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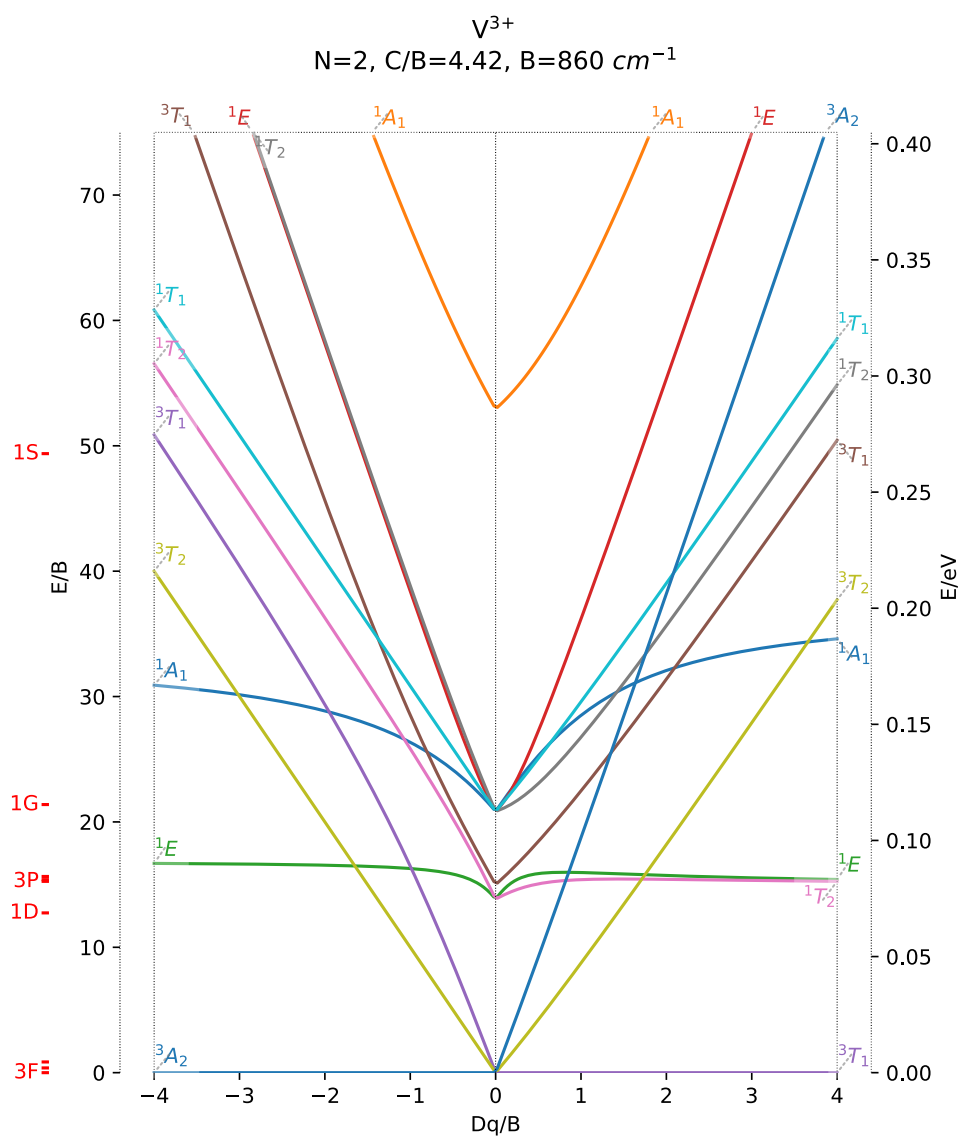
Data used for creating this figures can be found in the binary file `./calculations/all_terms.pkl`, and the script `./tsk_diagrams.py` can be used to generate them.

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

Contents

V^{3+}
N=2, C/B=4.42, B=860 cm^{-1}

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

$$
\begin{array}{cc}
 & \begin{array}{cc} t_2^2 & e^2 \end{array} \\
\begin{bmatrix}
10B + 5C - 8Dq & 2\sqrt{6}B + \sqrt{6}C \\
2\sqrt{6}B + \sqrt{6}C & 8B + 4C + 12Dq
\end{bmatrix}
\end{array}
\tag{1}
$$

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

$$
\begin{array}{cc}
 & \begin{array}{cc} t_2^2 & e^2 \end{array} \\
\begin{bmatrix}
B + 2C - 8Dq & -2\sqrt{3}B \\
-2\sqrt{3}B & 2C + 12Dq
\end{bmatrix}
\end{array}
\tag{2}
$$

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

$$
\begin{array}{cc}
 & \begin{array}{cc} t_2^2 & t_2e \end{array} \\
\begin{bmatrix}
-5B - 8Dq & -6B \\
-6B & 4B + 2Dq
\end{bmatrix}
\end{array}
\tag{3}
$$

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

$$
\begin{array}{cc}
 & \begin{array}{cc} t_2^2 & t_2e \end{array} \\
\begin{bmatrix}
B + 2C - 8Dq & 2\sqrt{3}B \\
2\sqrt{3}B & 2C + 2Dq
\end{bmatrix}
\end{array}
\tag{4}
$$

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

$$
\begin{array}{c}
t_2e \\
\begin{bmatrix} -8B + 2Dq \end{bmatrix}
\end{array}
\tag{5}
$$

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

$$
\begin{array}{c}
t_2e \\
\begin{bmatrix} 4B + 2C + 2Dq \end{bmatrix}
\end{array}
\tag{6}
$$

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

$$
\begin{array}{c}
e^2 \\
\begin{bmatrix} -8B + 12Dq \end{bmatrix}
\end{array}
\tag{7}
$$

