

Article

# JJ2LSJ Transformation and Unique Labeling for Energy Levels

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**Abstract:** The JJ2LSJ program, which is important not only for the GRASP2K package but for the atom theory in general, is presented. The program performs the transformation of atomic state functions (ASFs) from a *jj*-coupled CSF basis into an *LSJ*-coupled CSF basis. In addition, the program implements a procedure that assigns a unique label to all energy levels. Examples of how to use the JJ2LSJ program are given. Several cases are presented where there is a unique labeling problem.

**Keywords:** energy levels; *LSJ*-coupling; *jj*-coupling; JJ2LSJ transformation; unique label

## 1. Introduction

In principle, any valid coupling scheme can be used to represent the wave function in atomic structure calculations. Levels of an energy spectrum are identified and labeled with the help of sets of quantum numbers describing the coupling scheme used for the wave function. However, these quantum numbers are exact only for the cases of pure coupling. In a calculations of energy spectra one has to start with the coupling scheme closest to reality [1]. The most frequently used coupling schemes in atomic theory are the *LSJ* and *jj*. In atomic spectroscopy, the standard *LSJ* notation of the levels is frequently applied for classifying the low-lying level structures of atoms or ions.

Calculations may be performed in the relativistic (*jj*-coupling) scheme in order to get more accurate data that include relativistic effects. Thus, after a multiconfiguration Dirac-Hartree-Fock (MCDHF) or relativistic configuration interaction (RCI) [2] calculation the transformation to *LSJ*-coupling is needed. The JJ2LSJ code in GRASP2K [3] does this by applying a unitary transformation to the relativistic configuration state function (CSF) basis set which preserves orthonormality. The unitary transformation selected is the coupling transformation that changes the order of coupling from *jj* to *LSJ*, a transformation that does not involve the radial factor, only the spin-angular factor.

An energy level is normally assigned the label of the leading CSF in the wave function expansion. For many systems, two or more wave functions have the same leading CSFs giving rise to non-unique labels for the energy levels. We have such a situation for Si-like ions [4] and some other systems [5]. The new JJ2LSJ program implements a procedure that resolves these problems, assigning a unique label to all energy levels.

## 2. Theory

### 2.1. Transformation from *jj*- to *LSJ*-Coupling

Each nonrelativistic *nl*-orbital (except for *ns*) is associated with two relativistic orbitals  $l_{\pm} \equiv j = l \pm 1/2$ . In the transformation of the spin-angular factor  $|l^w \alpha LS\rangle$  into a *jj*-coupled angular basis, two subshell states, one with  $l_- \equiv j = l - 1/2$  and another one with  $l_+ \equiv j = l + 1/2$ , may occur in the expansion. This shell-splitting

$$|l^w \alpha \nu LS\rangle \longrightarrow (|l_-^{w_1} \nu_1 J_1\rangle, |l_+^{w_2} \nu_2 J_2\rangle) , \quad (1)$$

obviously conserves the number of electrons, provided ( $w = w_1 + w_2$ ), with  $w_1(\max) = 2l$  and  $w_2(\max) = 2(l + 1)$ . Making use of this notation, the transformation between the subshell states in *LSJ*- and *jj*-coupling can be written as

$$|l^w \alpha \nu LSJ\rangle = \sum_{\nu_1 J_1 \nu_2 J_2 w_1} |(l_-^{w_1} \nu_1 J_1, l_+^{(w-w_1)} \nu_2 J_2) J\rangle \langle (l_-^{w_1} \nu_1 J_1, l_+^{(w-w_1)} \nu_2 J_2) J | l^w \alpha \nu LSJ\rangle, \quad (2)$$

$$|(l_-^{w_1} \nu_1 J_1, l_+^{(w-w_1)} \nu_2 J_2) J\rangle = \sum_{\alpha \nu LS} |l^w \alpha \nu LSJ\rangle \langle l^w \alpha \nu LSJ | (l_-^{w_1} \nu_1 J_1, l_+^{(w-w_1)} \nu_2 J_2) J\rangle, \quad (3)$$

which, in both cases, includes a summation over all the quantum numbers (except of *n*,  $l_-$ , and  $l_+$ ). Here,  $|(l_-^{w_1} \nu_1 J_1, l_+^{w_2} \nu_2 J_2) J\rangle$  is a coupled angular state with well-defined total angular momentum *J* which is built from the corresponding *jj*-coupled subshell states with  $j_1 = l_- = l - \frac{1}{2}$ ,  $j_2 = l_+ = l + \frac{1}{2}$  and the total subshell angular momenta  $J_1$  and  $J_2$ , respectively.

