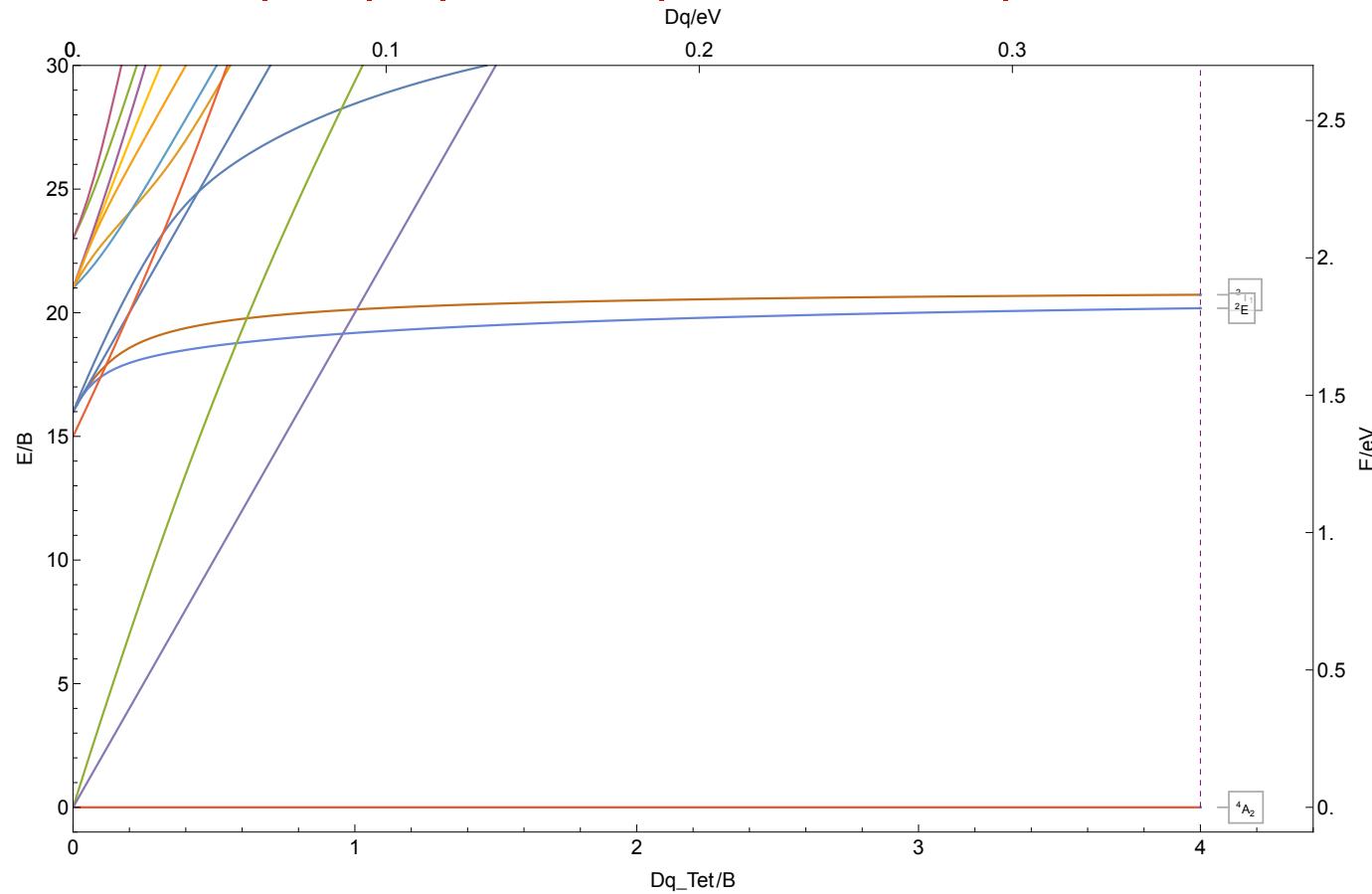
8.2.53 Ru<sup>6+</sup>

| 1,3 | d<sup>2</sup> | C/B ≈ 4.1 | B ≈ 819 cm<sup>-1</sup> | Ru<sup>6+</sup>



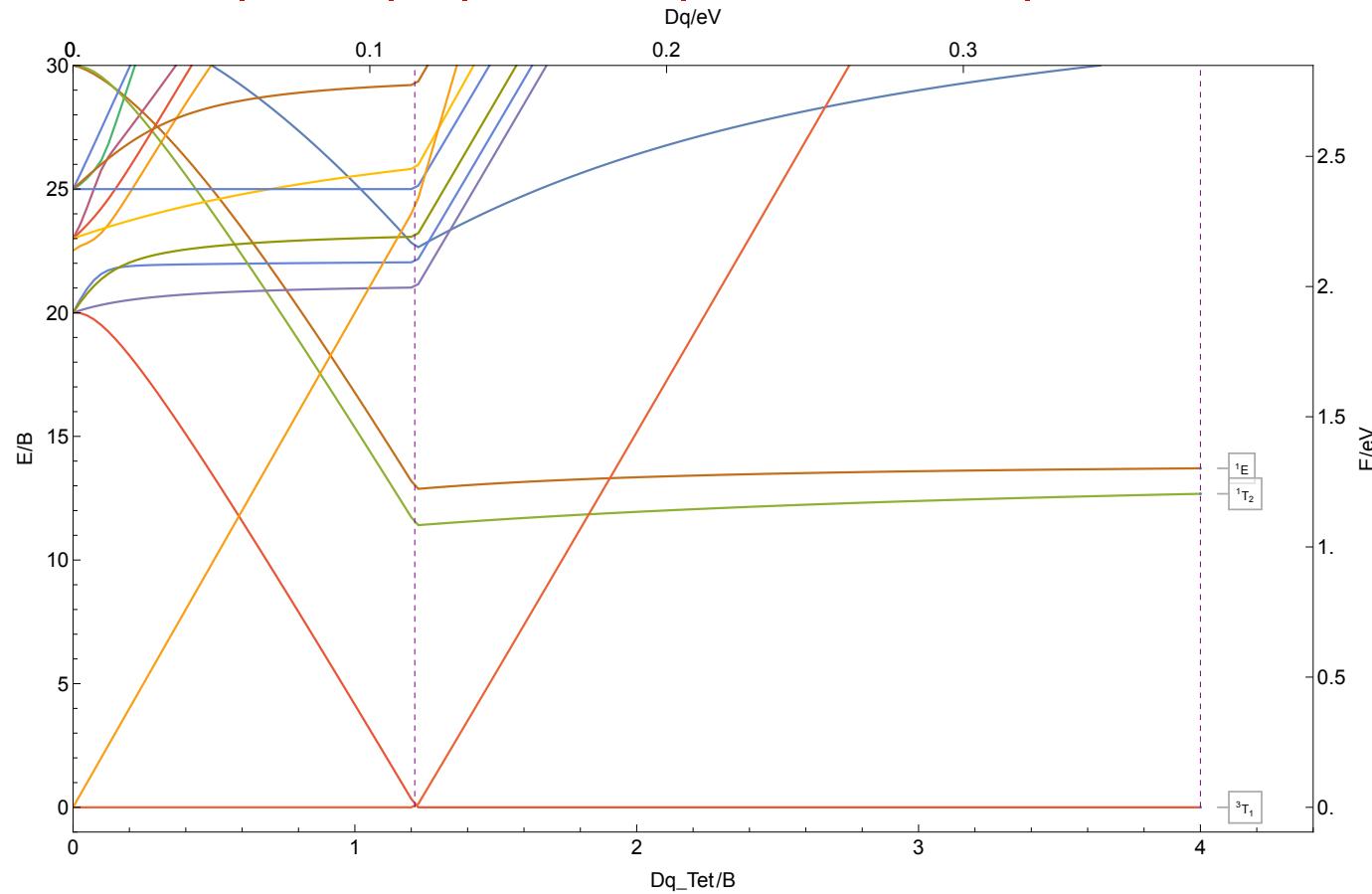
8.2.54 Rh<sup>2+</sup>

|2,4|d<sup>7</sup>| C/B ≈ 4. |B ≈ 726 cm<sup>-1</sup> | Rh<sup>2+</sup>



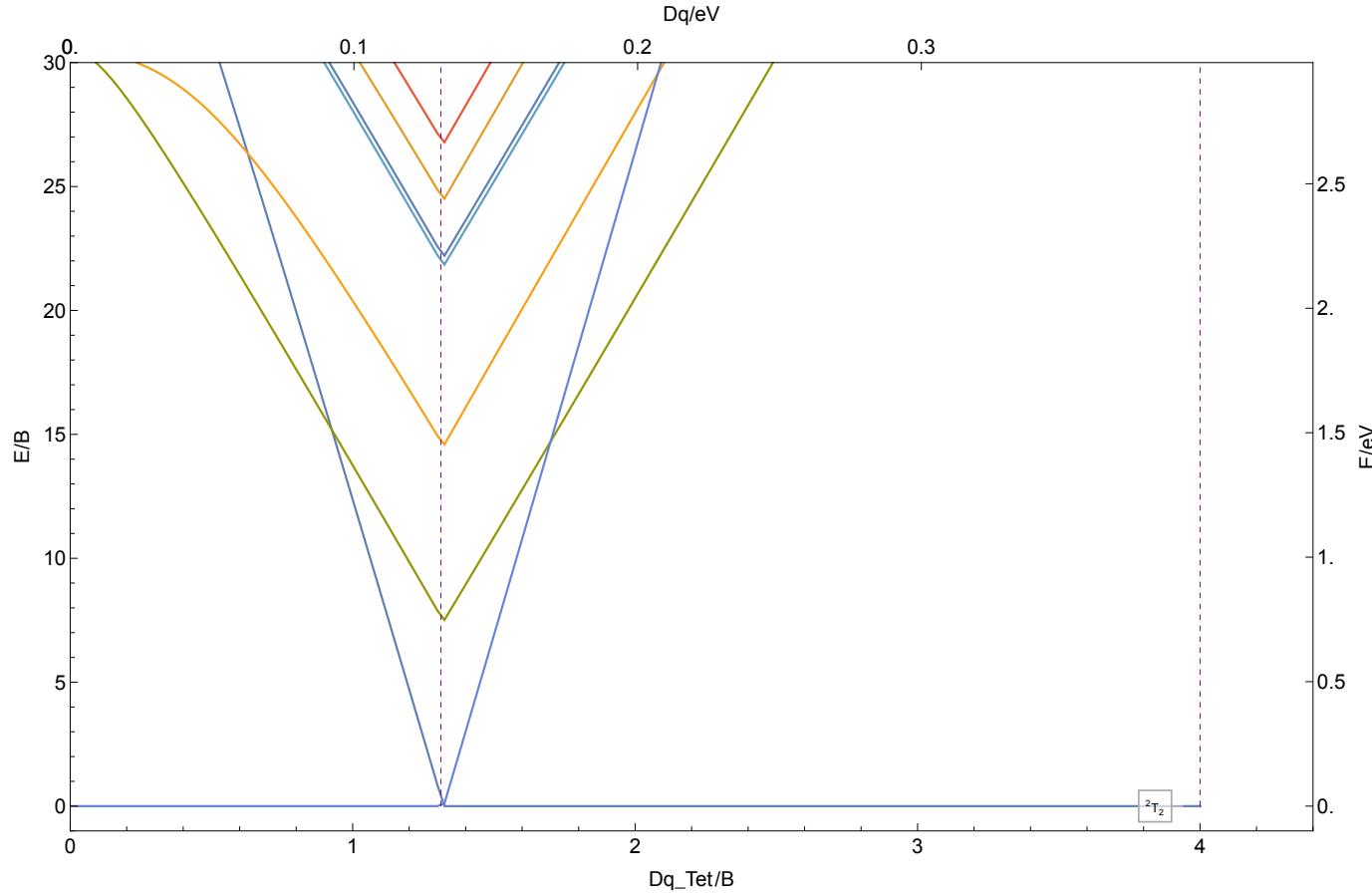
8.2.55 Rh<sup>3+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4. | B ≈ 766 cm<sup>-1</sup> | Rh<sup>3+</sup>



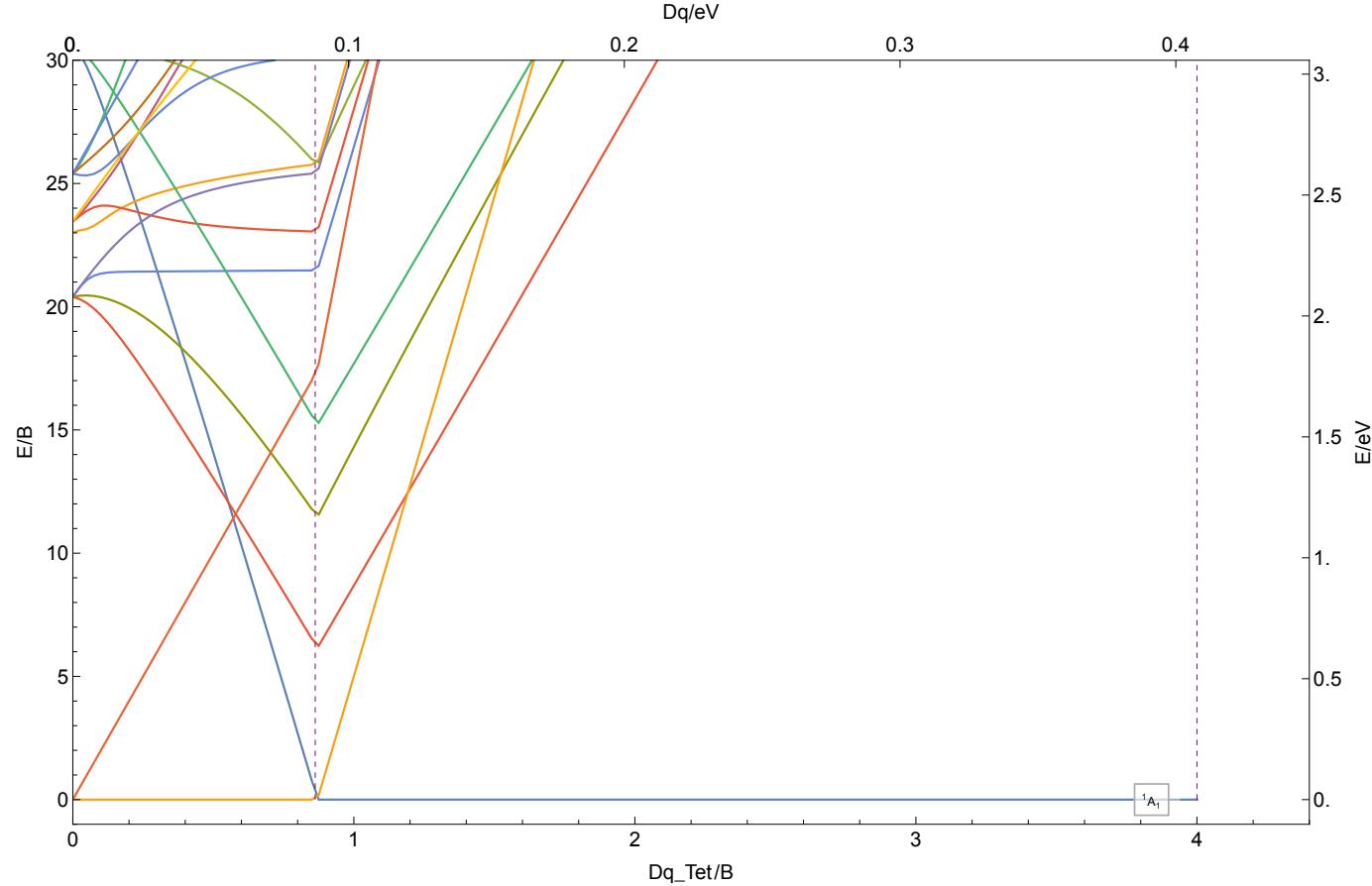
8.2.56 Rh<sup>4+</sup>

|2,4,6| d<sup>5</sup>| C/B ≈ 4.1| B ≈ 803 cm<sup>-1</sup> | Rh<sup>4+</sup>



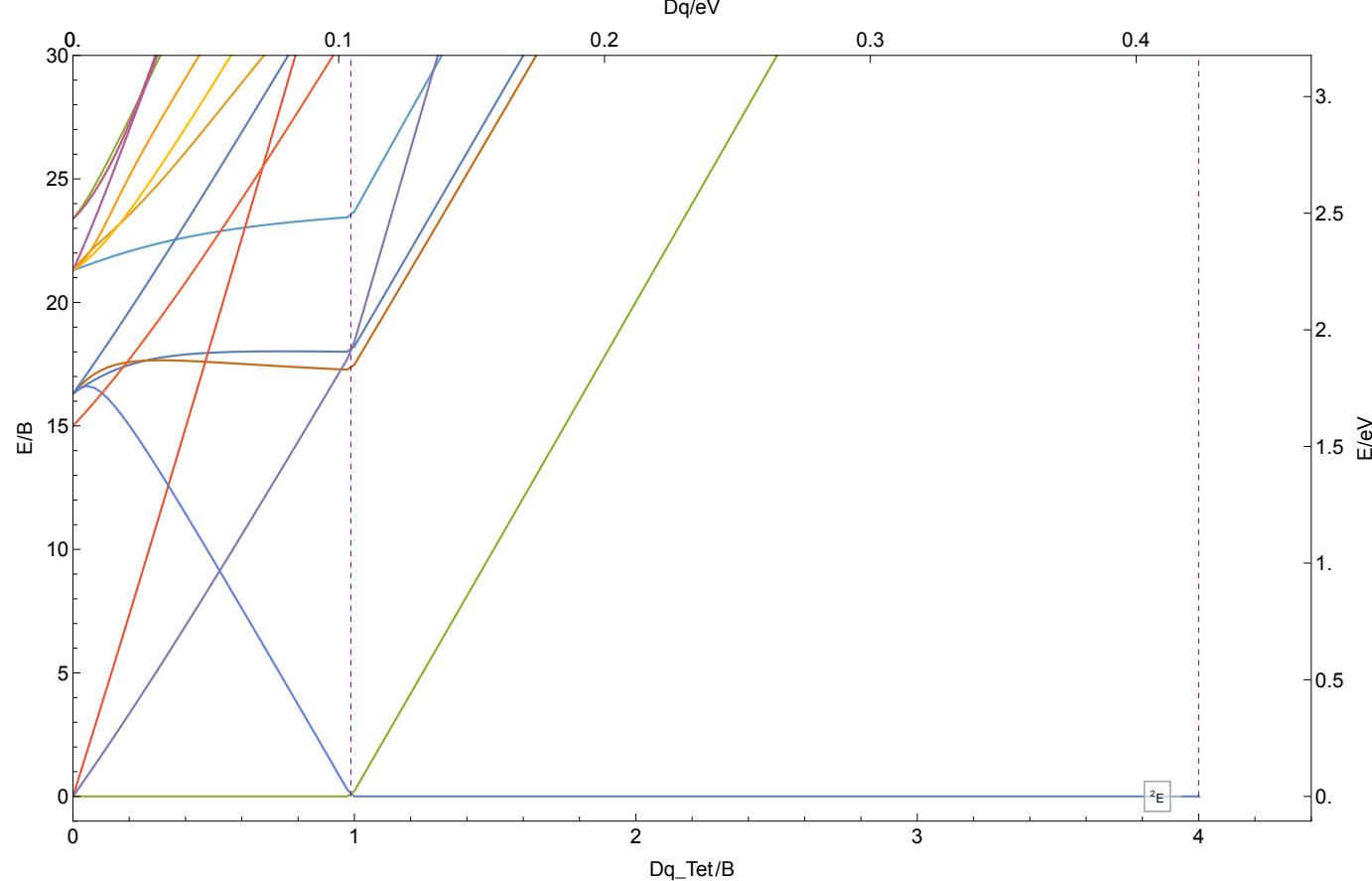
8.2.57 Rh<sup>5+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 4.1 | B ≈ 822 cm<sup>-1</sup> | Rh<sup>5+</sup>



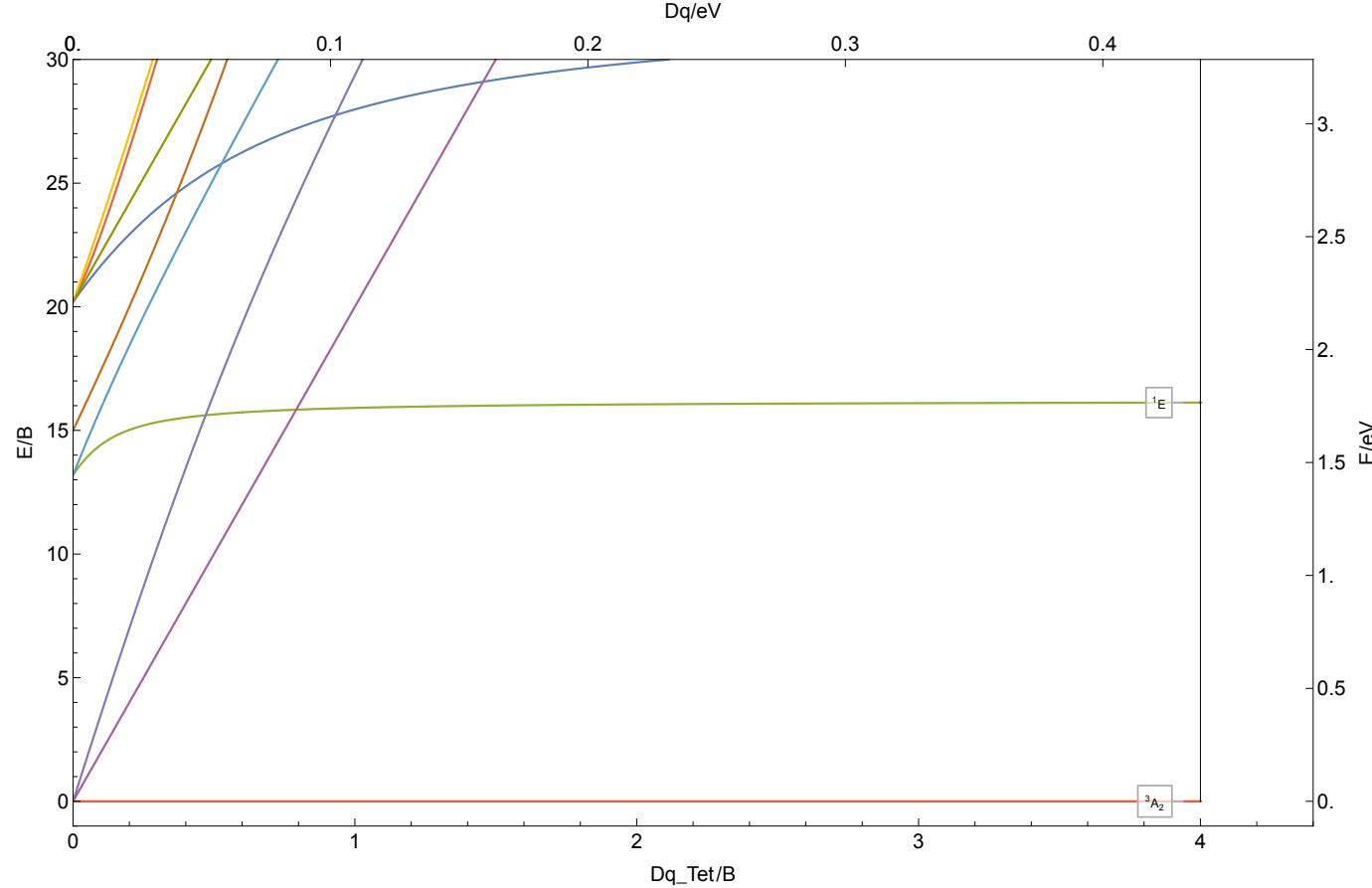
8.2.58 Rh<sup>6+</sup>

|2,4|d<sup>3</sup>| C/B ≈ 4.1| B ≈ 854 cm<sup>-1</sup> | Rh<sup>6+</sup>



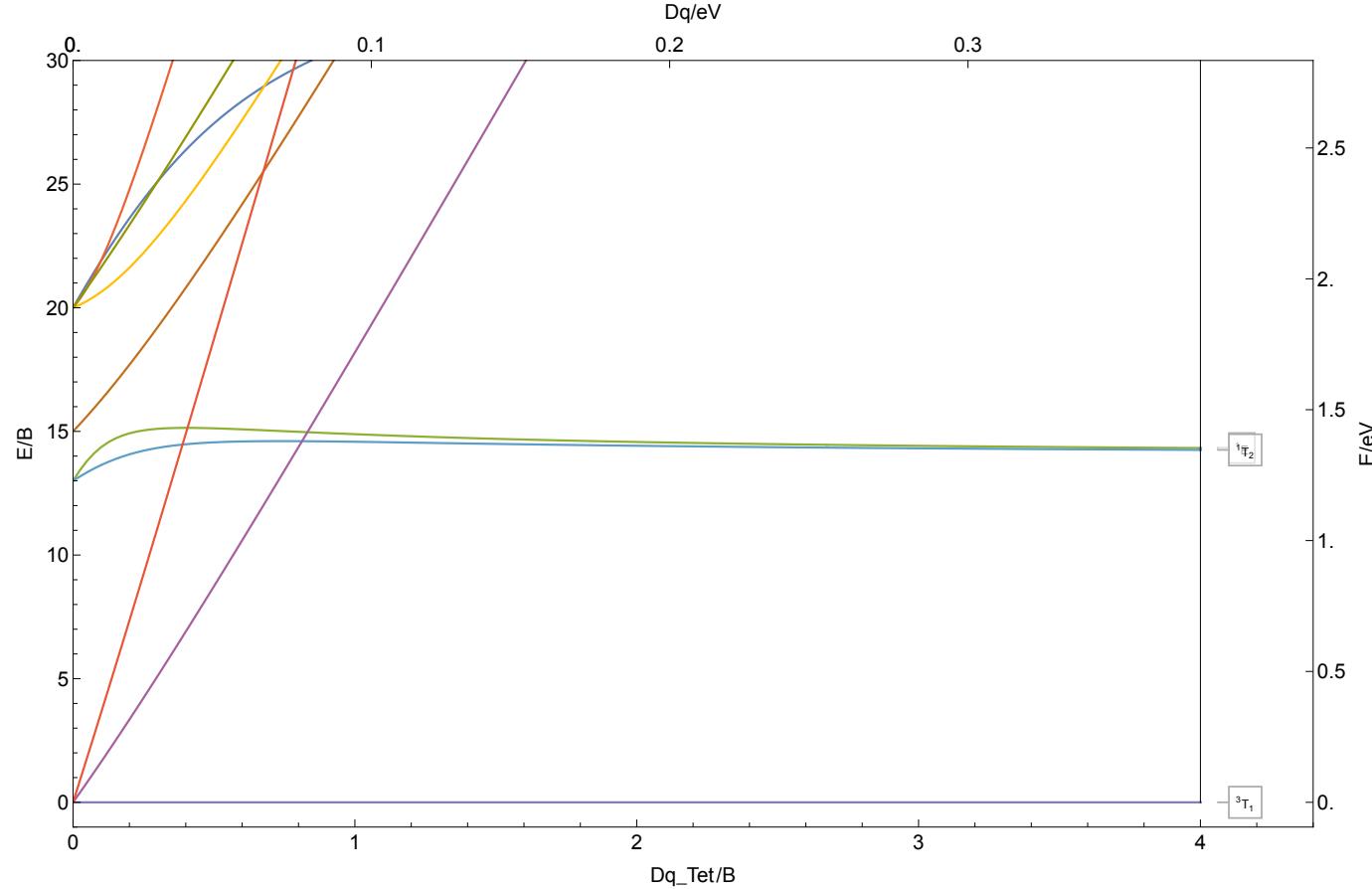
8.2.59 Rh<sup>7+</sup>

| 1,3 | d<sup>2</sup> | C/B ≈ 4.1 | B ≈ 883 cm<sup>-1</sup> | Rh<sup>7+</sup>



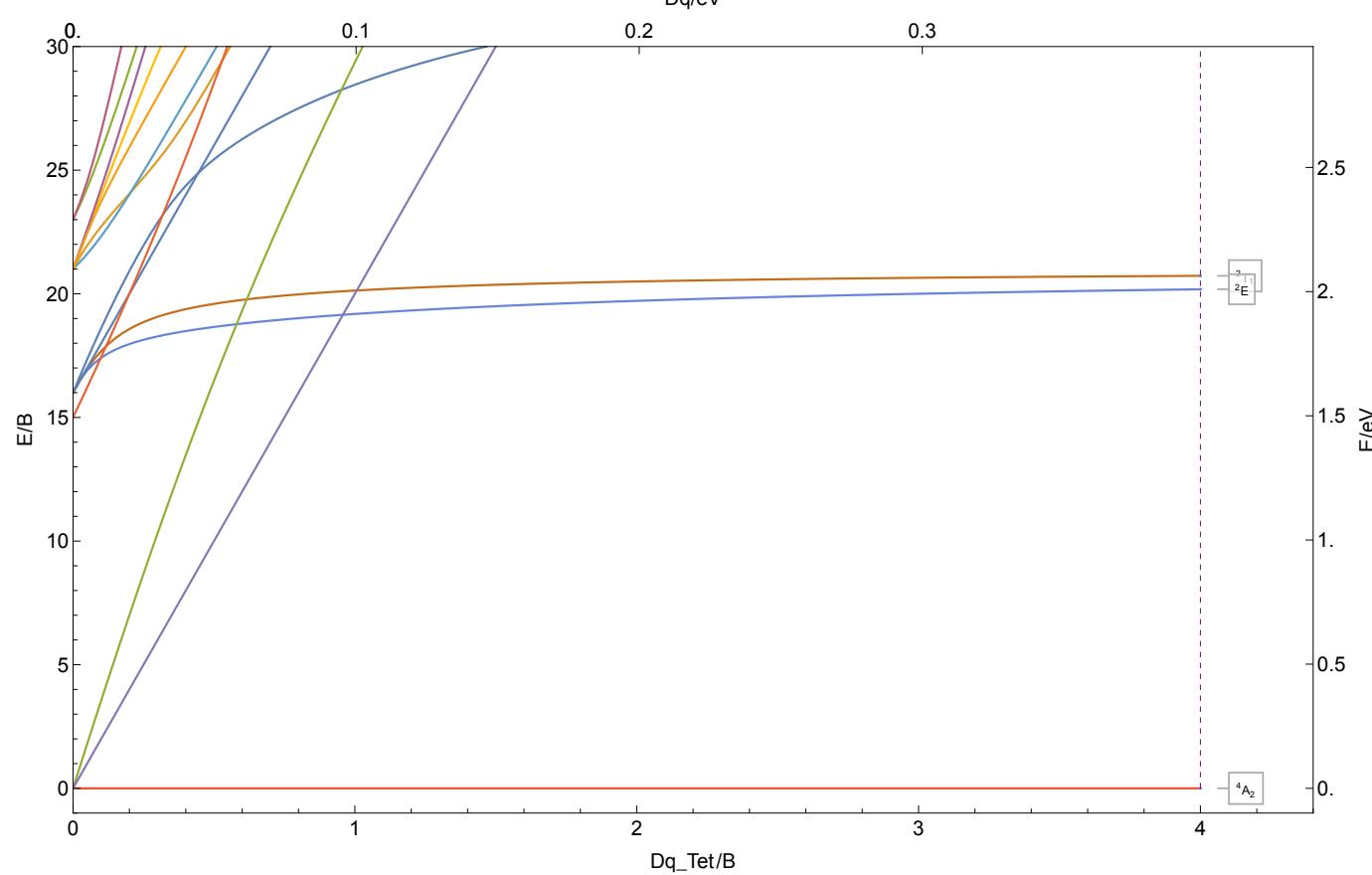
8.2.60 Pd<sup>2+</sup>

| 1,3 | d<sup>8</sup> | C/B ≈ 4. | B ≈ 762 cm<sup>-1</sup> | Pd<sup>2+</sup>



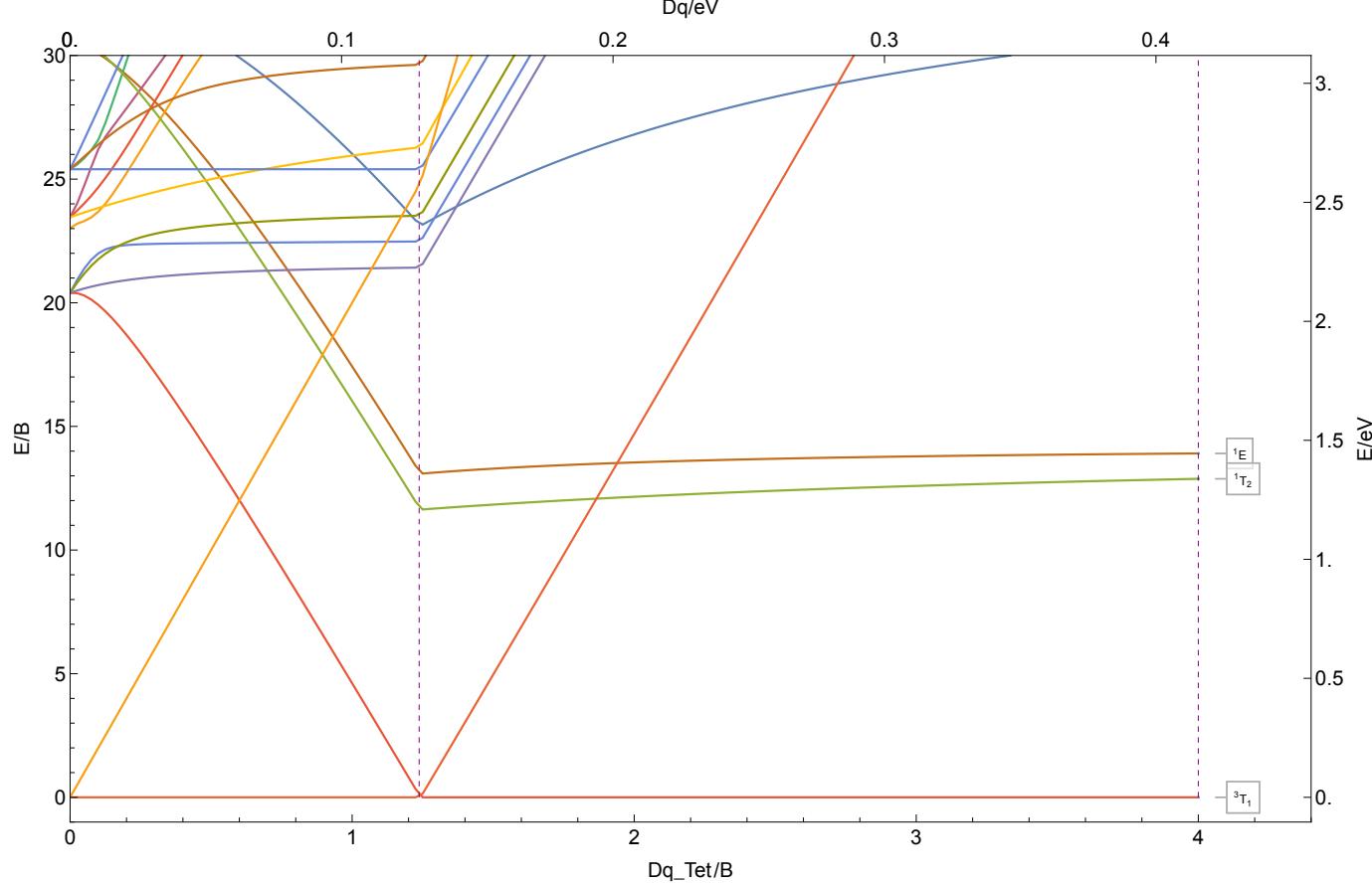
8.2.61 Pd<sup>3+</sup>

|2,4|d<sup>7</sup>| C/B ≈ 4. | B ≈ 803 cm<sup>-1</sup> | Pd<sup>3+</sup>



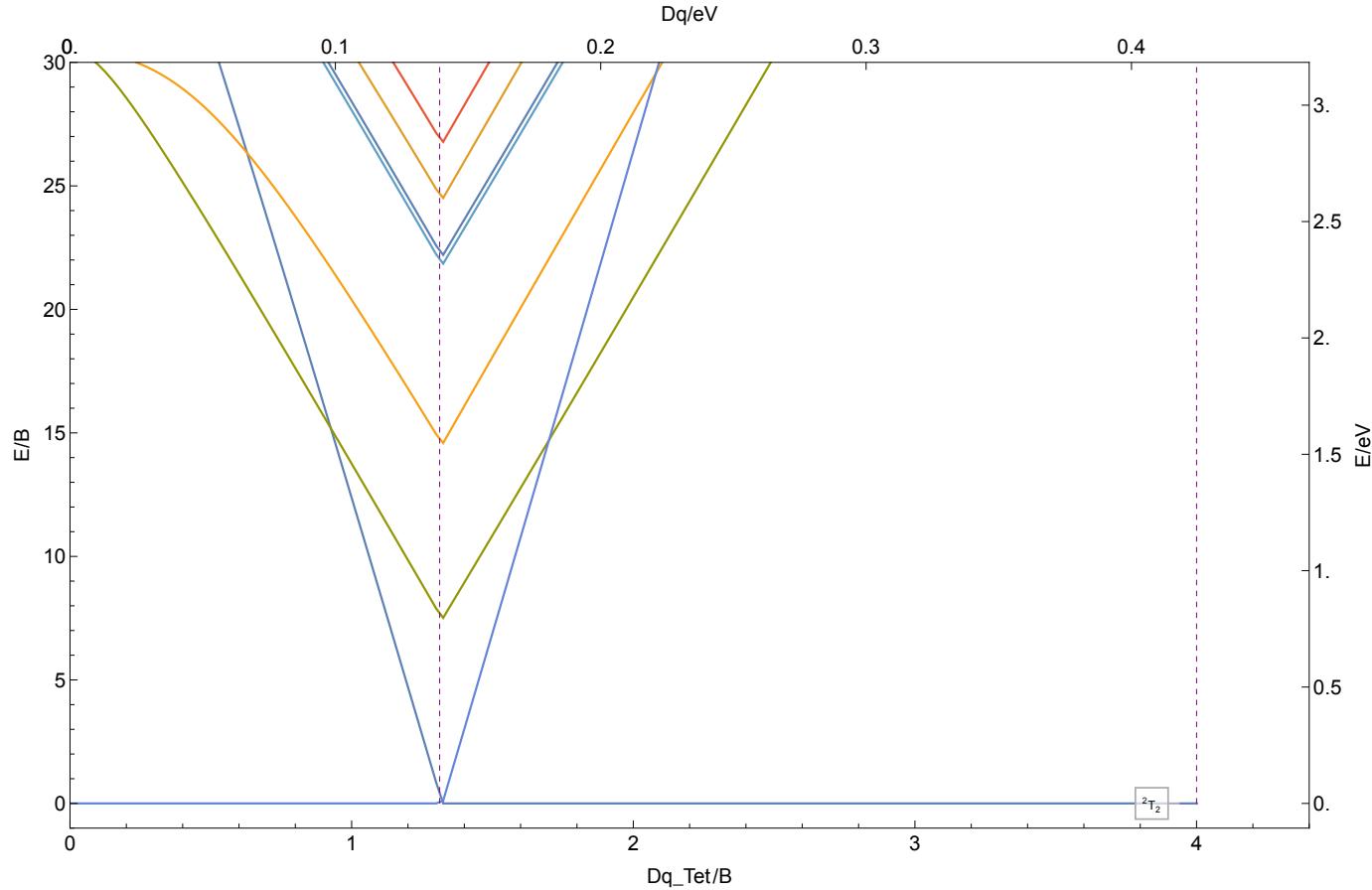
8.2.62 Pd<sup>4+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4.1 | B ≈ 838 cm<sup>-1</sup> | Pd<sup>4+</sup>



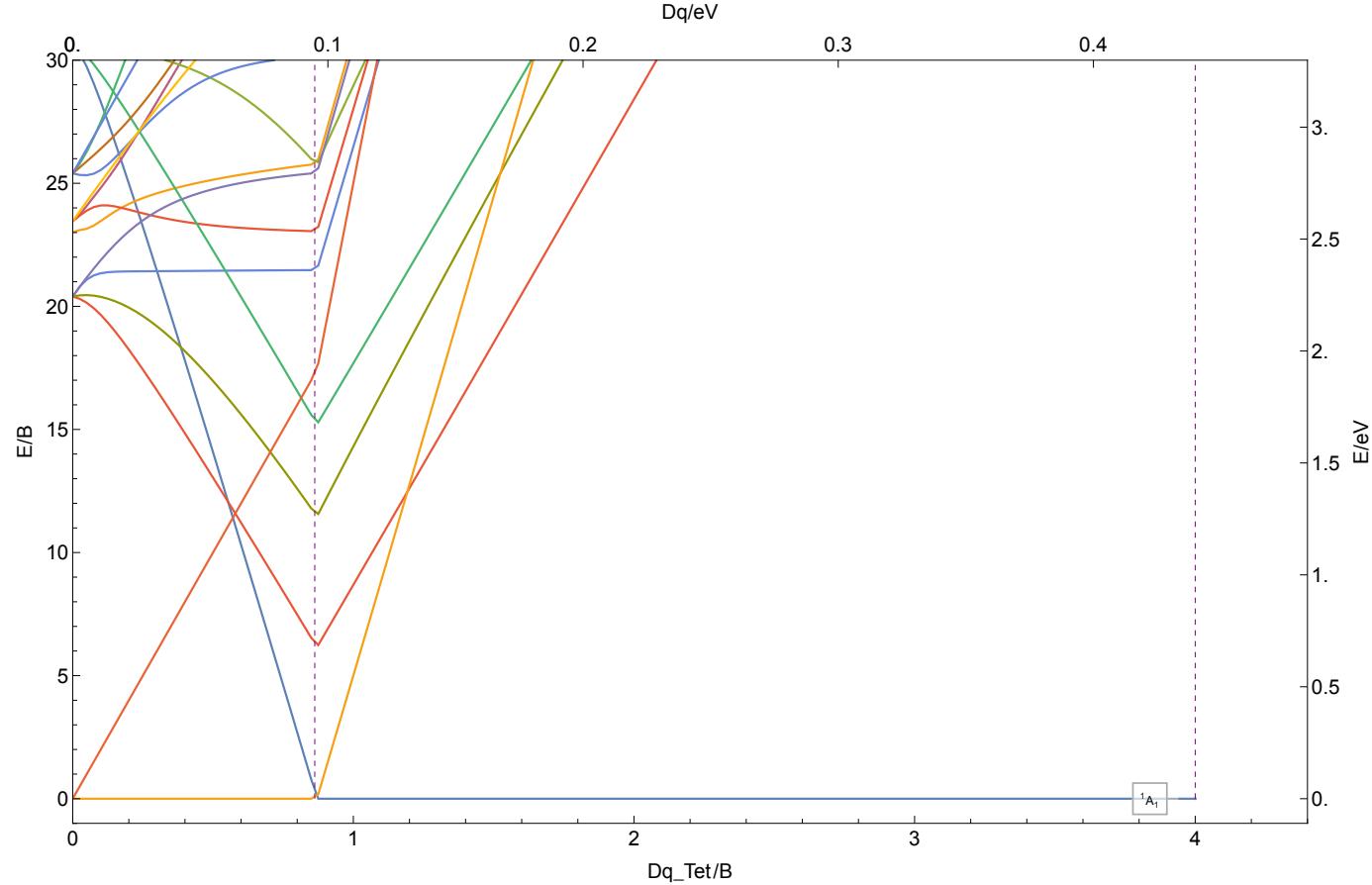
8.2.63 Pd<sup>5+</sup>

|2,4,6| d<sup>5</sup>| C/B ≈ 4.1| B ≈ 856 cm<sup>-1</sup> |Pd<sup>5+</sup>



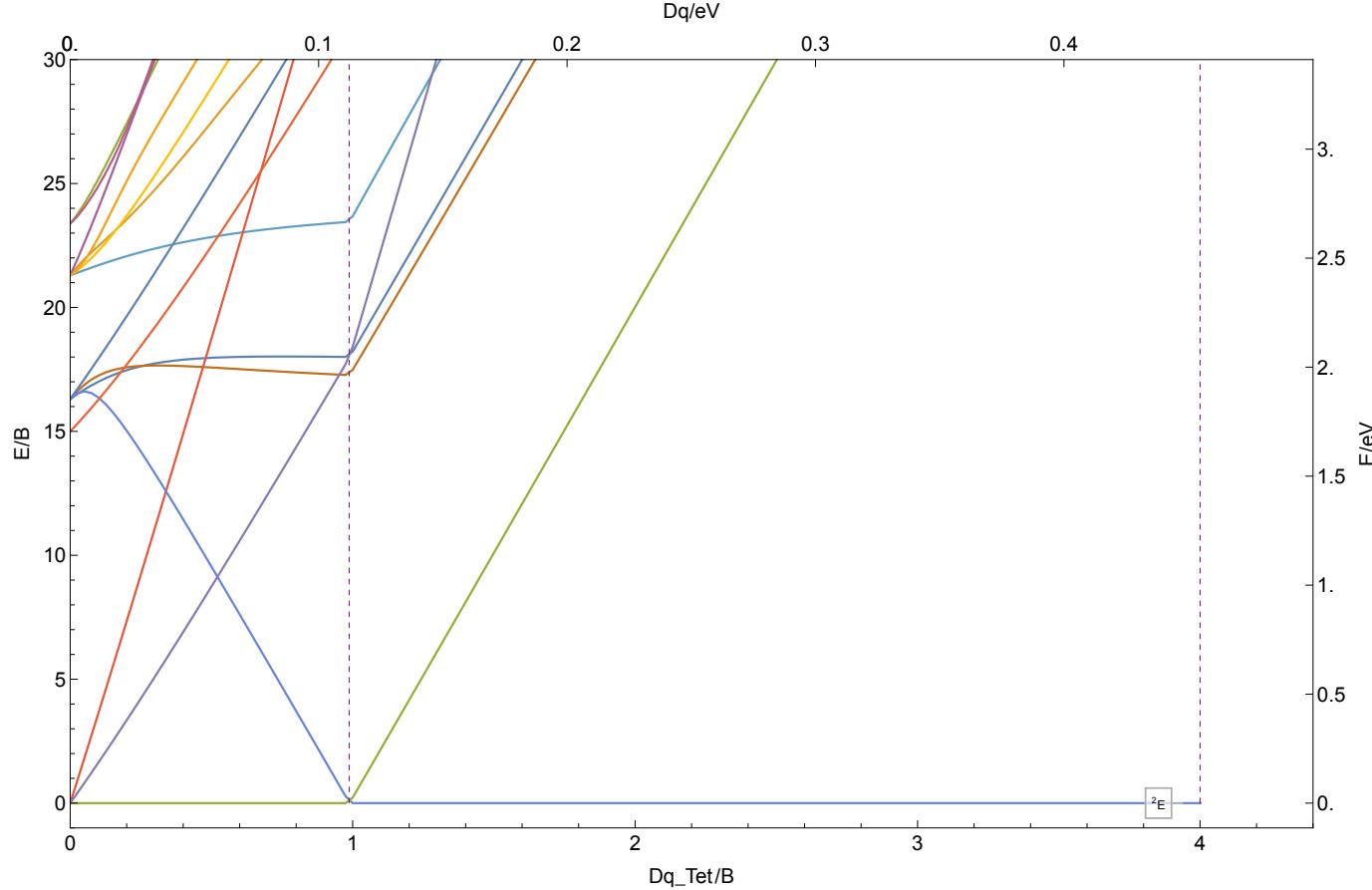
8.2.64 Pd<sup>6+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 4.1 | B ≈ 887 cm<sup>-1</sup> | Pd<sup>6+</sup>



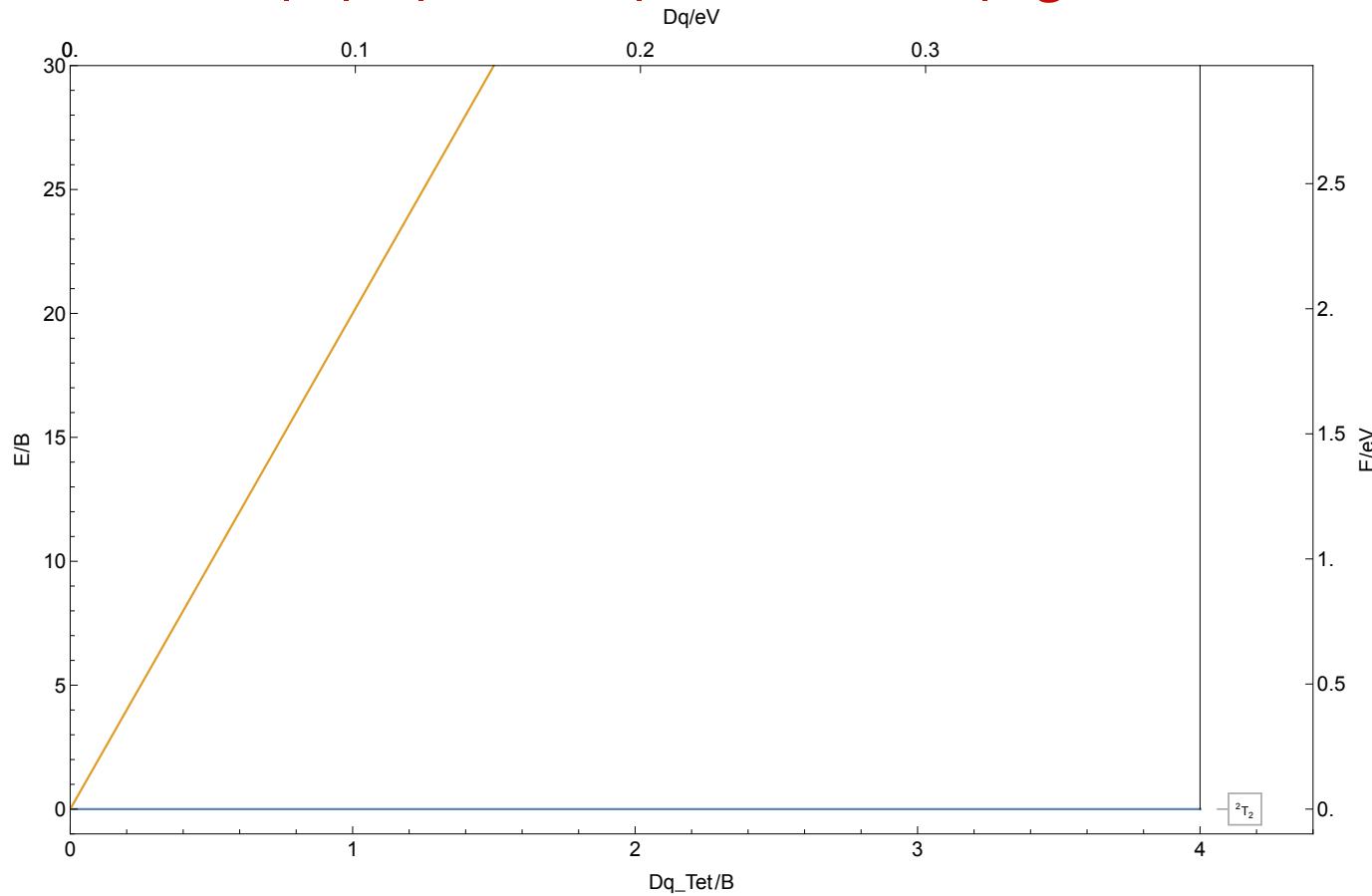
8.2.65 Pd<sup>7+</sup>

|2,4| d<sup>3</sup>| C/B ≈ 4.1| B ≈ 917 cm<sup>-1</sup> | Pd<sup>7+</sup>



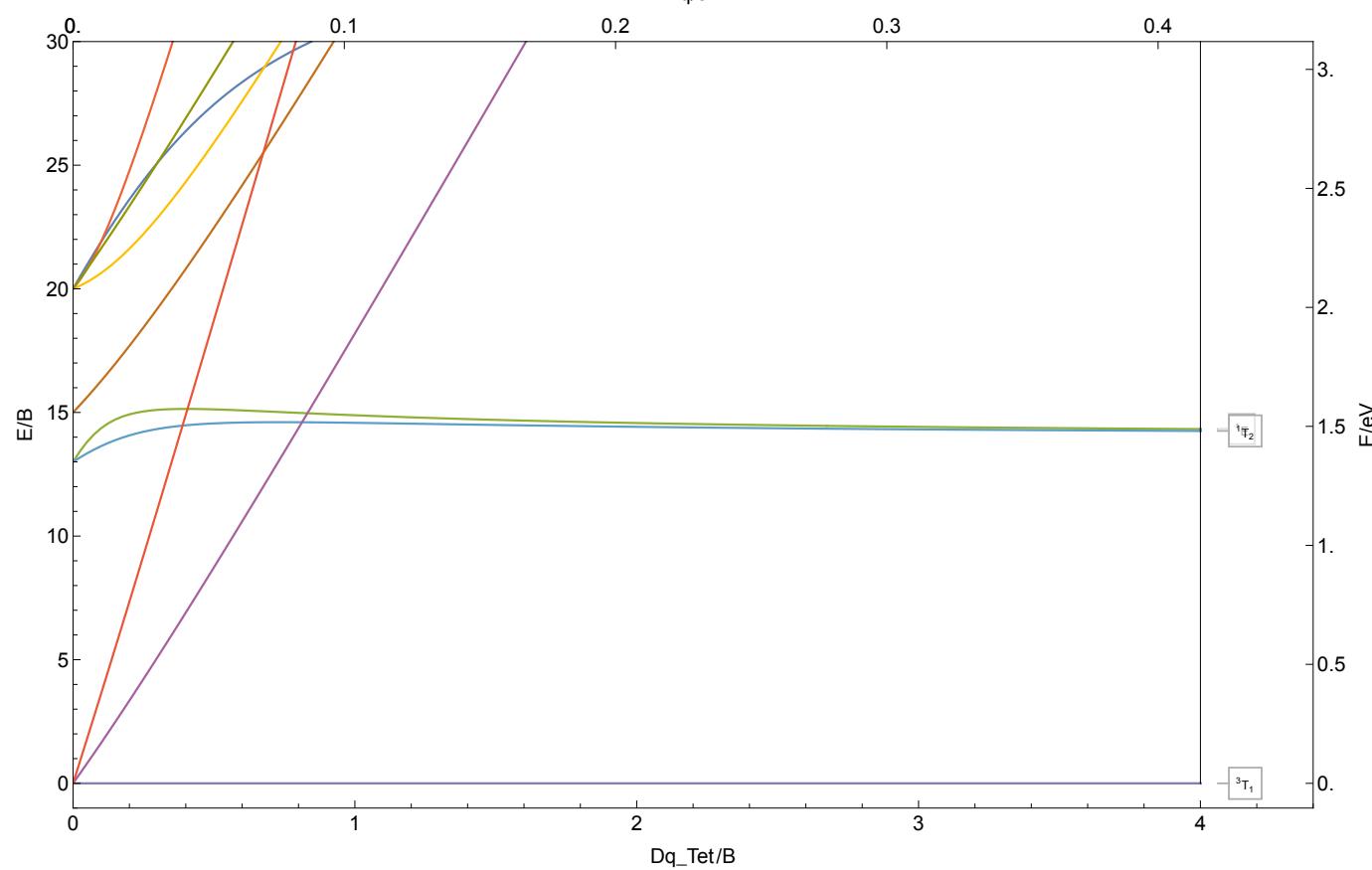
8.2.66  $\text{Ag}^{2+}$

$|2|d^9|C/B \approx 4. |B \approx 799 \text{ cm}^{-1}| \text{Ag}^{2+}$



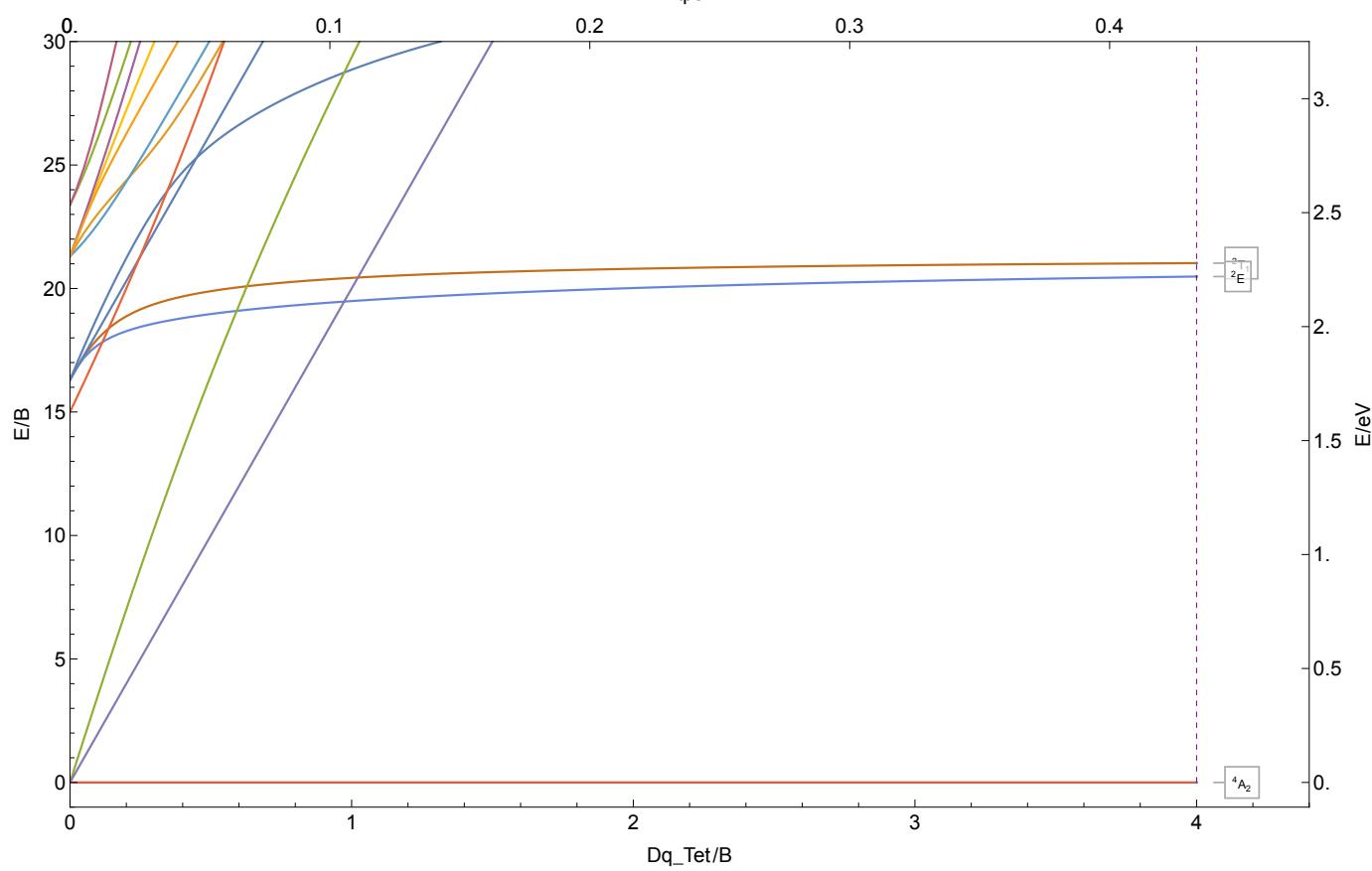
8.2.67  $\text{Ag}^{3+}$

$|1,3|d^8|C/B \approx 4.|B \approx 838 \text{ cm}^{-1}|Ag^{3+}$



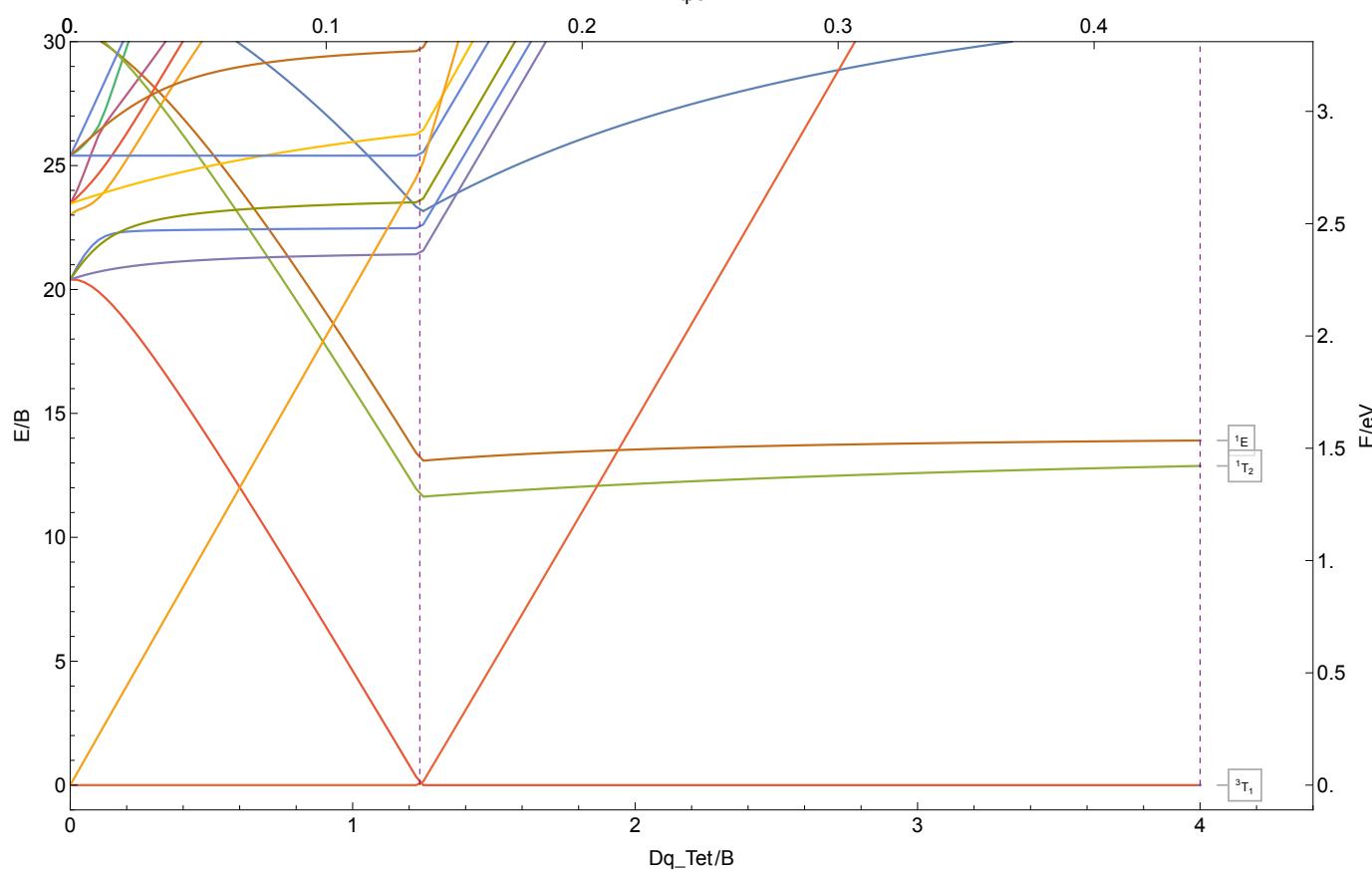
8.2.68 Ag<sup>4+</sup>

$$|2,4|d^7|C/B \approx 4.1|B \approx 874\text{ cm}^{-1}|Ag^{4+}$$



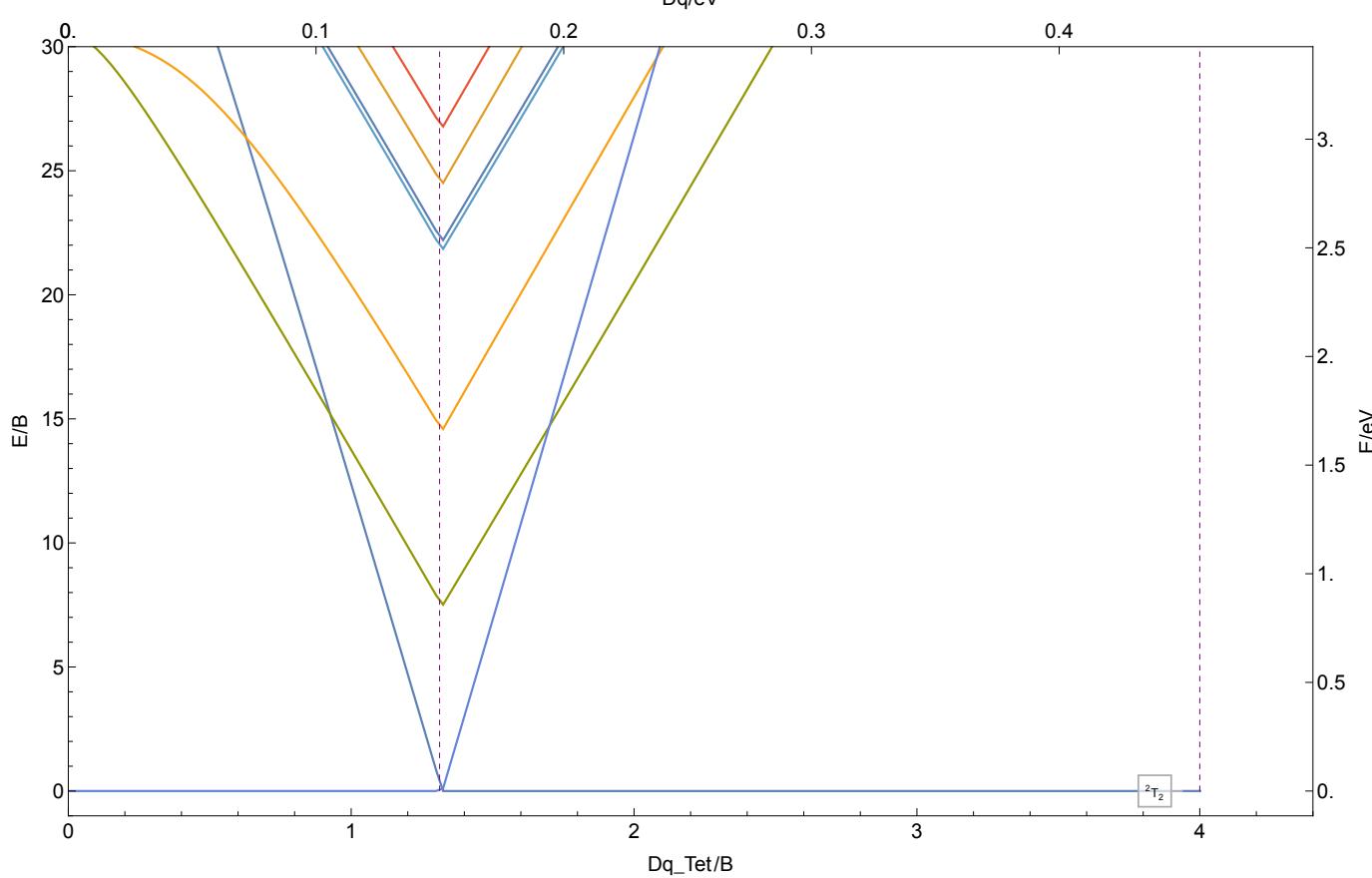
8.2.69 Ag<sup>5+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4.1 | B ≈ 890 cm<sup>-1</sup> | Ag<sup>5+</sup>



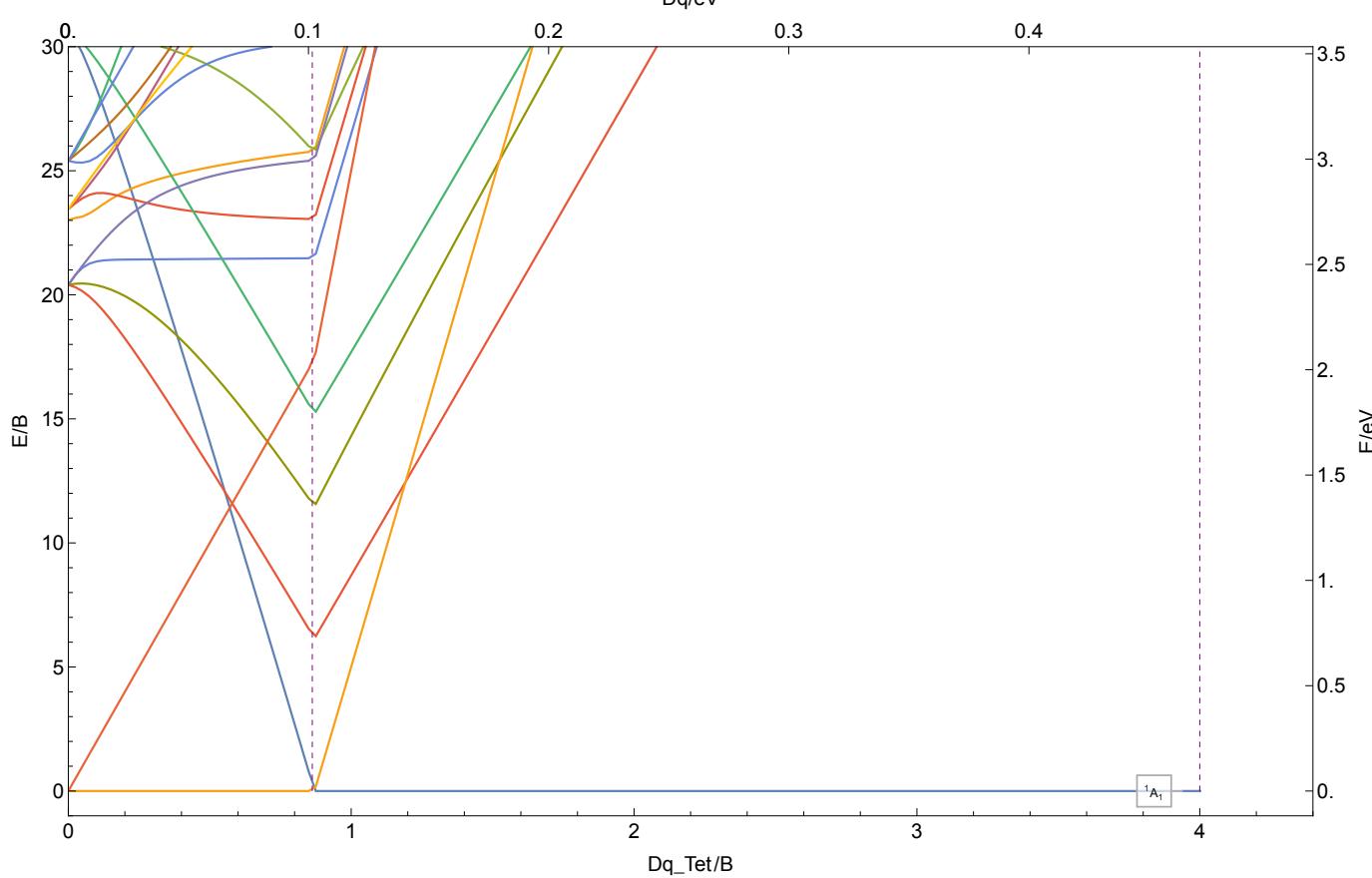
8.2.70 Ag<sup>6+</sup>

|2,4,6|d<sup>5</sup>|C/B ≈ 4.1|B ≈ 921 cm<sup>-1</sup>|Ag<sup>6+</sup>



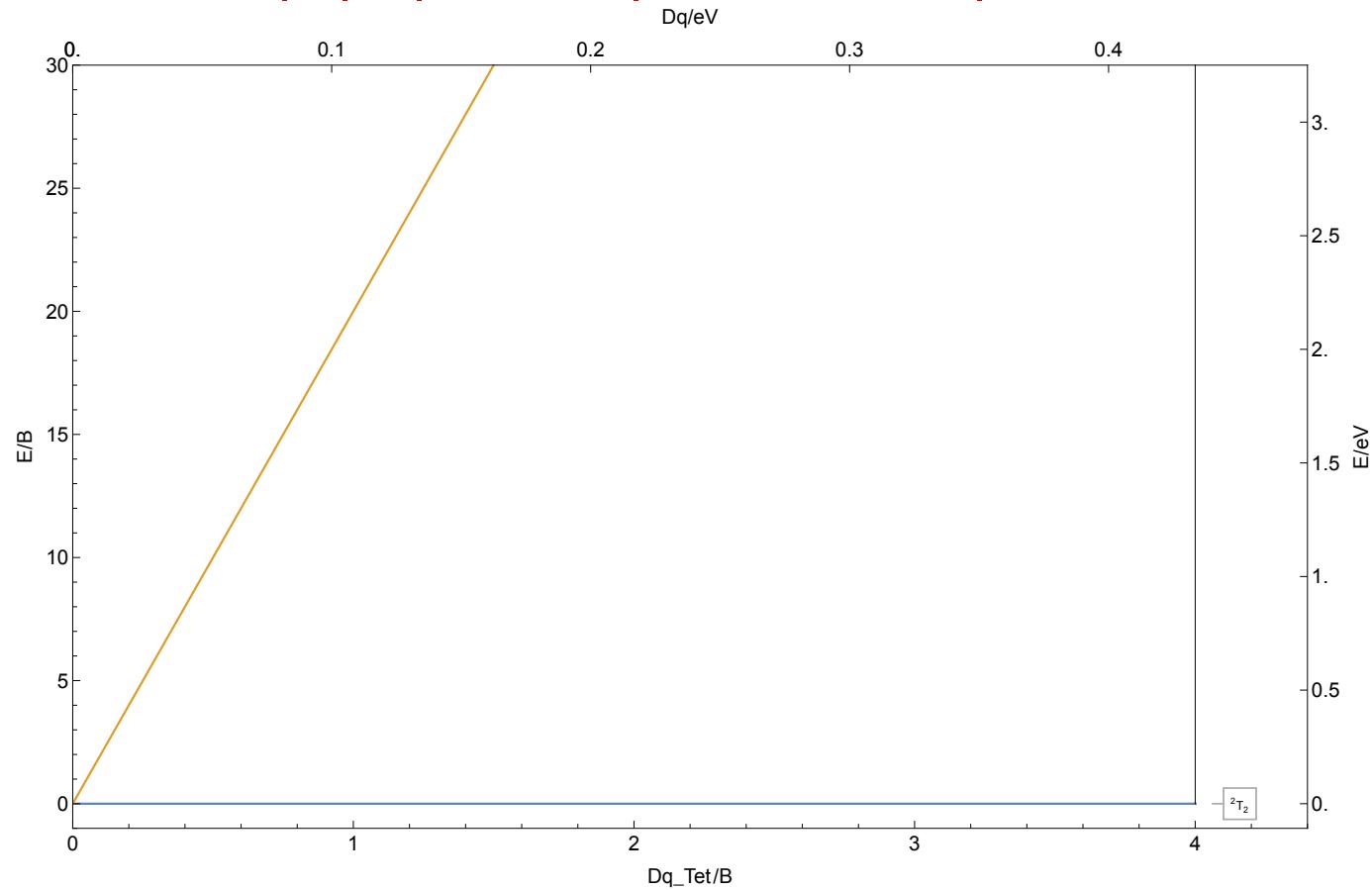
8.2.71 Ag<sup>7+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 4.1 | B ≈ 950 cm<sup>-1</sup> | Ag<sup>7+</sup>



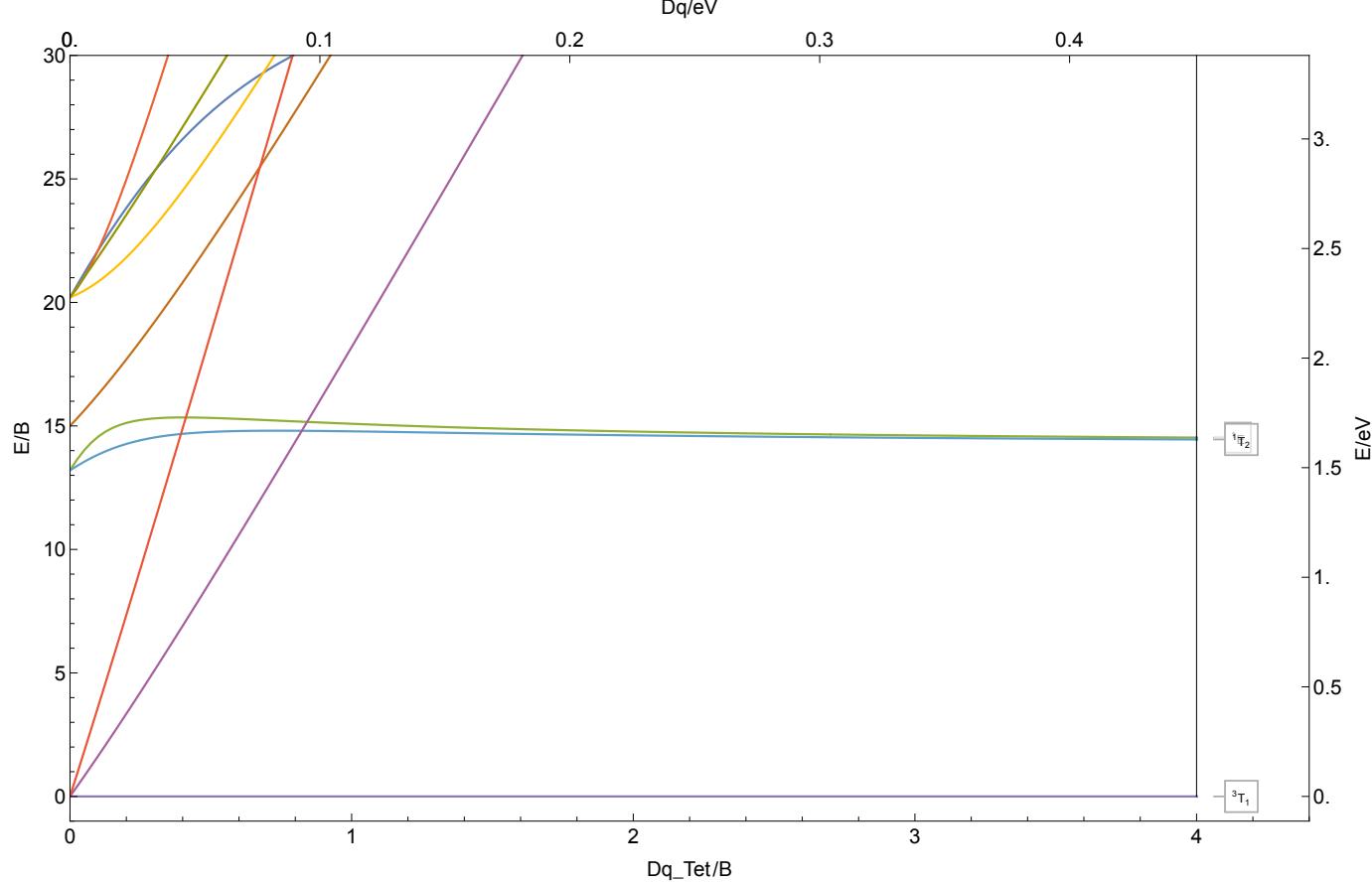
8.2.72 Cd<sup>3+</sup>

|2|d<sup>9</sup>| C/B ≈ 4. |B ≈ 874 cm<sup>-1</sup> |Cd<sup>3+</sup>



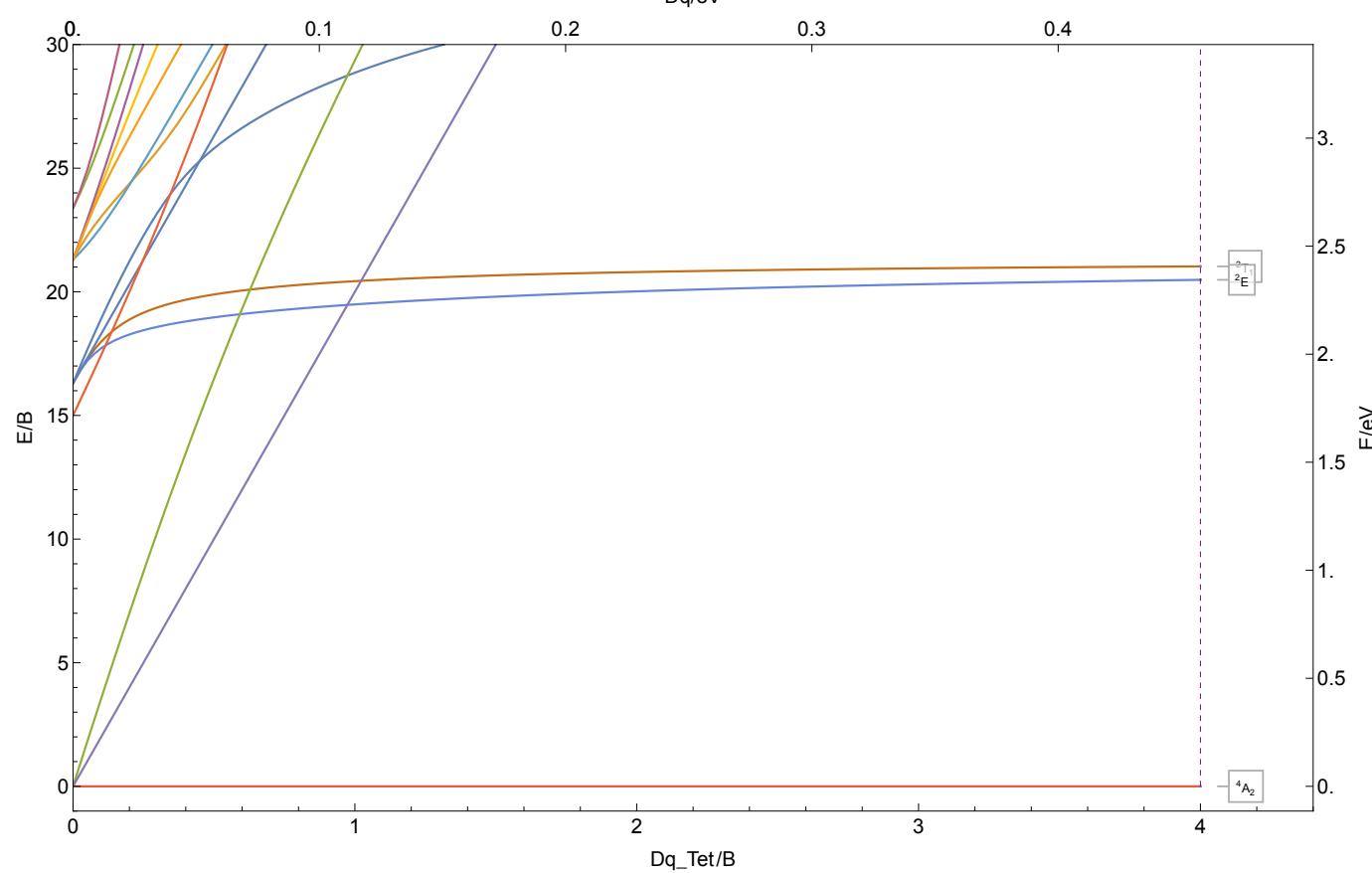
8.2.73 Cd<sup>4+</sup>

$|1,3|d^8|C/B \approx 4.1|B \approx 909\text{ cm}^{-1}|Cd^{4+}$



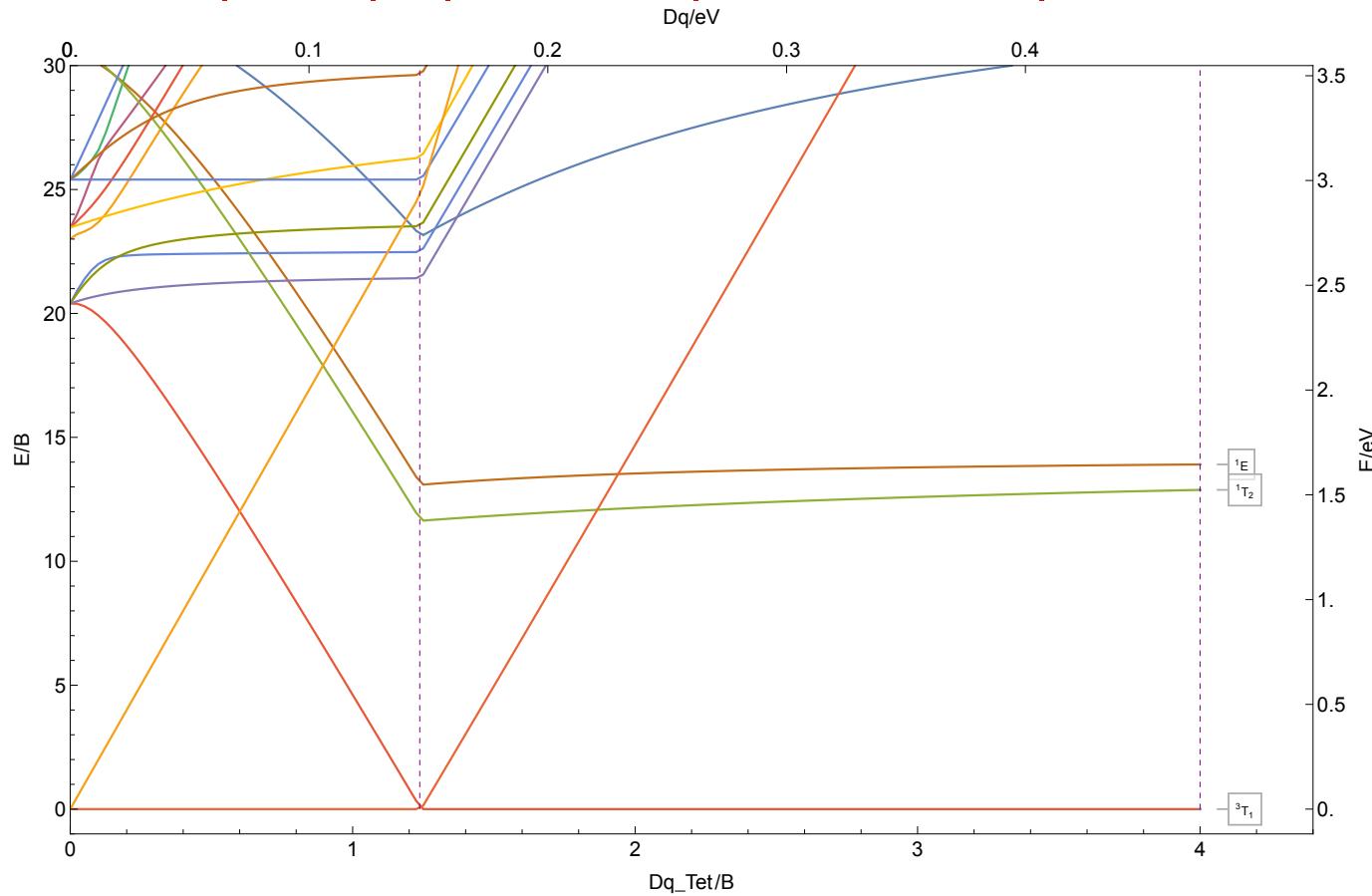
8.2.74 Cd<sup>5+</sup>

|2,4|d<sup>7</sup>| C/B ≈ 4.1| B ≈ 923 cm<sup>-1</sup> |Cd<sup>5+</sup>



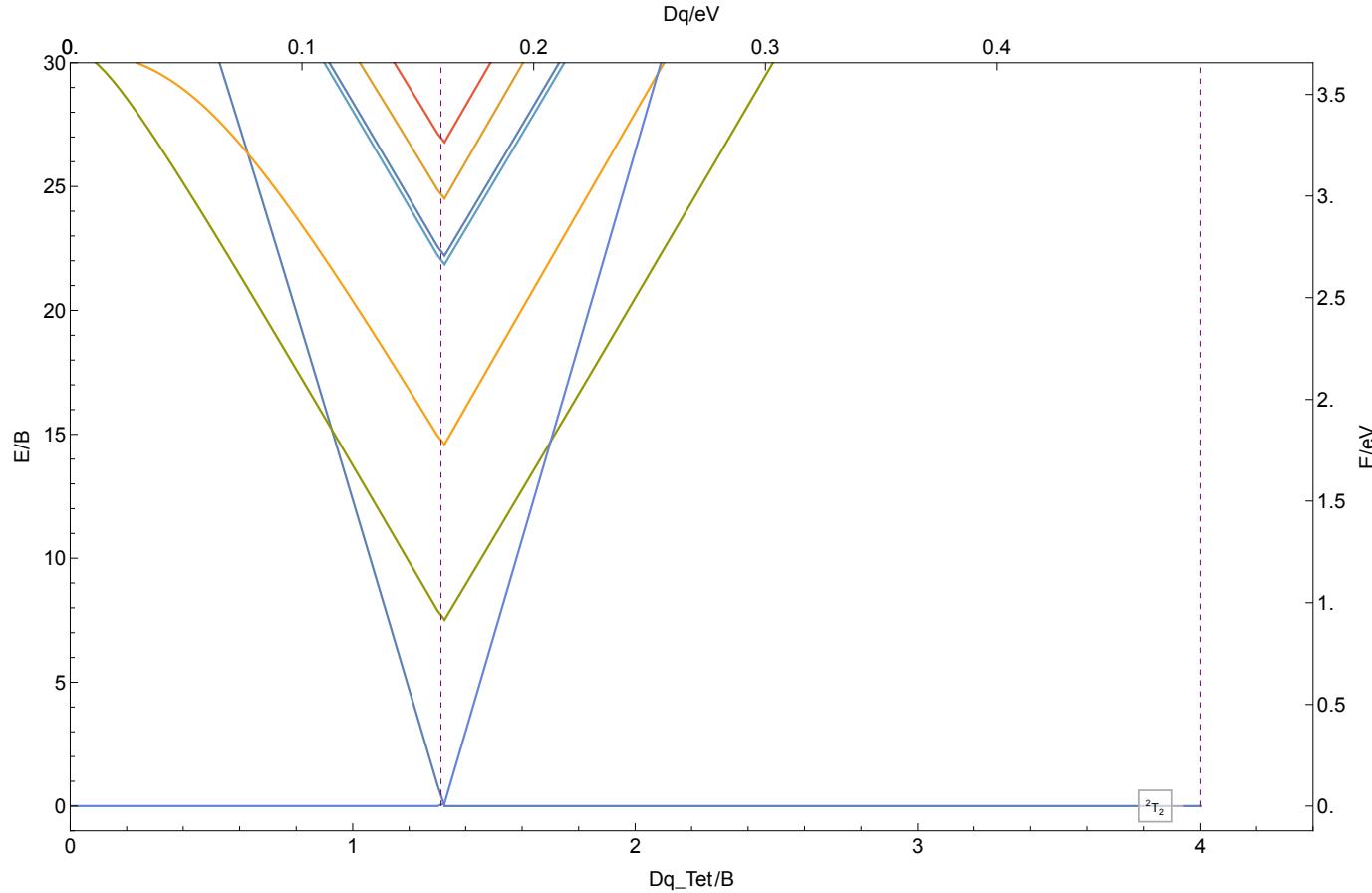
8.2.75 Cd<sup>6+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4.1 | B ≈ 954 cm<sup>-1</sup> | Cd<sup>6+</sup>