Cr^{3+}
N=3, C/B=4.50, B=918 cm^{-1}
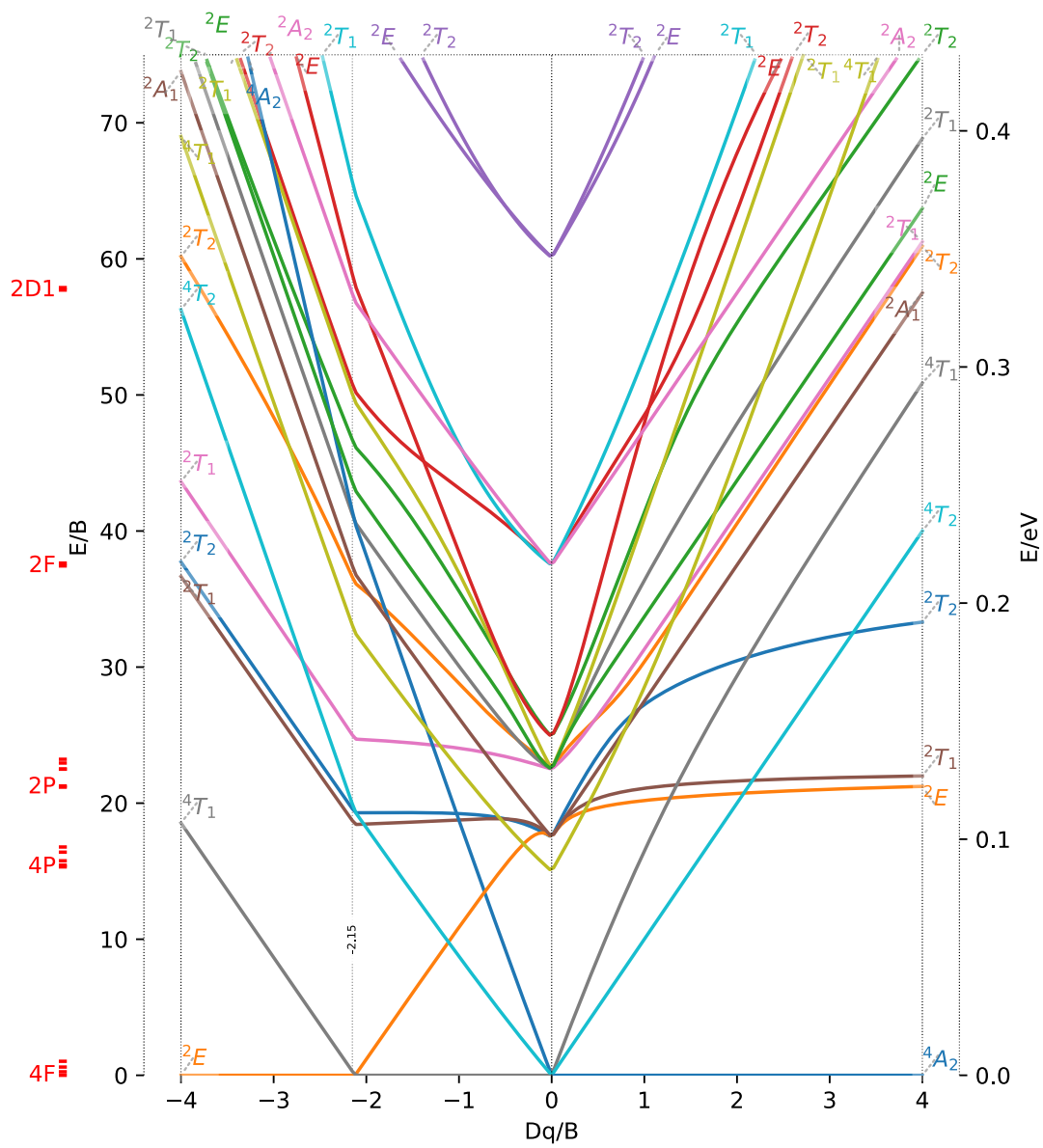
$$^2T_2(^2D, {}^2D, {}^2F, {}^2G, {}^2H)$$

