Sample Calculation: Spectroscopy Analysis Program

This document shows a sample input and output of my crystal field theory program.

Raw Input:

```
#Popova M N, Chukalina E P, Stanislavchuk T N, et al, 2007. Optical
   ↪ spectra, crystal-field parameters, and magnetic susceptibility of
   ↪ multiferroic NdFe3(BO3)4[J/OL]. Physical Review B, 75(22): 224435.
   ↪ DOI:10.1103/PhysRevB.75.224435.

ion ND3+

SYMMETRY D3

time 15

**************************

4I9/2
0.0
8.05897287
17.481771918
27.400507758
39.922911756

4F9/2
1809.177417216
1813.0209273540002
1814.012800938
1825.419347154
1837.44581436

4G7/2
2337.1021323
2342.3094686160002
2347.764773328
2354.831872614
```

Raw Output:

```
************************************************************
**beta program for spectroscopy analysis with crystal field**
**author: Qi Dawei                                         **
**Powered by PyCrystalField                                **
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 ********************************************************
 *                PyCrystalField 2.3.11                 *
```

```
 *  Please cite  J. Appl. Cryst. (2021). 54, 356-362   *
 *    <https://doi.org/10.1107/S160057672001554X>      *
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The following term symbols will be fitted:
['4F9/2', '4G7/2', '4I9/2']
Ion: ND3+
Energy unit: mev

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************************Resuls************************************

Fitted Crystal Field Parameters:
Ar20: 31.5158086018825
Ar40: -16.911661234029147
Ar43: -222.88865726665648
Ar60: 4.769473864736957
Ar63: -33.10401997471025
Ar66: -35.78089352092562

Sum of Squared Differences: 34.69375262517639

Comparison between theoretical and experimental energies:
Theoretical      Experimental
4F9/2
  0.000000  :    0.000000
  2.779131  :    3.843510
  5.724535  :    4.835384
 12.717900  :   16.241930
 27.542482  :   28.268397

4G7/2
  0.000000  :    0.000000
  6.369339  :    5.207336
 12.658573  :   10.662641
 15.443154  :   17.729740

4I9/2
  0.000000  :    0.000000
  5.766333  :    8.058973
 18.578504  :   17.481772
 26.874177  :   27.400508
 38.333570  :   39.922912
```