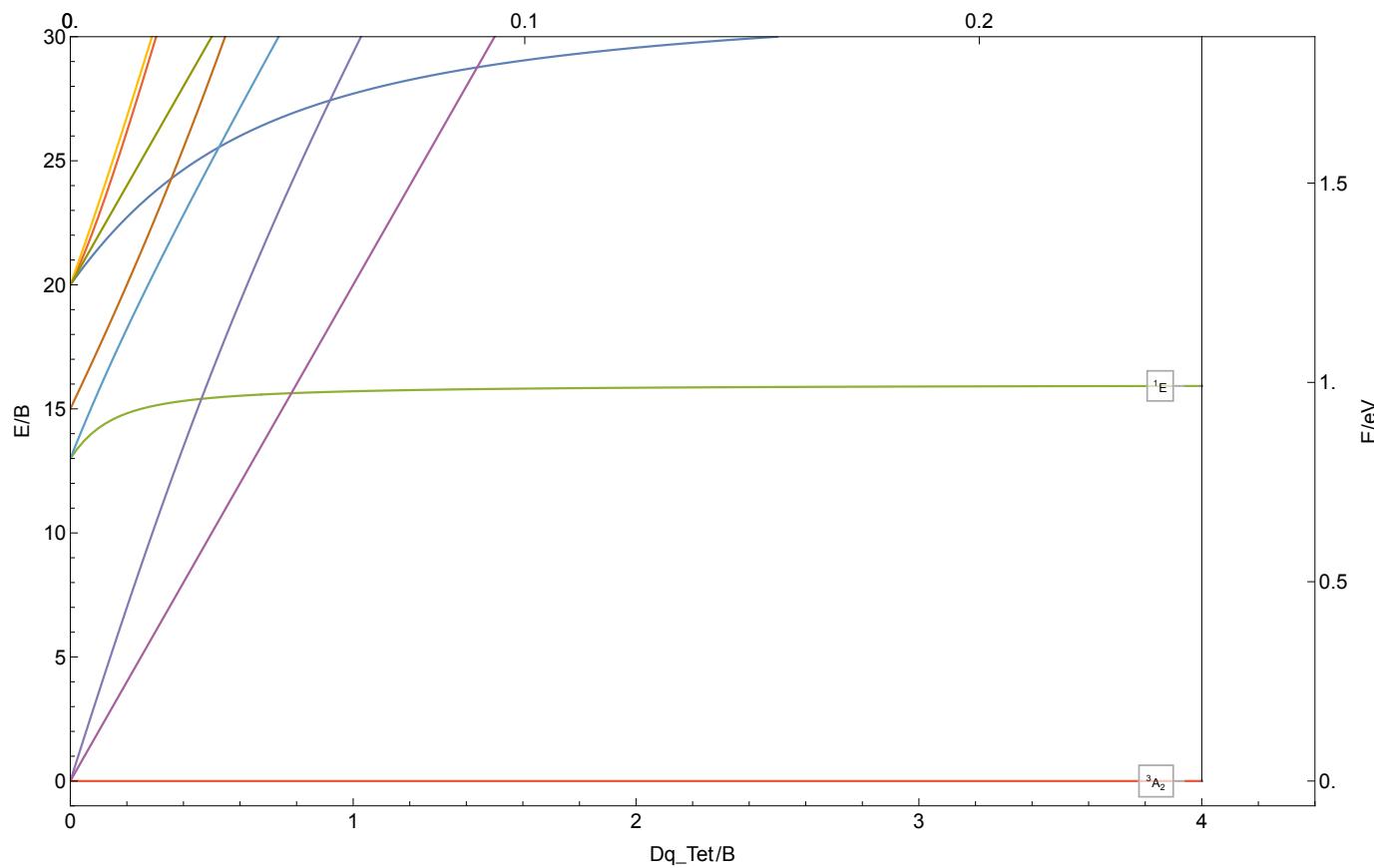
8.2.76 Cd<sup>7+</sup>

|2,4,6| d<sup>5</sup>| C/B ≈ 4.1| B ≈ 983 cm<sup>-1</sup> |Cd<sup>7+</sup>



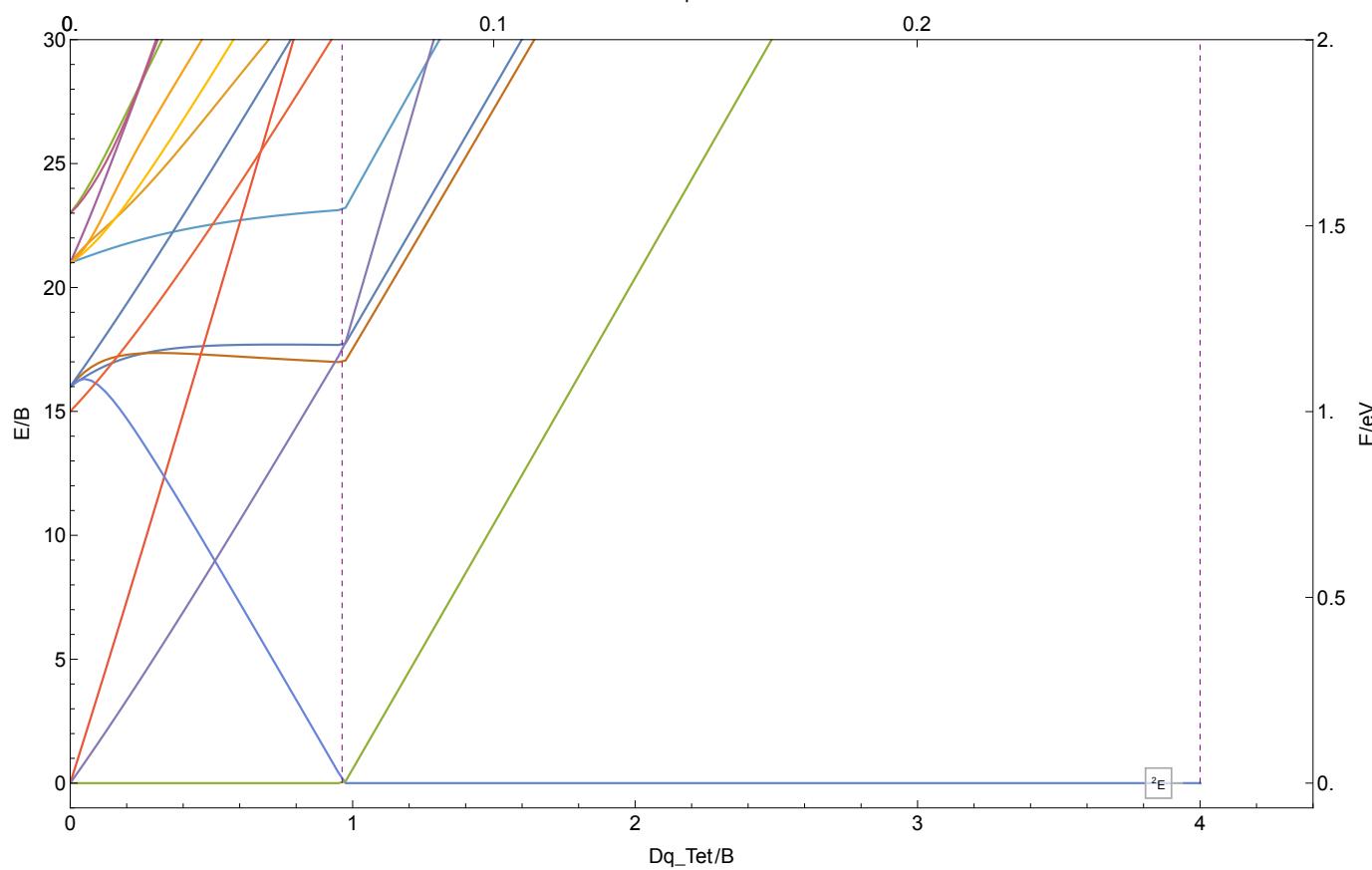
8.2.77  $\text{Hf}^{2+}$

$|1,3|d^2|$  C/B  $\approx 4.$  | B  $\approx 502 \text{ cm}^{-1}$  |  $\text{Hf}^{2+}$



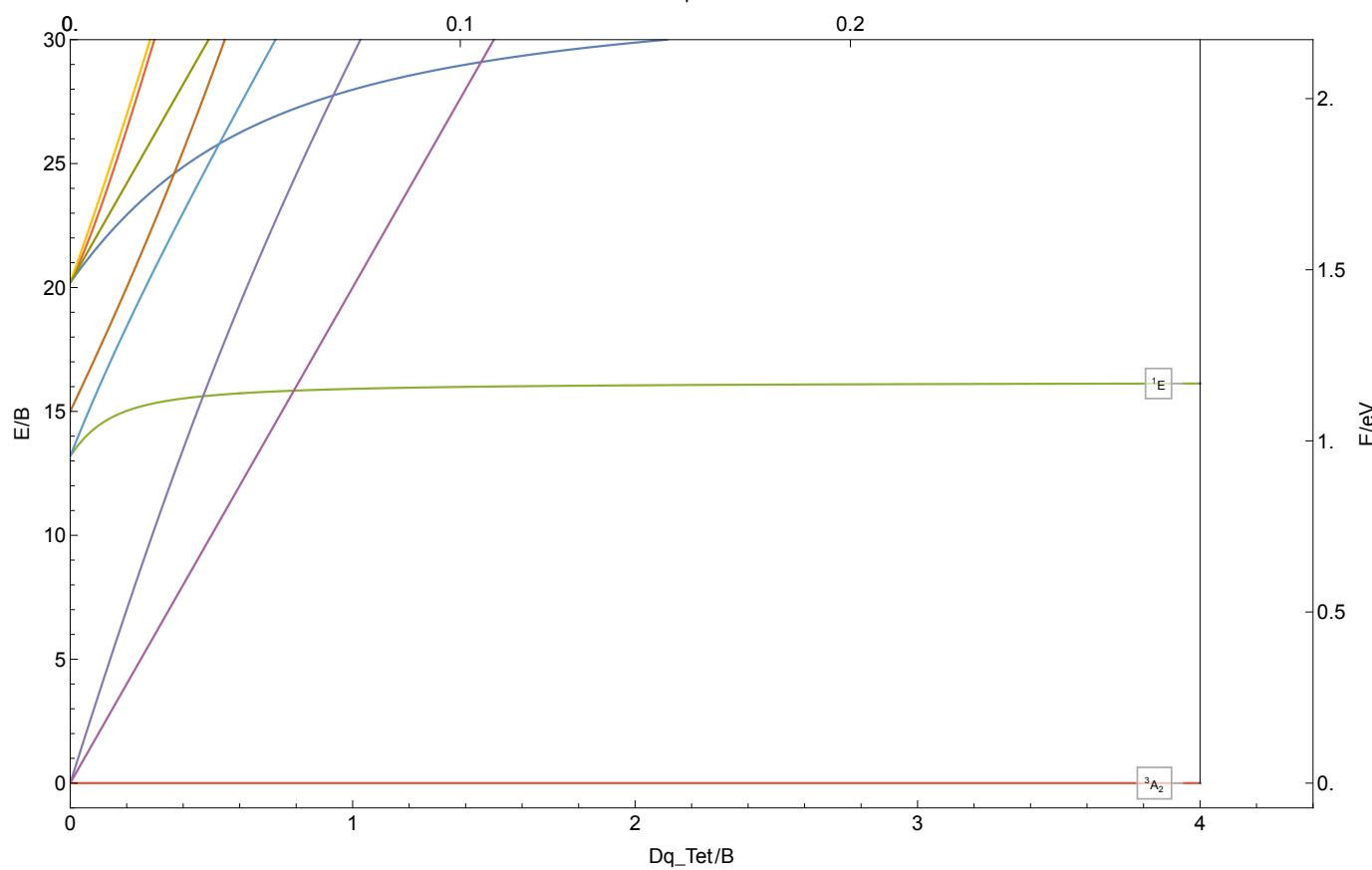
8.2.78  $Ta^{2+}$

$|2,4|d^3|C/B \approx 4. |B \approx 538\text{ cm}^{-1}|Ta^{2+}$



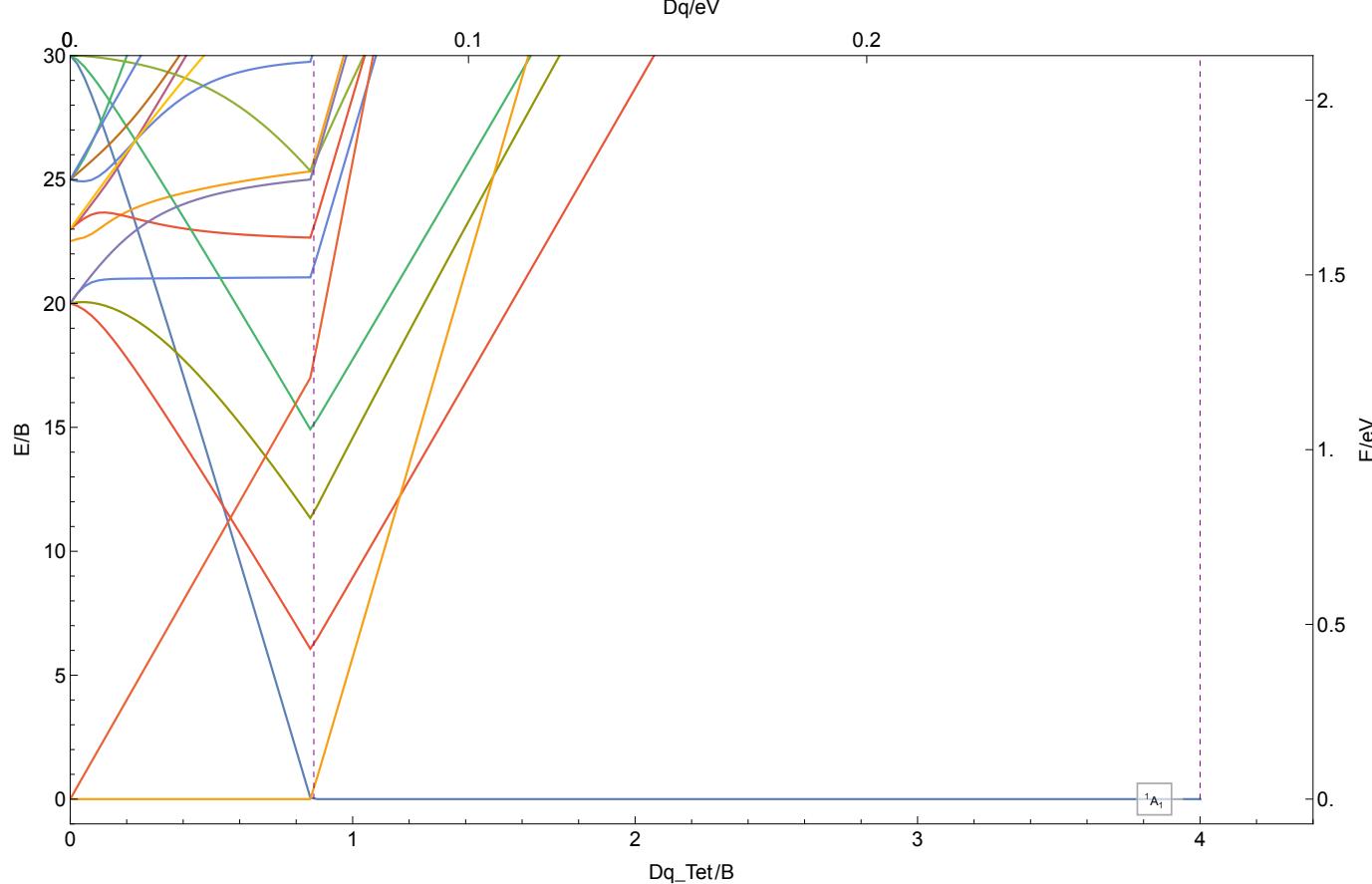
8.2.79 Ta<sup>3+</sup>

| 1,3 | d<sup>2</sup> | C/B ≈ 4.1 | B ≈ 584 cm<sup>-1</sup> | Ta<sup>3+</sup>



8.2.80  $W^{2+}$

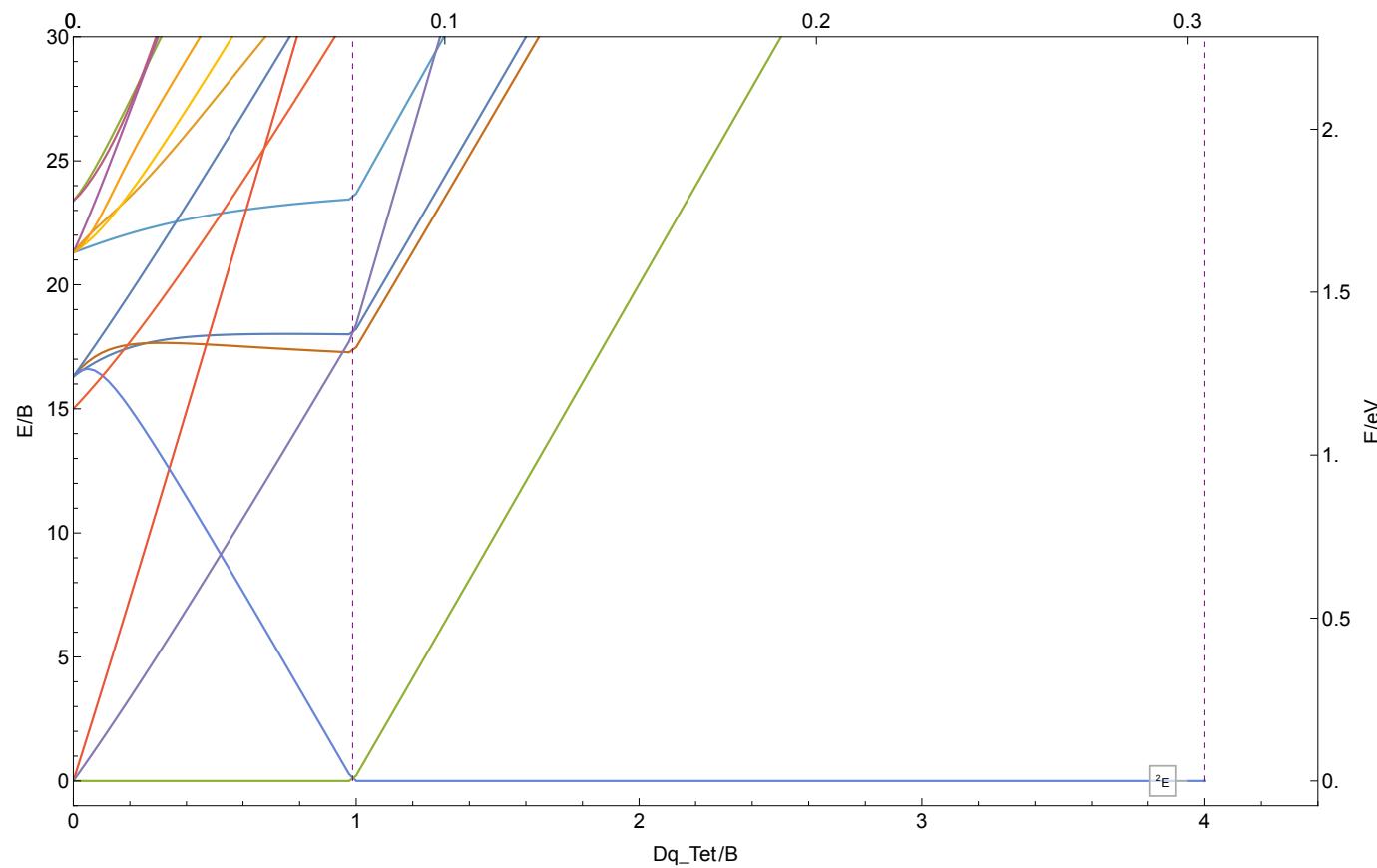
$|1,3,5|d^4|C/B \approx 4. |B \approx 572\text{ cm}^{-1}|W^{2+}$



8.2.81  $\text{W}^{3+}$

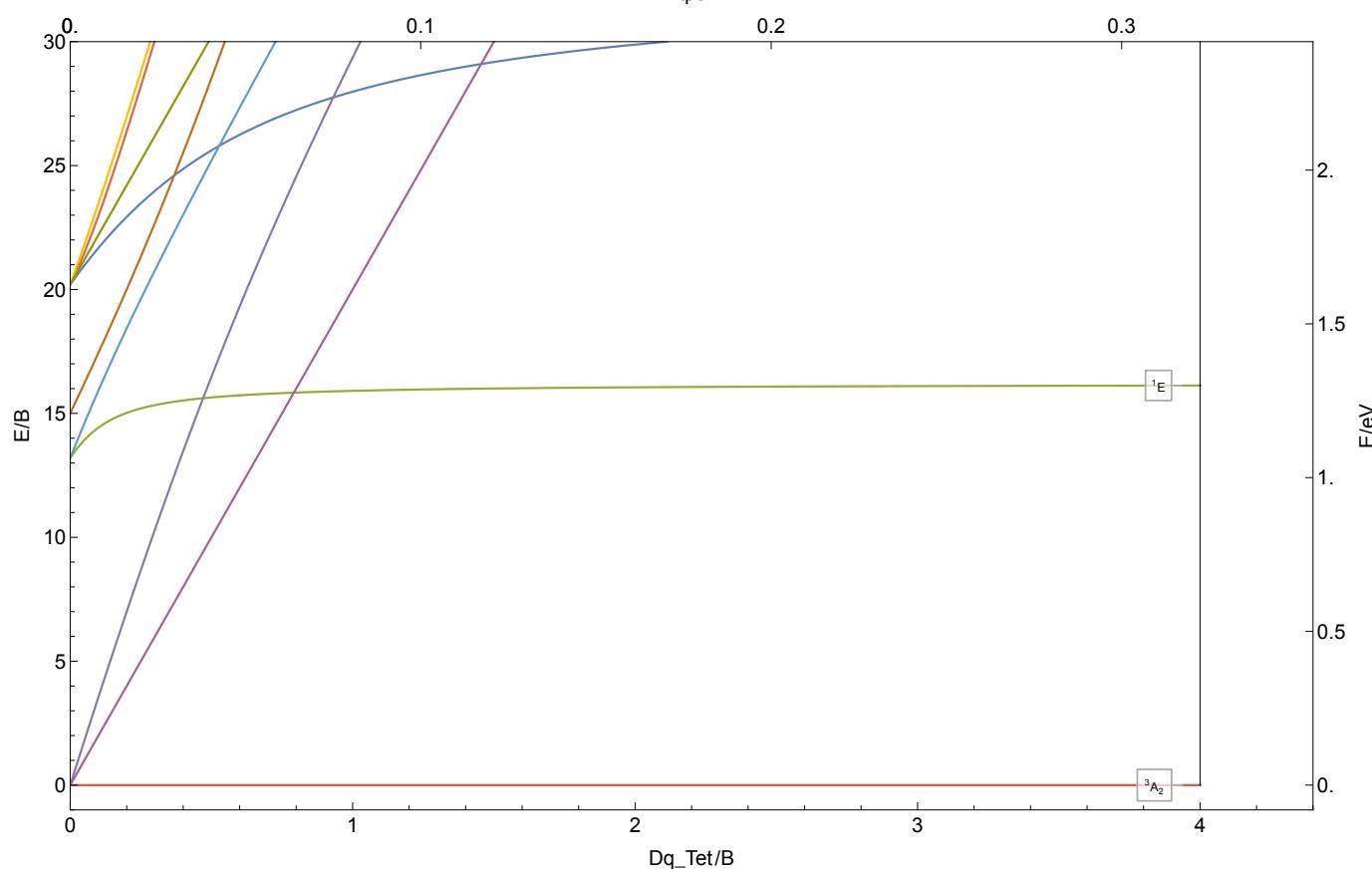
$$|2,4|\text{d}^3|\text{C/B} \approx 4.1|\text{B} \approx 614\text{ cm}^{-1}| \text{W}^{3+}$$

Dq/eV



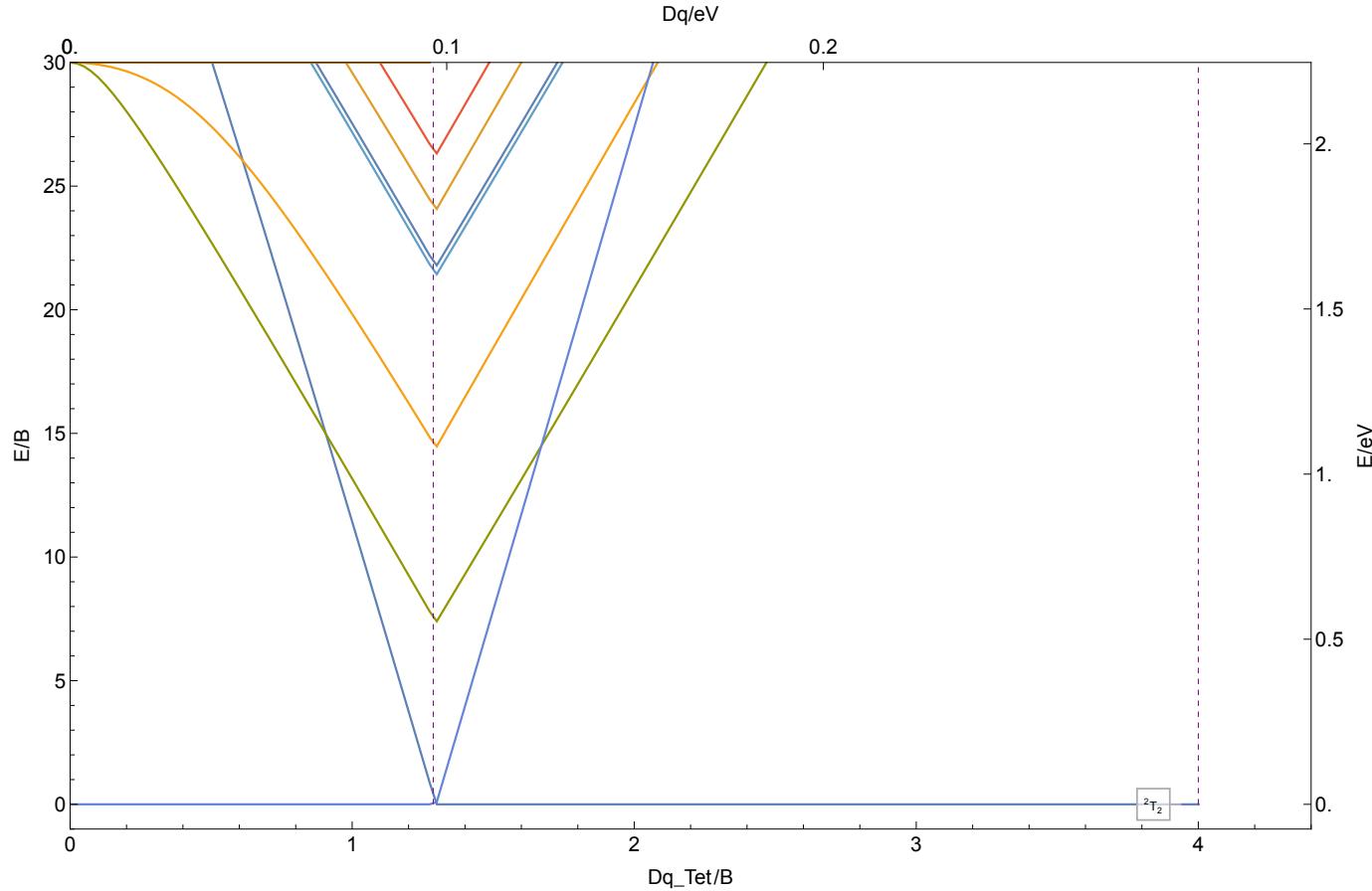
8.2.82 W<sup>4+</sup>

$$|1,3|d^2|C/B \approx 4.1|B \approx 650\text{ cm}^{-1}|W^{4+}$$



8.2.83  $\text{Re}^{2+}$

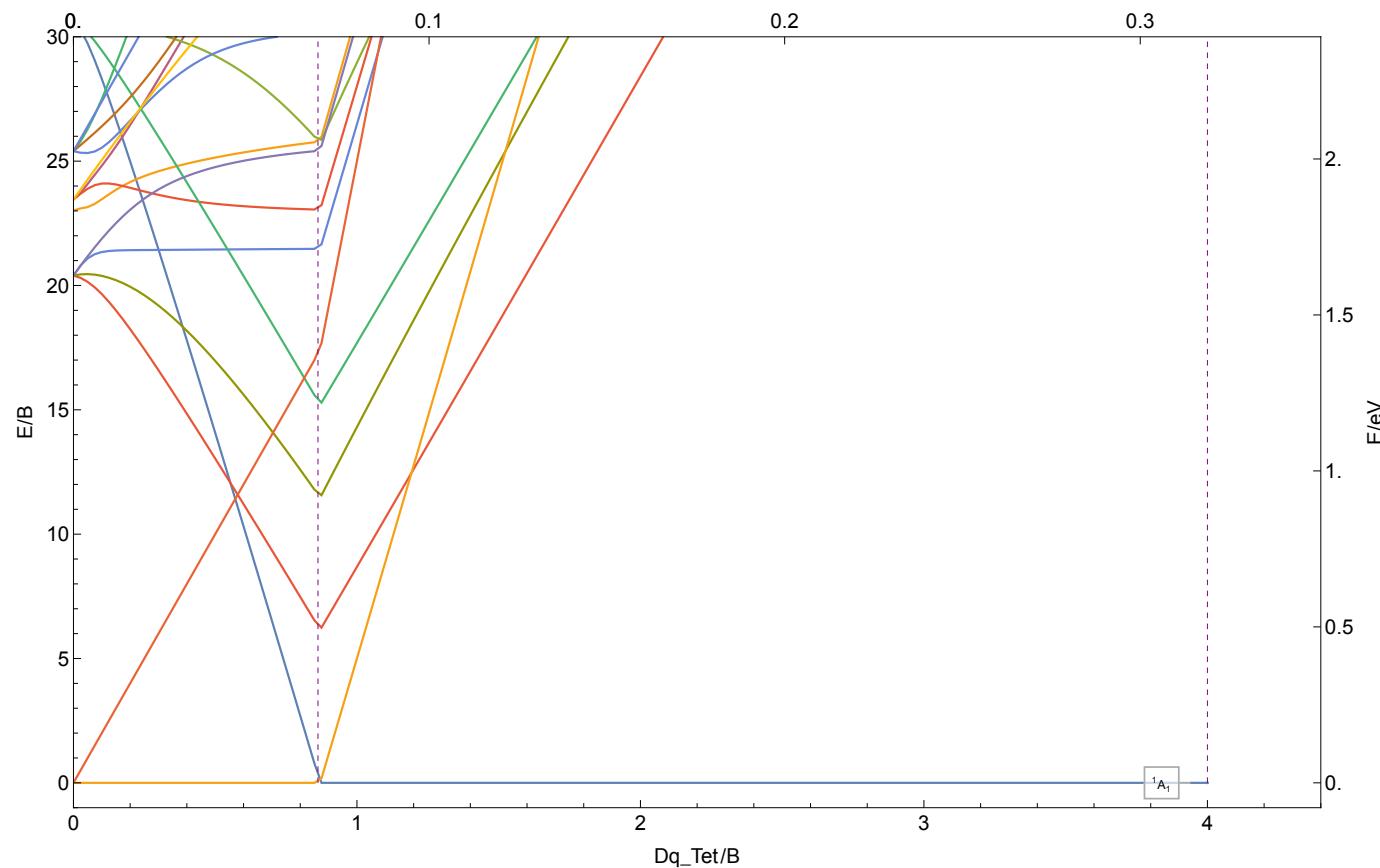
$|2,4,6|d^5|C/B \approx 4. | B \approx 604 \text{ cm}^{-1}| \text{Re}^{2+}$



8.2.84  $\text{Re}^{3+}$

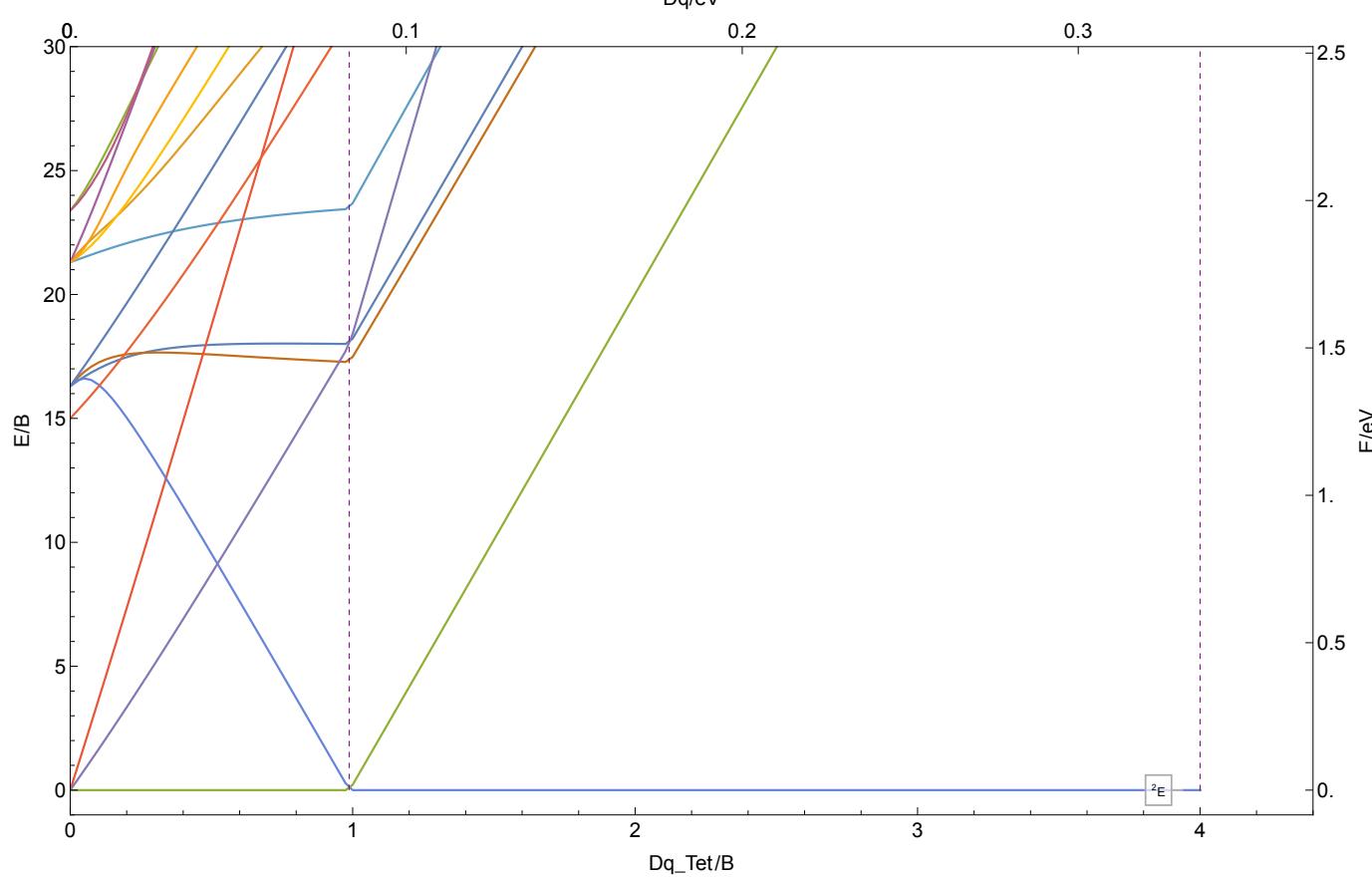
$|1,3,5|d^4|C/B \approx 4.1|B \approx 643 \text{ cm}^{-1}| \text{Re}^{3+}$

$Dq/\text{eV}$



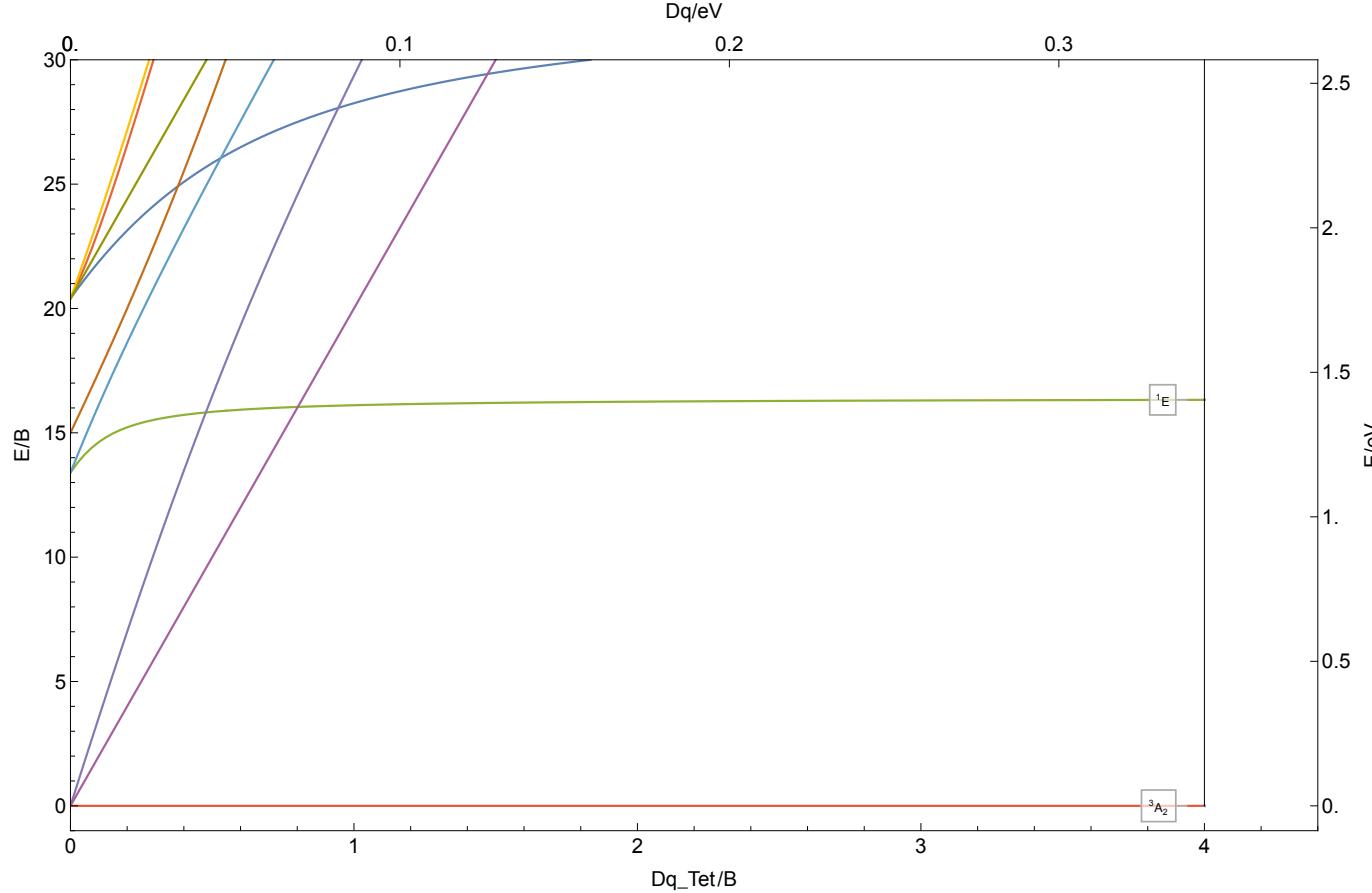
8.2.85 Re<sup>4+</sup>

|2,4|d<sup>3</sup>| C/B ≈ 4.1| B ≈ 678 cm<sup>-1</sup> |Re<sup>4+</sup>



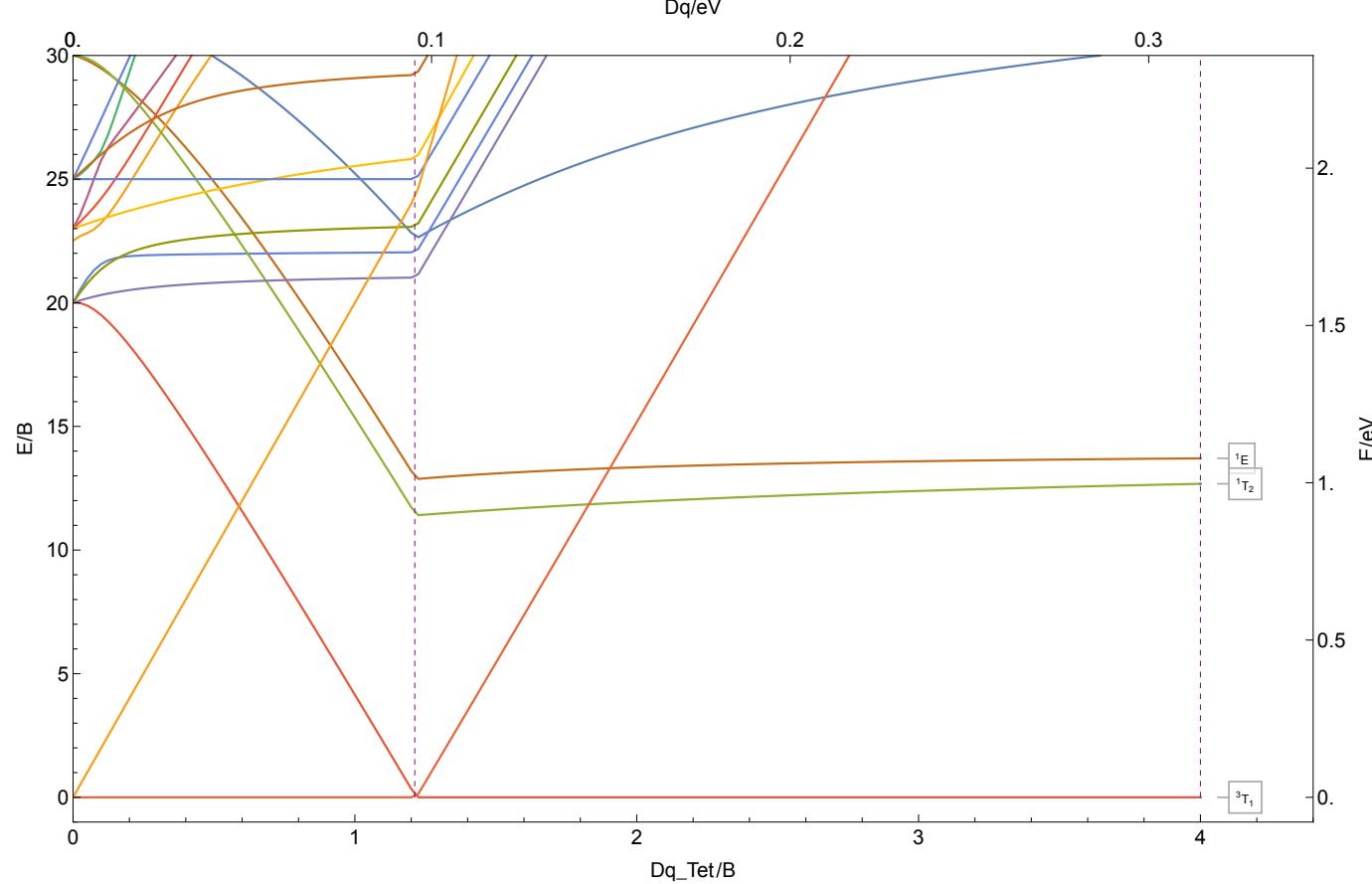
8.2.86 Re<sup>5+</sup>

$$|1,3|d^2|C/B \approx 4.2|B \approx 694\text{ cm}^{-1}|Re^{5+}$$



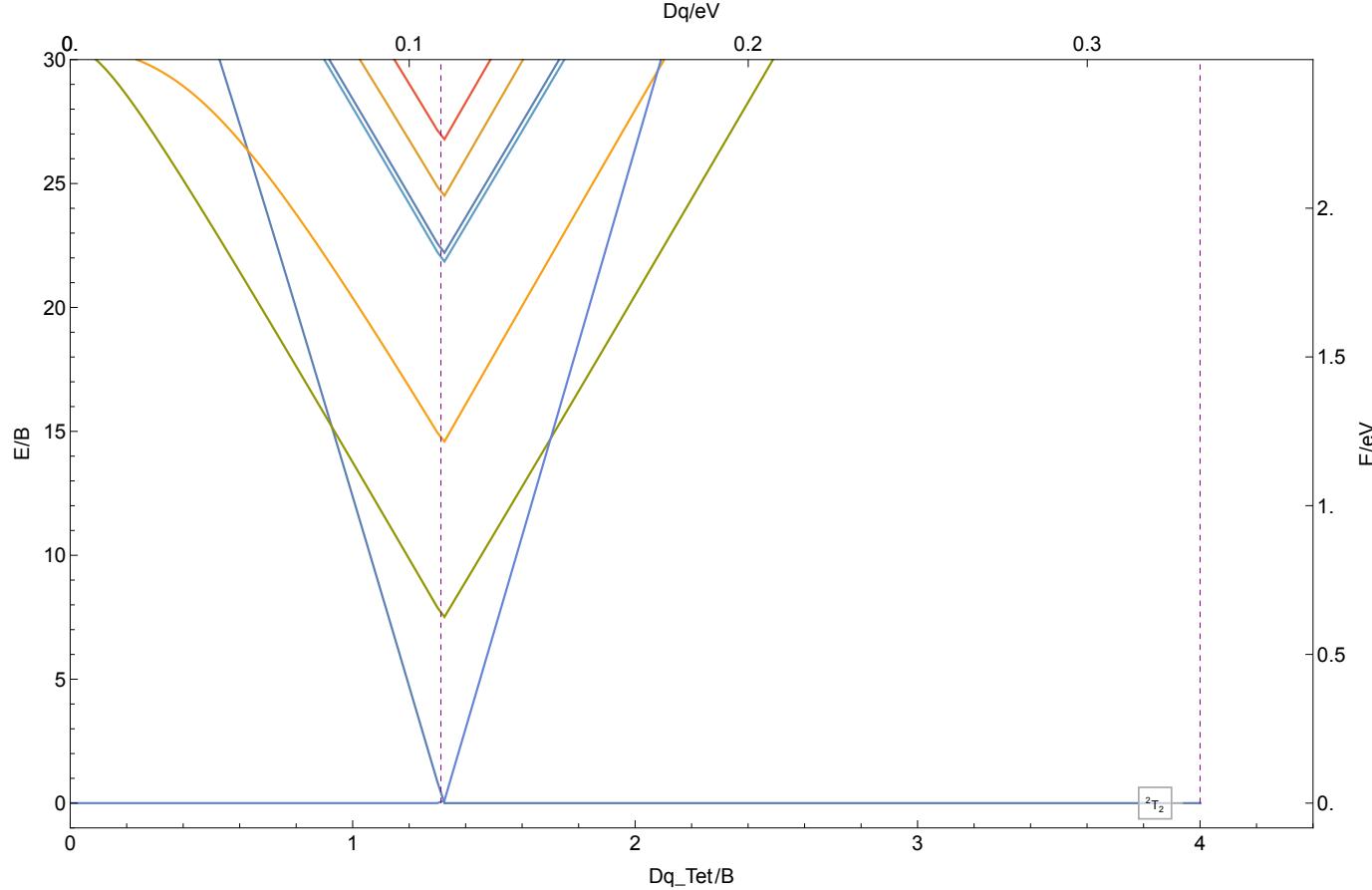
8.2.87 Os<sup>2+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4. | B ≈ 634 cm<sup>-1</sup> | Os<sup>2+</sup>



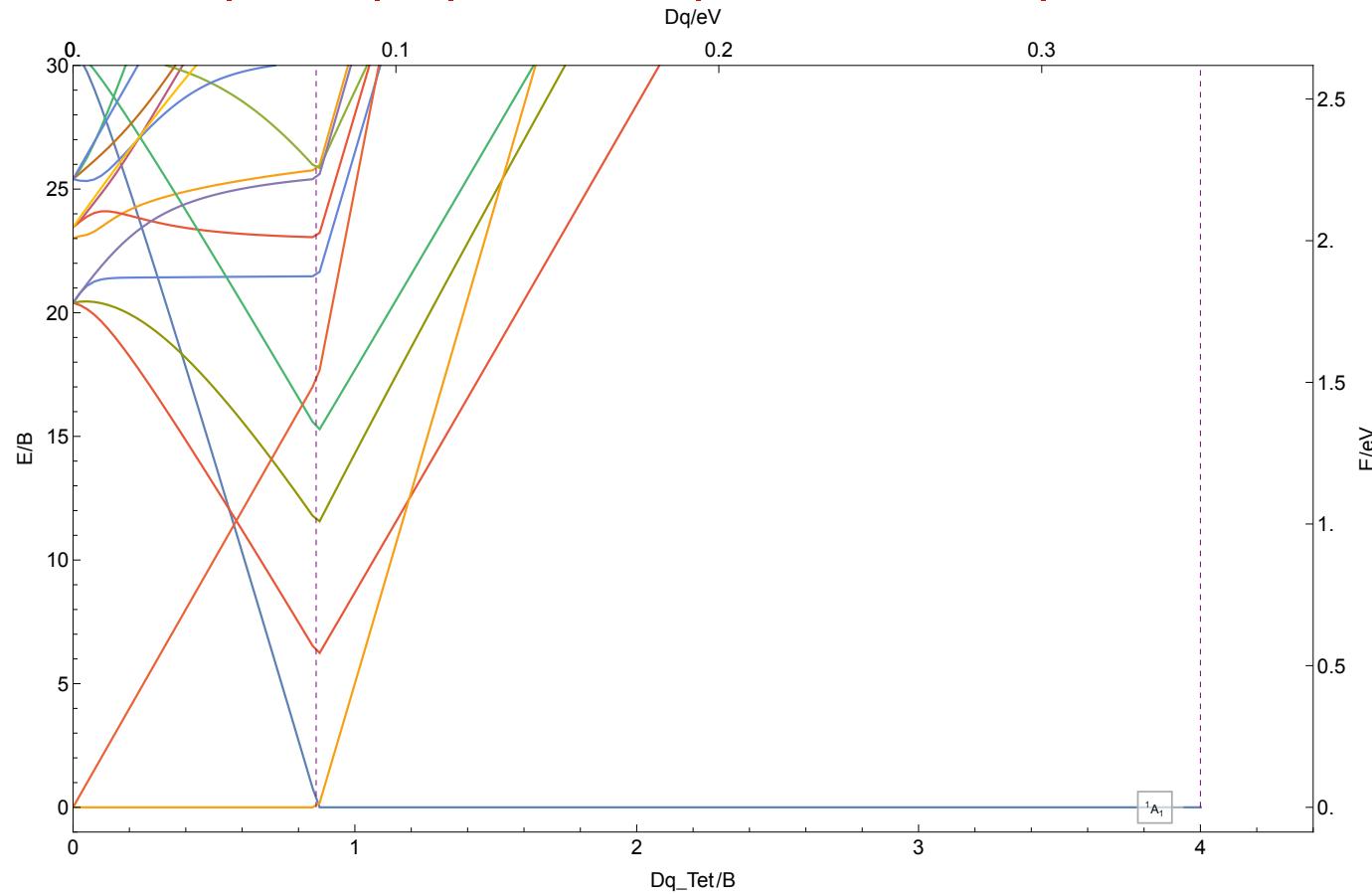
8.2.88 Os<sup>3+</sup>

|2,4,6| d<sup>5</sup>| C/B ≈ 4.1| B ≈ 672 cm<sup>-1</sup> | Os<sup>3+</sup>



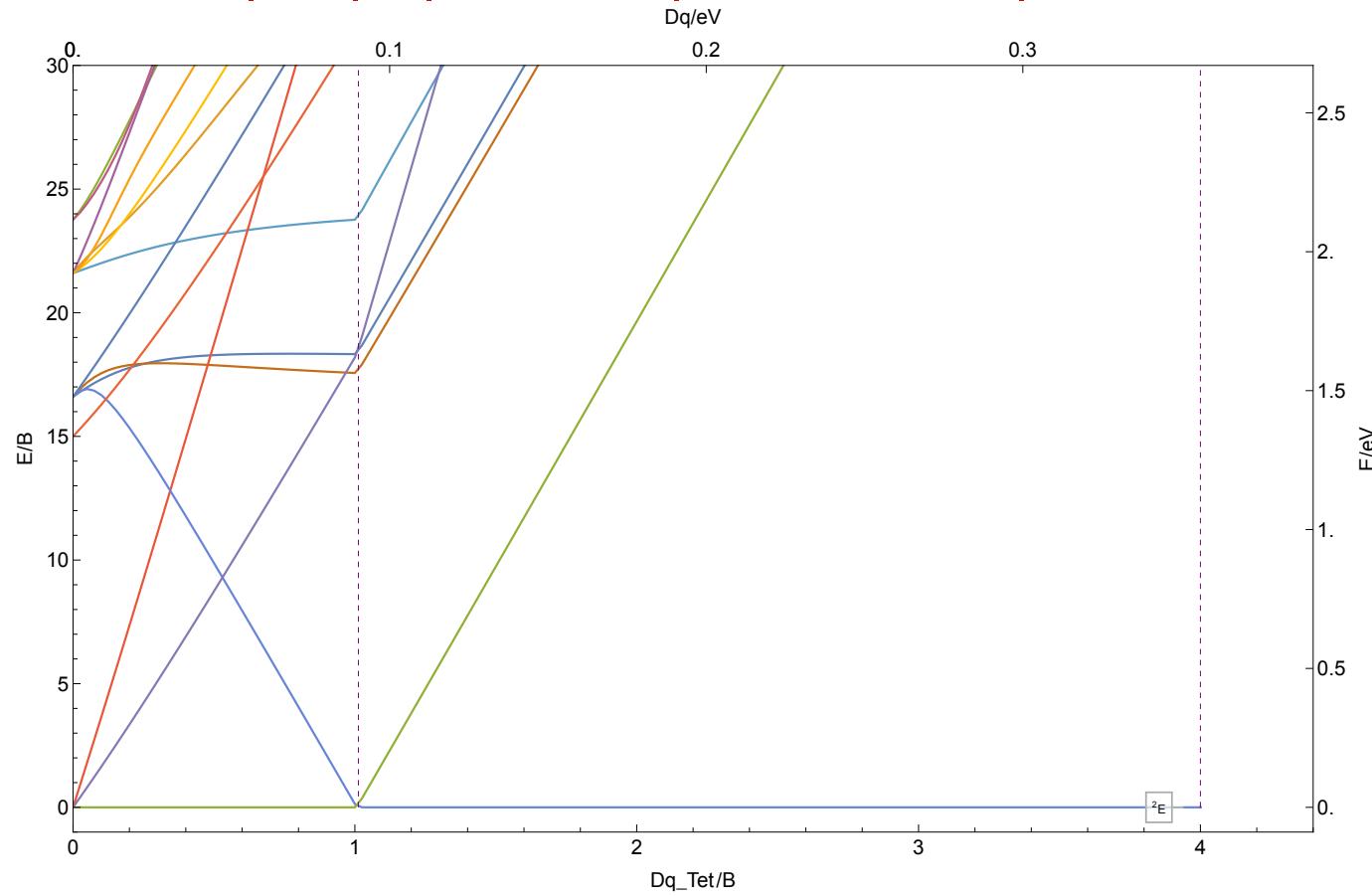
8.2.89 Os<sup>4+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 4.1 | B ≈ 704 cm<sup>-1</sup> | Os<sup>4+</sup>



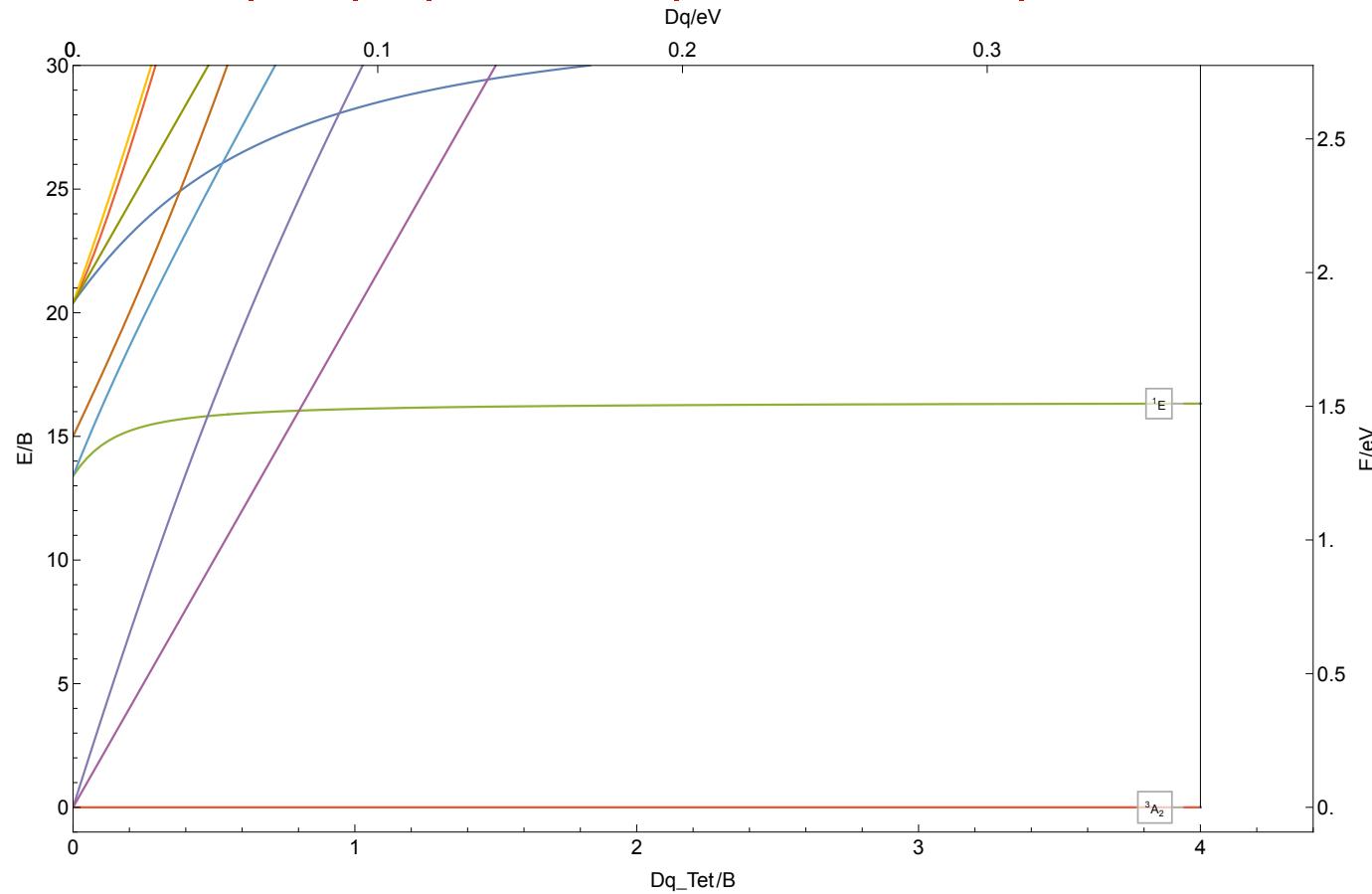
8.2.90 Os<sup>5+</sup>

|2,4|d<sup>3</sup>| C/B ≈ 4.2| B ≈ 718 cm<sup>-1</sup> |Os<sup>5+</sup>



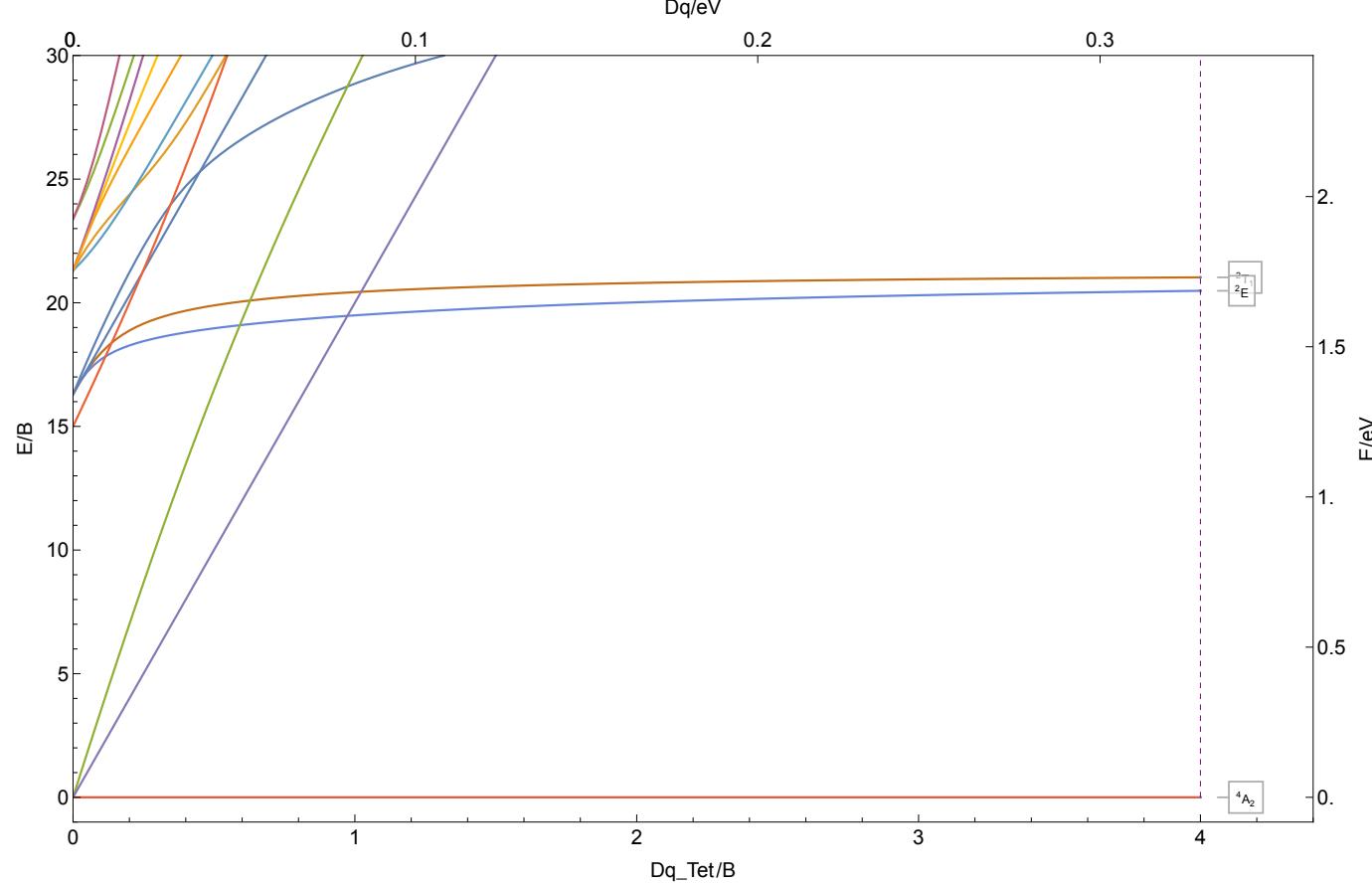
8.2.91 Os<sup>6+</sup>

| 1,3 | d<sup>2</sup> | C/B ≈ 4.2 | B ≈ 746 cm<sup>-1</sup> | Os<sup>6+</sup>



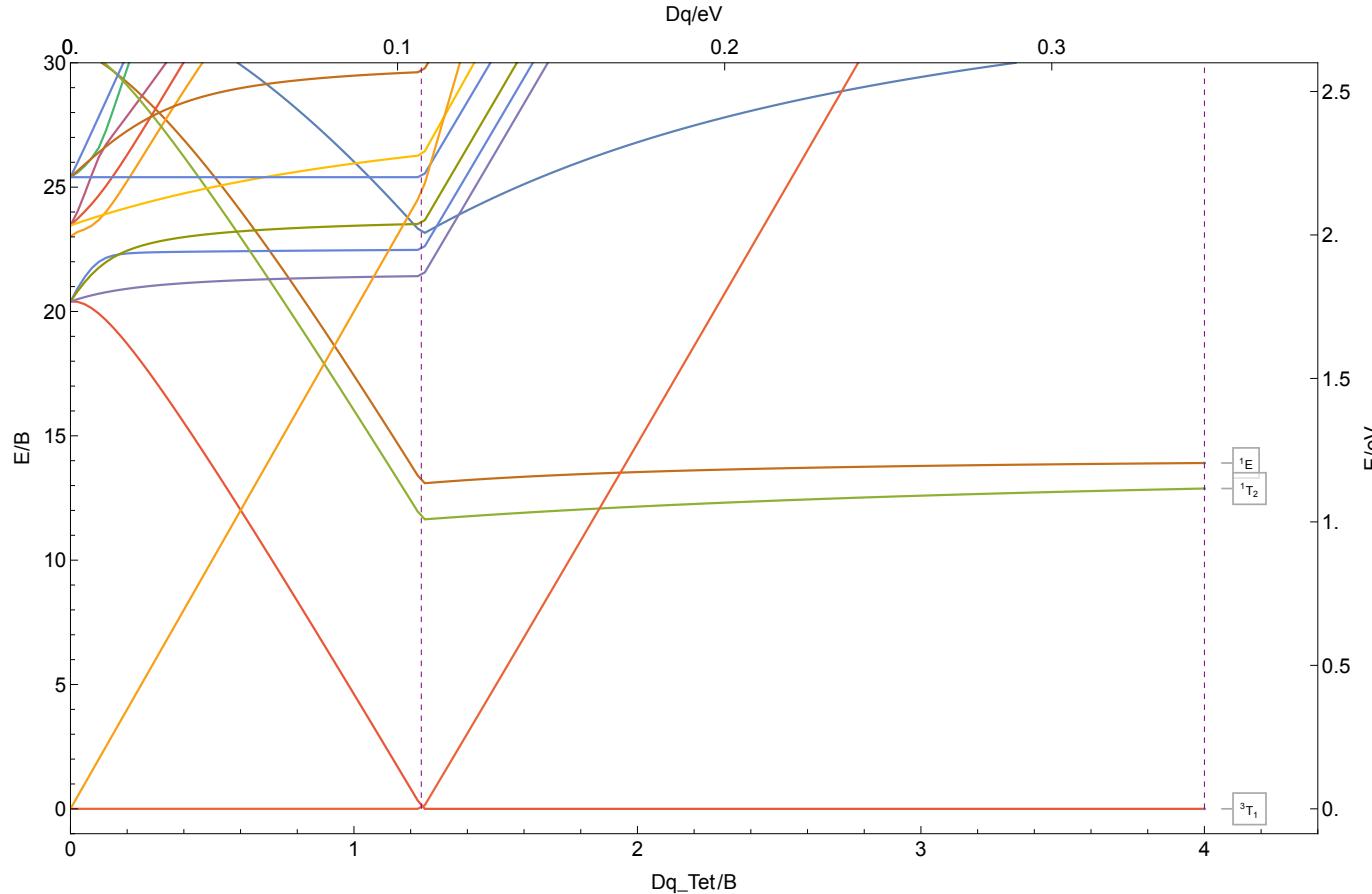
8.2.92 Ir<sup>2+</sup>

|2,4|d<sup>7</sup>|C/B ≈ 4.1|B ≈ 664 cm<sup>-1</sup>||Ir<sup>2+</sup>



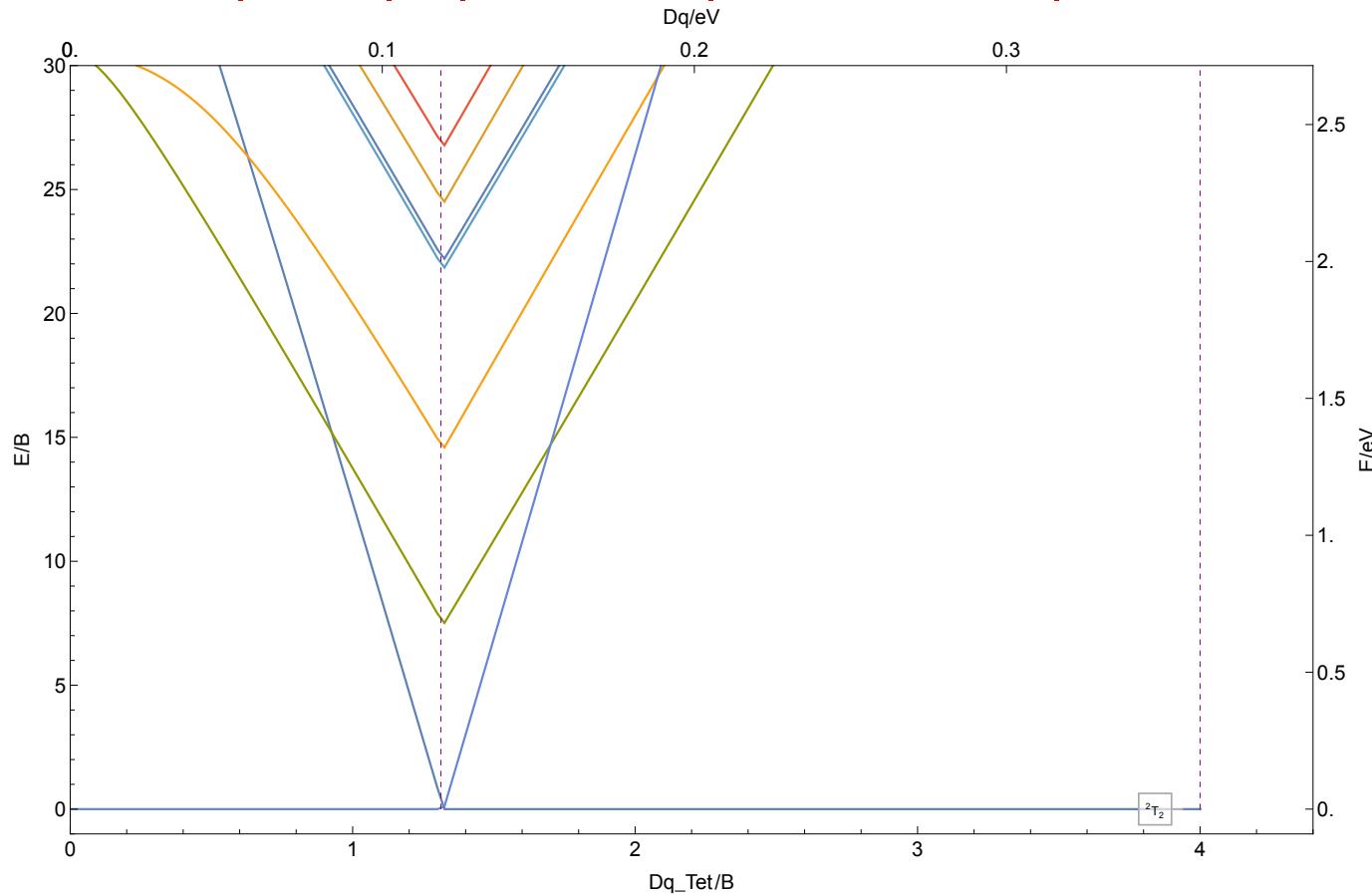
8.2.93 Ir<sup>3+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4.1 | B ≈ 699 cm<sup>-1</sup> | Ir<sup>3+</sup>



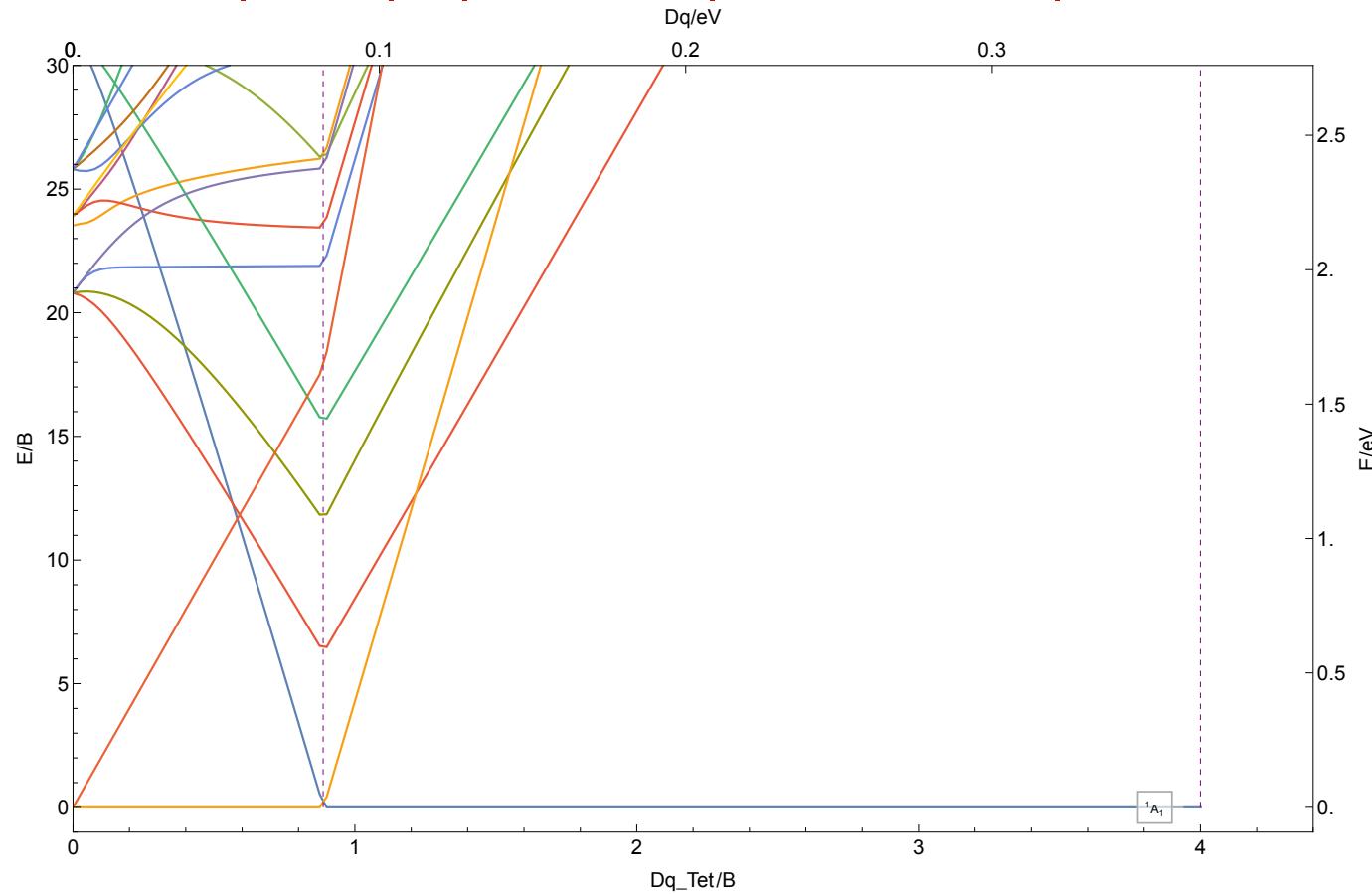
8.2.94 Ir<sup>4+</sup>

|2,4,6|d<sup>5</sup>|C/B ≈ 4.1|B ≈ 730 cm<sup>-1</sup>|Ir<sup>4+</sup>



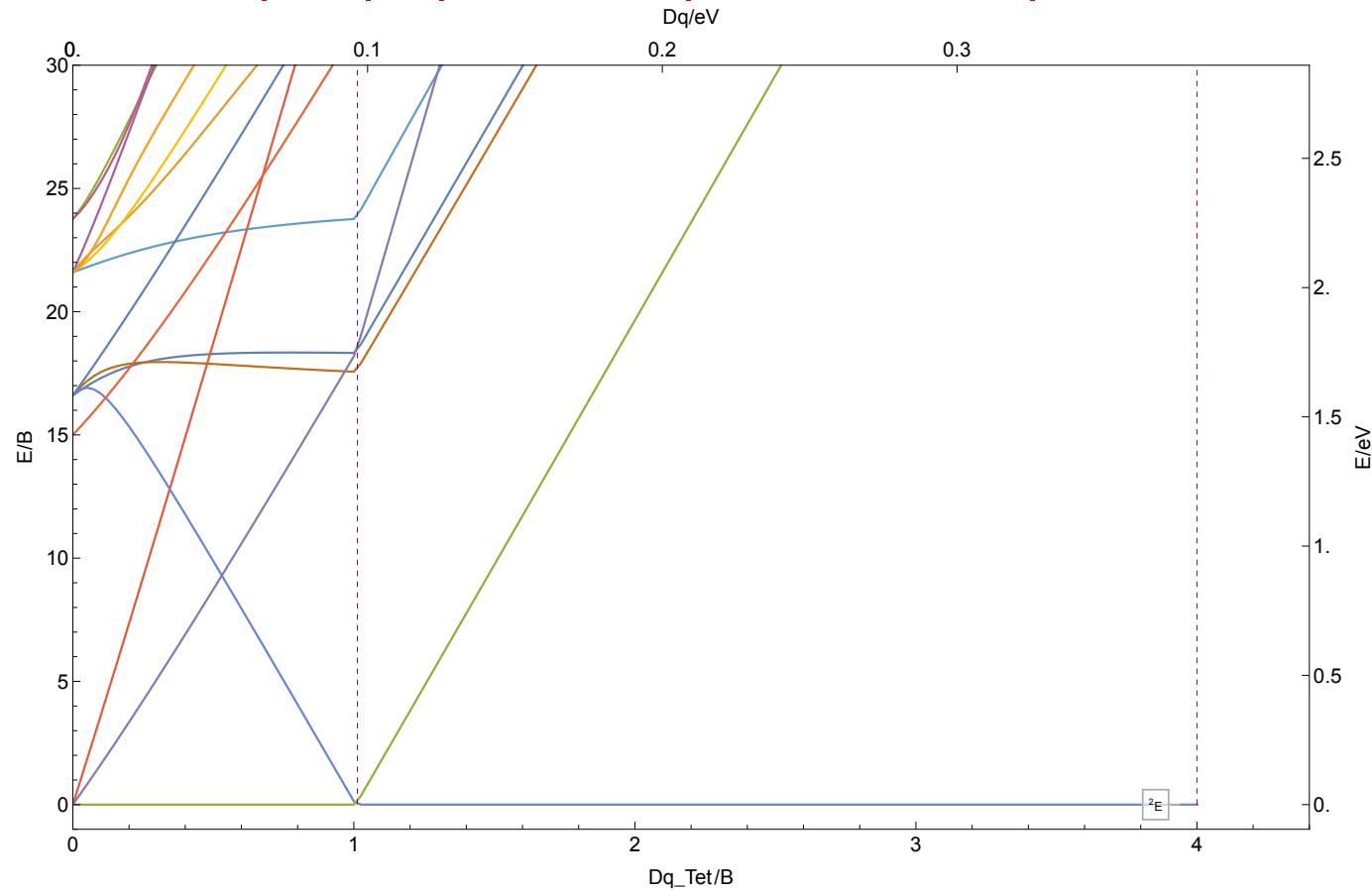
8.2.95 Ir<sup>5+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 4.2 | B ≈ 742 cm<sup>-1</sup> | Ir<sup>5+</sup>



