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 nd3+

symmetry C1H

time 5

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4G7/2
2336.606195508
2345.7810261600002
2355.327809406
2366.85833982

4G9/2
2400.4580574780002
None
2408.269061952
2417.319908406
None
```

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:
['4G7/2', '4G9/2']
```

```
Ion: ND3+
Energy unit: mev

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

Fitted Crystal Field Parameters:
Ar20: -142.98044776985853
Ar22: -194.29633059111381
Ar40: -10.745368524381611
Ar42: -59.387015258660895
Ar4-2: 45.28040859408949
Ar44: -1.5858845910550148
Ar4-4: -27.00894171543997
Ar60: 9.831741412062415
Ar62: -3.128751589586352
Ar6-2: 16.024718665025524
Ar64: -50.52444721398157
Ar6-4: 25.07625885844527
Ar66: -45.69990599037913
Ar6-6: -9.567872264025667

Sum of Squared Differences: 6.62902424082586

Comparison between theoretical and experimental energies:
Theoretical      Experimental
4G7/2
  0.000000  :    0.000000
  9.687222  :    9.174831
 17.676409  :   18.721614
 31.441037  :   30.252144

4G9/2
  0.000000  :    0.000000
  7.172047  :   None
  9.772359  :    7.811004
 16.745030  :   16.861851
 27.419319  :   None
```