2p-1s Cm-248 analysis

Stella Vogiatzi, 06.05.2022

E/RI vs dQ vs dR dependence

The new energy and relative intensity theoretical predictions of Natalia sent on 08/04/2022 are calculated for the $\mathrm{dR} = \frac{\mathrm{R}}{\mathrm{R}_0}$ and $\mathrm{dQ} = \frac{\mathrm{Q}}{\mathrm{Q}_0}$ values — where R_0 is the value of Angeli et al and Q_0 is the 12.04 b — in a 5 x 5 grid of (dR,dQ) where, dR = 1.01 +/- {0.001,0.1} & dQ = 1.00 +/- {0.001,0.1}, meaning for:

- dR = [1.0, 1.009, 1.01, 1.011, 1.02]
- dQ = [0.99, 0.999, 1.0, 1.001, 1.01]

in all combinations of dQ and dR, e.g. (dQ, dR) = (0.99, 1.), (0.99, 1.009), …, (0.99, 1.02), (0.999, 1.), …, (1.01, 1.02).

The question is → what is the relation that describes the energy / relative intensity dependence on both dQ and dR? ⇒ see next slide

E/RI vs dQ vs dR dependence

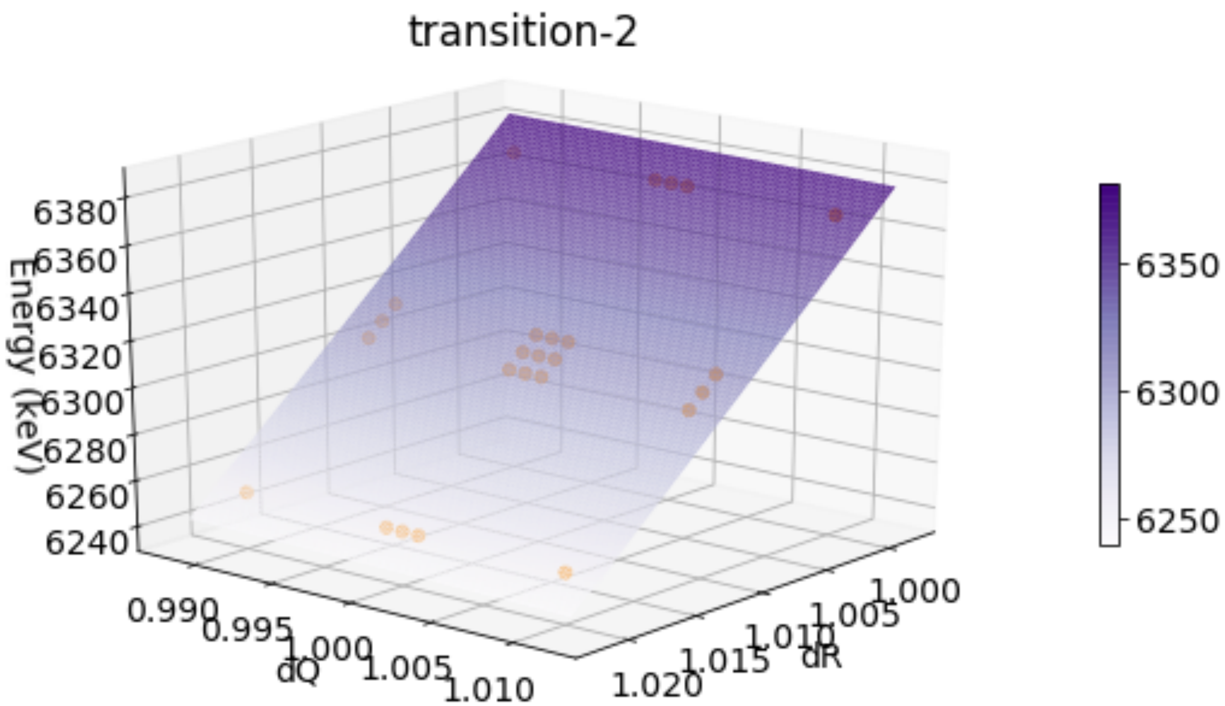
Using the script in /psi/home/vogiatzi_s/248Cm_dRvsdQ_dependencies/: EnergyVSdQVSdRSpace.ipynb (or versions/EnergyVSdQVSdRSpace-v3.ipynb), I load Natalia's values (sent on 08/04/2022) after I have manually ordered the transitions in the file.

Below I plot the energy as a function of the dR and dQ values. A 2nd degree polynomial function on both the dR and dQ values is fitted:

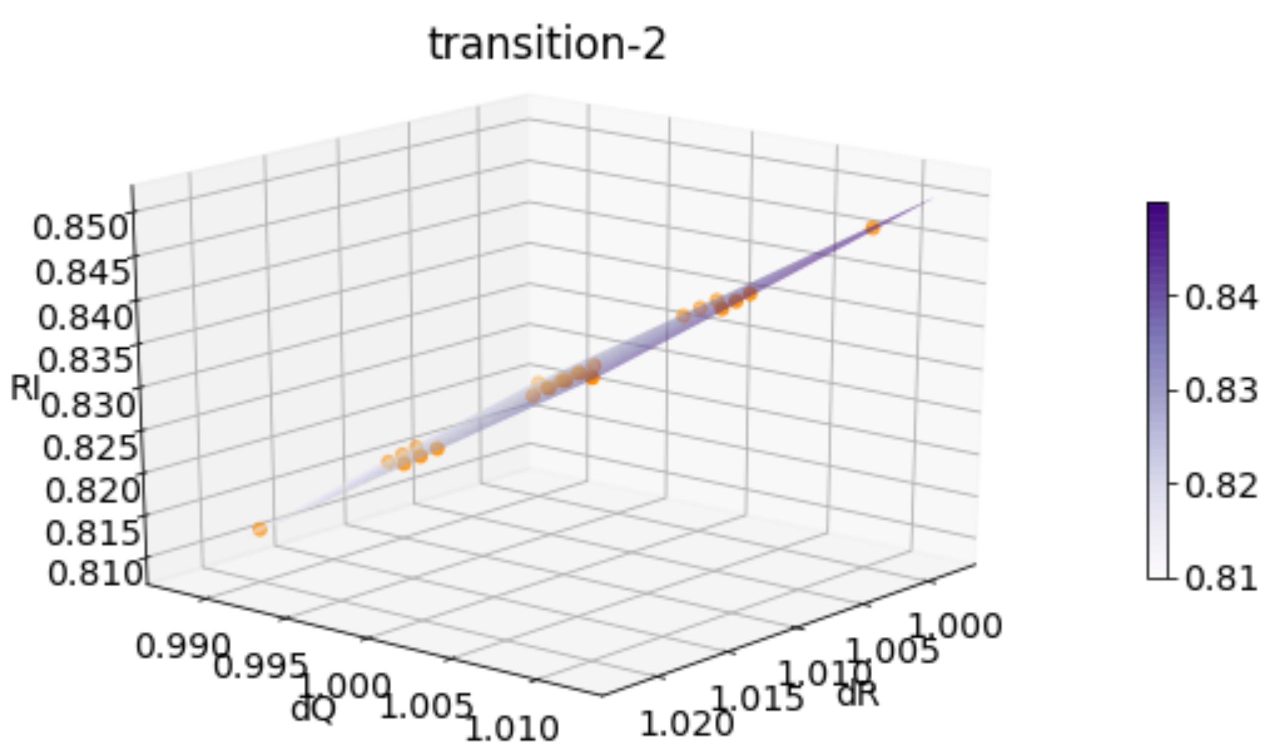
$$\mathrm{En} = c_0 \cdot 1 + c_1 \cdot dR + c_2 \cdot dQ + c_3 \cdot dR^2 + c_4 \cdot dR^2 \cdot dQ + c_5 \cdot dR^2 \cdot dQ^2 + c_6 \cdot dQ^2 + c_7 \cdot dR \cdot dQ^2 + c_8 \cdot dR \cdot dQ$$

This actually corresponds to

$E = E0 + E1 \cdot dR + E2 \cdot dR^2 = (a_{00} + a_{01} \cdot dQ + a_{02} \cdot dQ^2) + (a_{10} + a_{11} \cdot dQ + a_{12} \cdot dQ^2) \cdot dR + (a_{20} + a_{21} \cdot dQ + a_{22} \cdot dQ^2) \cdot dR^2$, where $a_{00} = c_0, a_{01} = c_2, a_{02} = c_6, a_{10} = c_1, a_{11} = c_8, a_{12} = c_7, a_{20} = c_3, a_{21} = c_4, a_{22} = c_5$. The surface with the obtained $c_0 - c_8$ coefficients is plotted in purple colour. The orange points are Natalia's values. Similarly for the relative intensity.