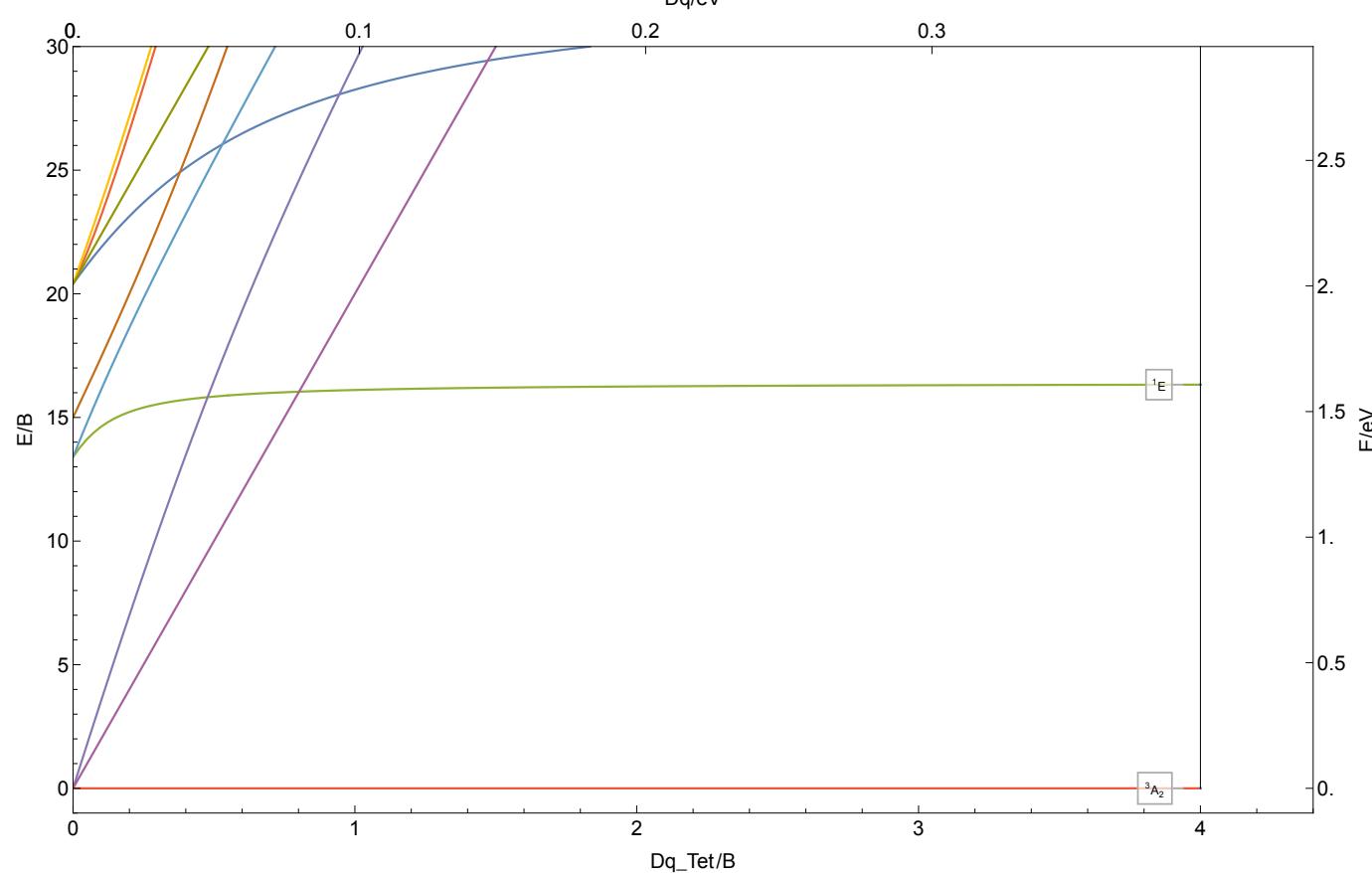
8.2.96 Ir<sup>6+</sup>

|2,4|d<sup>3</sup>| C/B ≈ 4.2 | B ≈ 769 cm<sup>-1</sup> | Ir<sup>6+</sup>



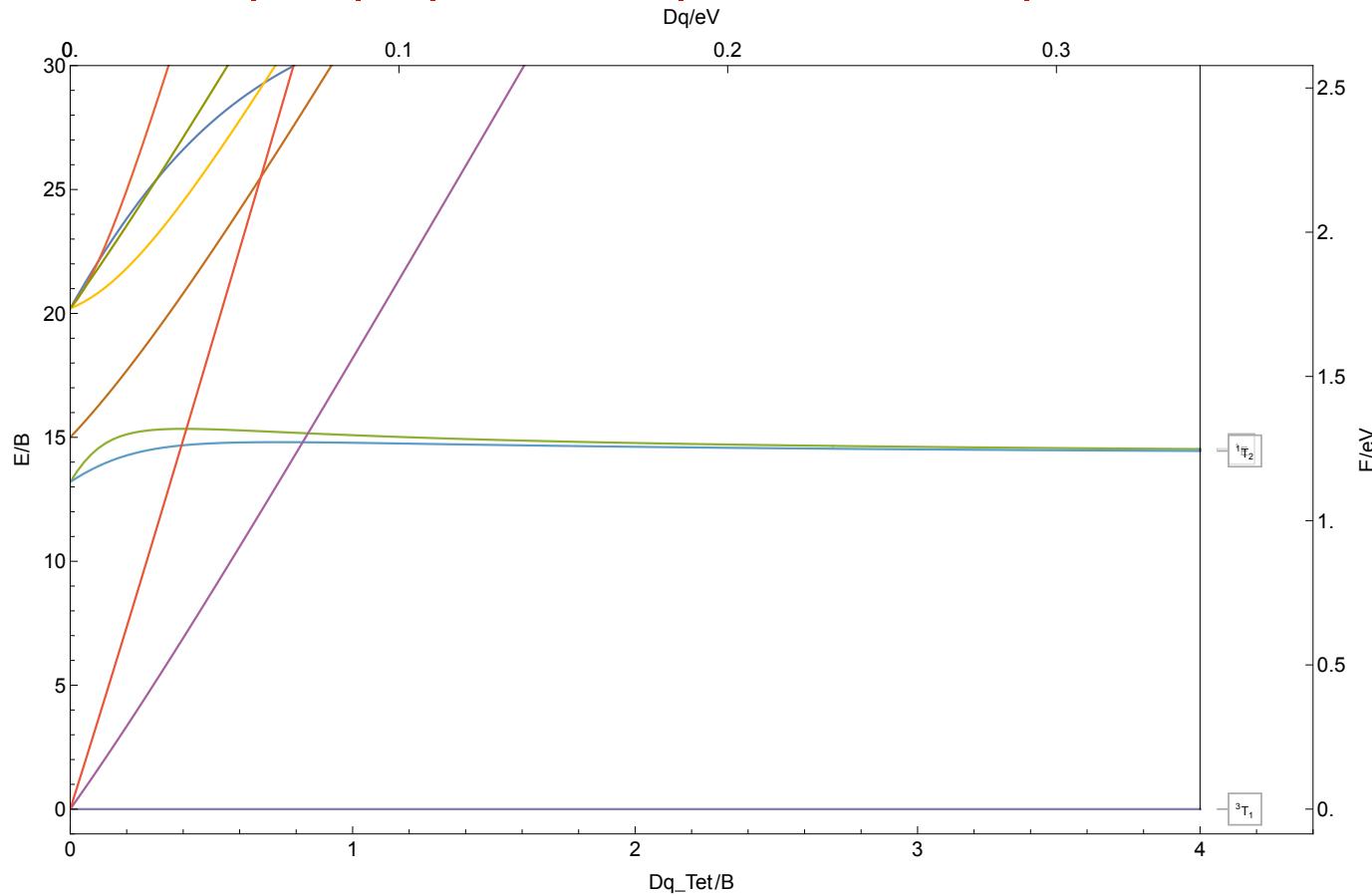
8.2.97 Ir<sup>7+</sup>

| 1,3 | d<sup>2</sup> | C/B ≈ 4.2 | B ≈ 794 cm<sup>-1</sup> | Ir<sup>7+</sup>



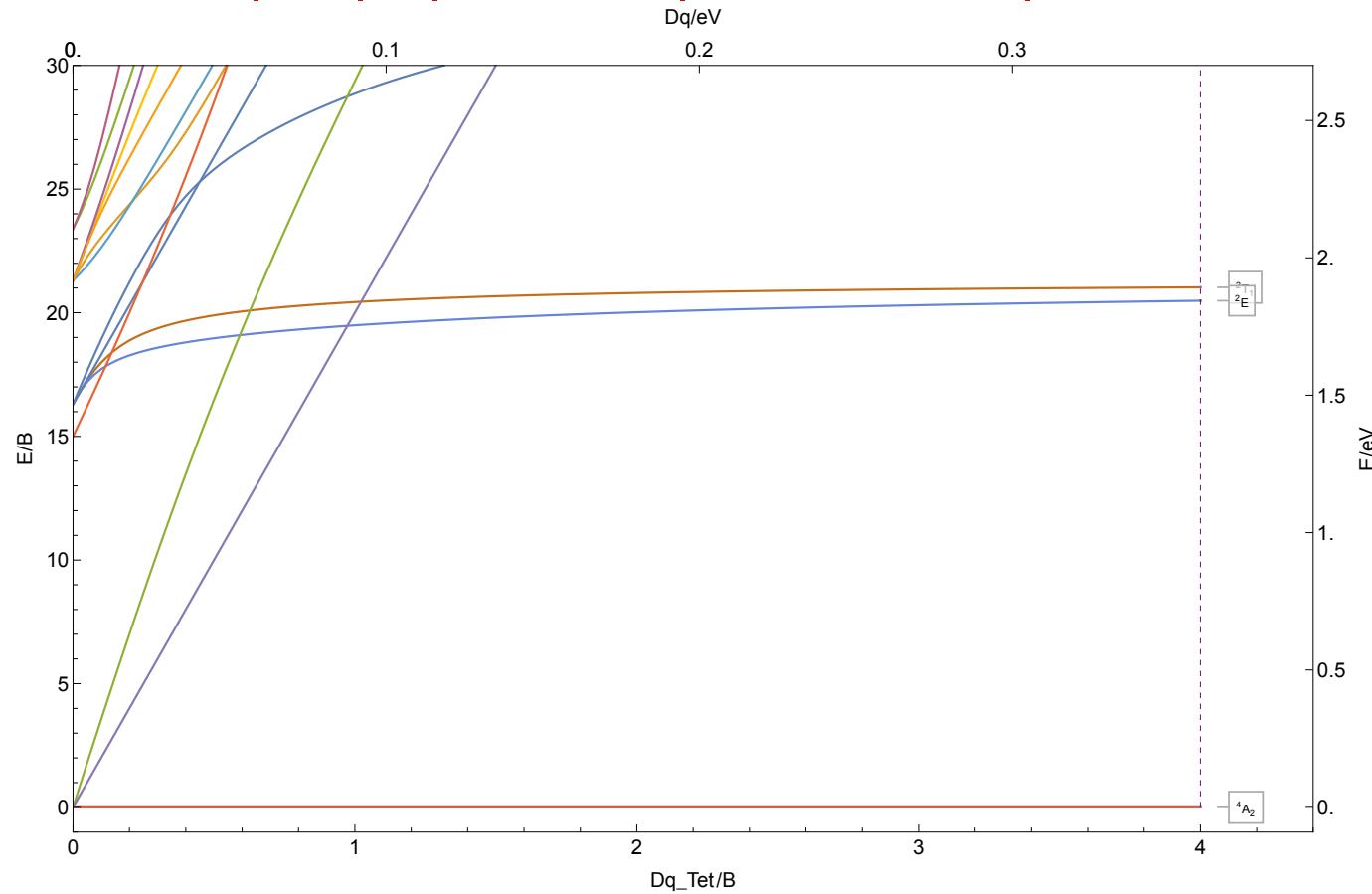
8.2.98 Pt<sup>2+</sup>

| 1,3 | d<sup>8</sup> | C/B ≈ 4.1 | B ≈ 693 cm<sup>-1</sup> | Pt<sup>2+</sup>



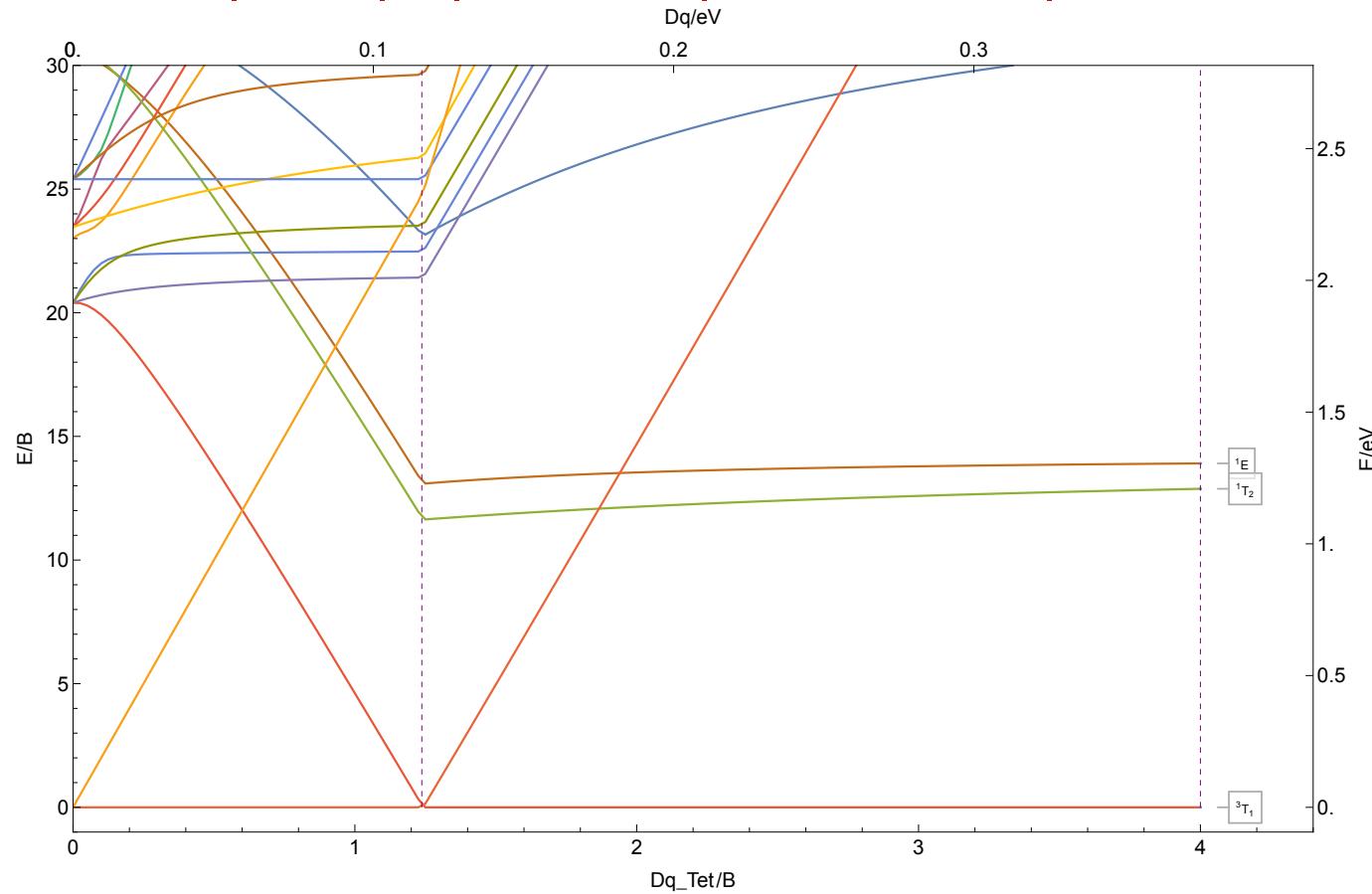
8.2.99 Pt<sup>3+</sup>

|2,4|d<sup>7</sup>|C/B ≈ 4.1|B ≈ 726 cm<sup>-1</sup>|Pt<sup>3+</sup>



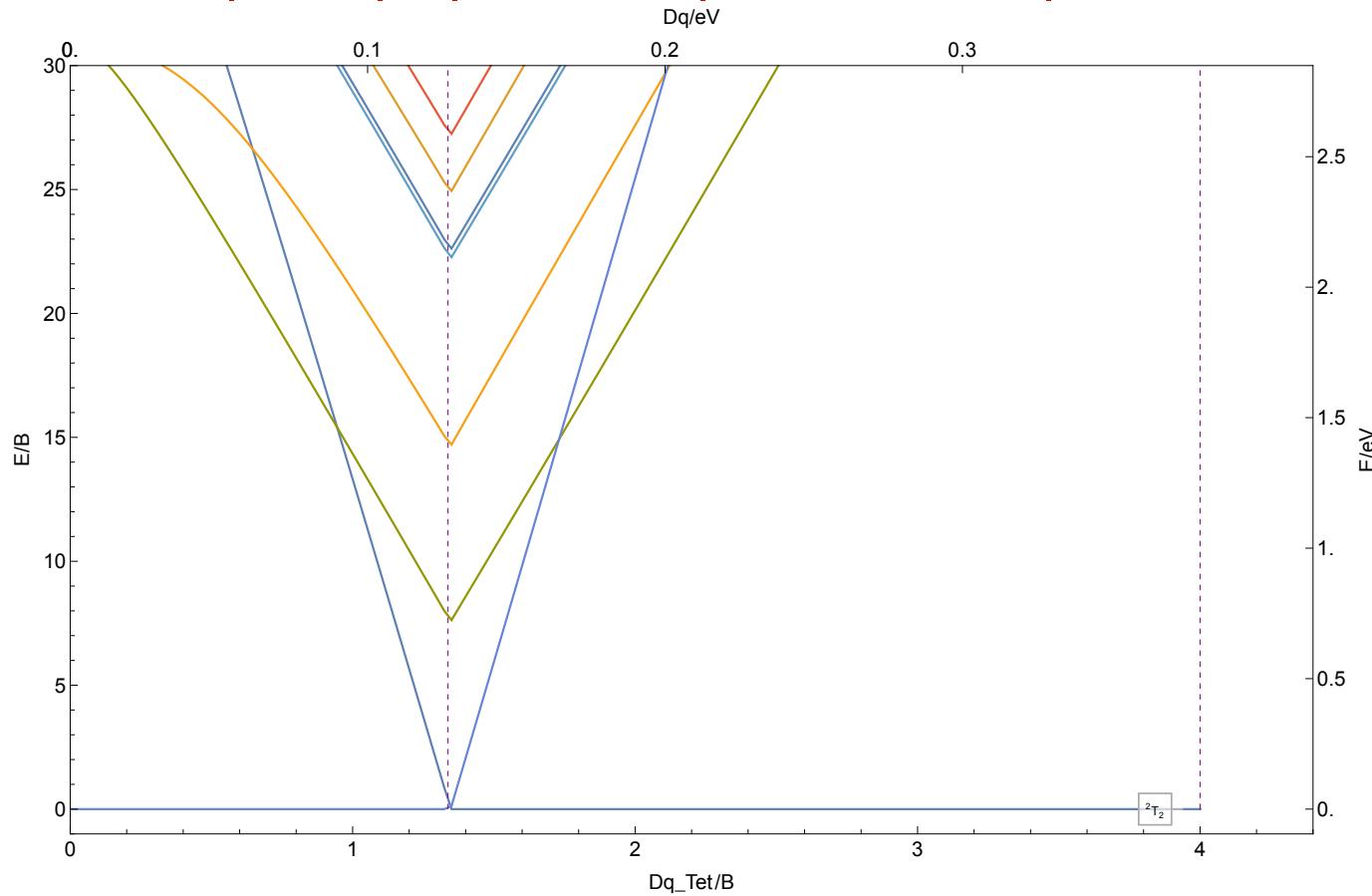
8.2.100 Pt<sup>4+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4.1 | B ≈ 757 cm<sup>-1</sup> | Pt<sup>4+</sup>



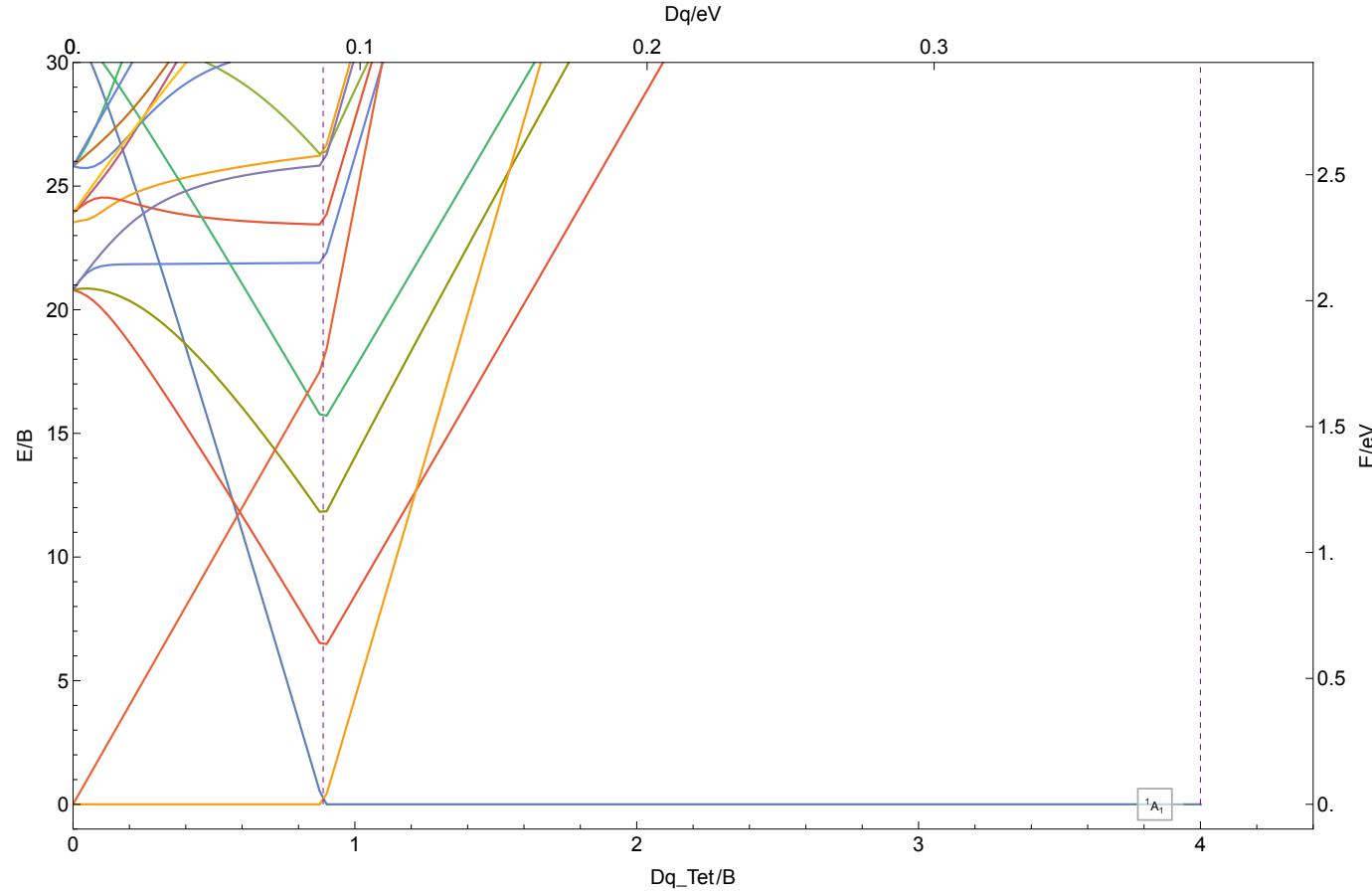
8.2.101 Pt<sup>5+</sup>

|2,4,6| d<sup>5</sup>| C/B ≈ 4.2| B ≈ 766 cm<sup>-1</sup> | Pt<sup>5+</sup>



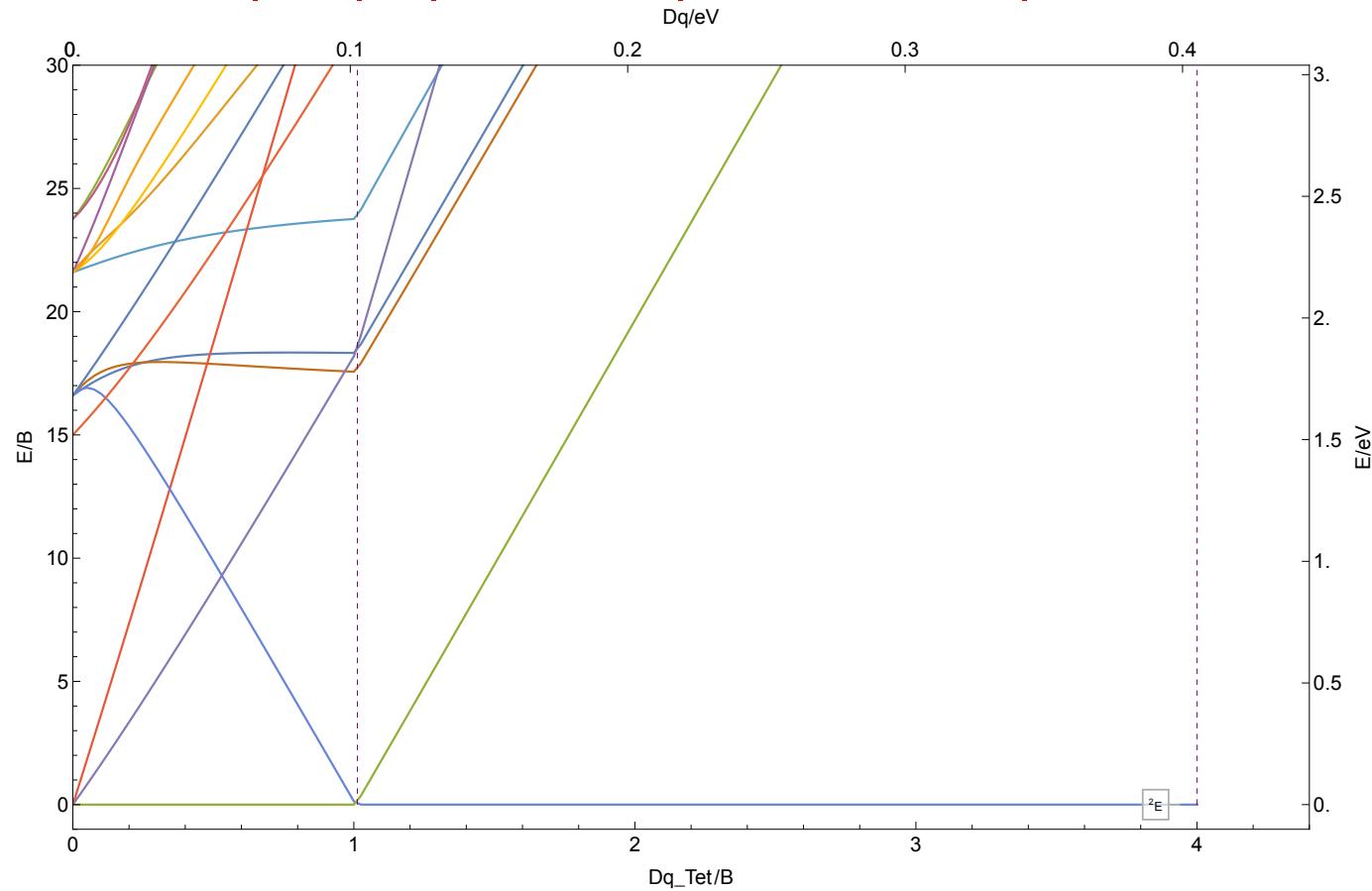
8.2.102 Pt<sup>6+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 4.2 | B ≈ 792 cm<sup>-1</sup> | Pt<sup>6+</sup>



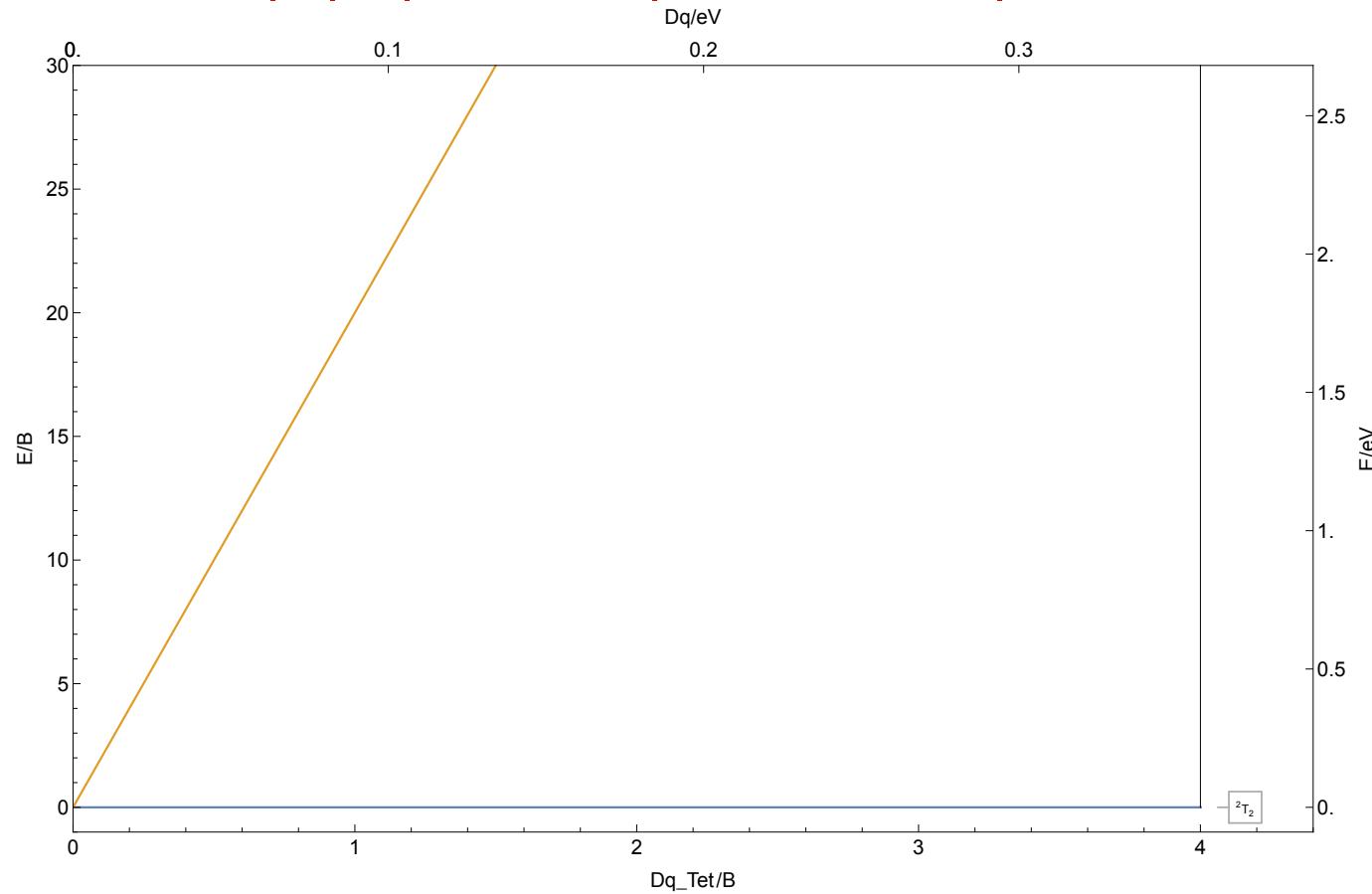
8.2.103 Pt<sup>7+</sup>

|2,4|d<sup>3</sup>|C/B ≈ 4.2|B ≈ 817 cm<sup>-1</sup>|Pt<sup>7+</sup>



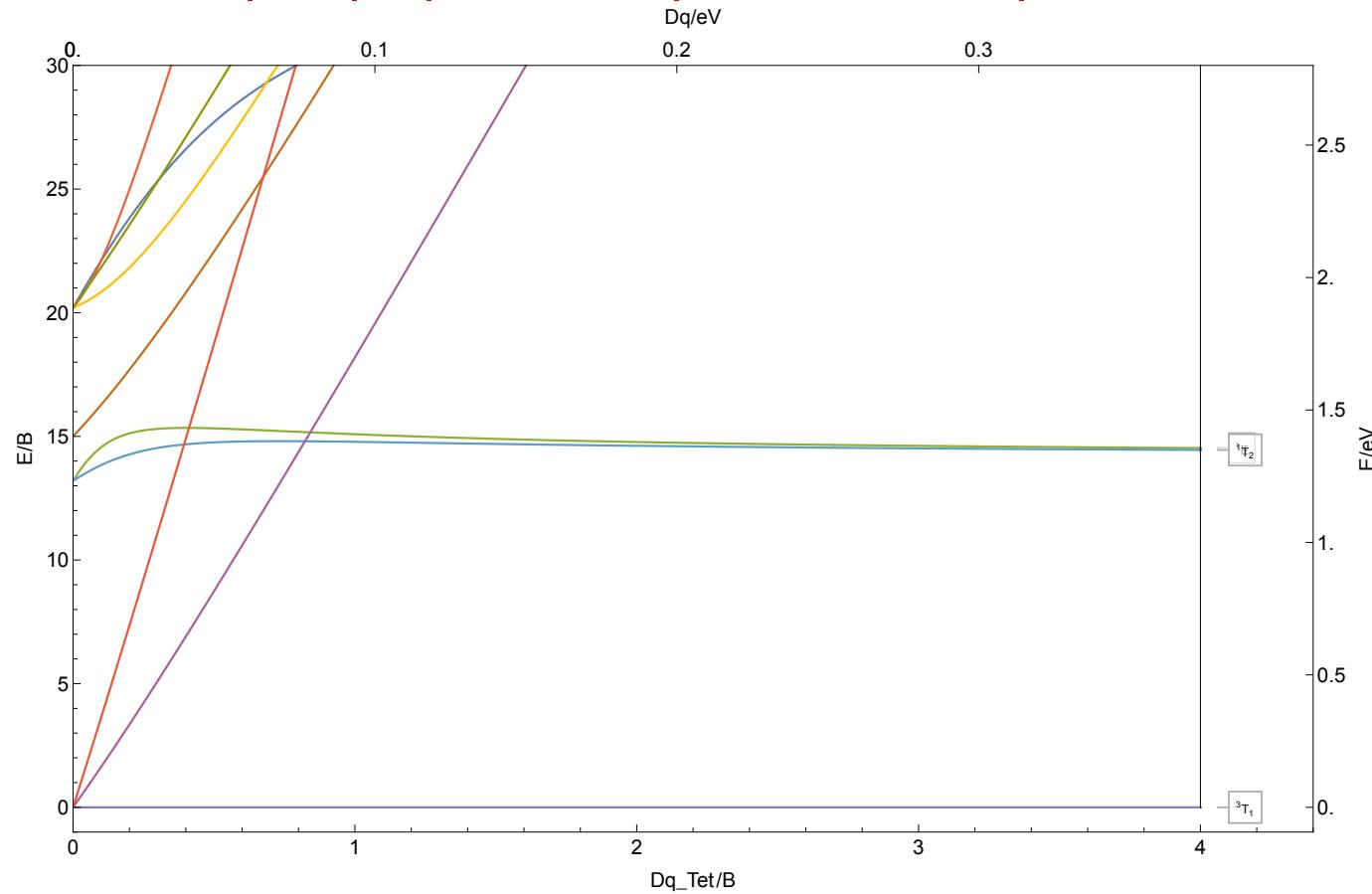
8.2.104 Au<sup>2+</sup>

|2|d<sup>9</sup>|C/B ≈ 4.1|B ≈ 721 cm<sup>-1</sup>|Au<sup>2+</sup>



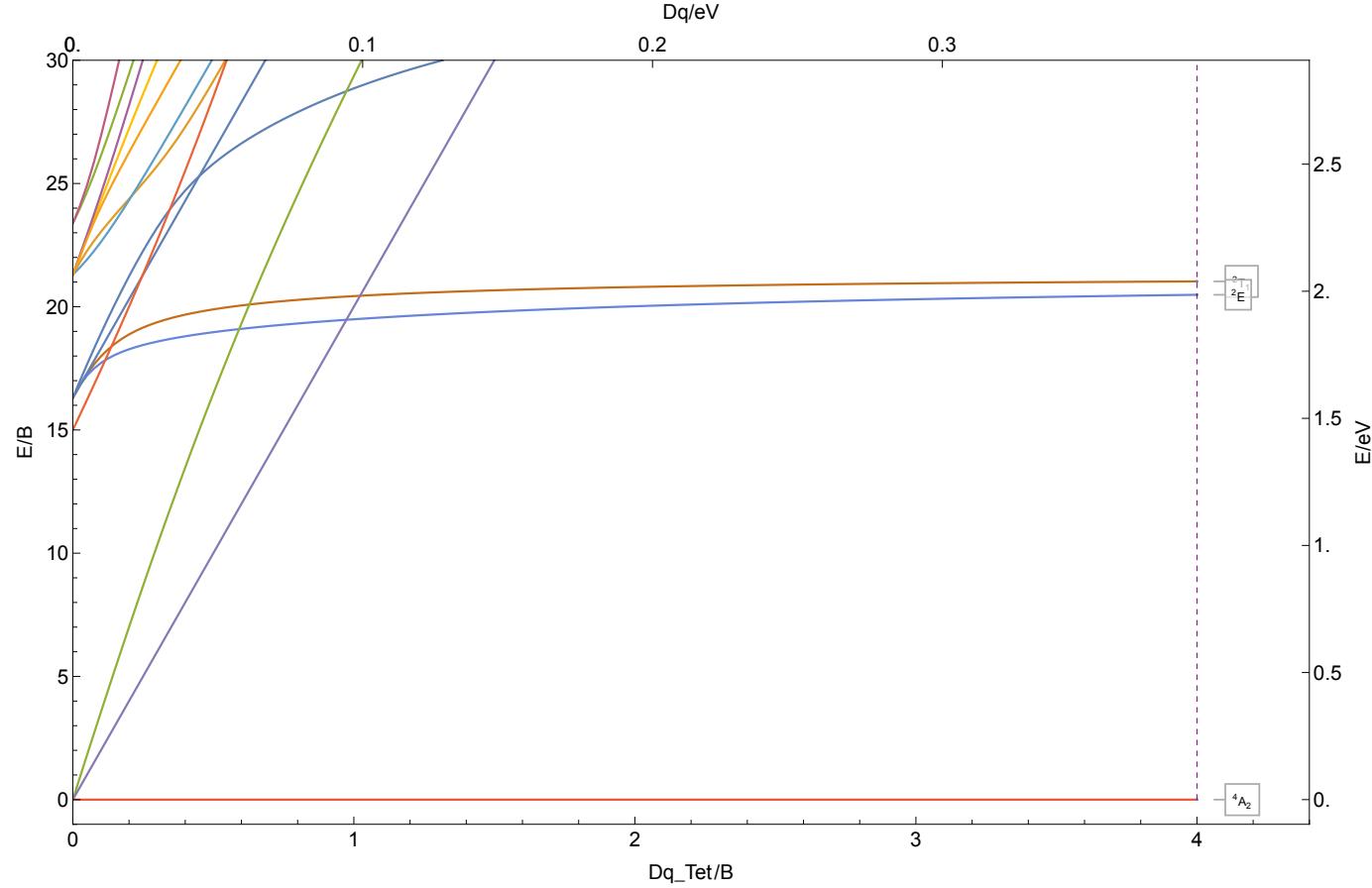
8.2.105 Au<sup>3+</sup>

| 1,3 | d<sup>8</sup> | C/B ≈ 4.1 | B ≈ 753 cm<sup>-1</sup> | Au<sup>3+</sup>



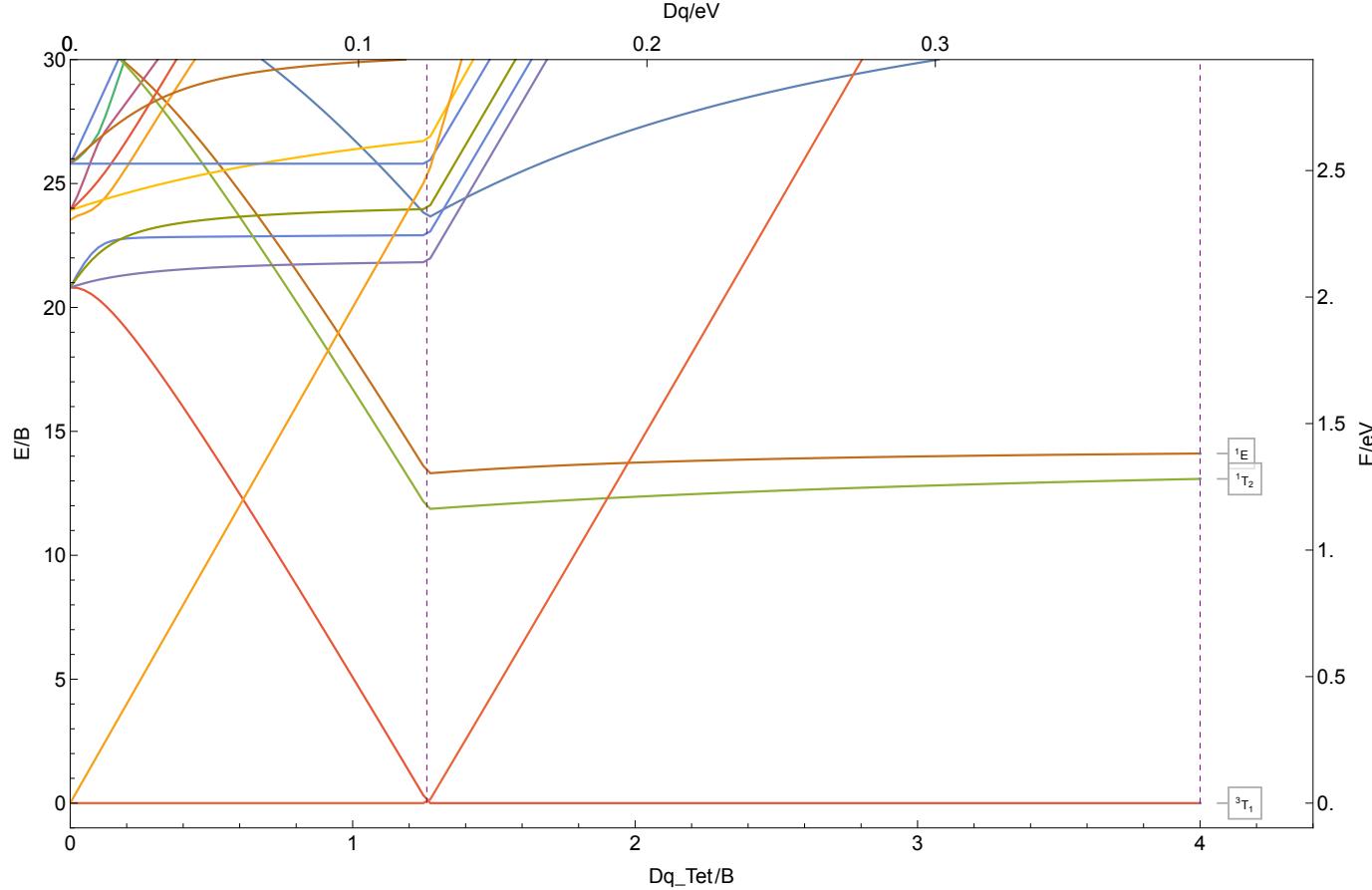
8.2.106 Au<sup>4+</sup>

|2,4|d<sup>7</sup>| C/B ≈ 4.1| B ≈ 782 cm<sup>-1</sup> |Au<sup>4+</sup>



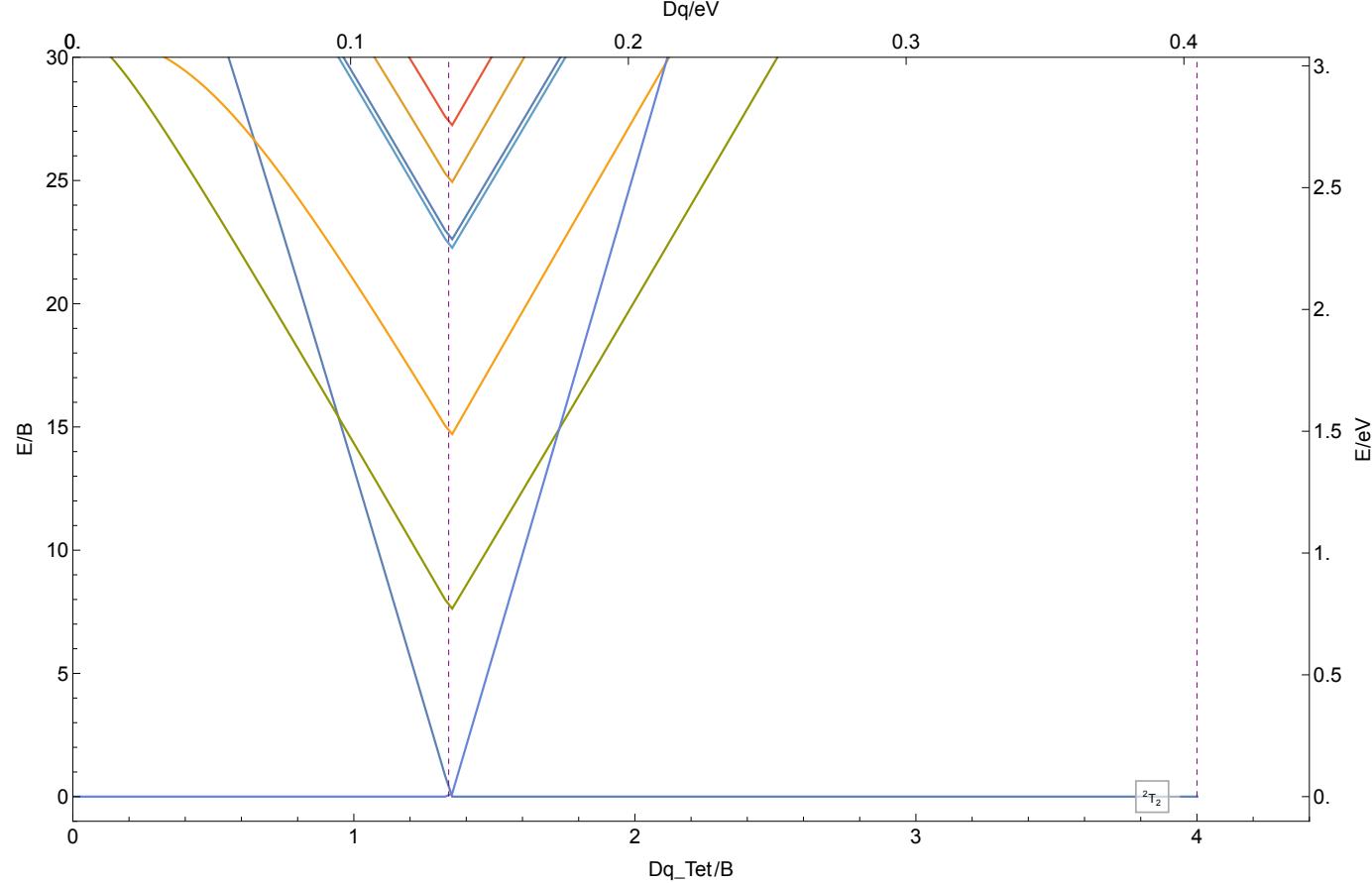
8.2.107 Au<sup>5+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4.2 | B ≈ 790 cm<sup>-1</sup> | Au<sup>5+</sup>



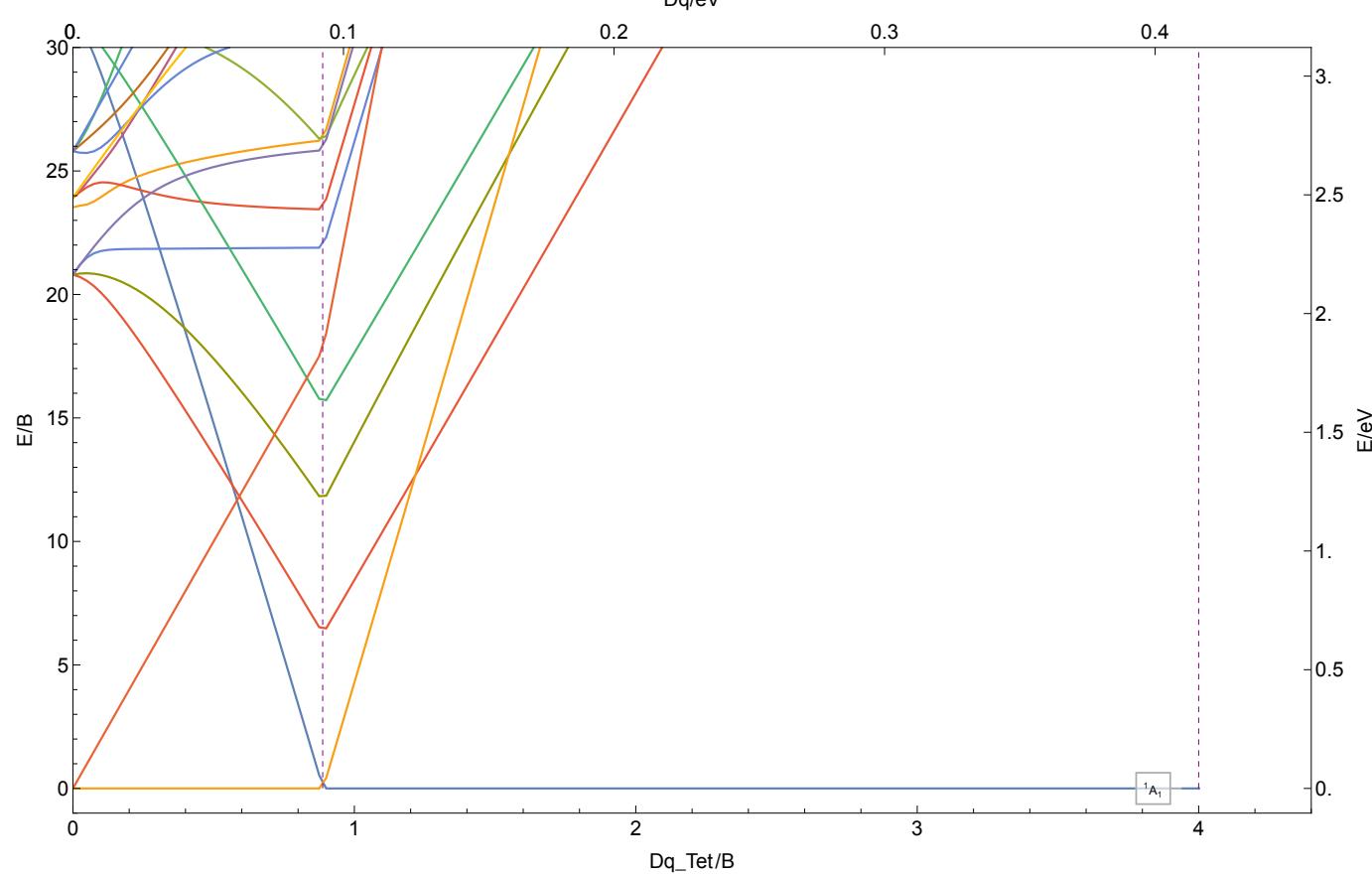
8.2.108 Au<sup>6+</sup>

|2,4,6|d<sup>5</sup>|C/B ≈ 4.2|B ≈ 816 cm<sup>-1</sup>|Au<sup>6+</sup>



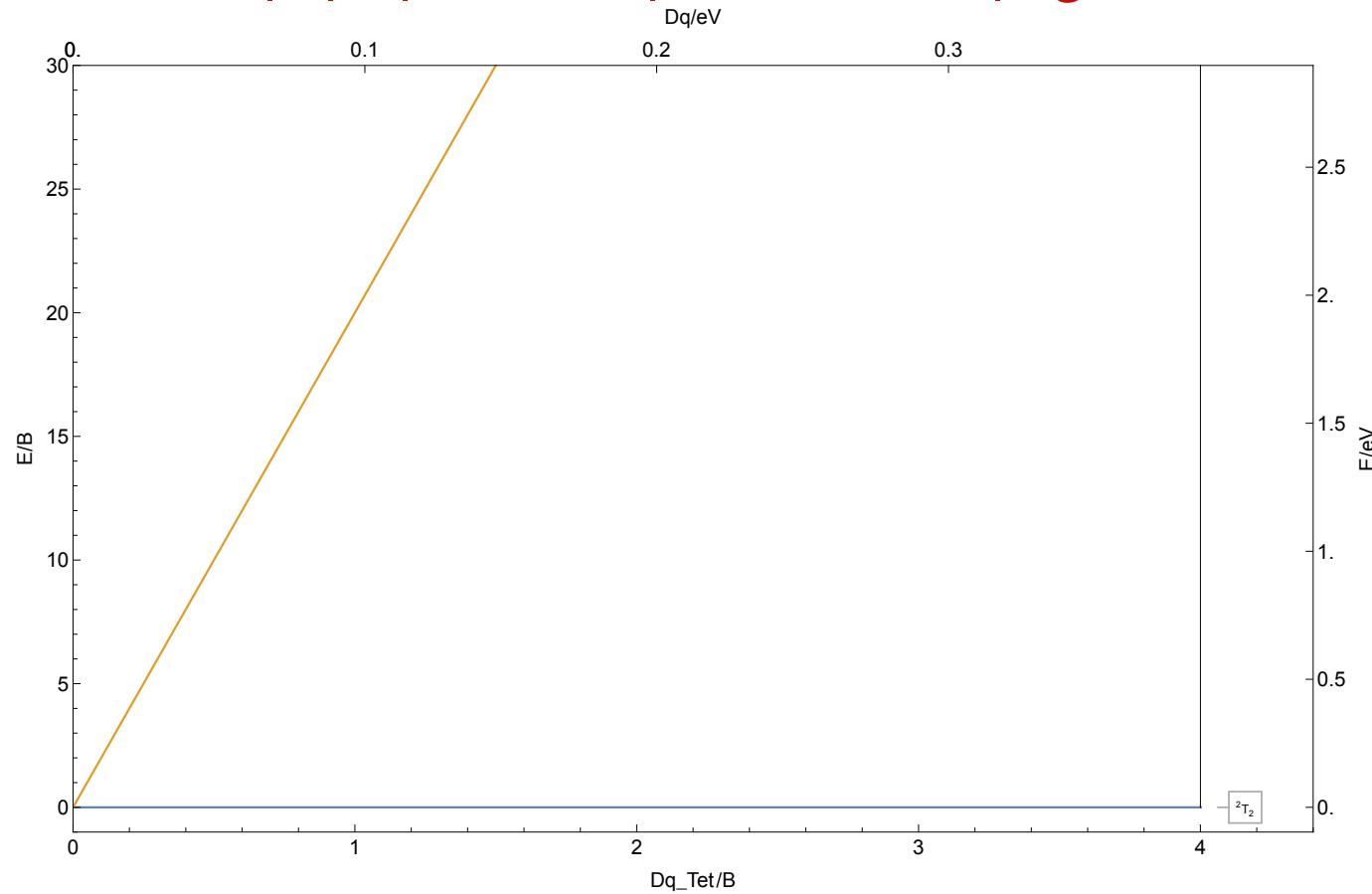
8.2.109 Au<sup>7+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 4.2 | B ≈ 839 cm<sup>-1</sup> | Au<sup>7+</sup>



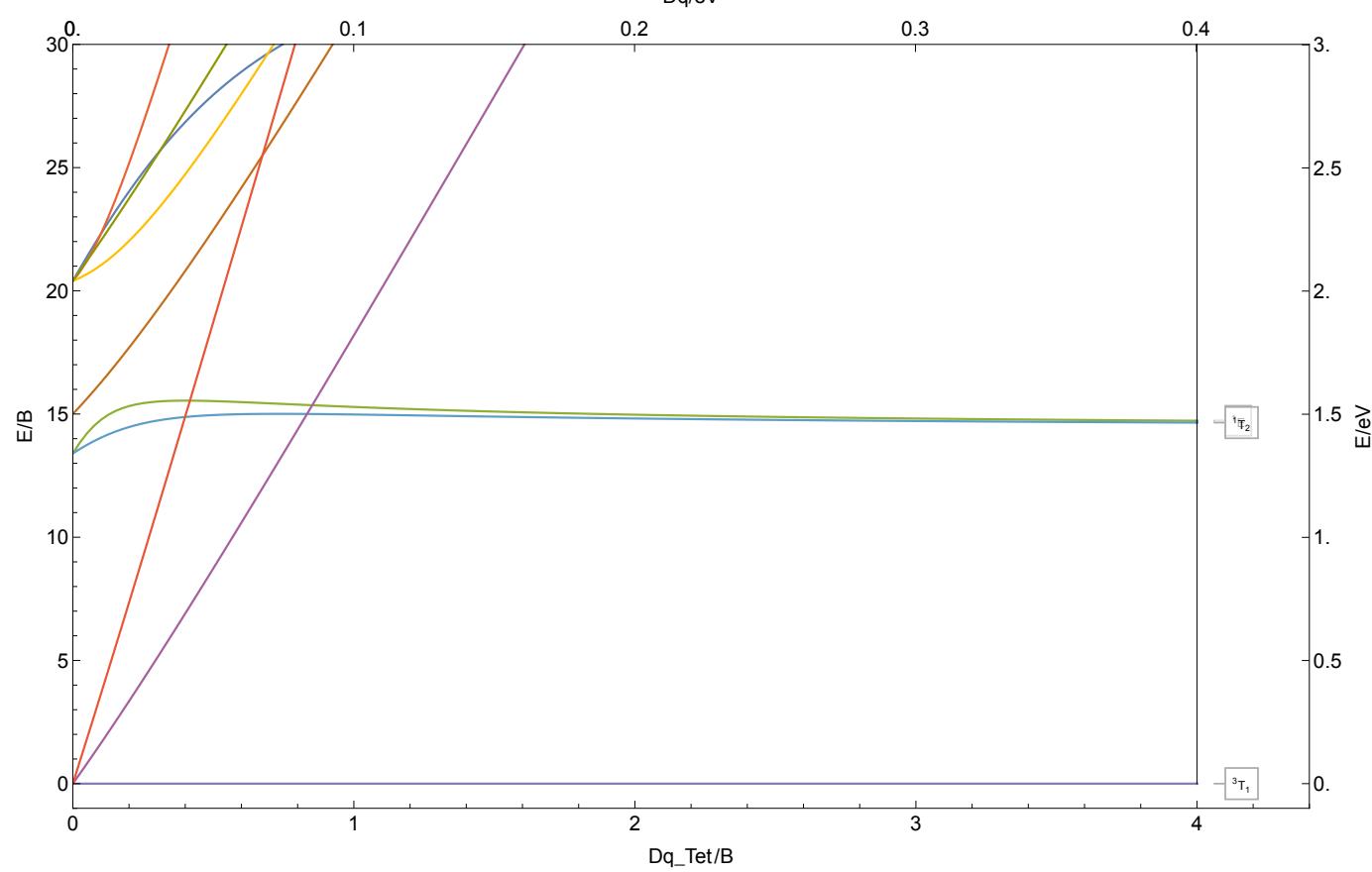
8.2.110 Hg<sup>3+</sup>

|2|d<sup>9</sup>|C/B ≈ 4.1|B ≈ 779 cm<sup>-1</sup>|Hg<sup>3+</sup>



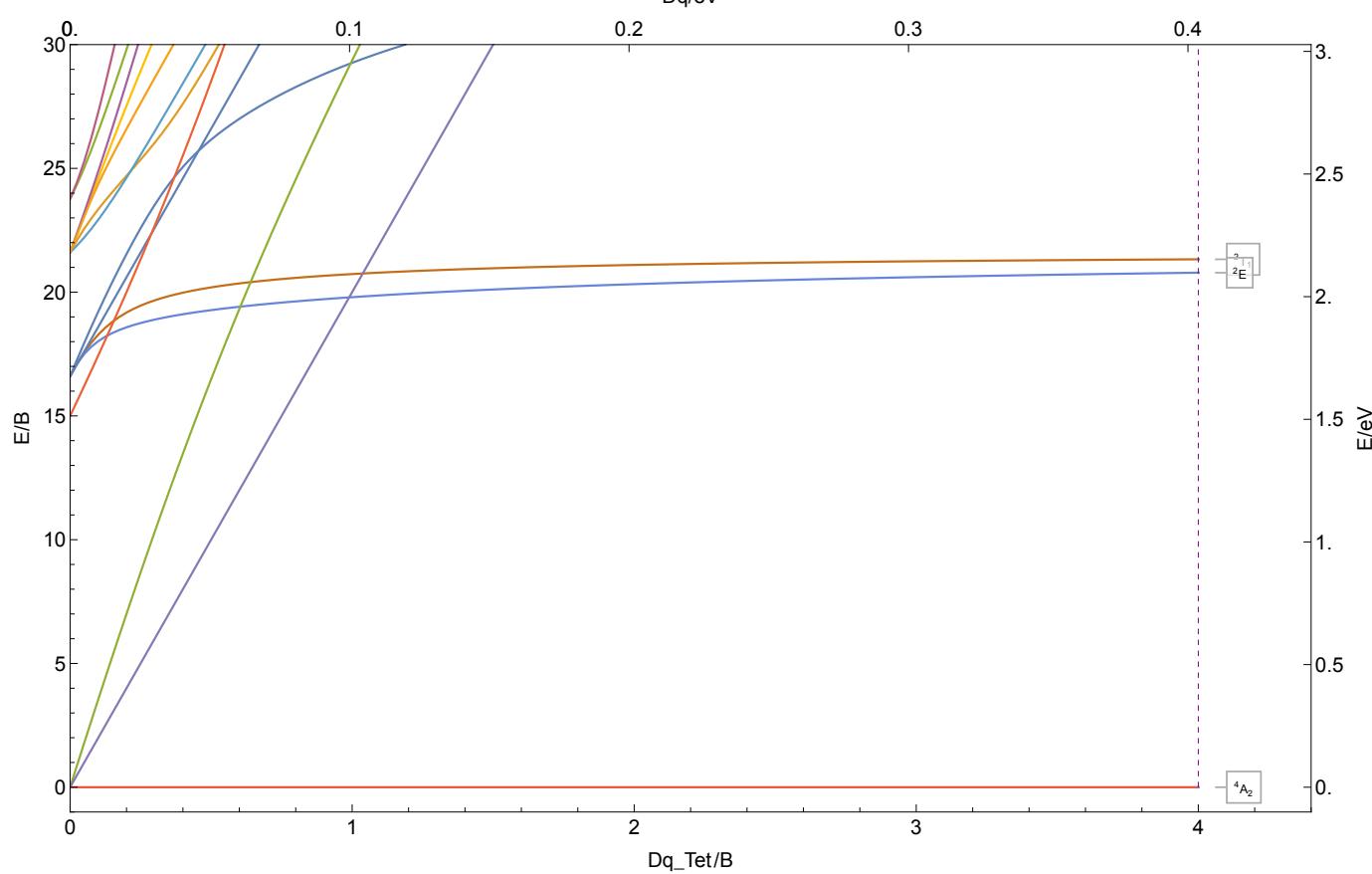
8.2.111 Hg<sup>4+</sup>

$|1,3|d^8|C/B \approx 4.2|B \approx 807\text{ cm}^{-1}|Hg^{4+}$



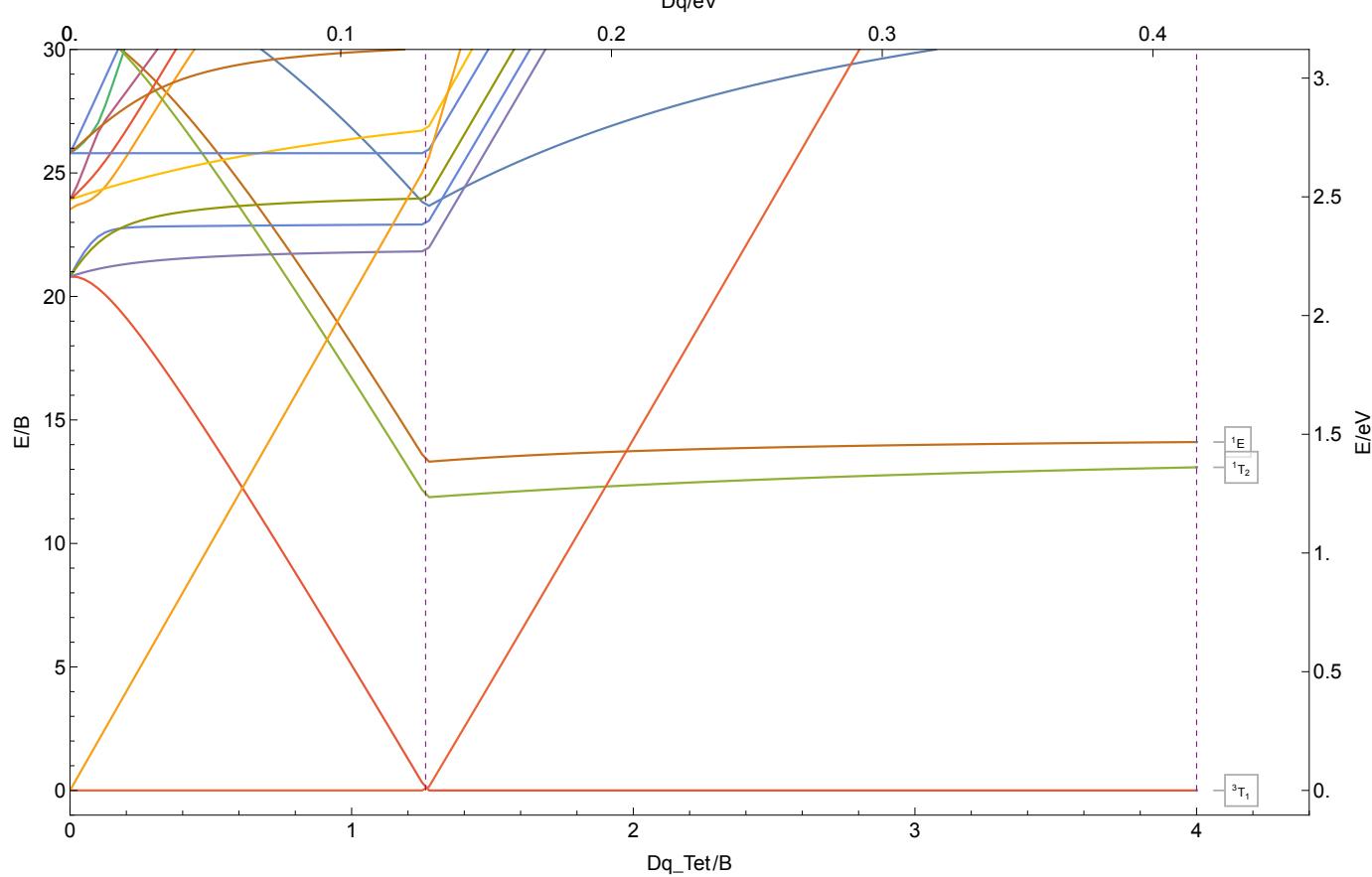
8.2.112 Hg<sup>5+</sup>

$|2,4|d^7|C/B \approx 4.2|B \approx 814\text{ cm}^{-1}|Hg^{5+}$



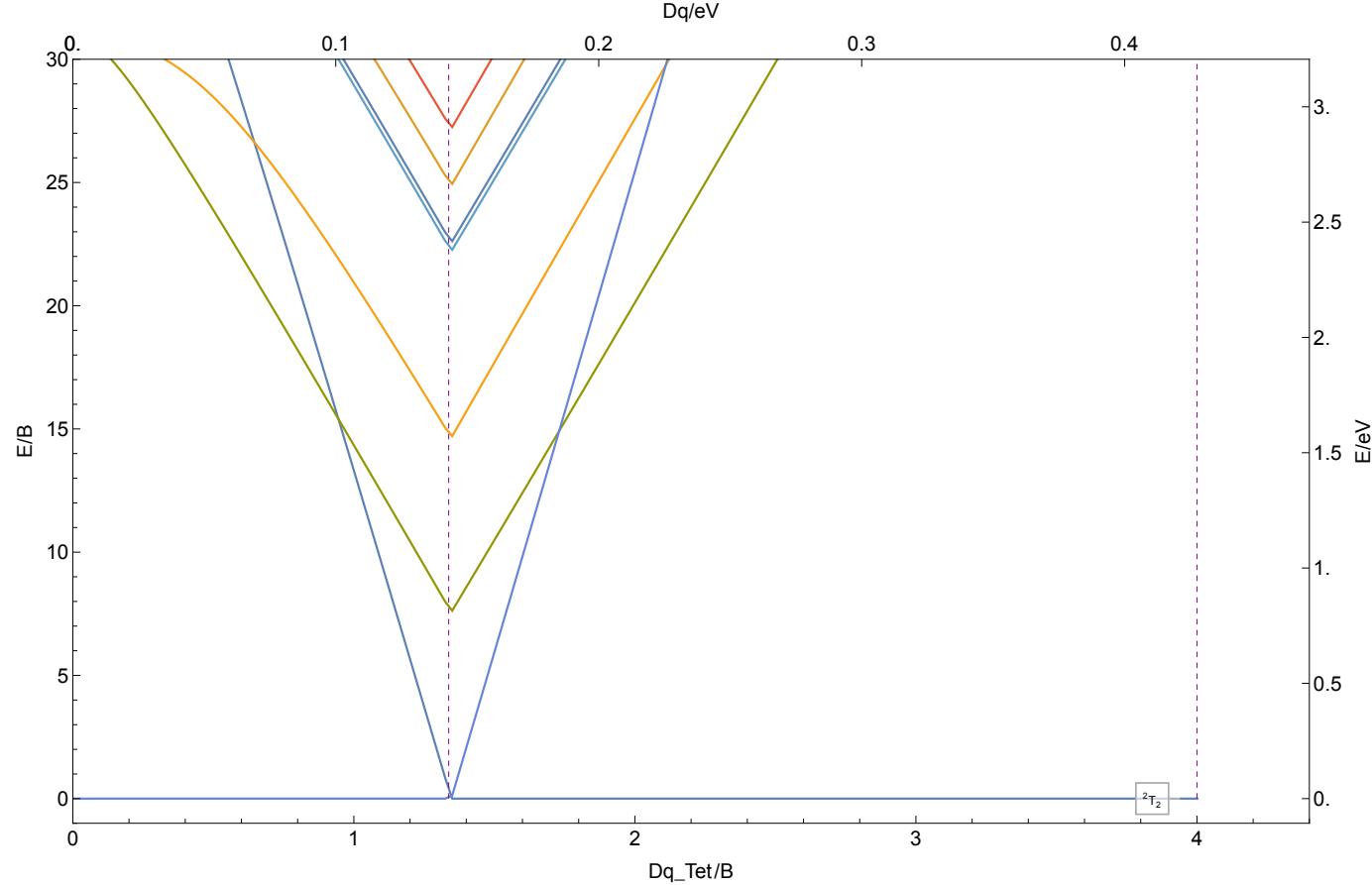
8.2.113 Hg<sup>6+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4.2 | B ≈ 839 cm<sup>-1</sup> | Hg<sup>6+</sup>



8.2.114 Hg<sup>7+</sup>

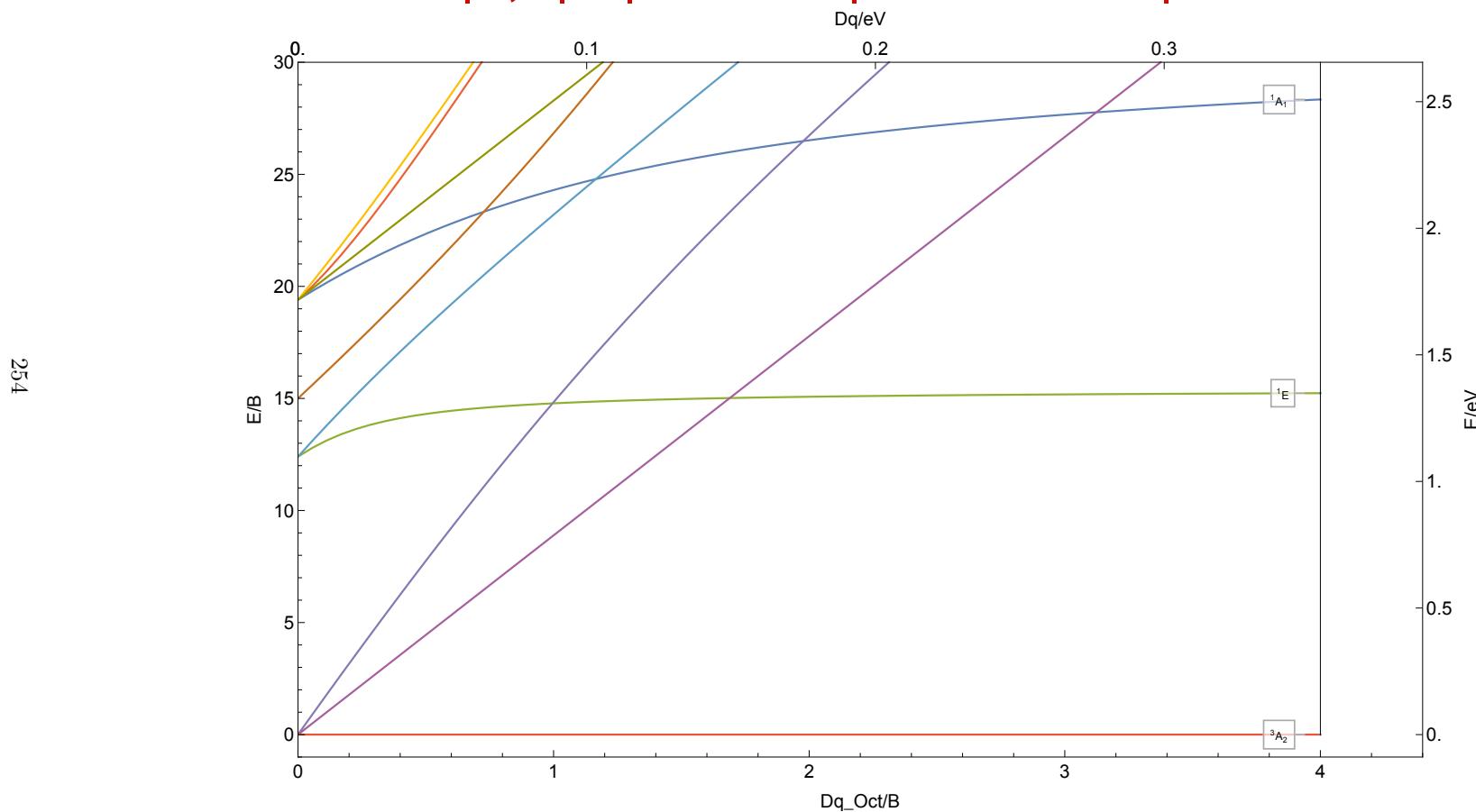
|2,4,6|d<sup>5</sup>| C/B ≈ 4.2 | B ≈ 862 cm<sup>-1</sup> | Hg<sup>7+</sup>



## 8.3 Octahedral field

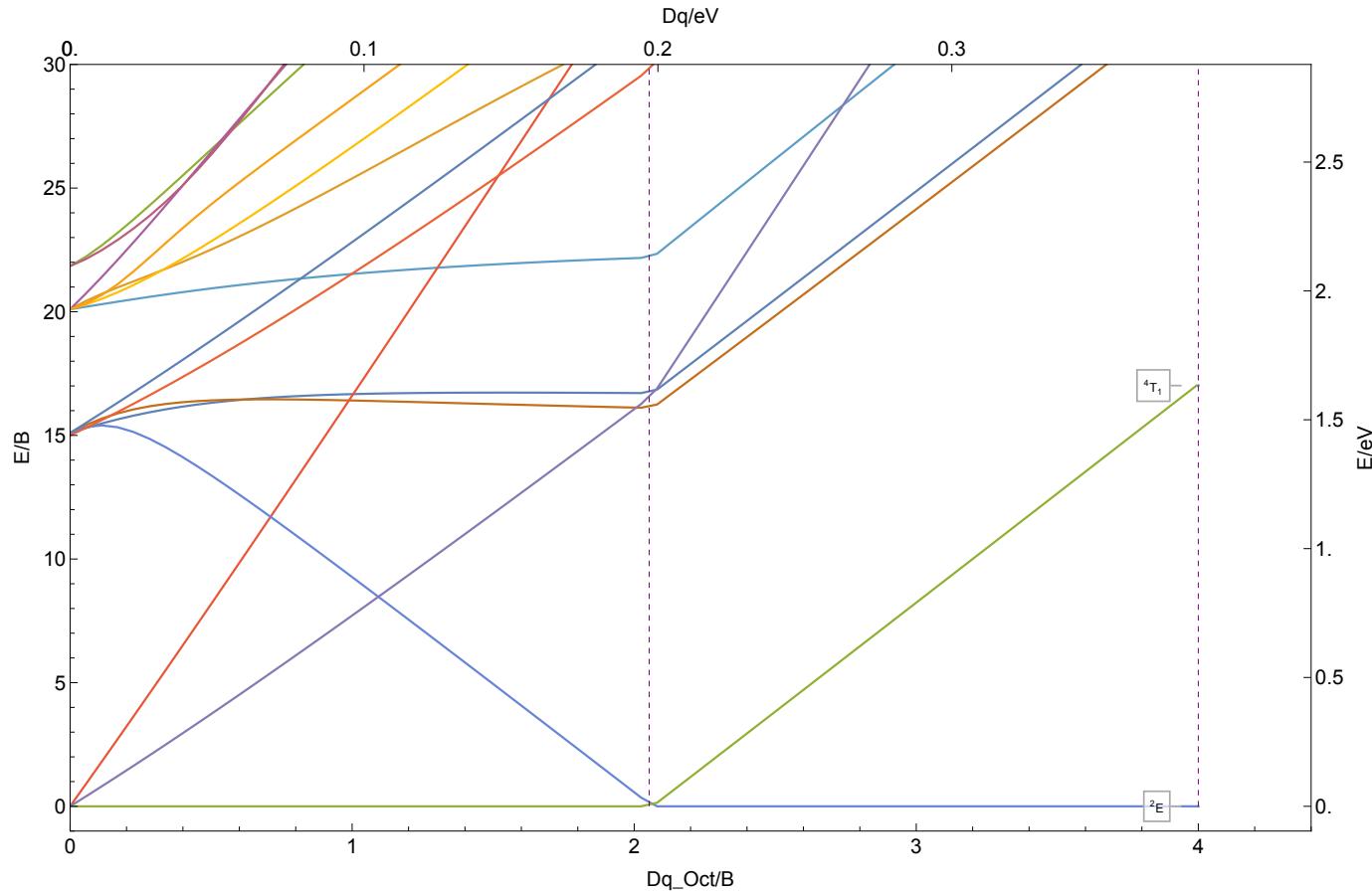
### 8.3.1 $\text{Ti}^{2+}$

$|1,3|d^2|C/B \approx 3.7|B \approx 714\text{ cm}^{-1}| \text{Ti}^{2+}$



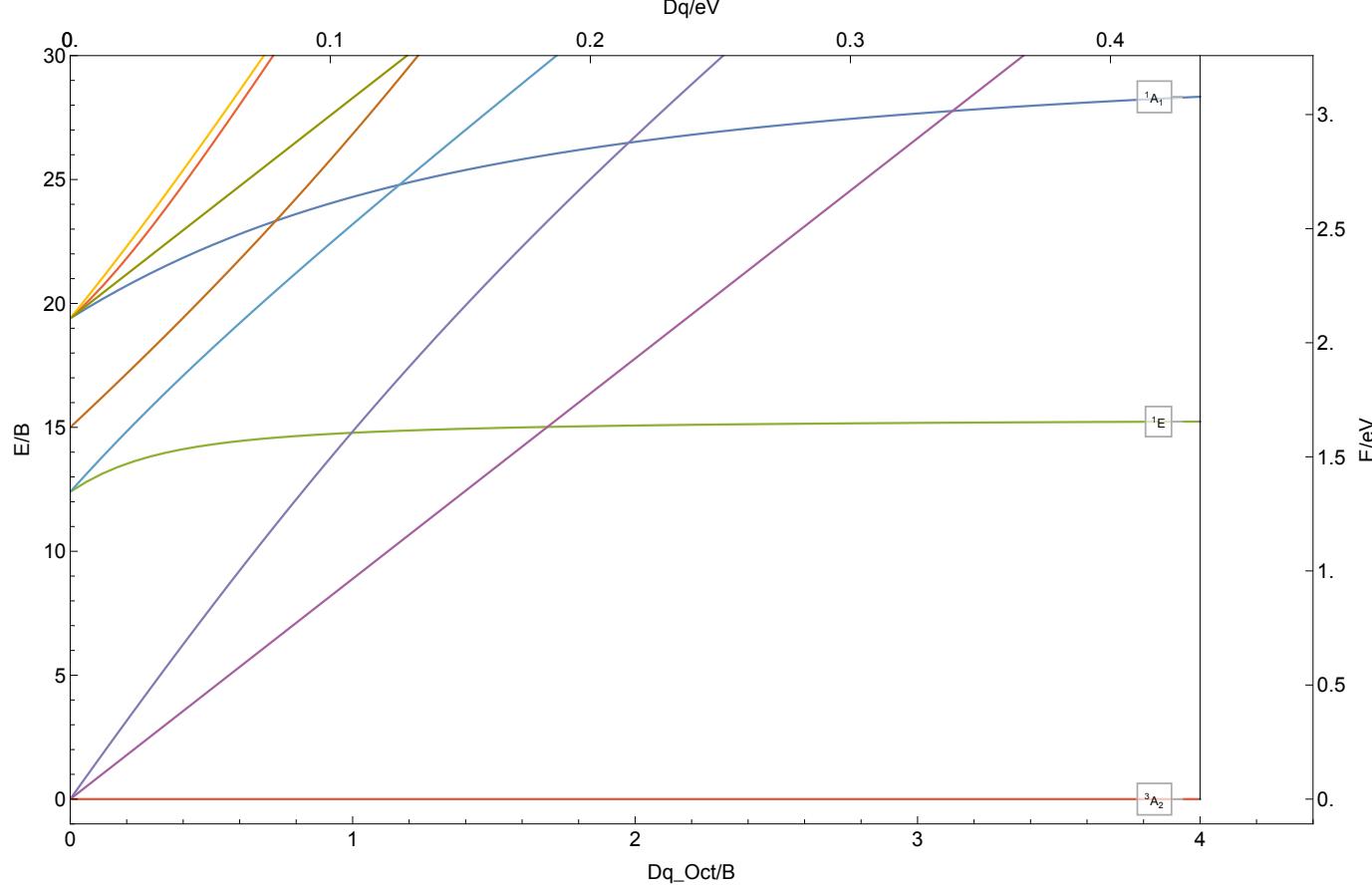
### 8.3.2 V<sup>2+</sup>

|2,4|d<sup>3</sup>| C/B ≈ 3.7 | B ≈ 774 cm<sup>-1</sup> | V<sup>2+</sup>



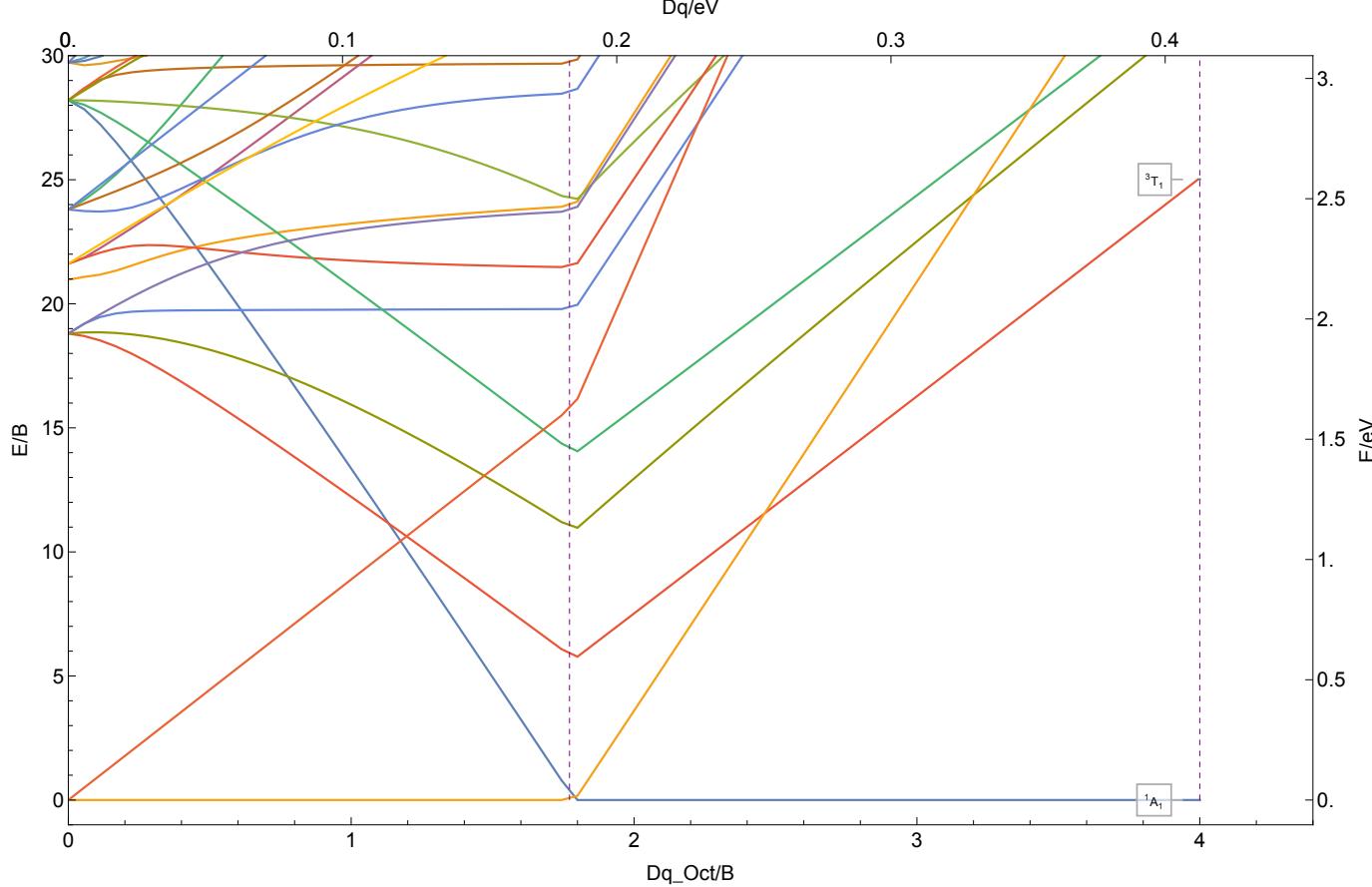
### 8.3.3 V<sup>3+</sup>

$|1,3|d^2| C/B \approx 3.7 | B \approx 876 \text{ cm}^{-1} | V^{3+}$



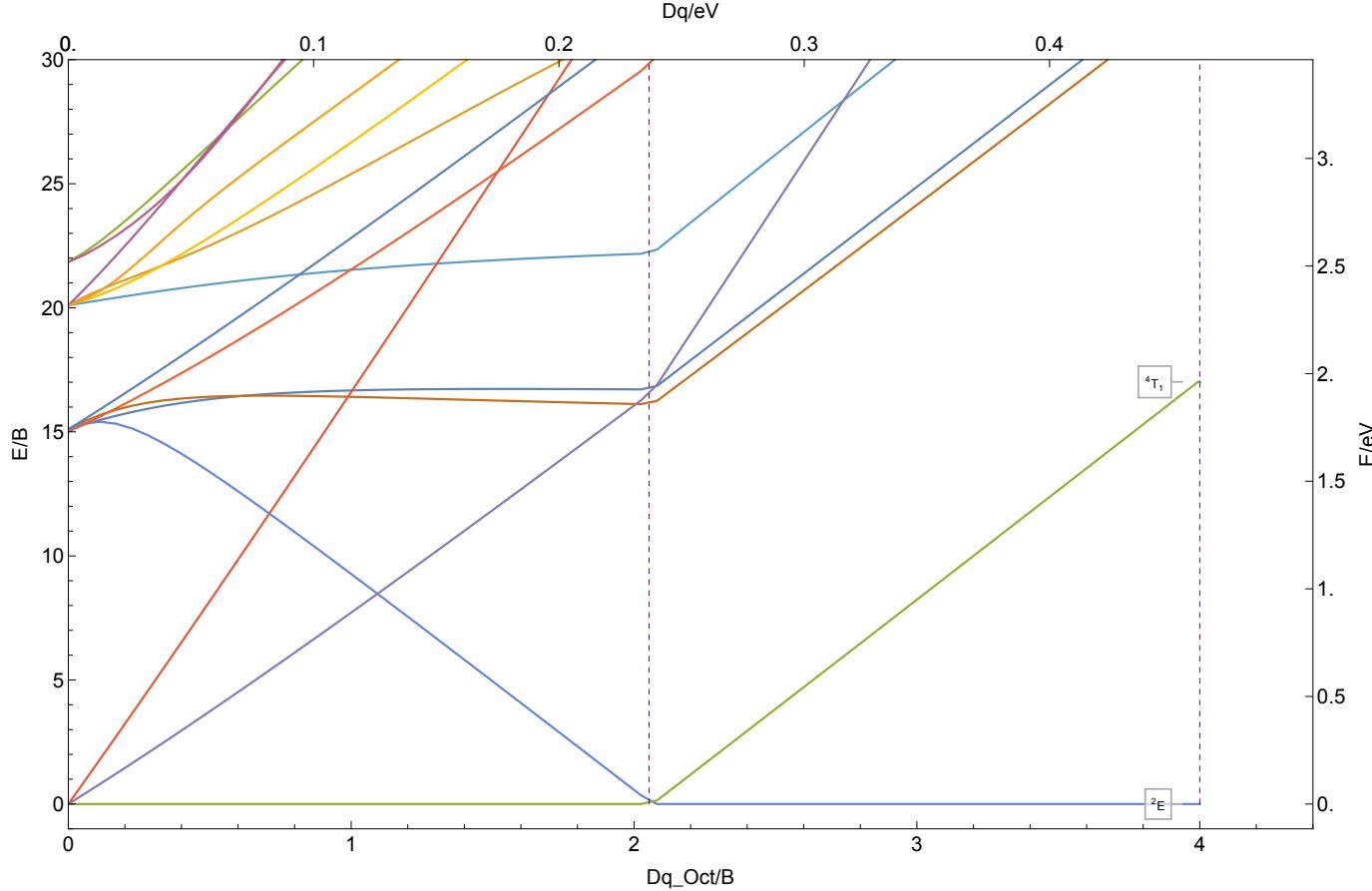
### 8.3.4 Cr<sup>2+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 3.7 | B ≈ 832 cm<sup>-1</sup> | Cr<sup>2+</sup>