An explicit expression for the coupling transformation coefficients

$$\langle (l_-^{w_1} \nu_1 J_1, l_+^{(w-w_1)} \nu_2 J_2) J | l^w \alpha \nu LSJ\rangle = \langle l^w \alpha \nu LSJ | (l_-^{w_1} \nu_1 J_1, l_+^{(w-w_1)} \nu_2 J_2) J\rangle \quad (4)$$

in (2) and (3) can be obtained only if we take the construction of the subshell states of *w* equivalent electrons from their corresponding *parent states* with  $w - 1$  electrons into account. In general, however, the *recursive* definition of the subshell states, out of their parent states, also leads to a recursive generation of the transformation matrices (4). These transformation coefficients can be chosen *real*: they occur very frequently as the *building blocks* in the transformation of all symmetry functions. The expressions and values of these coefficients are published in [6,7].

These transformation matrices, which are applied internally by the program JJ2LSJ, are consistent with the definition of the coefficients of fractional parentage [8,9] and with the phase system used in the [10]. So the program presented in the paper supports transformation from *jj*- to *LSJ*-coupling if ASF (which needs transformation) was created using the approach [7–10]. Otherwise the program may perform the transformation incorrectly.

### 2.2. Unique Labeling

An energy level is often given the label of the leading CSF in the wave function expansion. But it sometimes happens that two wave functions have the same largest CSF in *LSJ*- or *jj*-coupling, and then classification in energy spectra is not unique. The simplest way to have a unique identification of an energy level would be use a position number (POS) and symmetry *J*. But to get the energy spectra with unique labels in *LSJ*-coupling we should re-classify levels. For that purpose JJ2LSJ transformation with the unique labeling option can be used. To obtain unique labels the algorithm proposed in [11,12] is used: for a given set of wave functions with the same *J* and parity, the CSF with largest expansion coefficient is used as the label for the function containing this largest component. Once a label is assigned, the corresponding CSF is removed from consideration in the determination of the next label. In such a way we will get energy levels with unique labels. In this process, cases where

one CSF is dominant (defines more than 50 % of the wave function composition) that CSF will give the label for the corresponding energy level, but when the composition is spread over a number of CSFs, and none particularly large, the label is defined by the algorithm. Thus labeling is done by blocks of levels, each of the same  $J$  and parity. The first step is to order the levels by energy and assign the POS (position) identifier with the lowest having POS = 1, the second POS = 2, etc. and then proceed with determining the label.

In the Section 4 we will present a few examples where wave functions have the same dominant term and where the unique labeling algorithm is needed.

### 3. The JJ2LSJ Program

JJ2LSJ program is intended to perform the transformation of ASFs from a  $jj$ -coupled CSF basis into an  $LSJ$ -coupled CSF basis. This program is written in FORTRAN90 and is included in the GRASP2K package [3]. It uses the same libraries as other programs in GRASP2K. The program is based on the earlier published LSJ program [13], but modified for speed up. The new program transforms only the most important components of large expansions. In addition, the new program provides an option to choose unique labeling versus labeling by the leading CSF in the wave function expansion.