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

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

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

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

$$
\begin{bmatrix}
t_2^3 \\
-15B-12Dq
\end{bmatrix}
\tag{10}
$$

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

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

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

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

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

$$
\begin{bmatrix}
t_2^2(^1E)e \\
9B+3C-2Dq
\end{bmatrix}
\tag{13}
$$
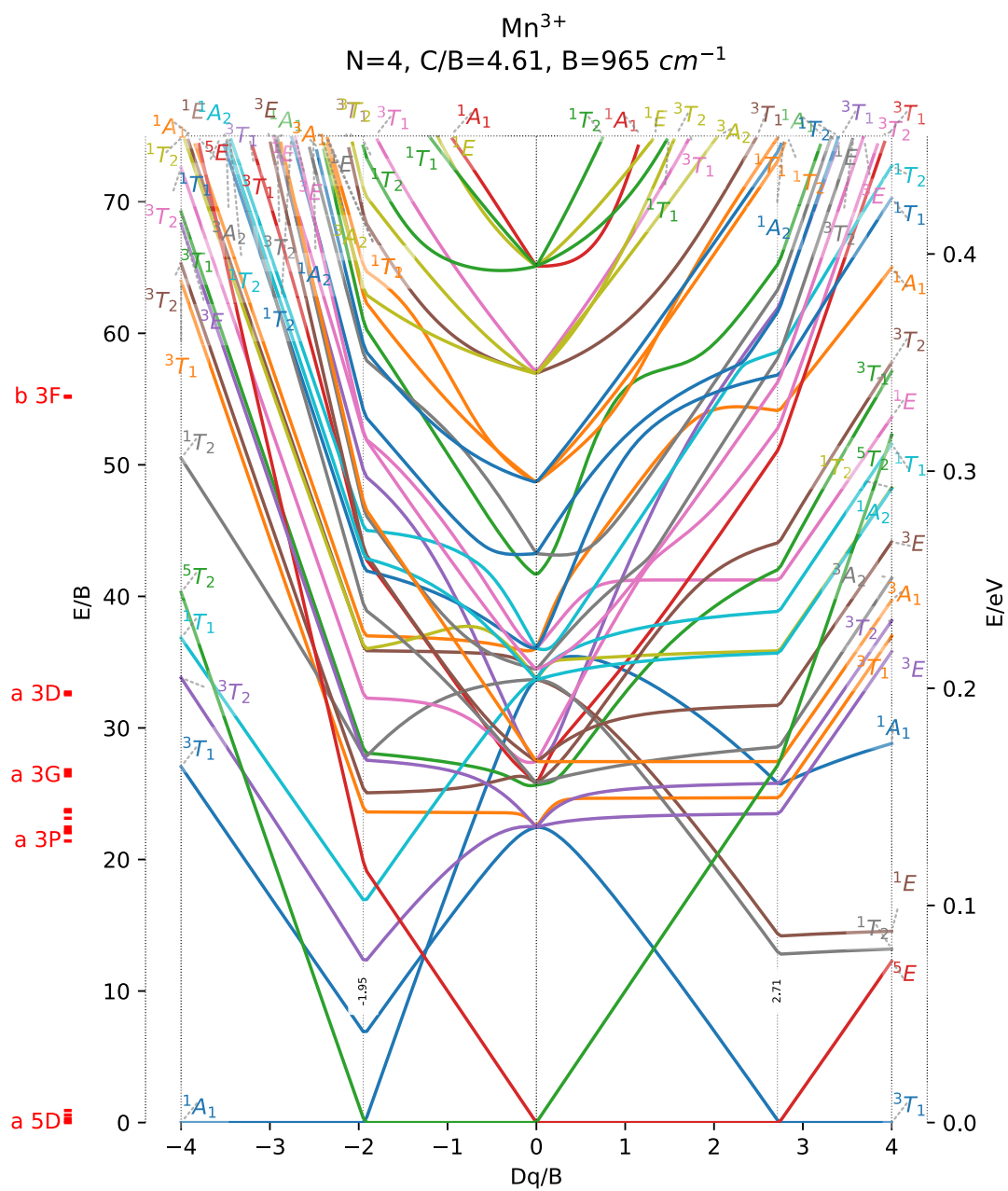
$$^4T_1(^4F, {}^4P)$$

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

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

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

Mn^{3+}
N=4, C/B=4.61, B=965 cm^{-1}

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

columns: $t_2^4\ \mid\ t_2^3(^2E)e\ \mid\ t_2^2(^1E)e^2(^1A_1)\ \mid\ t_2^2(^1A_1)e^2(^1E)\ \mid\ e^4$

$$\begin{bmatrix}
10C-16Dq & -12\sqrt2\,B & 4\sqrt2\,B+2\sqrt2\,C & 2\sqrt2\,B & 0\\
 & 6C-6Dq & -12B & -6B & 0\\
 & & 14B+11C+4Dq & 20B & 2\sqrt6\,B+\sqrt6\,C\\
 & & & -3B+6C+4Dq & 2\sqrt6\,B\\
 & & & & -16B+8C+24Dq
\end{bmatrix}\tag{16}$$

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

columns: $t_2^4\ \mid\ t_2^3(^2E)e\ \mid\ t_2^2(^1E)e^2(^1A_1)\ \mid\ t_2^2(^1A_1)e^2(^1E)\ \mid\ t_2^2(^1E)e^2(^1E)$

$$\begin{bmatrix}
-9B+7C-16Dq & 6B & 2\sqrt2\,B+\sqrt2\,C & -2B & -4B\\
 & -6B+6C-6Dq & -3\sqrt2\,B & -3B & 0\\
 & & 5B+8C+4Dq & 10\sqrt2\,B & -10\sqrt2\,B\\
 & & & 6B+9C+4Dq & 0\\
 & & & & -3B+6C+4Dq
\end{bmatrix}\tag{17}$$

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

columns: $t_2^4\ \mid\ t_2^3(^2E)e\ \mid\ t_2^3(^2T_1)e\ \mid\ t_2^2(^3T_1)e^2(^1E)\ \mid\ t_2^2(^1T_2)e^2(^3A_2)\ \mid\ t_2e^3(^2E)$

$$\begin{bmatrix}
-15B+5C-16Dq & 3\sqrt2\,B & 3\sqrt6\,B & 2\sqrt2\,B+\sqrt2\,C & -2\sqrt2\,B & 0\\
 & -11B+4C-6Dq & \sqrt6\,B & \sqrt3\,B & 5\sqrt3\,B & \sqrt2\,B\\
 & & -3B+6C+4Dq & 3B & -3B & -3\sqrt3\,B\\
 & & & -11B+4C+4Dq & 0 & -6B\\
 & & & & -11B+4C+4Dq & -3\sqrt6\,B\\
 & & & & & -16B+5C+14Dq
\end{bmatrix}\tag{18}$$

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

columns: $t_2^4\ \mid\ t_2^3(^2T_1)e\ \mid\ t_2^2(^1T_2)e^2(^1A_1)\ \mid\ t_2^2(^3T_1)e^2(^1E)\ \mid\ t_2^2(^1T_2)e^2(^1E)\ \mid\ t_2e^3(^2E)$

$$\begin{bmatrix}
-9B+7C-16Dq & 3\sqrt2\,B & 2\sqrt2\,B+\sqrt2\,C & -2\sqrt2\,B & 0 & 0\\
 & 3B+8C-6Dq & -5\sqrt3\,B & -5\sqrt3\,B & -3\sqrt3\,B & 3\sqrt2\,B+\sqrt2\,C\\
 & & -B+6C+4Dq & 3\sqrt3\,B & 3B & -5\sqrt3\,B\\
 & & & 5B+8C+4Dq & -10B & -6B\\
 & & & & -9B+4C+4Dq & -3\sqrt6\,B\\
 & & & & & 7C+14Dq
\end{bmatrix}\tag{19}$$