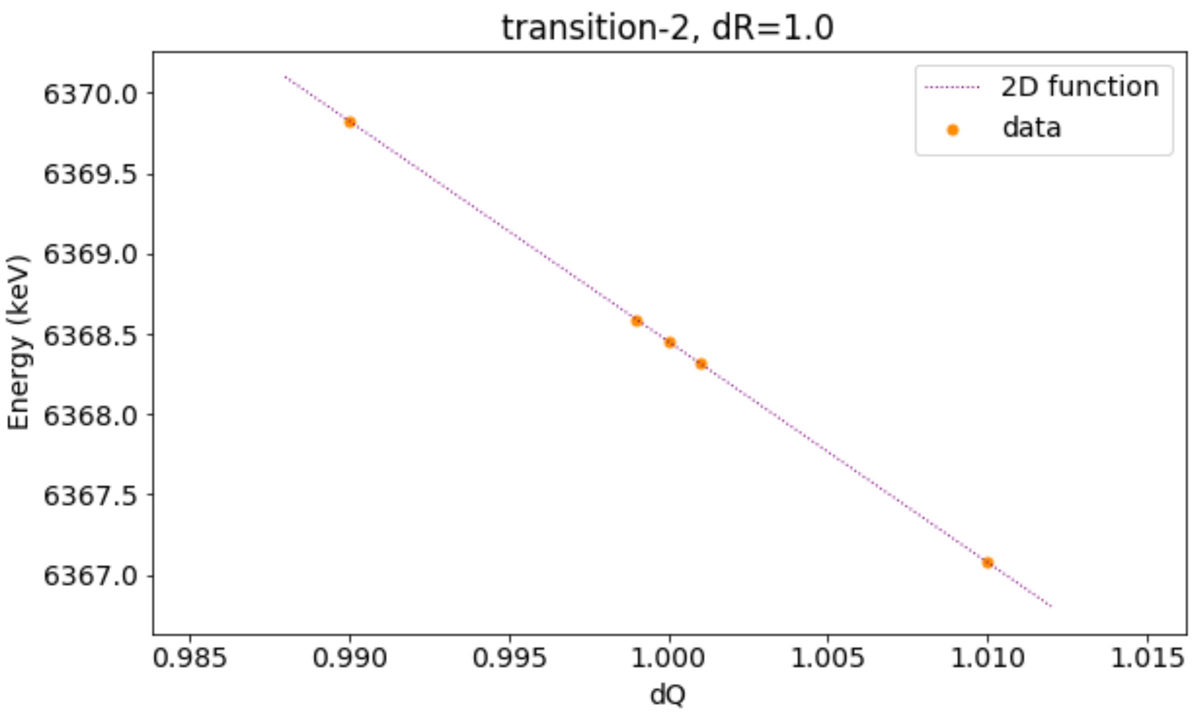


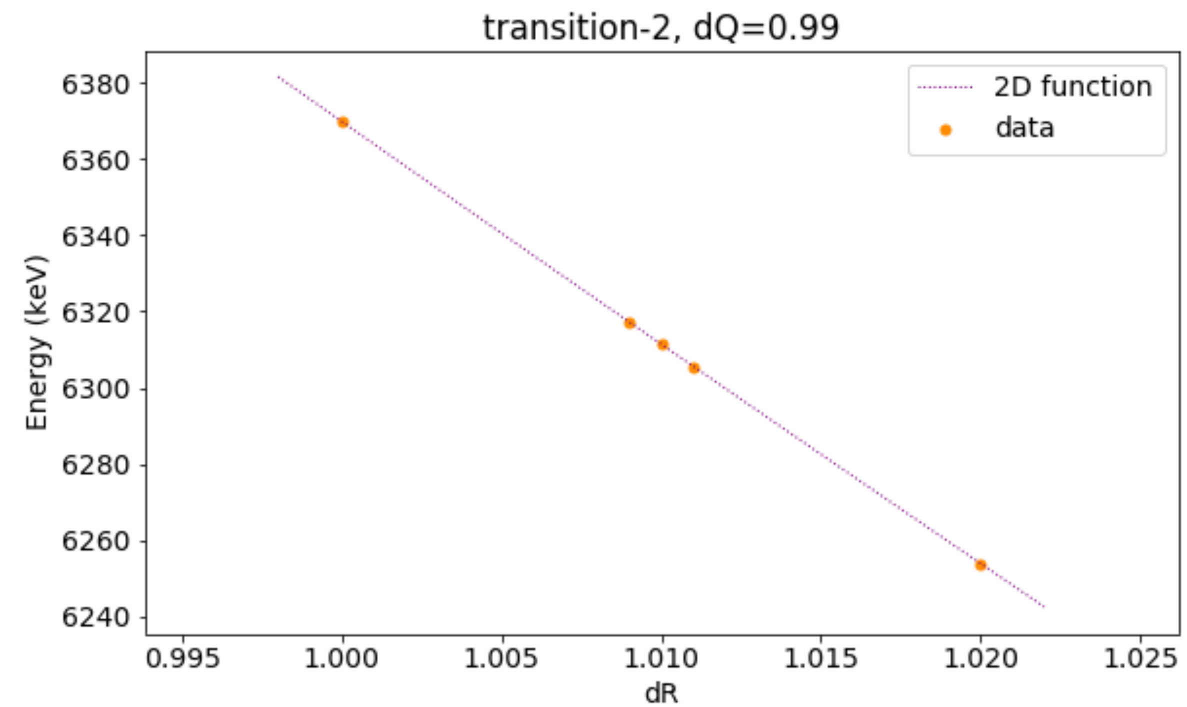
There is a different set of $c_0 - c_8$ coefficients for each transition for energy and a different one for relative intensity.

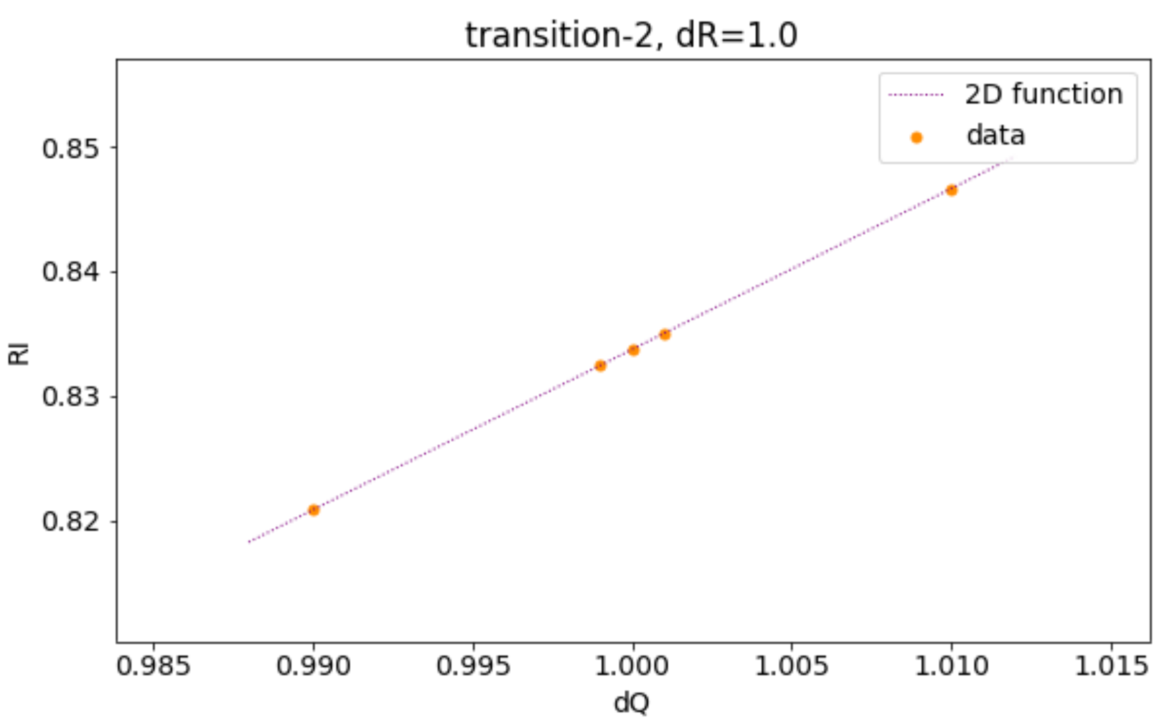


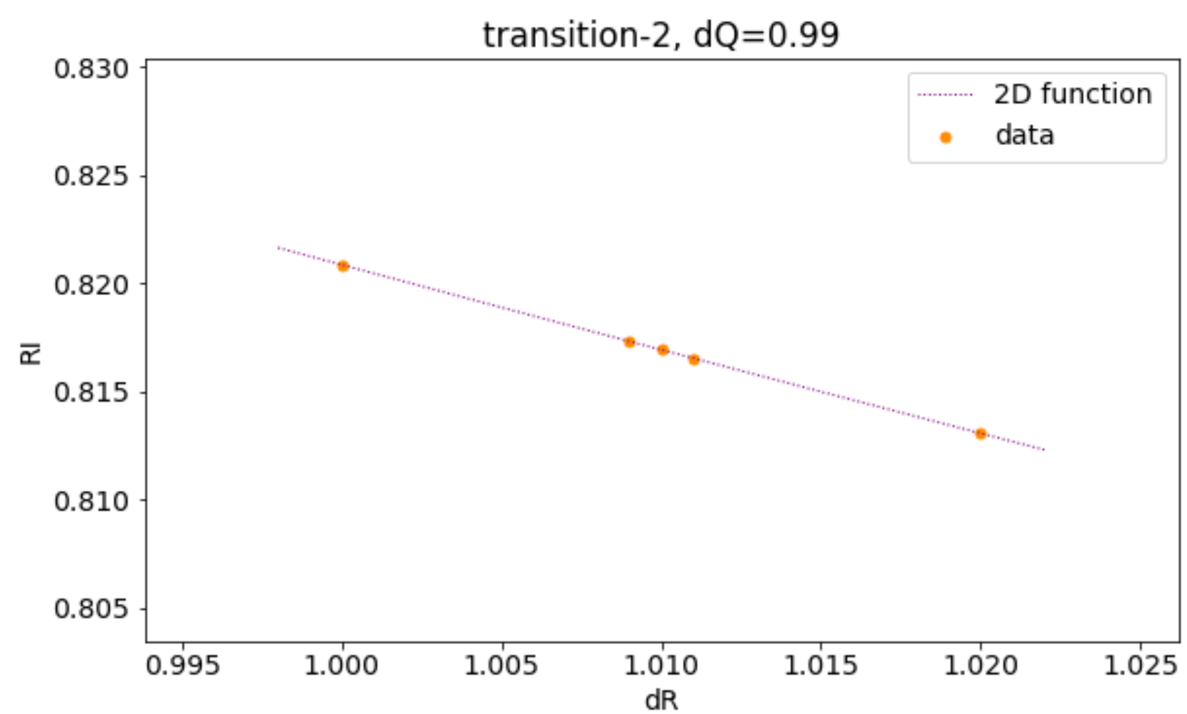
E/RI vs dQ vs dR dependence

Below I plot the energy / relative intensity as a function of dQ for dR=1.0 and as a function of dR for dQ=0.99 for transition-2 as an example; Natalia's energies (orange points) and $\mathrm{En/RI} = c_0 \cdot 1 + c_1 \cdot dR + c_2 \cdot dQ + c_3 \cdot dR^2 + c_4 \cdot dR^2 \cdot dQ + c_5 \cdot dR^2 \cdot dQ^2 + c_6 \cdot dQ^2 + c_7 \cdot dR \cdot dQ^2 + c_8 \cdot dR \cdot dQ$ function (purple line).