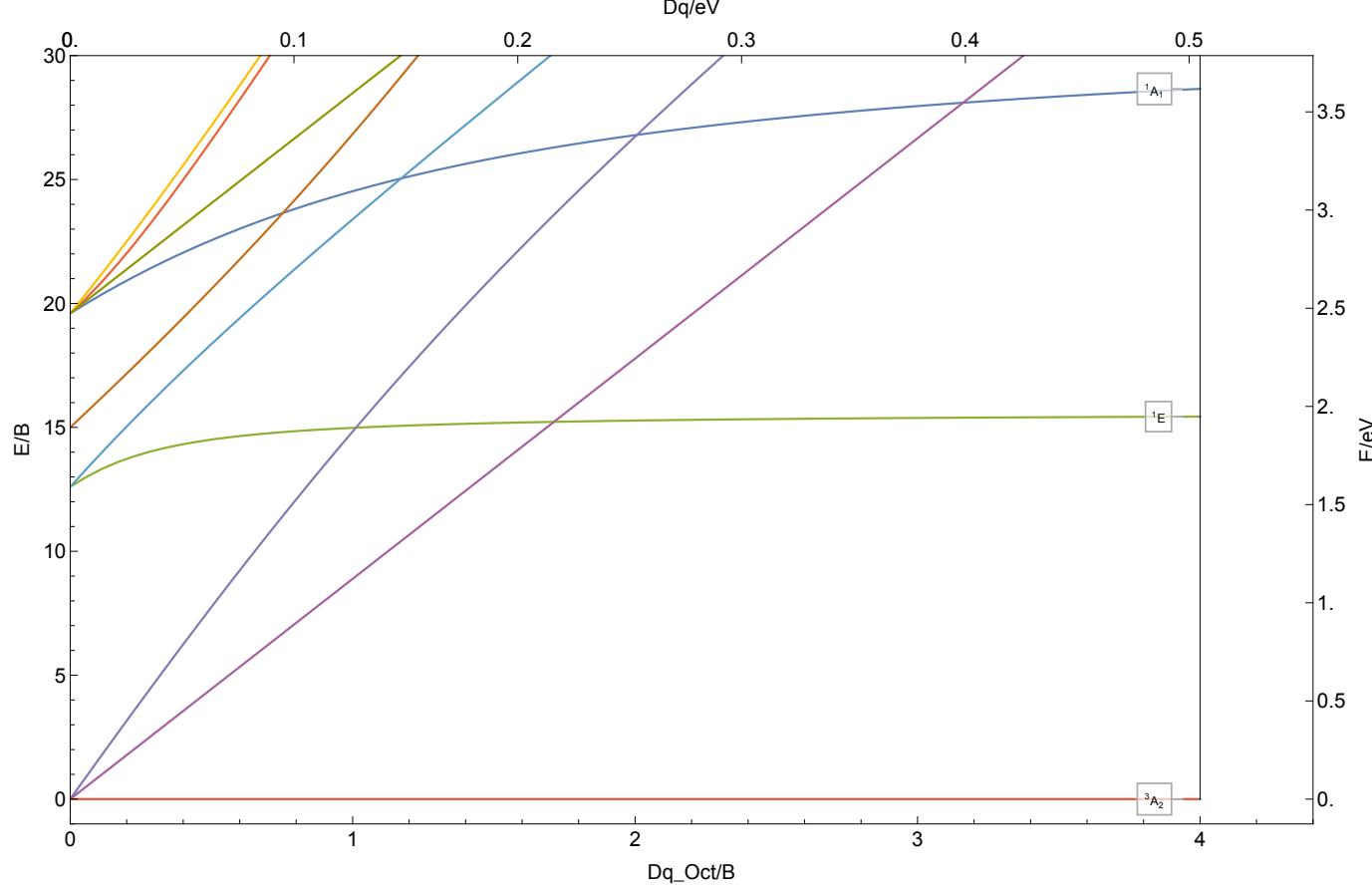
### 8.3.5 Cr<sup>3+</sup>

$|2,4|d^3|C/B \approx 3.7|B \approx 930\text{ cm}^{-1}|Cr^{3+}$



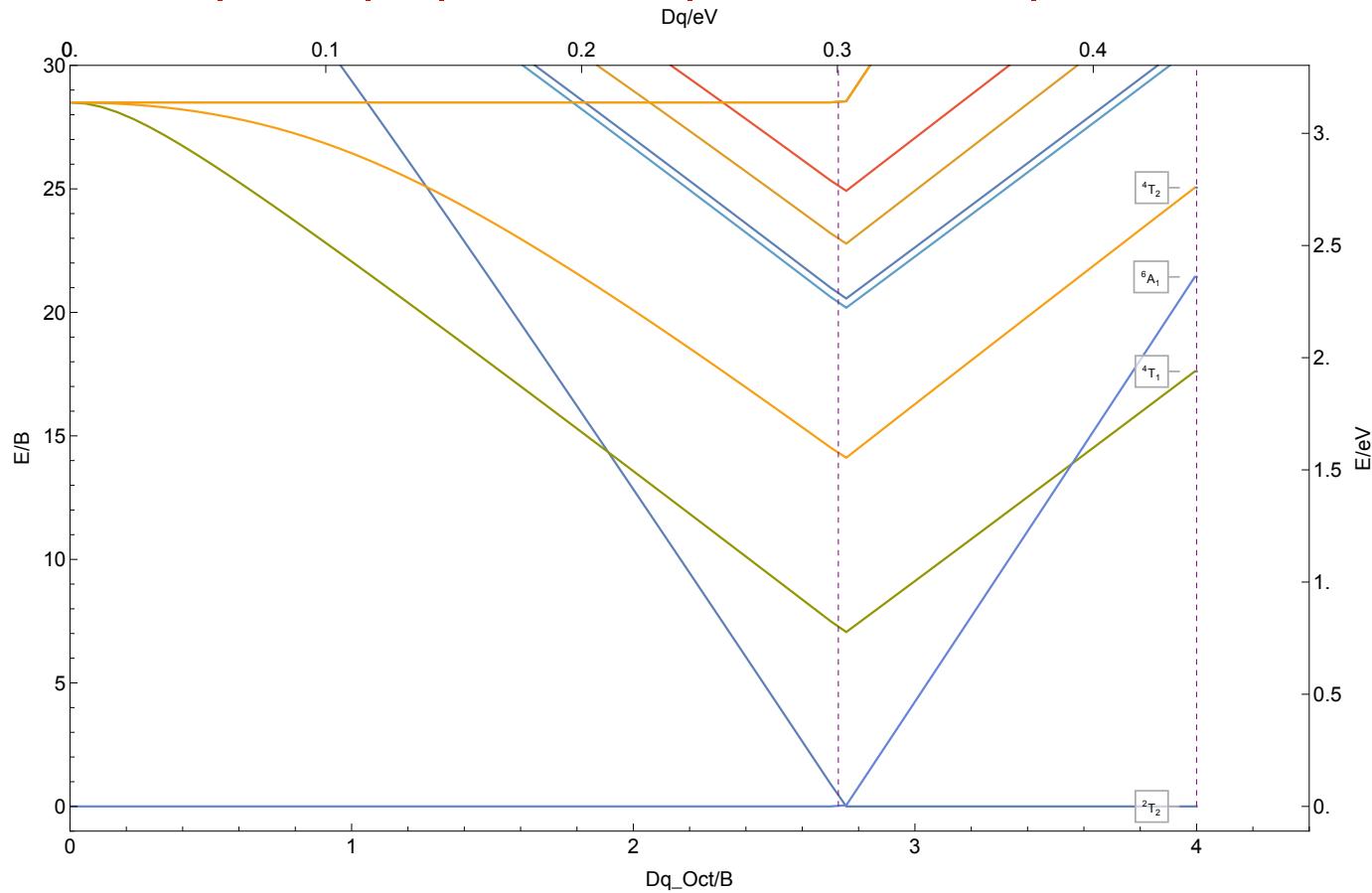
### 8.3.6 Cr<sup>4+</sup>

|1,3|d<sup>2</sup>| C/B ≈ 3.8 | B ≈ 1018 cm<sup>-1</sup> |Cr<sup>4+</sup>



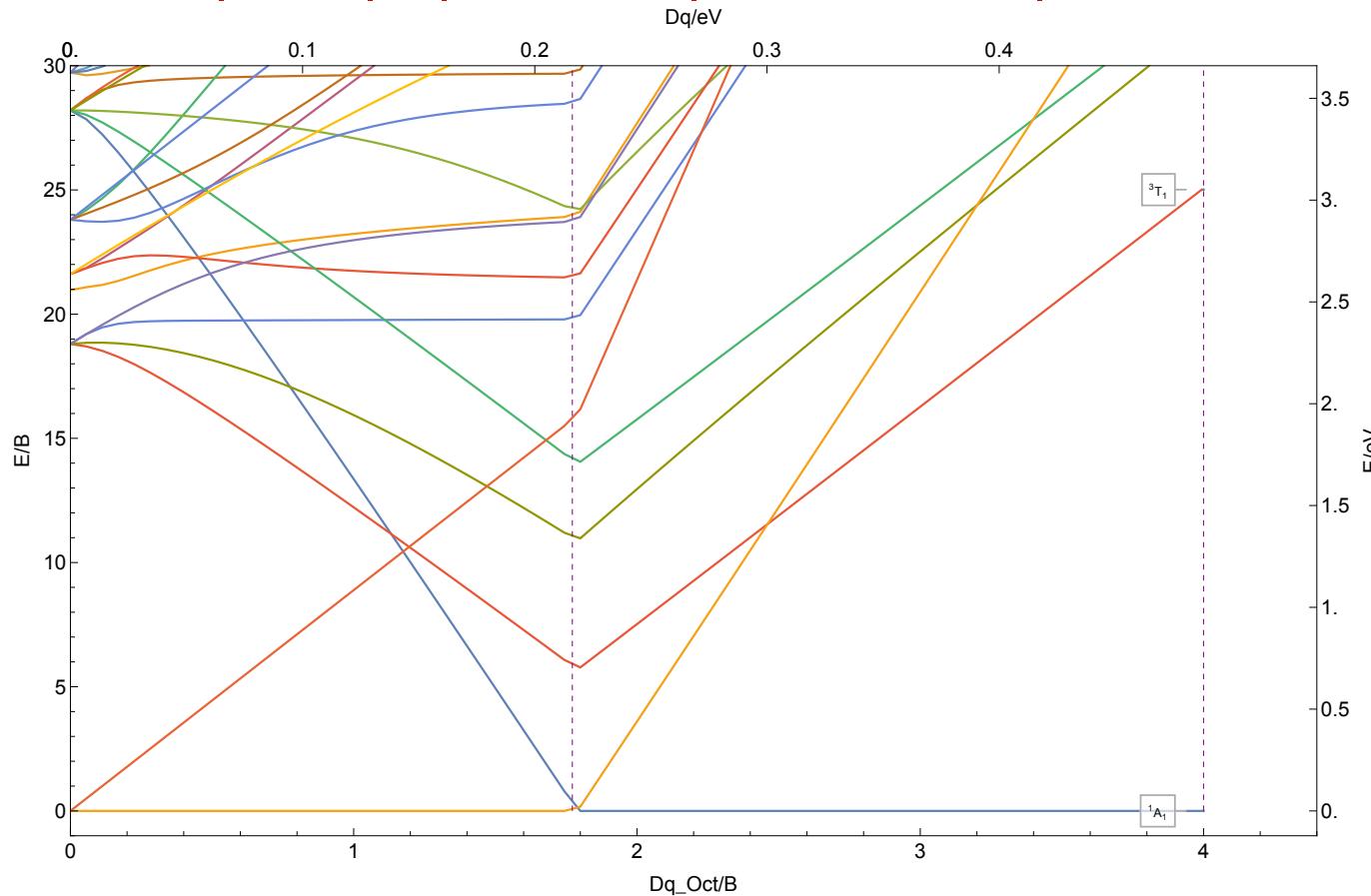
### 8.3.7 Mn<sup>2+</sup>

$|2,4,6|d^5|C/B \approx 3.7|B \approx 888\text{ cm}^{-1}|Mn^{2+}$



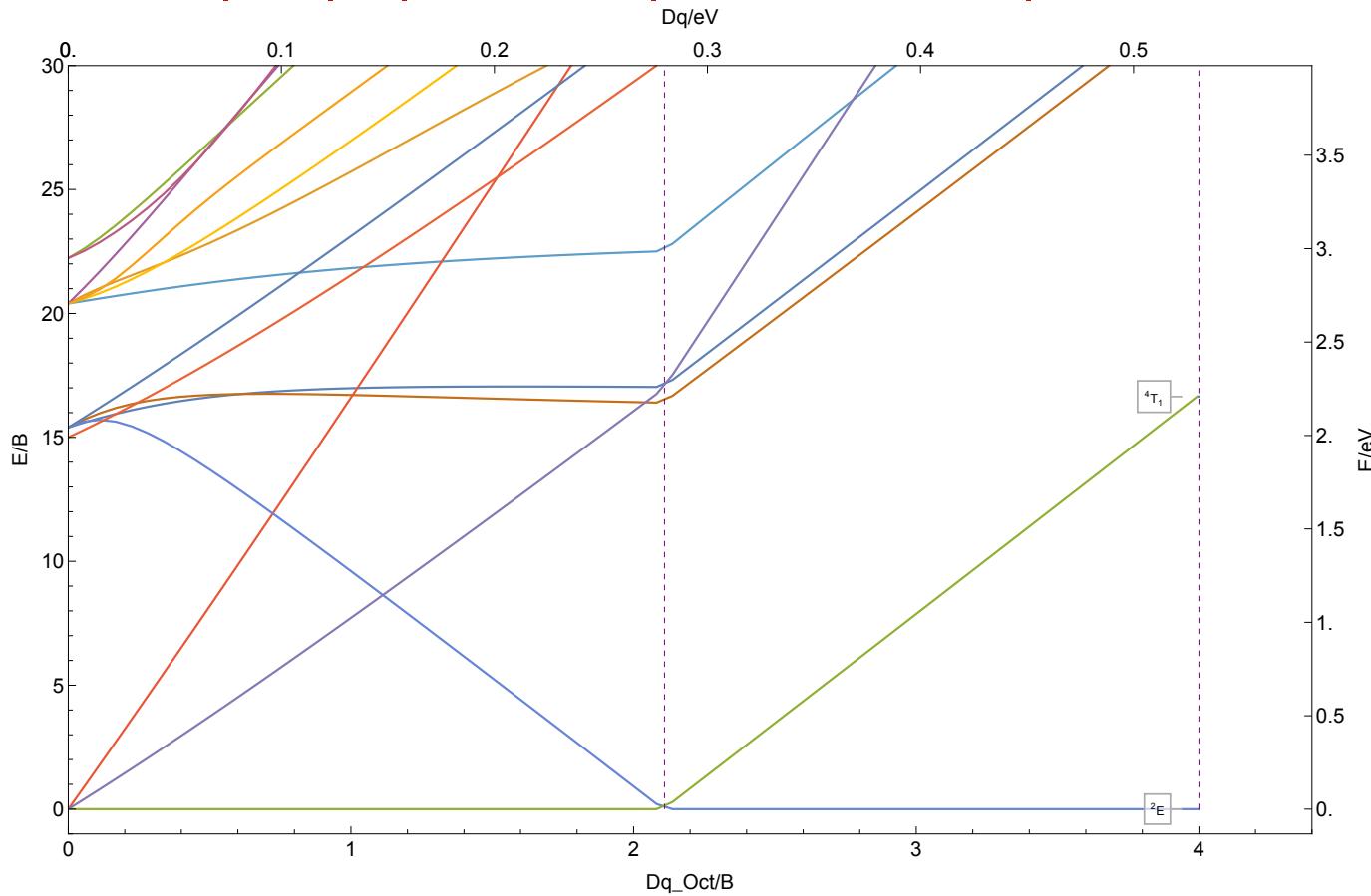
### 8.3.8 Mn<sup>3+</sup>

$|1,3,5|d^4|C/B \approx 3.7|B \approx 984\text{ cm}^{-1}|Mn^{3+}$



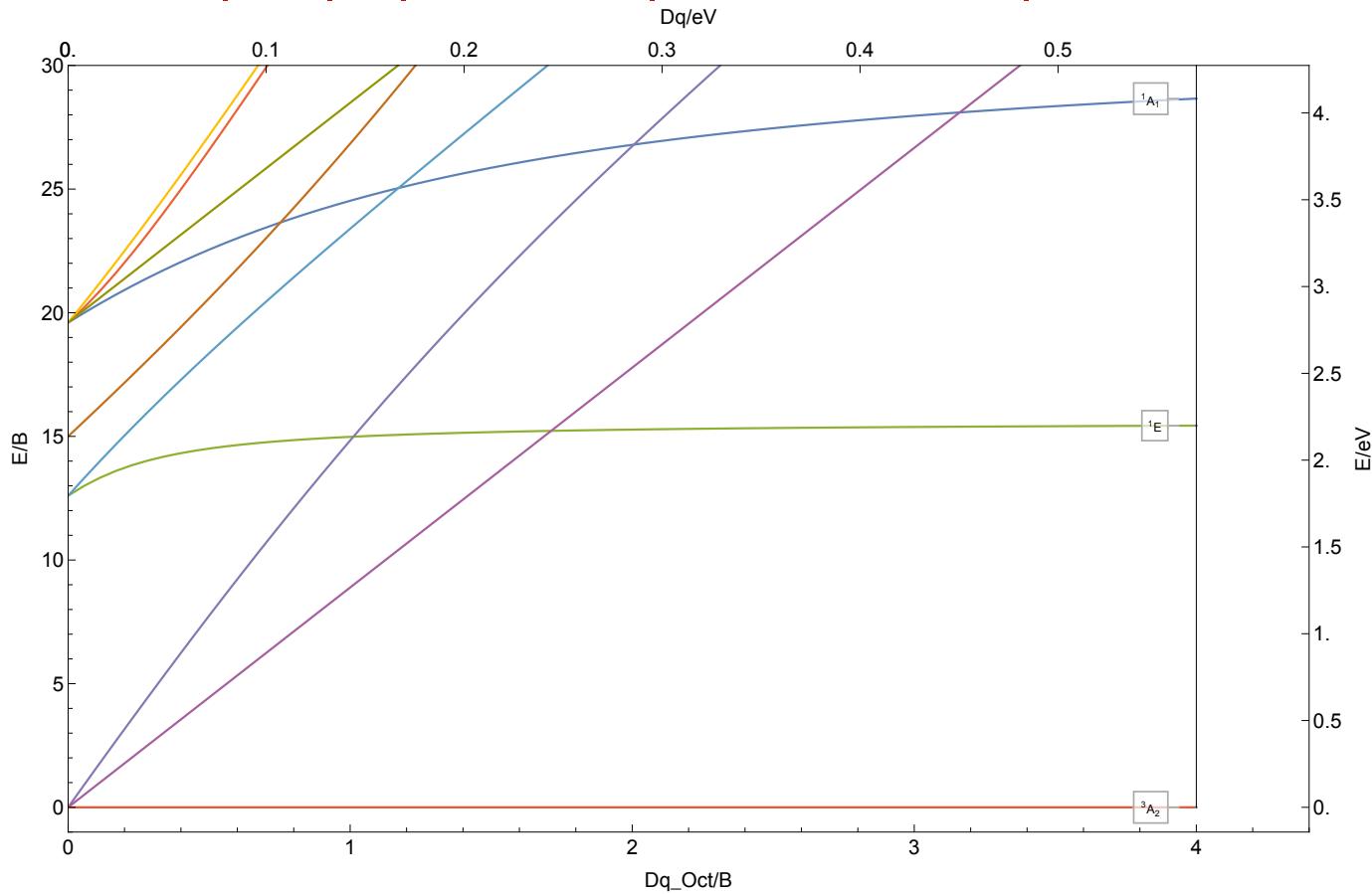
### 8.3.9 Mn<sup>4+</sup>

$|2,4|d^3|C/B \approx 3.8|B \approx 1070\text{ cm}^{-1}|Mn^{4+}$



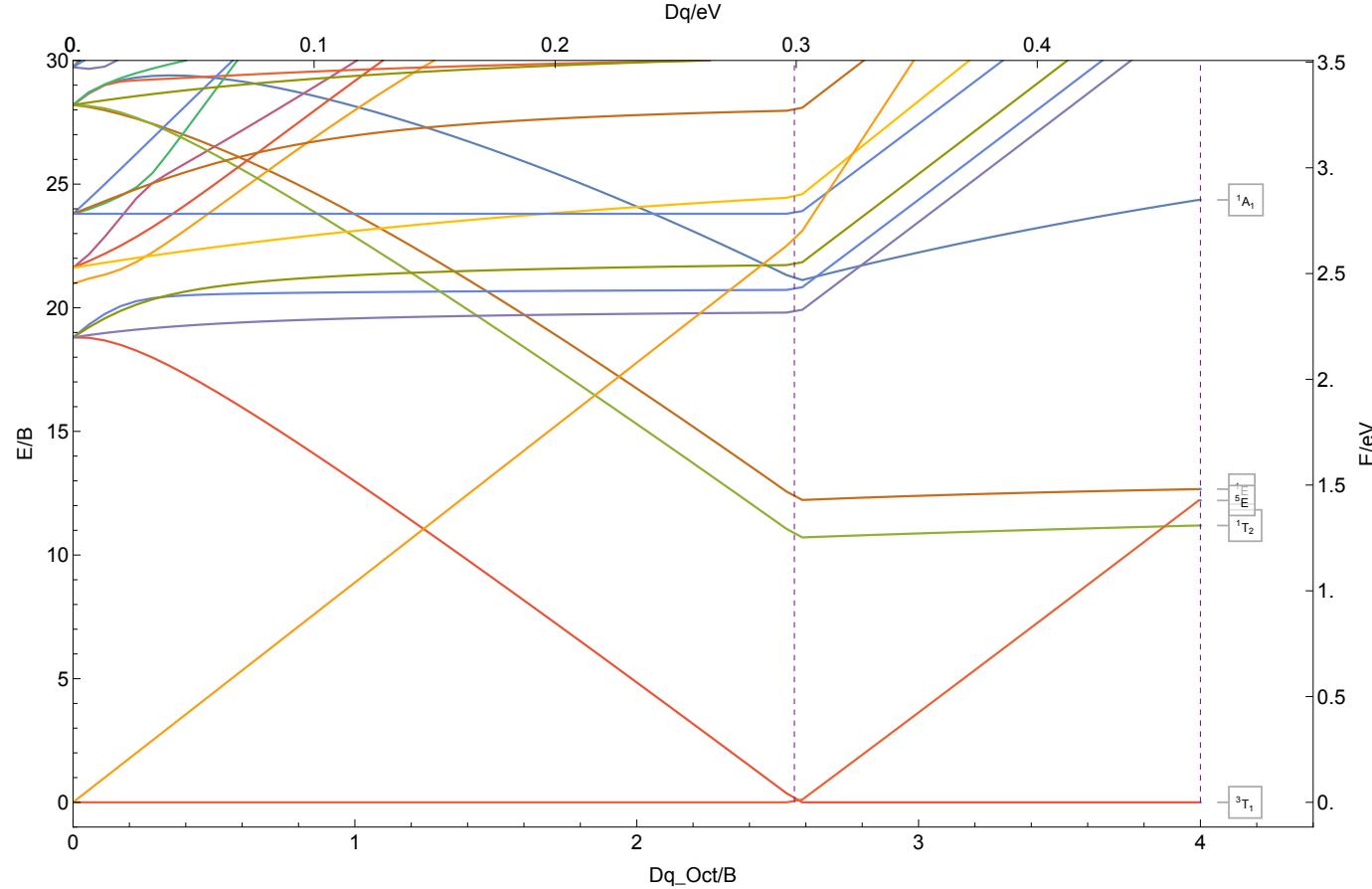
### 8.3.10 Mn<sup>5+</sup>

$|1,3|d^2|C/B \approx 3.8|B \approx 1149\text{ cm}^{-1}|Mn^{5+}$



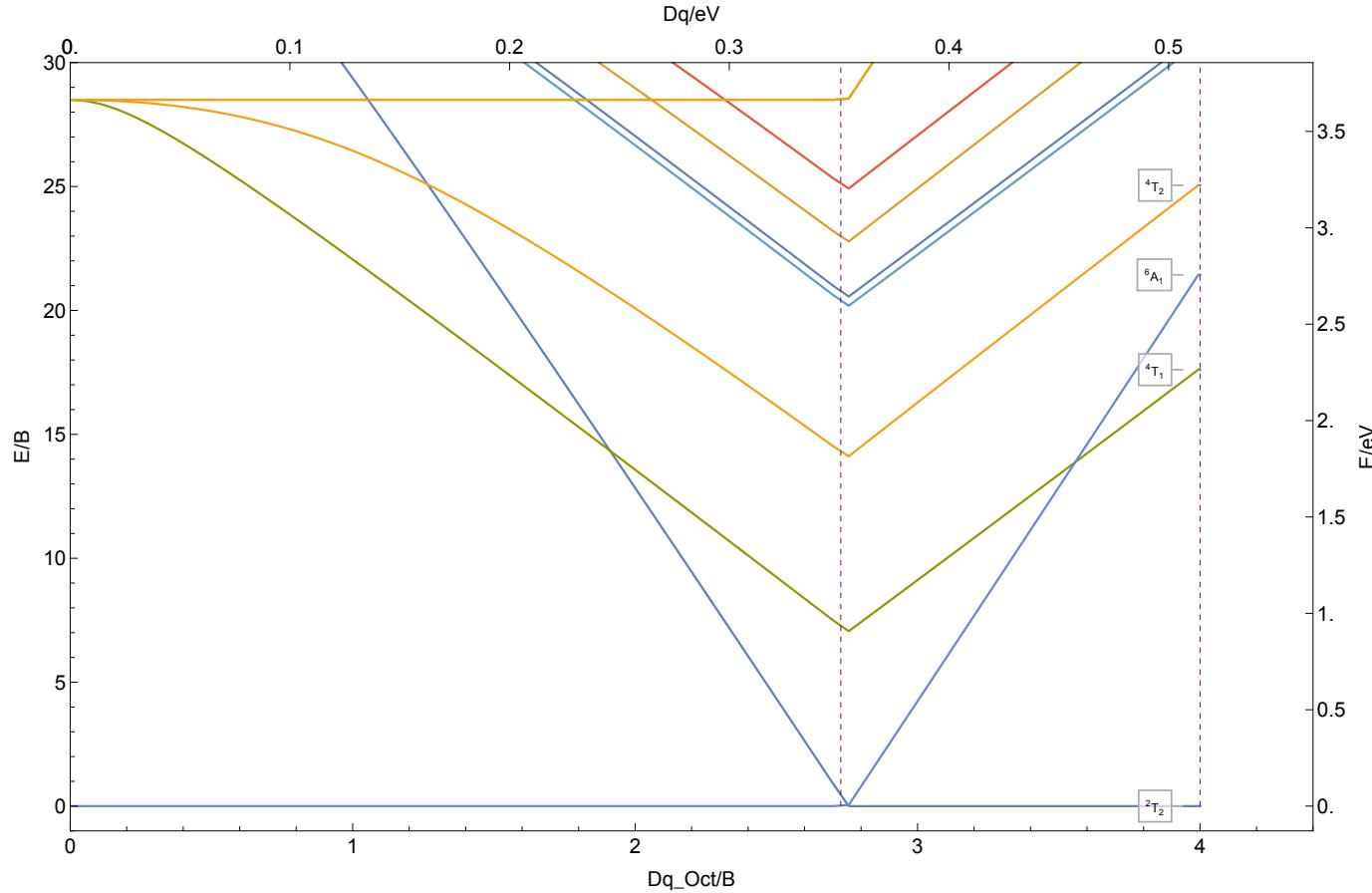
### 8.3.11 Fe<sup>2+</sup>

$|1,3,5|d^6|C/B \approx 3.7|B \approx 943\text{ cm}^{-1}|Fe^{2+}$



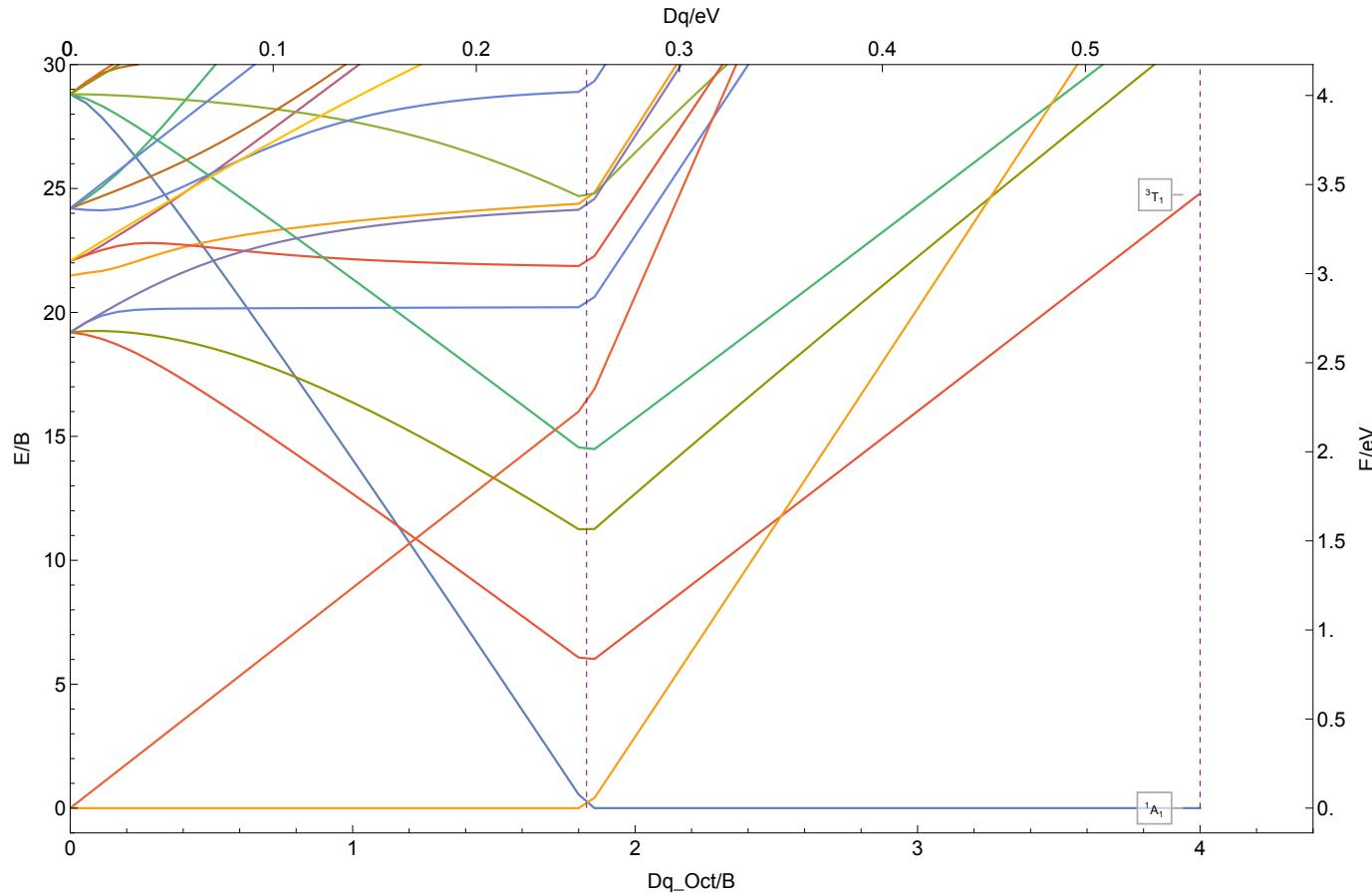
### 8.3.12 Fe<sup>3+</sup>

$|2,4,6|d^5|C/B \approx 3.7|B \approx 1037\text{cm}^{-1}|Fe^{3+}$



8.3.13 Fe<sup>4+</sup>

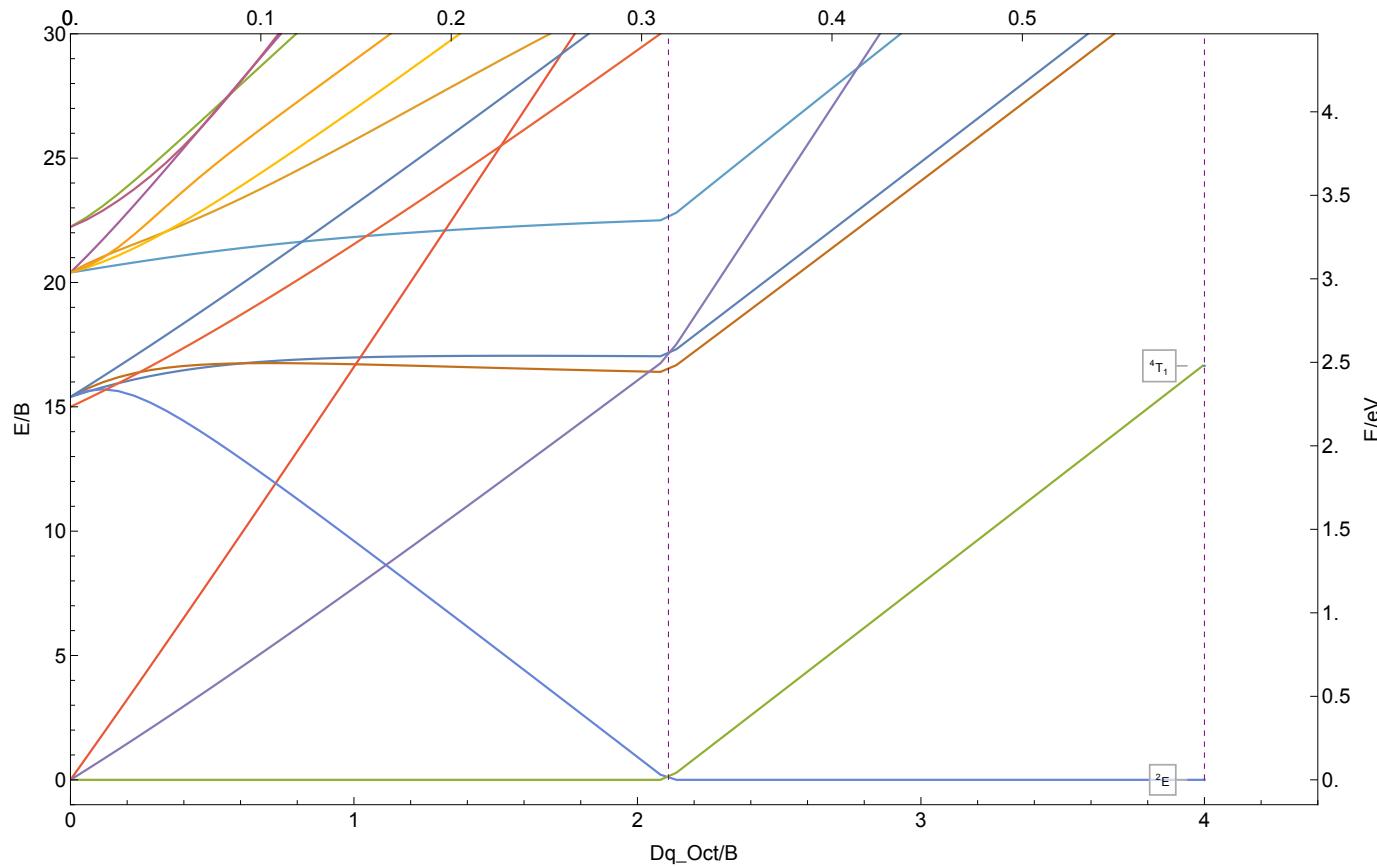
| 1,3,5 | d<sup>4</sup> | C/B ≈ 3.8 | B ≈ 1122 cm<sup>-1</sup> | Fe<sup>4+</sup>



8.3.14 Fe<sup>5+</sup>

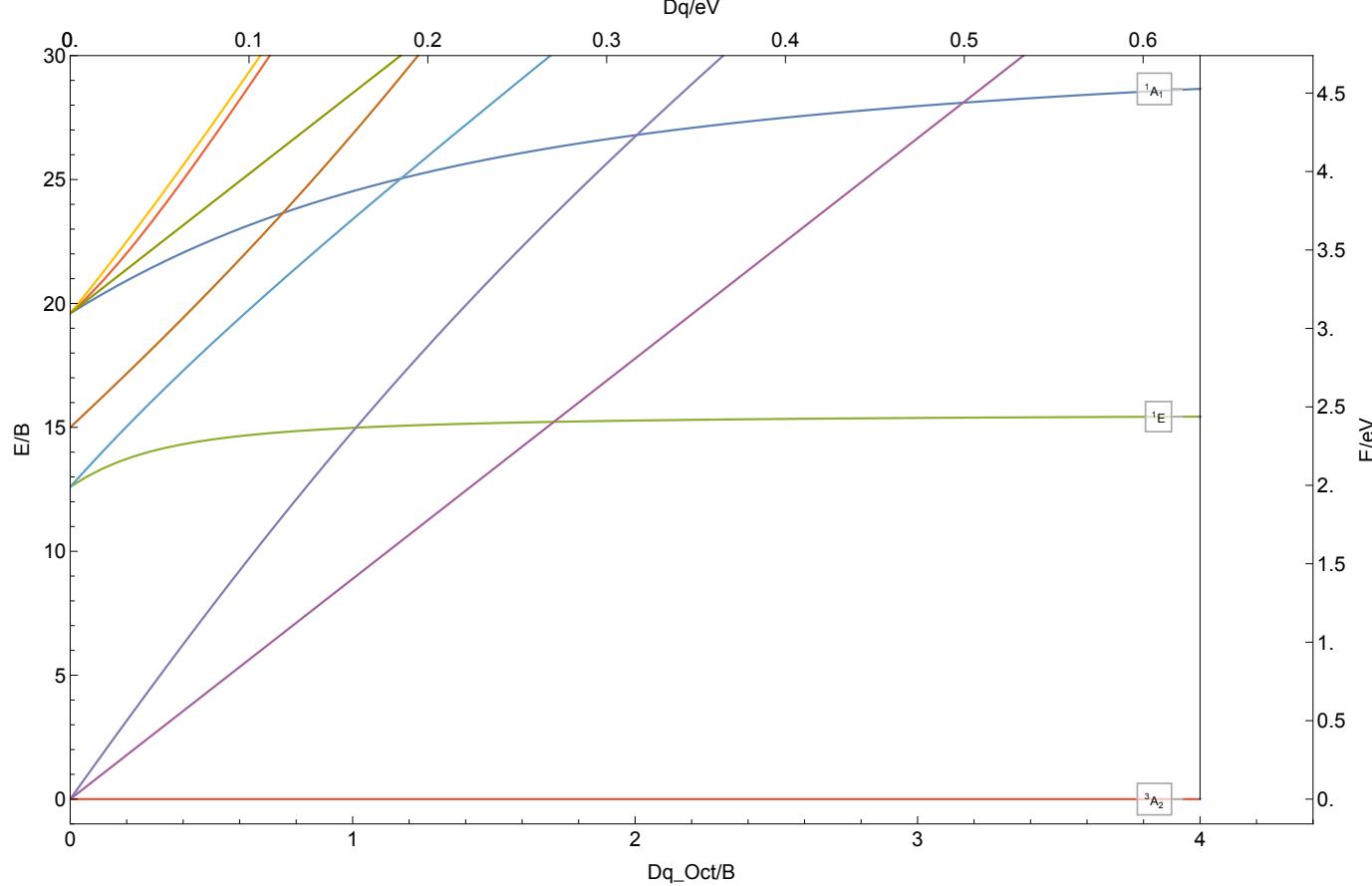
|2,4|d<sup>3</sup>|C/B ≈ 3.8|B ≈ 1201 cm<sup>-1</sup>|Fe<sup>5+</sup>

Dq/eV



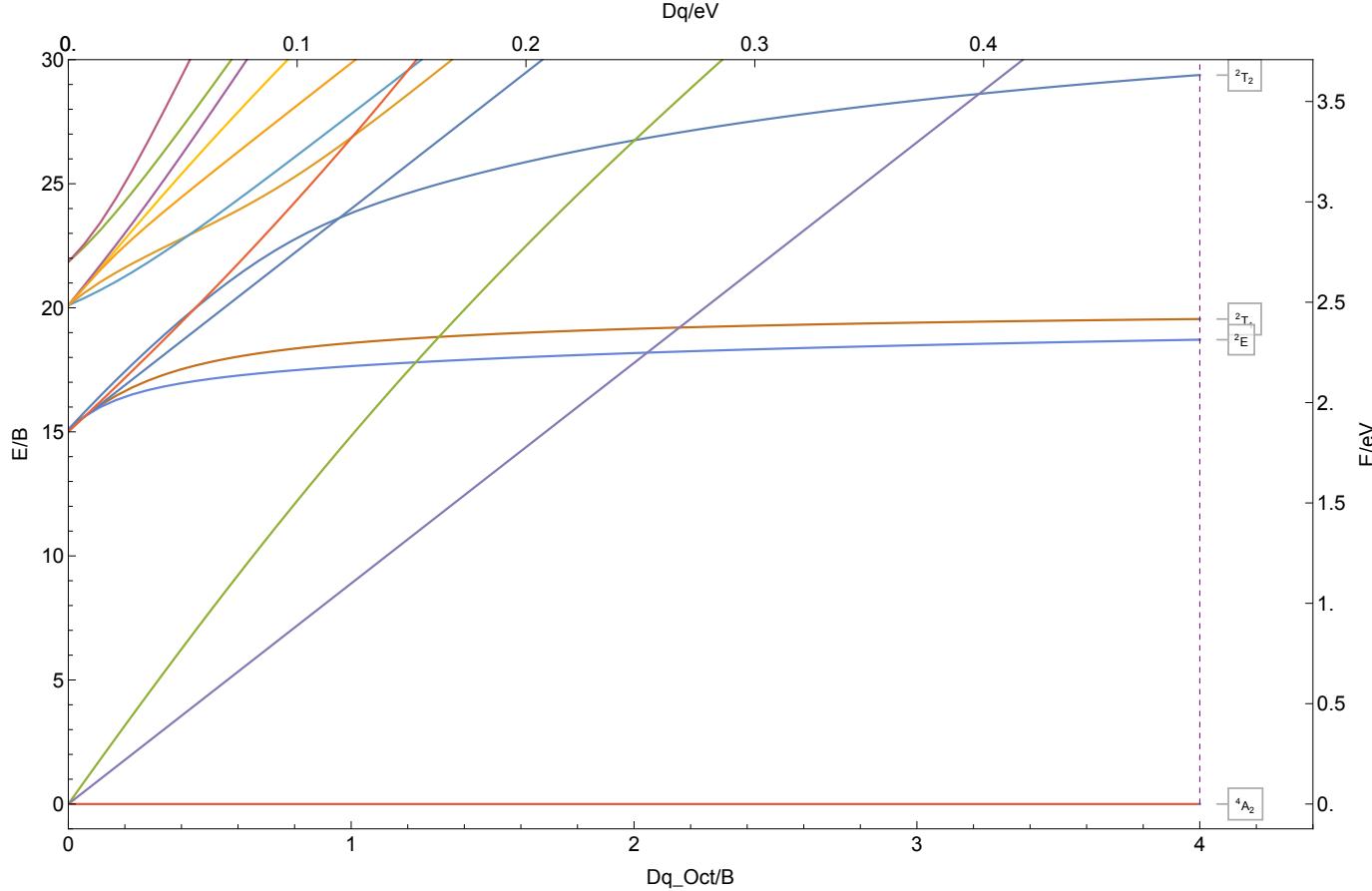
8.3.15 Fe<sup>6+</sup>

$|1,3|d^2|C/B \approx 3.8|B \approx 1274\text{ cm}^{-1}|Fe^{6+}$



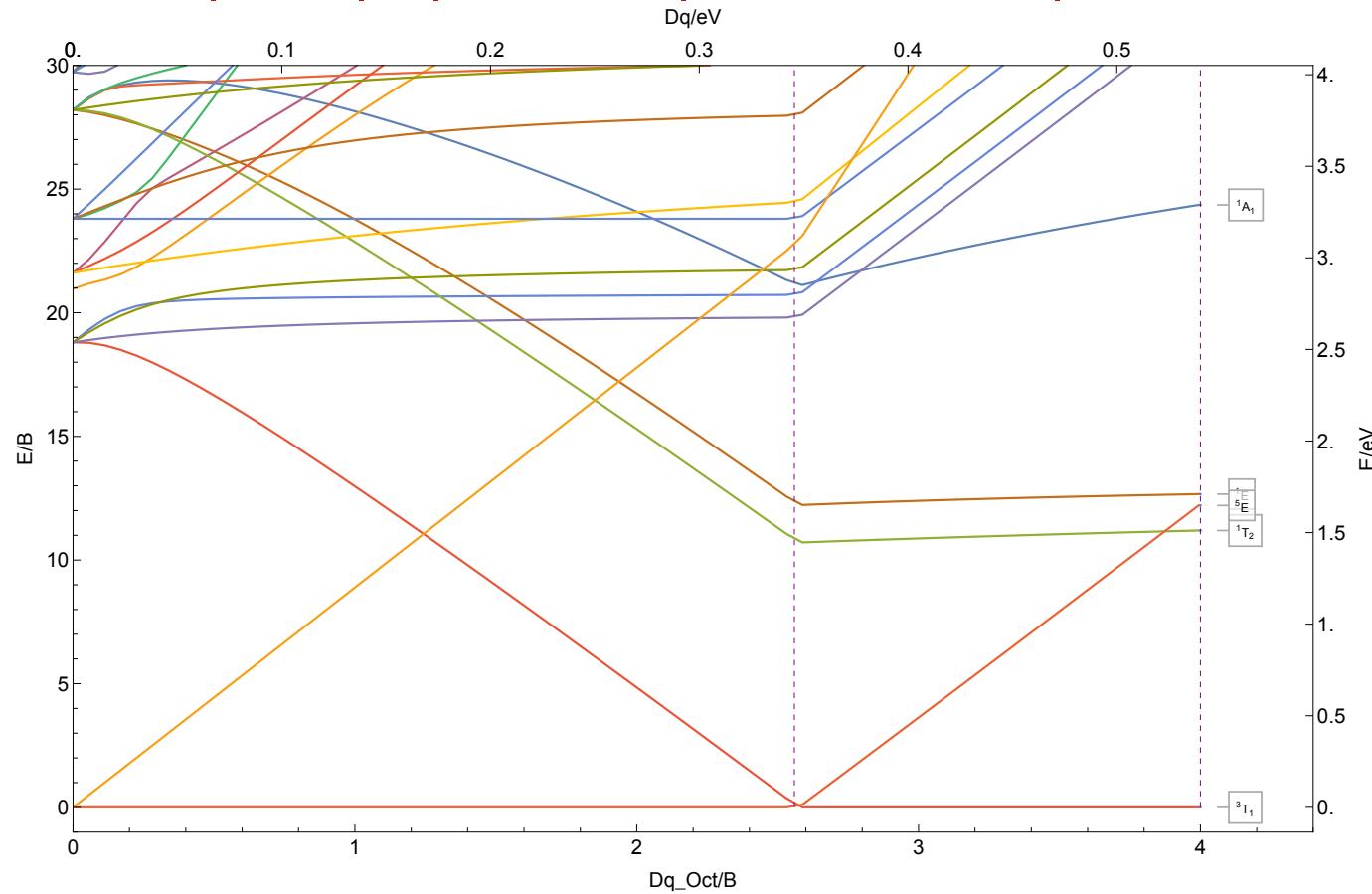
### 8.3.16 $\text{Co}^{2+}$

$|2,4| \text{d}^7| \text{C/B} \approx 3.7 | \text{B} \approx 997 \text{ cm}^{-1} | \text{Co}^{2+}$



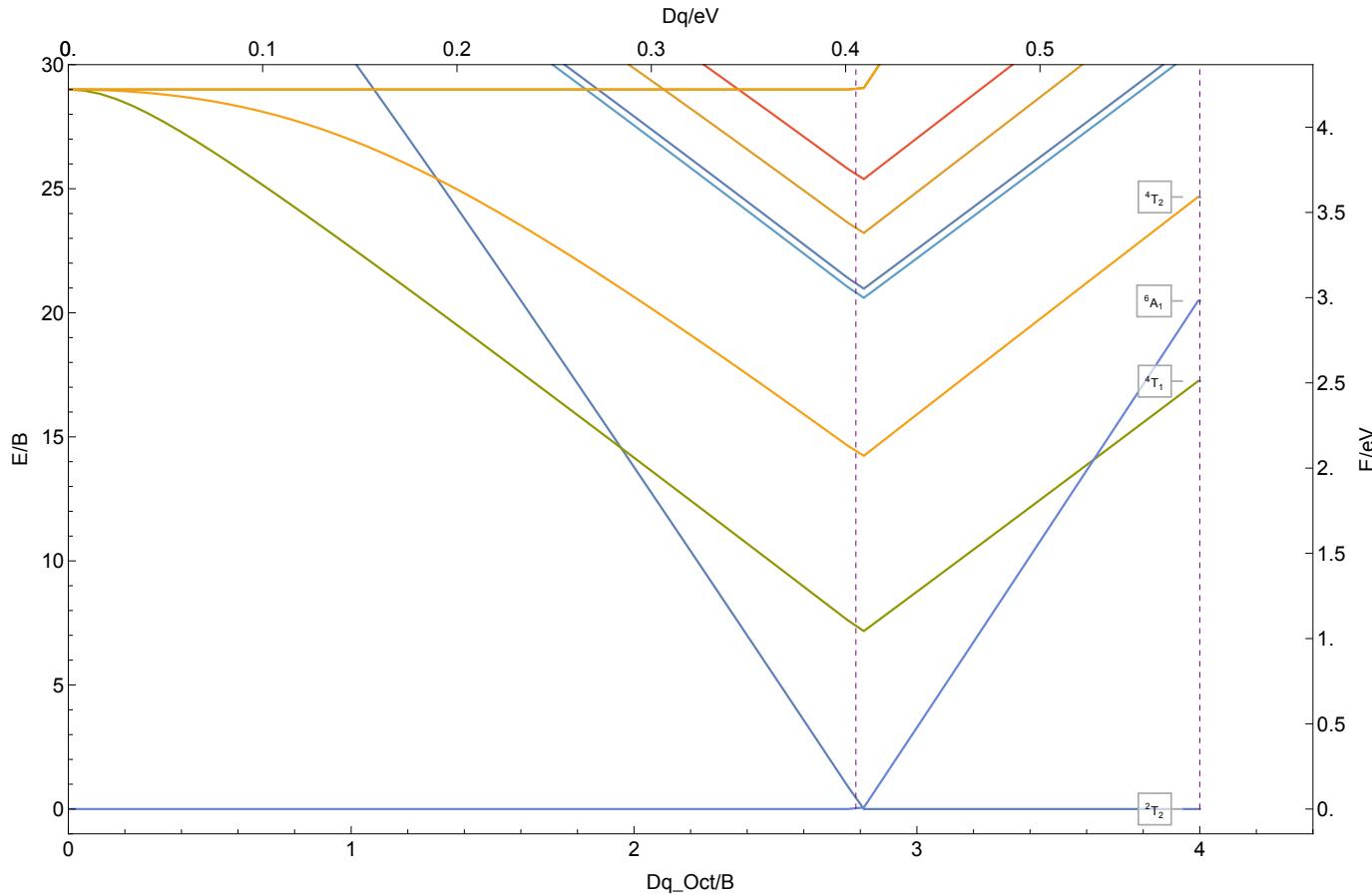
8.3.17  $\text{Co}^{3+}$

$|1,3,5| \text{d}^6 | \text{C/B} \approx 3.7 | \text{B} \approx 1089 \text{ cm}^{-1} | \text{Co}^{3+}$



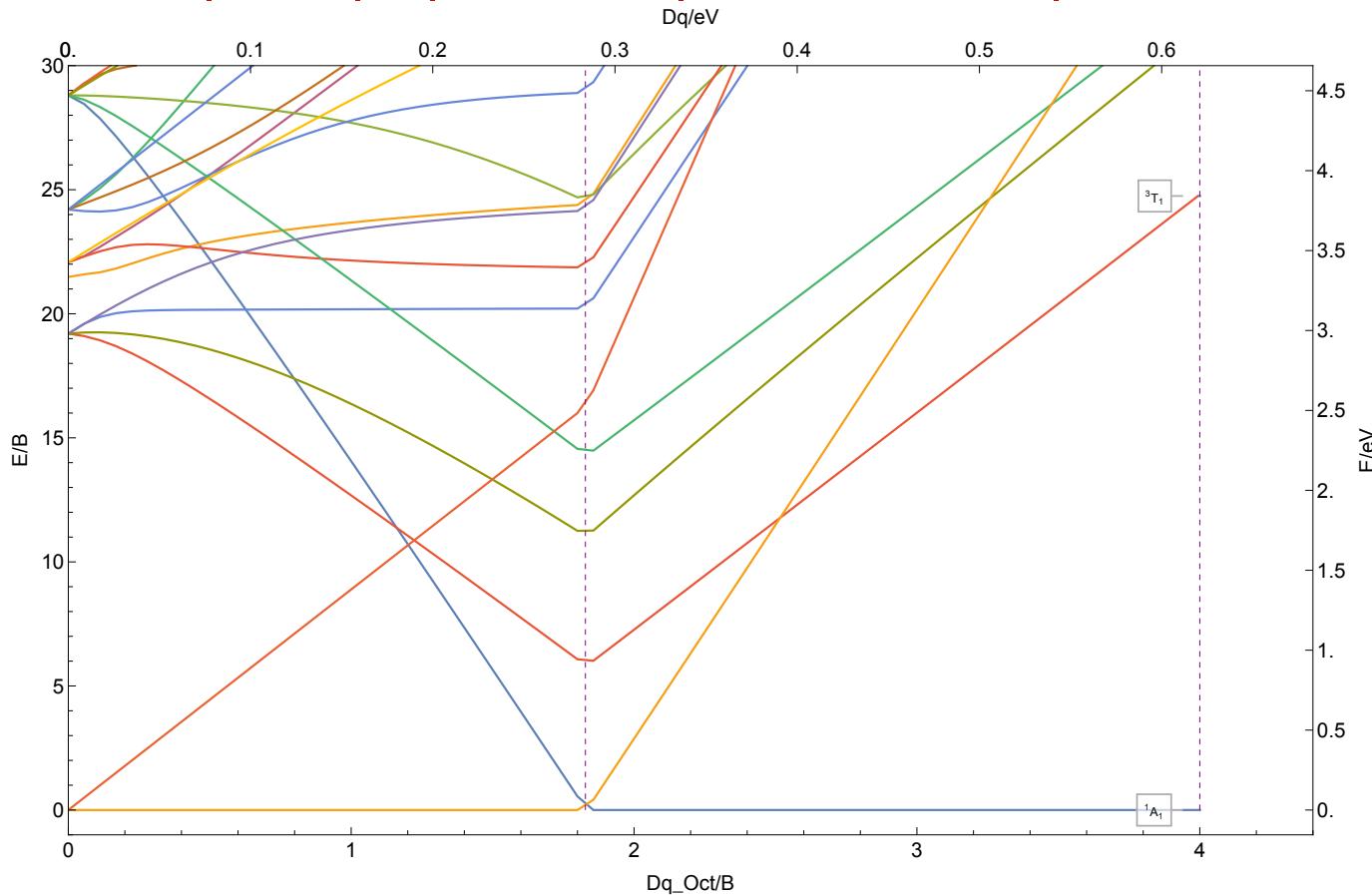
8.3.18  $\text{Co}^{4+}$

$|2,4,6| \text{d}^5 | \text{C/B} \approx 3.8 | \text{B} \approx 1174 \text{ cm}^{-1} | \text{Co}^{4+}$



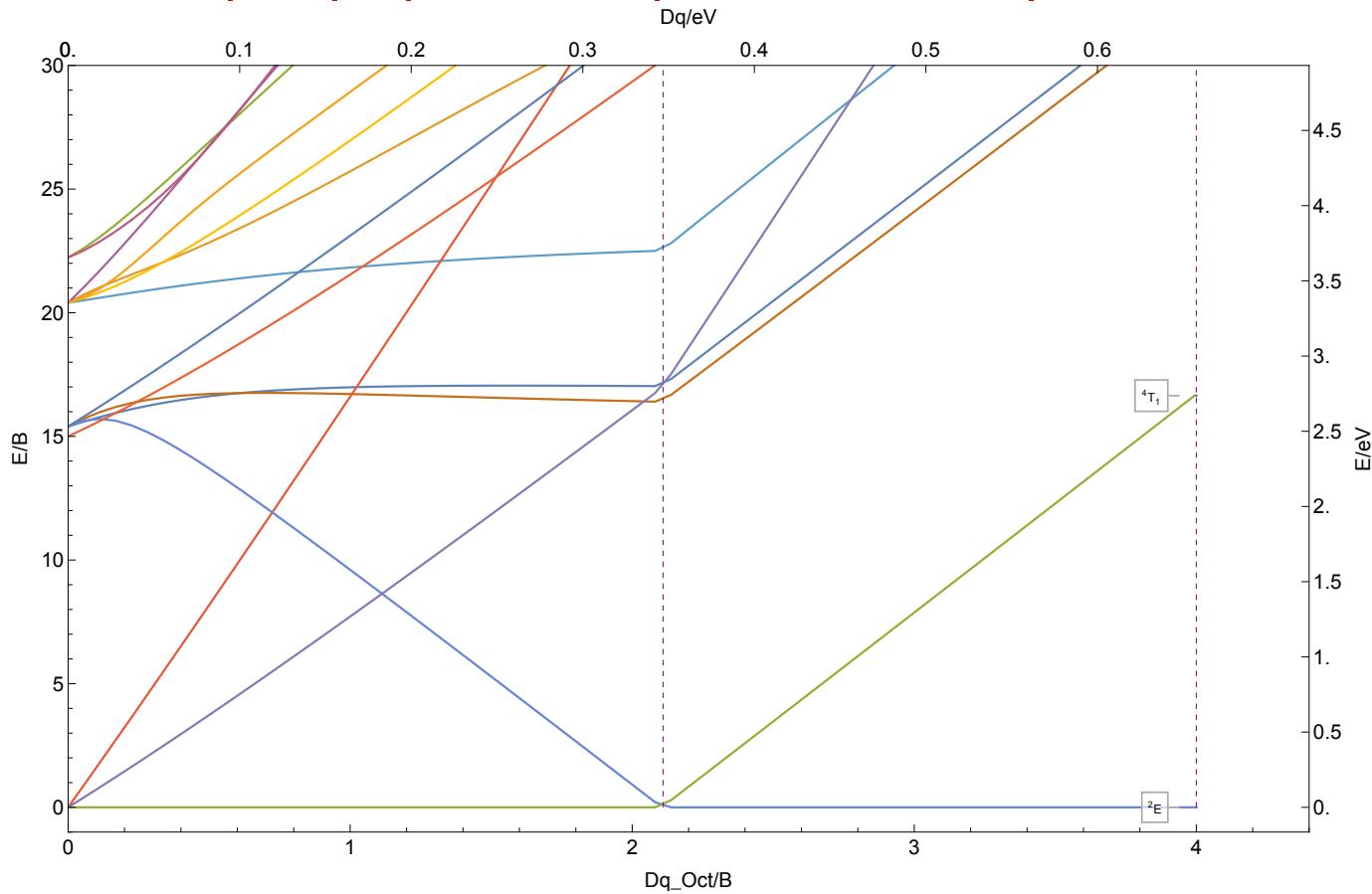
8.3.19  $\text{Co}^{5+}$

$|1,3,5|d^4|C/B \approx 3.8|B \approx 1252\text{ cm}^{-1}|Co^{5+}$



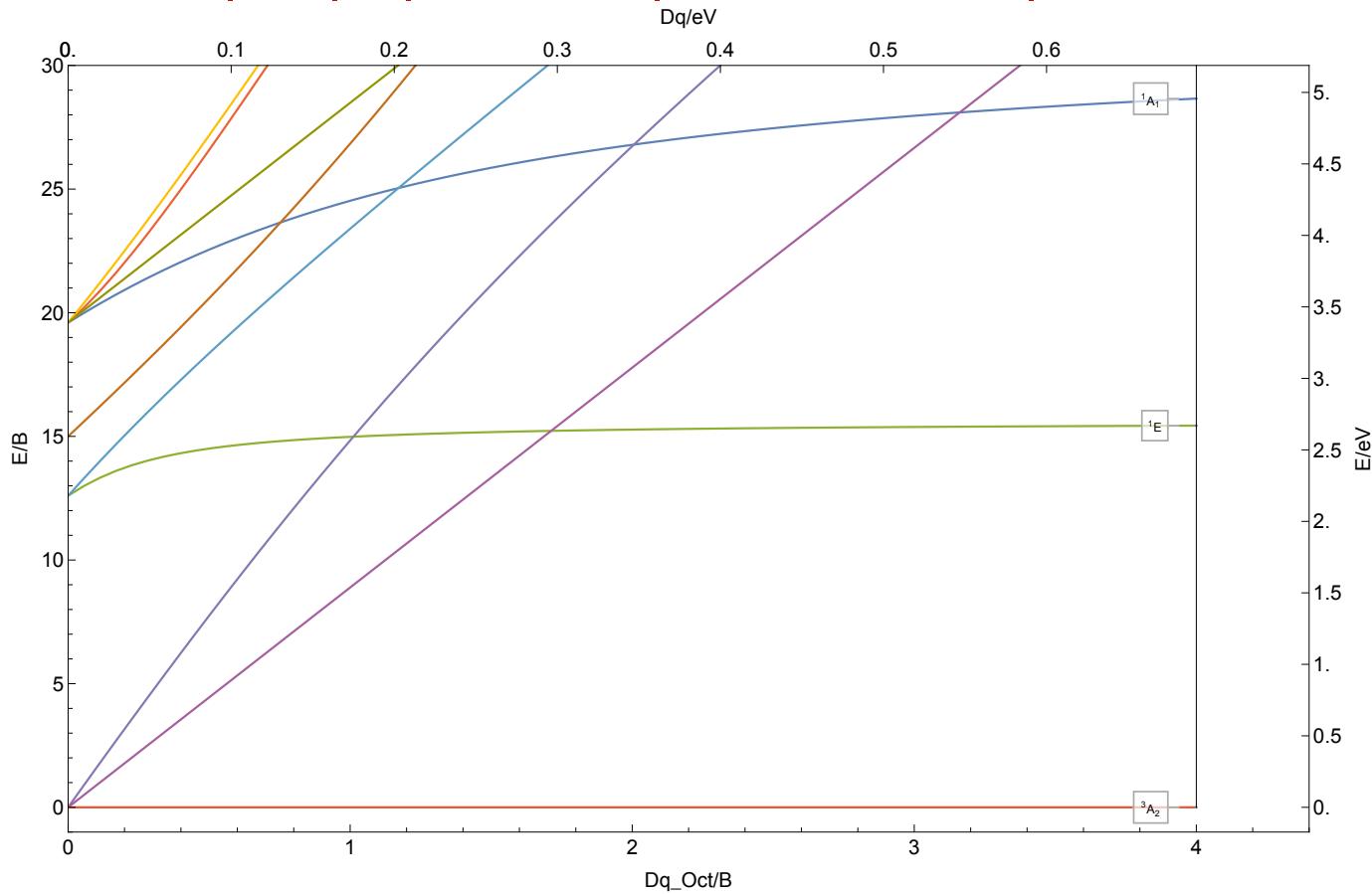
8.3.20  $\text{Co}^{6+}$

$|2,4|d^3|C/B \approx 3.8|B \approx 1326\text{ cm}^{-1}|Co^{6+}$



### 8.3.21 Co<sup>7+</sup>

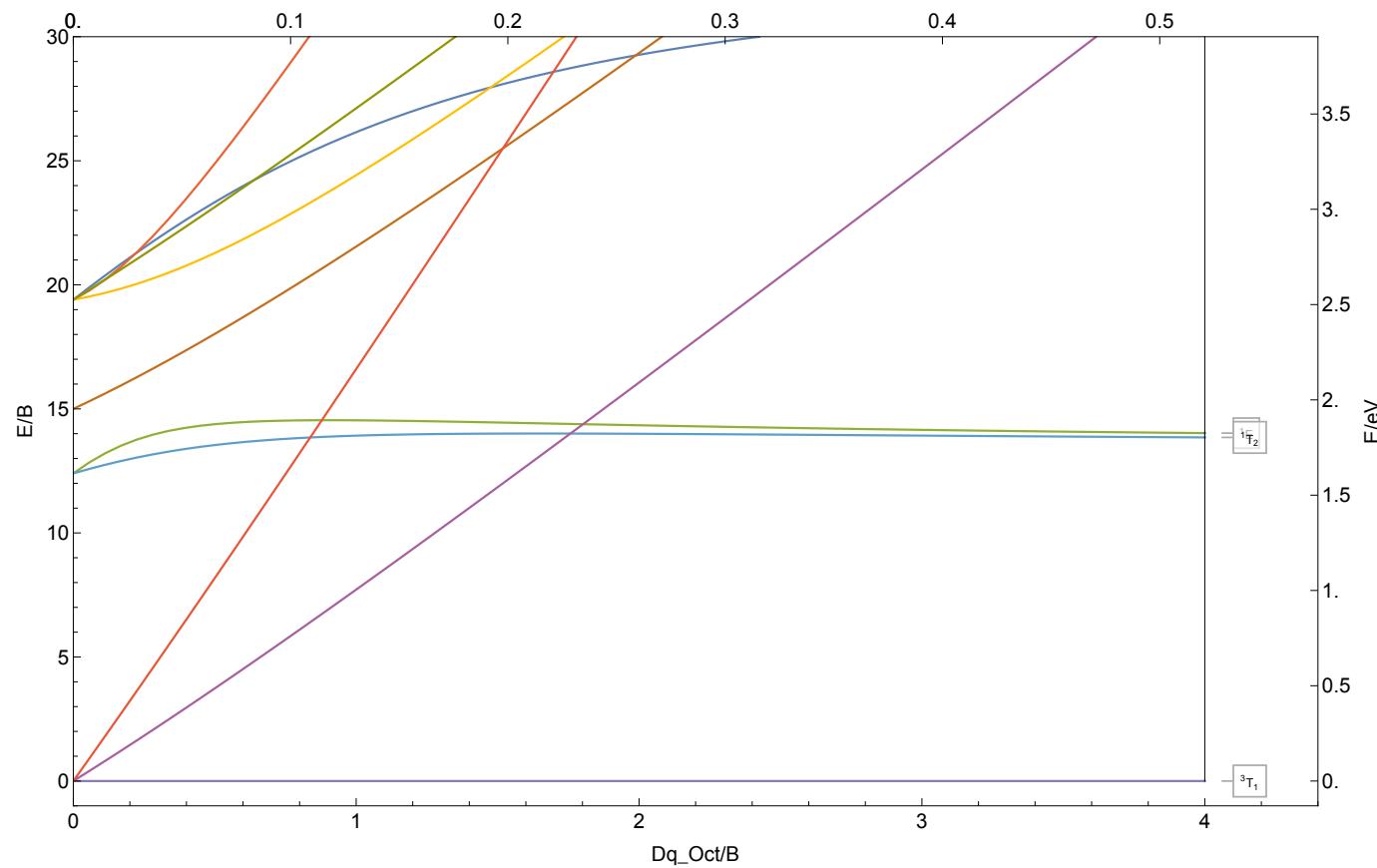
$|1,3|d^2|C/B \approx 3.8|B \approx 1395\text{ cm}^{-1}|Co^{7+}$



8.3.22  $\text{Ni}^{2+}$

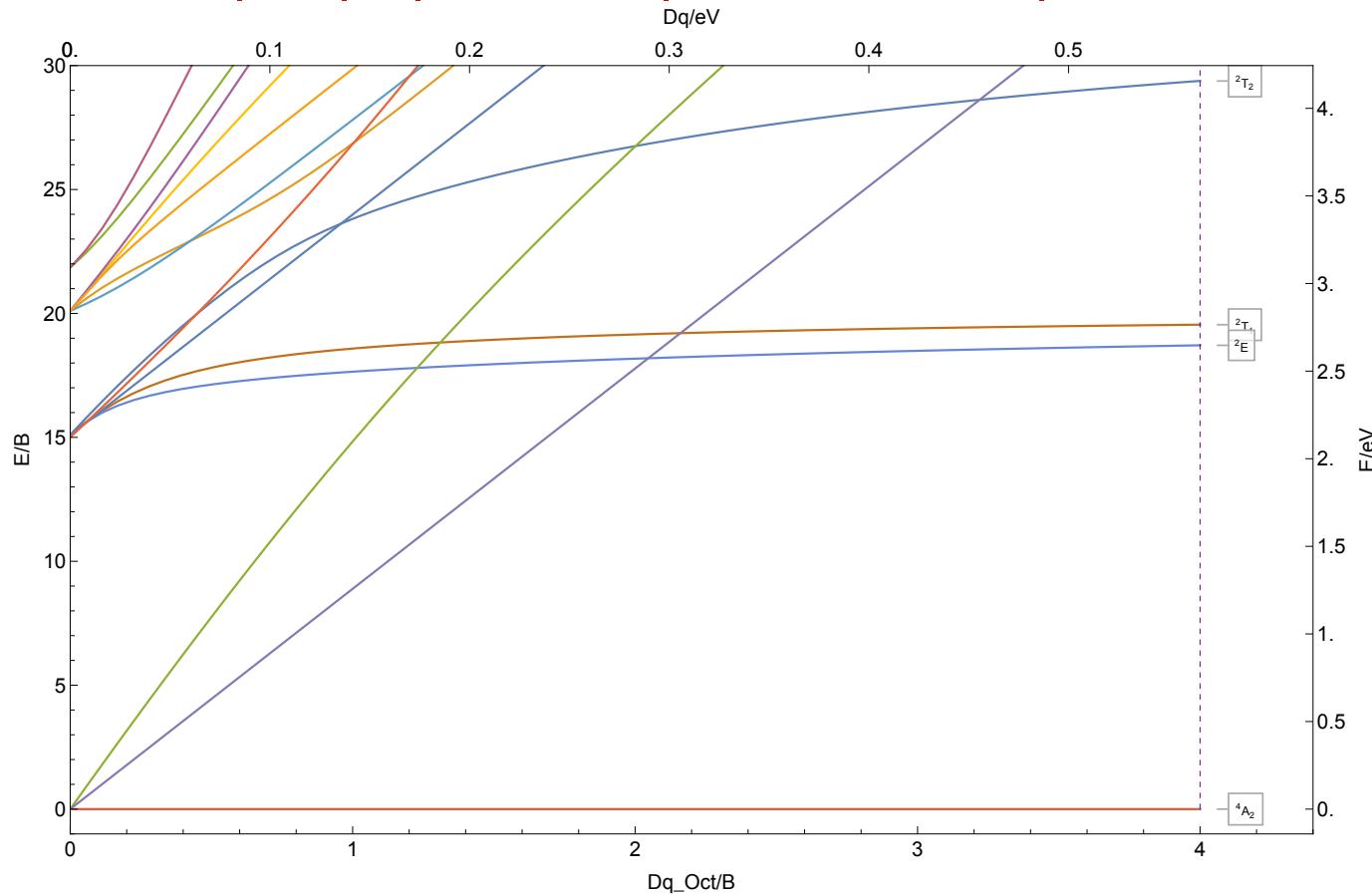
$|1,3|d^8|C/B \approx 3.7|B \approx 1050\text{ cm}^{-1}| \text{Ni}^{2+}$