For running the JJ2LSJ program we need several input files generated with the GRASP2K package: the CSFs list file (name.c) and the mixing coefficients file after MCDHF (name.m) or after RCI calculations (name.cm). The example below shows the execution of the JJ2LSJ program for the odd states of Si-like Sr (Sr XXV) ion, built on a CSF basis containing orbitals with principal quantum numbers up to  $n = 7$  and expansion coefficients from RCI calculations. In the following example, the unique labeling option is chosen and the program is run in default mode. It should be remembered that the contribution to the wave function composition from a particular CSF is the square of the expansion coefficient. Thus a CSF with an expansion coefficient of 0.10 contributes 1% to the wave function composition.

```
>>jj2lsj

jj2lsj: Transformation of ASFs from a jj-coupled CSF basis
      into an LSJ-coupled CSF basis (Fortran 95 version)
      (C) Copyright by G. Gaigalas and Ch. F. Fischer,
      (2017).

Input files: name.c, name.(c)m
Output files: name.lsj.lbl,
      (optional) name.lsj.c, name.lsj.j,
      name.uni.lsj.lbl, name.uni.lsj.sum

Name of state
>>odd7
Loading Configuration Symmetry List File ...
There are 49 relativistic subshells;
There are 4420742 relativistic CSFs;
... load complete;

Mixing coefficients from a CI calc.?
>>y
Do you need a unique labeling? (y/n)
>>y
      nelec =          14
      ncftot =       4420742
      nw      =          49
      nblock =           5

      block   ncf     nev   2j+1  parity
         1  190132     2     1     -1
         2  703411     7     3     -1
         3 1095473     8     5     -1
```

```

      4 1276414      4      7      -1
      5 1155312      1      9      -1
Default settings? (y/n)
>>y
Maximum % of omitted composition is 1.000
Below 5.0E-03 the eigenvector component is to be neglected for calculating
Below 1.0E-03 the eigenvector composition is to be neglected for printing

. . . . .
Under investigation is the block:      1      The number of eigenvectors: 2
The number of CSF (in jj-coupling): 190132      The number of CSF (in LS-coupling): 184
Weights of major contributors to ASF in jj-coupling:

Level J Parity      CSF contributions

  1  0  -      0.89670 of      2  0.08762 of      1  0.00642 of      7  0.00250 of      13
           0.00204 of      9
      Total sum over weight (in jj) is: 0.99907840477285059

Definition of leading CSF:

      2) 2s ( 2)  2p-( 2)  2p ( 4)  3s ( 1)  3p-( 1)  3p ( 2)
                1/2      1/2
                1/2
                0

Weights of major contributors to ASF in LS-coupling:

Level J Parity      CSF contributions

  1  0  -      0.89670 of      2  0.08762 of      1  0.00821 of      4  0.00441 of      11
           0.00354 of      10
      Total sum over weight (in LSJ) is: 0.99862429376844597

Definition of leading CSF:

      1)  2s( 2)  2p( 6)  3s( 2)  3p( 1)  3d( 1)
           1S0      1S0      1S0      2P1      2D1      1S      1S      2P      3P      0
      2)  2s( 2)  2p( 6)  3s( 1)  3p( 3)
           1S0      1S0      2S1      2P1      1S      2S      3P      0
      4)  2s( 2)  2p( 6)  3s( 1)  3p( 1)  3d( 2)
           1S0      1S0      2S1      2P1      1S0      1S      2S      3P      3P      0
     11)  2s( 2)  2p( 6)  3p( 3)  3d( 1)
           1S0      1S0      2P1      2D1      1S      2P      3P      0

. . . . .
The new level is under investigation.
Weights of major contributors to ASF in jj-coupling:

Level J Parity      CSF contributions

  2  0  -      0.88679 of      1  0.08724 of      2  0.00640 of      4  0.00505 of      13
           0.00354 of      10
      Total sum over weight (in jj) is: 0.99887286591520896

Definition of leading CSF:

      1) 2s ( 2)  2p-( 2)  2p ( 4)  3s ( 2)  3p ( 1)  3d-( 1)
                3/2      3/2
                3/2
                0
    
```

Weights of major contributors to ASF in LS-coupling:

| Level | J | Parity | CSF contributions                                      |   |            |   |            |    |            |   |  |  |  |  |  |  |  |  |
|-------|---|--------|--|---|------------|---|------------|----|------------|---|--|--|--|--|--|--|--|--|
| 2     | 0 | -      | 0.88679 of   | 1 | 0.08724 of | 2 | 0.00852 of | 11 | 0.00670 of | 3 |  |  |  |  |  |  |  |  |
|       |   |        | 0.00537 of   | 8 | 0.00251 of | 6 |            |    |            |   |  |  |  |  |  |  |  |  |
|       |   |        | Total sum over weight (in LSJ) is: 0.99726815958280934 |   |            |   |            |    |            |   |  |  |  |  |  |  |  |  |