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

columns: $t_2^3(^2T_2)e\ \mid\ t_2^3(^2T_1)e\ \mid\ t_2^2(^3T_1)e^2(^1E)\ \mid\ t_2^2(^1T_2)e^2(^3A_2)\ \mid\ t_2e^3(^2E)$

$$\begin{bmatrix}
-5B+6C-6Dq & 5\sqrt3\,B & -3B & -3\sqrt2\,B & 3\sqrt2\,B+\sqrt2\,C\\
 & -9B+4C-6Dq & -\sqrt3\,B & 2\sqrt2\,B & -\sqrt6\,B\\
 & & -9B+4C+4Dq & -3B & \sqrt6\,B\\
 & & & -13B+4C+4Dq & -6B\\
 & & & & -8B+5C+14Dq
\end{bmatrix}\tag{20}$$

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

columns: $t_2^3(^2T_1)e\ \mid\ t_2^2(^1T_2)e^2(^1E)\ \mid\ t_2^2(^3T_1)e^2(^3A_2)\ \mid\ t_2e^3(^2E)$

$$\begin{bmatrix}
-3B+6C-6Dq & -5\sqrt3\,B & 3B & \sqrt6\,B\\
 & -3B+6C+4Dq & -3B & \sqrt6\,B\\
 & & -9B+4C+4Dq & -\sqrt6\,B\\
 & & & -16B+7C+14Dq
\end{bmatrix}\tag{21}$$

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

$$\begin{bmatrix}
 t_2^3(^4A_2)e\\
 -21B-6Dq
\end{bmatrix}\tag{22}$$

7

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

$$
\begin{bmatrix}
t_2^3(^2E)e & t_2^3(^4A_2)e & t_2(^1E)e^2(^3A_2) \\
-10B+4C-6Dq & 4B & 3\sqrt{2}B \\
3\sqrt{2}B & -13B+4C-6Dq & 0 \\
 & 0 & -11B+4C+4Dq
\end{bmatrix}
\tag{23}
$$

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

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

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

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

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

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

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

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

Mn^{2+}
N=5, C/B=4.48, B=860 cm^{-1}

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

$$
\begin{array}{c|cccccccccc}
 & t_2^5 & t_2^4(^3T_1)e & t_2^4(^1T_2)e & t_2^3(^2T_2)e^2(^1A_1) & t_2^3(^2T_2)e^2(^1E) & t_2^3(^2T_1)e^2(^1E) & t_2^3(^2T_1)e^2(^3A_2) & t_2^2(^3T_1)e^3(^2E) & t_2^2(^1T_2)e^3(^2E) & t_2e^4(^1A_1) \\
\hline
 & -20B+10C-20Dq & -3\sqrt6 B & \sqrt6 B & 4B+2C & 2B & -2\sqrt3 B & 0 & 0 & 0 & 0 \\
 & & -8B+9C-10Dq & -3B & -\frac{3\sqrt6 B}{2} & -\frac{3\sqrt6 B}{2} & \frac{3\sqrt2 B}{2} & \frac{\sqrt6 B}{2} & 4B+C & 0 & 0 \\
 & & & -18B+9C-10Dq & \frac{5\sqrt6 B}{2} & -\frac{5\sqrt6 B}{2} & -\frac{3\sqrt2 B}{2} & -\frac{3\sqrt6 B}{2} & 0 & C & 0 \\
 & & & & 2B+12C & 0 & -10\sqrt3 B & 0 & \frac{3\sqrt6 B}{2} & -\frac{5\sqrt6 B}{2} & -2B \\
 & & & & & -6B+10C & 0 & 0 & -\frac{3\sqrt6 B}{2} & -\frac{5\sqrt6 B}{2} & -2B \\
 & & & & & & -6B+10C & 0 & -2\sqrt3 B & 0 & 0 \\
 & & & & & & & -16B+8C & -\frac{\sqrt6 B}{2} & \frac{3\sqrt6 B}{2} & 0 \\
 & & & & & & & & -8B+9C+10Dq & -3B & 3\sqrt6 B \\
 & & & & & & & & & -18B+9C+10Dq & -\sqrt6 B \\
 & & & & & & & & & & -20B+10C+20Dq
\end{array}
$$
(28)

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

$$
\begin{array}{c|ccccccc}
 & t_2^4(^1A_1)e & t_2^4(^1E)e & t_2^3(^2E)e^2(^1A_1) & t_2^3(^2E)e^2(^1E) & t_2^3(^2E)e^2(^3A_2) & t_2^2(^3T_1)e^3(^2E) & t_2^2(^1E)e^3(^2E) \\
\hline
 & -4B+12C-10Dq & 10B & 6B & 6\sqrt2 B & -6\sqrt3 B & 4B+2C & -2B \\
 & & -13B+9C-10Dq & -3B & 0 & -3\sqrt3 B & 2B & 2B+C \\
 & & & -4B+10C & 0 & 0 & -6B & -3B \\
 & & & & -12B+8C & -2\sqrt6 B & -6\sqrt6 B & 3\sqrt2 B \\
 & & & & & -16B+8C & -6\sqrt3 B & 3\sqrt3 B \\
 & & & & & & -8B+9C+10Dq & -10B \\
 & & & & & & & -13B+9C+10Dq
\end{array}
$$
(29)

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

$$
\begin{array}{c|cccc}
 & t_2^4(^1E)e & t_2^3(^2E)e^2(^1E) & t_2^3(^4A_2)e^2(^3A_2) & t_2^2(^1A_1)e^3(^2E) \\
\hline
 & -3B+9C-10Dq & -3\sqrt2 B & 0 & 6B+C \\
 & & -12B+8C & -4\sqrt3 B & 3\sqrt2 B \\
 & & & -19B+8C & 0 \\
 & & & & -3B+9C+10Dq
\end{array}
$$
(30)