Dq/eV



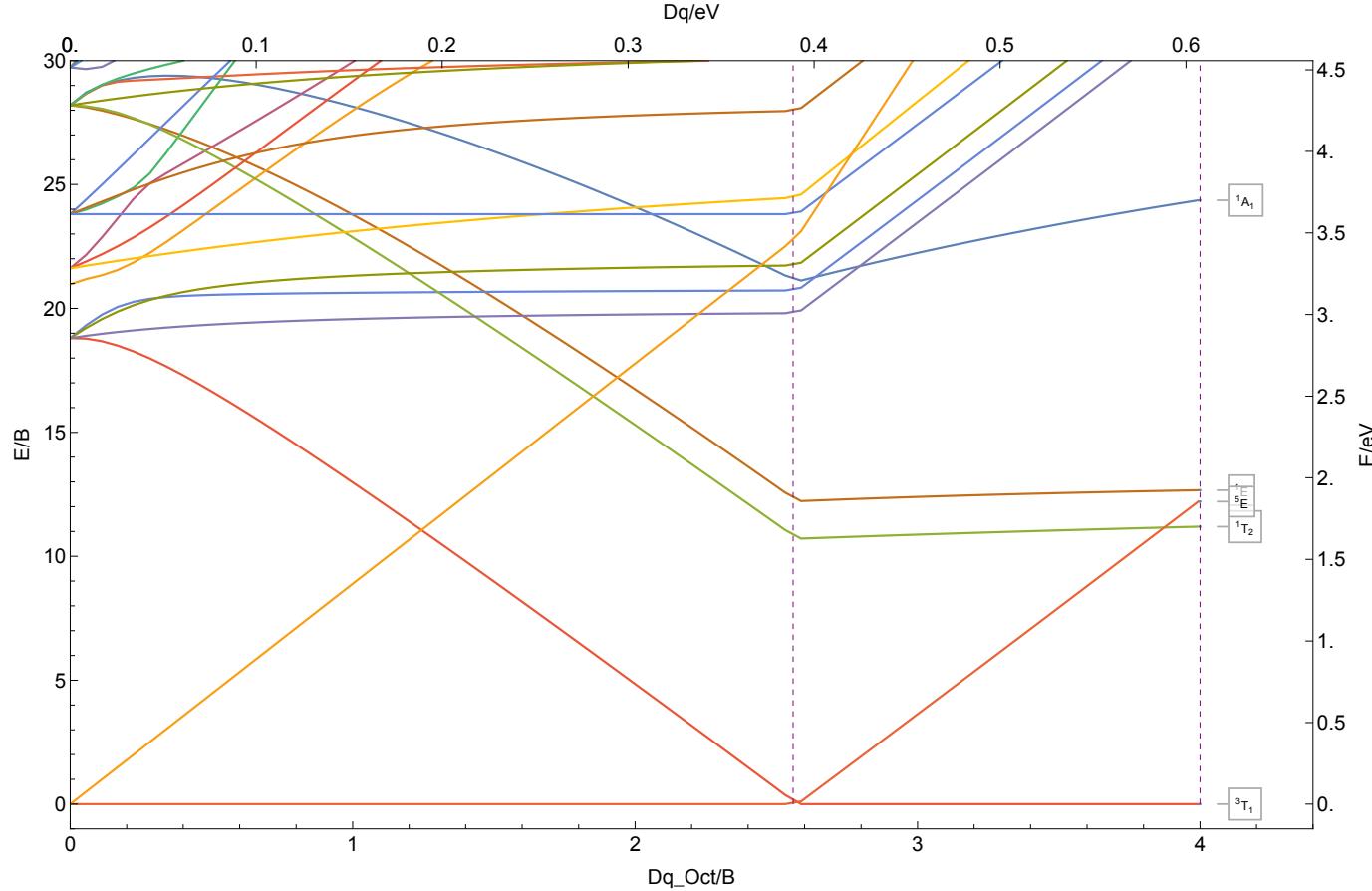
### 8.3.23 Ni<sup>3+</sup>

$|2,4|d^7| C/B \approx 3.7 | B \approx 1141\text{ cm}^{-1} | \text{Ni}^{3+}$



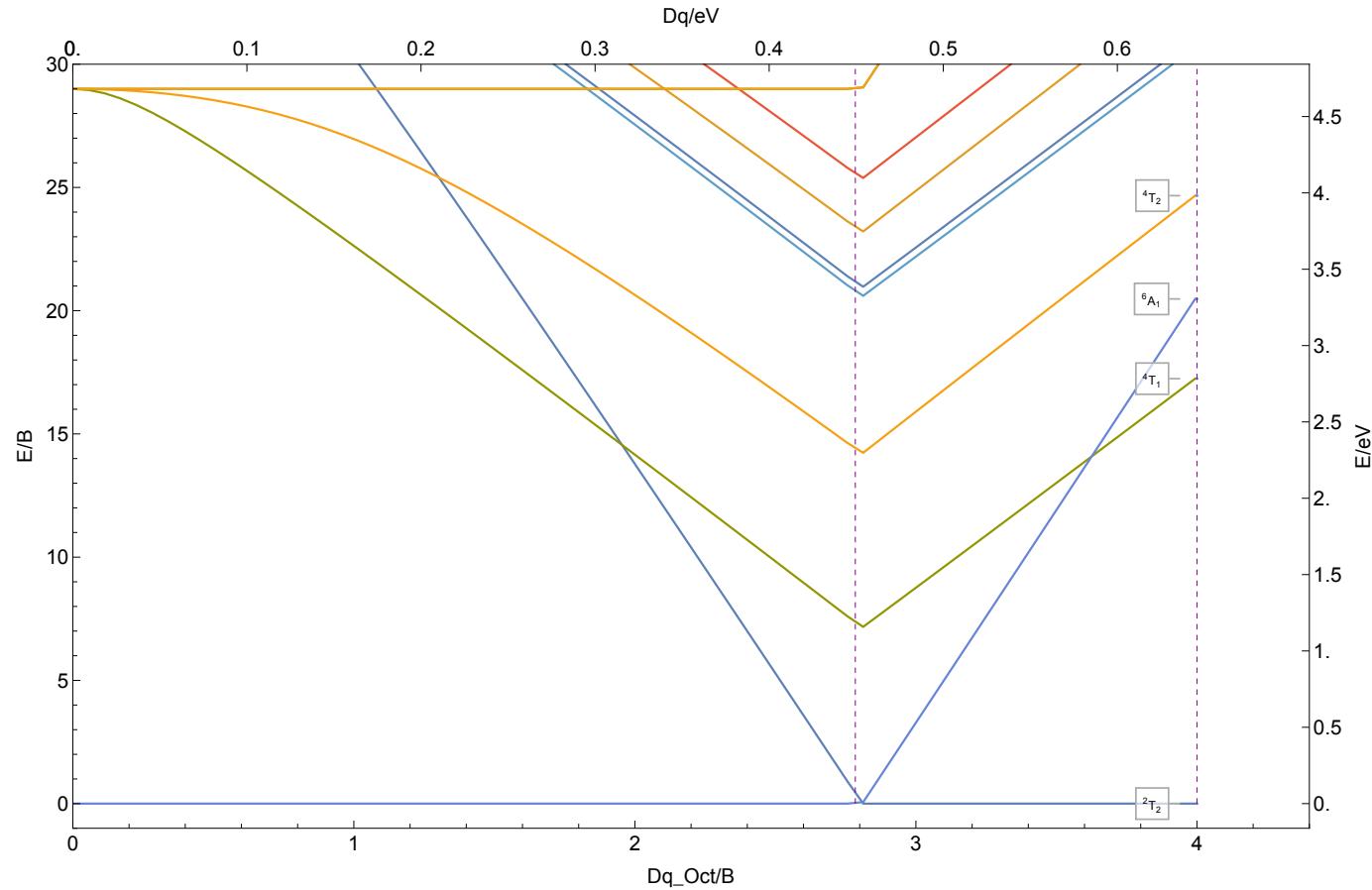
8.3.24 Ni<sup>4+</sup>

$|1,3,5|d^6|C/B \approx 3.7|B \approx 1225\text{ cm}^{-1}|Ni^{4+}$



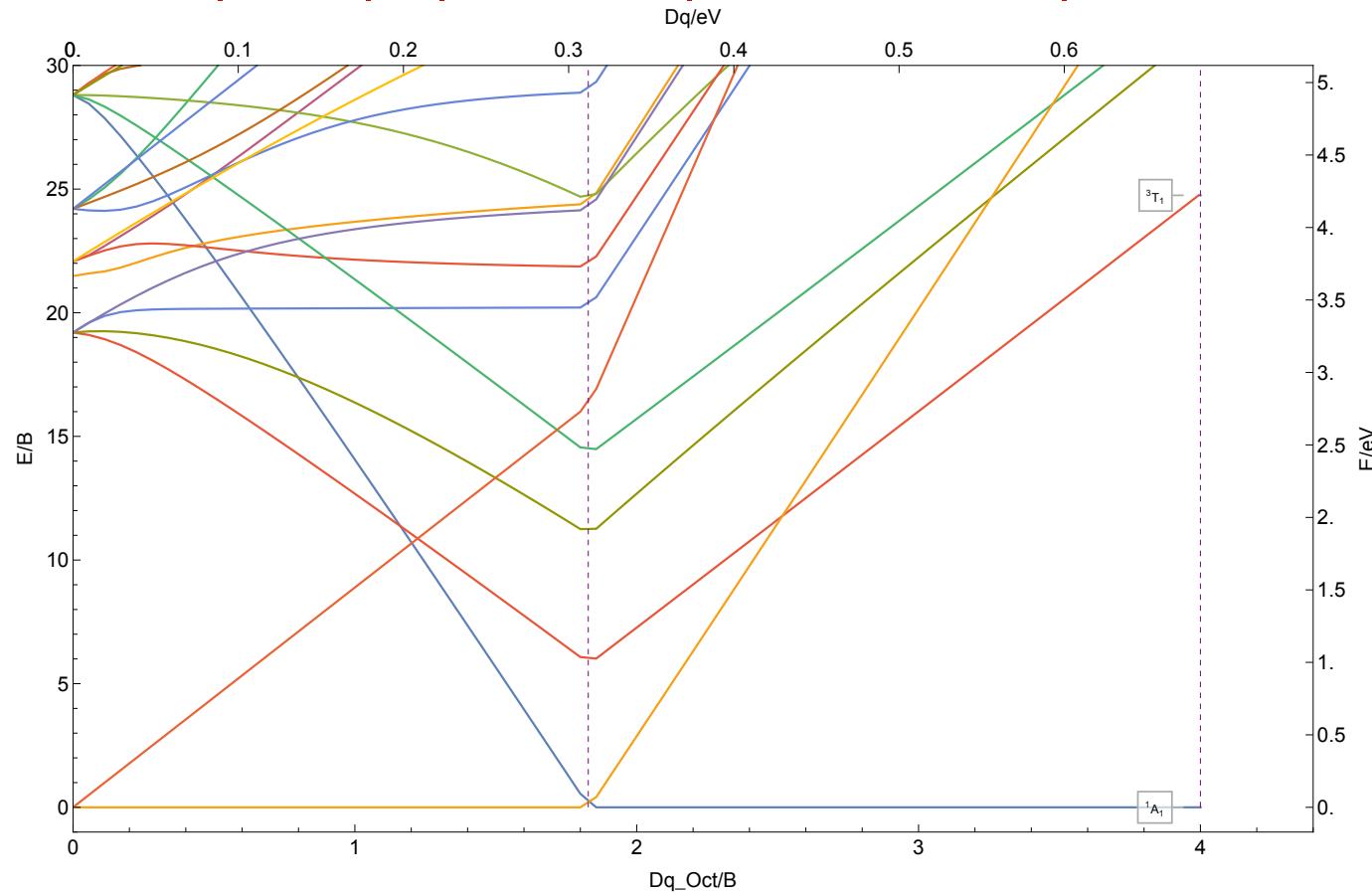
8.3.25 Ni<sup>5+</sup>

|2,4,6|d<sup>5</sup>|C/B ≈ 3.8|B ≈ 1302 cm<sup>-1</sup>|Ni<sup>5+</sup>



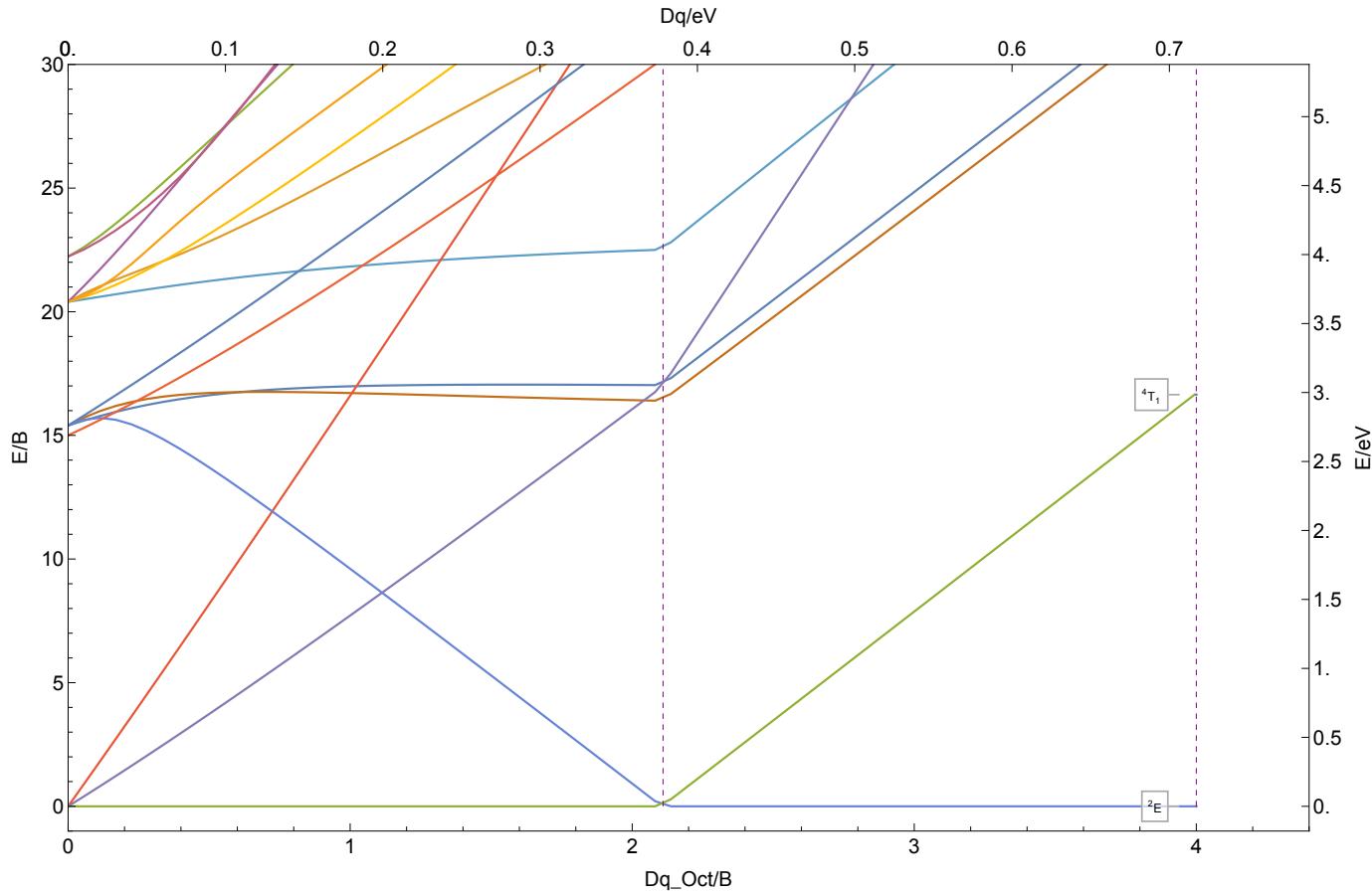
8.3.26 Ni<sup>6+</sup>

$|1,3,5|d^4|C/B \approx 3.8|B \approx 1376\text{ cm}^{-1}|Ni^{6+}$



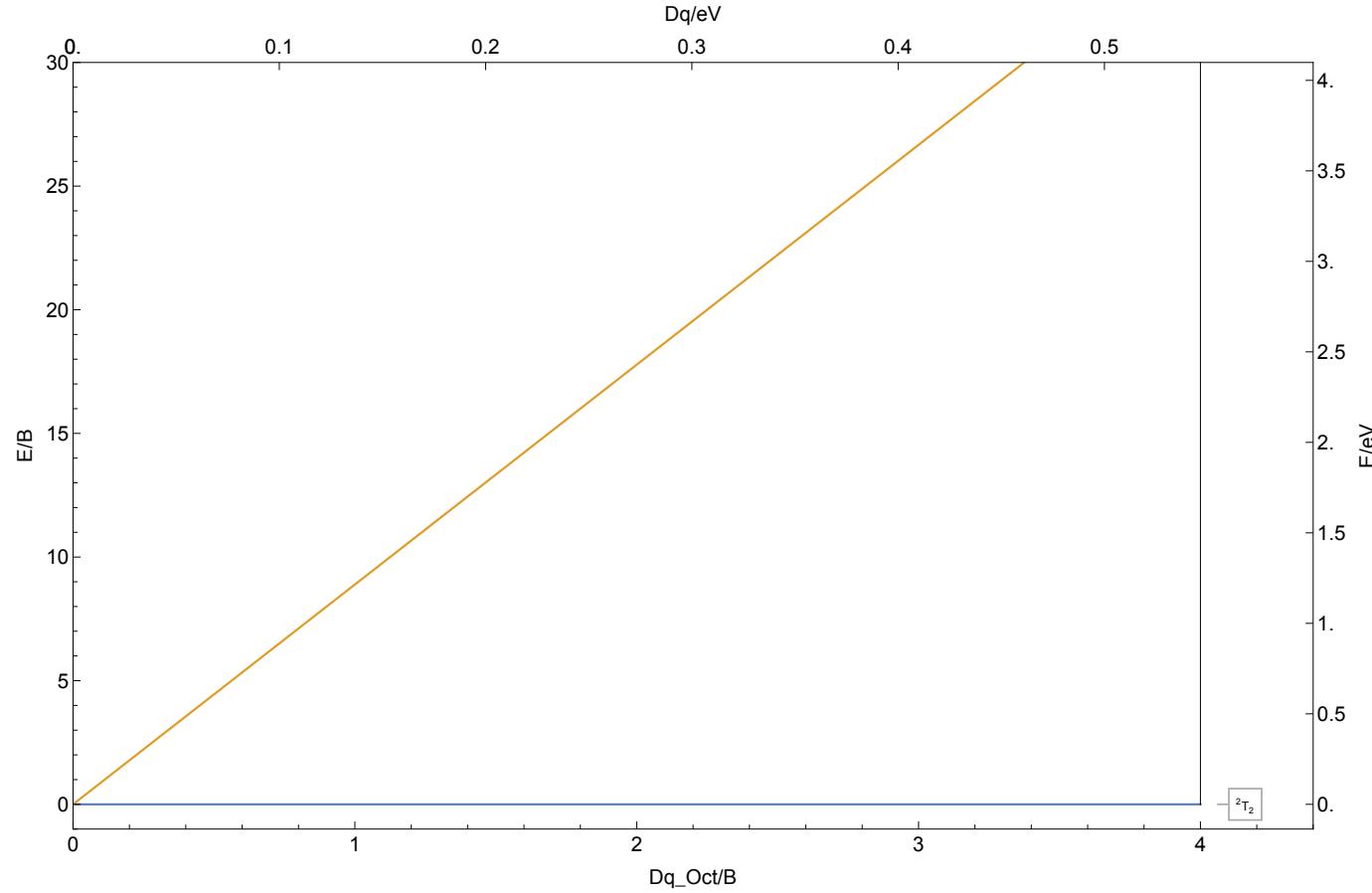
8.3.27 Ni<sup>7+</sup>

|2,4|d<sup>3</sup>| C/B ≈ 3.8 | B ≈ 1446 cm<sup>-1</sup> | Ni<sup>7+</sup>



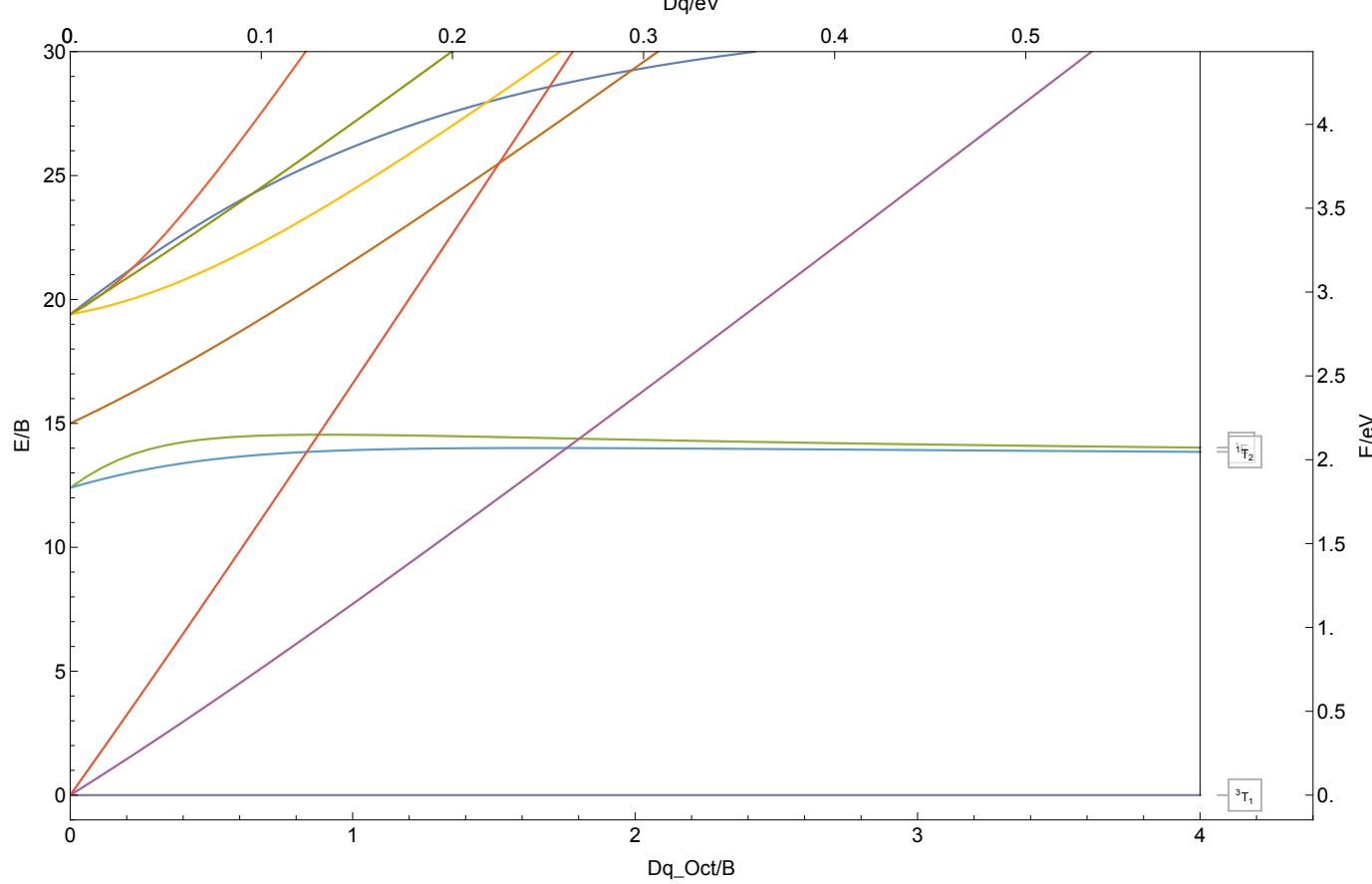
8.3.28 Cu<sup>2+</sup>

|2|d<sup>9</sup>| C/B ≈ 3.7 | B ≈ 1102 cm<sup>-1</sup> | Cu<sup>2+</sup>



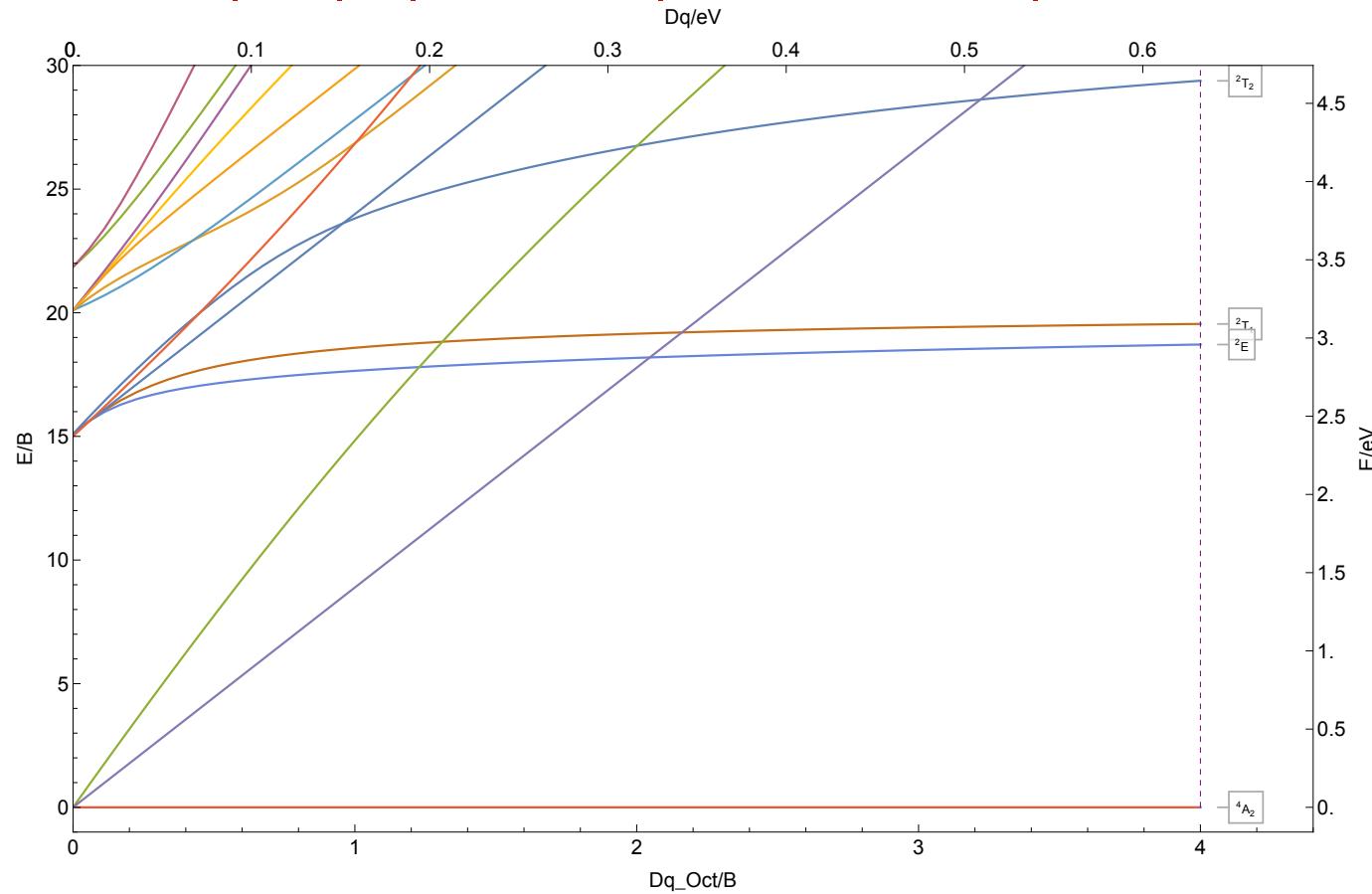
8.3.29 Cu<sup>3+</sup>

|1,3|d<sup>8</sup>|C/B ≈ 3.7|B ≈ 1192 cm<sup>-1</sup>|Cu<sup>3+</sup>



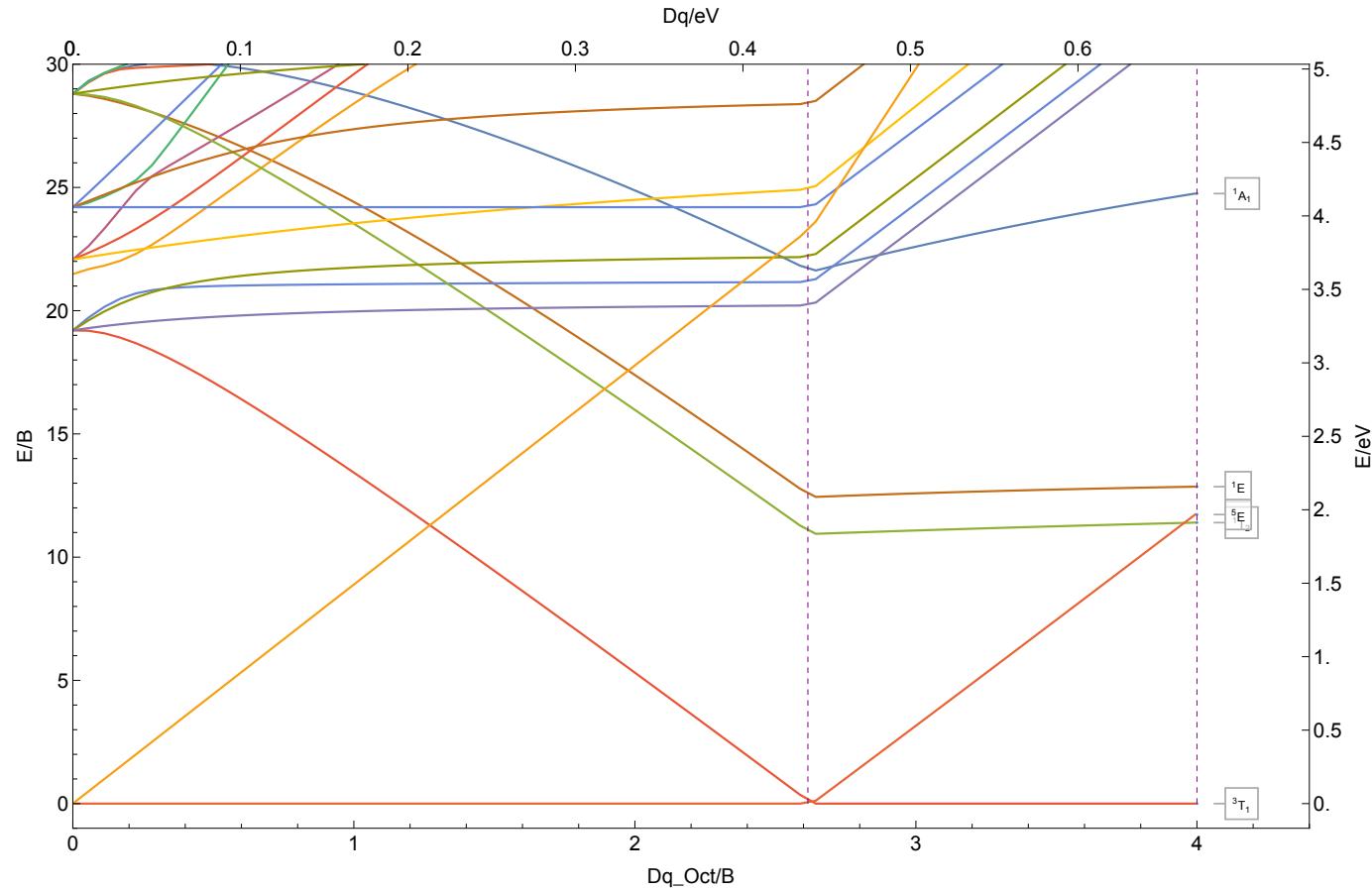
### 8.3.30 Cu<sup>4+</sup>

|2,4|d<sup>7</sup>|C/B ≈ 3.7|B ≈ 1275 cm<sup>-1</sup>|Cu<sup>4+</sup>



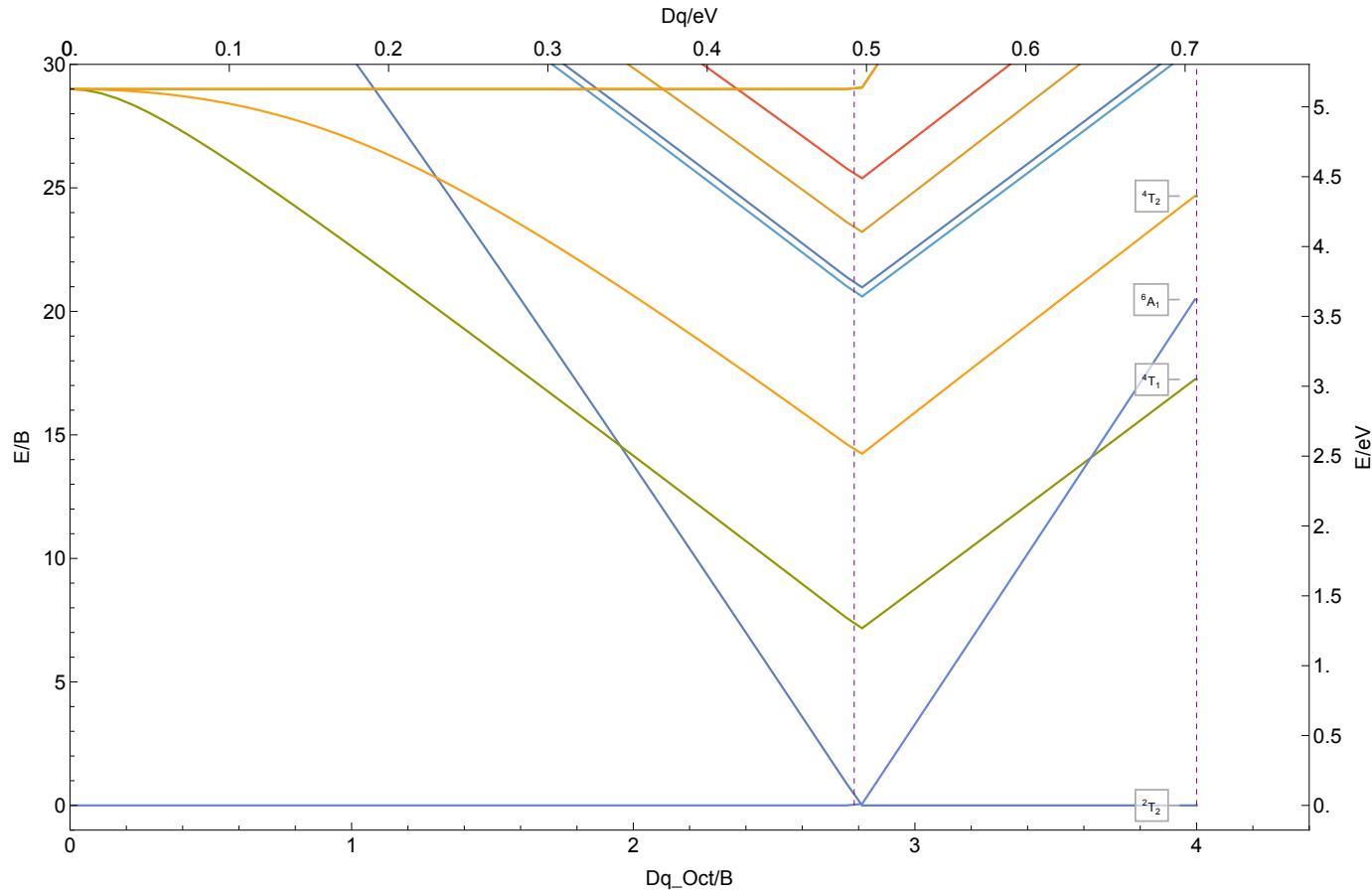
### 8.3.31 Cu<sup>5+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 3.8 | B ≈ 1353 cm<sup>-1</sup> | Cu<sup>5+</sup>



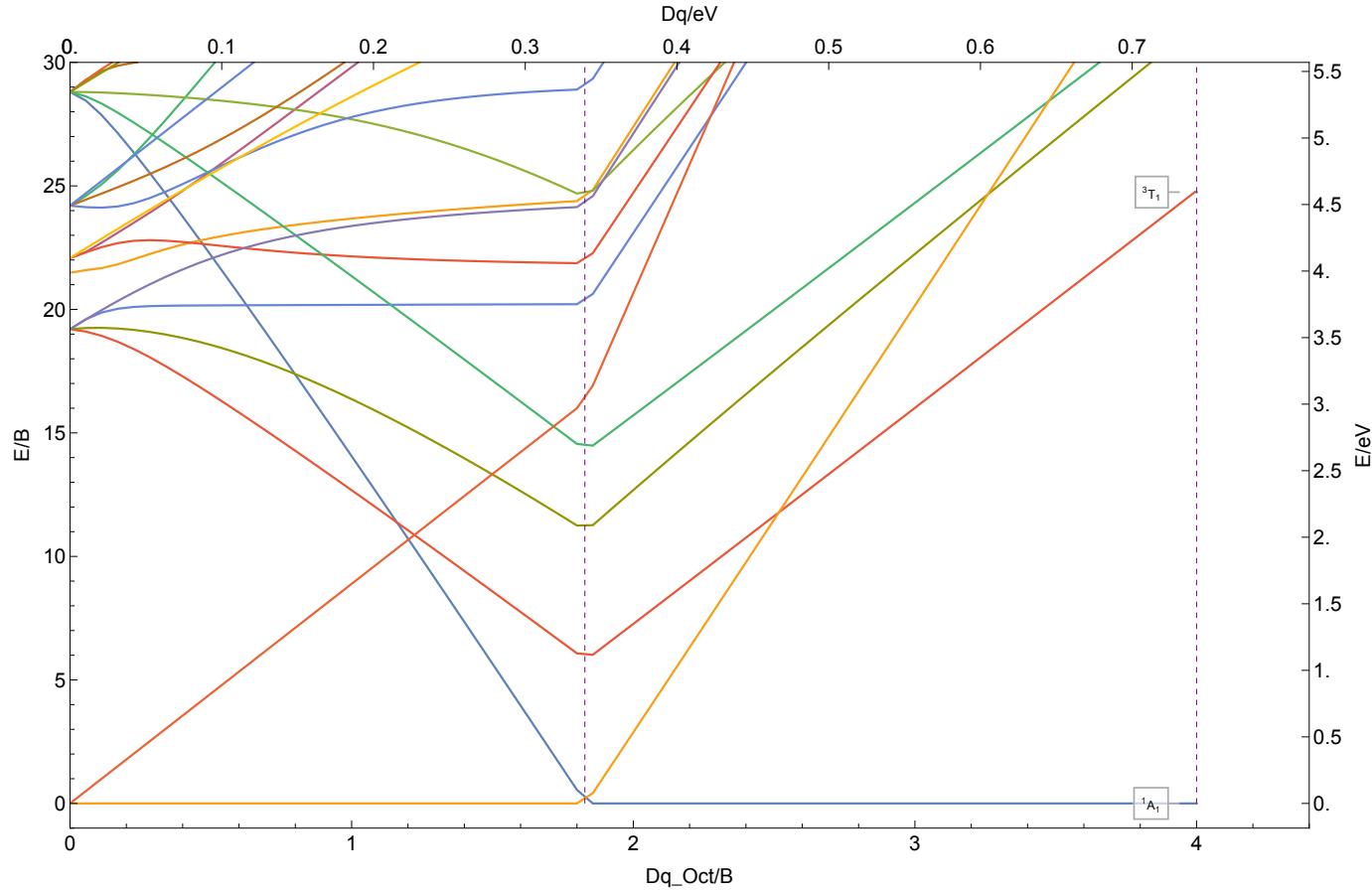
8.3.32 Cu<sup>6+</sup>

|2,4,6|d<sup>5</sup>|C/B ≈ 3.8|B ≈ 1426 cm<sup>-1</sup>|Cu<sup>6+</sup>



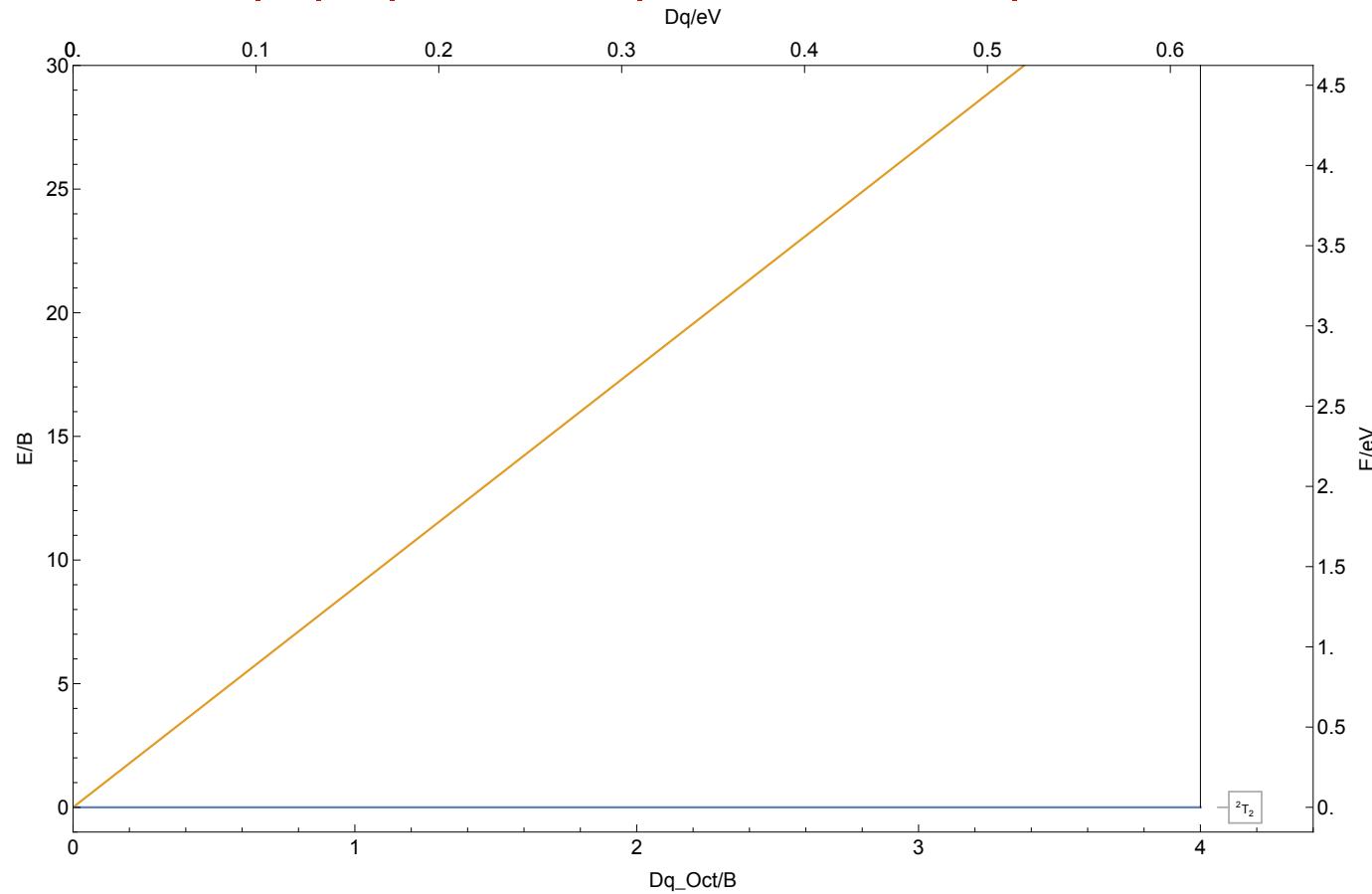
8.3.33 Cu<sup>7+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 3.8 | B ≈ 1497 cm<sup>-1</sup> | Cu<sup>7+</sup>



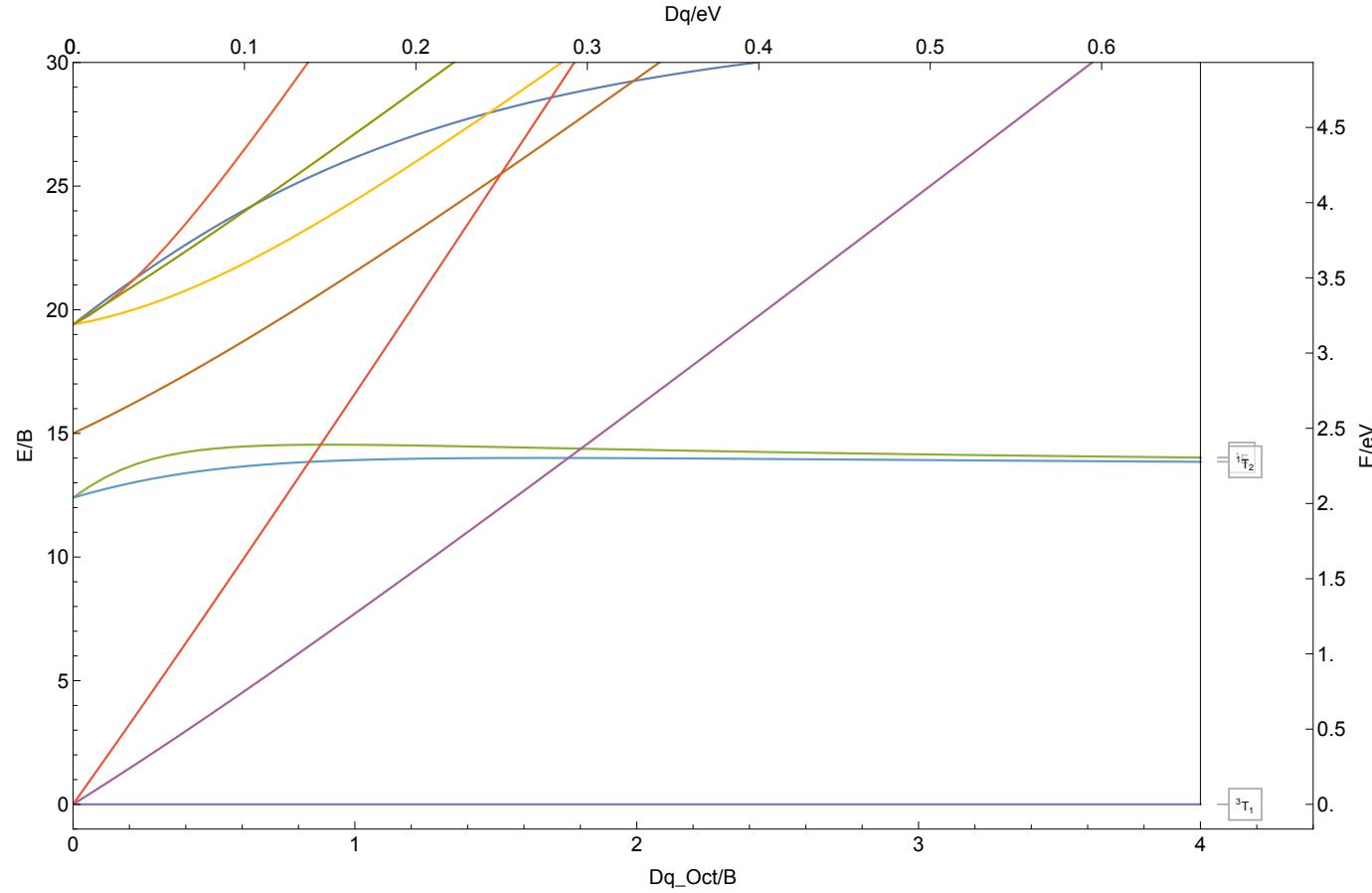
8.3.34 Zn<sup>3+</sup>

$$|2|d^9|C/B \approx 3.7|B \approx 1243\text{ cm}^{-1}|Zn^{3+}$$



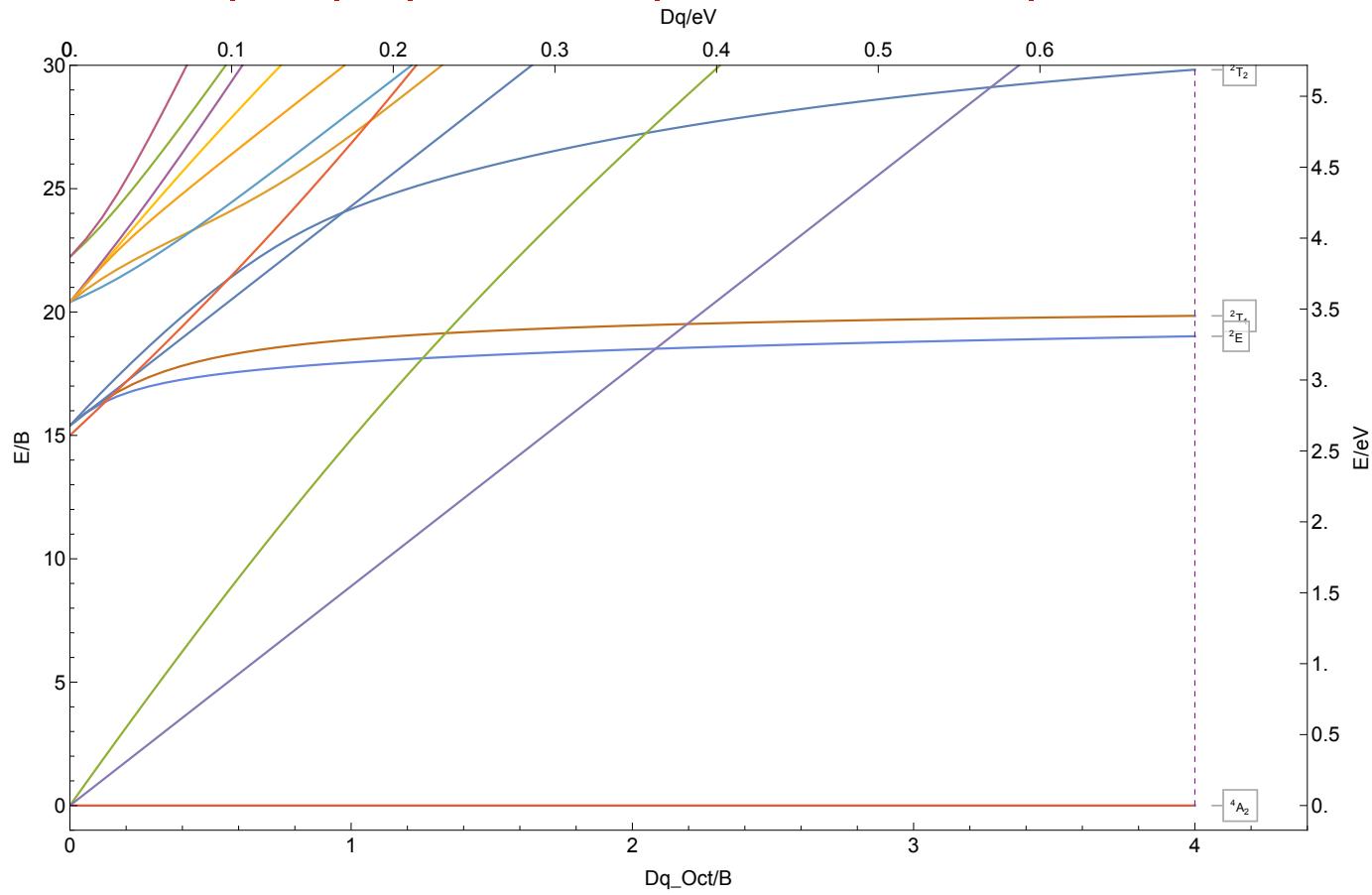
8.3.35 Zn<sup>4+</sup>

| 1,3 | d<sup>8</sup> | C/B ≈ 3.7 | B ≈ 1326 cm<sup>-1</sup> | Zn<sup>4+</sup>



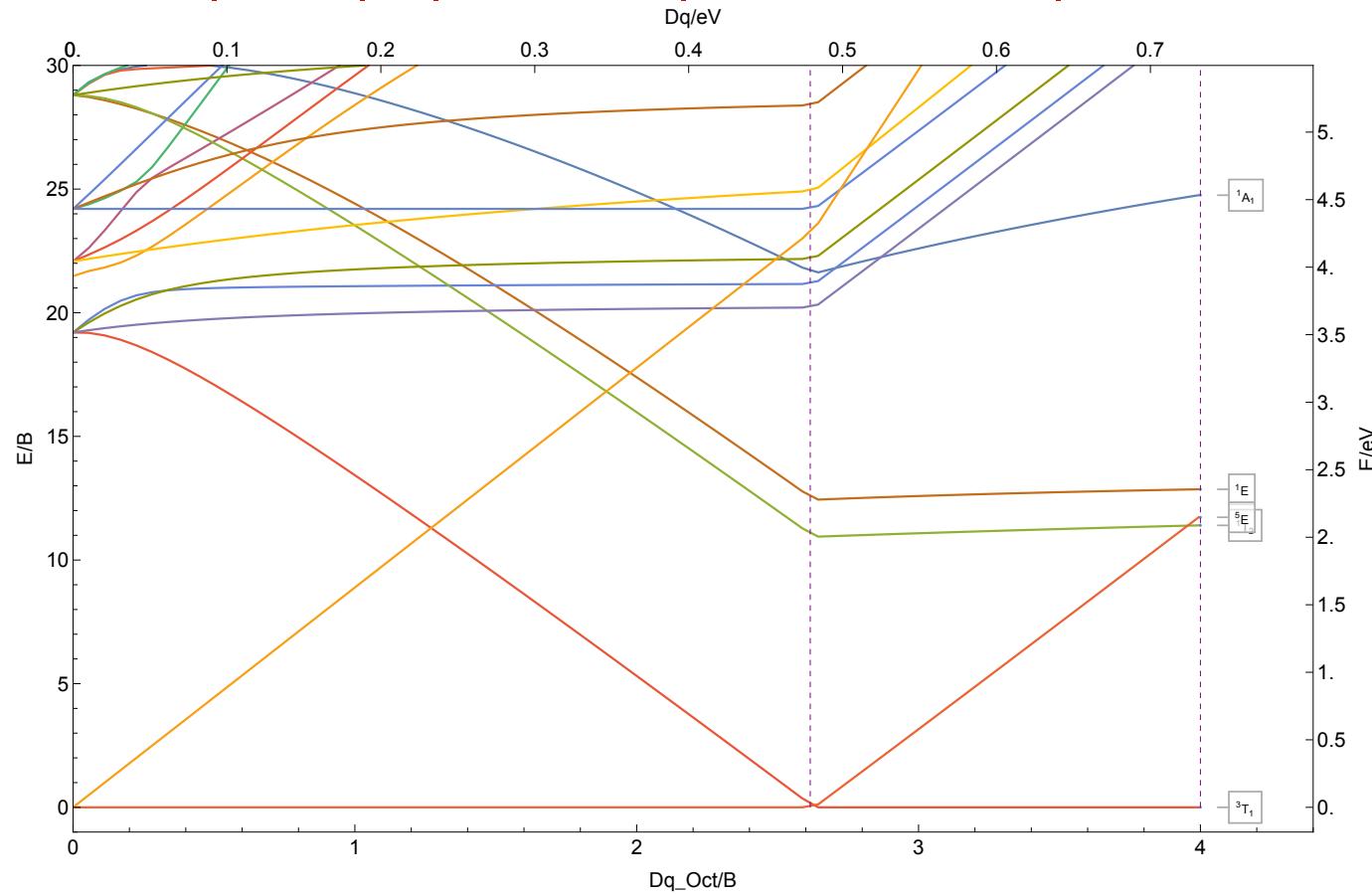
8.3.36 Zn<sup>5+</sup>

|2,4|d<sup>7</sup>| C/B ≈ 3.8 | B ≈ 1403 cm<sup>-1</sup> | Zn<sup>5+</sup>



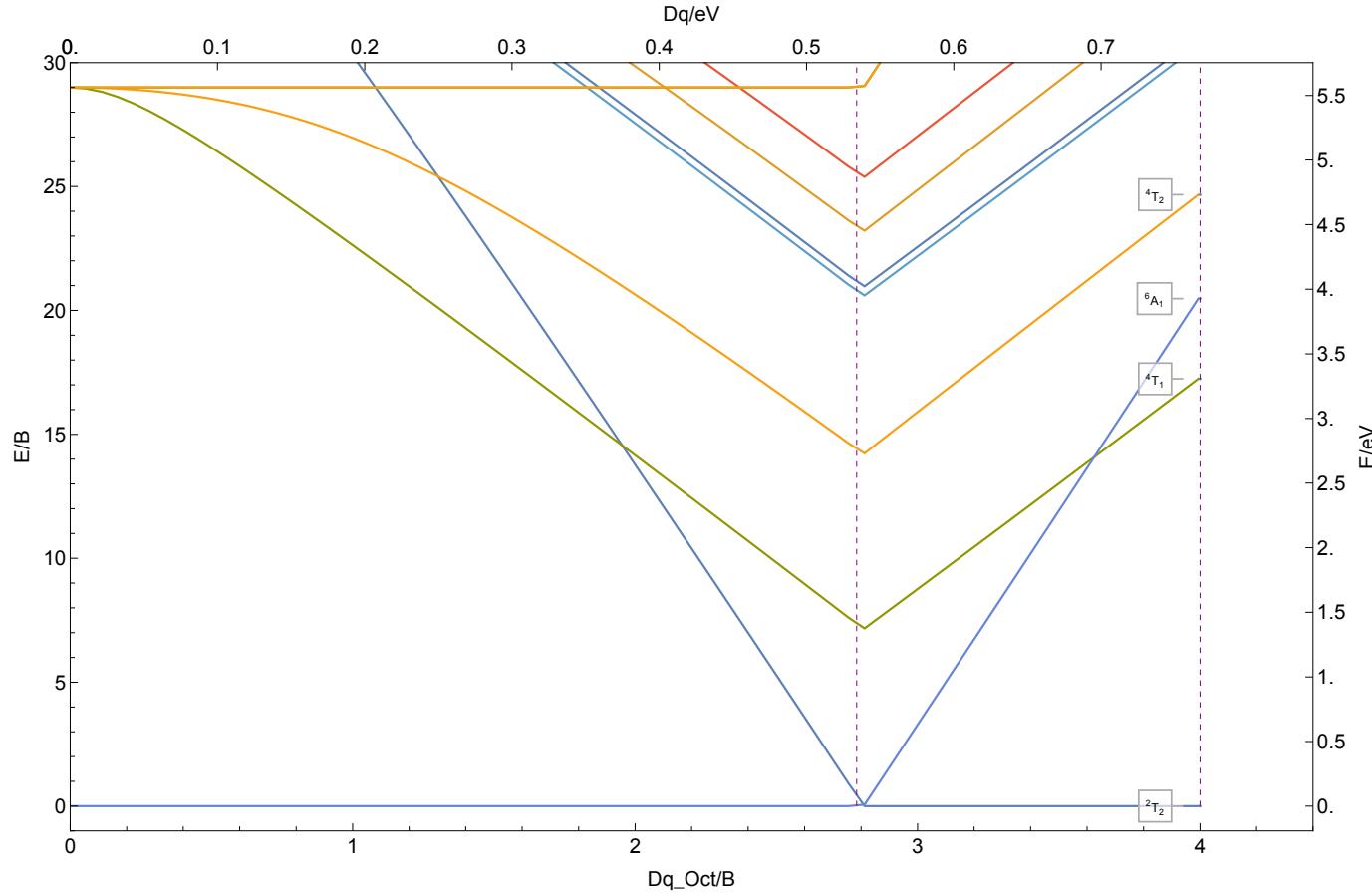
8.3.37 Zn<sup>6+</sup>

$|1,3,5|d^6|C/B \approx 3.8|B \approx 1477\text{ cm}^{-1}|Zn^{6+}$



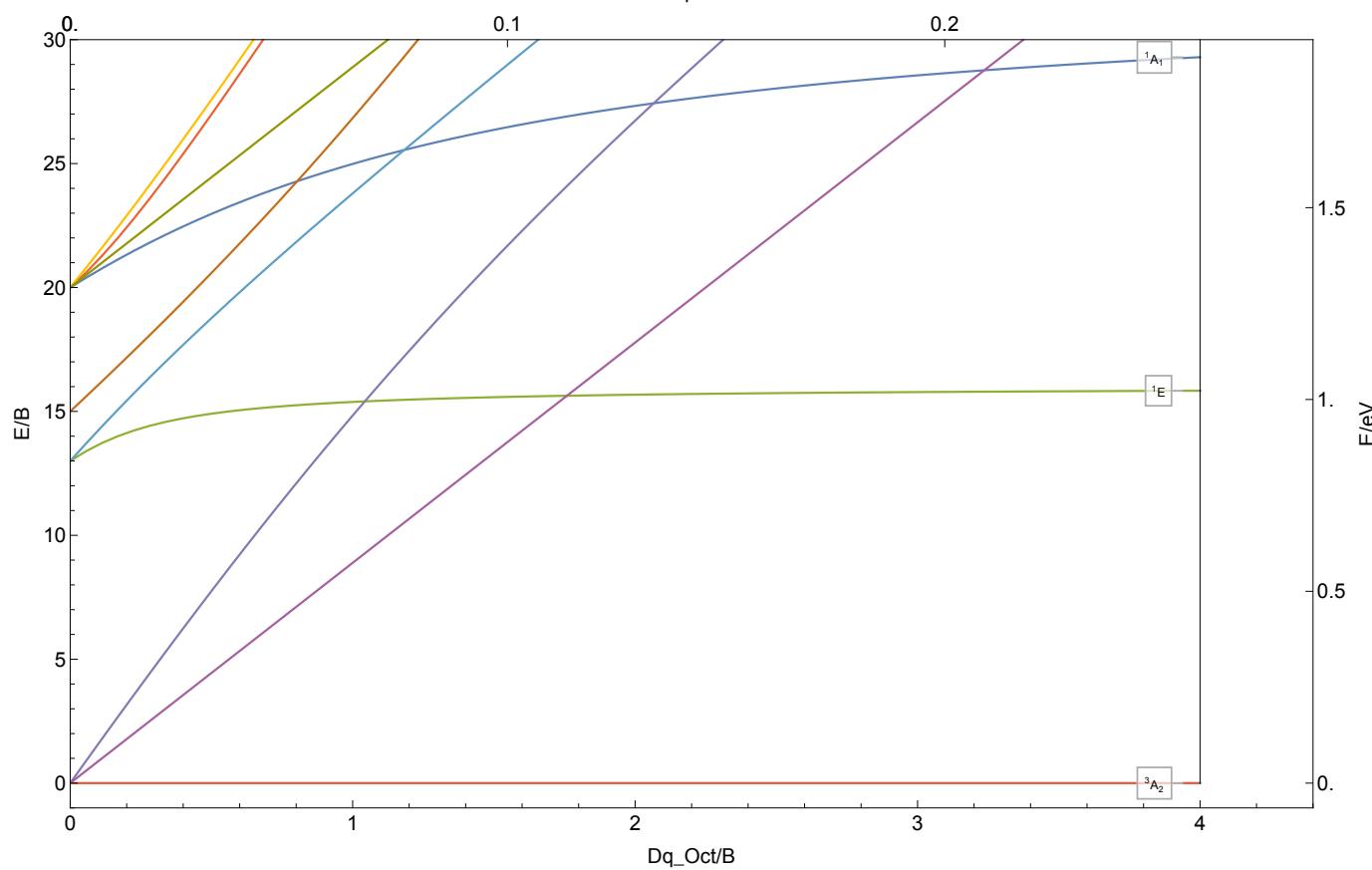
8.3.38 Zn<sup>7+</sup>

|2,4,6| d<sup>5</sup>| C/B ≈ 3.8| B ≈ 1547 cm<sup>-1</sup> | Zn<sup>7+</sup>



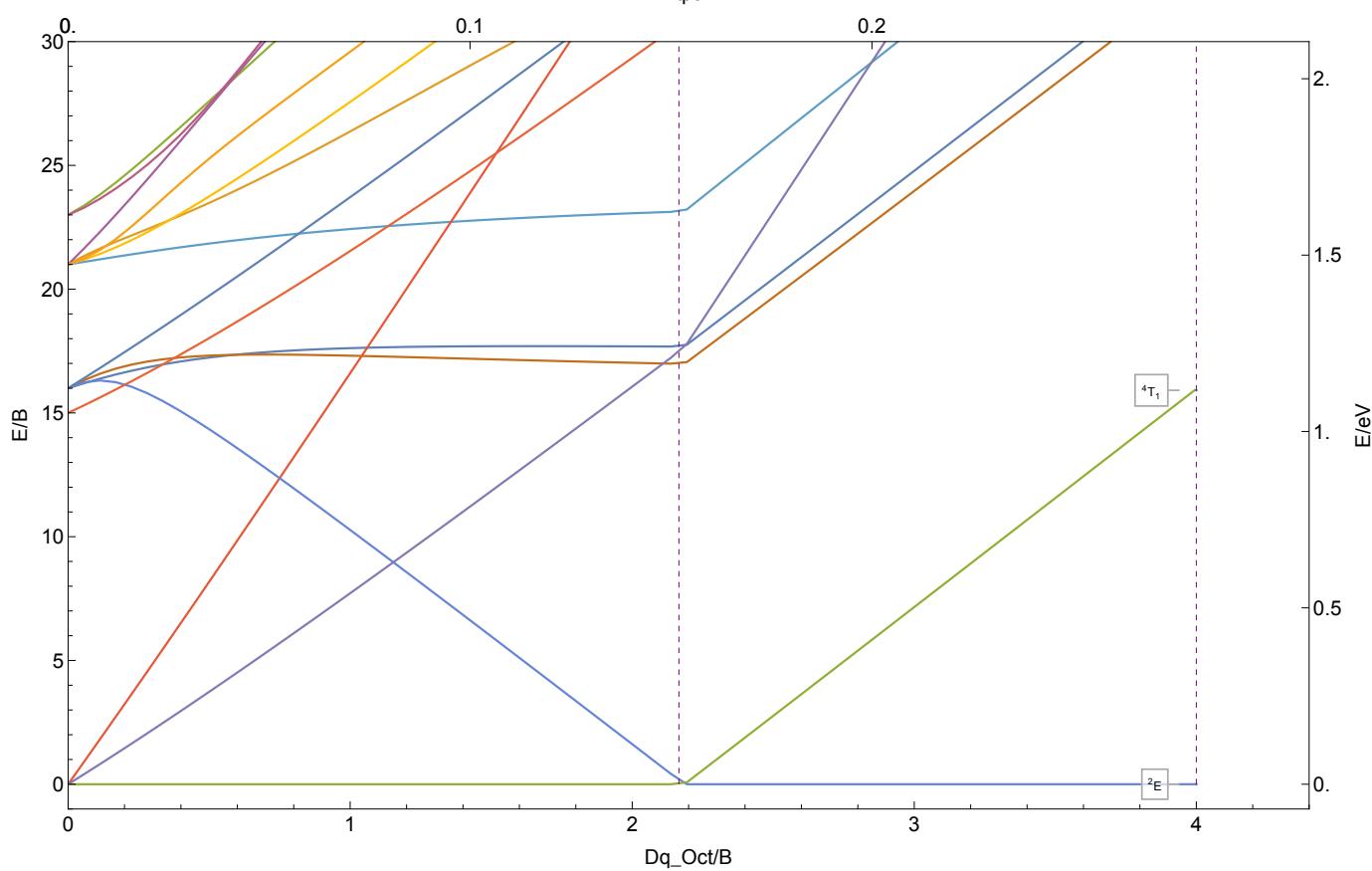
8.3.39 Zr<sup>2+</sup>

$|1,3|d^2|C/B \approx 4.|B \approx 521\text{ cm}^{-1}|Zr^{2+}$



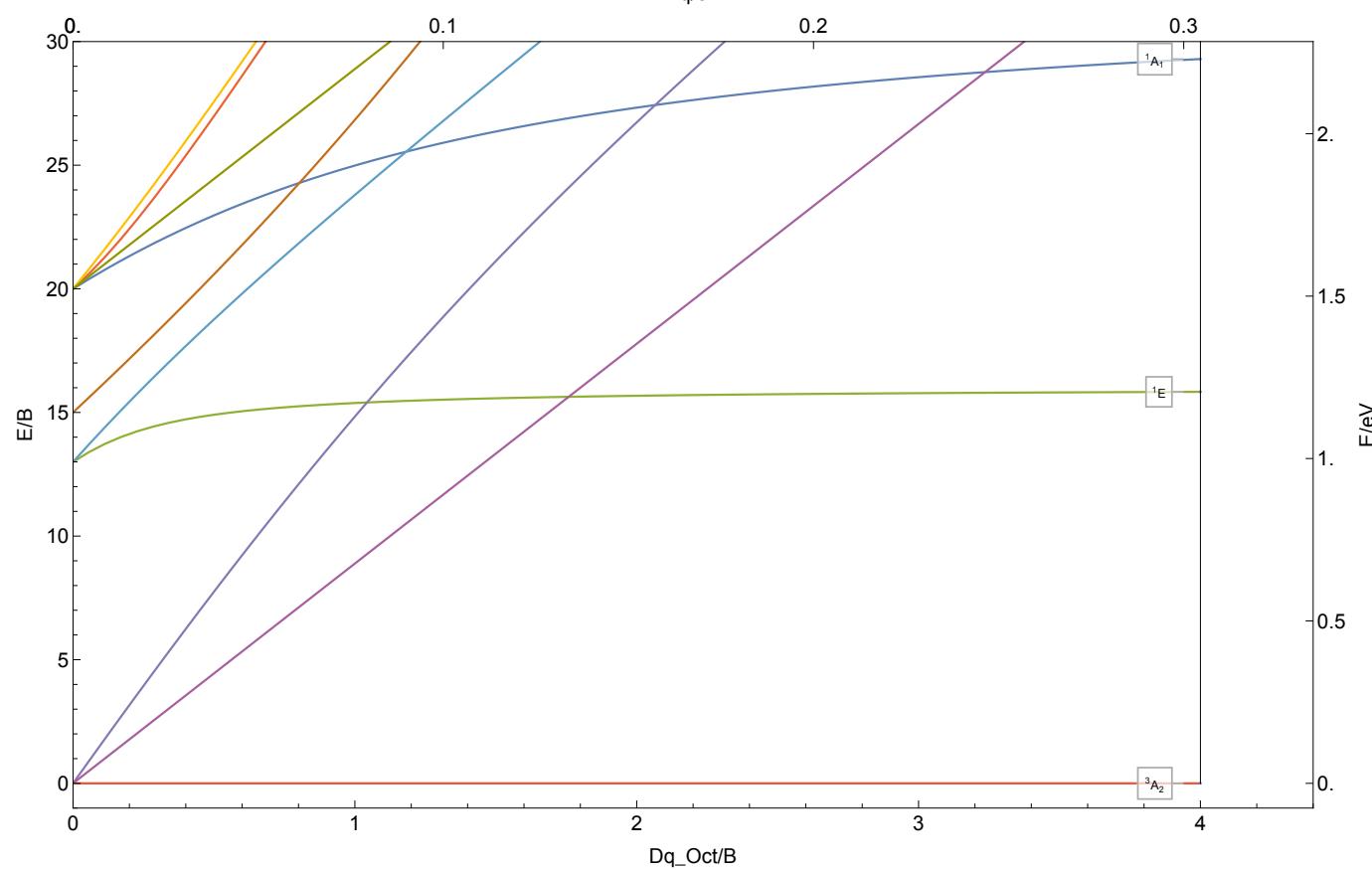
8.3.40  $\text{Nb}^{2+}$

$|2,4|d^3|C/B \approx 4.|B \approx 566 \text{ cm}^{-1}|Nb^{2+}$



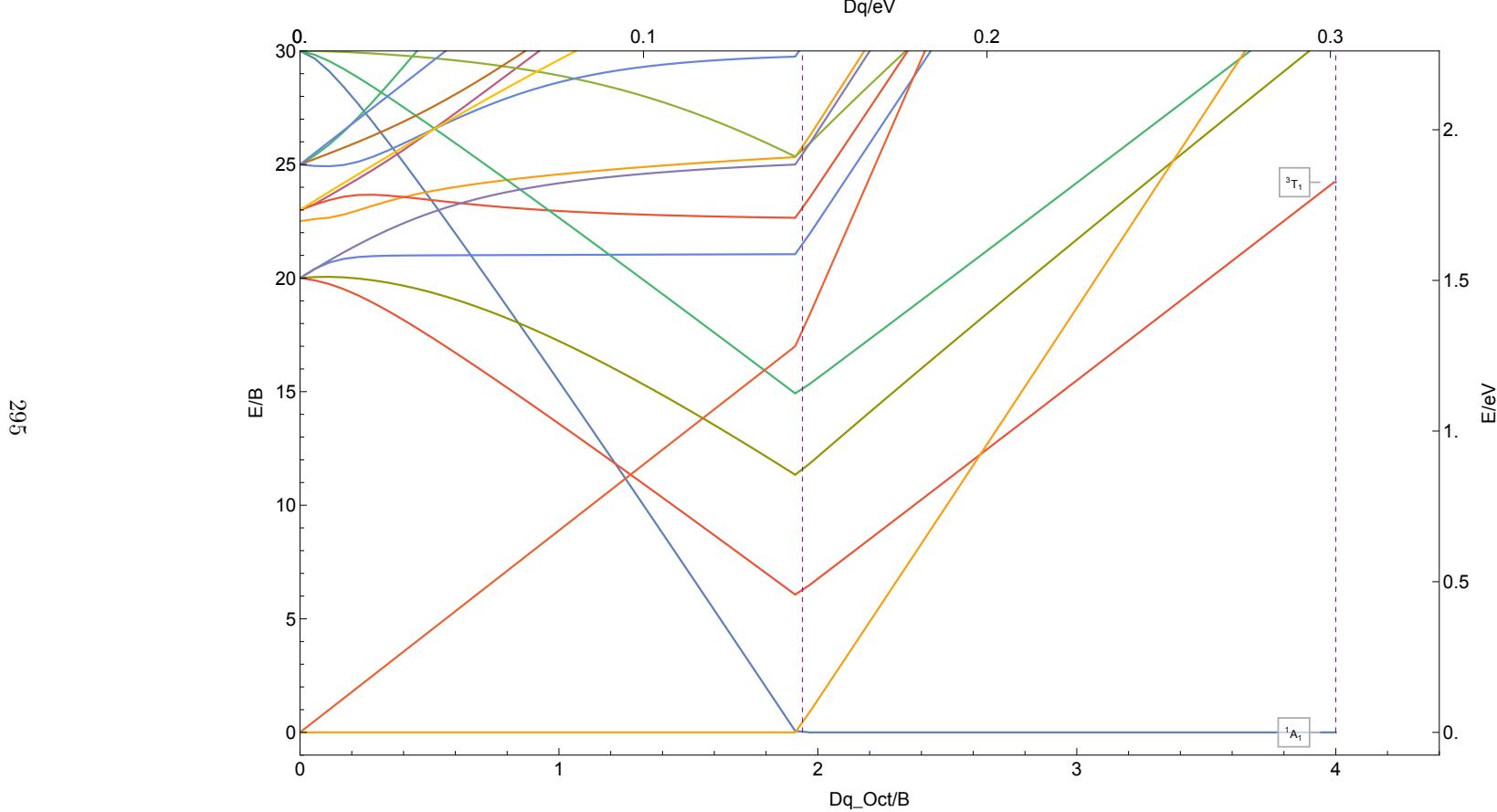
8.3.41 Nb<sup>3+</sup>

| 1,3 | d<sup>2</sup> | C/B ≈ 4. | B ≈ 614 cm<sup>-1</sup> | Nb<sup>3+</sup>



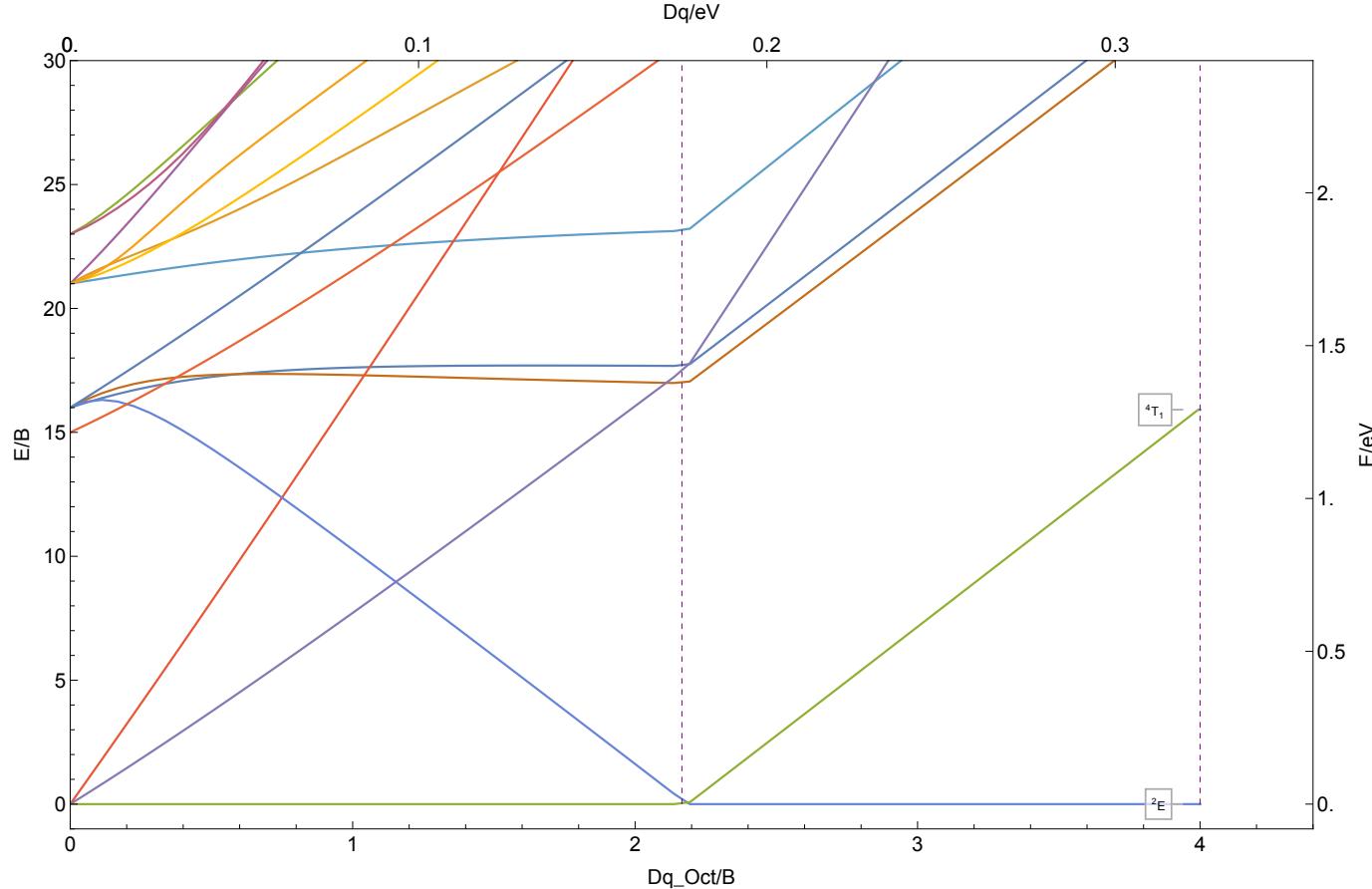
8.3.42 Mo<sup>2+</sup>

|1,3,5|d<sup>4</sup>| C/B ≈ 4. | B ≈ 608 cm<sup>-1</sup> | Mo<sup>2+</sup>



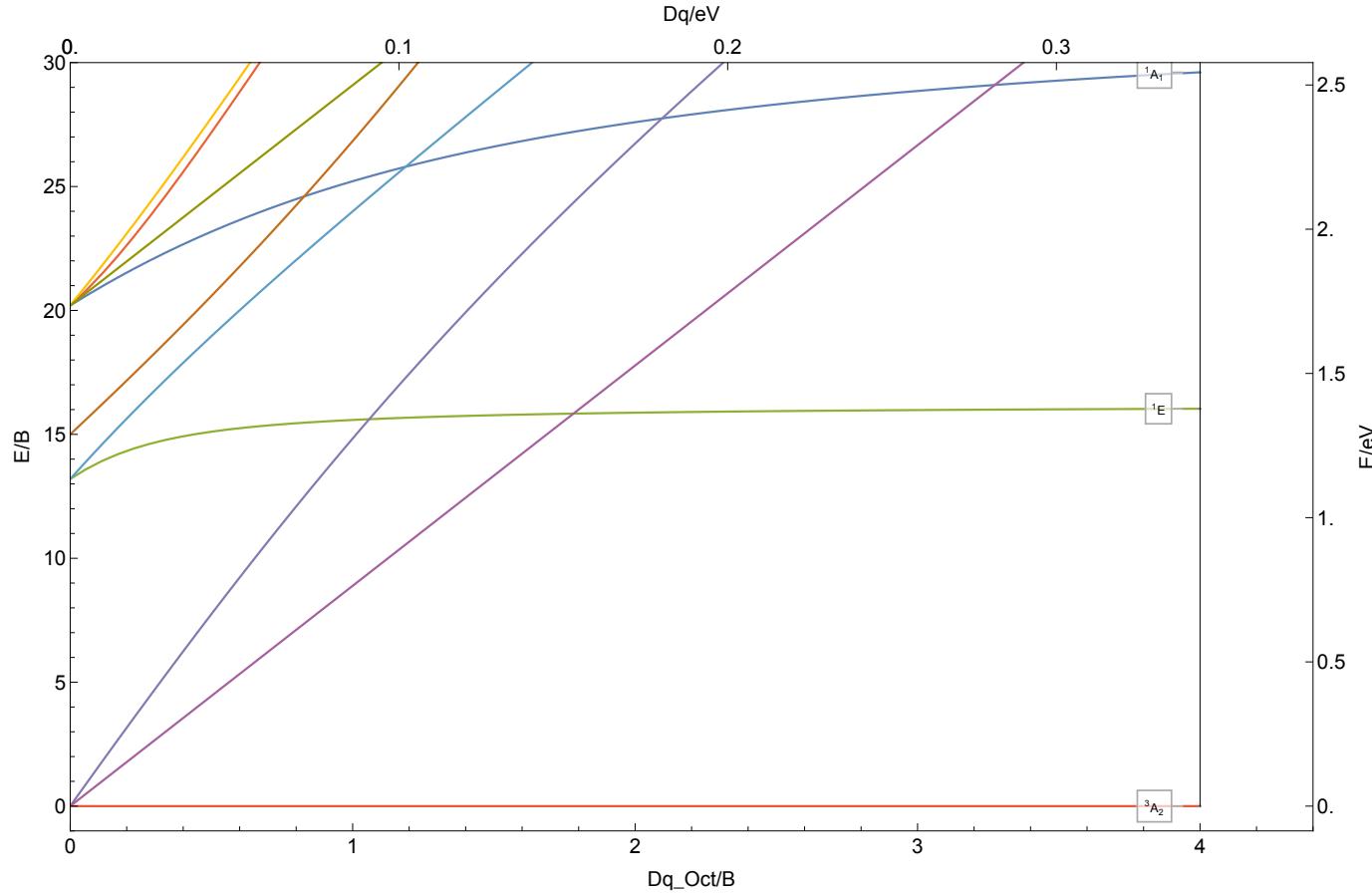
8.3.43 Mo<sup>3+</sup>

|2,4|d<sup>3</sup>|C/B ≈ 4.|B ≈ 654 cm<sup>-1</sup>|Mo<sup>3+</sup>



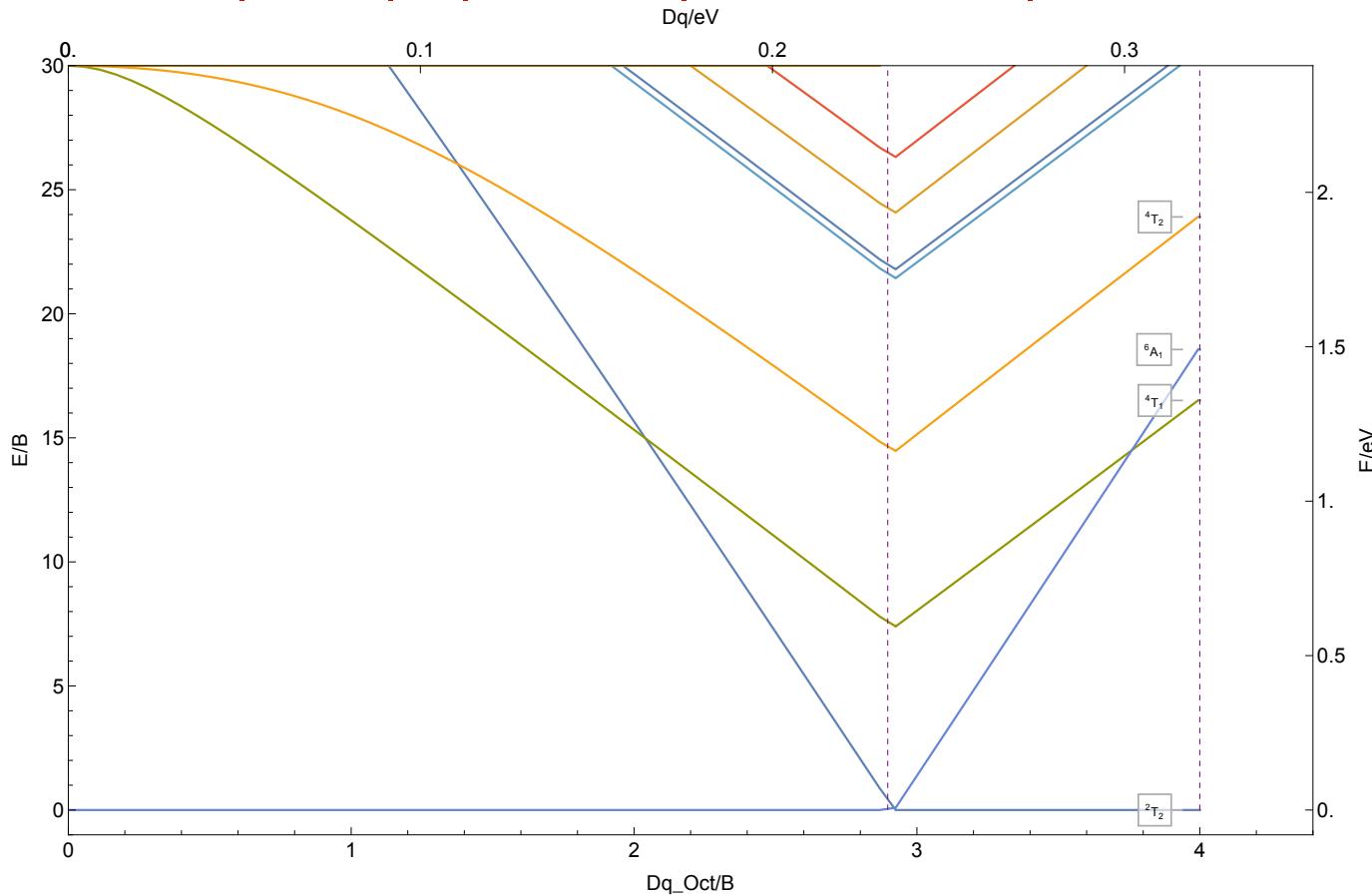
8.3.44 Mo<sup>4+</sup>

|1,3|d<sup>2</sup>| C/B ≈ 4.1| B ≈ 693 cm<sup>-1</sup>| Mo<sup>4+</sup>



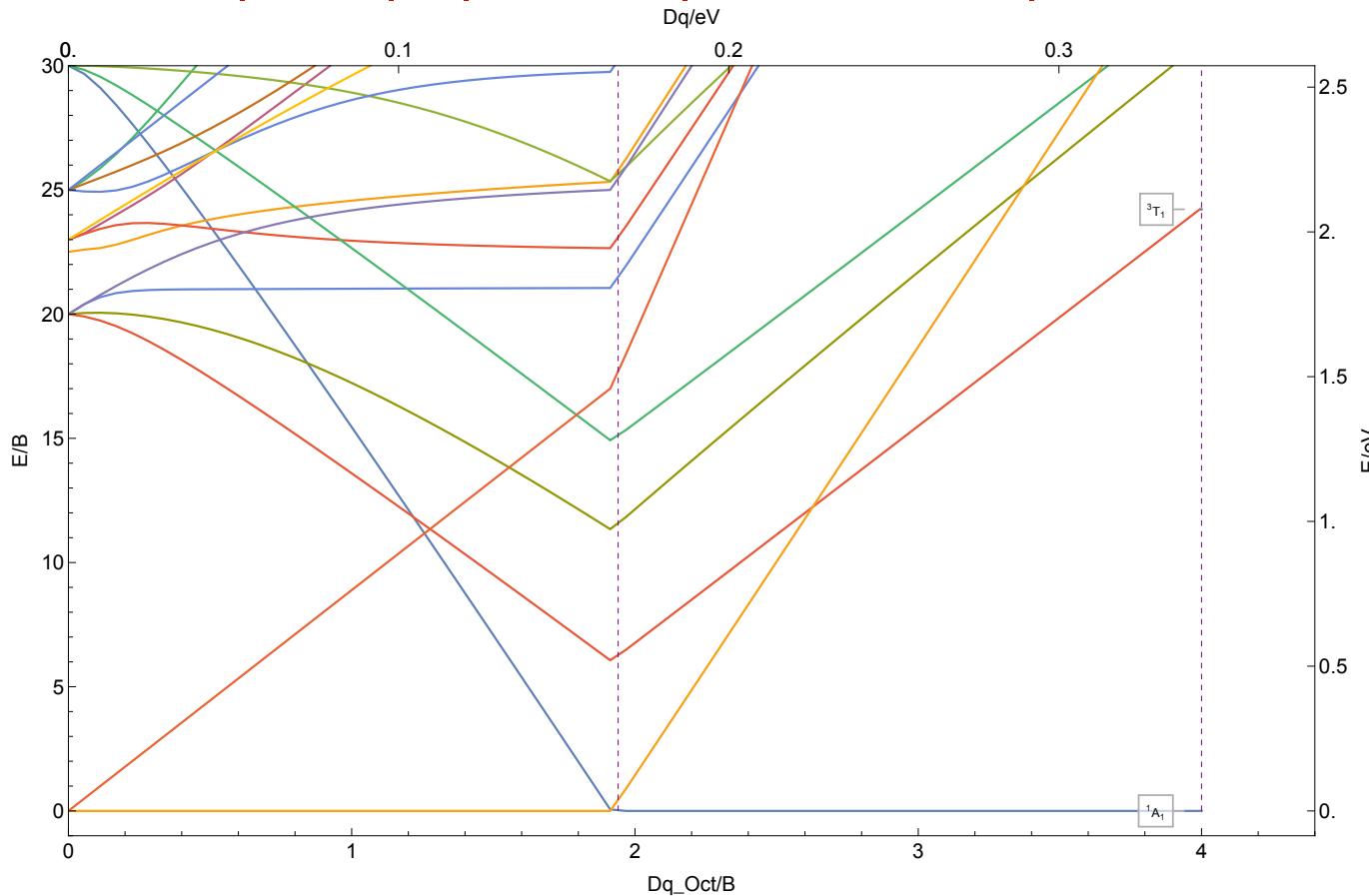
8.3.45 Tc<sup>2+</sup>

|2,4,6|d<sup>5</sup>|C/B ≈ 4.|B ≈ 648 cm<sup>-1</sup>|Tc<sup>2+</sup>



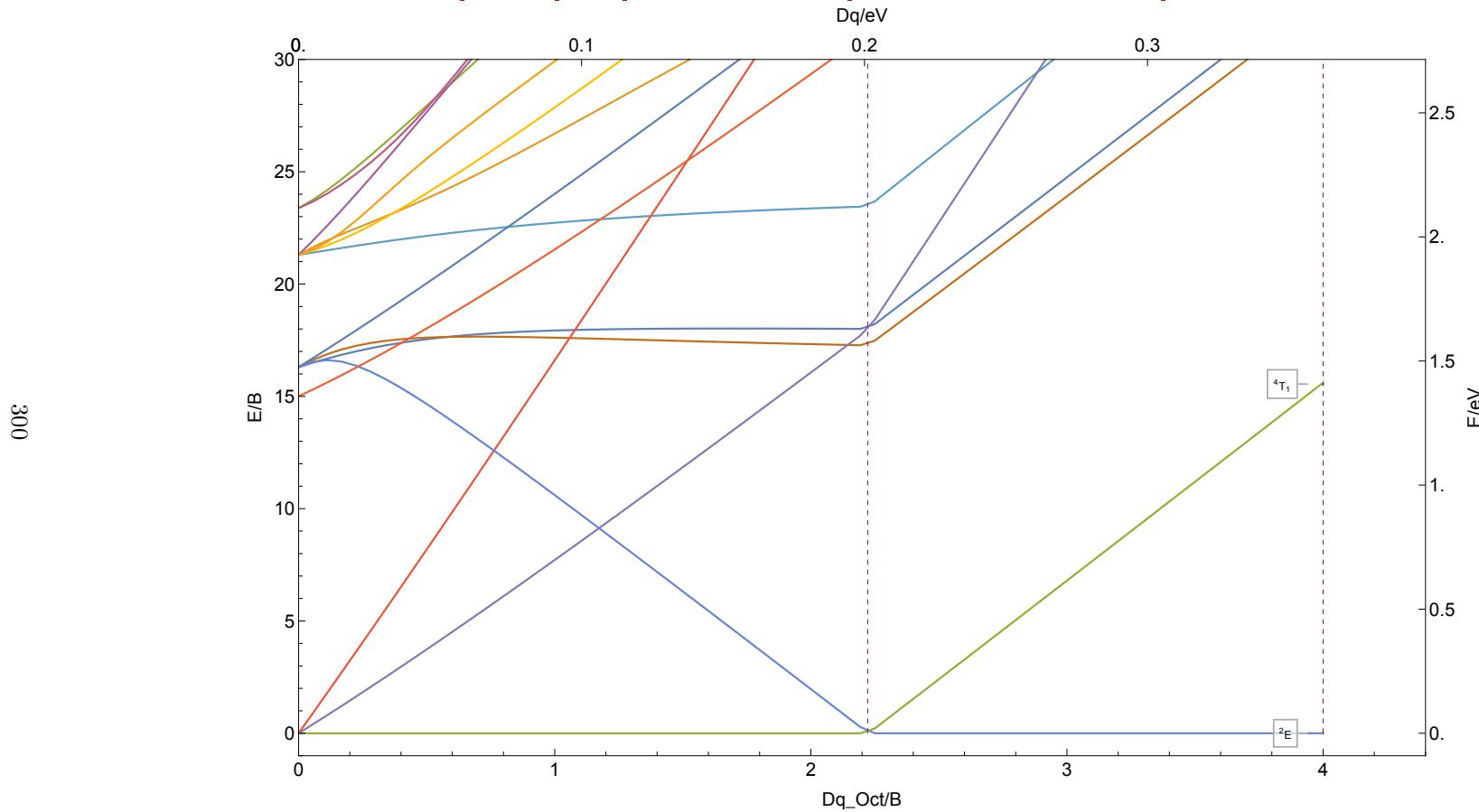
8.3.46 Tc<sup>3+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 4. | B ≈ 692 cm<sup>-1</sup> | Tc<sup>3+</sup>



8.3.47 Tc<sup>4+</sup>

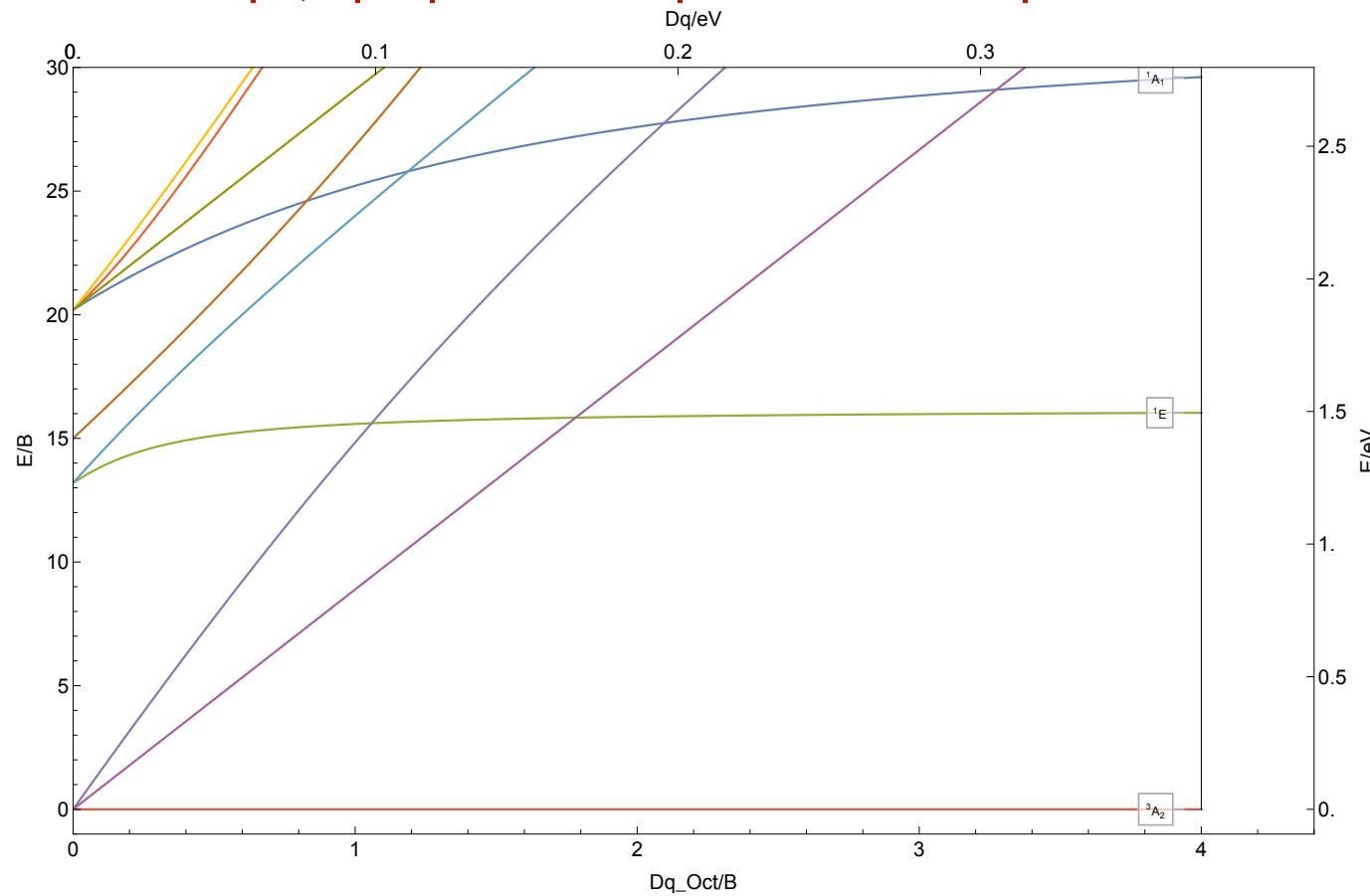
|2,4|d<sup>3</sup>| C/B ≈ 4.1| B ≈ 730 cm<sup>-1</sup> | Tc<sup>4+</sup>