Definition of leading CSF:

|     |        |        |        |        |        |     |    |    |    |    |  |  |  |  |  |  |  |  |  |  |   |
|-----|--------|--------|--------|--------|--------|-----|----|----|----|----|--|--|--|--|--|--|--|--|--|--|---|
| 1)  | 2s( 2) | 2p( 6) | 3s( 2) | 3p( 1) | 3d( 1) |     |    |    |    |    |  |  |  |  |  |  |  |  |  |  |   |
|     |        | 1S0    | 1S0    | 1S0    | 2P1    | 2D1 | 1S | 1S | 2P | 3P |  |  |  |  |  |  |  |  |  |  | 0 |
| 2)  | 2s( 2) | 2p( 6) | 3s( 1) | 3p( 3) |        |     |    |    |    |    |  |  |  |  |  |  |  |  |  |  |   |
|     |        | 1S0    | 1S0    | 2S1    | 2P1    | 1S  | 2S | 3P | 0  |    |  |  |  |  |  |  |  |  |  |  |   |
| 3)  | 2s( 2) | 2p( 6) | 3s( 1) | 3p( 1) | 3d( 2) |     |    |    |    |    |  |  |  |  |  |  |  |  |  |  |   |
|     |        | 1S0    | 1S0    | 2S1    | 2P1    | 3P2 | 1S | 2S | 1P | 3P |  |  |  |  |  |  |  |  |  |  | 0 |
| 6)  | 2s( 2) | 2p( 6) | 3s( 1) | 3p( 1) | 3d( 2) |     |    |    |    |    |  |  |  |  |  |  |  |  |  |  |   |
|     |        | 1S0    | 1S0    | 2S1    | 2P1    | 3P2 | 1S | 2S | 3P | 3P |  |  |  |  |  |  |  |  |  |  | 0 |
| 8)  | 2s( 2) | 2p( 6) | 3s( 1) | 3p( 1) | 3d( 2) |     |    |    |    |    |  |  |  |  |  |  |  |  |  |  |   |
|     |        | 1S0    | 1S0    | 2S1    | 2P1    | 1D2 | 1S | 2S | 3P | 3P |  |  |  |  |  |  |  |  |  |  | 0 |
| 11) | 2s( 2) | 2p( 6) | 3p( 3) | 3d( 1) |        |     |    |    |    |    |  |  |  |  |  |  |  |  |  |  |   |
|     |        | 1S0    | 1S0    | 2P1    | 2D1    | 1S  | 2P | 3P | 0  |    |  |  |  |  |  |  |  |  |  |  |   |

.....  
 .....  
 jj2lsj: Execution complete.

The program, in default mode, produces the name .lsj.lbl file in which, for each ASF, the position, J, parity, total energy (in hartrees), and percentage of the wave function compositions are provided, followed by a list of expansion coefficients, their squares (compositions), and the CSF in LSJ-coupling. The example for odd7.lsj.lbl is given below. The label of the ASF is given by the notation of the first line. So the level with total energy -2794.938367562 is labeled 2s(2).2p(6).3s(2).3p\_2P.3d\_3F.