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

$$
\begin{array}{c|ccc}
 & t_2^4(^1E)e & t_2^3(^2E)e^2(^1E) & t_2^2(^1E)e^3(^2E) \\
\hline
 & -23B+9C-10Dq & 3\sqrt2 B & -2B+C \\
 & & -12B+8C & -3\sqrt2 B \\
 & & & -23B+9C+10Dq
\end{array}
$$
(31)

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

$$
\begin{array}{c|ccc}
 & t_2^4(^3T_1)e & t_2^3(^2T_2)e^2(^3A_2) & t_2^2(^3T_1)e^3(^2E) \\
\hline
 & -25B+6C-10Dq & -3\sqrt2 B & C \\
 & & -16B+7C & -3\sqrt2 B \\
 & & & -25B+6C+10Dq
\end{array}
$$
(32)

$$^4T_2(^4D, \, ^4F, \, ^4G)$$

$$
\begin{array}{c|ccc}
 & t_2^4(^3T_1)e & t_2^3(^2T_1)e^2(^3A_2) & t_2^3(^3T_1)e^3(^2E) \\
\hline
 & -17B+6C-10Dq & \sqrt6 B & 4B+C \\
 & & -22B+5C & -\sqrt6 B \\
 & & & -17B+6C+10Dq
\end{array}
$$
(33)

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

$$\left[\begin{array}{cccccccc}
 & t_2^4(^3T_1)e & t_2^4(^1T_2)e & t_2^3(^2T_1)e^2(^1A_1) & t_2^3(^2T_2)e^2(^1E) & t_2^3(^2T_1)e^2(^1E) & t_2^3(^2T_2)e^2(^3A_2) & t_2^2(^3T_1)e^3(^2E) & t_2^2(^1T_2)e^3(^2E) \\
t_2^4(^3T_1)e & -22B+9C-10Dq & 3B & \frac{3\sqrt{2}B}{2} & \frac{3\sqrt{6}B}{2} & -\frac{3\sqrt{2}B}{2} & -\frac{3\sqrt{2}B}{2} & C & 0 \\
 & 3B & -8B+9C-10Dq & \frac{3\sqrt{2}B}{2} & \frac{5\sqrt{6}B}{2} & \frac{3\sqrt{2}B}{2} & -\frac{15\sqrt{2}B}{2} & 0 & 4B+C \\
 & \frac{3\sqrt{2}B}{2} & \frac{3\sqrt{2}B}{2} & -4B+10C & 10\sqrt{3}B & 0 & 0 & \frac{3\sqrt{2}B}{2} & \frac{3\sqrt{2}B}{2} \\
 & \frac{3\sqrt{6}B}{2} & \frac{5\sqrt{6}B}{2} & 10\sqrt{3}B & -6B+10C & 0 & -2\sqrt{3}B & \frac{3\sqrt{6}B}{2} & \frac{5\sqrt{6}B}{2} \\
 & -\frac{3\sqrt{2}B}{2} & \frac{3\sqrt{2}B}{2} & 0 & 0 & -12B+8C & 0 & \frac{3\sqrt{2}B}{2} & -\frac{3\sqrt{2}B}{2} \\
 & -\frac{3\sqrt{2}B}{2} & -\frac{15\sqrt{2}B}{2} & 0 & -2\sqrt{3}B & 0 & -10B+10C & -\frac{3\sqrt{2}B}{2} & -\frac{15\sqrt{2}B}{2} \\
 & C & 0 & \frac{3\sqrt{2}B}{2} & \frac{3\sqrt{6}B}{2} & \frac{3\sqrt{2}B}{2} & -\frac{3\sqrt{2}B}{2} & -22B+9C+10Dq & 3B \\
 & 0 & 4B+C & \frac{3\sqrt{2}B}{2} & \frac{5\sqrt{6}B}{2} & -\frac{3\sqrt{2}B}{2} & -\frac{15\sqrt{2}B}{2} & 3B & -8B+9C+10Dq
\end{array}\right]$$

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

$$\left[\begin{array}{c} t_2^3(^4A_2)e^2(^1A_1) \\ -13B+7C \end{array}\right]$$

$$^4E(^4D,\,^4G)$$

$$\left[\begin{array}{cc} t_2^3(^2E)e^2(^3A_2) & t_2^3(^4A_2)e^2(^1E) \\ -22B+5C & -2\sqrt{3}B \\ -2\sqrt{3}B & -21B+5C \end{array}\right]$$