8.3.48 Tc<sup>5+</sup>

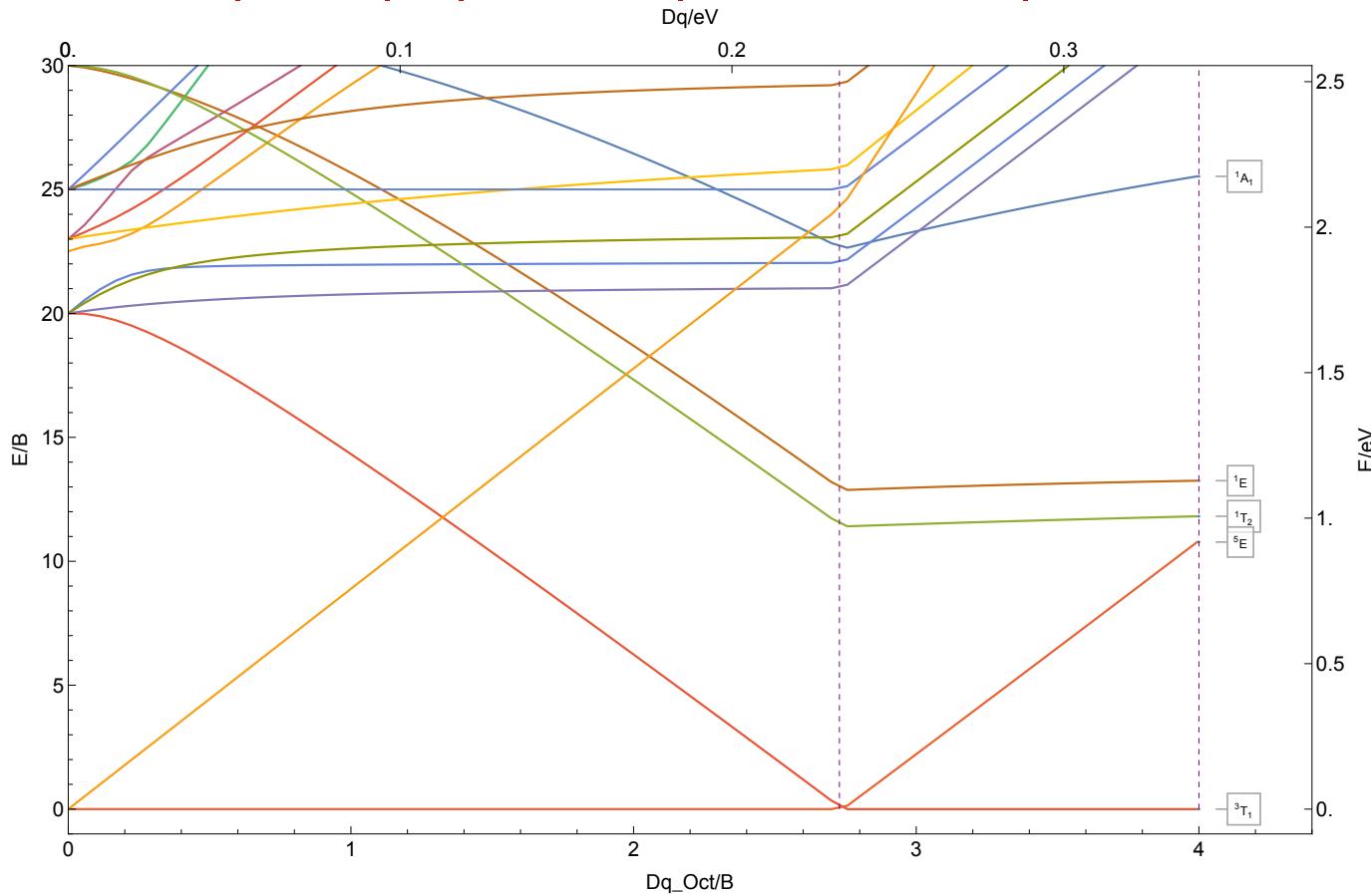
| 1,3 | d<sup>2</sup> | C/B ≈ 4.1 | B ≈ 752 cm<sup>-1</sup> | Tc<sup>5+</sup>

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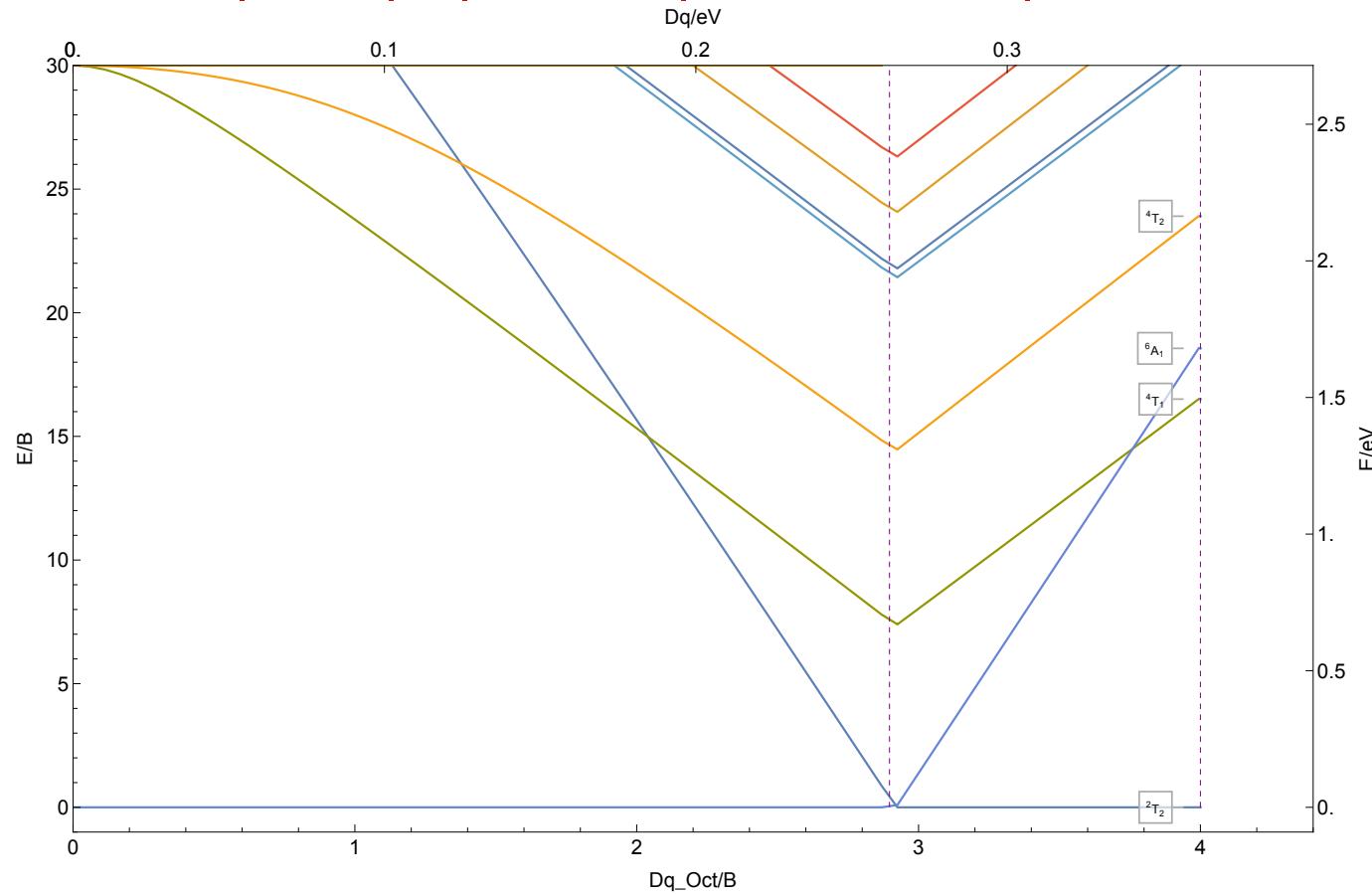
8.3.49 Ru<sup>2+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4. | B ≈ 687 cm<sup>-1</sup> | Ru<sup>2+</sup>



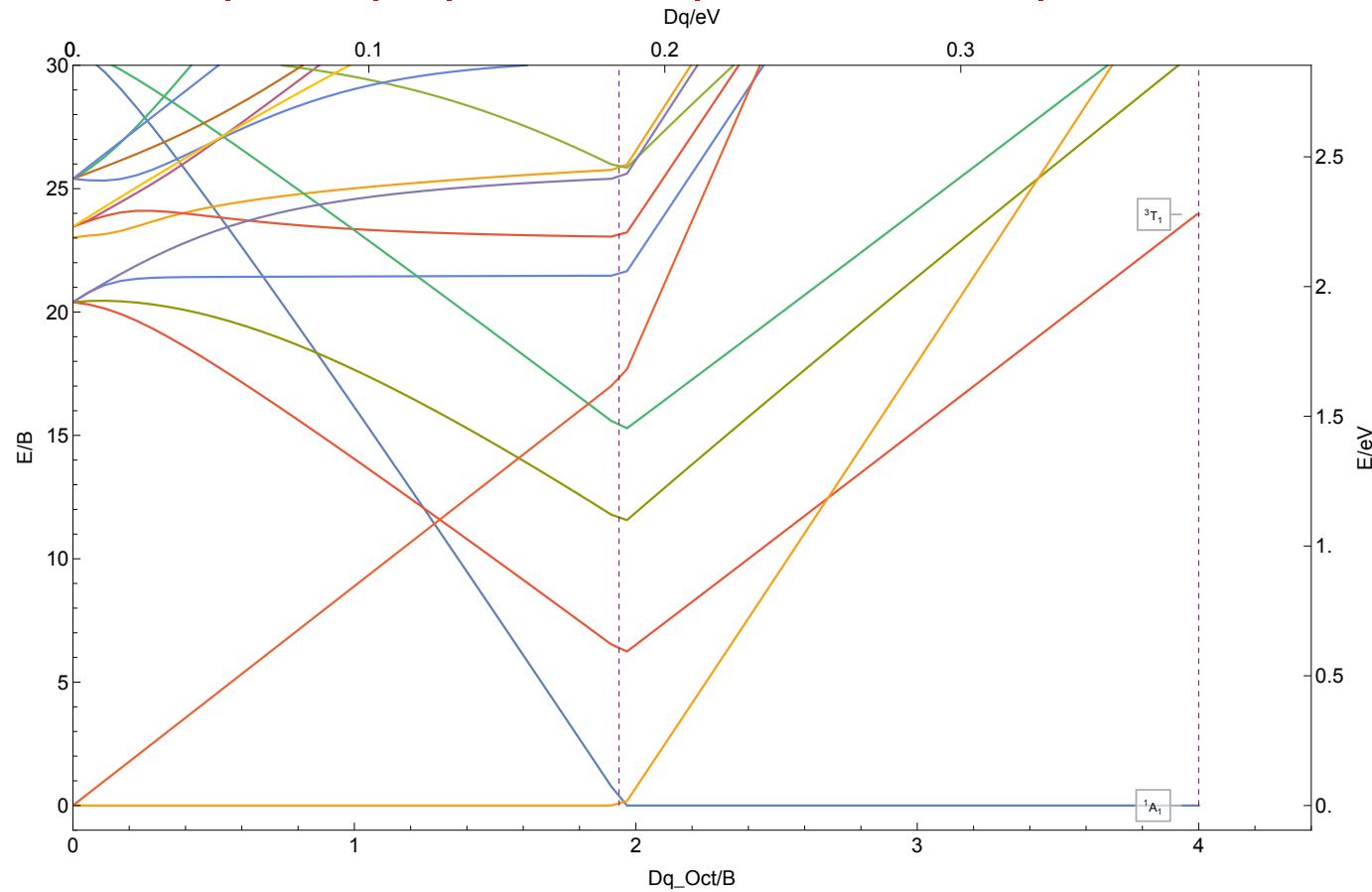
8.3.50 Ru<sup>3+</sup>

|2,4,6|d<sup>5</sup>|C/B ≈ 4.|B ≈ 730 cm<sup>-1</sup>|Ru<sup>3+</sup>



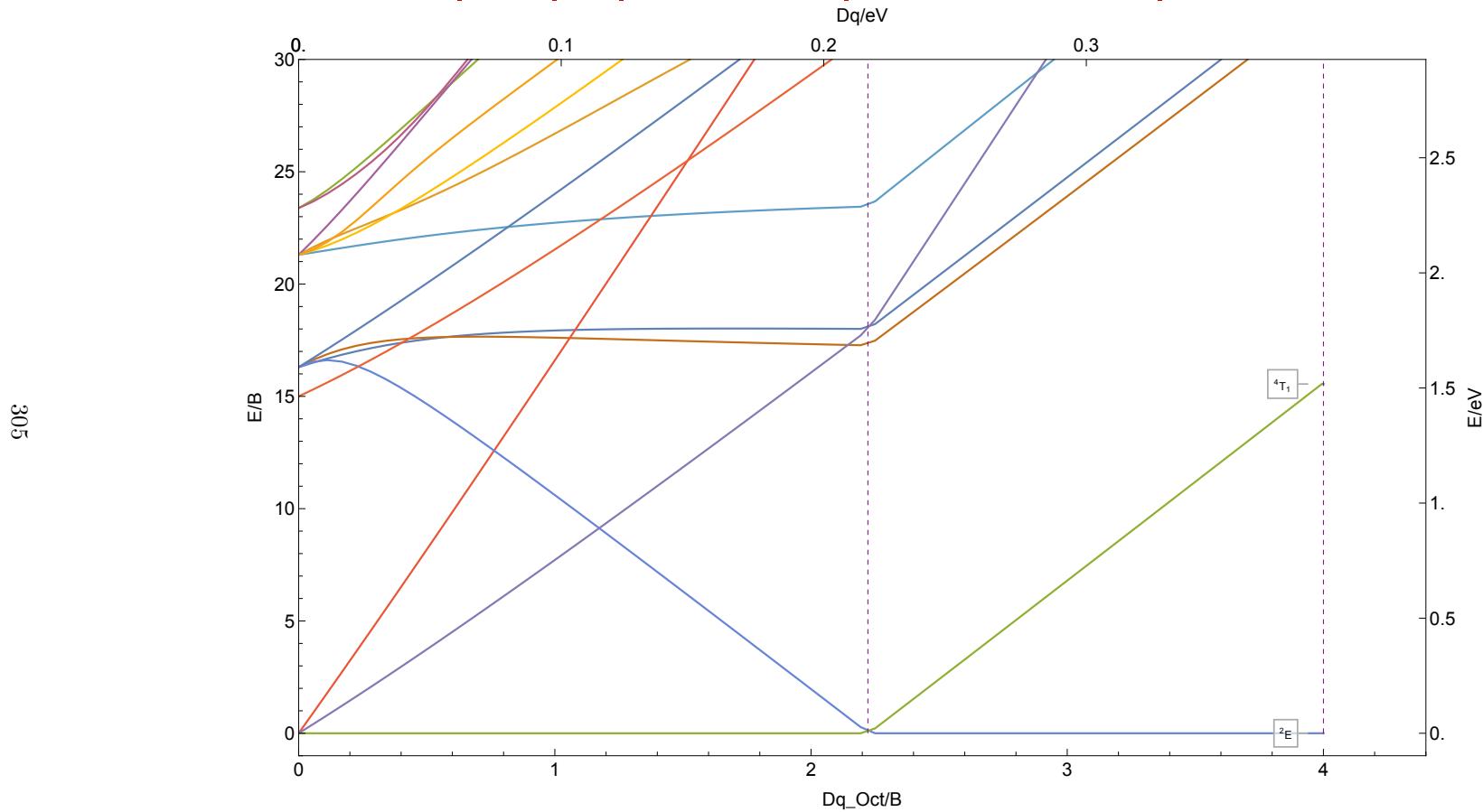
### 8.3.51 Ru<sup>4+</sup>

$|1,3,5|d^4| C/B \approx 4.1 | B \approx 767 \text{ cm}^{-1} | \text{Ru}^{4+}$



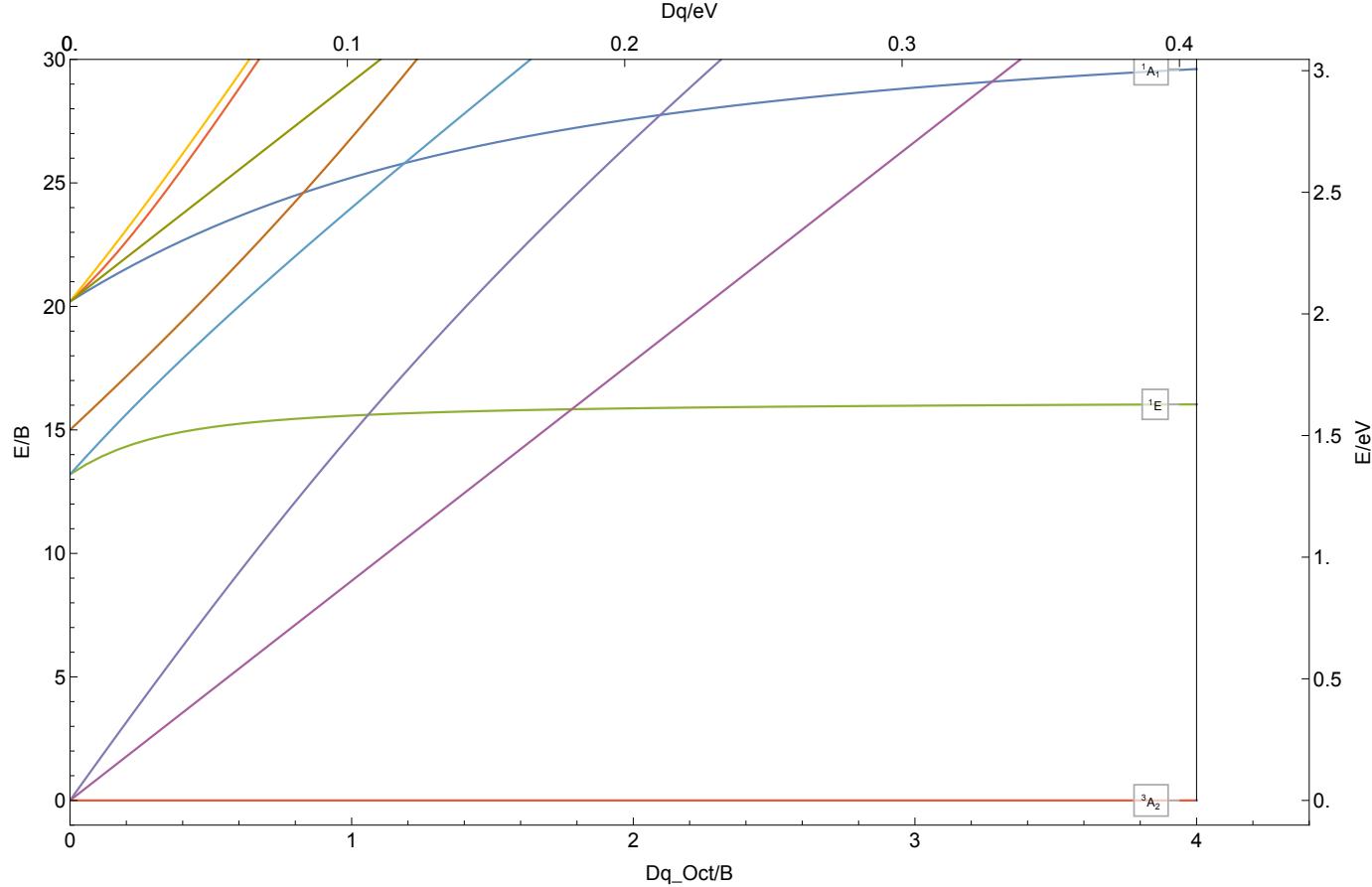
8.3.52 Ru<sup>5+</sup>

|2,4|d<sup>3</sup>| C/B ≈ 4.1| B ≈ 787 cm<sup>-1</sup> | Ru<sup>5+</sup>



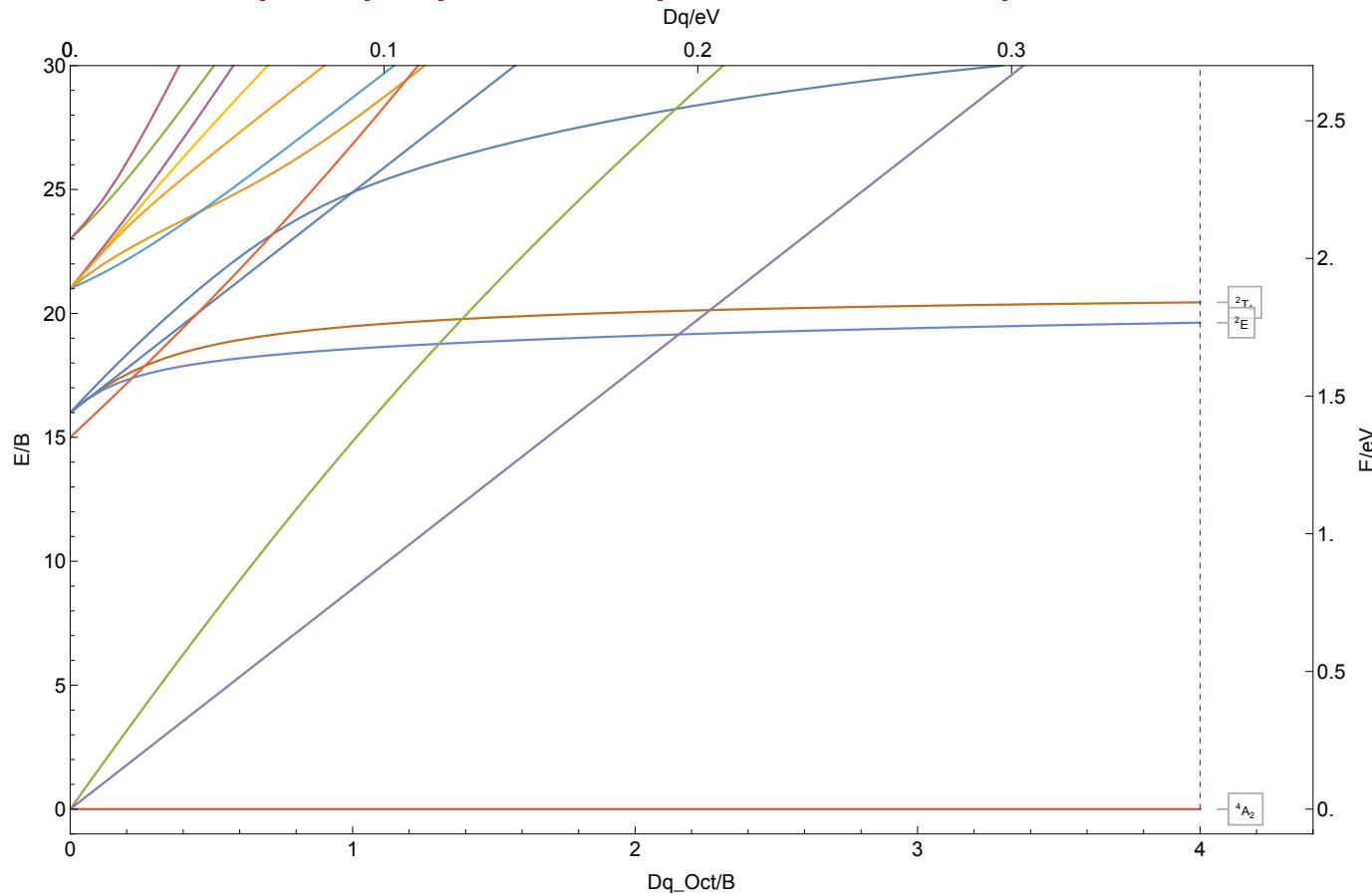
8.3.53 Ru<sup>6+</sup>

| 1,3 | d<sup>2</sup> | C/B ≈ 4.1 | B ≈ 819 cm<sup>-1</sup> | Ru<sup>6+</sup>



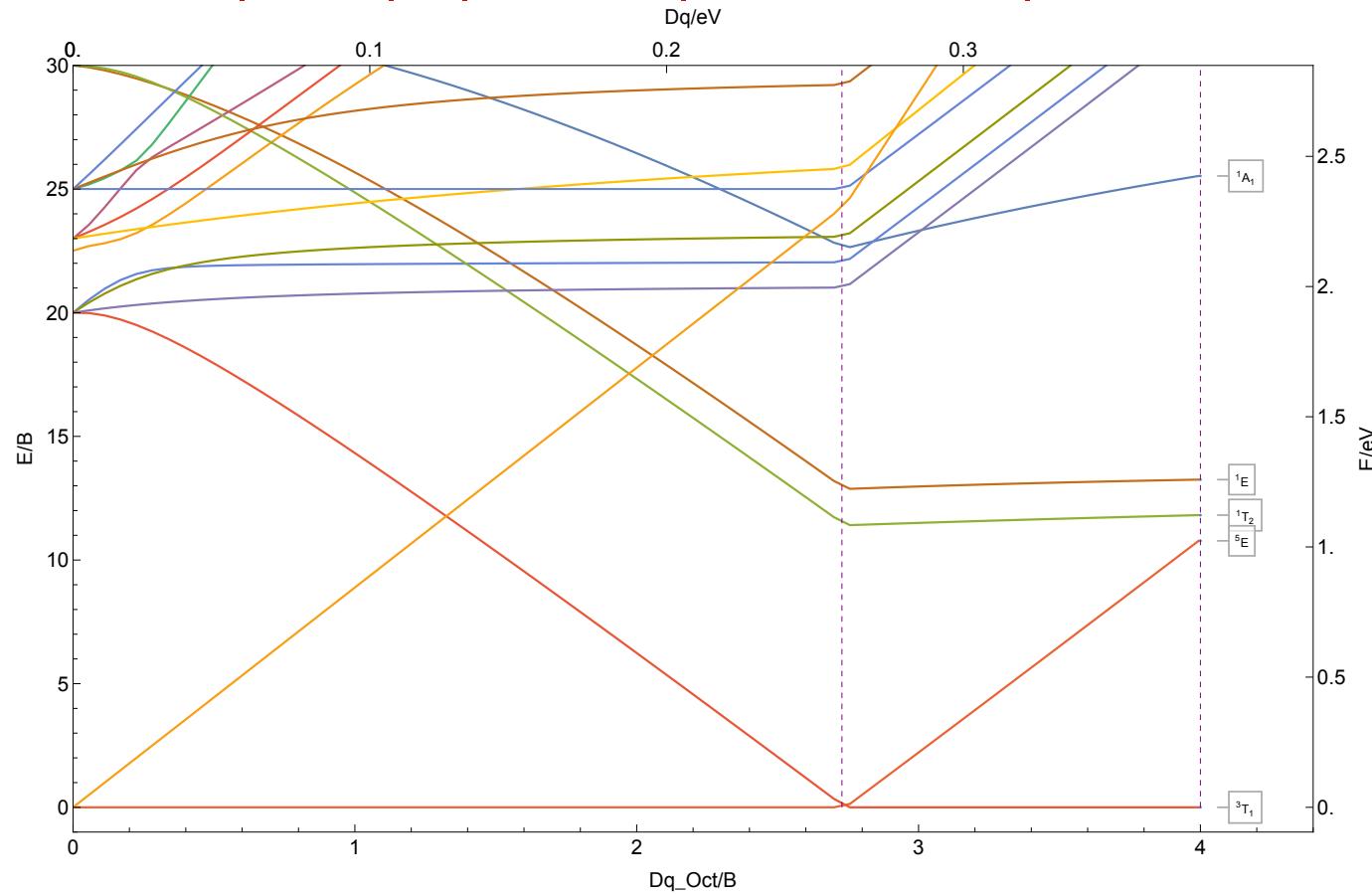
8.3.54 Rh<sup>2+</sup>

|2,4|d<sup>7</sup>| C/B ≈ 4. | B ≈ 726 cm<sup>-1</sup> | Rh<sup>2+</sup>



### 8.3.55 Rh<sup>3+</sup>

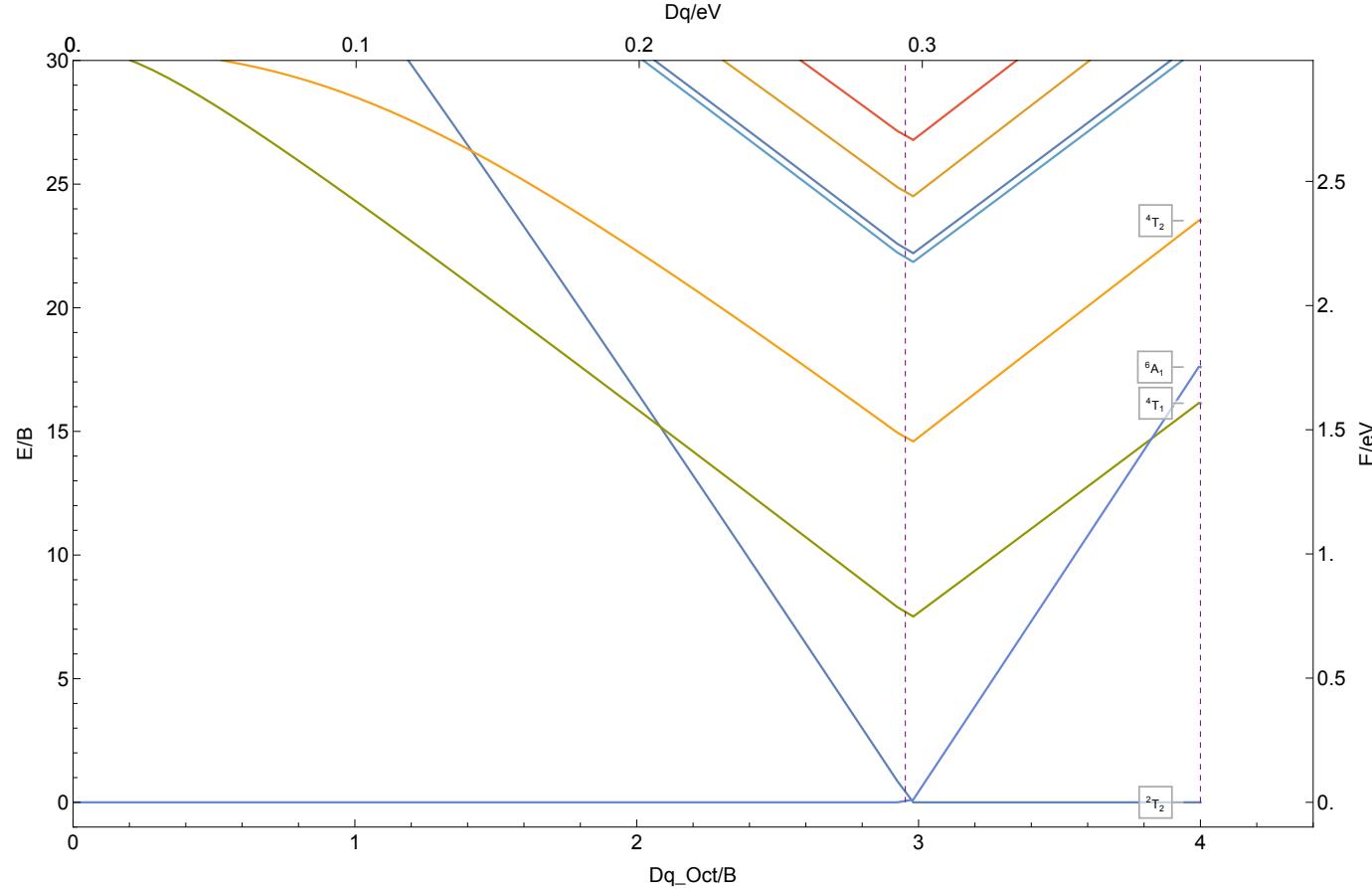
| 1,3,5 | d<sup>6</sup> | C/B ≈ 4. | B ≈ 766 cm<sup>-1</sup> | Rh<sup>3+</sup>



8.3.56 Rh<sup>4+</sup>

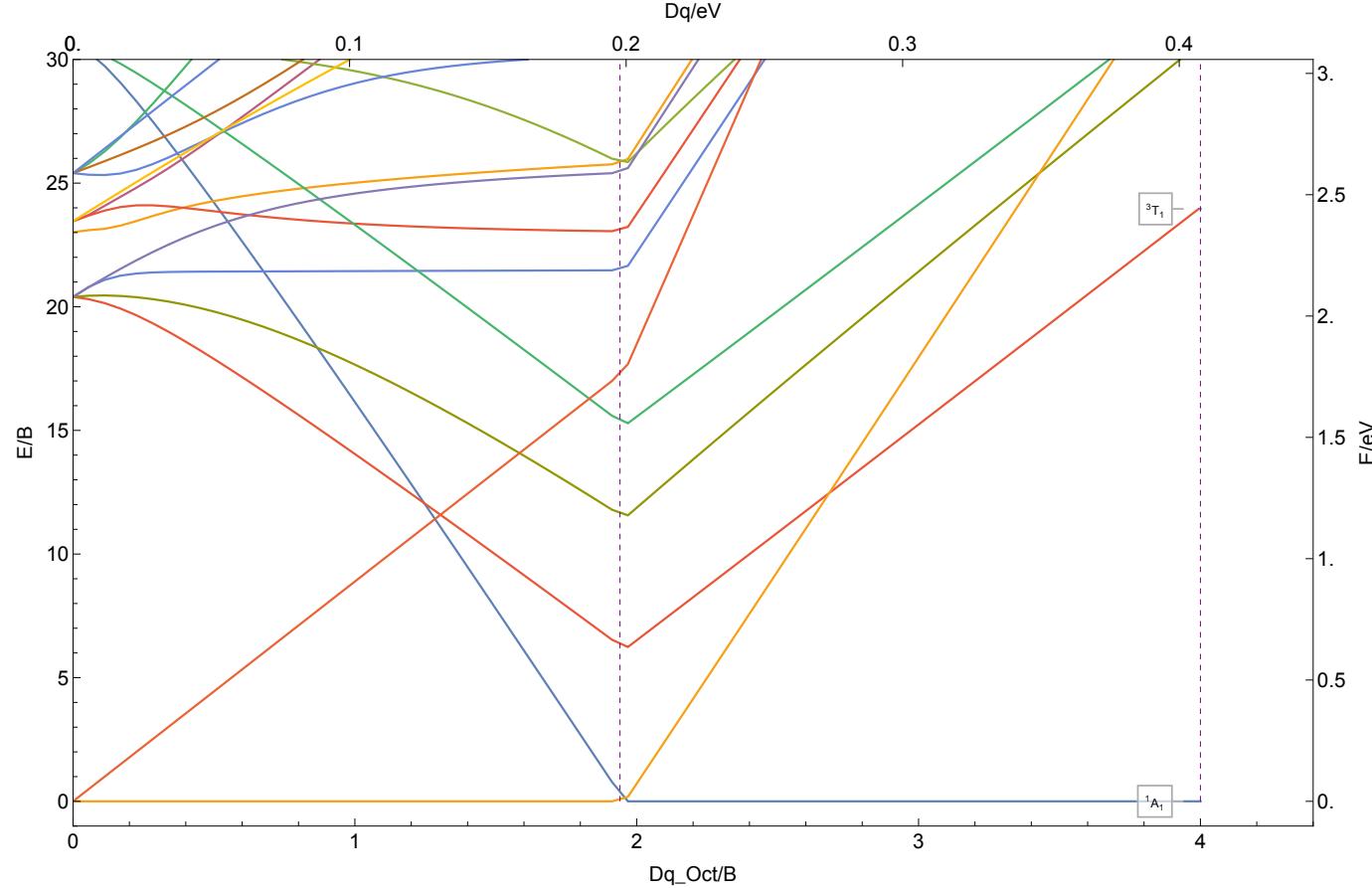
|2,4,6| d<sup>5</sup>| C/B ≈ 4.1| B ≈ 803 cm<sup>-1</sup> | Rh<sup>4+</sup>

60ε



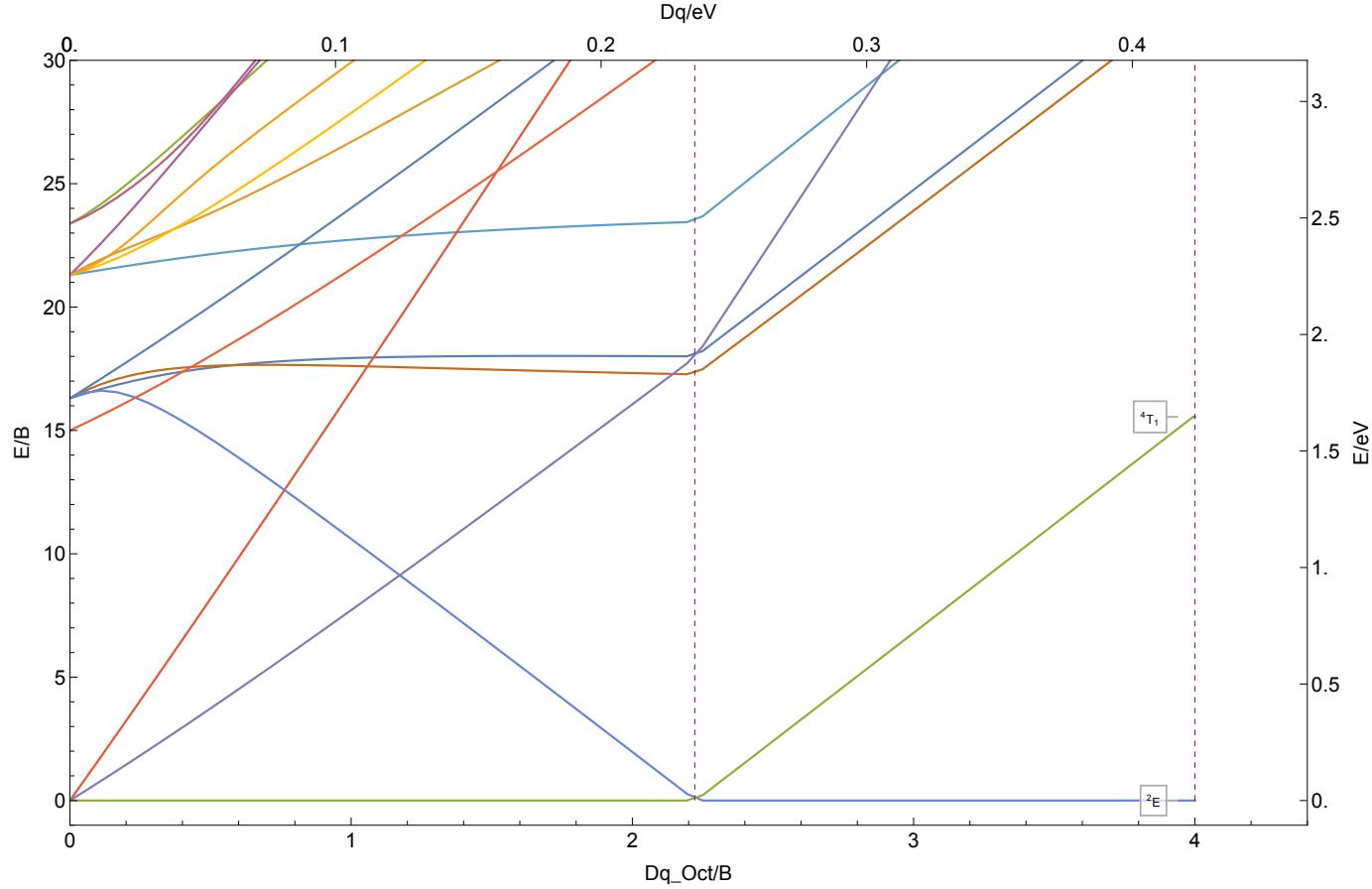
8.3.57 Rh<sup>5+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 4.1 | B ≈ 822 cm<sup>-1</sup> | Rh<sup>5+</sup>



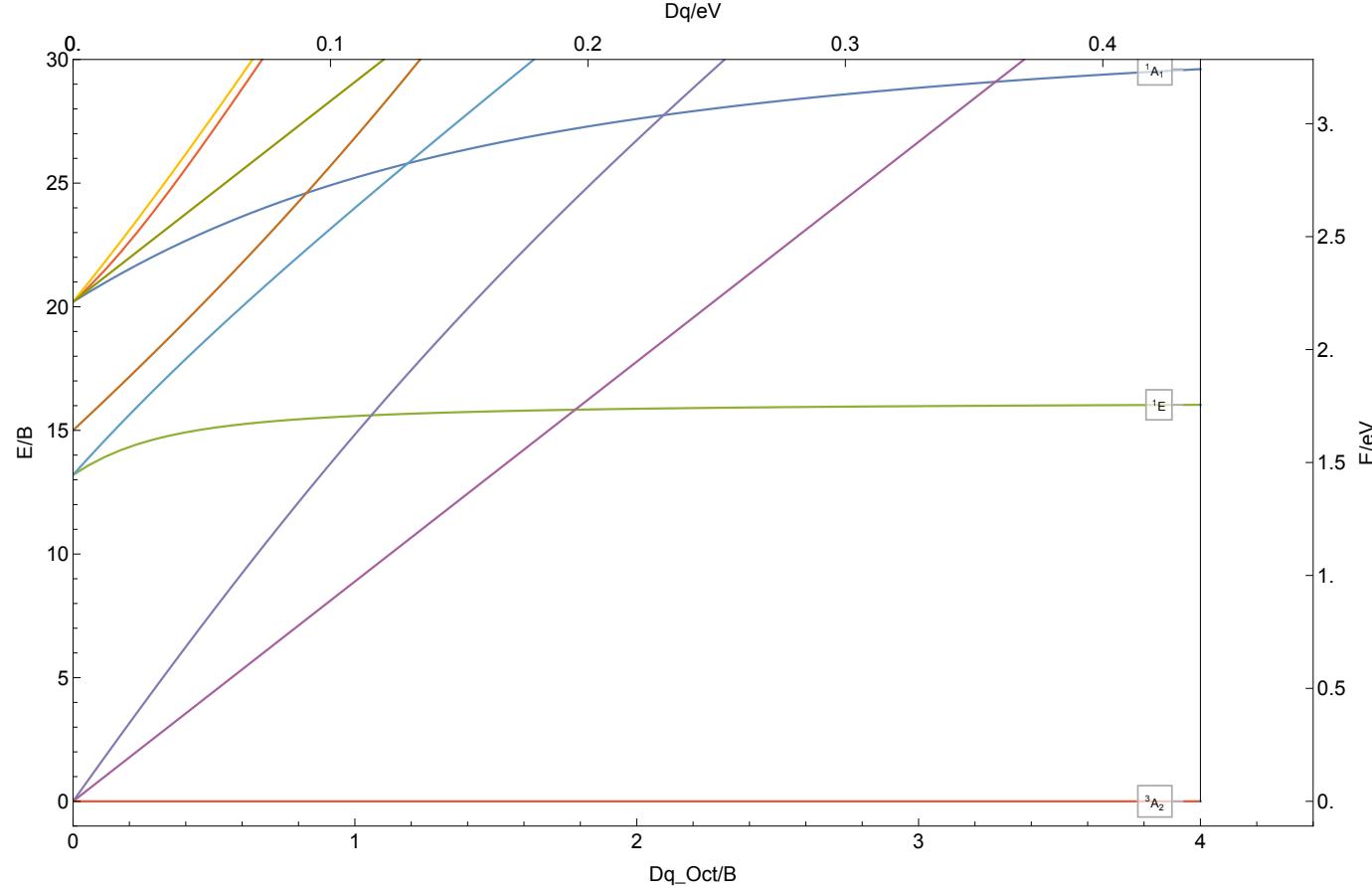
8.3.58 Rh<sup>6+</sup>

|2,4|d<sup>3</sup>| C/B ≈ 4.1| B ≈ 854 cm<sup>-1</sup> | Rh<sup>6+</sup>



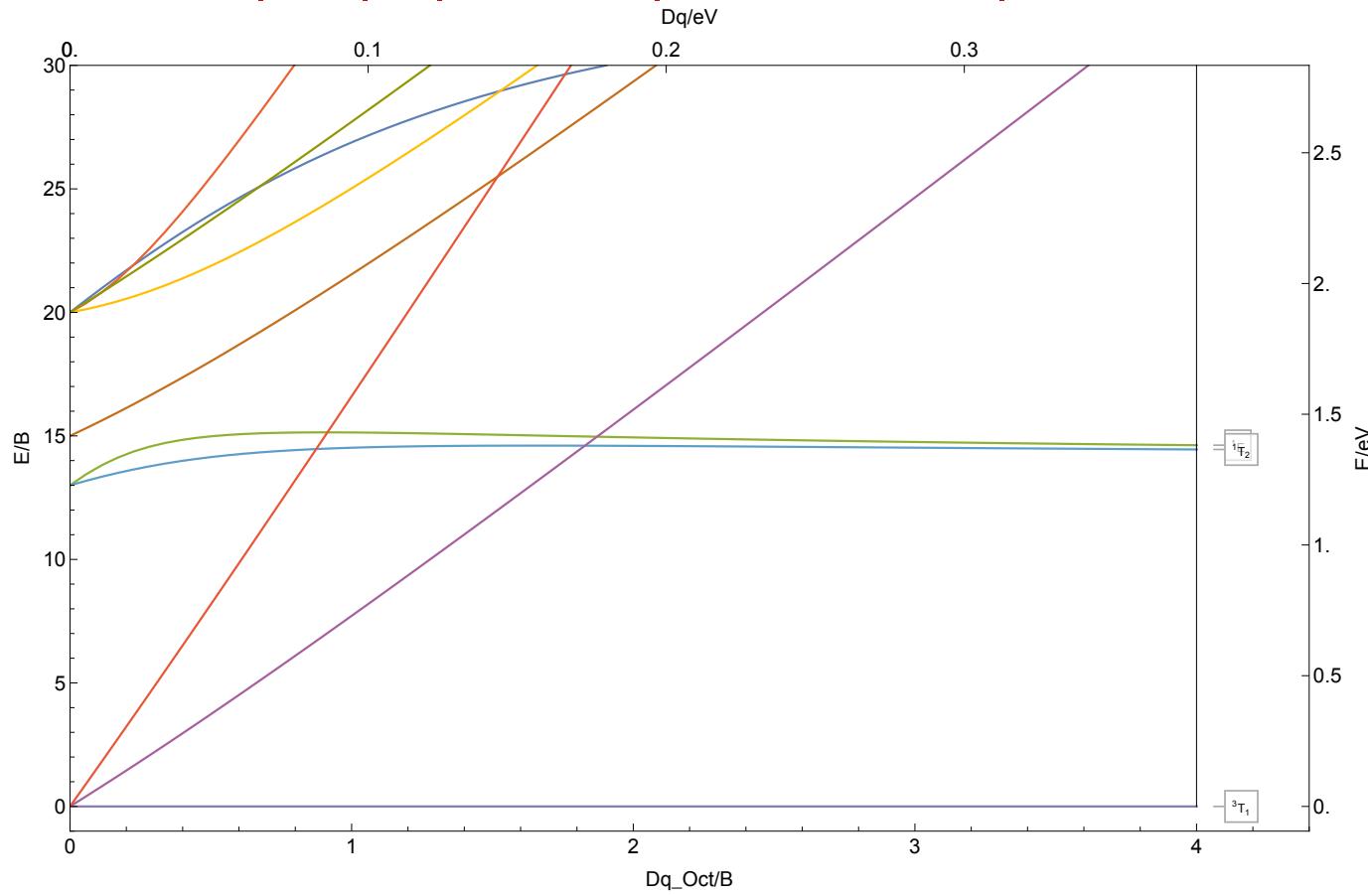
8.3.59 Rh<sup>7+</sup>

| 1,3 | d<sup>2</sup> | C/B ≈ 4.1 | B ≈ 883 cm<sup>-1</sup> | Rh<sup>7+</sup>



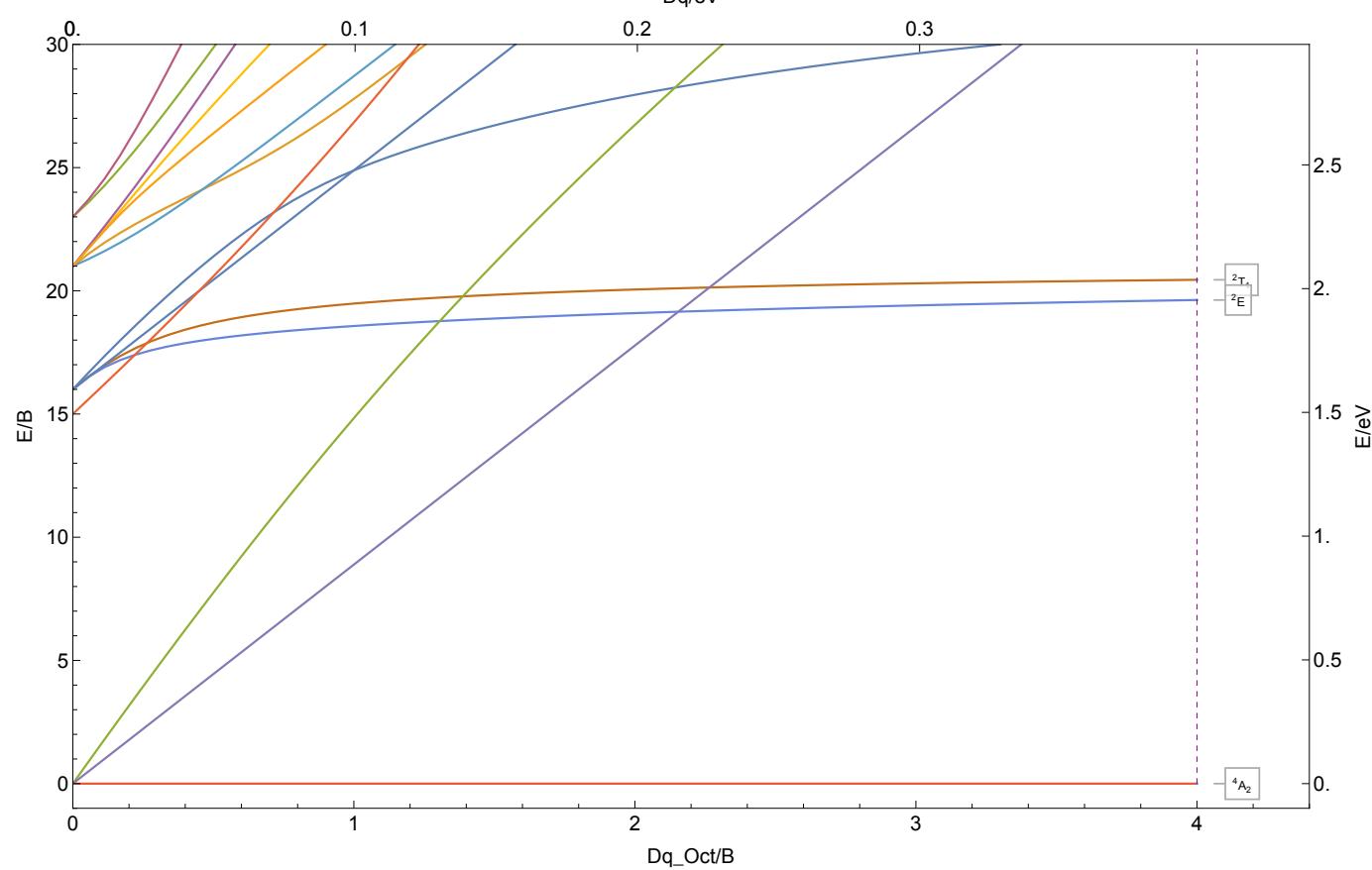
8.3.60 Pd<sup>2+</sup>

| 1,3 | d<sup>8</sup> | C/B ≈ 4. | B ≈ 762 cm<sup>-1</sup> | Pd<sup>2+</sup>



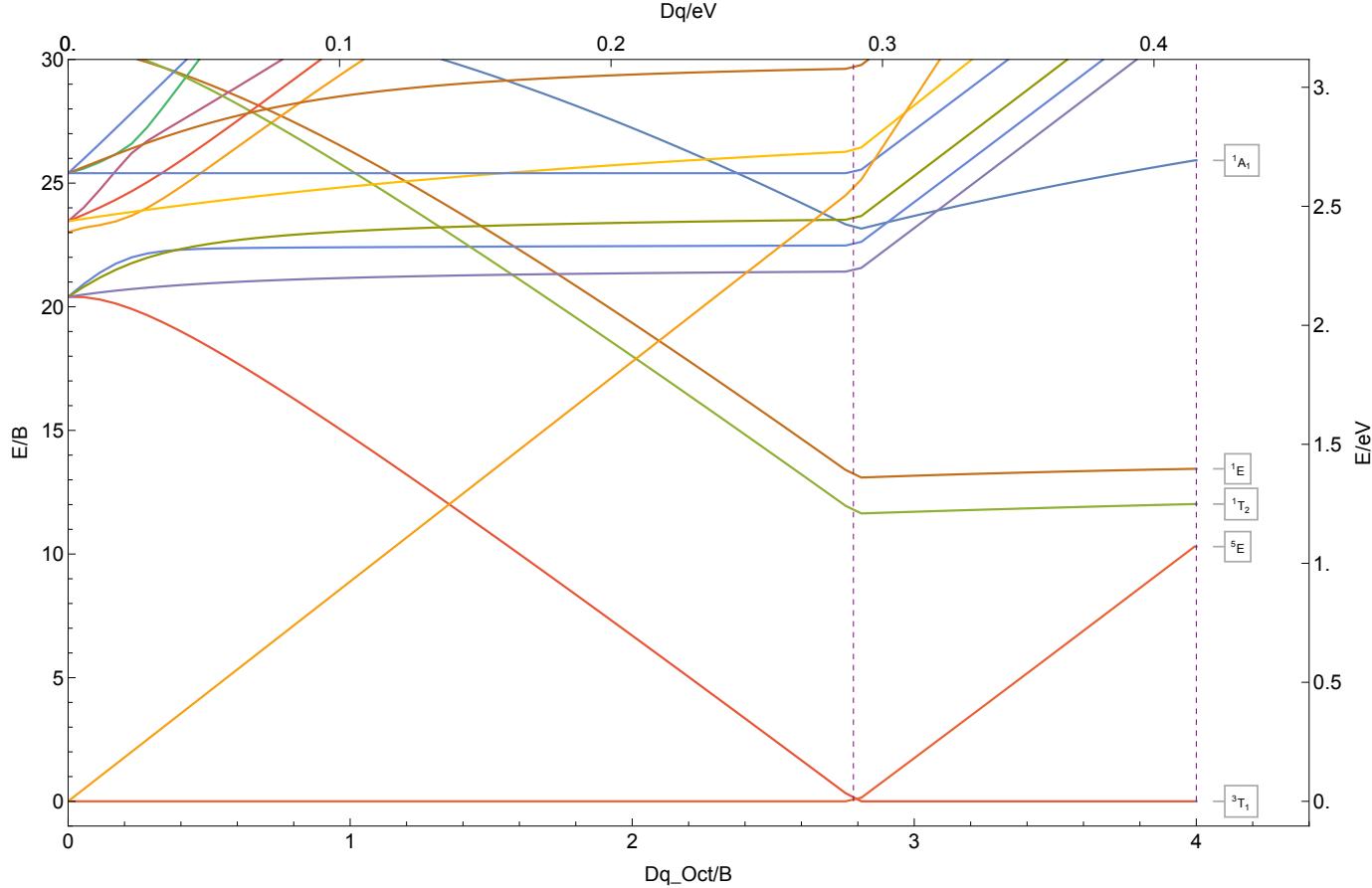
8.3.61 Pd<sup>3+</sup>

|2,4|d<sup>7</sup>| C/B ≈ 4. | B ≈ 803 cm<sup>-1</sup> | Pd<sup>3+</sup>



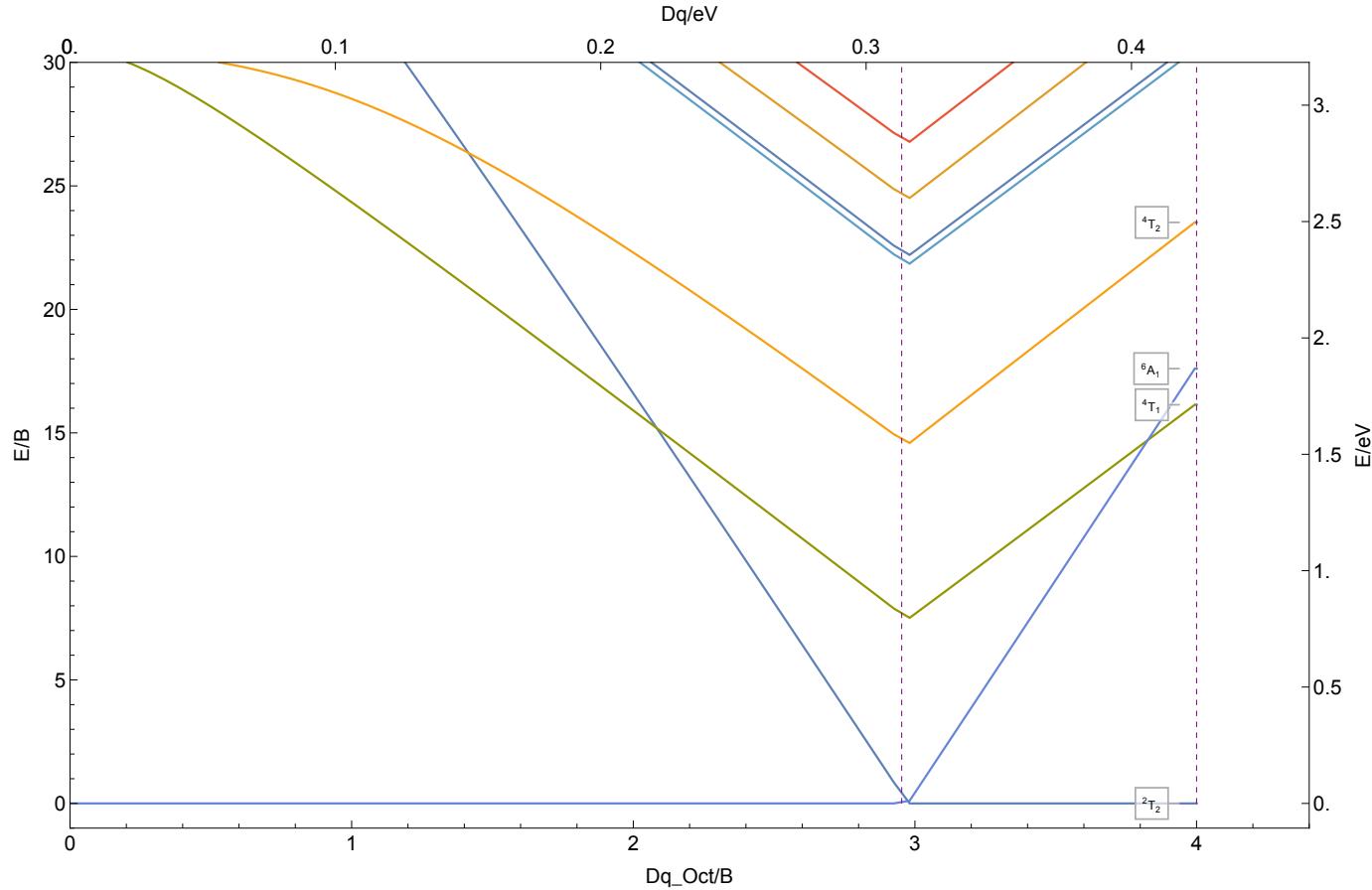
8.3.62 Pd<sup>4+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4.1 | B ≈ 838 cm<sup>-1</sup> | Pd<sup>4+</sup>



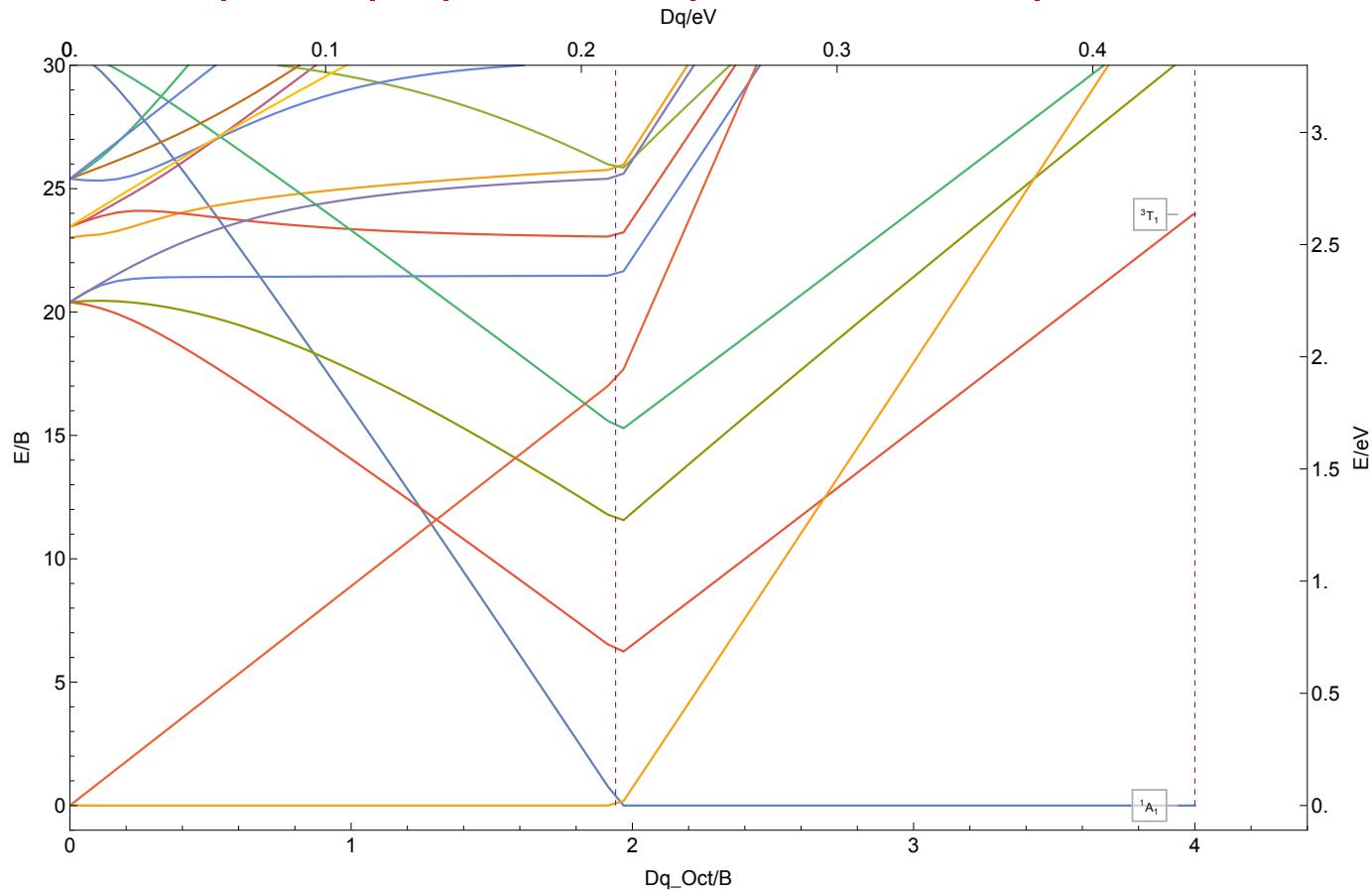
8.3.63 Pd<sup>5+</sup>

|2,4,6| d<sup>5</sup>| C/B ≈ 4.1| B ≈ 856 cm<sup>-1</sup> | Pd<sup>5+</sup>



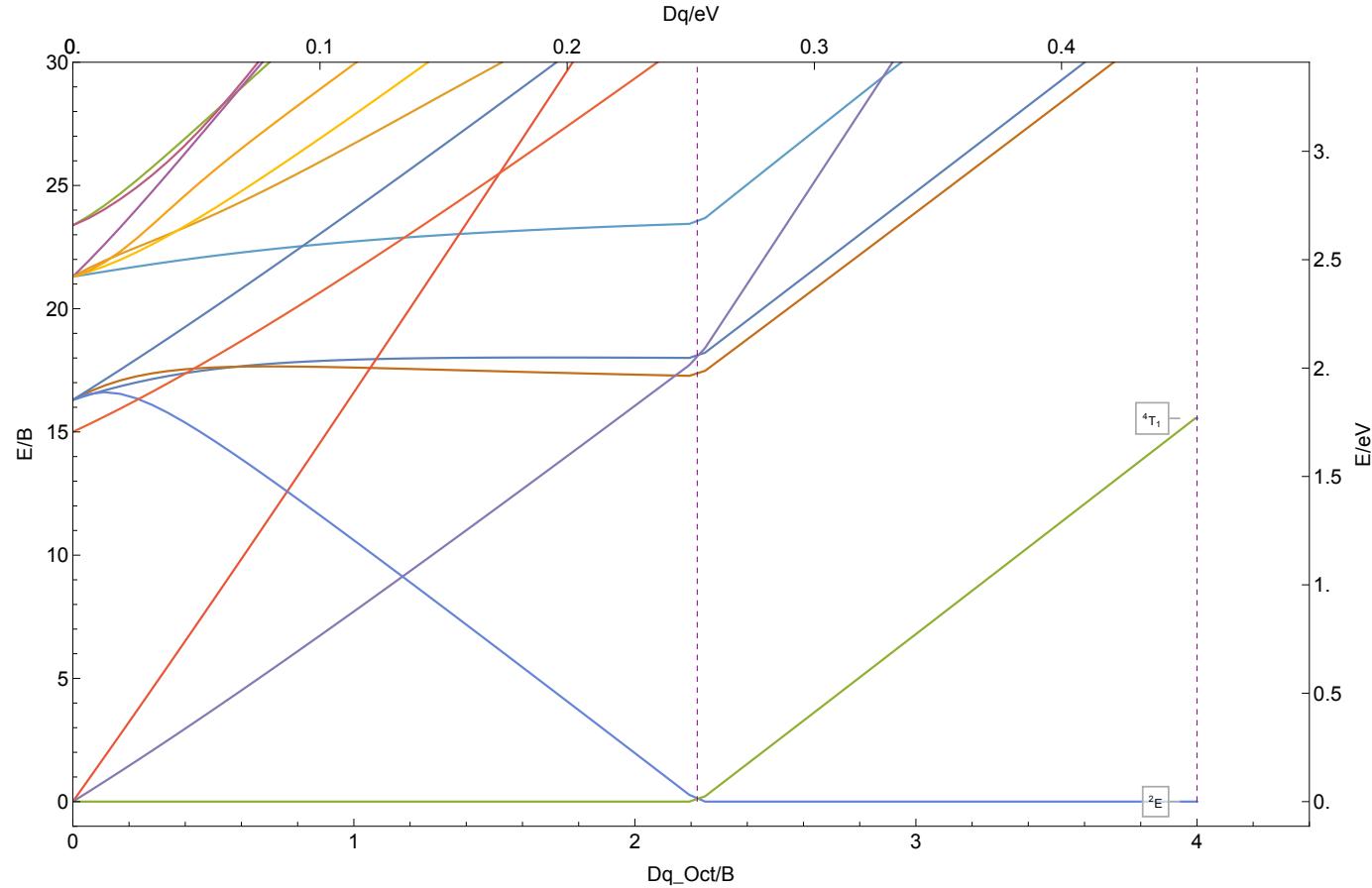
8.3.64 Pd<sup>6+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 4.1 | B ≈ 887 cm<sup>-1</sup> | Pd<sup>6+</sup>



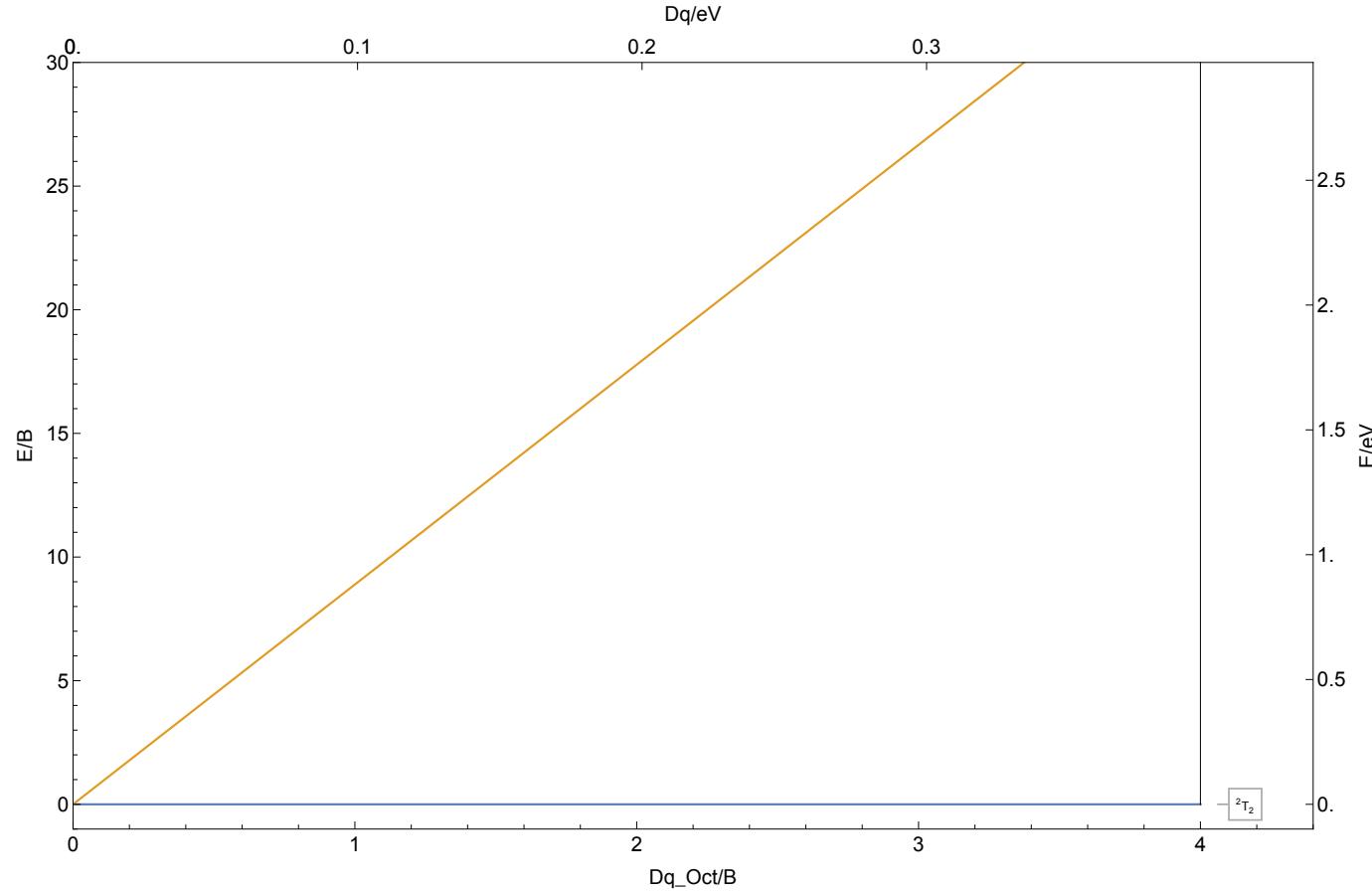
8.3.65 Pd<sup>7+</sup>

|2,4|d<sup>3</sup>| C/B ≈ 4.1| B ≈ 917 cm<sup>-1</sup> |Pd<sup>7+</sup>



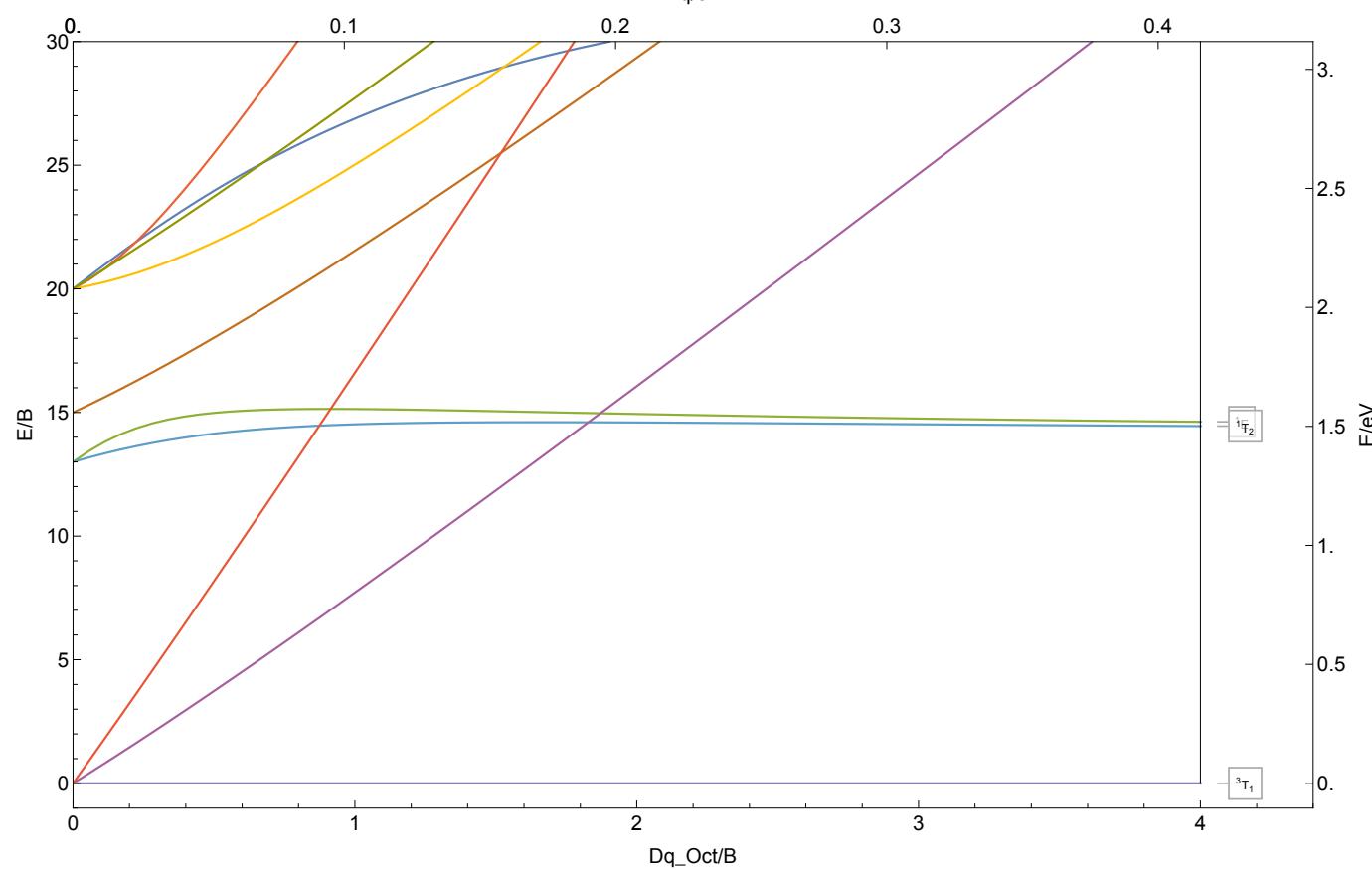
8.3.66  $\text{Ag}^{2+}$

$|2|d^9|C/B \approx 4. |B \approx 799 \text{ cm}^{-1}| \text{Ag}^{2+}$



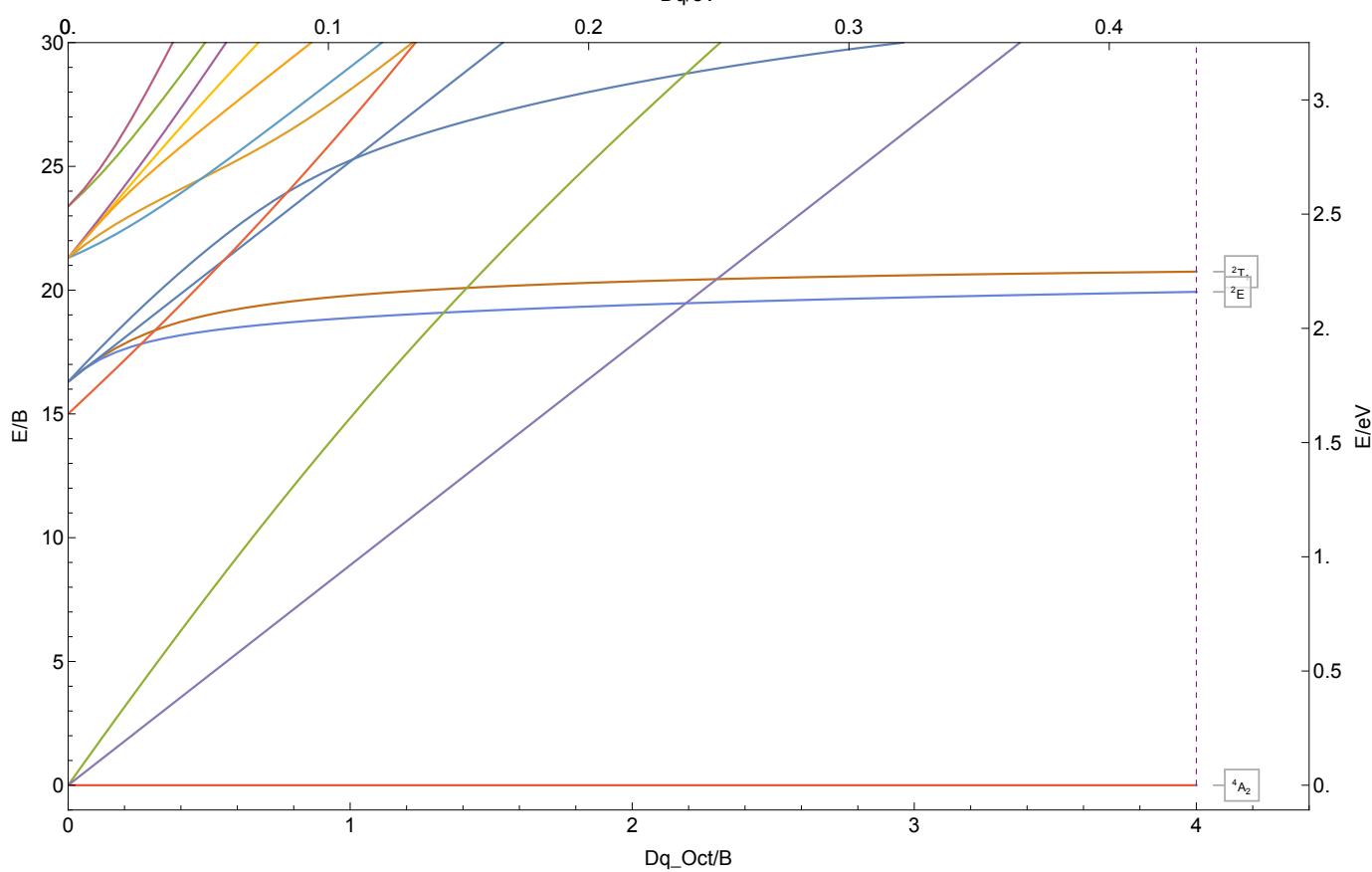
8.3.67  $\text{Ag}^{3+}$

$|1,3|d^8|C/B \approx 4.|B \approx 838 \text{ cm}^{-1}|Ag^{3+}$



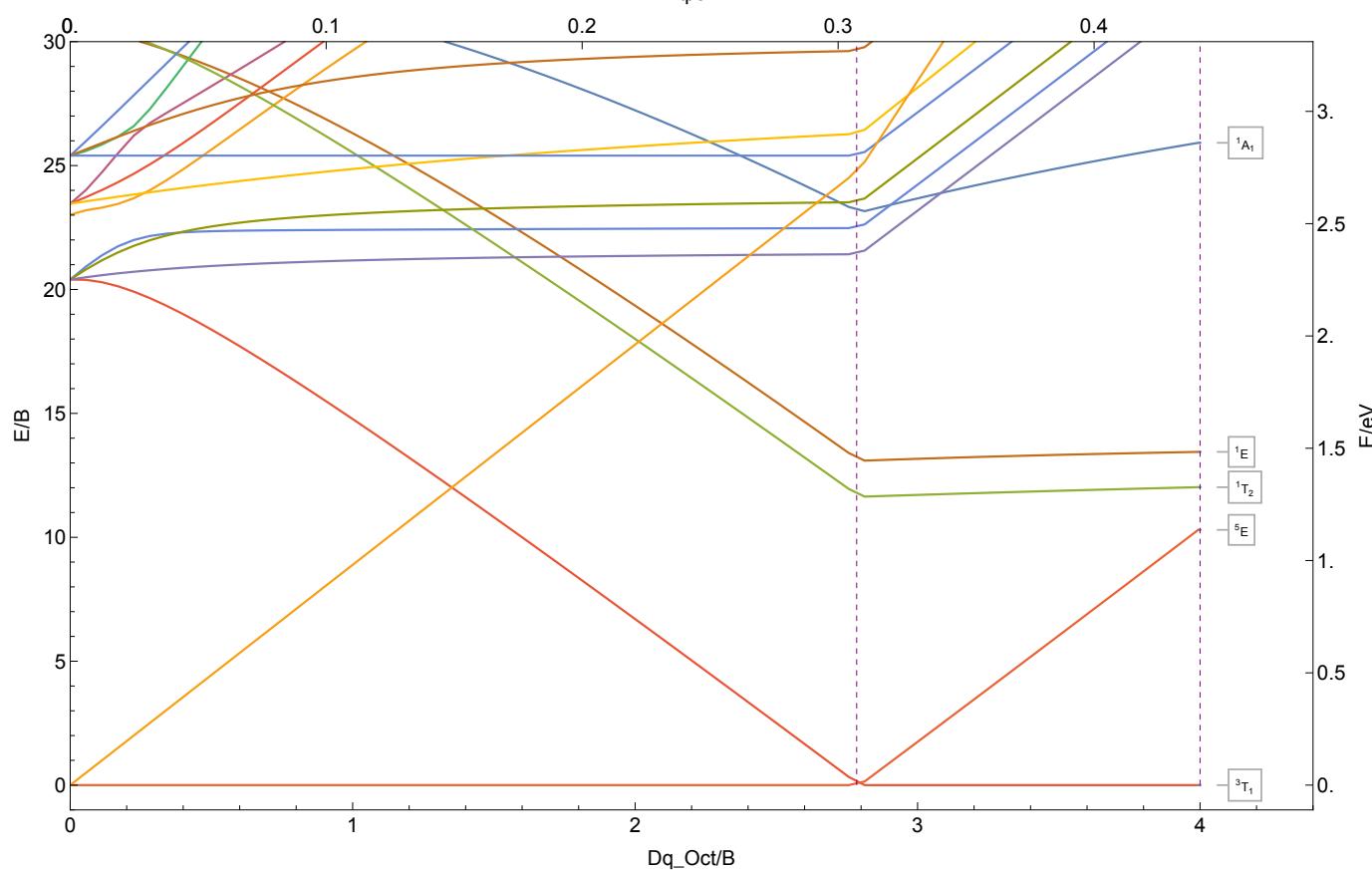
8.3.68  $\text{Ag}^{4+}$

$$|2,4|d^7|C/B \approx 4.1|B \approx 874 \text{ cm}^{-1}| \text{Ag}^{4+}$$



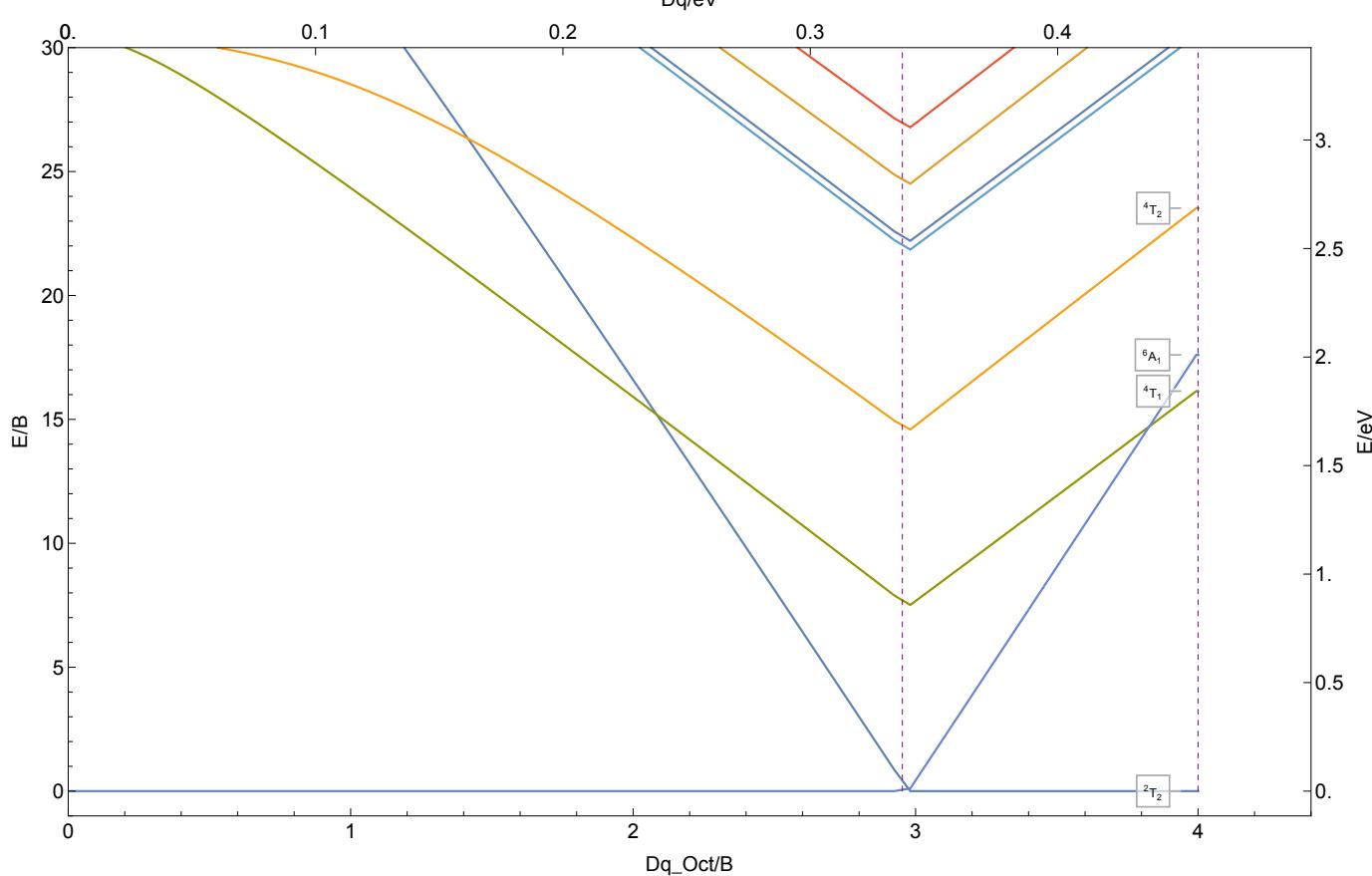
8.3.69 Ag<sup>5+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4.1 | B ≈ 890 cm<sup>-1</sup> | Ag<sup>5+</sup>