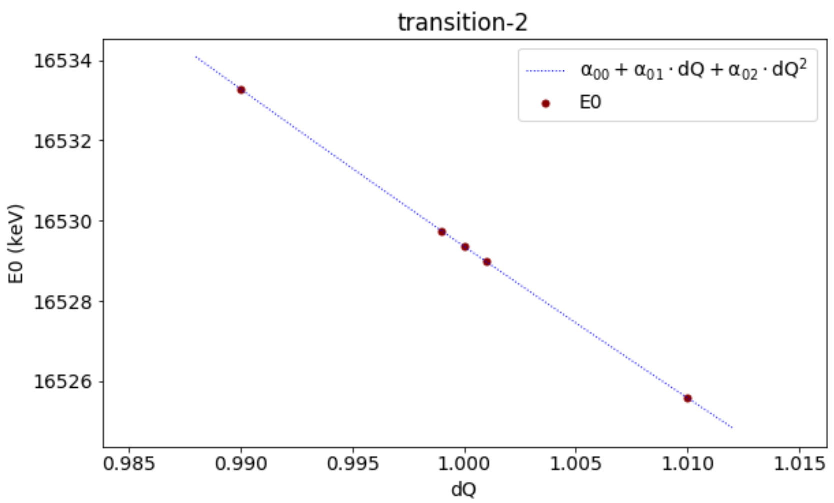


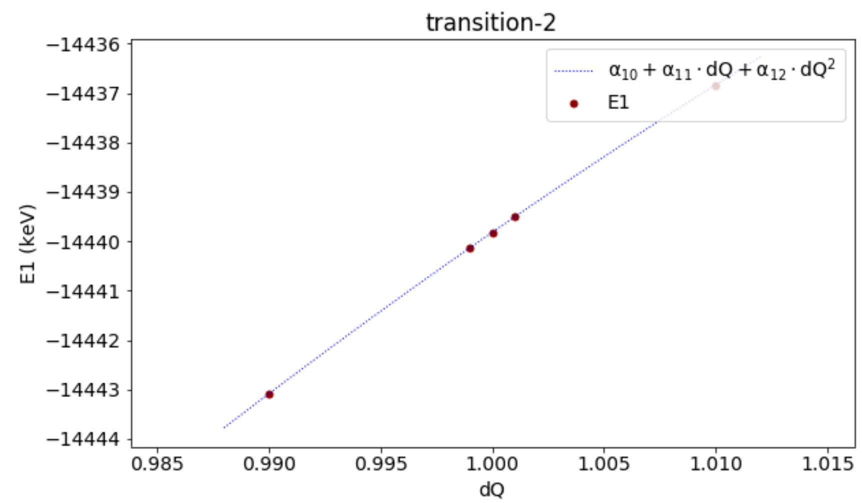


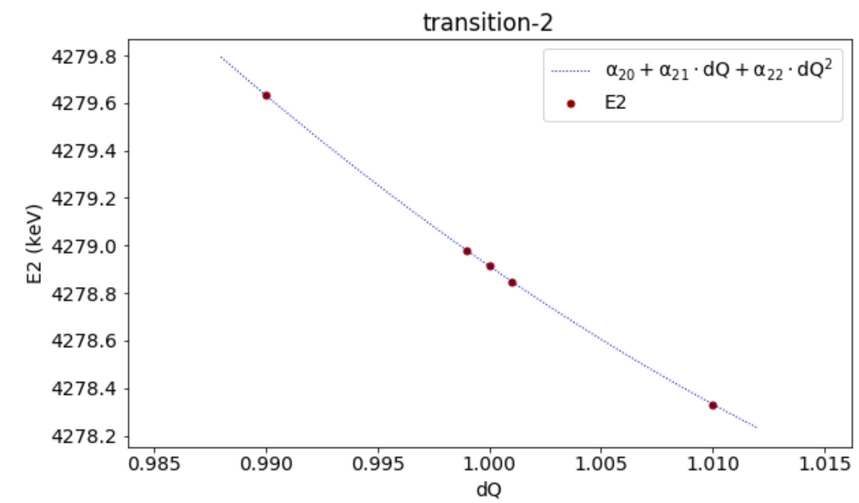


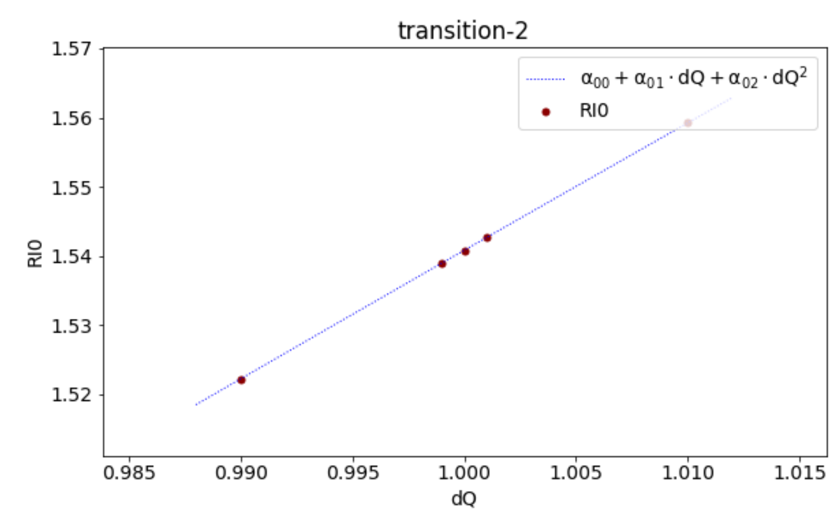
E/RI vs dQ vs dR dependence

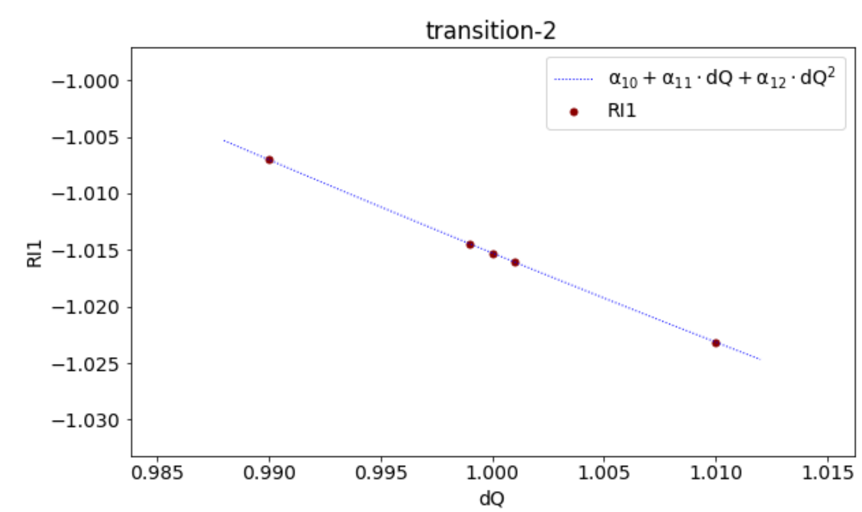
Below I plot the dependence of E0 / E1 / E2 on the dQ value as $(a_{00} + a_{01} \cdot dQ + a_{02} \cdot dQ^2)$ / $(a_{10} + a_{11} \cdot dQ + a_{12} \cdot dQ^2)$ / $(a_{20} + a_{21} \cdot dQ + a_{22} \cdot dQ^2)$, respectively, for transition-2. Similarly for the RI0, RI1, RI2.

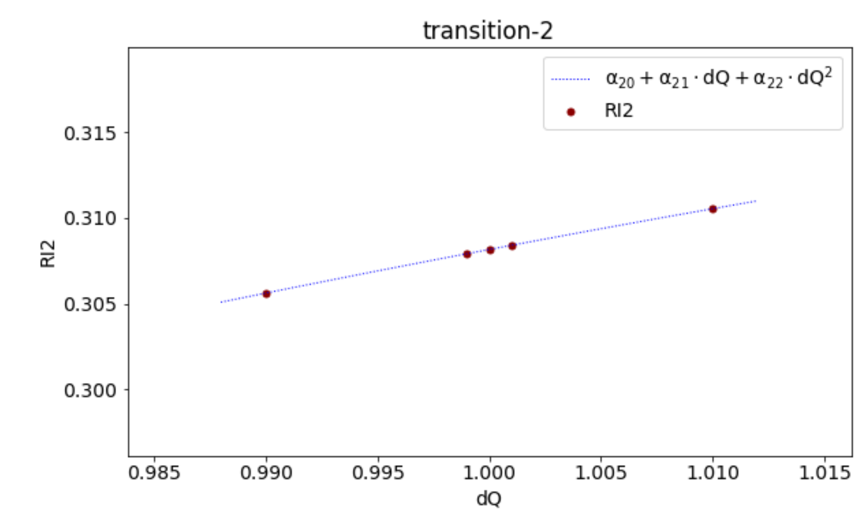












Fitting Cm-248

For each transition, I use the following formulas:

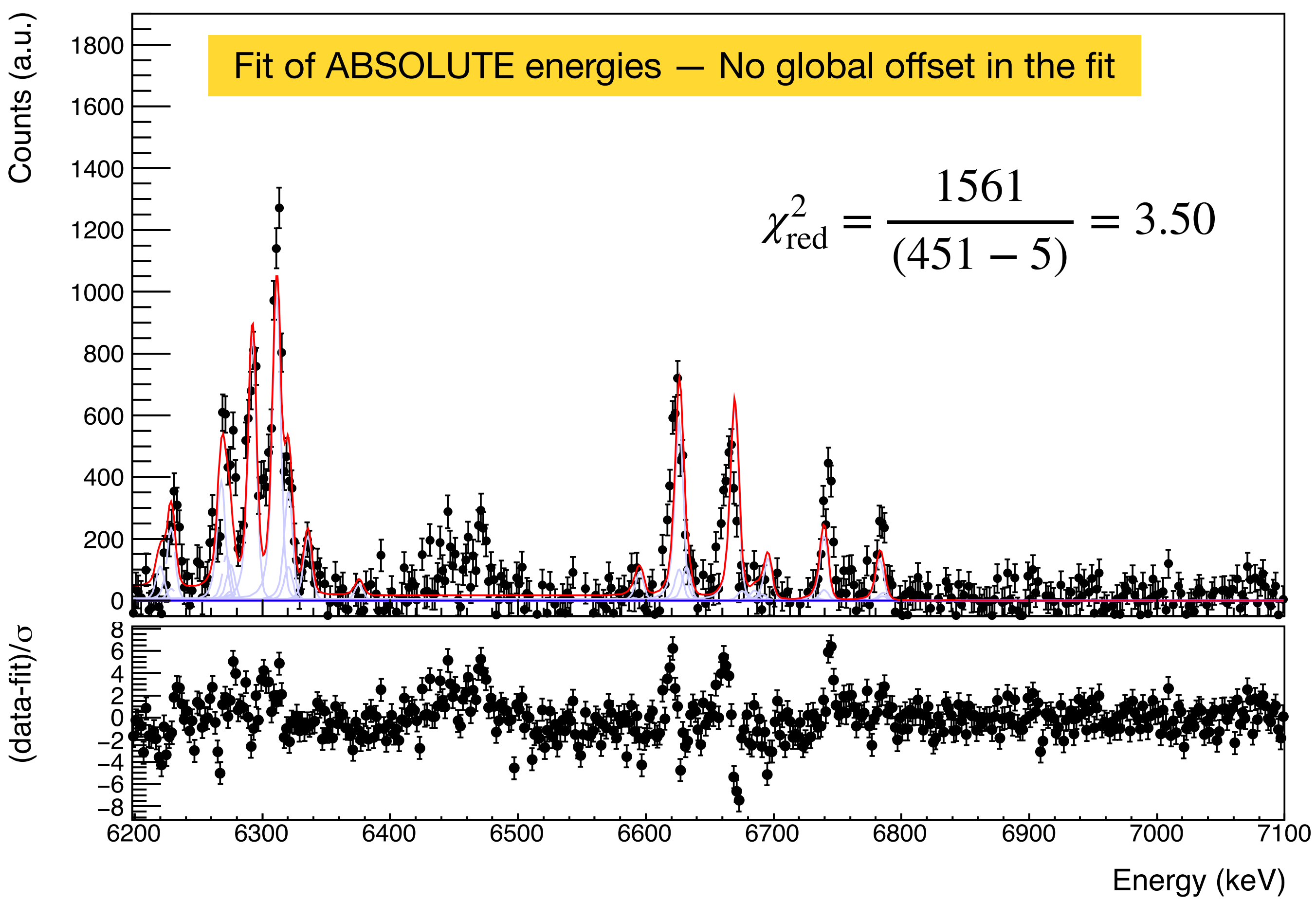
$$\mathrm{En} = c_0 \cdot 1 + c_1 \cdot \mathrm{dR} + c_2 \cdot \mathrm{dQ} + c_3 \cdot \mathrm{dR}^2 + c_4 \cdot \mathrm{dR}^2 \cdot \mathrm{dQ} + c_5 \cdot \mathrm{dR}^2 \cdot \mathrm{dQ}^2 + c_6 \cdot \mathrm{dQ}^2 + c_7 \cdot \mathrm{dR} \cdot \mathrm{dQ}^2 + c_8 \cdot \mathrm{dR} \cdot \mathrm{dQ}$$