$$^6A_1(^6S)$$

$$\left[\begin{array}{c} t_2^3(^4A_2)e^2(^3A_2) \\ -35B \end{array}\right]$$

$$^4A_1(^4G)$$

$$\left[\begin{array}{c} t_2^3(^4A_2)e^2(^3A_2) \\ -25B+5C \end{array}\right]$$

11

Co^{3+}

N=6, C/B=4.81, B=1065 cm^{-1}

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

Basis: $t_2^6,\ t_2^5(^2T_2)e,\ t_2^4(^3T_1)e^2(^1A_1),\ t_2^4(^1A_1)e^2(^1A_1),\ t_2^3(^2E)e^3(^2E),\ t_2^2(^1A_1)e^4(^1A_1)$
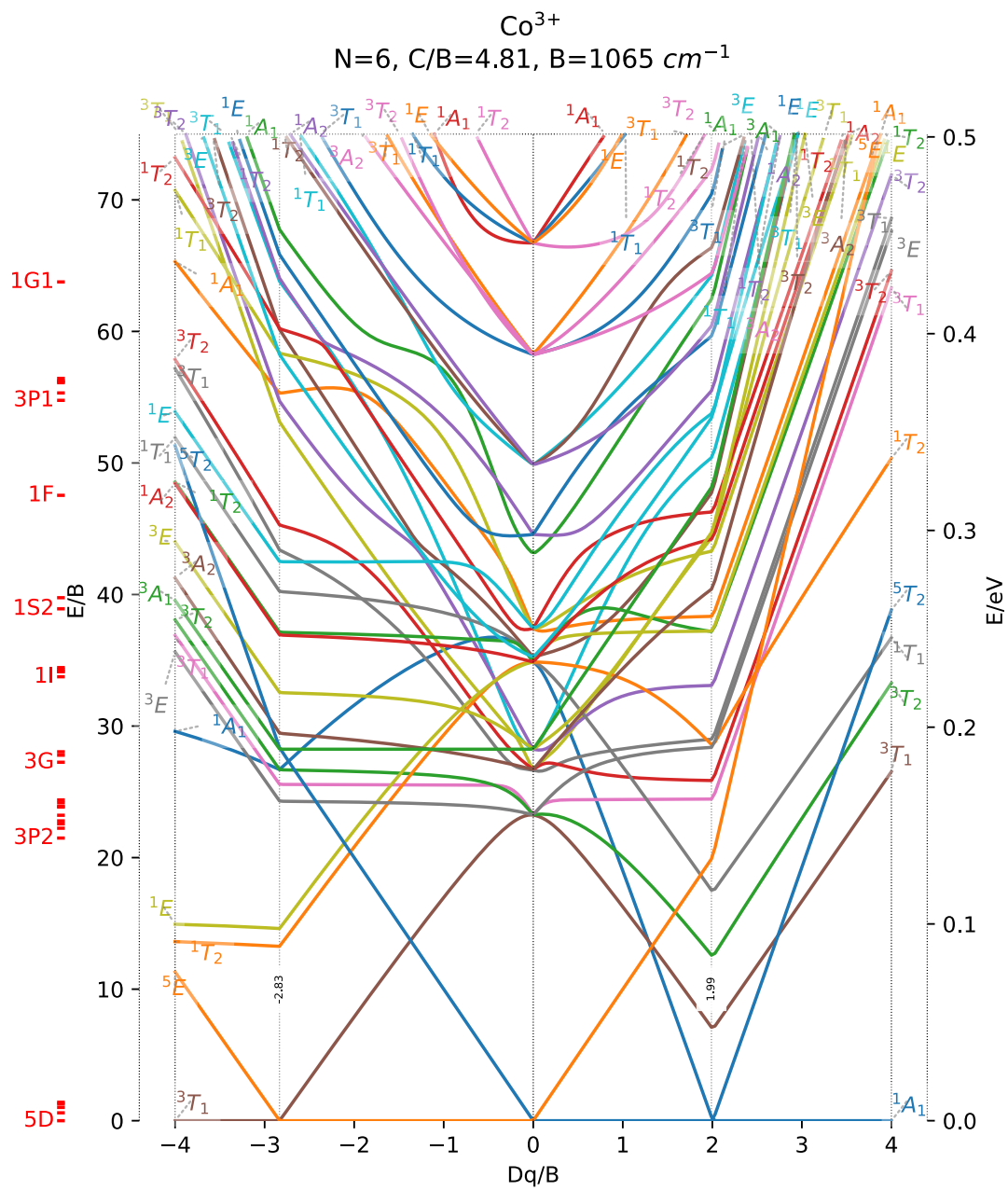
$$\begin{bmatrix}
-30B+15C-24Dq & 2\sqrt{6}B+\sqrt{6}C & 2\sqrt{6}B+\sqrt{6}C & 0 & 0 & 0\\
 & -30B+12C-14Dq & -3\sqrt{2}B & -3\sqrt{2}B & \sqrt{6}B & \sqrt{2}B+\sqrt{2}C\\
 & & -15B+13C-4Dq & 10B & 0 & 3B\\
 & & & 18C-4Dq & 20B & 4\sqrt{2}B+2\sqrt{2}C\\
 & & & & -14B+17C+16Dq & -12\sqrt{2}B\\
 & & & & & -14B+17C+16Dq
\end{bmatrix} \quad (39)$$

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

Basis: $t_2^5(^2T_2)e,\ t_2^4(^3T_1)e^2(^1A_1),\ t_2^4(^3T_1)e^2(^1E),\ t_2^3(^2T_1)e^3(^2E),\ t_2^3(^2E)e^3(^2E),\ t_2^2(^3T_1)e^4(^1A_1)$

$$\begin{bmatrix}
-30B+12C-14Dq & -3\sqrt{2}B & -3\sqrt{2}B & \sqrt{6}B & -\sqrt{6}B & 0\\
 & -15B+13C-4Dq & 10B & 0 & \sqrt{3}B & 2\sqrt{2}B+\sqrt{2}C\\
 & & -23B+11C-4Dq & -2\sqrt{3}B & \sqrt{3}B & 2\sqrt{2}B\\
 & & & -25B+11C+6Dq & -3B & 3\sqrt{2}B\\
 & & & & -25B+11C+6Dq & -\sqrt{6}B\\
 & & & & & -29B+12C+16Dq
\end{bmatrix} \quad (40)$$

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

Basis: $t_2^5(^2T_2)e,\ t_2^4(^3T_1)e^2(^1E),\ t_2^4(^1T_2)e^2(^3A_2),\ t_2^3(^2T_1)e^3(^2E),\ t_2^3(^2T_2)e^3(^2E)$

$$\begin{bmatrix}
-22B+12C-14Dq & 3\sqrt{2}B & 6B & 6B & 3\sqrt{2}B+\sqrt{2}C\\
 & -23B+11C-4Dq & 2\sqrt{2}B & 2\sqrt{2}B & 3\sqrt{2}B\\
 & & -27B+11C-4Dq & 3\sqrt{2}B & 3\sqrt{2}B\\
 & & & -19B+13C+6Dq & 5\sqrt{3}B\\
 & & & & -23B+13C+6Dq
\end{bmatrix} \quad (41)$$