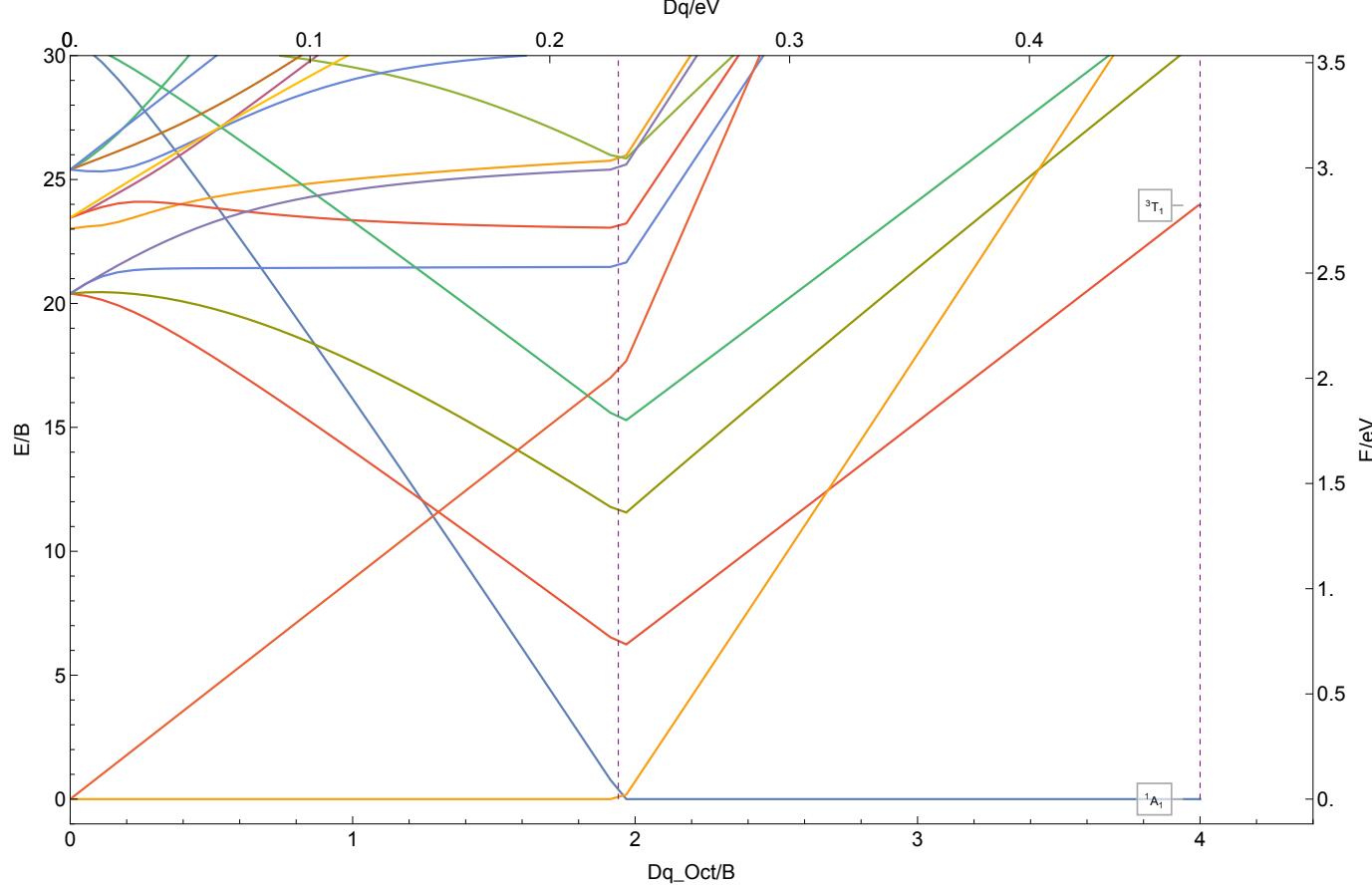
8.3.70 Ag<sup>6+</sup>

|2,4,6|d<sup>5</sup>|C/B ≈ 4.1|B ≈ 921 cm<sup>-1</sup>|Ag<sup>6+</sup>



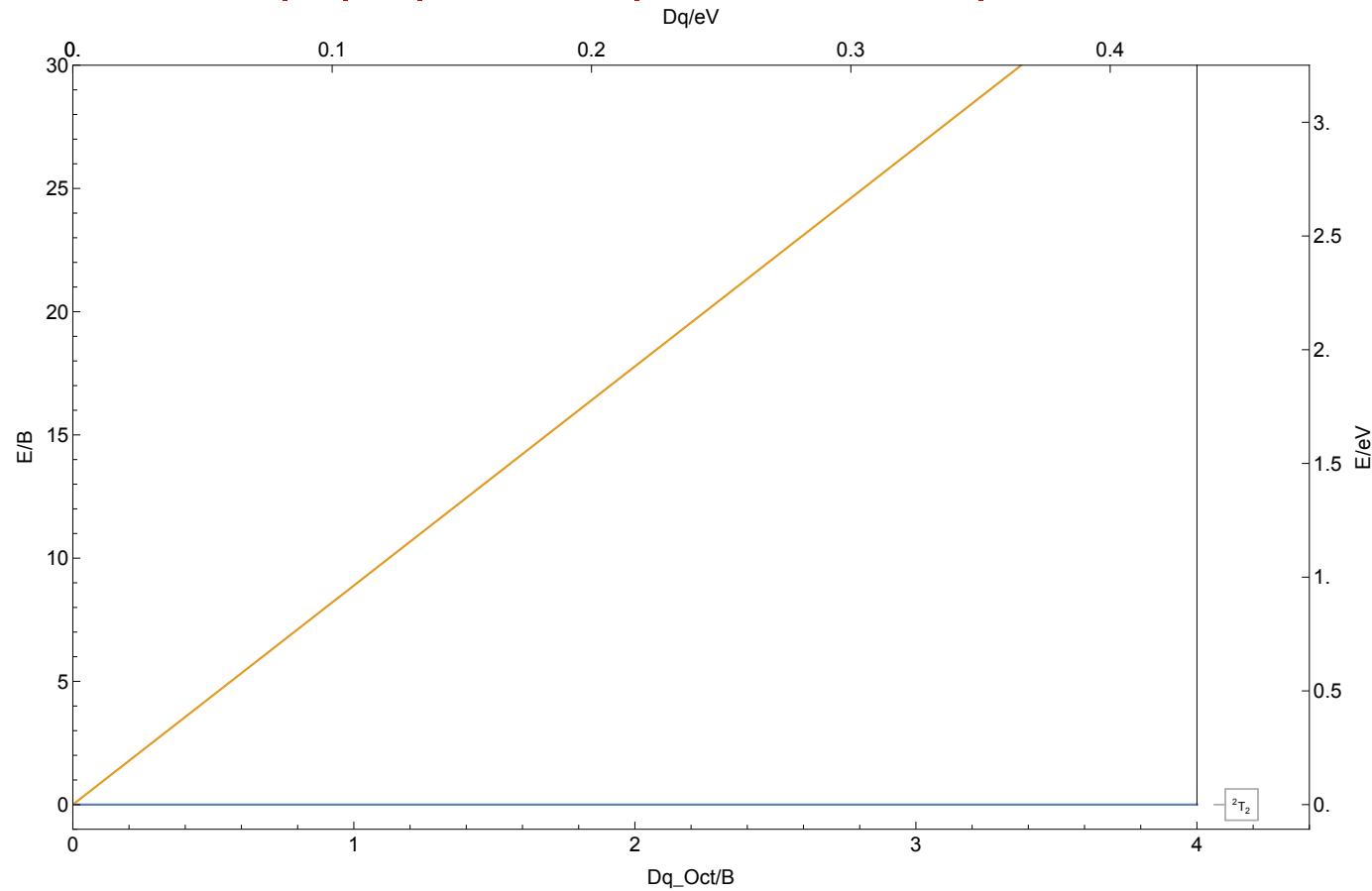
8.3.71 Ag<sup>7+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 4.1 | B ≈ 950 cm<sup>-1</sup> | Ag<sup>7+</sup>



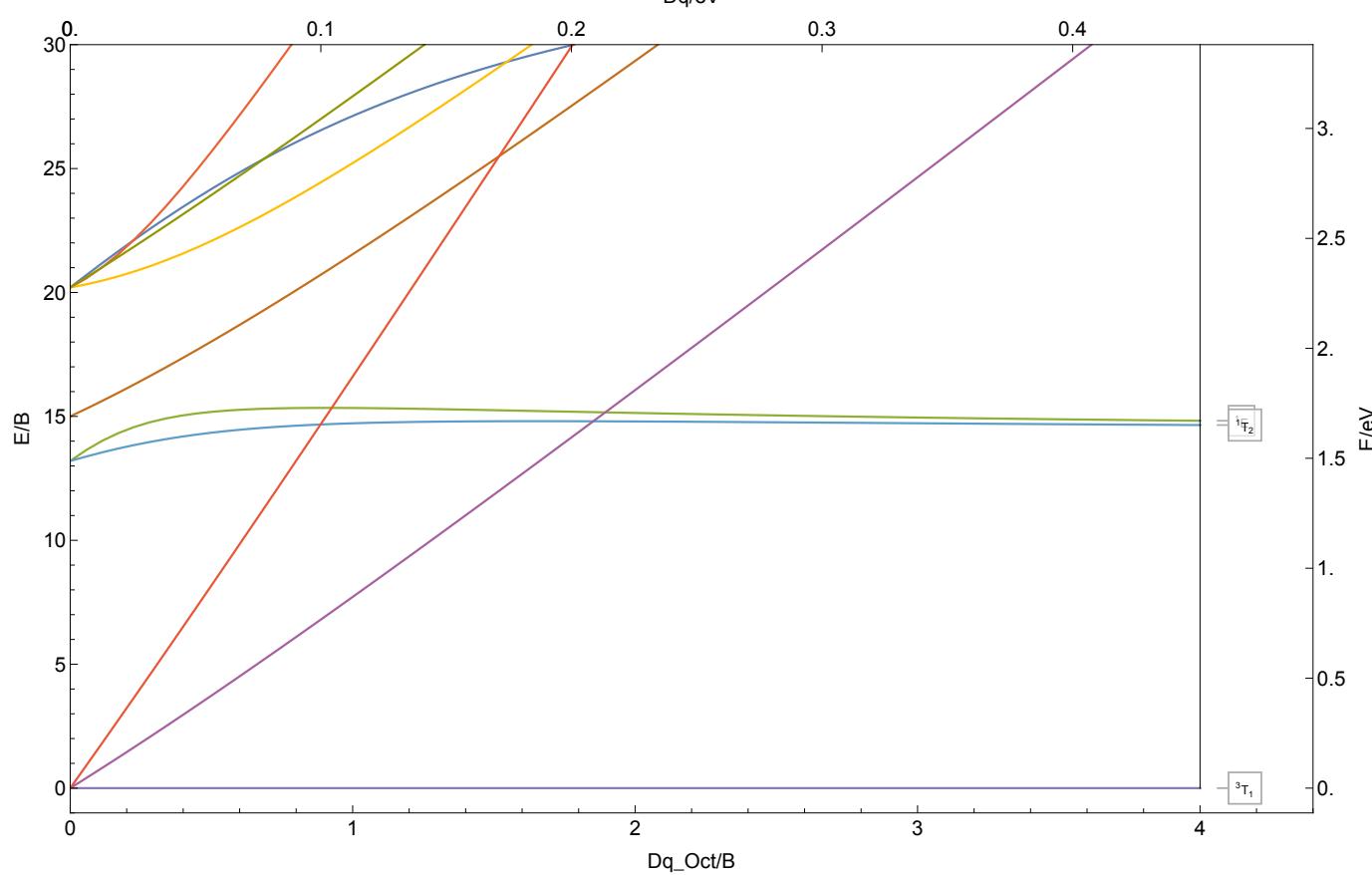
8.3.72 Cd<sup>3+</sup>

|2|d<sup>9</sup>| C/B ≈ 4. |B ≈ 874 cm<sup>-1</sup> |Cd<sup>3+</sup>



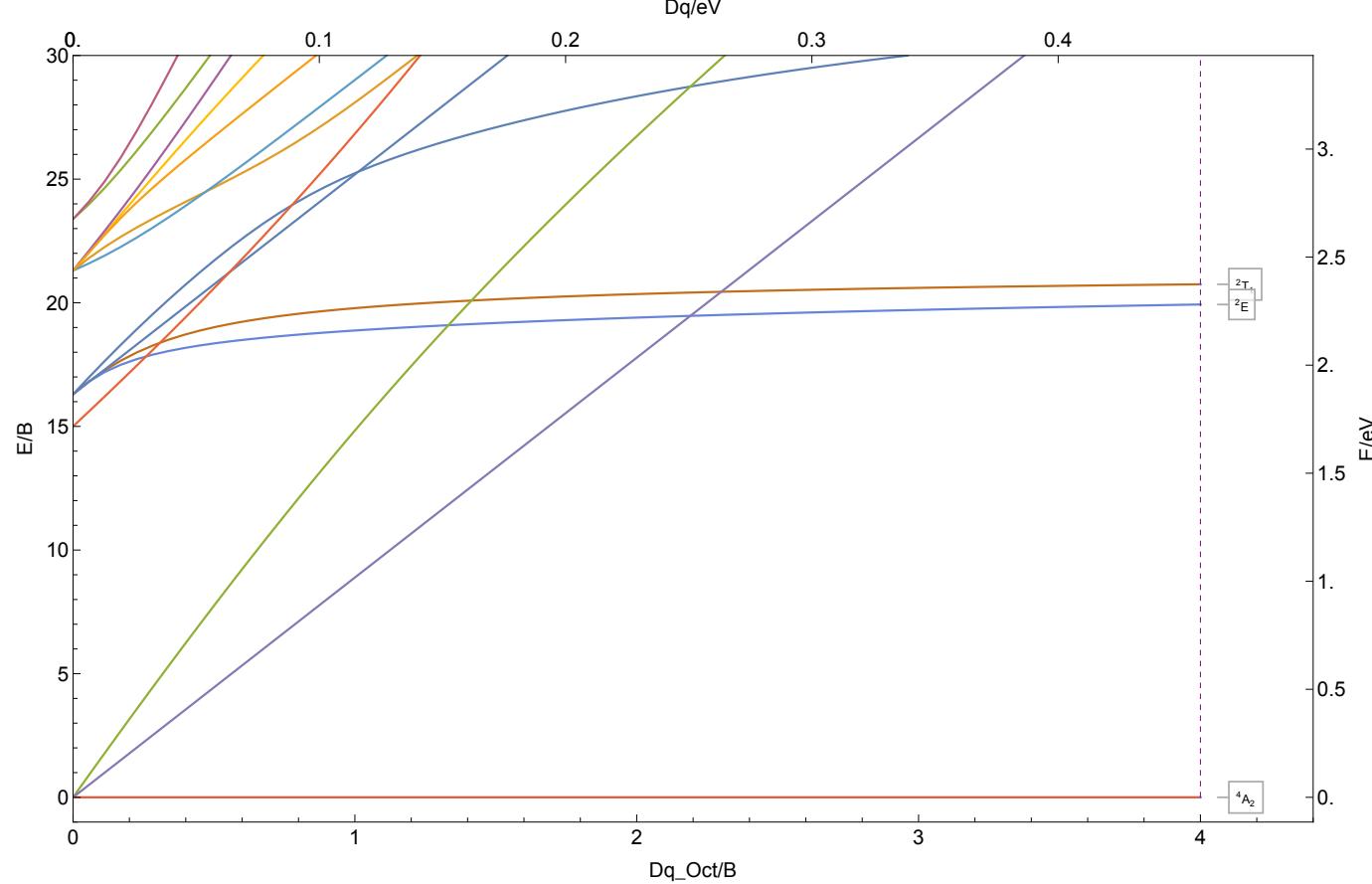
### 8.3.73 Cd<sup>4+</sup>

$|1,3|d^8|C/B \approx 4.1|B \approx 909\text{ cm}^{-1}|Cd^{4+}$



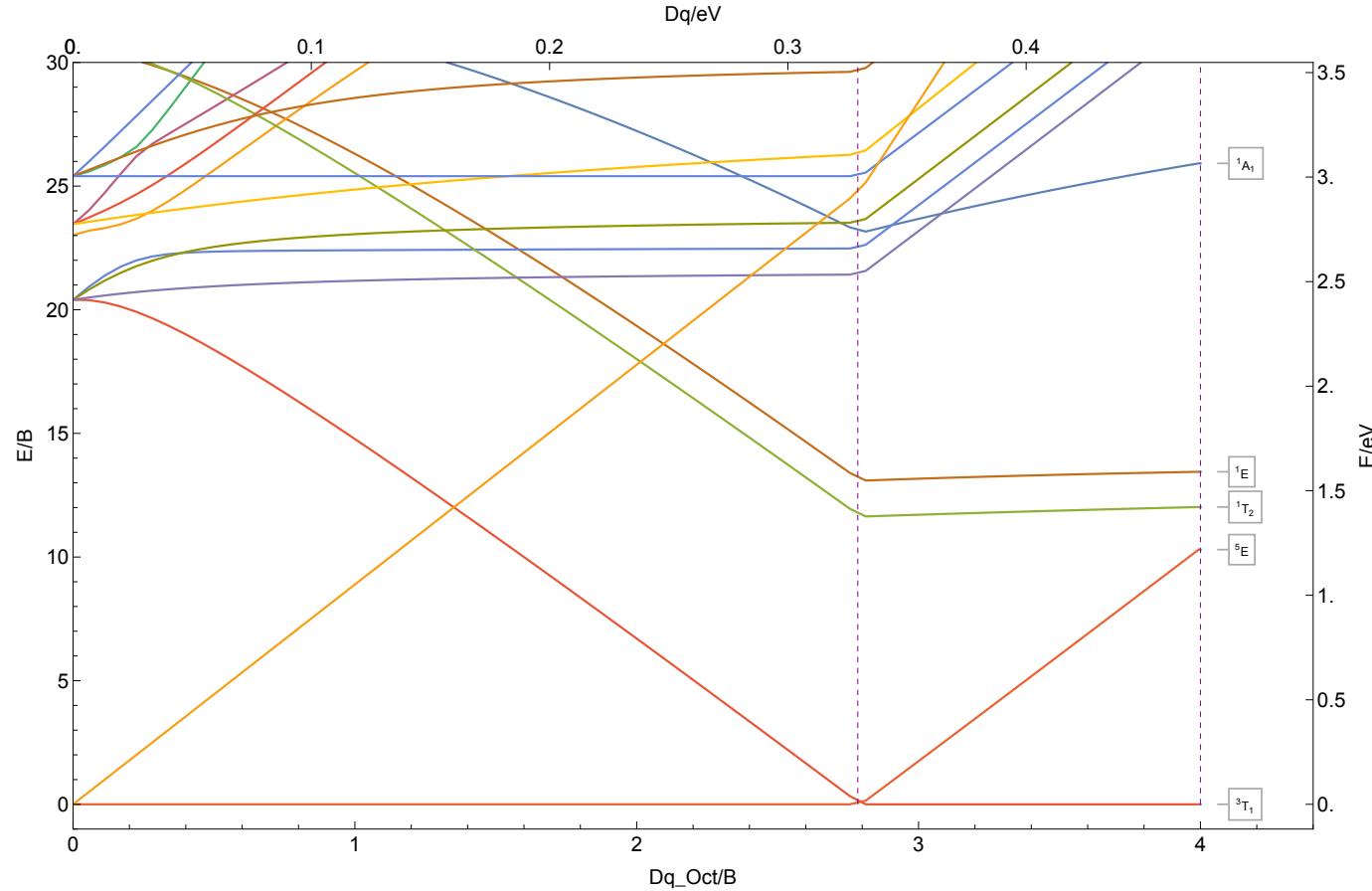
8.3.74 Cd<sup>5+</sup>

$|2,4|d^7|C/B \approx 4.1|B \approx 923\text{ cm}^{-1}|Cd^{5+}$



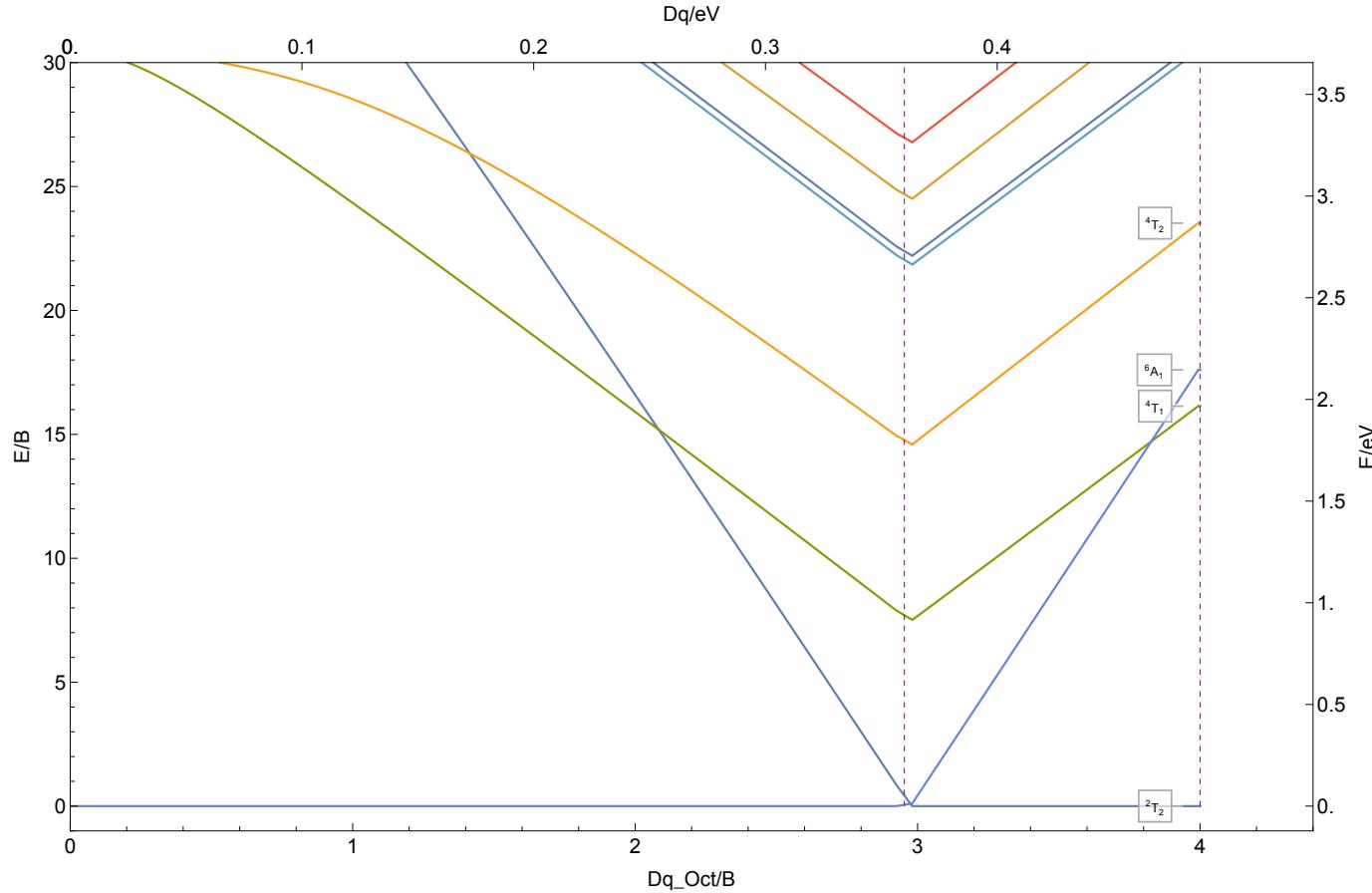
8.3.75 Cd<sup>6+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4.1 | B ≈ 954 cm<sup>-1</sup> | Cd<sup>6+</sup>



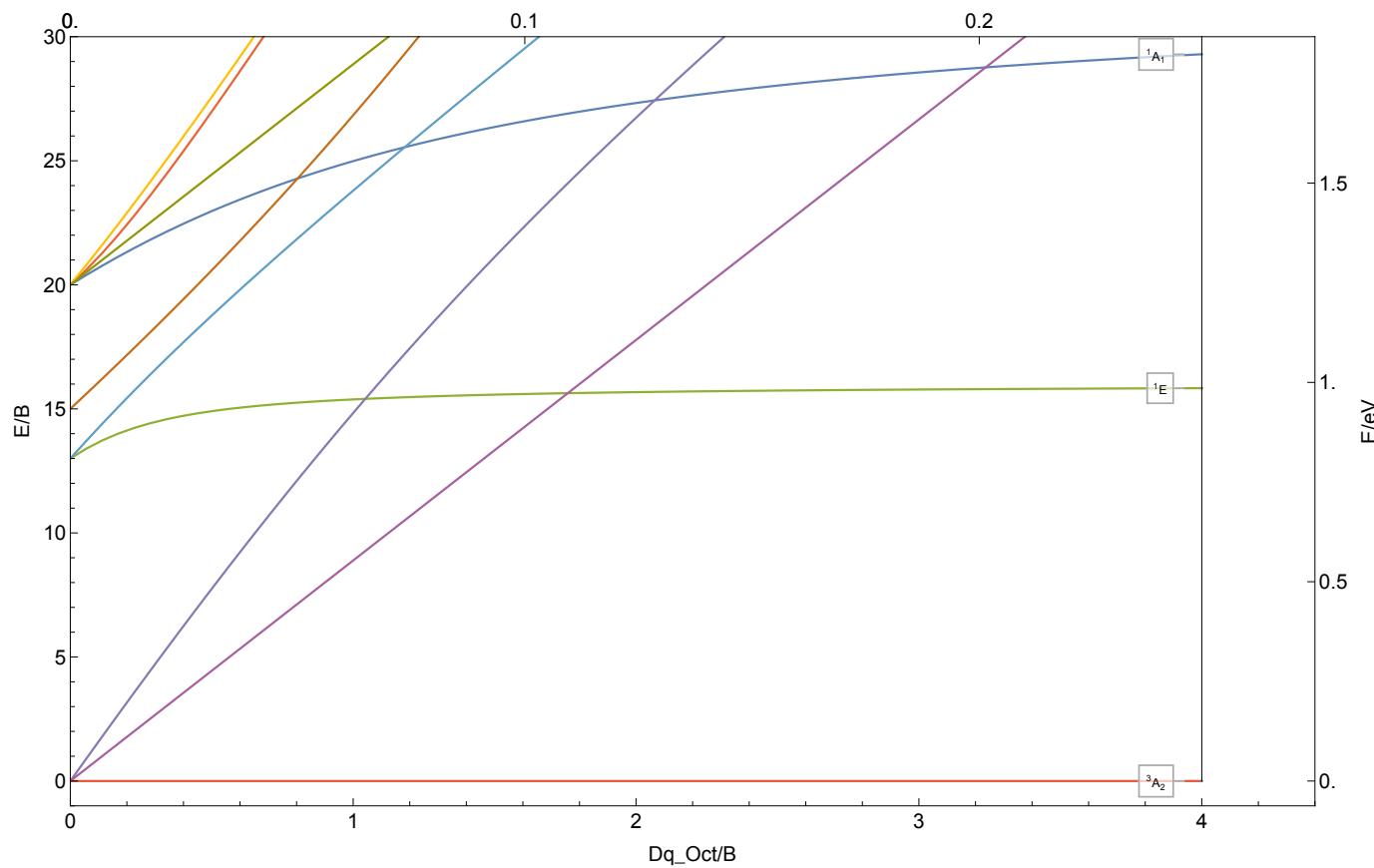
8.3.76 Cd<sup>7+</sup>

|2,4,6| d<sup>5</sup>| C/B ≈ 4.1| B ≈ 983 cm<sup>-1</sup> |Cd<sup>7+</sup>



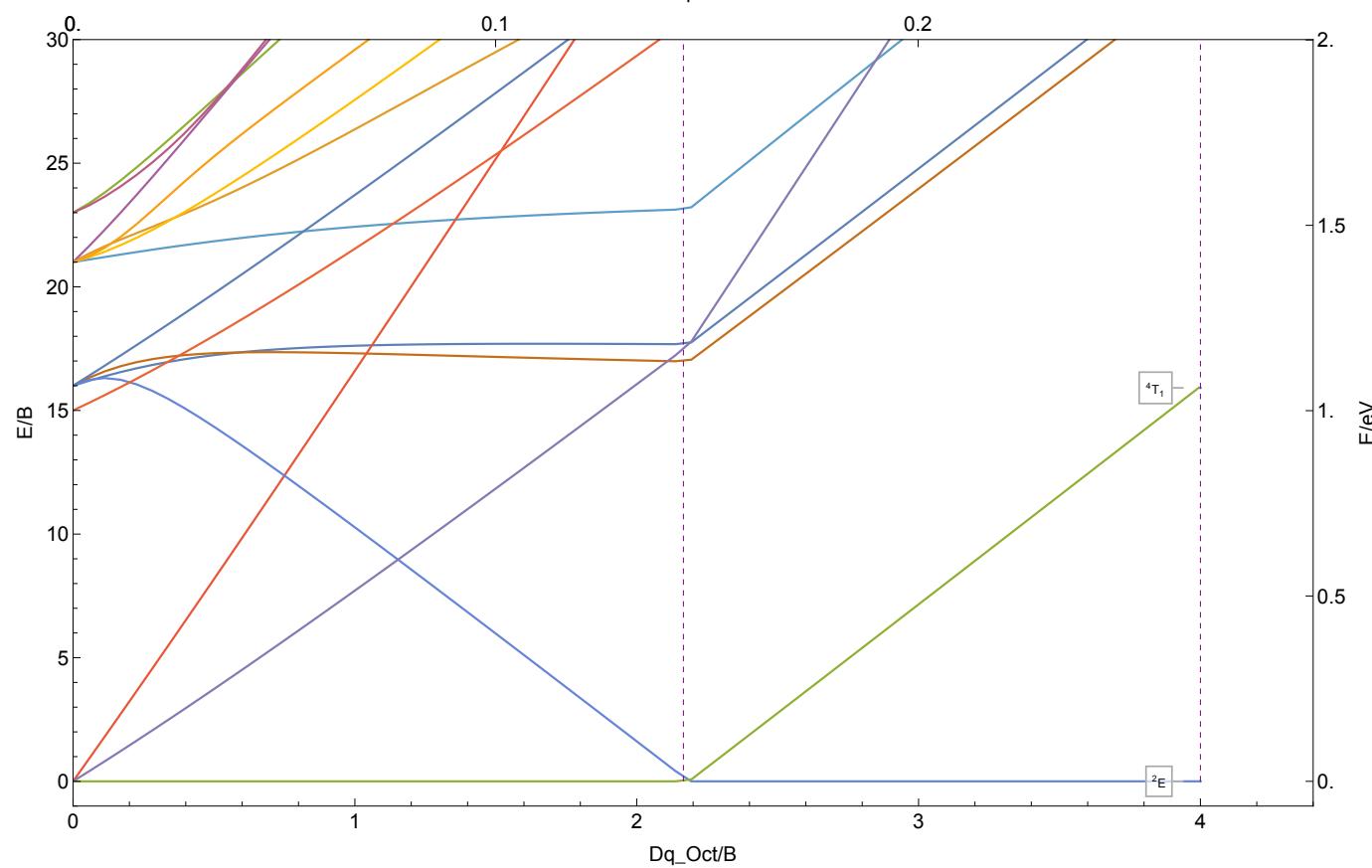
8.3.77  $\text{Hf}^{2+}$

$|1,3|d^2|$  C/B  $\approx 4.$  | B  $\approx 502 \text{ cm}^{-1}$  |  $\text{Hf}^{2+}$



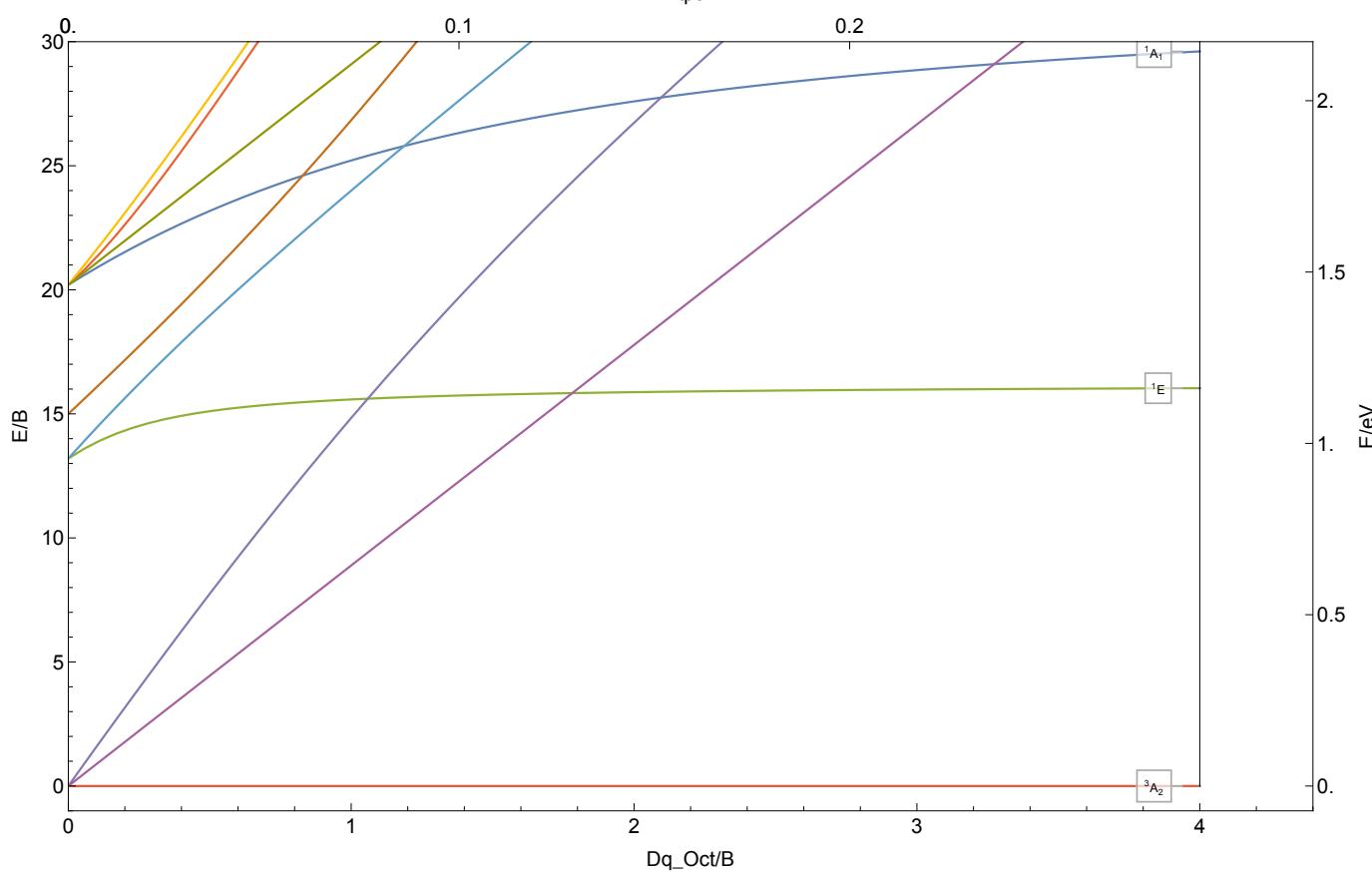
8.3.78  $Ta^{2+}$

$|2,4|d^3|C/B \approx 4.|B \approx 538\text{ cm}^{-1}|Ta^{2+}$



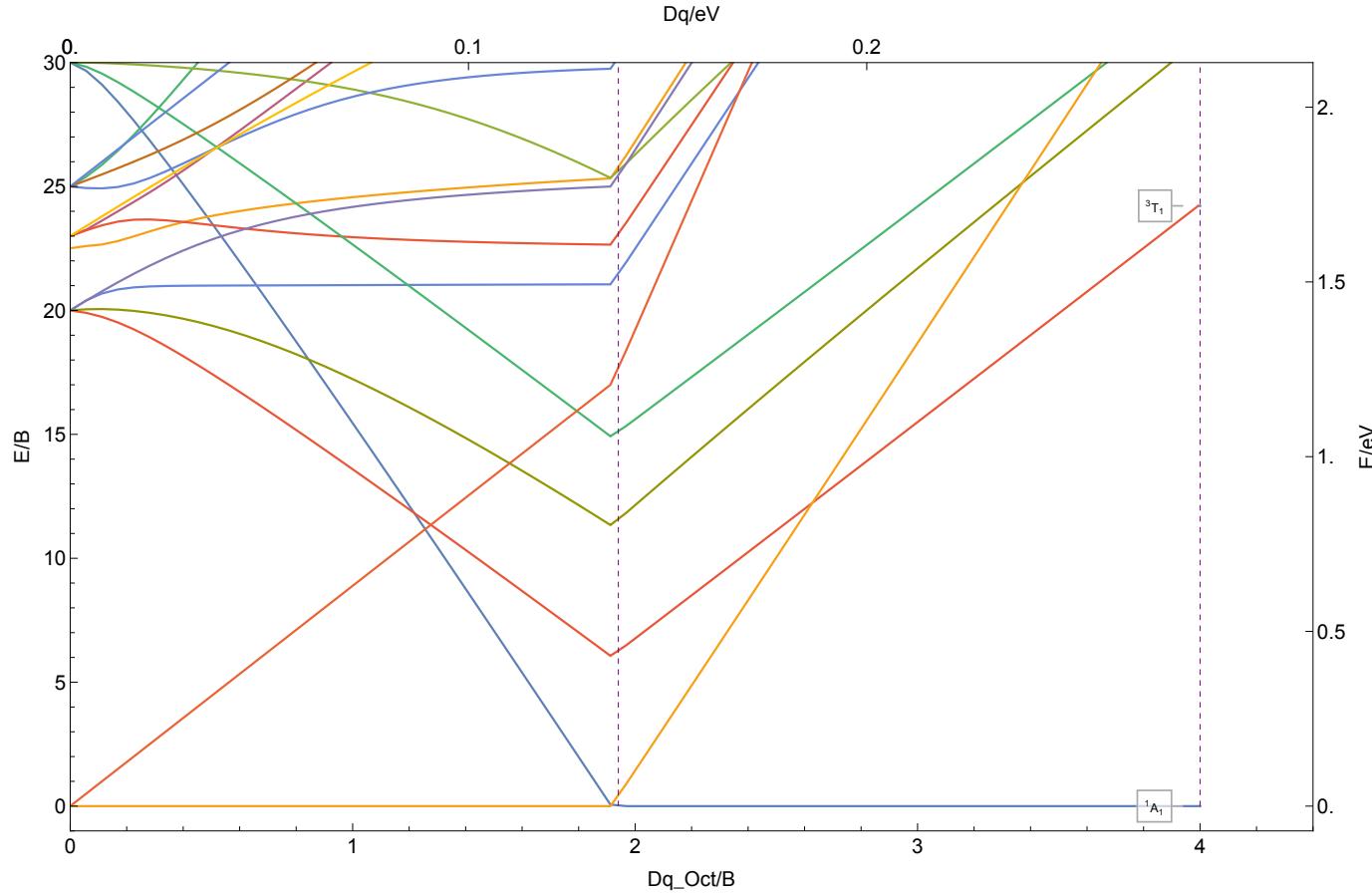
8.3.79 Ta<sup>3+</sup>

| 1,3 | d<sup>2</sup> | C/B ≈ 4.1 | B ≈ 584 cm<sup>-1</sup> | Ta<sup>3+</sup>



8.3.80  $W^{2+}$

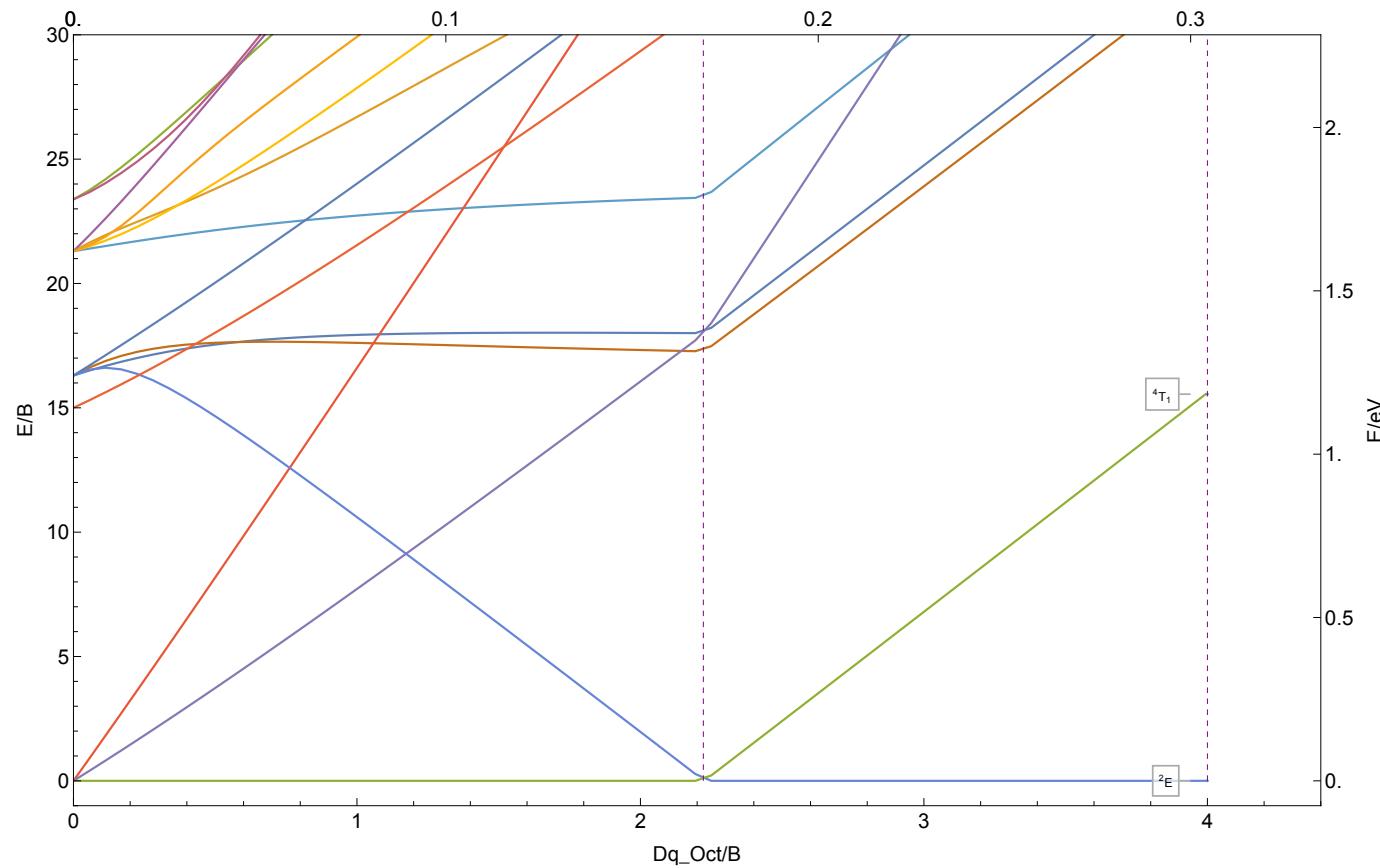
$|1,3,5|d^4|C/B \approx 4. |B \approx 572\text{ cm}^{-1}|W^{2+}$



8.3.81  $\text{W}^{3+}$

$$|2,4|\text{d}^3|\text{C/B} \approx 4.1|\text{B} \approx 614\text{ cm}^{-1}| \text{W}^{3+}$$

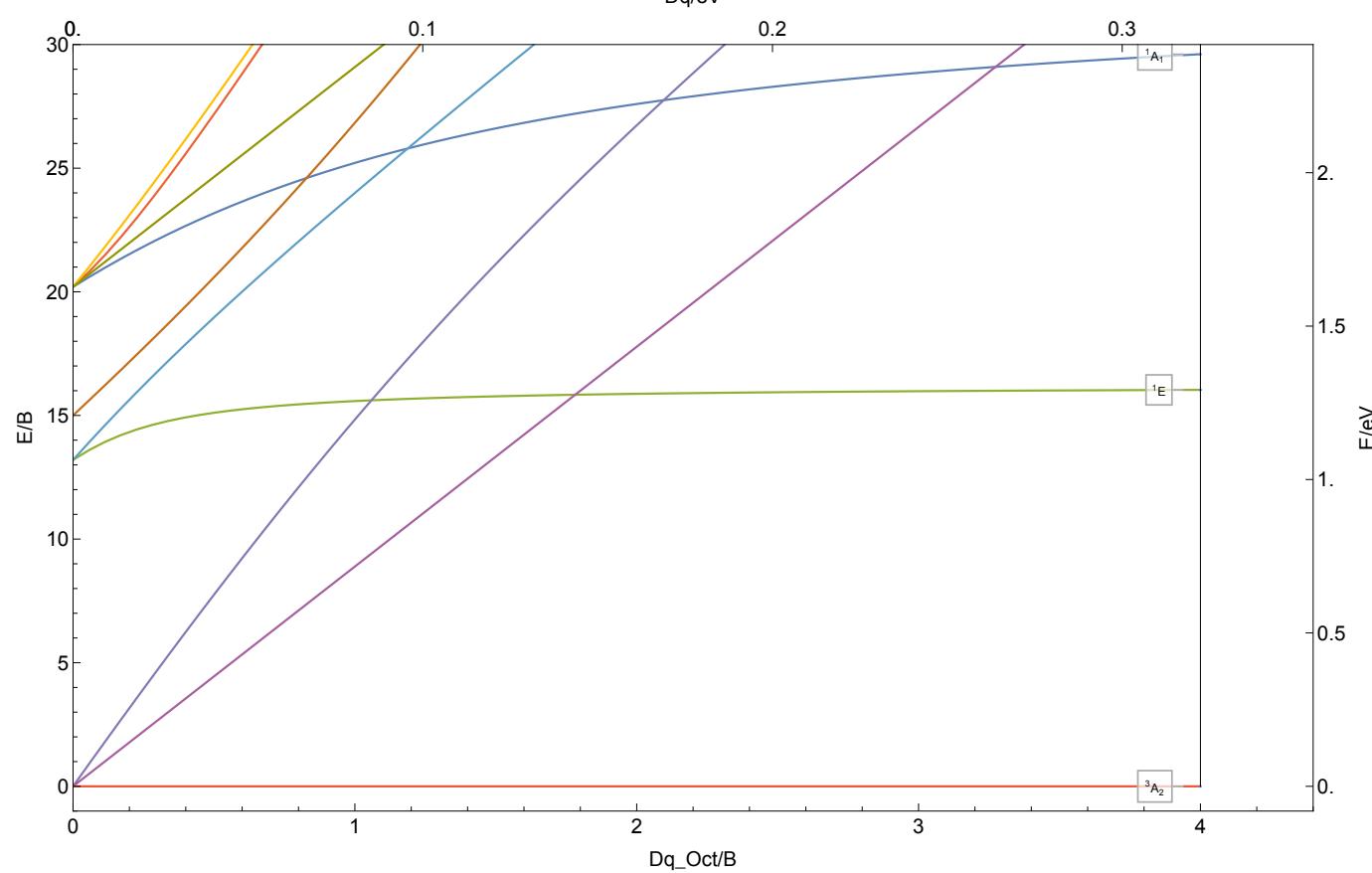
Dq/eV



8.3.82 W<sup>4+</sup>

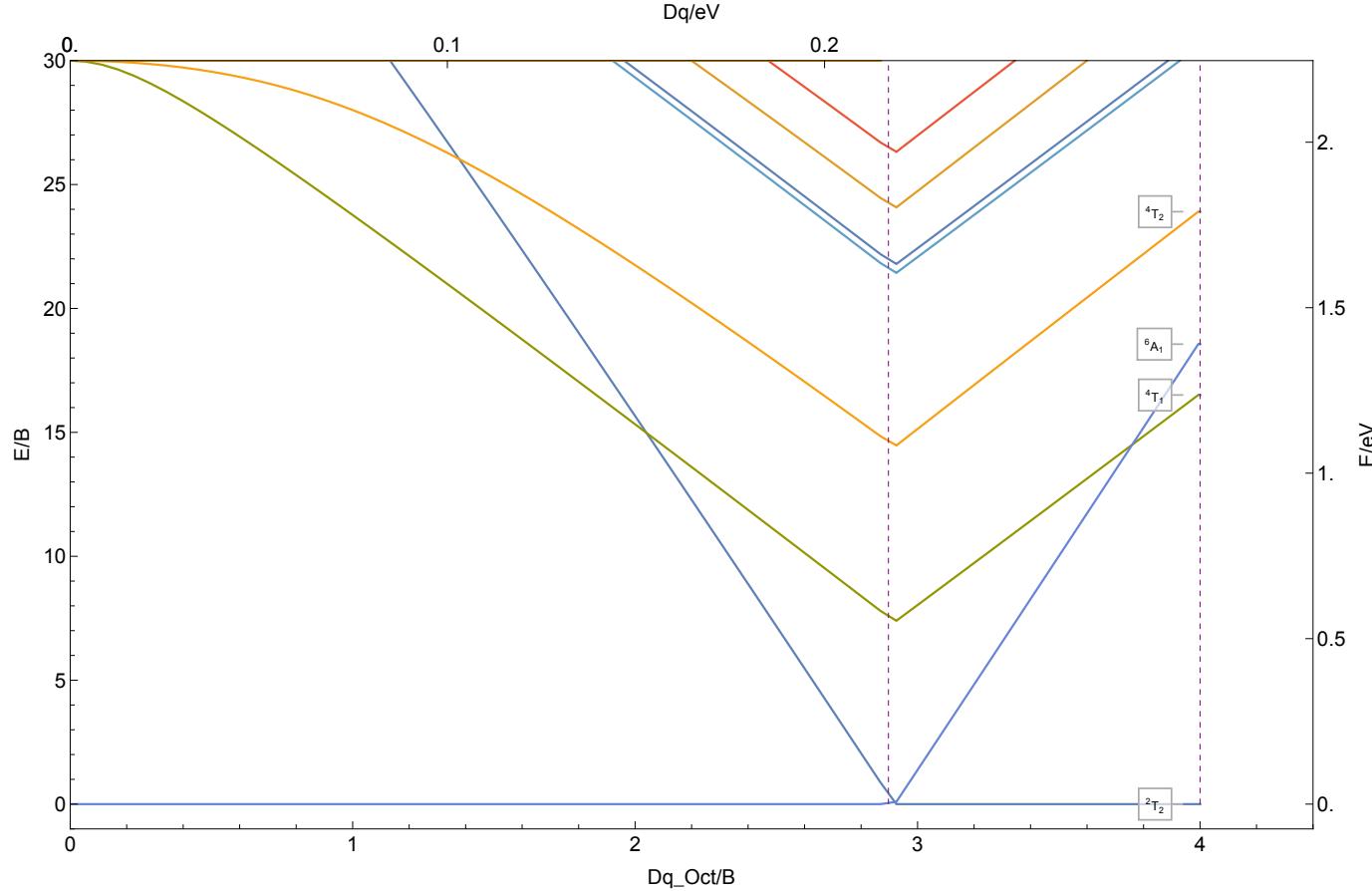
$$|1,3|d^2|C/B \approx 4.1|B \approx 650\text{ cm}^{-1}|W^{4+}$$

933



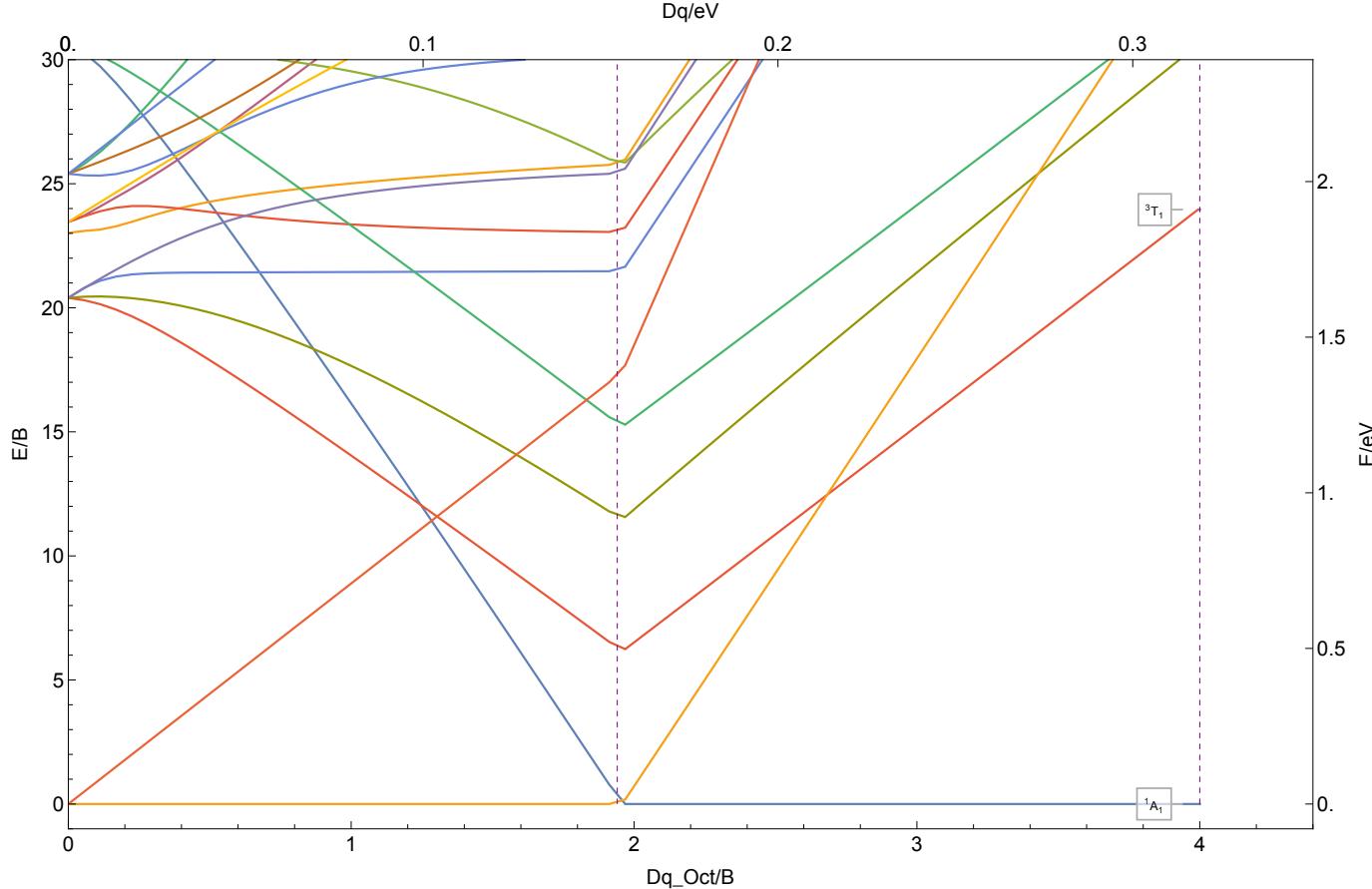
8.3.83  $\text{Re}^{2+}$

$|2,4,6| \text{d}^5 | \text{C/B} \approx 4. | \text{B} \approx 604 \text{ cm}^{-1} | \text{Re}^{2+}$



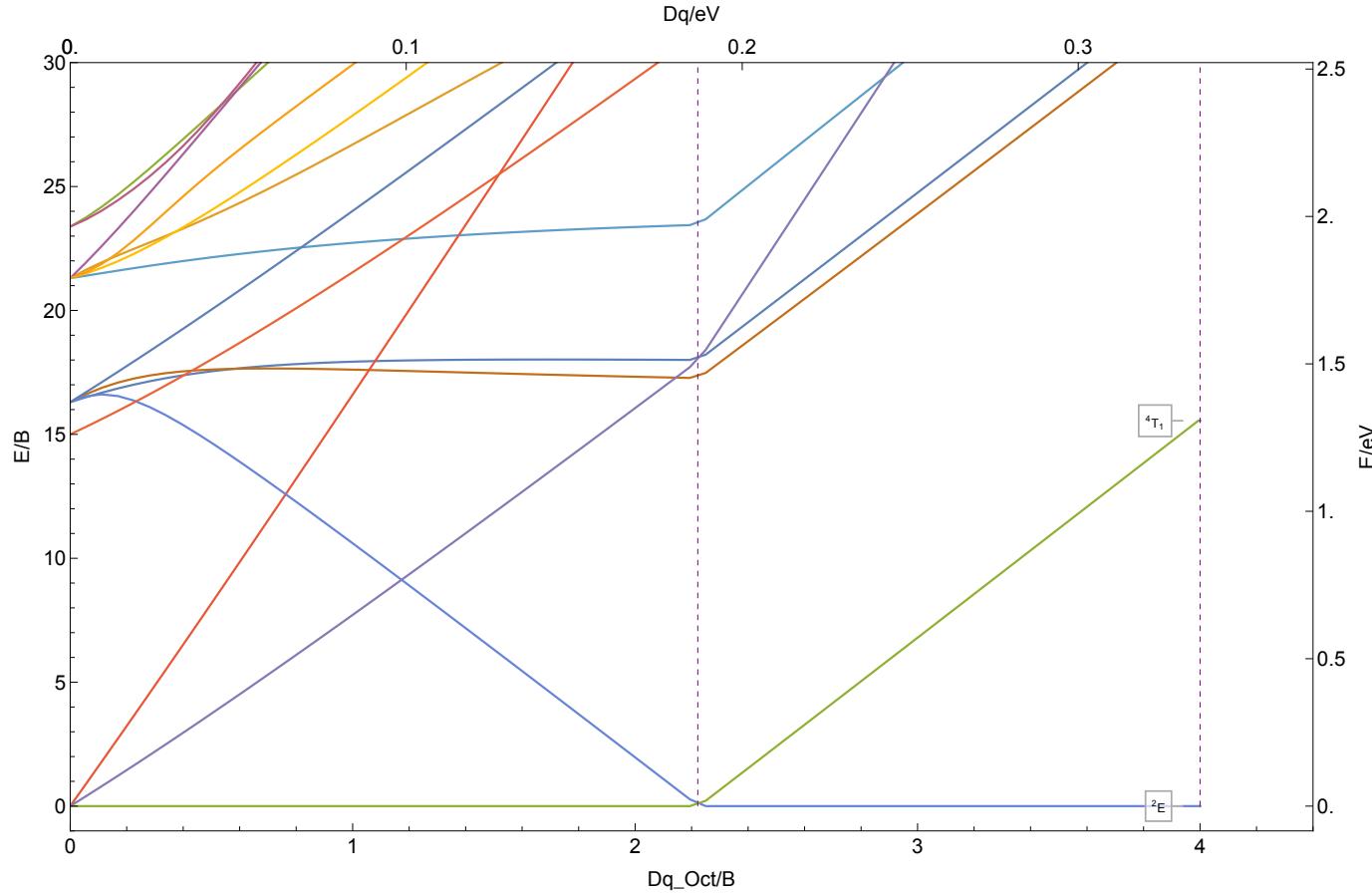
8.3.84  $\text{Re}^{3+}$

$|1,3,5|d^4|C/B \approx 4.1|B \approx 643\text{ cm}^{-1}| \text{Re}^{3+}$



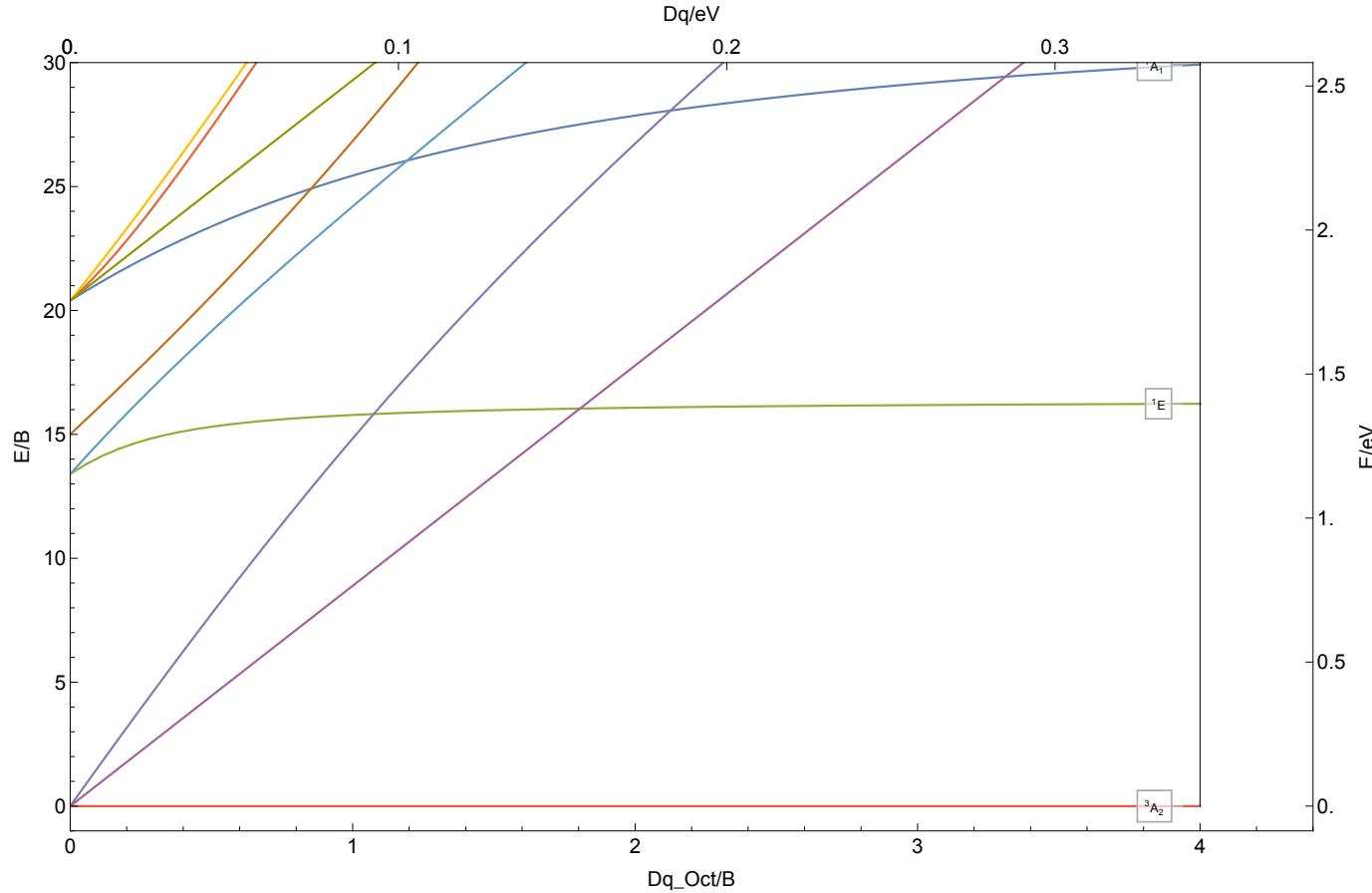
8.3.85 Re<sup>4+</sup>

|2,4|d<sup>3</sup>| C/B ≈ 4.1| B ≈ 678 cm<sup>-1</sup> |Re<sup>4+</sup>



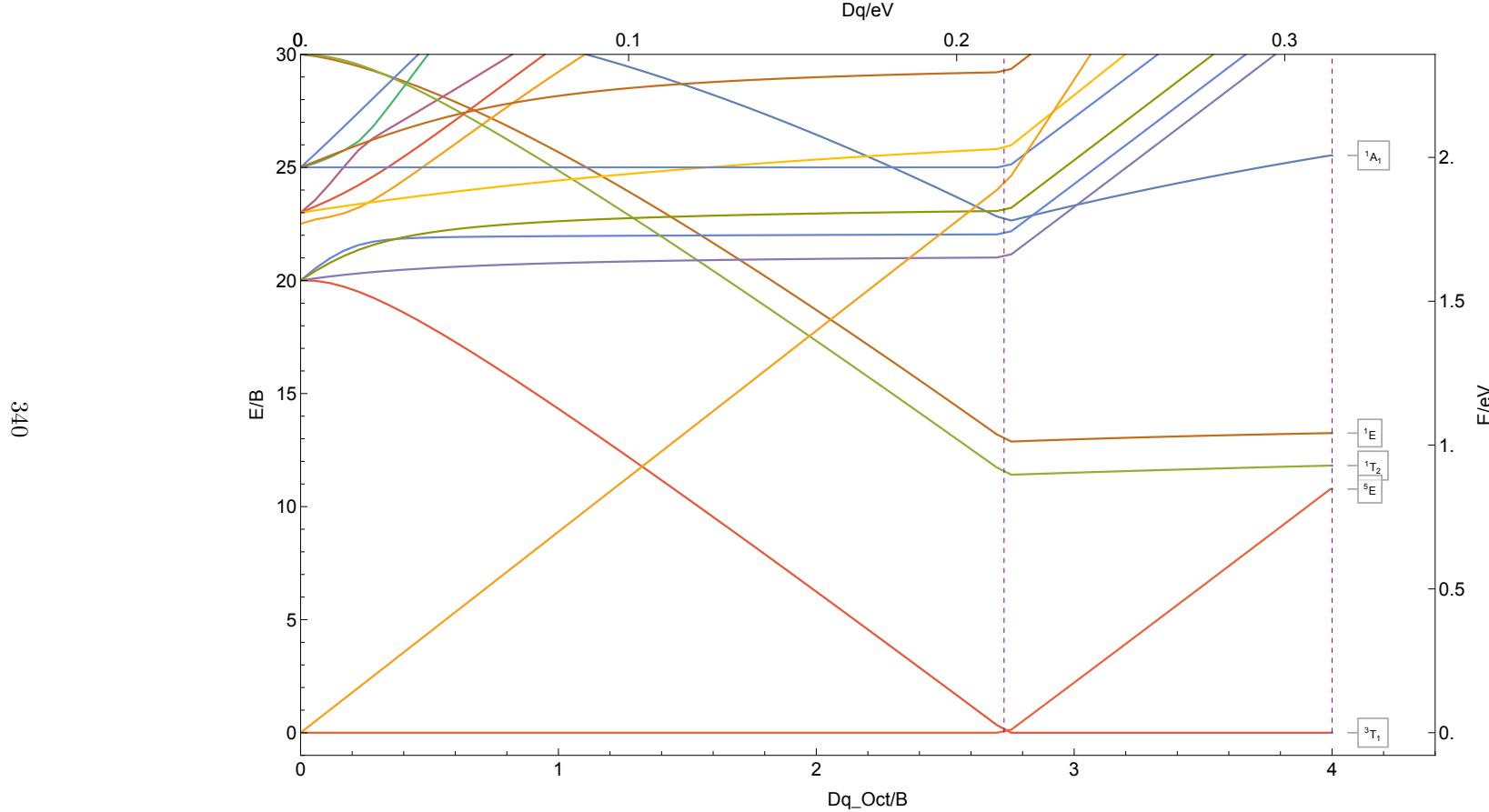
8.3.86  $\text{Re}^{5+}$

$$|1,3|d^2|C/B \approx 4.2|B \approx 694 \text{ cm}^{-1}| \text{Re}^{5+}$$



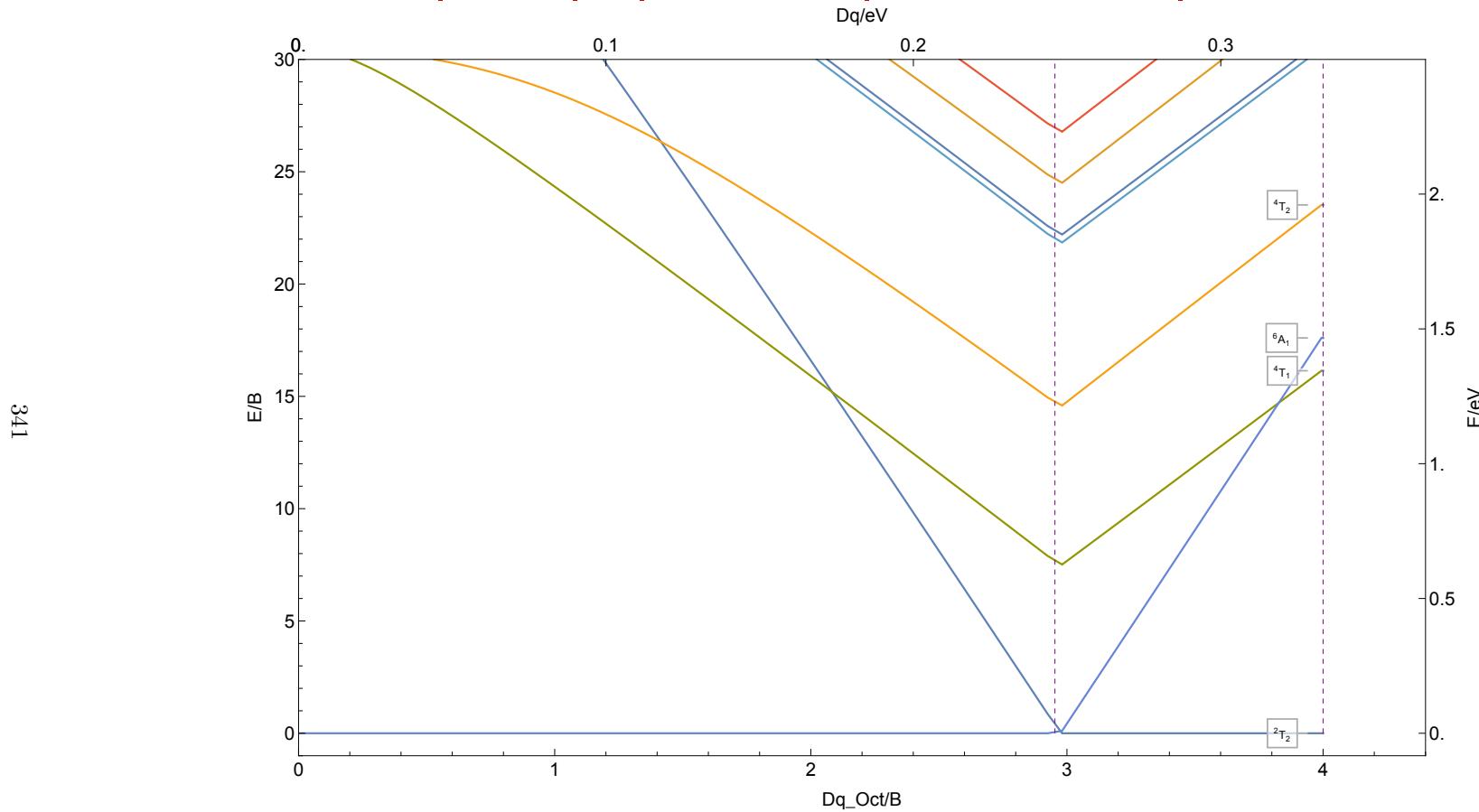
8.3.87 Os<sup>2+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4. | B ≈ 634 cm<sup>-1</sup> | Os<sup>2+</sup>



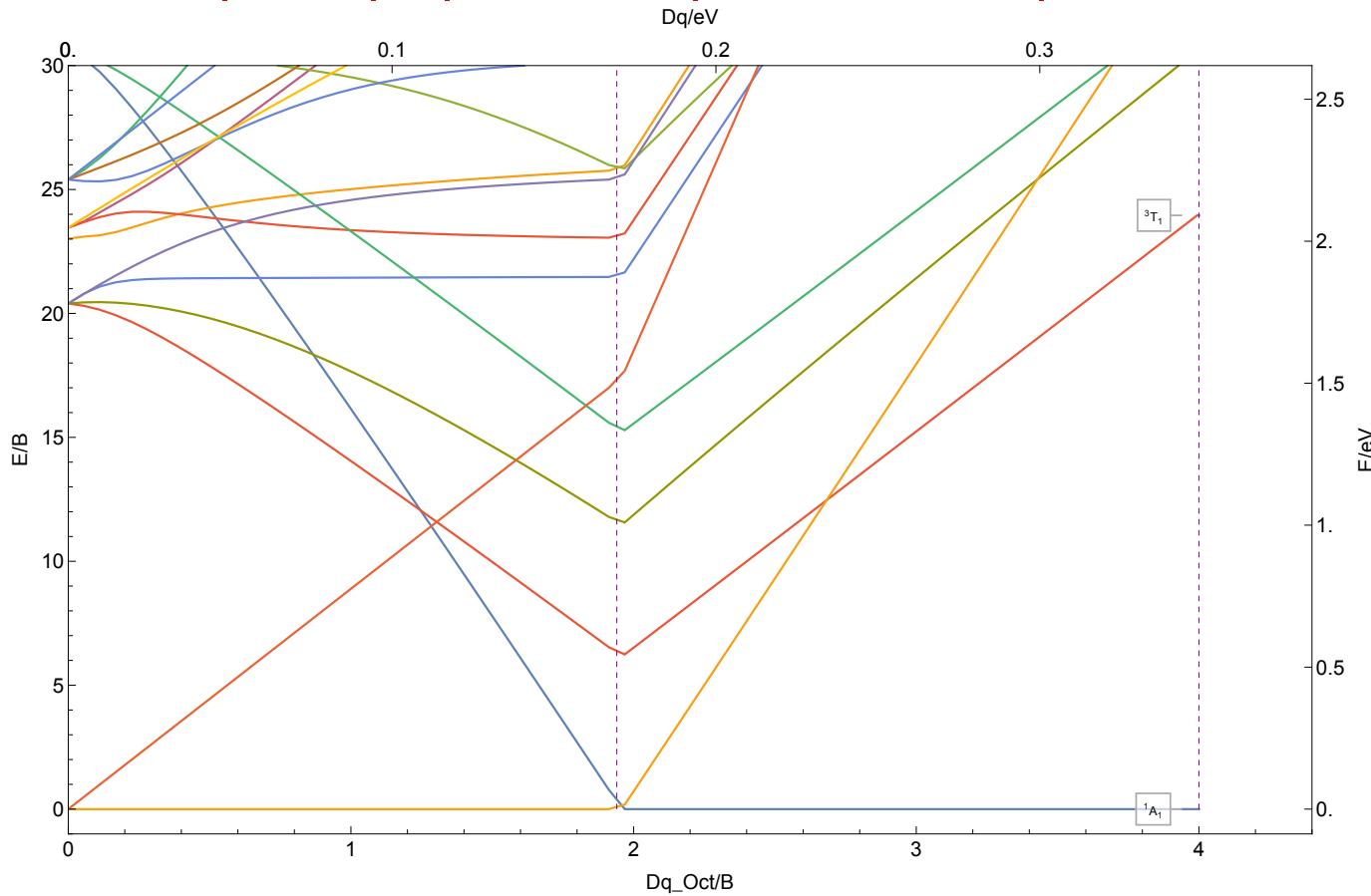
8.3.88 Os<sup>3+</sup>

|2,4,6| d<sup>5</sup>| C/B ≈ 4.1| B ≈ 672 cm<sup>-1</sup> | Os<sup>3+</sup>



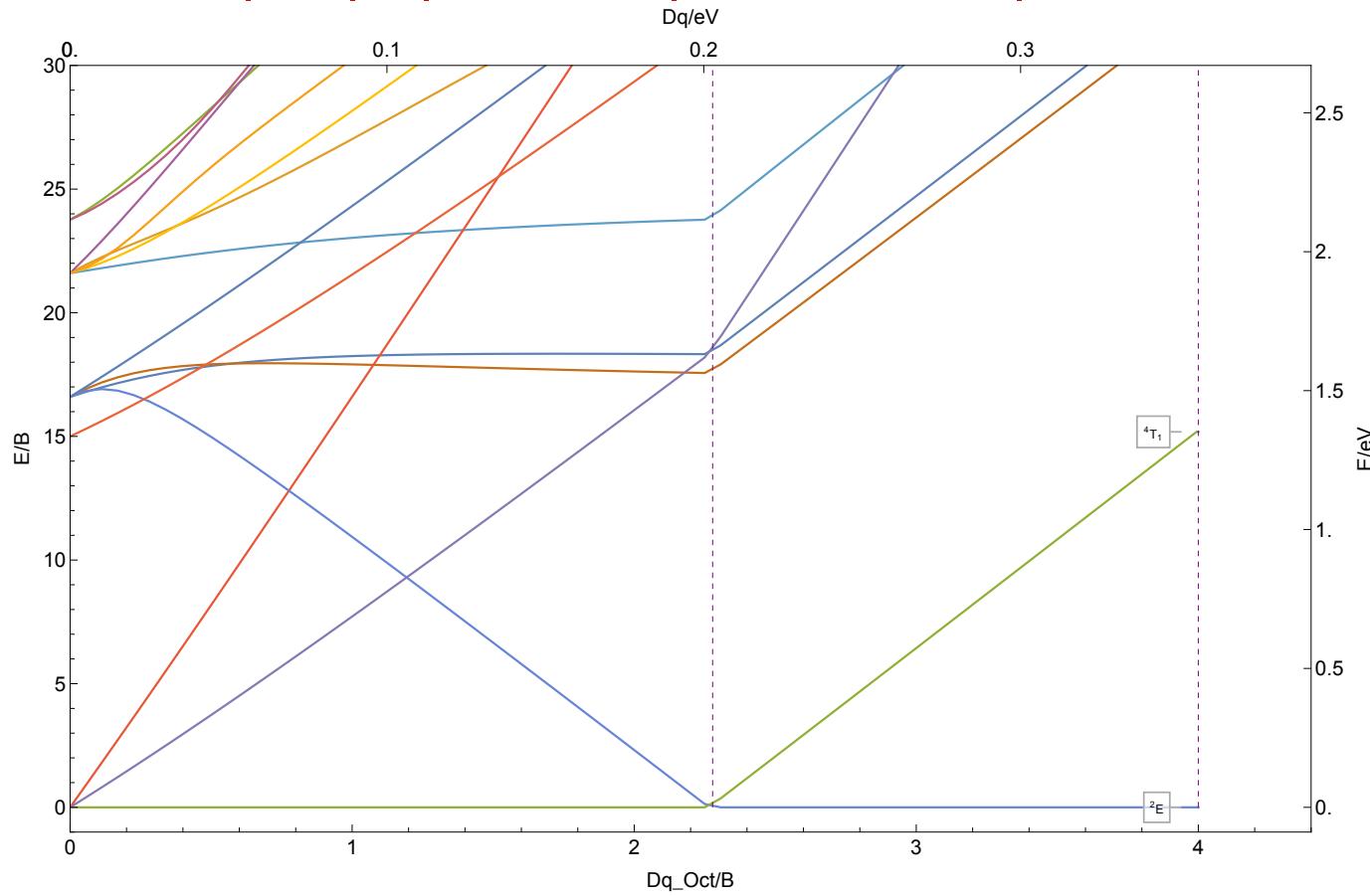
8.3.89 Os<sup>4+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 4.1 | B ≈ 704 cm<sup>-1</sup> | Os<sup>4+</sup>