$$\mathrm{RI} = c_0 \cdot 1 + c_1 \cdot \mathrm{dR} + c_2 \cdot \mathrm{dQ} + c_3 \cdot \mathrm{dR}^2 + c_4 \cdot \mathrm{dR}^2 \cdot \mathrm{dQ} + c_5 \cdot \mathrm{dR}^2 \cdot \mathrm{dQ}^2 + c_6 \cdot \mathrm{dQ}^2 + c_7 \cdot \mathrm{dR} \cdot \mathrm{dQ}^2 + c_8 \cdot \mathrm{dR} \cdot \mathrm{dQ}$$

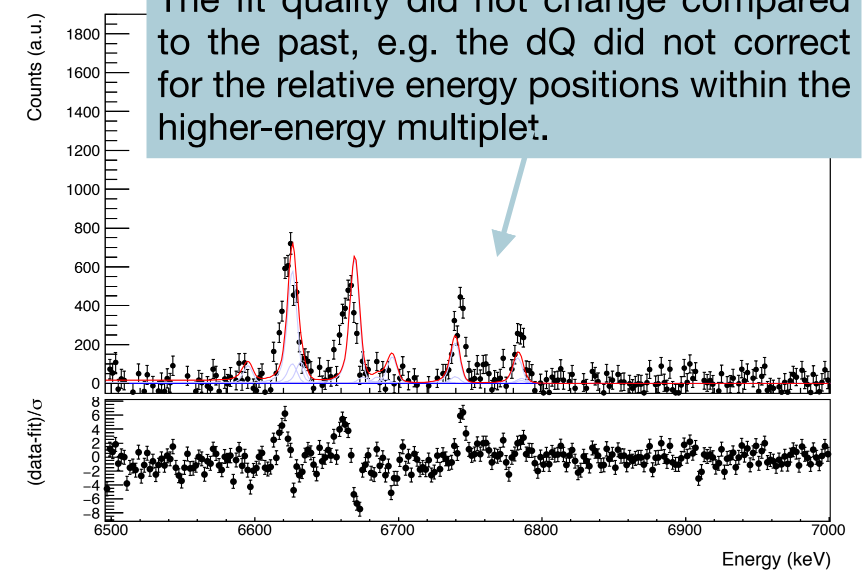
# of transitions = 30

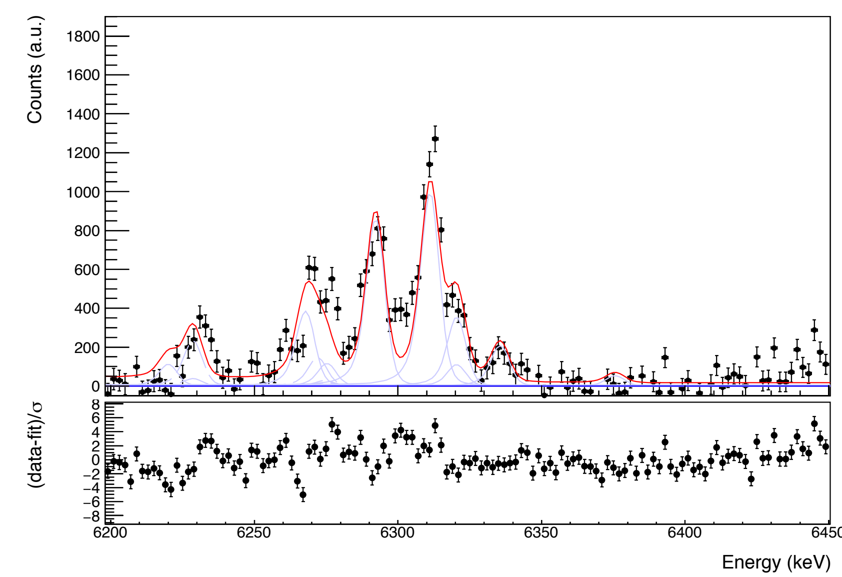
Definition of dR: $\mathrm{dR} = \dfrac{\mathrm{R}}{\mathrm{R}_0}$

Definition of dQ: $\mathrm{dQ} = \dfrac{\mathrm{Q}}{\mathrm{Q}_0}$



The fit quality did not change compared to the past, e.g. the dQ did not correct for the relative energy positions within the higher-energy multiplet.





- Using above formulas
- Free dQ and dR in [0.98, 1.02]
- En range: 6198 to 7100
- Transitions included: all 30 FE + SE (tr 7, 9,18, 21, 23, 26, 28, 29)

Line-shape: (Voigt + Tail + Step)

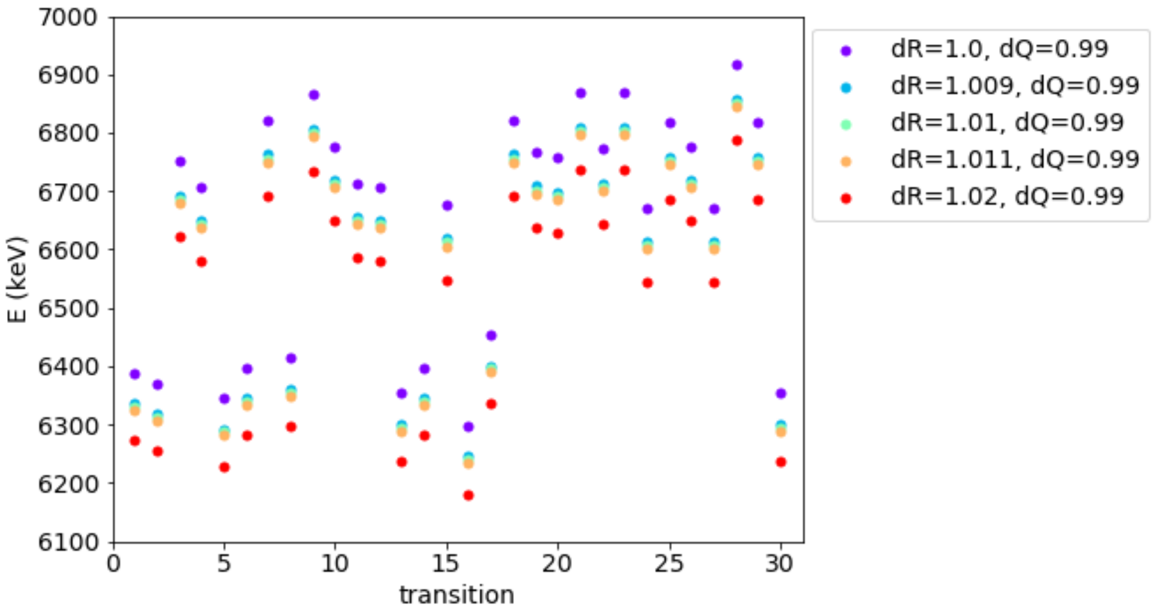
- Parameters as obtained in slide 33
- Same sigma for FE and SE (slide 33)
- A (step) free
- Natural line-width as calculated by Natalia (lw_2p32~1.628 keV, lw_2p12~1.482keV)

