Sample Calculation: Spectroscopy Analysis Program

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

Raw Input:

```
#Capobianco J A, Kabro P, Ermeneux F S, et al, 1997. Optical spectroscopy,
   ↪  fluorescence dynamics and crystal field analysis of Er3+ in YVO4[J/
   ↪ OL]. Chemical Physics, 214(2): 329-340. DOI:10.1016/S0301-0104(96)
   ↪ 00318-7.

ion er3+

symmetry d2d

time 5

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

4I15/2
0.0
4.711399524
5.0833521180000005
7.934988672
17.729740314
30.624096906000002
33.227765064
37.1952594

4I13/2
810.980639118
811.352591712
816.43594383
817.05586482
822.759137928
830.07420561
832.181936976

4I11/2
1262.655072432
1263.6469460160001
1264.762803798
1268.606313936
1270.094124312
1273.565681856

4I9/2
1530.832892706
None
None
```

```
None
1558.977305652

4F9/2
1885.303714788
1888.651288134
1894.354561242
1899.685881756
1902.165565716

4S3/2
2275.72995429
2276.34987528

2H11/2
2360.03920893
2365.61849784
2370.825834156
2374.2973917
2375.289265284
2380.868554194

4F7/2
2534.1130229220003
2539.568327634
2544.2797271580002
2545.39558494

4F5/2
2742.6544439580002
2745.382096314
2749.9695116400003

4F3/2
2787.040786842
2793.611949336
```

Raw Output:

```
************************************************************
**beta program for spectroscopy analysis with crystal field**
**author: Qi Dawei                                        **
**Powered by PyCrystalField                               **
************************************************************
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']
Ion: ER3+
Energy unit: mev

============================================================
```

```
************************Resuls************************************

Fitted Crystal Field Parameters:
Ar20: 18.24644022115434
Ar40: 23.75006350758516
Ar44: -72.43264517955416
Ar60: -1.1479712622025853
Ar64: 3.4479837772568334

Sum of Squared Differences: 216.9567651716691

Comparison between theoretical and experimental energies:
Theoretical      Experimental
4I15/2
  0.000000  :    0.000000
  3.711092  :    4.711400
  4.319350  :    5.083352
 10.090448  :    7.934989
 17.452314  :   17.729740
 27.046633  :   30.624097
 30.209278  :   33.227765
 36.904743  :   37.195259

4I13/2
  0.000000  :    0.000000
  1.632832  :    0.371953
  4.618629  :    5.455305
  8.598081  :    6.075226
 16.984992  :   11.778499
 19.647542  :   19.093566
 26.566464  :   21.201298

4I11/2
  0.000000  :    0.000000
  0.890926  :    0.991874
  2.973512  :    2.107731
  6.121109  :    5.951242
  8.033370  :    7.439052
 12.471179  :   10.910609

4F9/2
  0.000000  :    0.000000
  4.015220  :    3.347573
 11.527573  :    9.050846
 15.529818  :   14.382167
 18.952285  :   16.861851

4I9/2
  0.000000  :    0.000000
  3.974268  :   None
 13.582893  :   None
```

```
 15.418996  :   None
 20.873354  :   28.144413

4S3/2
  0.000000  :    0.000000
  4.541831  :    0.619921

2H11/2
  0.000000  :    0.000000
  2.477028  :    5.579289
  9.575160  :   10.786625
 11.153058  :   14.258183
 16.883041  :   15.250056
 19.811415  :   20.829345

4F7/2
  0.000000  :    0.000000
  8.099417  :    5.455305
  8.649881  :   10.166704
 11.299532  :   11.282562

4F5/2
  0.000000  :    0.000000
  1.777979  :    2.727652
  5.222356  :    7.315068

4F3/2
  0.000000  :    0.000000
  5.735914  :    6.571162
```