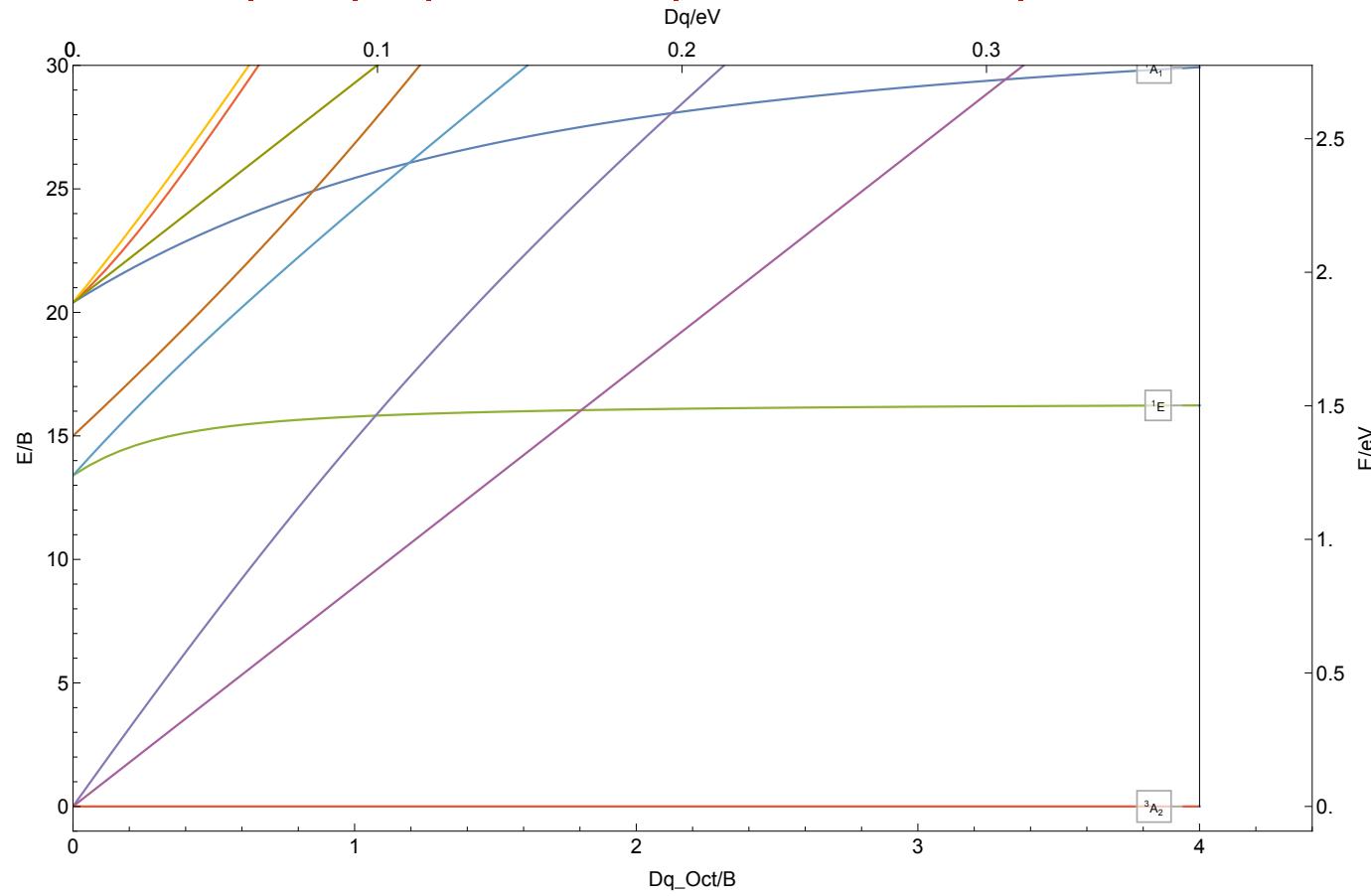
8.3.90 Os<sup>5+</sup>

$$|2,4|d^3|C/B \approx 4.2|B \approx 718\text{ cm}^{-1}|Os^{5+}$$



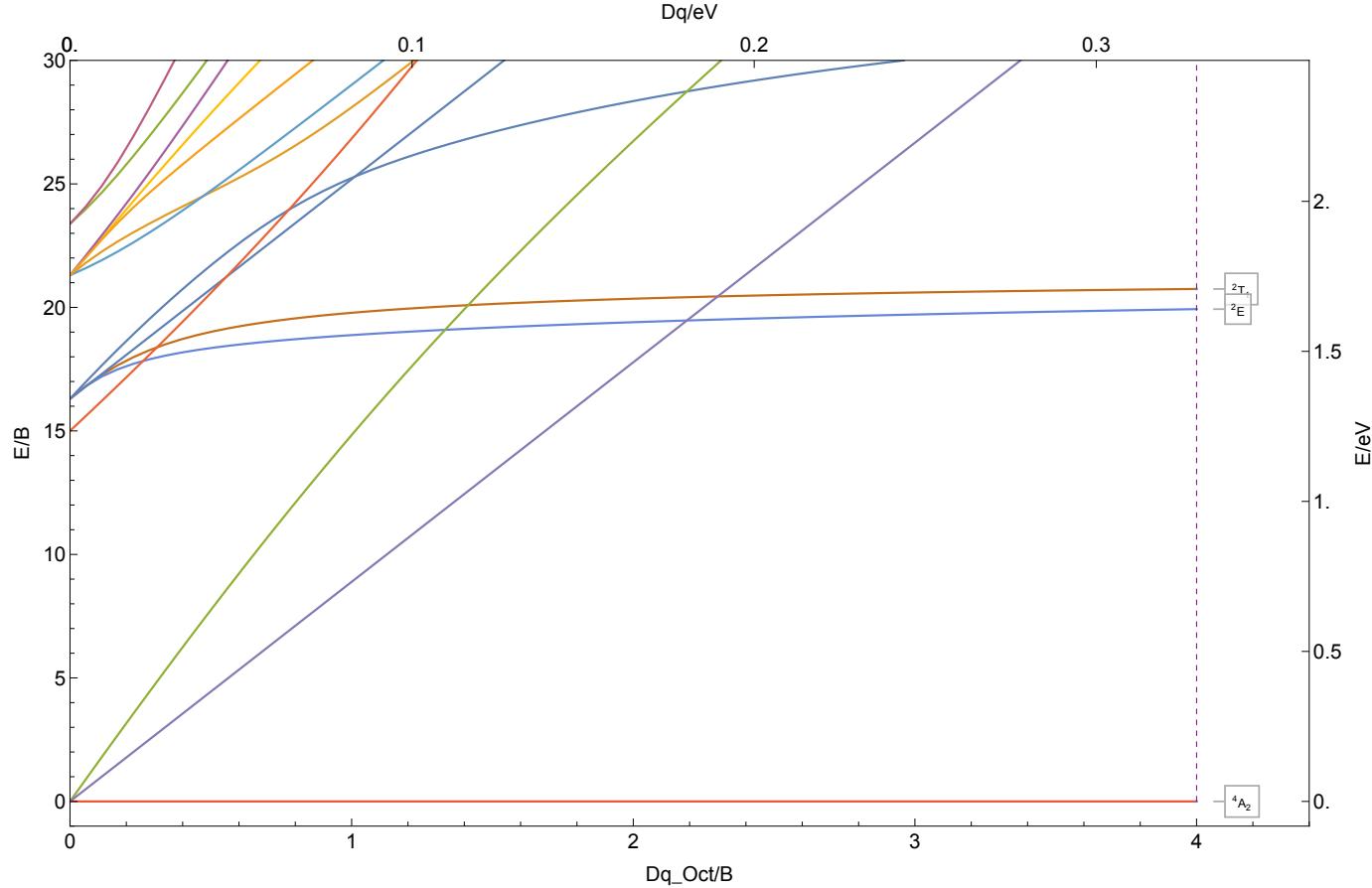
8.3.91 Os<sup>6+</sup>

| 1,3 | d<sup>2</sup> | C/B ≈ 4.2 | B ≈ 746 cm<sup>-1</sup> | Os<sup>6+</sup>



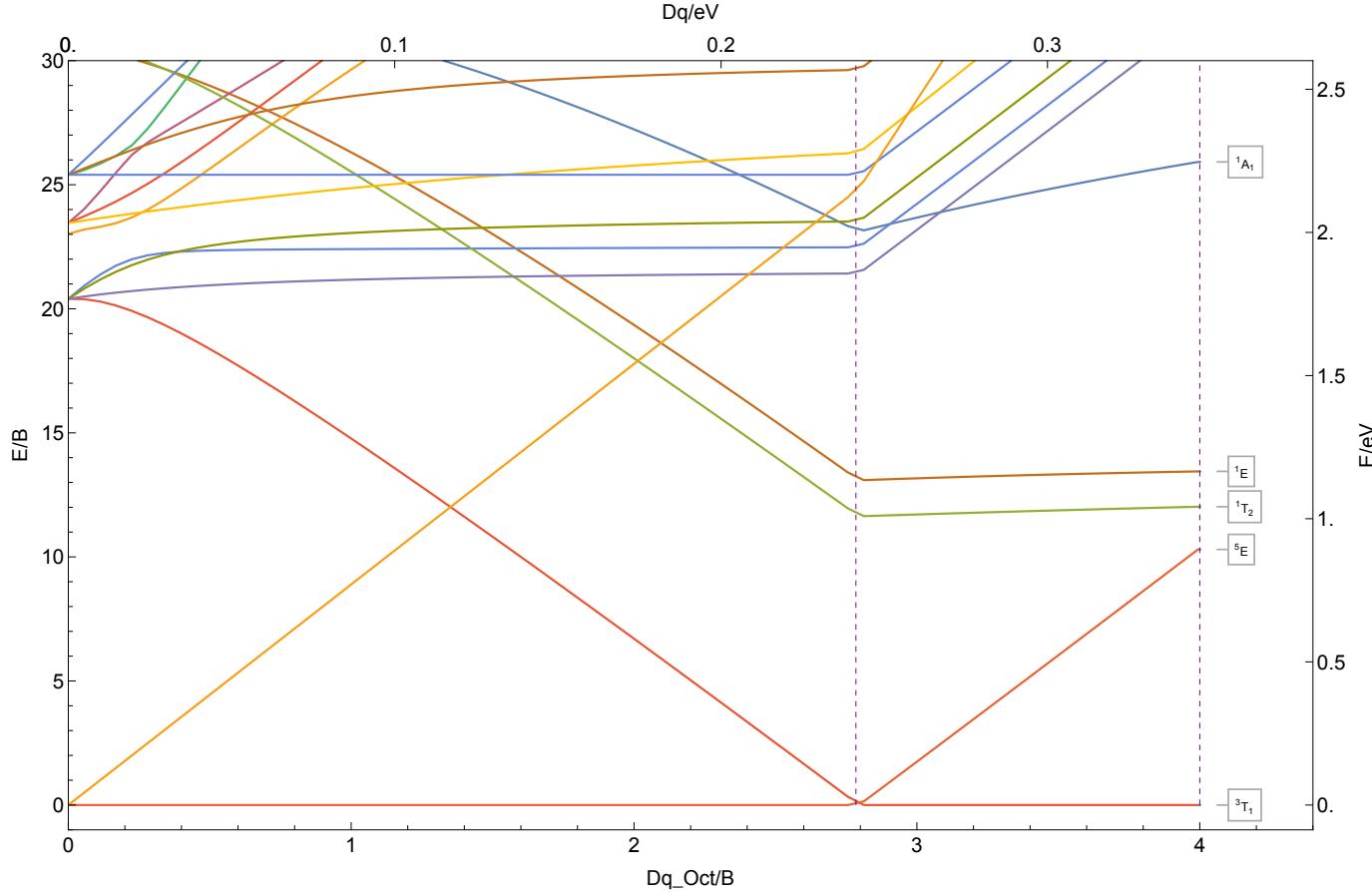
8.3.92 Ir<sup>2+</sup>

|2,4|d<sup>7</sup>| C/B ≈ 4.1 | B ≈ 664 cm<sup>-1</sup> | Ir<sup>2+</sup>



8.3.93  $\text{Ir}^{3+}$

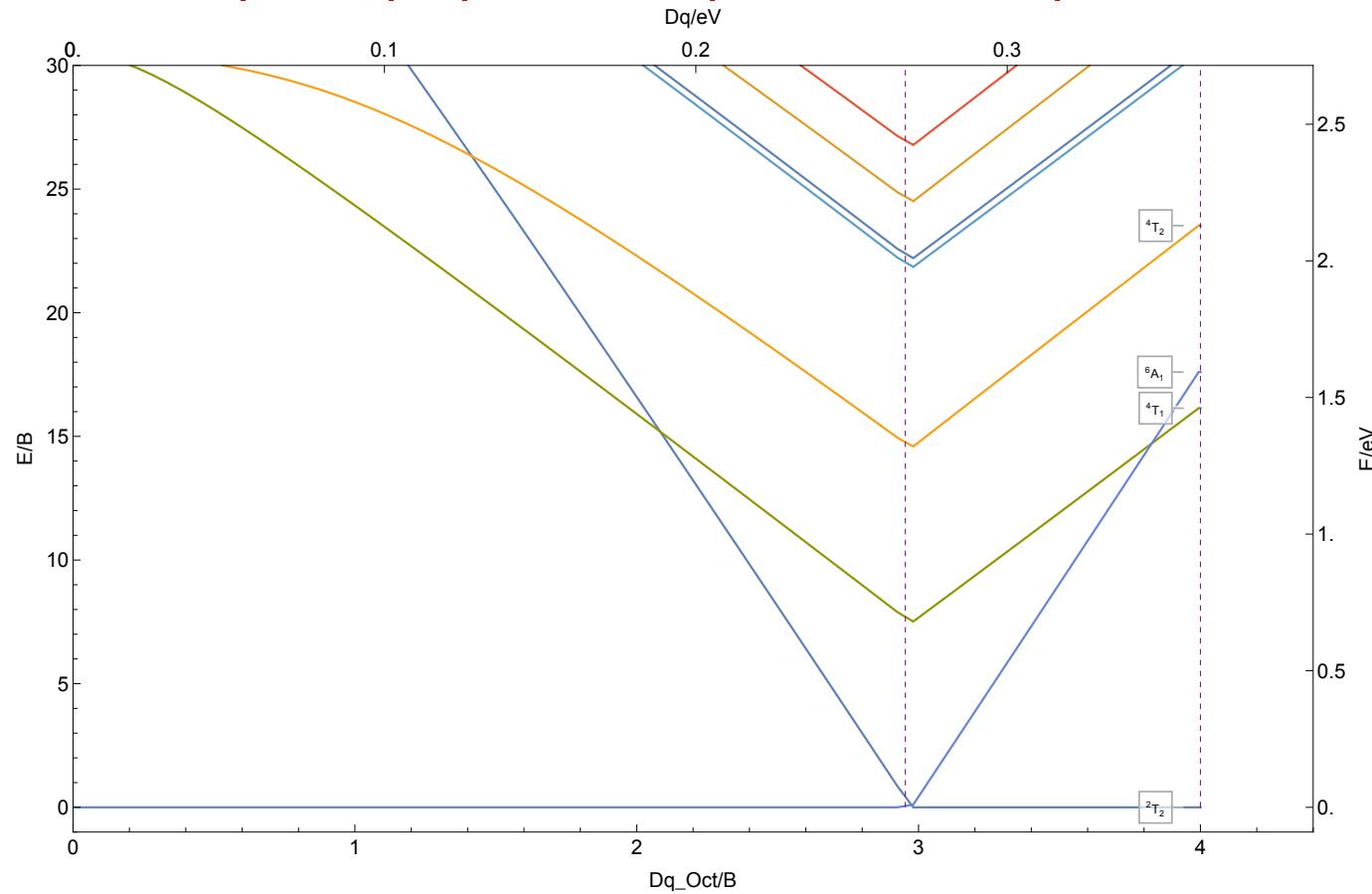
$|1,3,5|d^6|C/B \approx 4.1|B \approx 699 \text{ cm}^{-1}| \text{Ir}^{3+}$



8.3.94 Ir<sup>4+</sup>

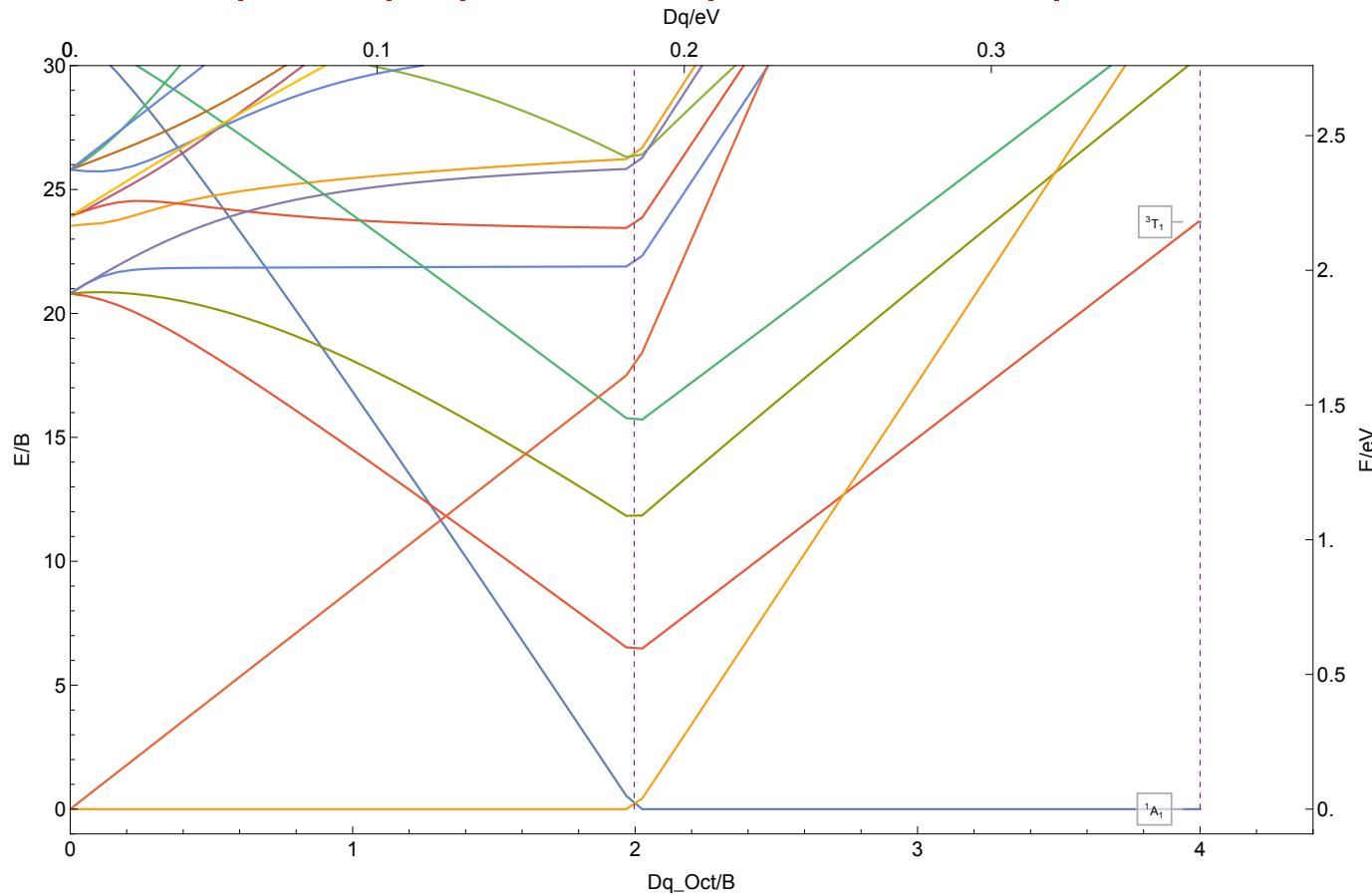
|2,4,6|d<sup>5</sup>| C/B ≈ 4.1| B ≈ 730 cm<sup>-1</sup> |Ir<sup>4+</sup>

EF



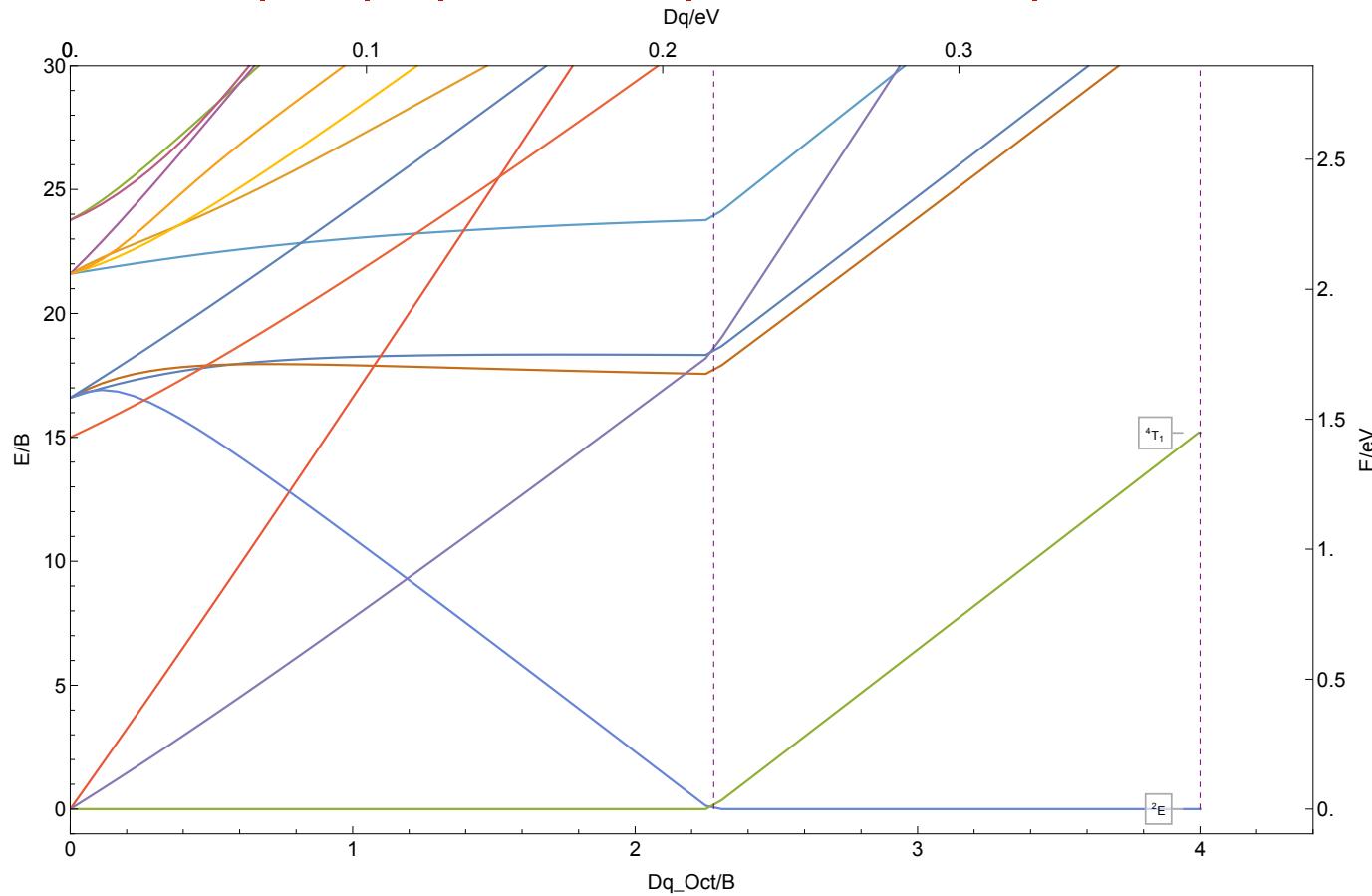
8.3.95  $\text{Ir}^{5+}$

$|1,3,5|d^4|C/B \approx 4.2|B \approx 742 \text{ cm}^{-1}| \text{Ir}^{5+}$



8.3.96  $\text{Ir}^{6+}$

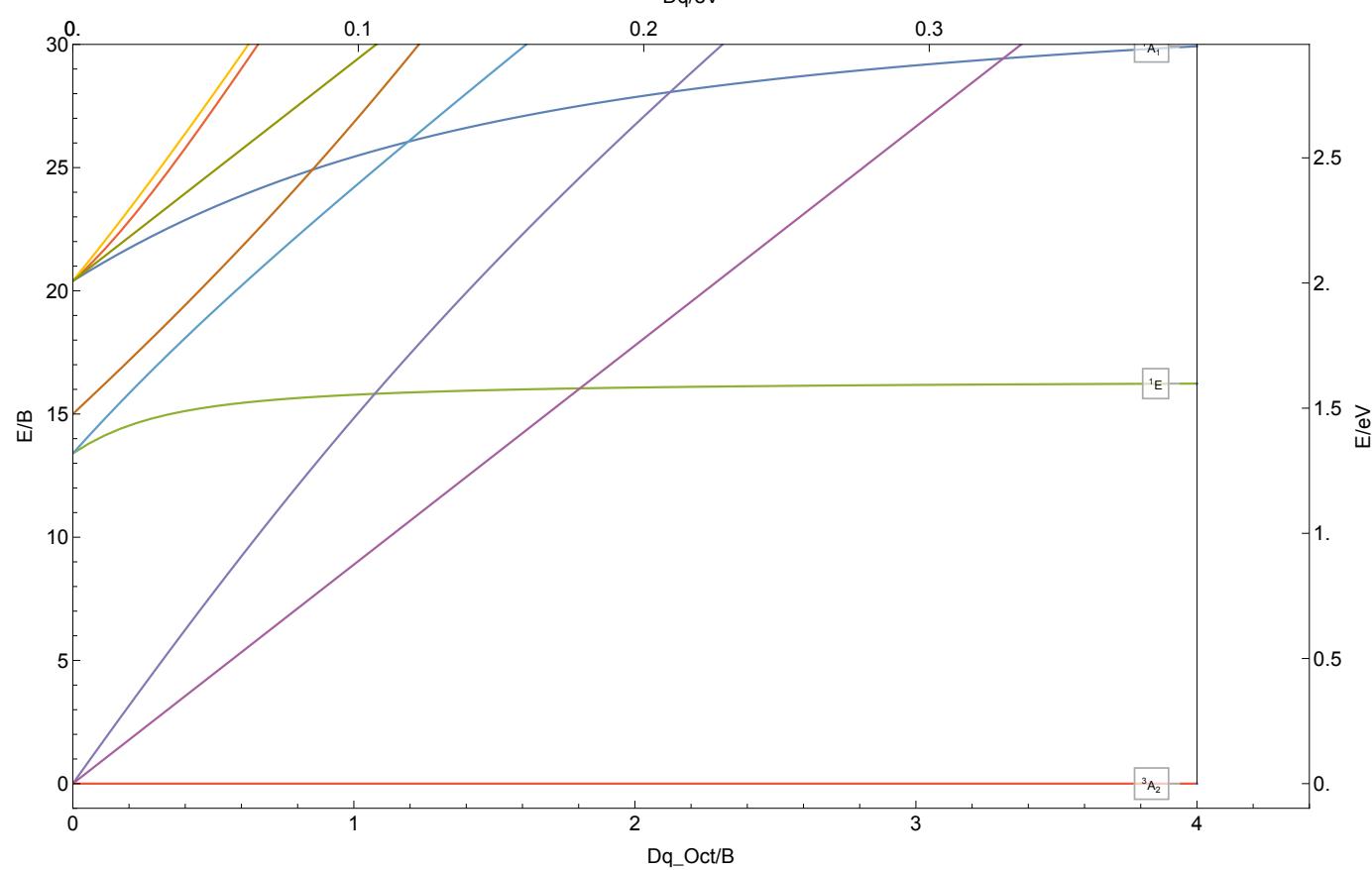
$|2,4|d^3|C/B \approx 4.2|B \approx 769 \text{ cm}^{-1}| \text{Ir}^{6+}$



8.3.97 Ir<sup>7+</sup>

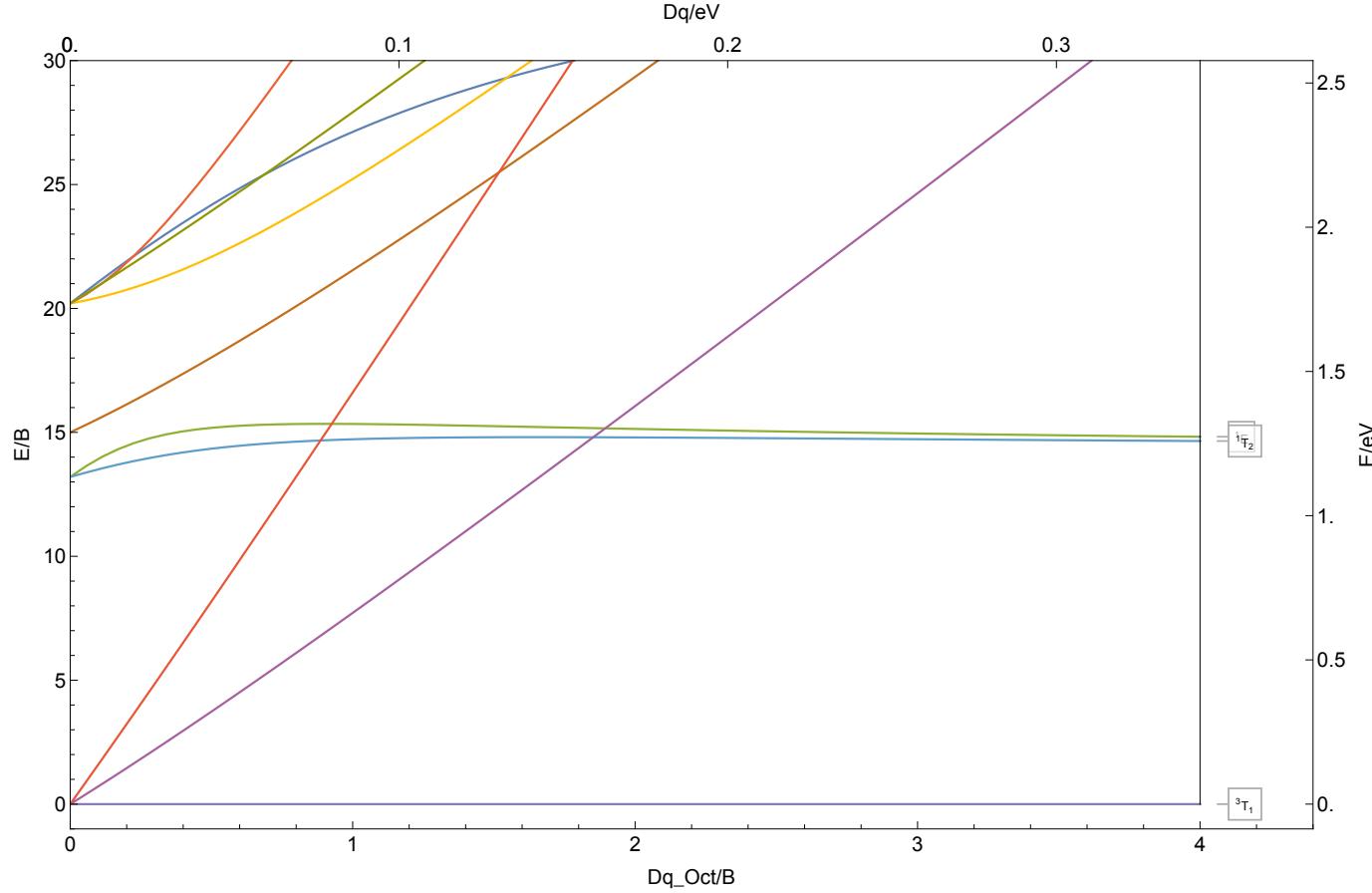
| 1,3 | d<sup>2</sup> | C/B ≈ 4.2 | B ≈ 794 cm<sup>-1</sup> | Ir<sup>7+</sup>

0.2



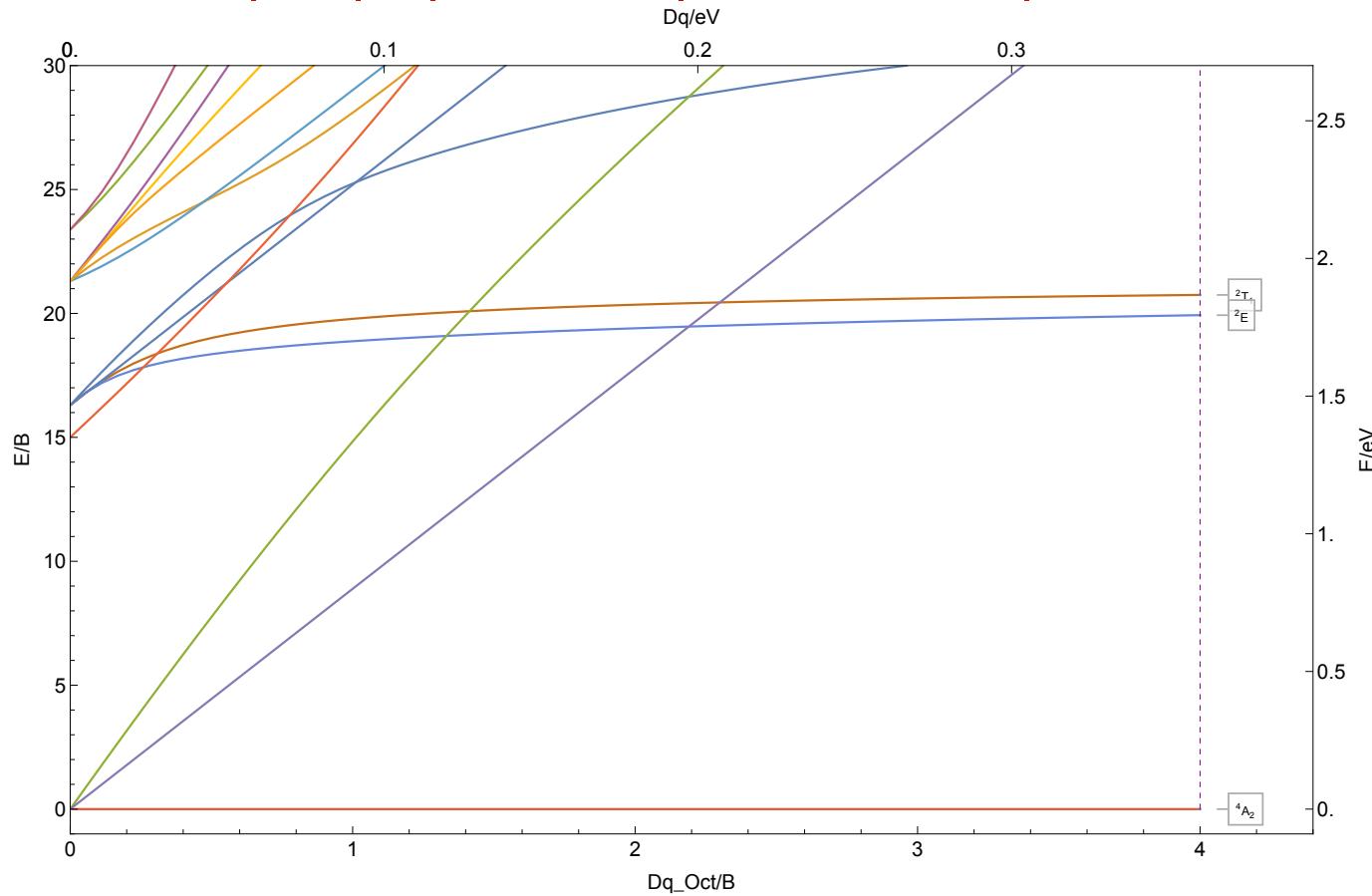
8.3.98 Pt<sup>2+</sup>

| 1,3 | d<sup>8</sup> | C/B ≈ 4.1 | B ≈ 693 cm<sup>-1</sup> | Pt<sup>2+</sup>



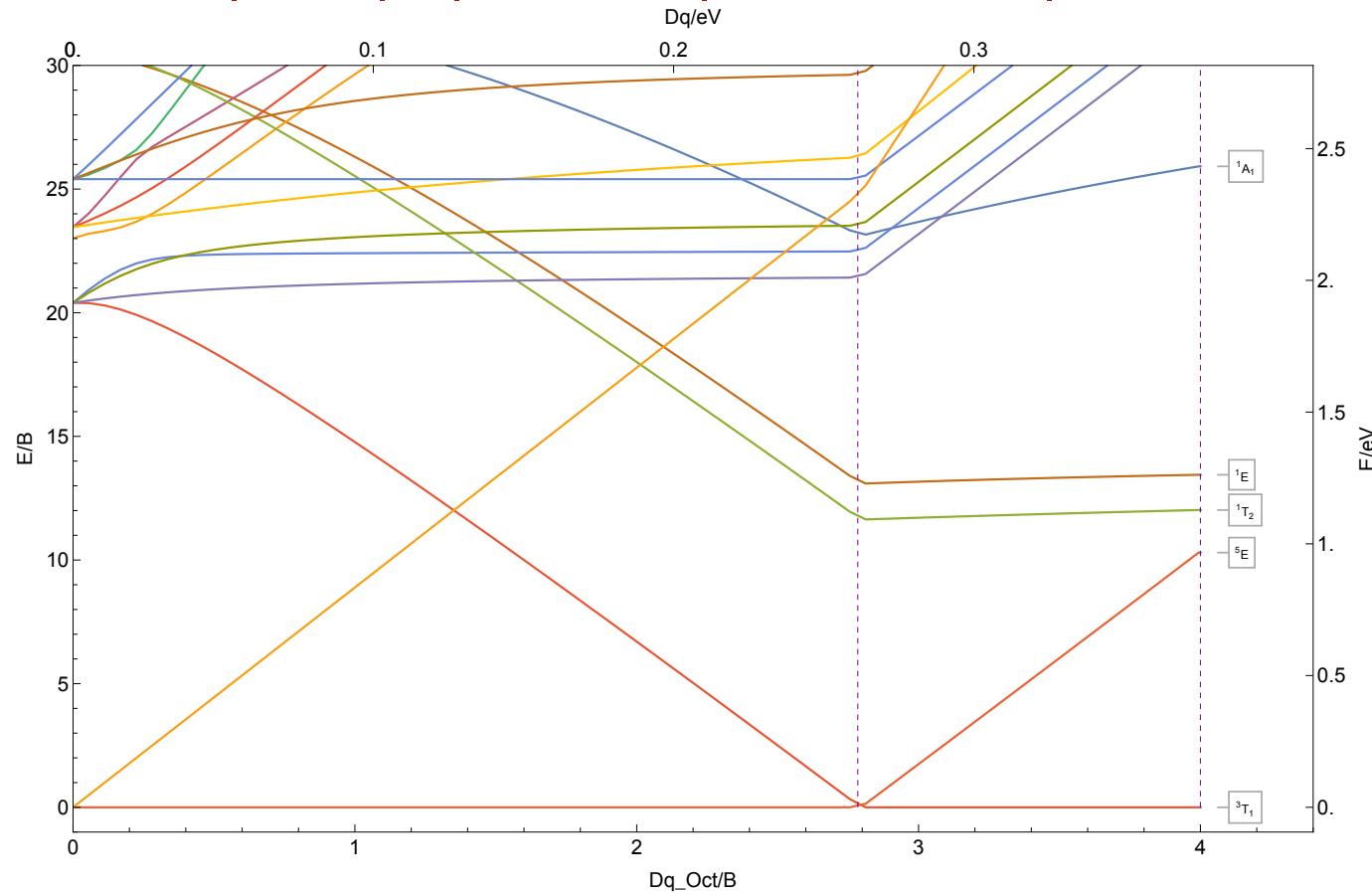
8.3.99 Pt<sup>3+</sup>

|2,4|d<sup>7</sup>|C/B ≈ 4.1|B ≈ 726 cm<sup>-1</sup>|Pt<sup>3+</sup>



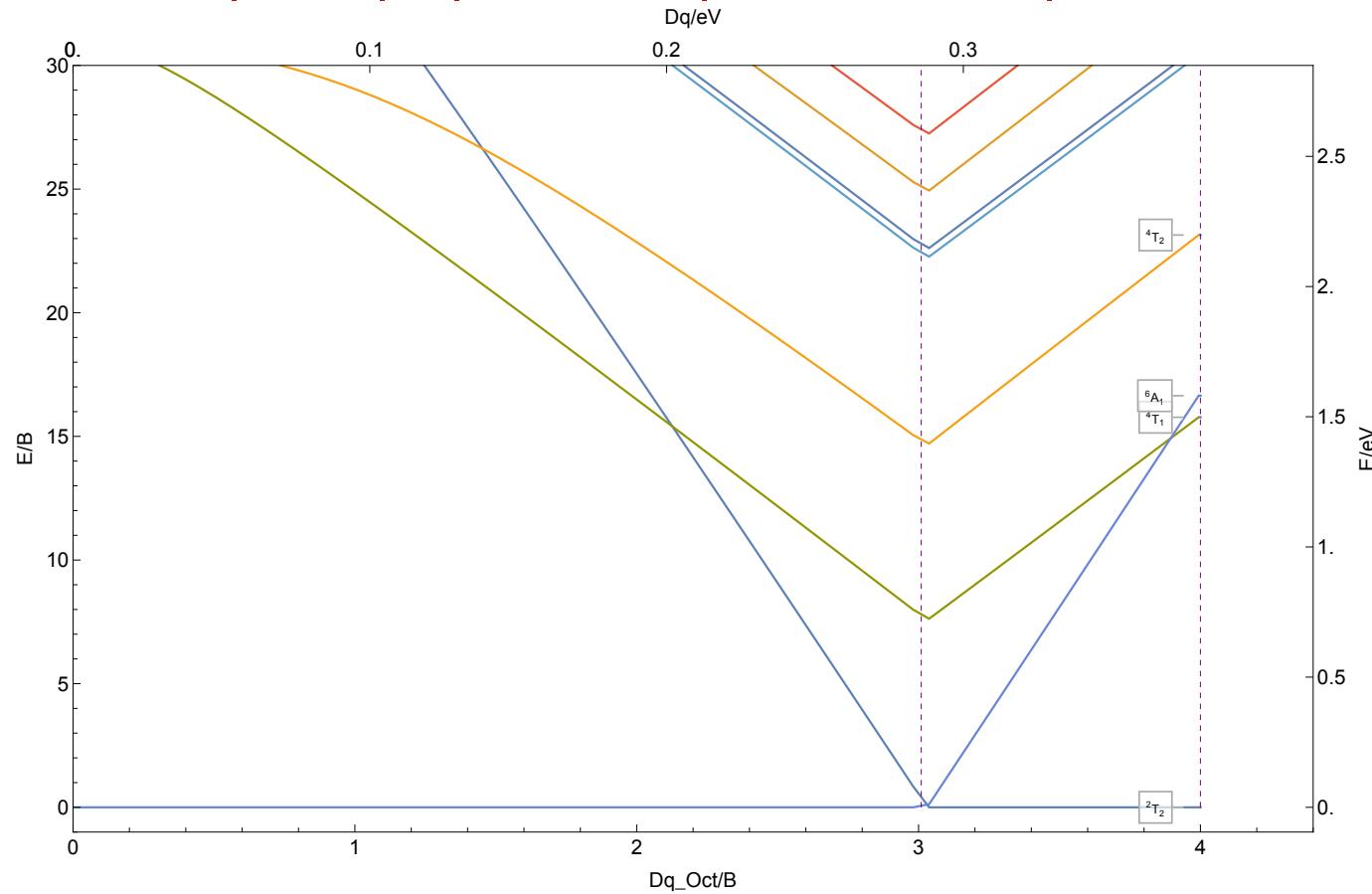
8.3.100 Pt<sup>4+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4.1 | B ≈ 757 cm<sup>-1</sup> | Pt<sup>4+</sup>



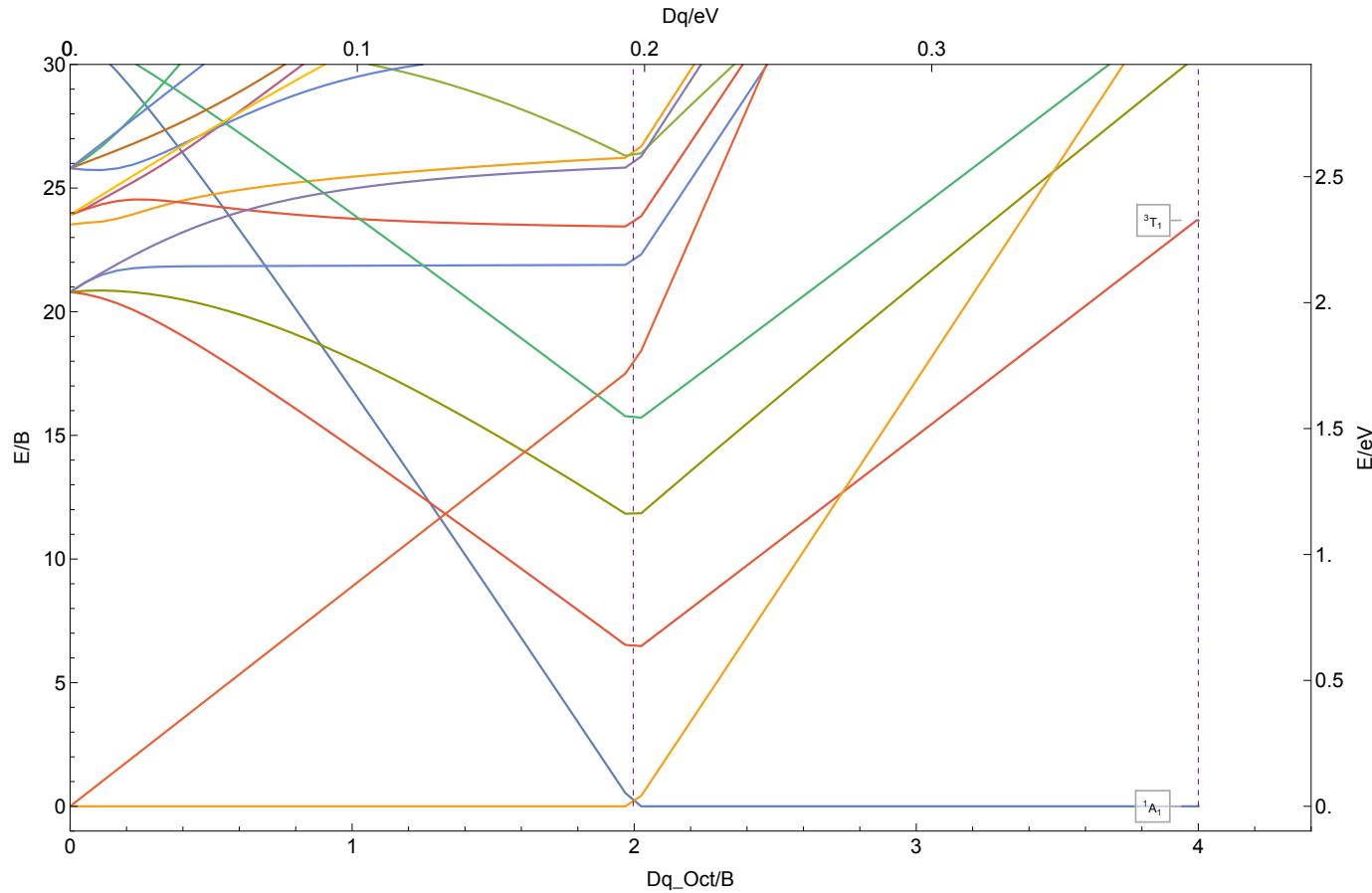
8.3.101 Pt<sup>5+</sup>

|2,4,6| d<sup>5</sup>| C/B ≈ 4.2| B ≈ 766 cm<sup>-1</sup> | Pt<sup>5+</sup>



8.3.102 Pt<sup>6+</sup>

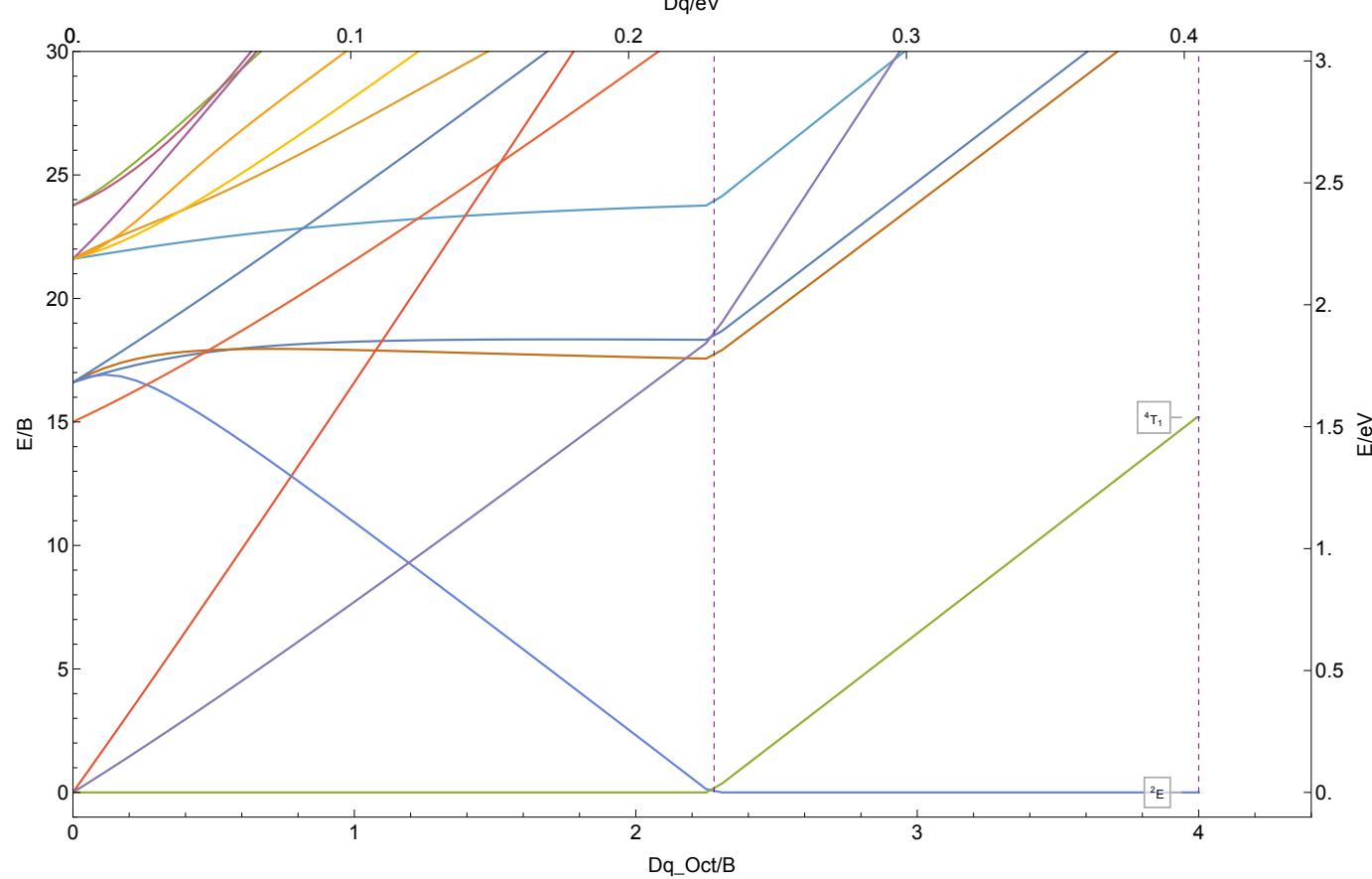
| 1,3,5 | d<sup>4</sup> | C/B ≈ 4.2 | B ≈ 792 cm<sup>-1</sup> | Pt<sup>6+</sup>



8.3.103 Pt<sup>7+</sup>

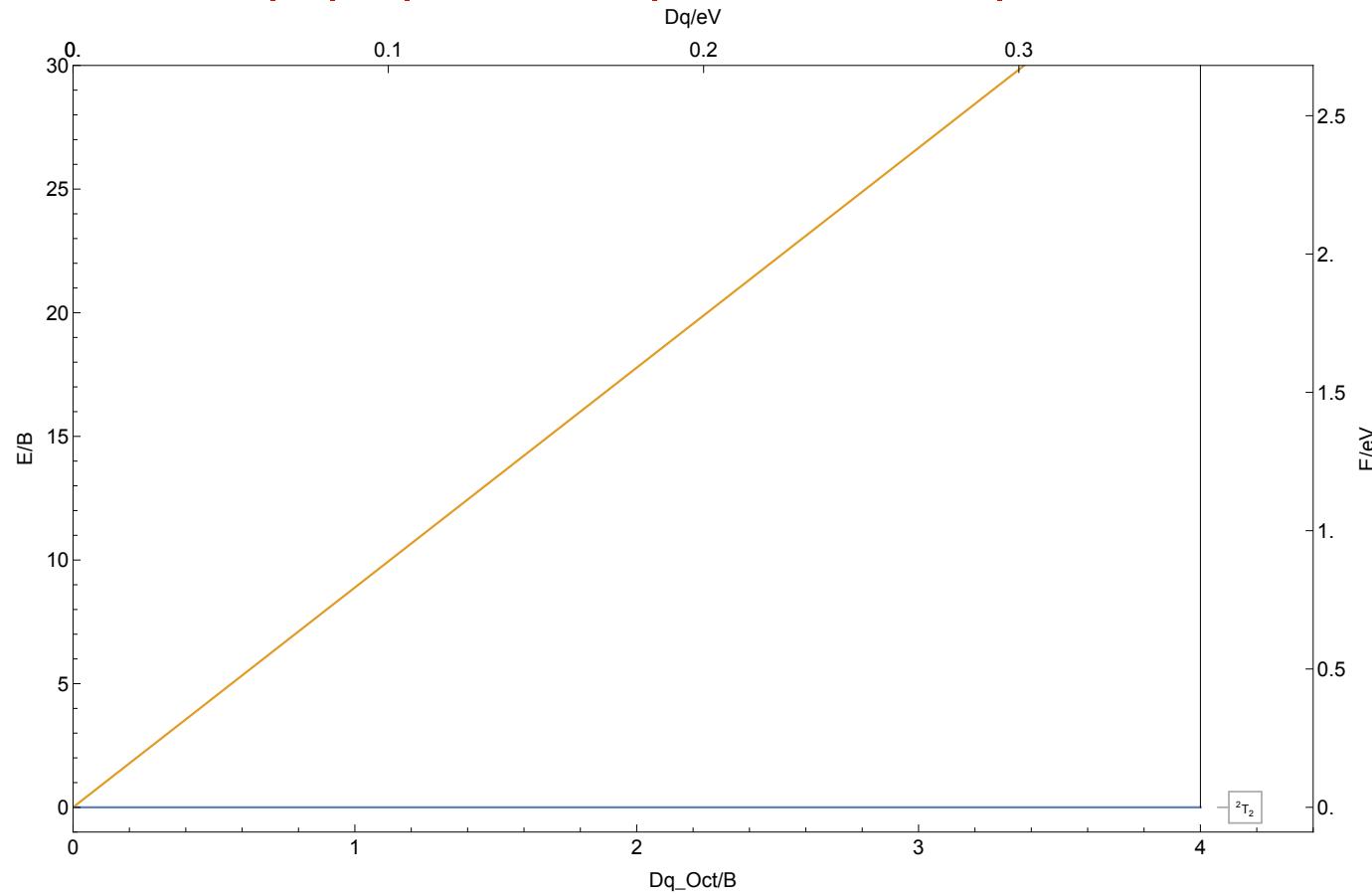
|2,4|d<sup>3</sup>|C/B ≈ 4.2|B ≈ 817 cm<sup>-1</sup>|Pt<sup>7+</sup>

953



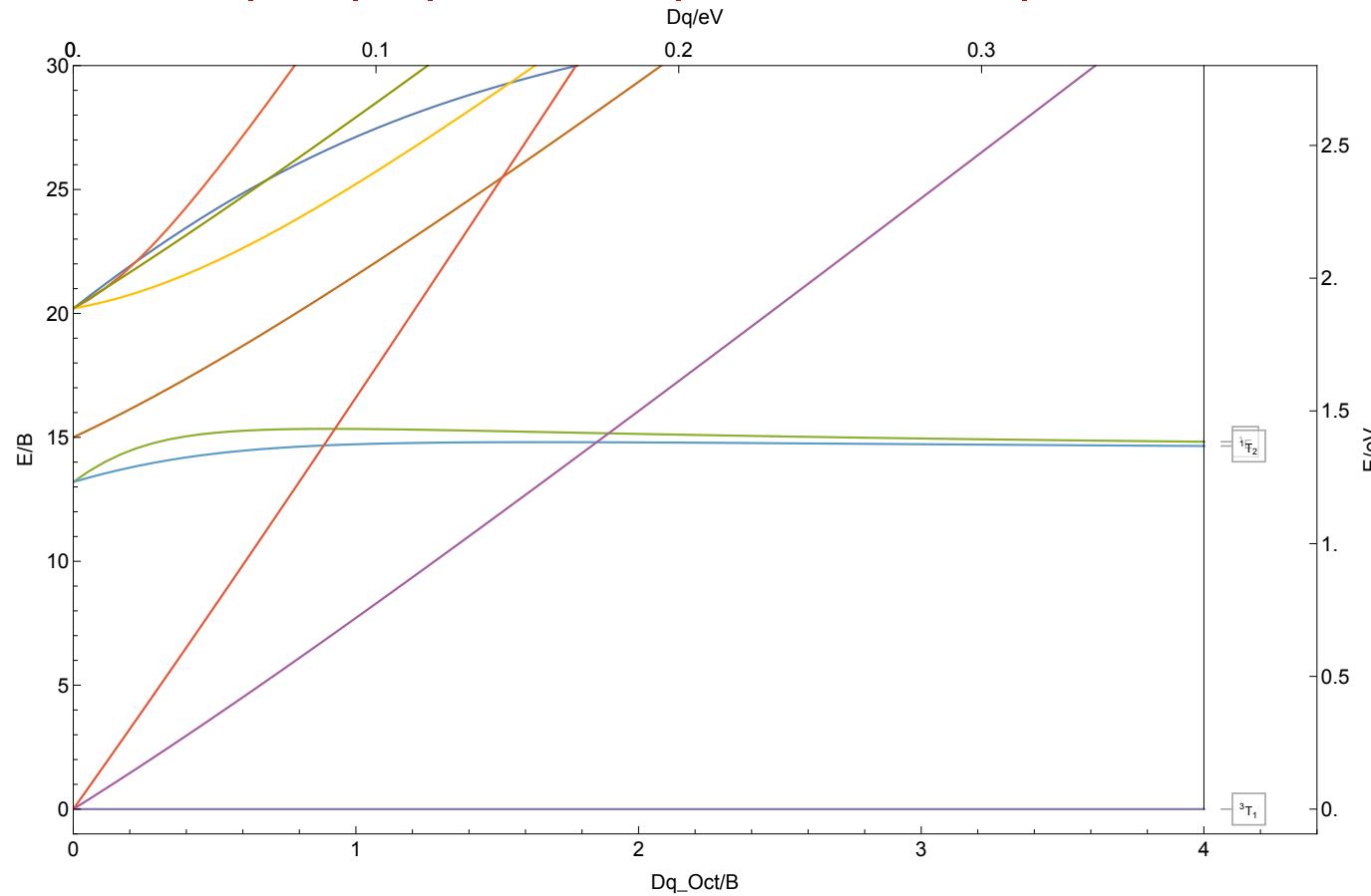
8.3.104  $\text{Au}^{2+}$

$|2|d^9|C/B \approx 4.1|B \approx 721\text{ cm}^{-1}| \text{Au}^{2+}$



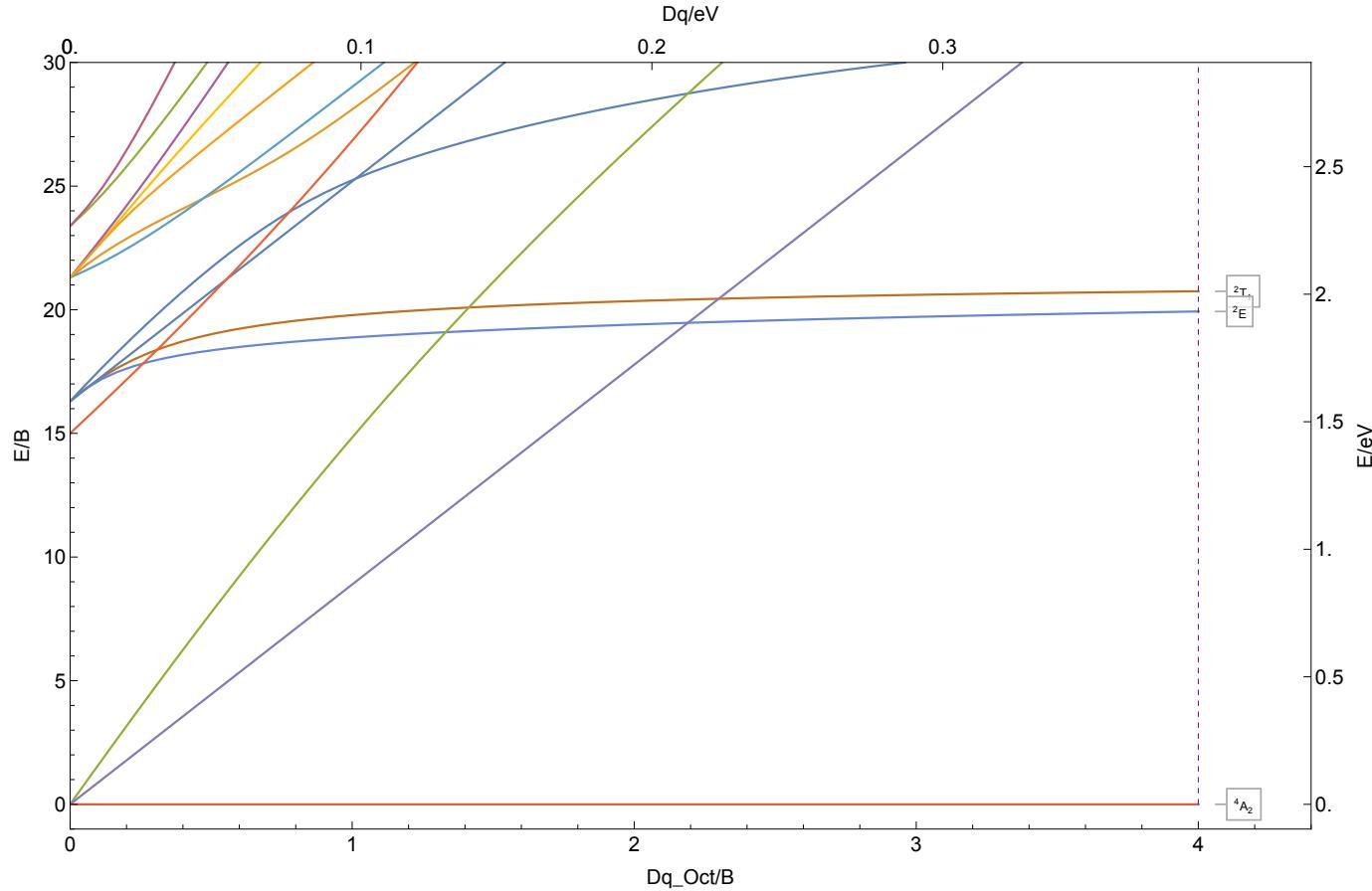
8.3.105 Au<sup>3+</sup>

| 1,3 | d<sup>8</sup> | C/B ≈ 4.1 | B ≈ 753 cm<sup>-1</sup> | Au<sup>3+</sup>



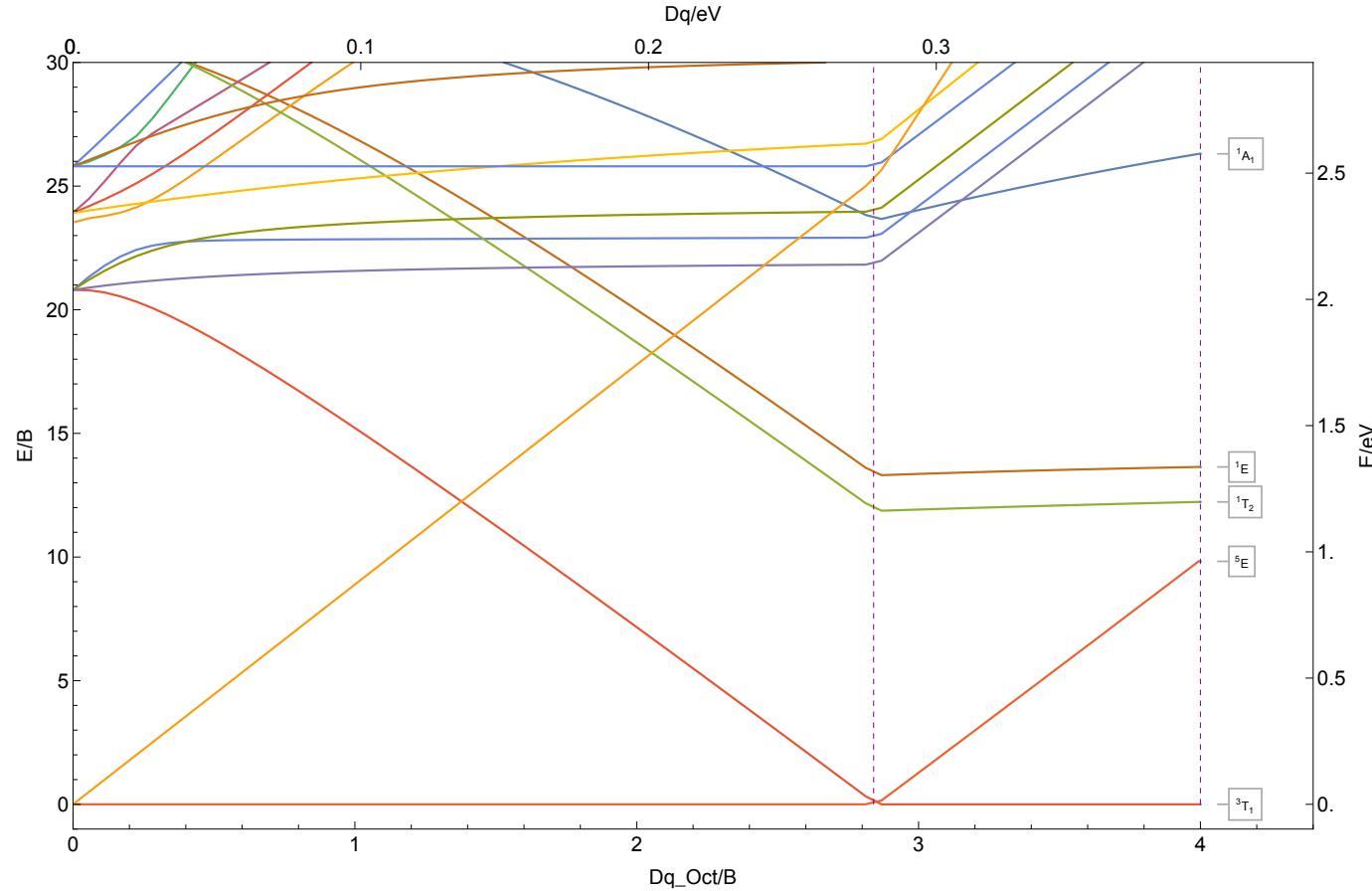
### 8.3.106 Au<sup>4+</sup>

|2,4|d<sup>7</sup>| C/B ≈ 4.1| B ≈ 782 cm<sup>-1</sup> |Au<sup>4+</sup>



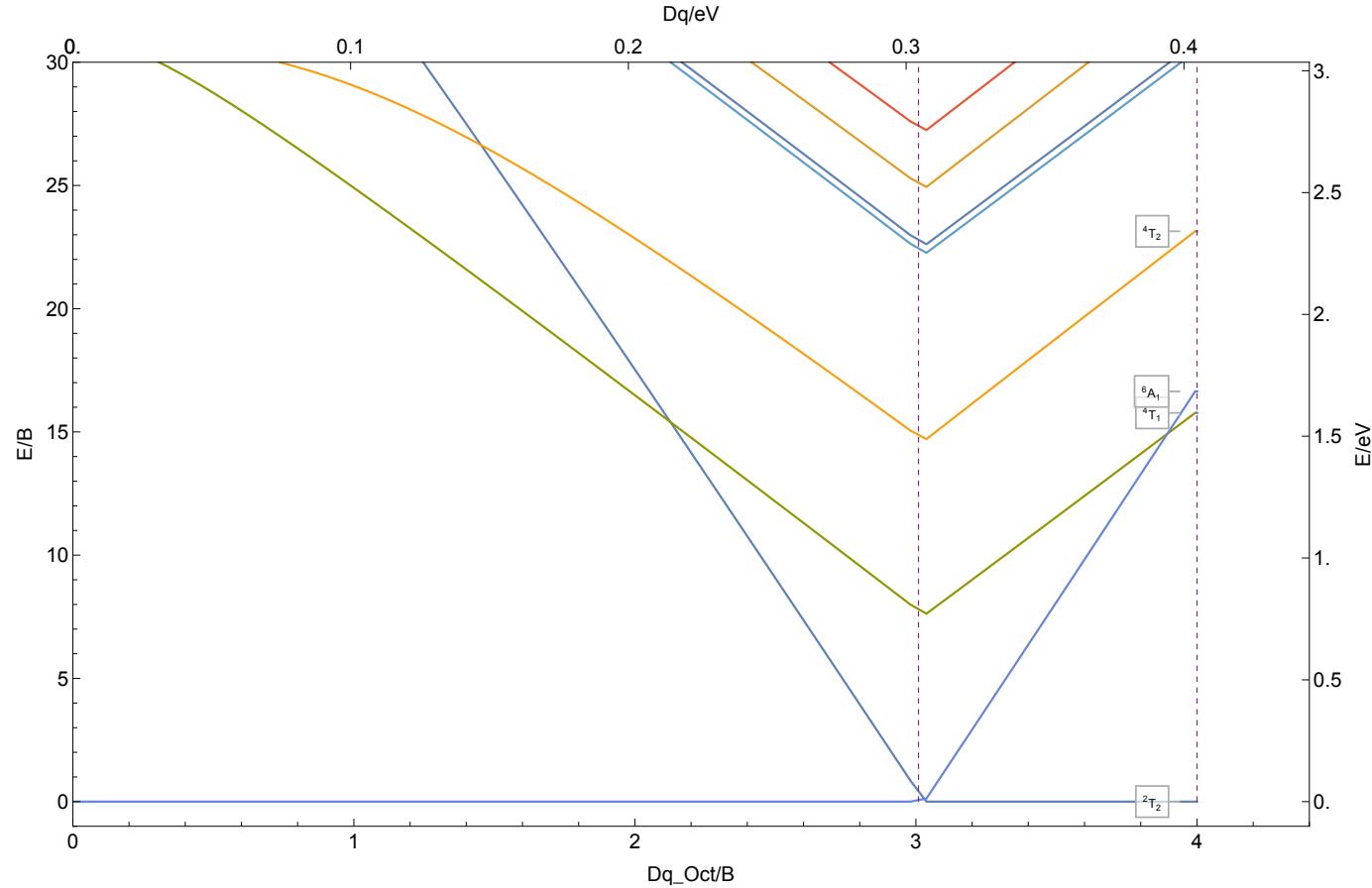
8.3.107 Au<sup>5+</sup>

| 1,3,5 | d<sup>6</sup> | C/B ≈ 4.2 | B ≈ 790 cm<sup>-1</sup> | Au<sup>5+</sup>



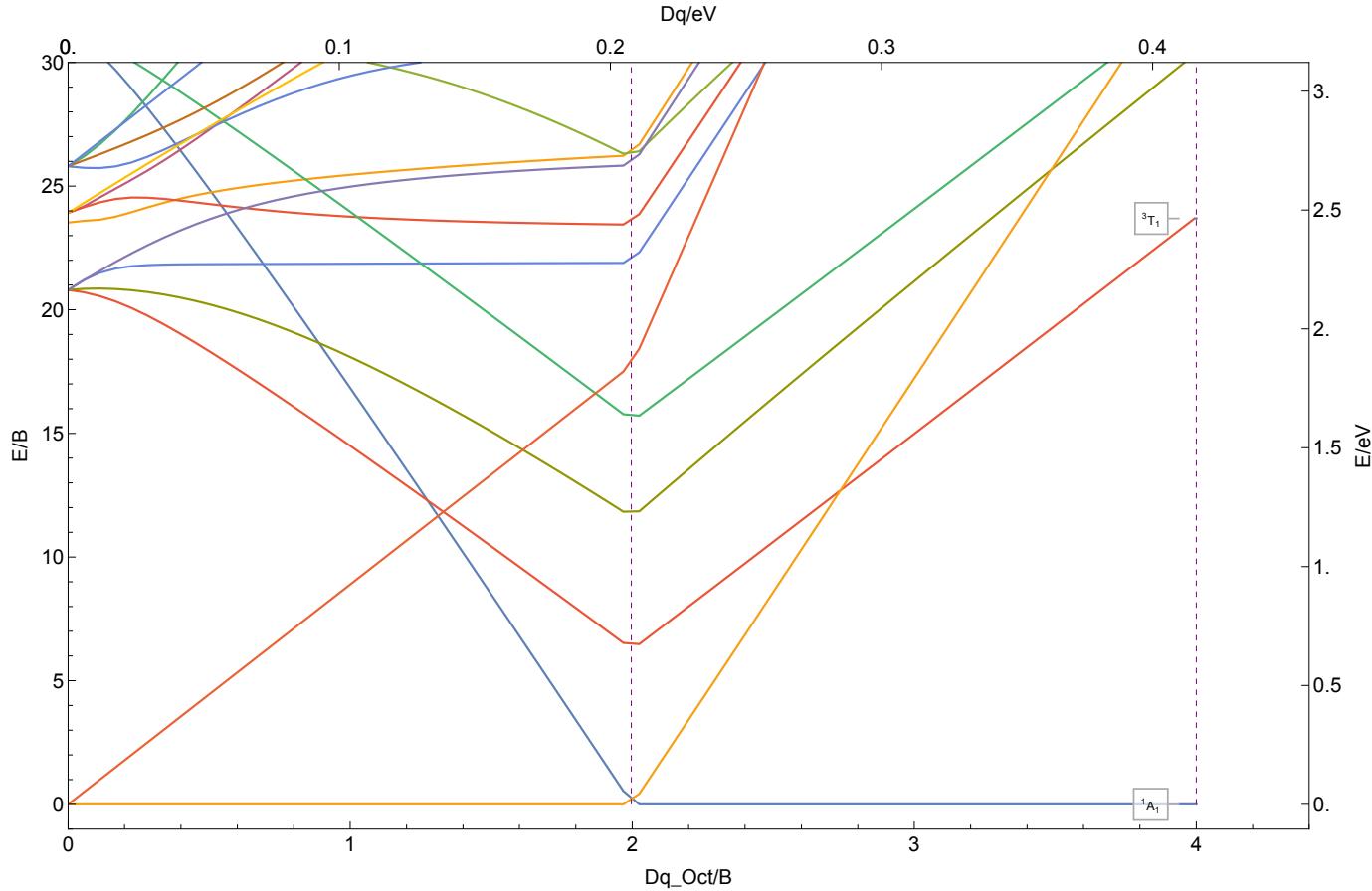
8.3.108 Au<sup>6+</sup>

|2,4,6| d<sup>5</sup>| C/B ≈ 4.2| B ≈ 816 cm<sup>-1</sup> |Au<sup>6+</sup>



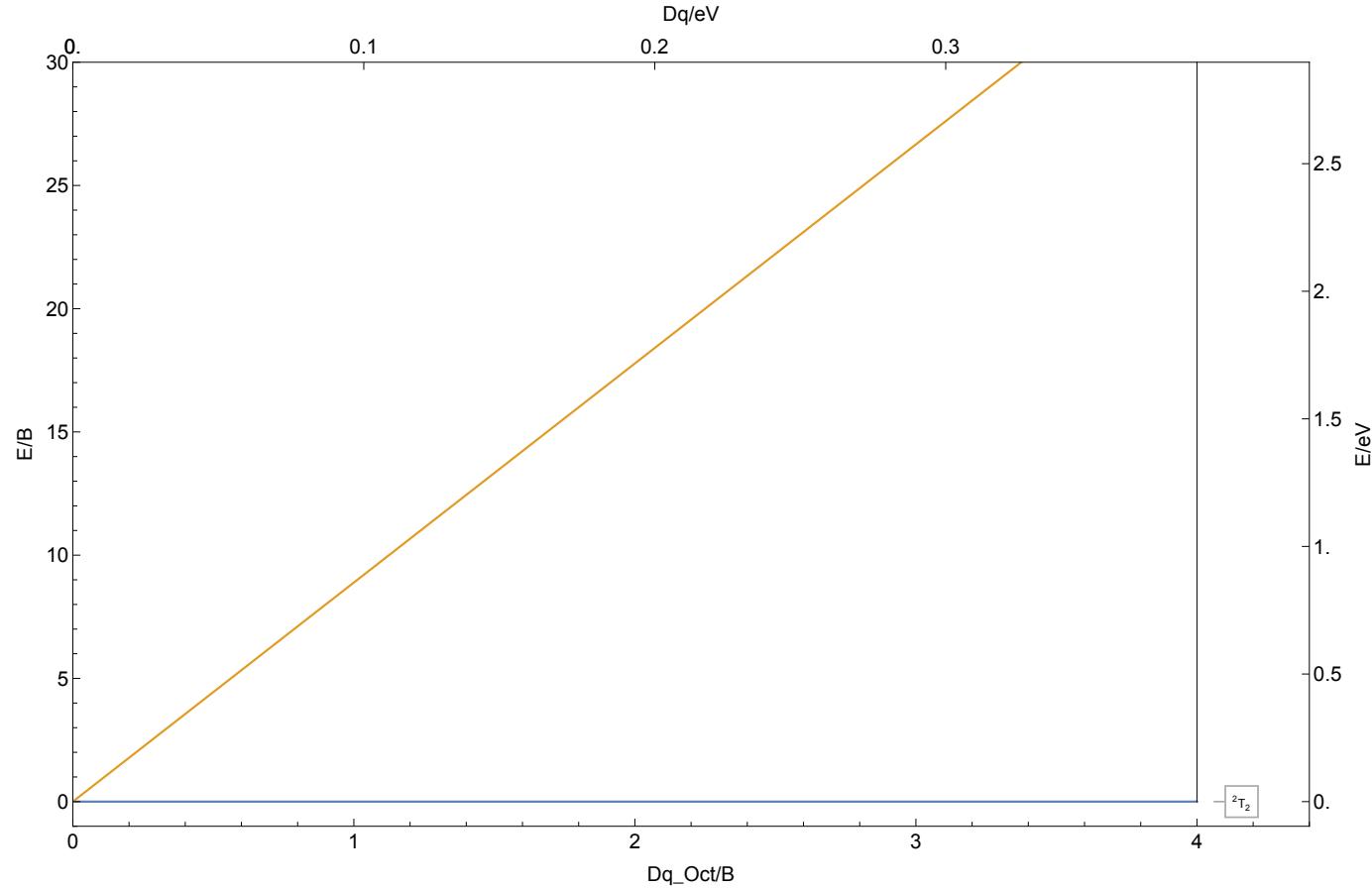
8.3.109 Au<sup>7+</sup>

| 1,3,5 | d<sup>4</sup> | C/B ≈ 4.2 | B ≈ 839 cm<sup>-1</sup> | Au<sup>7+</sup>



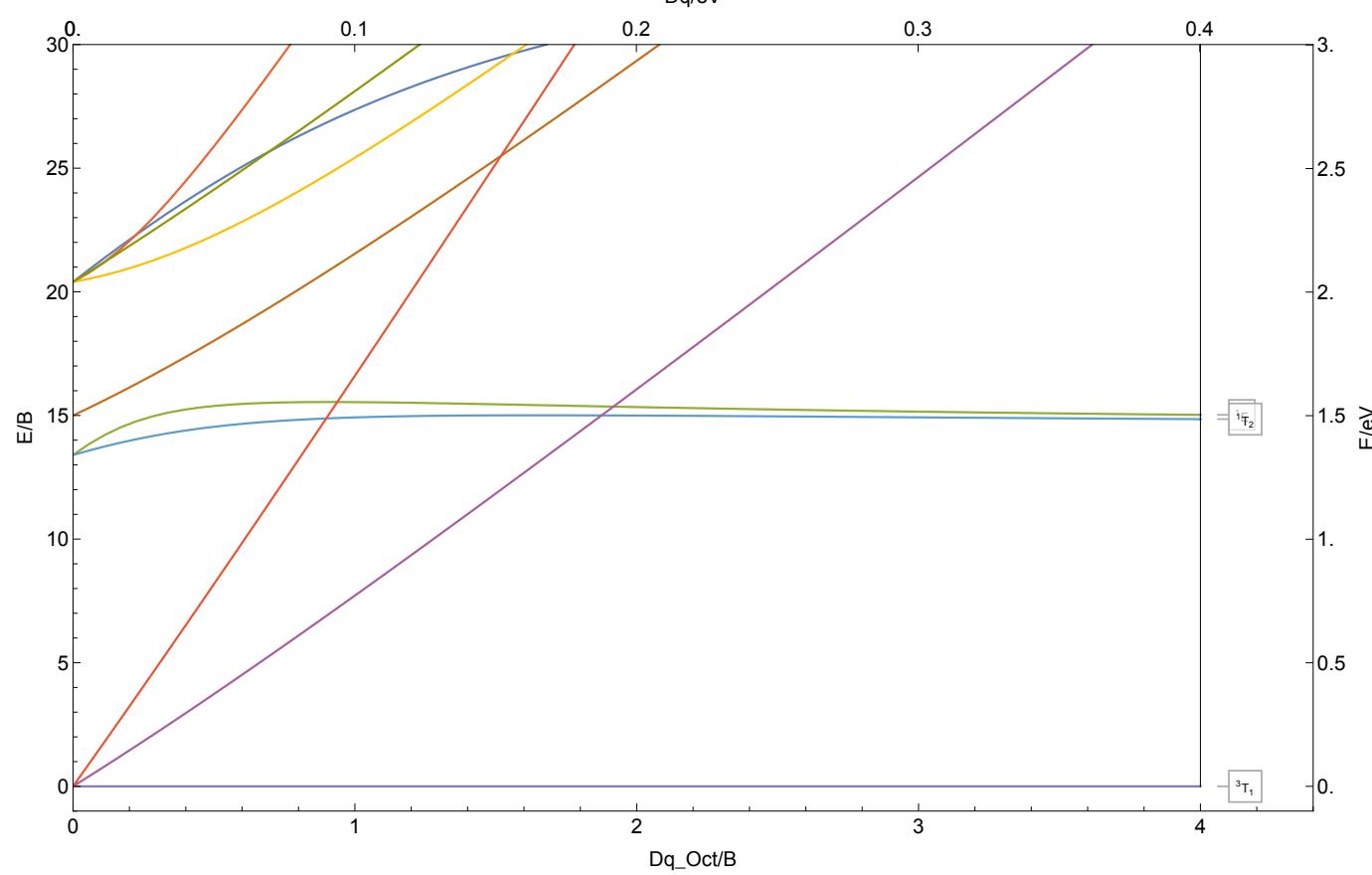
8.3.110 Hg<sup>3+</sup>

|2|d<sup>9</sup>|C/B ≈ 4.1|B ≈ 779 cm<sup>-1</sup>|Hg<sup>3+</sup>



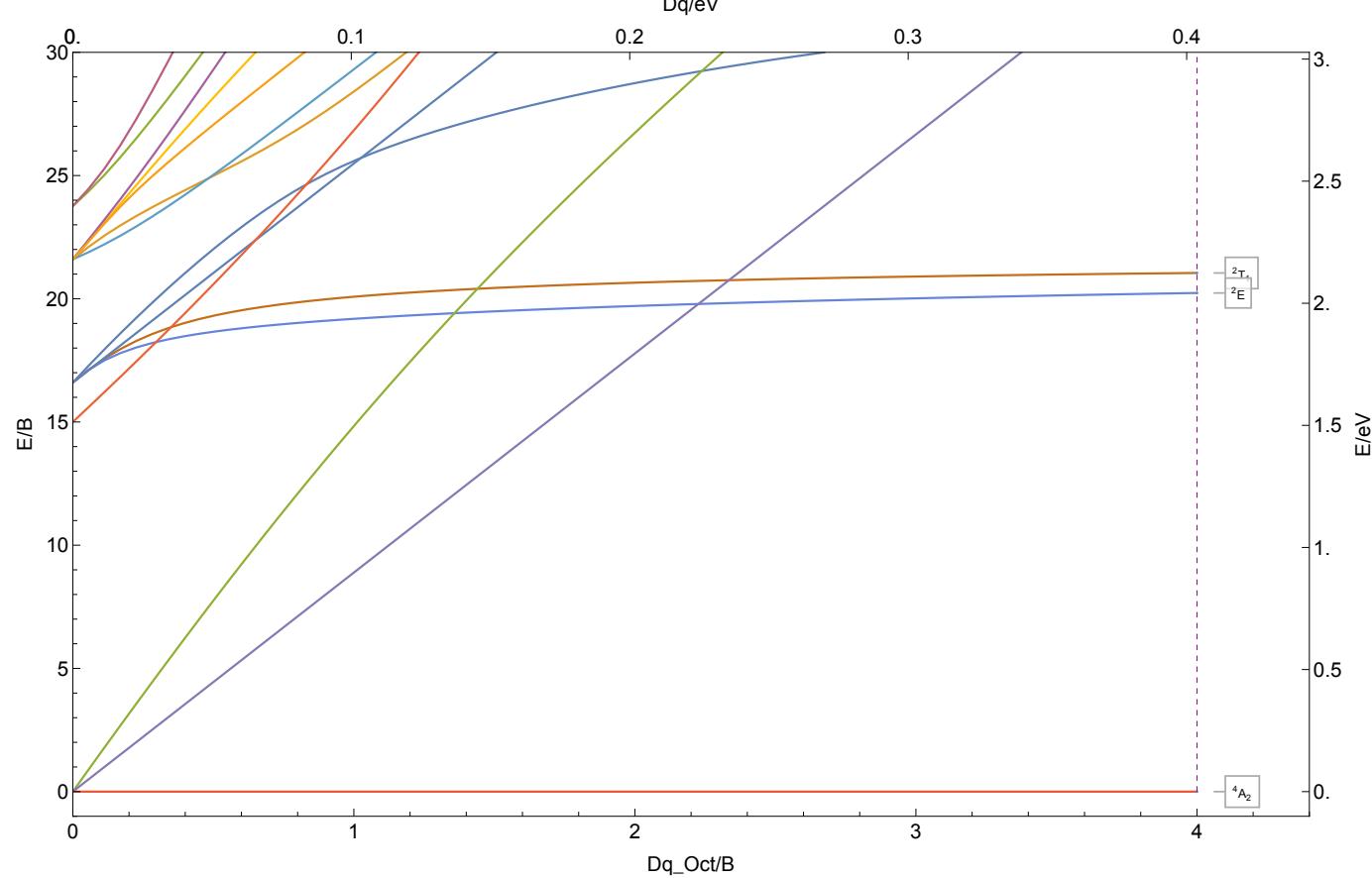
### 8.3.111 Hg<sup>4+</sup>

$|1,3|d^8|C/B \approx 4.2|B \approx 807\text{ cm}^{-1}|Hg^{4+}$



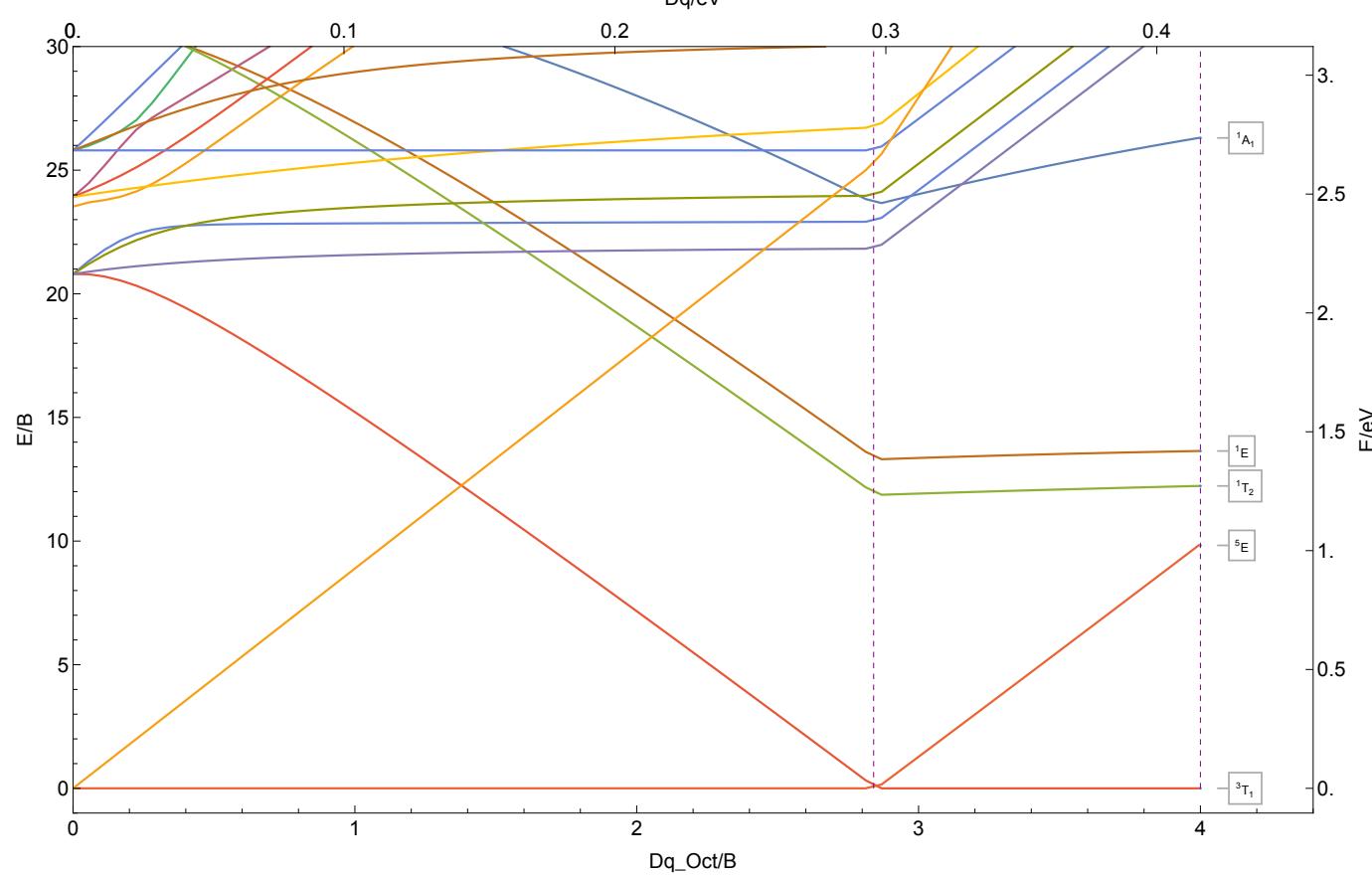
### 8.3.112 Hg<sup>5+</sup>

$|2,4|d^7|C/B \approx 4.2|B \approx 814\text{ cm}^{-1}|Hg^{5+}$



### 8.3.113 Hg<sup>6+</sup>

$|1,3,5|d^6| C/B \approx 4.2 | B \approx 839 \text{ cm}^{-1} | \text{Hg}^{6+}$



8.3.114 Hg<sup>7+</sup>

|2,4,6|d<sup>5</sup>| C/B ≈ 4.2 | B ≈ 862 cm<sup>-1</sup> | Hg<sup>7+</sup>