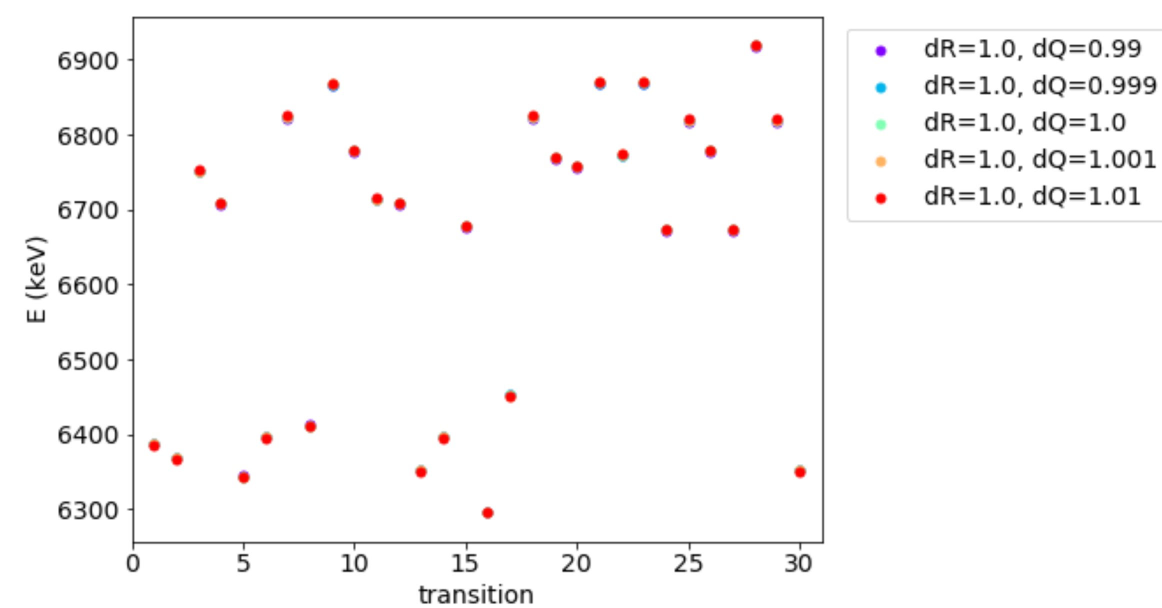
```
RooFitResult: minimized FCN value: -1.242e+05, estimated distance to minimum: 4.68e-06
                covariance matrix quality: Full, accurate covariance matrix
                Status : MIGRAD=0 HESSE=0

    Floating Parameter    InitialValue    FinalValue +/-  Error     GblCorr.
  --------------------  ------------  --------------------------  --------
                     A    1.0000e-04    7.9958e-04 +/-  1.71e-05  <none>
                Counts    2.0001e+05    5.0361e+03 +/-  2.81e+01  <none>
                  Nbkg    1.0000e+01    2.9548e+01 +/-  5.25e+00  <none>
                    dQ    1.0000e+00    1.0080e+00 +/-  2.73e-04  <none>
                    dR    1.0130e+00    1.0128e+00 +/-  5.78e-06  <none>
```

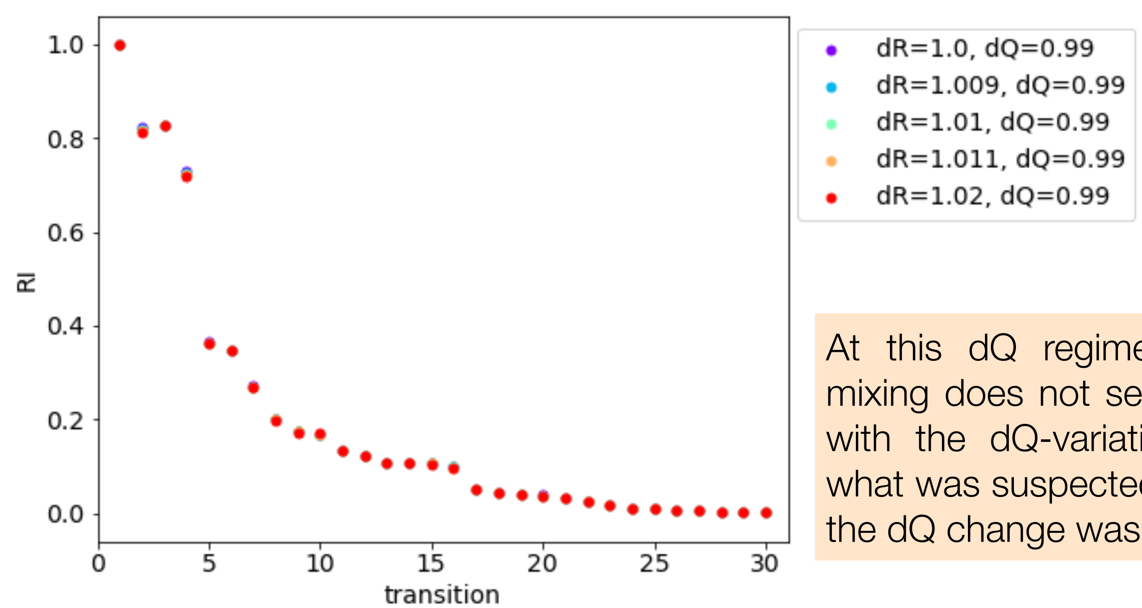
E/RI vs dQ vs dR dependence

Using the $\mathrm{En/RI} = c_0 \cdot 1 + c_1 \cdot \mathrm{dR} + c_2 \cdot \mathrm{dQ} + c_3 \cdot \mathrm{dR}^2 + c_4 \cdot \mathrm{dR}^2 \cdot \mathrm{dQ} + c_5 \cdot \mathrm{dR}^2 \cdot \mathrm{dQ}^2 + c_6 \cdot \mathrm{dQ}^2 + c_7 \cdot \mathrm{dR} \cdot \mathrm{dQ}^2 + c_8 \cdot \mathrm{dR} \cdot \mathrm{dQ}$ function, different plots are illustrated below.

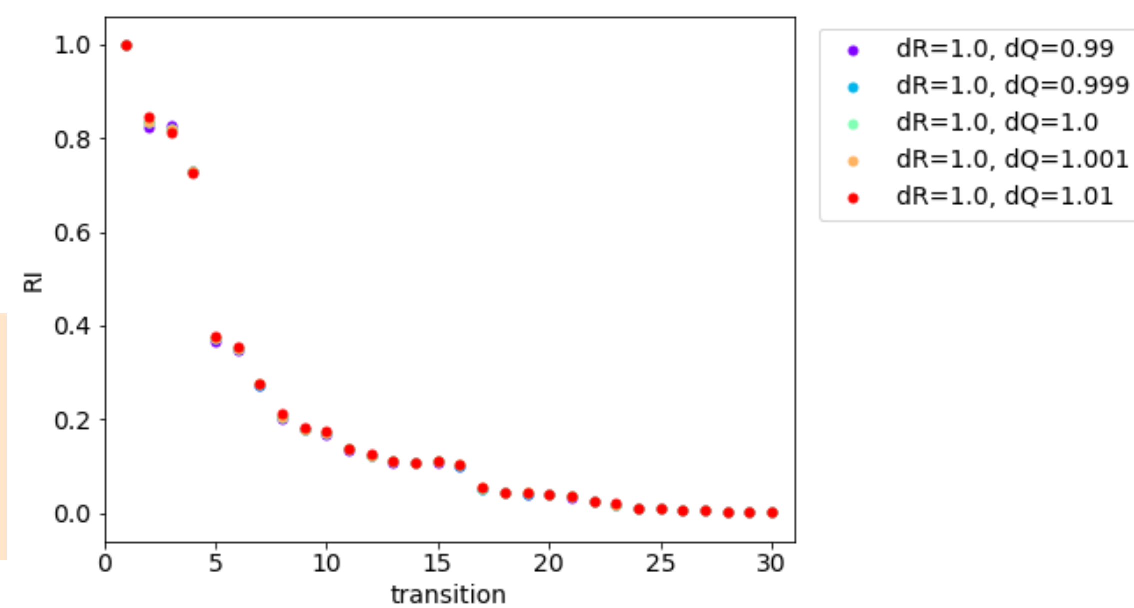




- The energy varies much more with the dR than with the dQ change.
- The dR variation shifts all transitions at the same direction, i.e. the dR increase shifts all transitions to lower energies, even - more or less - by the same amount.



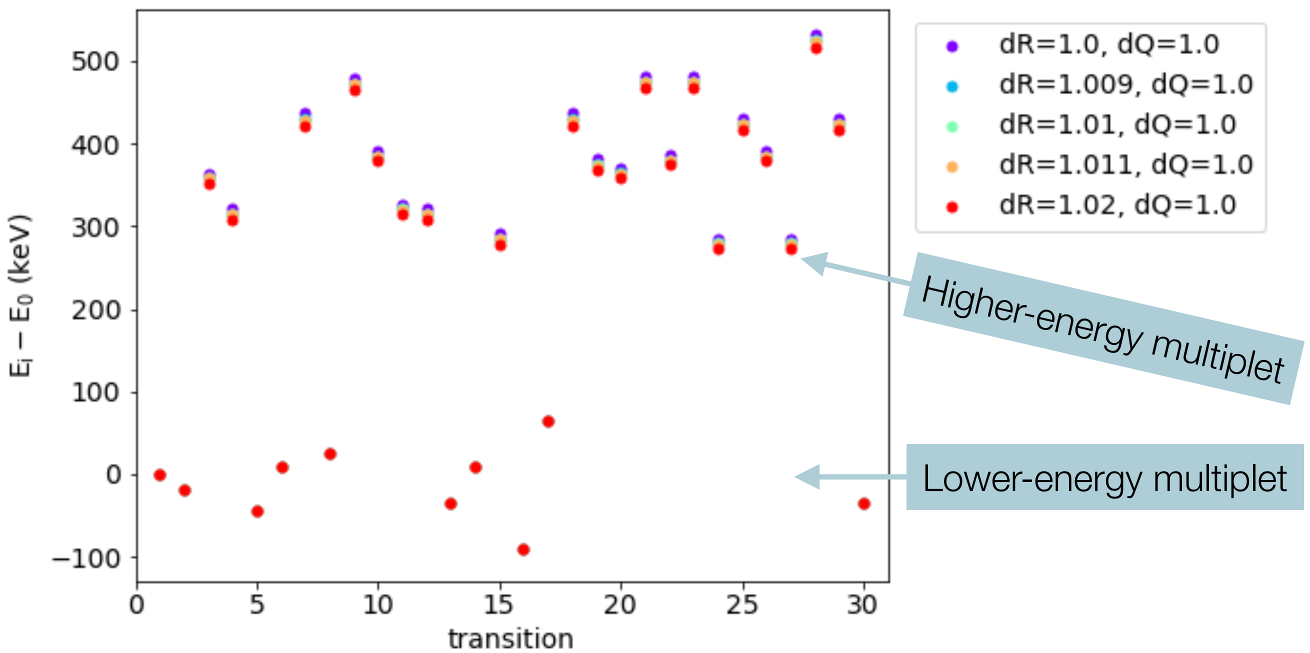
At this dQ regime, the transitions' mixing does not seem to be affected with the dQ-variation (compared to what was suspected in the past when the dQ change was more extreme)

