Sample Calculation: Spectroscopy Analysis Program

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

Raw Input:

```
#Duan C kui, Tanner P A, Makhov V N, et al, 2007. Vacuum ultraviolet spectra
   ↪ and crystal field analysis of YAlO3 doped with Nd3+ and Er3+[J/OL].
   ↪ Physical Review B, 75(19): 195130. DOI:10.1103/PhysRevB.75.195130.


ION er3+

symmetry C1H

time 300

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

4I15/2
0.0
6.323194098
21.201297858
27.028555164
32.979796668
48.105868824
54.924999714
63.975846168000004

4I13/2
818.543675196
823.379058918
826.8506164620001
832.55388957
839.7449730540001
844.8283251720001
851.523471864

4I11/2
1274.805523836
1276.169350014
1279.764891756
1282.864496706
1287.203943636
1289.683627596

4I9/2
1536.536165814
1543.107328308
1565.176515552
```

1568.1521363040001
1578.5668089360001

4F9/2
1892.370814074
1902.413534112
1906.133060052
1908.8607124080002
1919.399369238

4S3/2
2282.053148388
2292.095868426

2H11/2
2370.453881562
2375.785202076
2379.25675962
2385.45596952
2389.79541645
2393.266973994

4F7/2
2539.444343436
2548.49518989
2556.182210166
2564.61313563

4F5/2
2751.953258808
2755.796768946
2759.7642632820002

4F3/2
2792.868044148
2806.506305928

2G9/2
3035.009182842
3040.8364401480003
3058.194227868
3062.161722204
3070.592647668

4G11/2
3261.776280984
3263.5120597560003
3270.827127438
3280.4978948820003
3282.605626248
3288.804836148

Raw Output:

```
************************************************************
**beta program for spectroscopy analysis with crystal field**
**author: Qi Dawei                                         **
**Powered by PyCrystalField                                **
************************************************************
 ******************************************************
 *                PyCrystalField 2.3.11               *
 *  Please cite  J. Appl. Cryst. (2021). 54, 356-362   *
 *    <https://doi.org/10.1107/S160057672001554X>      *
 ******************************************************

The following term symbols will be fitted:
['4I15/2', '4I13/2', '4I11/2', '4F9/2', '4I9/2', '4S3/2', '2H11/2', '4F7/2',
   ↪ '4F5/2', '4F3/2', '2G9/2', '4G11/2']
Ion: ER3+
Energy unit: mev

======================================================================
************************Resuls************************************

Fitted Crystal Field Parameters:
Ar20: -30.47960685118962
Ar22: 61.35358765873905
Ar40: -3.360583706316399
Ar42: 75.98064600294201
Ar4-2: -85.3239932149706
Ar44: -52.31873880736281
Ar4-4: 4.259702912239502
Ar60: -4.248157792495738
Ar62: -28.276507563904648
Ar6-2: -3.415024115631354
Ar64: 19.076244182877826
Ar6-4: 13.370056359693368
Ar66: -10.9541258223984
Ar6-6: -18.18427882741528

Sum of Squared Differences: 1217.325821329331

Comparison between theoretical and experimental energies:
Theoretical      Experimental
4I15/2
  0.000000  :    0.000000
  7.692718  :    6.323194
 19.152384  :   21.201298
 25.236258  :   27.028555
 32.820952  :   32.979797
 43.122858  :   48.105869
 50.603322  :   54.925000
 60.303258  :   63.975846
```

```
4I13/2
  0.000000  :    0.000000
  5.660097  :    4.835384
 13.130281  :    8.306941
 18.281432  :   14.010214
 25.737684  :   21.201298
 29.633937  :   26.284650
 36.417980  :   32.979797

4I11/2
  0.000000  :    0.000000
  3.501239  :    1.363826
  7.919295  :    4.959368
 12.876316  :    8.058973
 14.276823  :   12.398420
 17.915491  :   14.878104

4F9/2
  0.000000  :    0.000000
  7.234806  :   10.042720
 16.556667  :   13.762246
 24.327675  :   16.489898
 35.778836  :   27.028555

4I9/2
  0.000000  :    0.000000
 11.810102  :    6.571162
 17.674642  :   28.640350
 21.324751  :   31.615970
 28.812322  :   42.030643

4S3/2
  0.000000  :    0.000000
 11.632025  :   10.042720

2H11/2
  0.000000  :    0.000000
  8.047581  :    5.331321
 10.784300  :    8.802878
 14.913199  :   15.002088
 22.518333  :   19.341535
 38.081599  :   22.813092

4F7/2
  0.000000  :    0.000000
 10.695892  :    9.050846
 16.886347  :   16.737867
 25.792223  :   25.168792

4F5/2
```

```
  0.000000  :    0.000000
  2.623656  :    3.843510
  7.660233  :    7.811004

4F3/2
  0.000000  :    0.000000
 14.690177  :   13.638262

2G9/2
  0.000000  :    0.000000
  7.088498  :    5.827257
 16.584936  :   23.185045
 22.007333  :   27.152539
 31.576225  :   35.583465

4G11/2
  0.000000  :    0.000000
  3.586235  :    1.735779
  8.630650  :    9.050846
 23.270059  :   18.721614
 27.746260  :   20.829345
 30.389769  :   27.028555
```