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

Basis: $t_2^5(^2T_2)e,\ t_2^4(^1T_2)e^2(^1E),\ t_2^3(^2T_2)e^3(^2E),\ t_2^3(^2T_1)e^3(^2E)$

$$\begin{bmatrix}
-30B+14C-14Dq & \sqrt{6}B & \sqrt{2}B+\sqrt{2}C & -\sqrt{6}B\\
 & -17B+13C-4Dq & 5\sqrt{3}B & 3B\\
 & & -17B+15C+6Dq & -5\sqrt{3}B\\
 & & & -17B+13C+6Dq
\end{bmatrix} \quad (42)$$

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

Basis: $t_2^4(^1T_2)e^2(^1A_1),\ t_2^4(^1T_2)e^2(^1E),\ t_2^4(^3T_1)e^2(^3A_2),\ t_2^3(^2T_2)e^3(^2E),\ t_2^3(^2T_1)e^3(^2E),\ t_2^2(^1T_2)e^4(^1A_1)$

$$\begin{bmatrix}
-9B+15C-4Dq & 10B & 3\sqrt{6}B & \sqrt{6}B & -\sqrt{6}B & 0\\
 & -17B+13C-4Dq & 0 & -3B & -5\sqrt{3}B & 2\sqrt{2}B+\sqrt{2}C\\
 & & -23B+13C-4Dq & 3B & 3\sqrt{3}B & 2\sqrt{2}B\\
 & & & -23B+13C+6Dq & 5\sqrt{3}B & 0\\
 & & & & -11B+15C+6Dq & -5\sqrt{6}B\\
 & & & & & -23B+14C+16Dq
\end{bmatrix} \quad (43)$$

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

Basis: $t_2^4(^1E)e^2(^1A_1),\ t_2^4(^1A_1)e^2(^1E),\ t_2^2(^1E)e^2(^1E),\ t_2^3(^2E)e^3(^2E),\ t_2^2(^1E)e^4(^1A_1)$

$$\begin{bmatrix}
-9B+15C-4Dq & 10\sqrt{2}B & 10\sqrt{2}B & 3\sqrt{2}B & 2\sqrt{2}B+\sqrt{2}C\\
 & -8B+16C-4Dq & 12B & 0 & -2B\\
 & & 12B & 0 & 4B\\
 & & & -20B+13C+6Dq & -6B\\
 & & & & -23B+14C+16Dq
\end{bmatrix} \quad (44)$$

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

Basis: $t_2^4(^1E)e^2(^1E),\ t_2^3(^2E)e^3(^2E)$

$$\begin{bmatrix}
-17B+13C-4Dq & 6B\\
6B & -26B+13C+6Dq
\end{bmatrix} \quad (45)$$

13

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

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

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

$$
\begin{bmatrix}
t_2^4(^1E)e^2(^3A_2) & t_2^3(^2E)e^3(^2E) & t_2^3(^4A_2)e^3(^2E) \\
-25B+11C-4Dq & 3\sqrt{2}B & 0 \\
3\sqrt{2}B & -24B+11C+6Dq & 4B \\
0 & 4B & -27B+11C+6Dq
\end{bmatrix}
\tag{47}
$$

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

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

$$^5E(^5D)$$
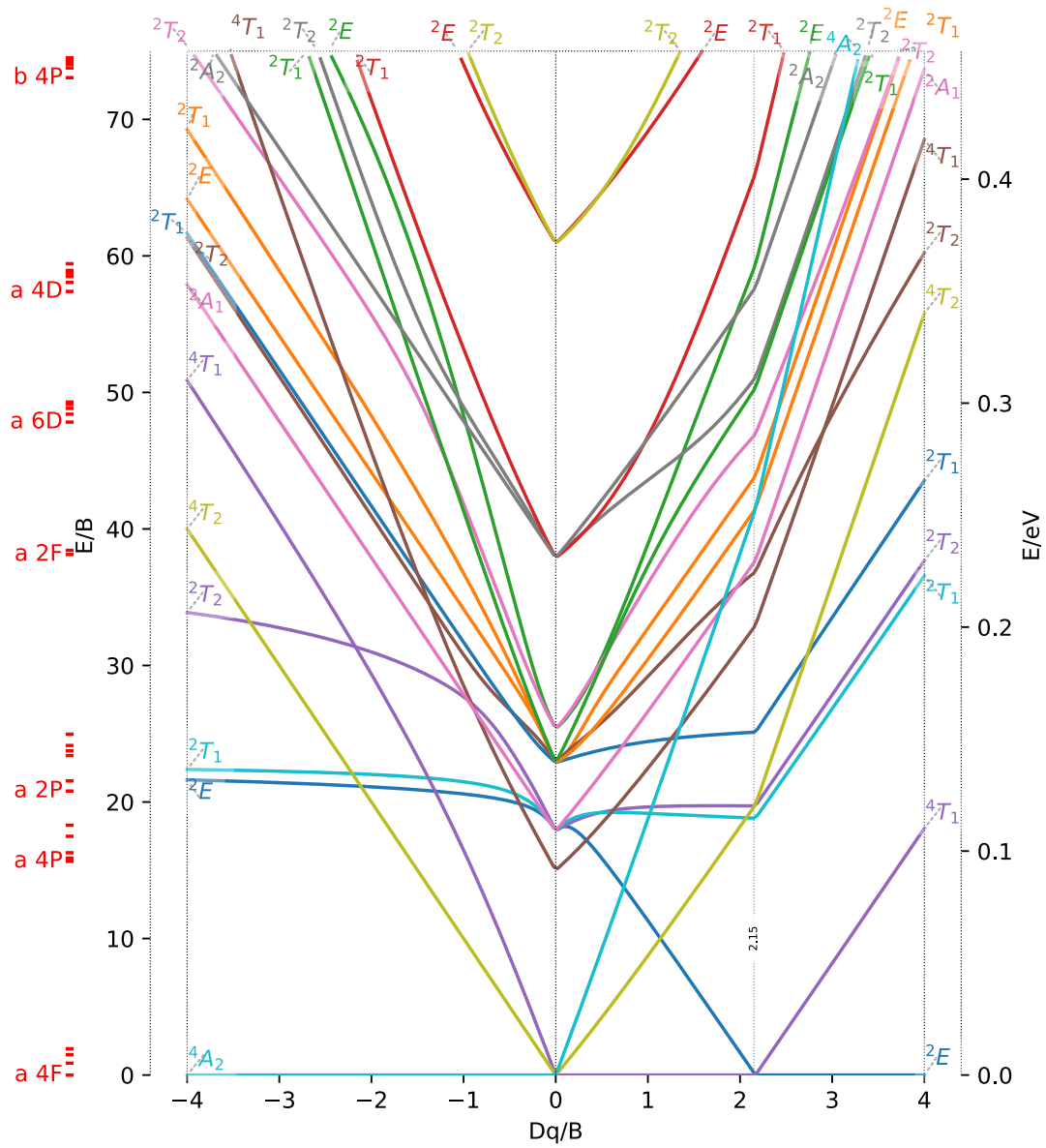
$$
\begin{bmatrix}
t_2^3(^4A_2)e^3(^2E) \\
-35B+7C+6Dq
\end{bmatrix}
\tag{49}
$$