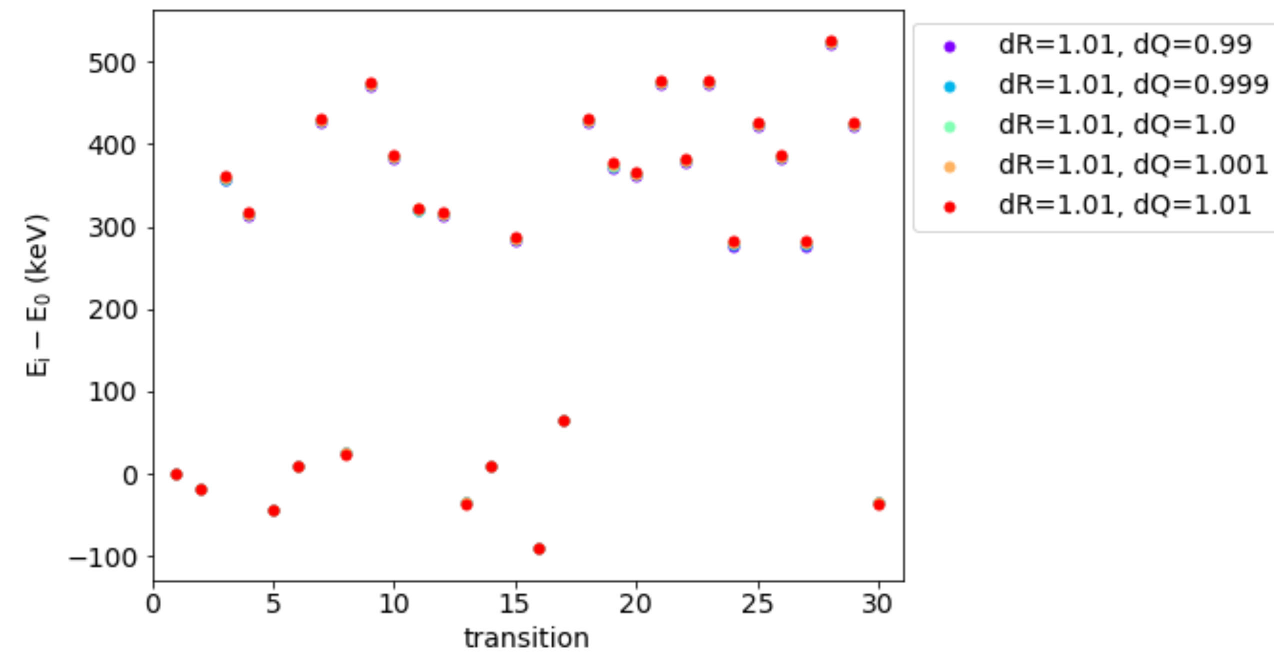


E/RI vs dQ vs dR dependence

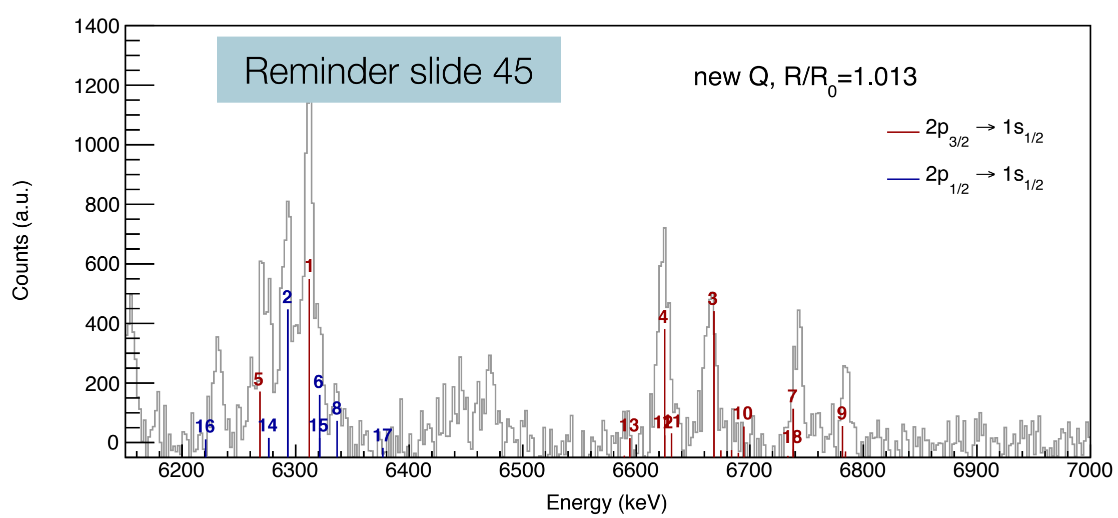
Using the $En/RI = c_0 \cdot 1 + c_1 \cdot dR + c_2 \cdot dQ + c_3 \cdot dR^2 + c_4 \cdot dR^2 \cdot dQ + c_5 \cdot dR^2 \cdot dQ^2 + c_6 \cdot dQ^2 + c_7 \cdot dR \cdot dQ^2 + c_8 \cdot dR \cdot dQ$ function, different plots are illustrated below.

E_0 is the most intense transition of the multiplet (transition-1)



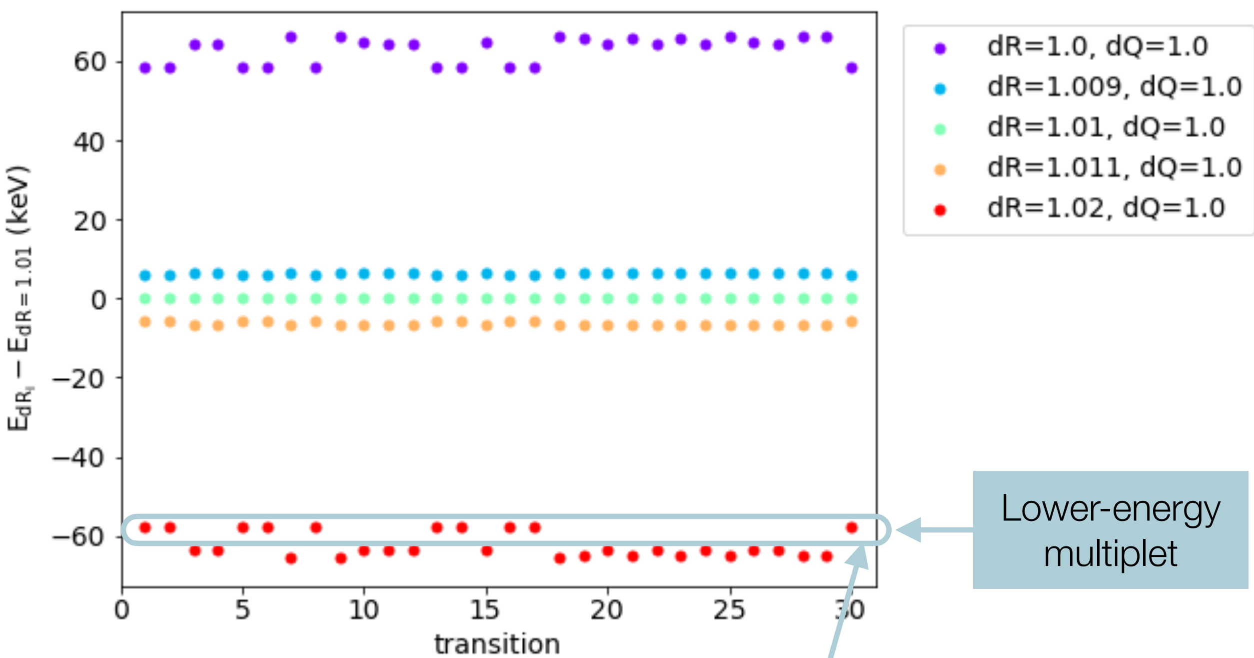


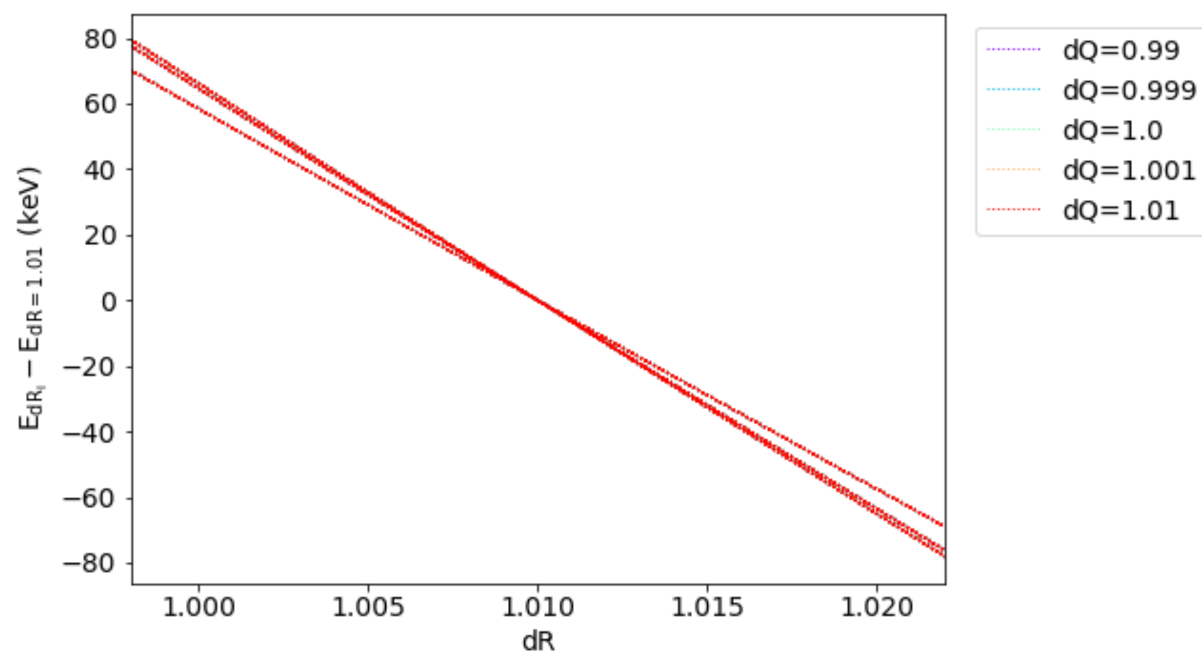
As expected from previous observations the dR variation has a bigger effect on the relative shift of the transitions than the dQ variation.



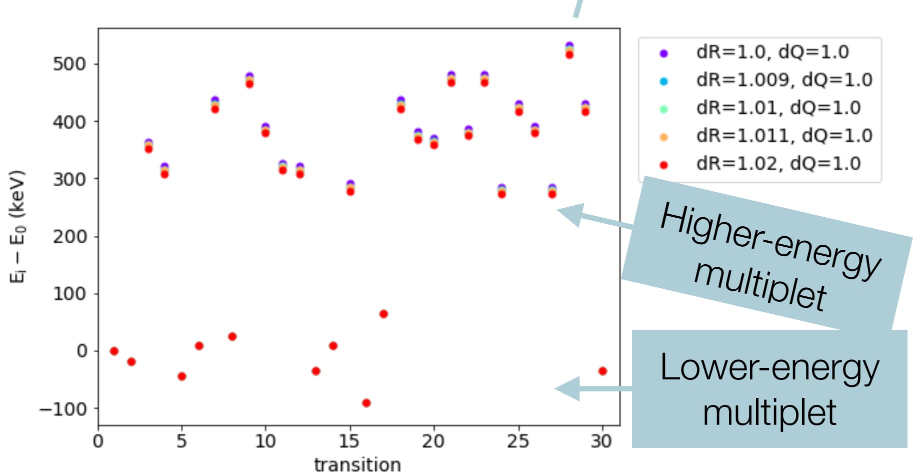
E/RI vs dQ vs dR dependence

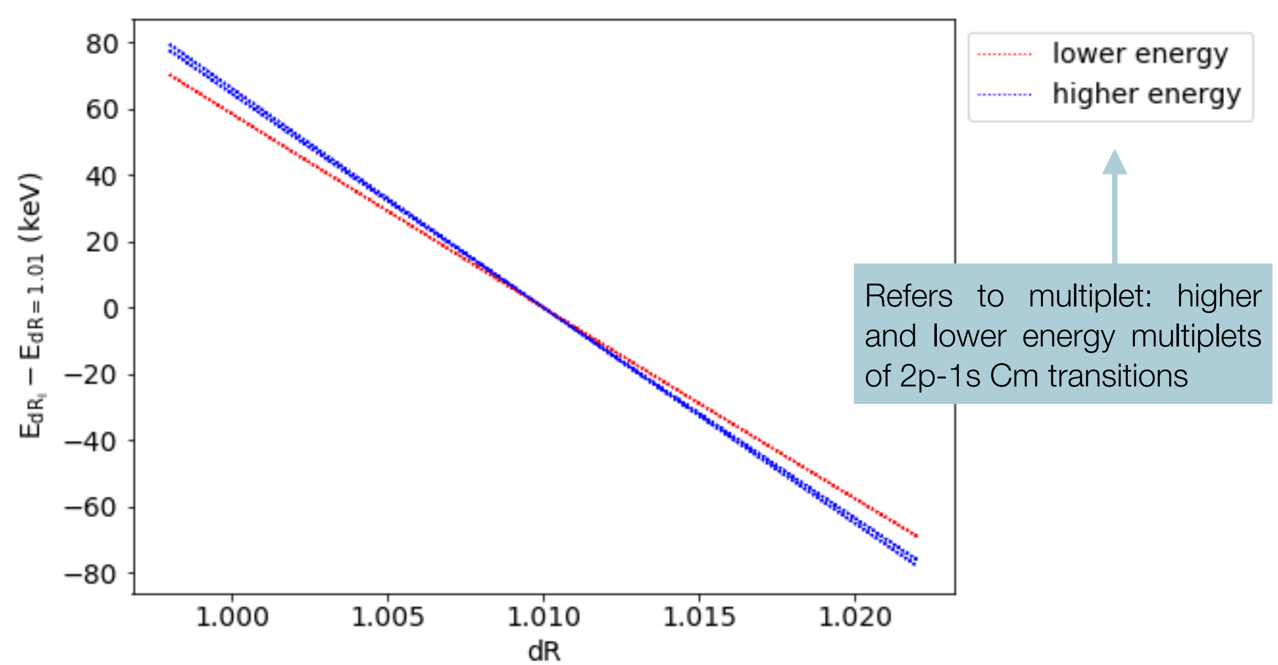
Using the $En/RI = c_0 \cdot 1 + c_1 \cdot dR + c_2 \cdot dQ + c_3 \cdot dR^2 + c_4 \cdot dR^2 \cdot dQ + c_5 \cdot dR^2 \cdot dQ^2 + c_6 \cdot dQ^2 + c_7 \cdot dR \cdot dQ^2 + c_8 \cdot dR \cdot dQ$ function, different plots are illustrated below.





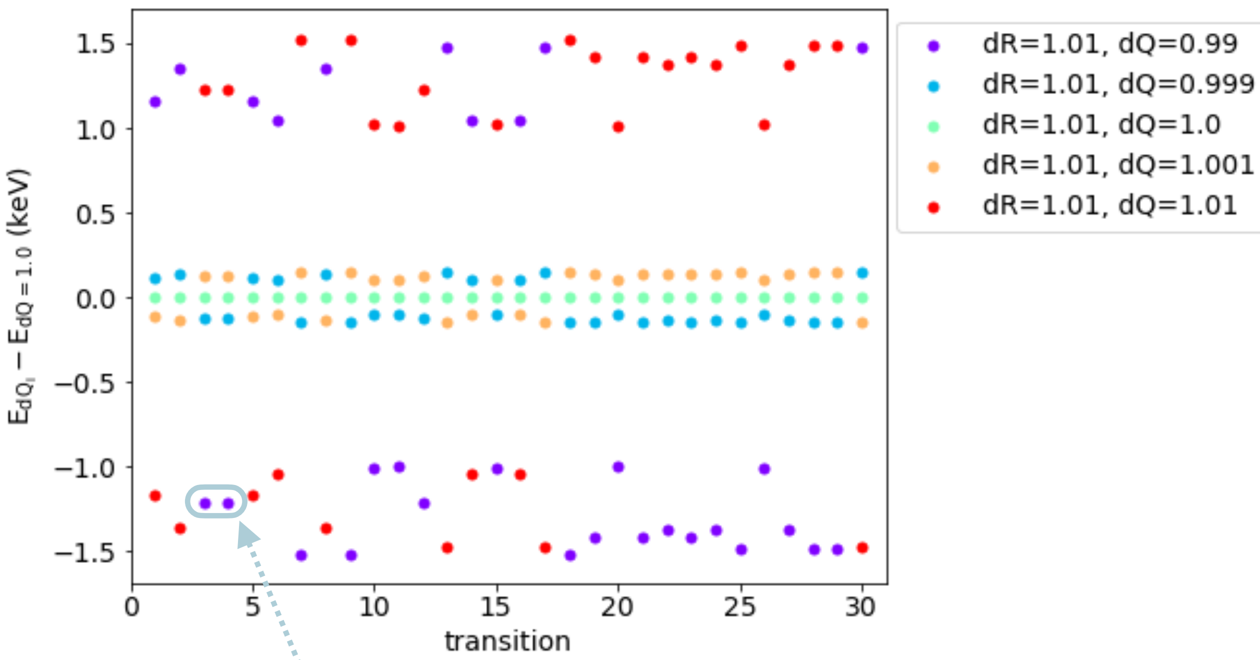
- The dR variation shifts all transitions at the same direction
- The energy change for all transitions belonging in the same multiplet (lower- or higher-energy one) is almost the same