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

$$
\begin{bmatrix}
t_2^3(^2E)e^3(^2E) \\
-26B+11C+6Dq
\end{bmatrix}
\tag{50}
$$

Co^{2+}
N=7, C/B=4.63, B=971 cm^{-1}

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

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

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

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

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

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

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

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

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

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

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

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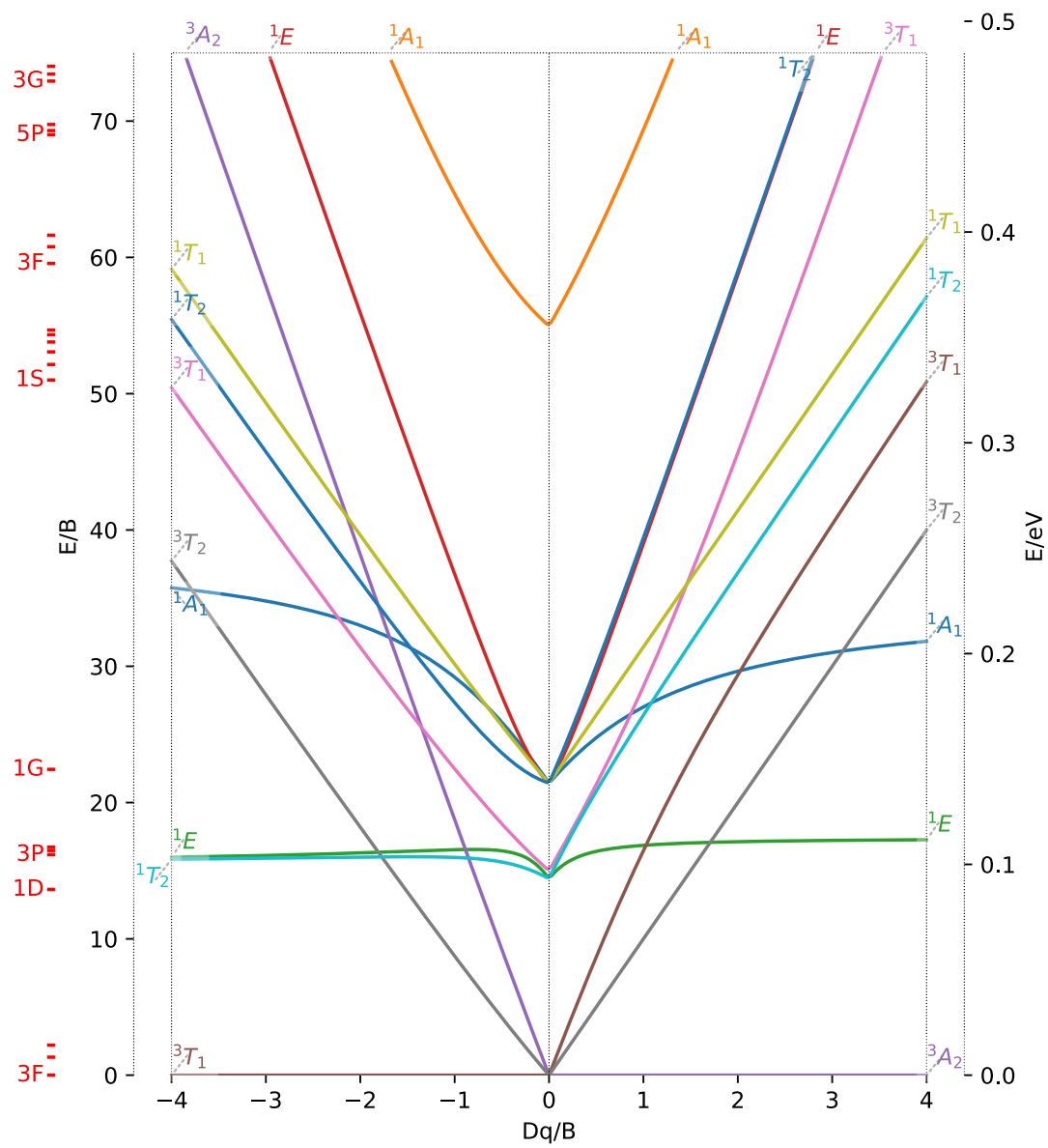-19B + 17C + 2Dq
\end{bmatrix}
\tag{56}
$$

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

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

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

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

Ni^{2+}
N=8, C/B=4.71, B=1030 cm^{-1}

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

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

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

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

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

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

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

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

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

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

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

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

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

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