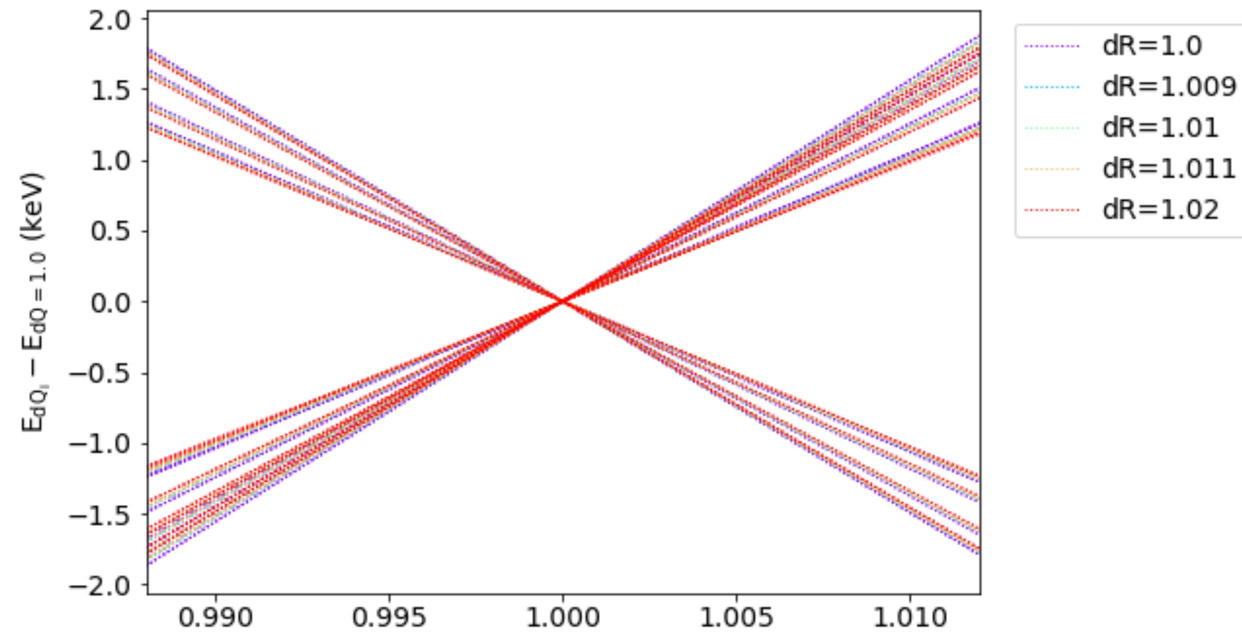




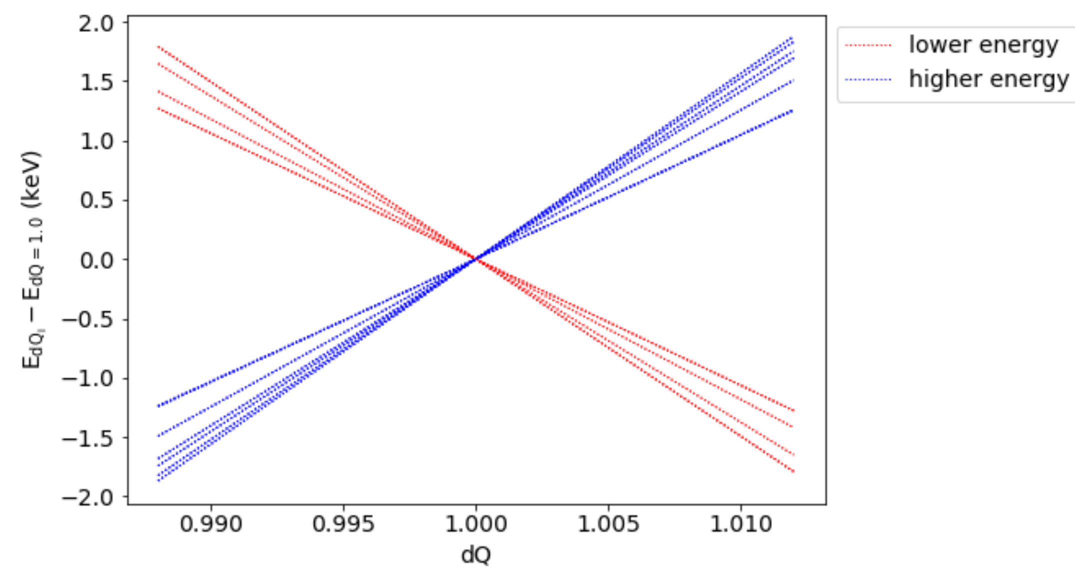
E/RI vs dQ vs dR dependence

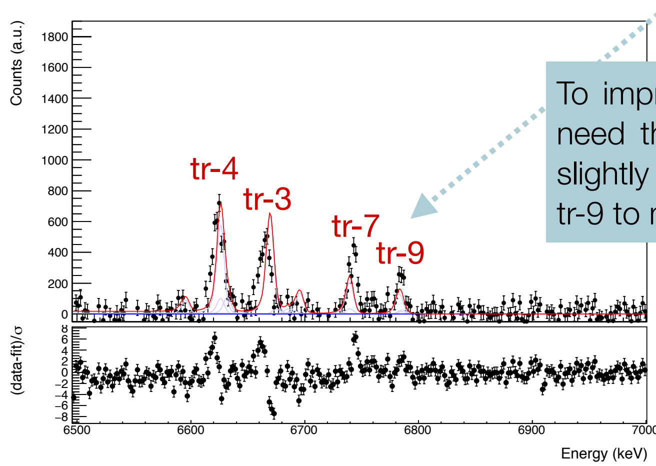
Using the $\mathrm{En/RI} = c_0 \cdot 1 + c_1 \cdot dR + c_2 \cdot dQ + c_3 \cdot dR^2 + c_4 \cdot dR^2 \cdot dQ + c_5 \cdot dR^2 \cdot dQ^2 + c_6 \cdot dQ^2 + c_7 \cdot dR \cdot dQ^2 + c_8 \cdot dR \cdot dQ$ function, different plots are illustrated below.





- The dQ variation shifts the transitions belonging in a different multiplet (lower- vs higher-energy) to a different energy direction, i.e. for the lower-energy multiplet's transitions, the energy decreases with the dQ increase while the for the higher-energy multiplet's transitions the energy increases with the dQ increase. However, the relative energy shift for a dQ value for transitions belonging in the same multiplet is very small, e.g. the energy shift of transitions 7 and 9 relative to transitions 3 and 4 is ~0.5 keV. This means that the dQ effect cannot correct for the bad reduced chi-square of the 2p-1s fit in that region which is bigger than 0.5 keV (sth like ~5 keV?).





To improve the pull distribution we need the tr-3 and tr-4 to move to slightly lower energies and tr-7 and tr-9 to move to higher energies.

E/RI vs dQ vs dR dependence

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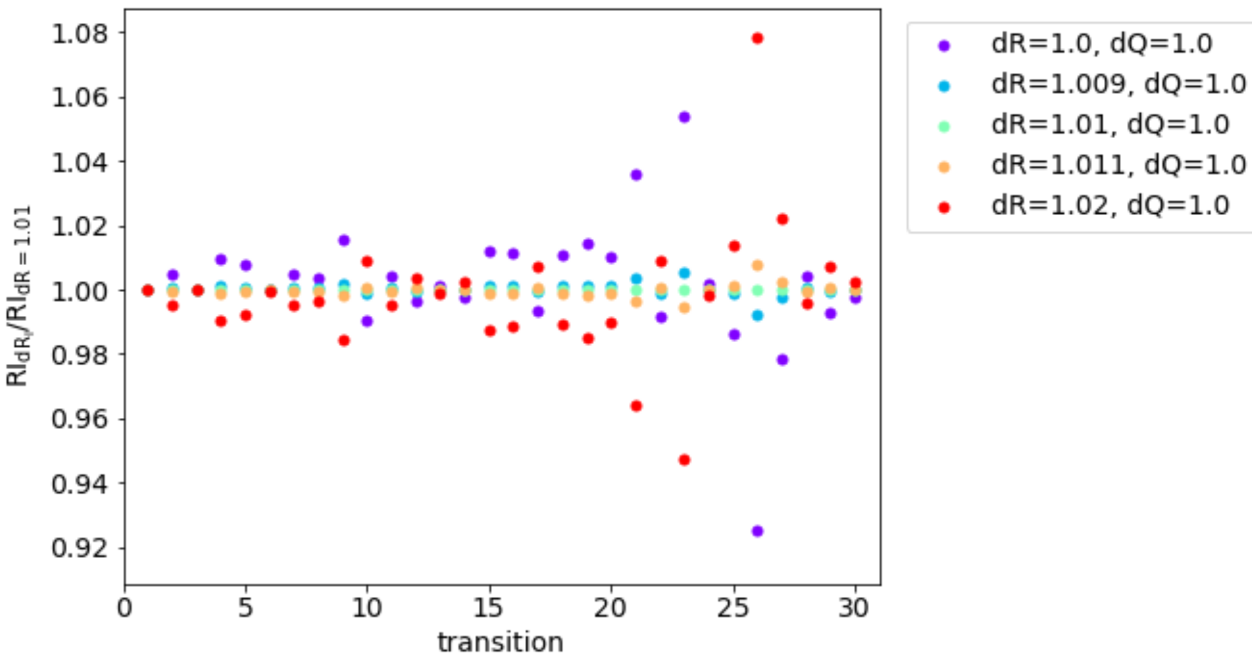

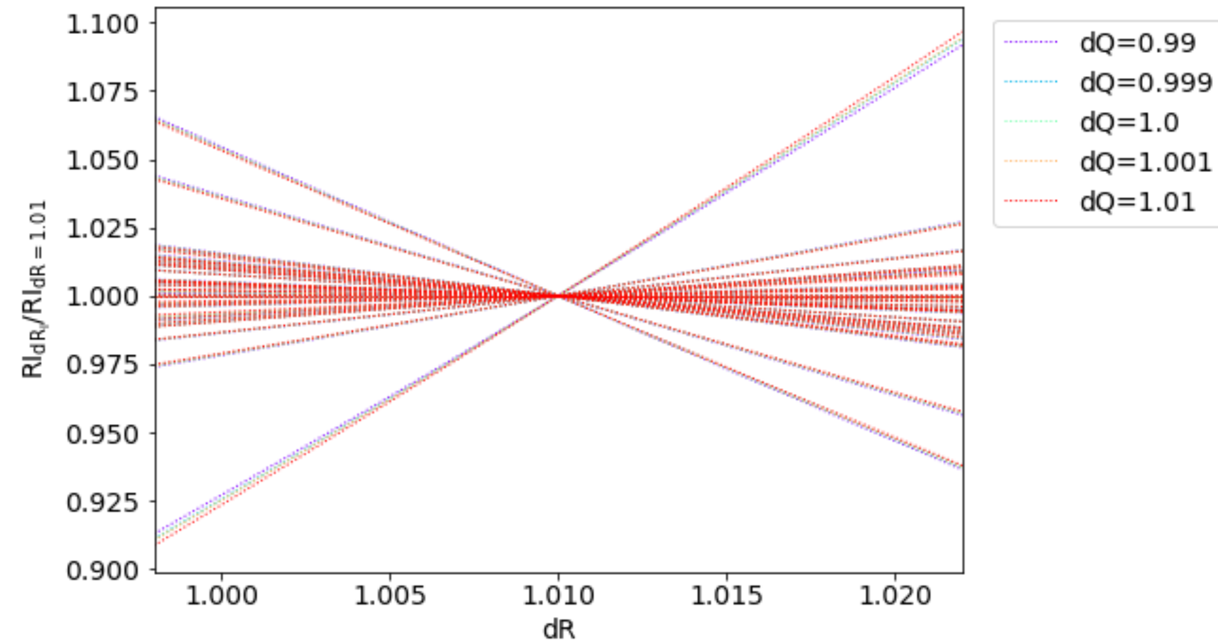

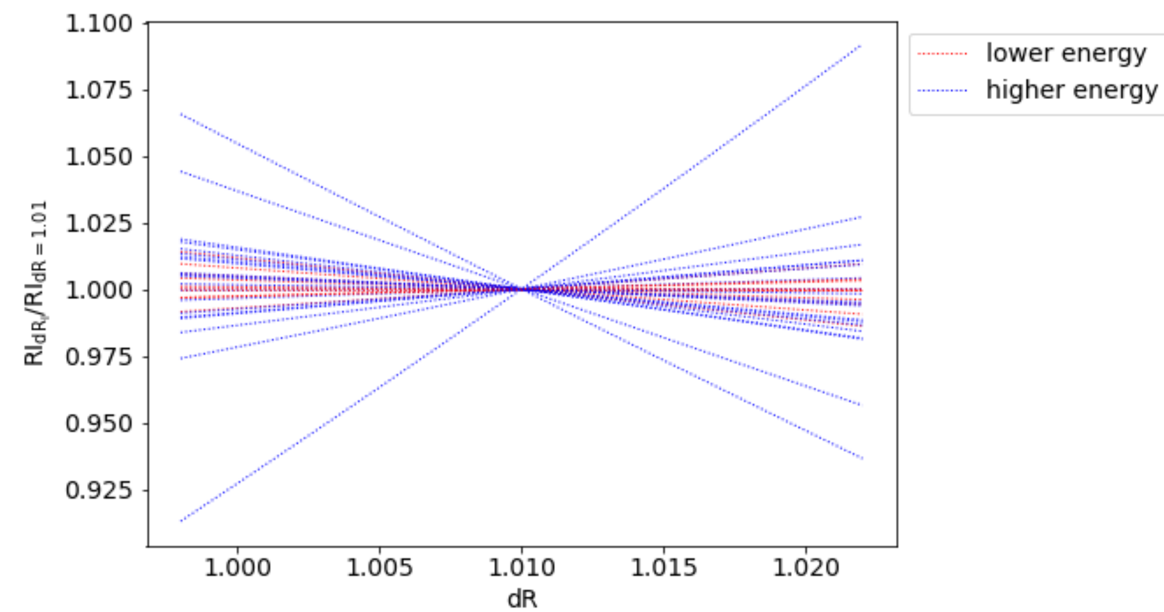

E/RI vs dQ vs dR dependence

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