Output file odd7.lsj.lbl

```
-----
```

| Pos   | J | Parity | Energy Total    | Comp. of ASF                                   |
|-------|---|--------|-----------------|--|
| 1     | 0 | -      | -2795.294072330 | 99.862%  |
|       |   |        | -0.94694267     | 0.89670042 2s(2).2p(6).3s_2S.3p(3)2P1_3P       |
|       |   |        | -0.29599906     | 0.08761544 2s(2).2p(6).3s(2).3p_2P.3d_3P       |
|       |   |        | -0.09062556     | 0.00821299 2s(2).2p(6).3s_2S.3p_3P.3d(2)1S0_3P |
|       |   |        | -0.06641103     | 0.00441042 2s(2).2p(6).3p(3)2P1_2P.3d_3P       |
| 2     | 0 | -      | -2793.959522946 | 99.727%  |
|       |   |        | -0.94169405     | 0.88678769 2s(2).2p(6).3s(2).3p_2P.3d_3P       |
|       |   |        | 0.29537085      | 0.08724394 2s(2).2p(6).3s_2S.3p(3)2P1_3P       |
|       |   |        | -0.09229288     | 0.00851798 2s(2).2p(6).3p(3)2P1_2P.3d_3P       |
|       |   |        | 0.08186357      | 0.00670164 2s(2).2p(6).3s_2S.3p_1P.3d(2)3P2_3P |
|       |   |        | -0.07330494     | 0.00537361 2s(2).2p(6).3s_2S.3p_3P.3d(2)1D2_3P |
|       |   |        | -0.05007114     | 0.00250712 2s(2).2p(6).3s_2S.3p_3P.3d(2)3P2_3P |
| ..... |   |        |                 |  |
| 4     | 2 | -      | -2794.938367562 | 99.746%  |
|       |   |        | 0.61826021      | 0.38224569 2s(2).2p(6).3s(2).3p_2P.3d_3F       |
|       |   |        | 0.54278368      | 0.29461412 2s(2).2p(6).3s_2S.3p(3)2P1_3P       |
|       |   |        | 0.37809496      | 0.14295580 2s(2).2p(6).3s(2).3p_2P.3d_1D       |
|       |   |        | 0.29469334      | 0.08684416 2s(2).2p(6).3s_2S.3p(3)2D3_3D       |
|       |   |        | 0.17060037      | 0.02910449 2s(2).2p(6).3s(2).3p_2P.3d_3P       |
|       |   |        | -0.16453825     | 0.02707283 2s(2).2p(6).3s_2S.3p(3)4S3_5S       |
|       |   |        | 0.12507106      | 0.01564277 2s(2).2p(6).3s_2S.3p(3)2D3_1D       |
|       |   |        | -0.06574377     | 0.00432224 2s(2).2p(6).3s(2).3p_2P.3d_3D       |
|       |   |        | 0.06041988      | 0.00365056 2s(2).2p(6).3p(3)2P1_2P.3d_3F       |

```

0.05069300 0.00256978 2s(2).2p(6).3s_2S.3p_3P.3d(2)1S0_3P
0.03868154 0.00149626 2s(2).2p(6).3p(3)2P1_2P.3d_3P
0.03576268 0.00127897 2s(2).2p(6).3p(3)2P1_2P.3d_1D
-0.03187628 0.00101610 2s(2).2p(6).3s_2S.3p_1P.3d(2)3F2_3F

```

When the unique labeling option is chosen, the name .uni.lsj.lbl and name .uni.lsj.sum files are produced. The format and information in the name .uni.lsj.lbl is the same as in name .lsj.lbl, but all the levels have unique labels. Please note that the third level, with total energy -2794.938367562, and a smaller largest component, was relabeled as 2s(2).2p(6).3s\_2S.3p(3)2P1\_3P since the <sup>3</sup>F label had already been assigned.

Output file odd7.uni.lsj.lbl

```

-----
Pos  J  Parity      Energy Total      Comp. of ASF
1    0  -          -2795.294072330    99.862%
   -0.94694267    0.89670042    2s(2).2p(6).3s_2S.3p(3)2P1_3P
   -0.29599906    0.08761544    2s(2).2p(6).3s(2).3p_2P.3d_3P
   -0.09062556    0.00821299    2s(2).2p(6).3s_2S.3p_3P.3d(2)1S0_3P
   -0.06641103    0.00441042    2s(2).2p(6).3p(3)2P1_2P.3d_3P
2    0  -          -2793.959522946    99.727%
   -0.94169405    0.88678769    2s(2).2p(6).3s(2).3p_2P.3d_3P
   0.29537085    0.08724394    2s(2).2p(6).3s_2S.3p(3)2P1_3P
   -0.09229288    0.00851798    2s(2).2p(6).3p(3)2P1_2P.3d_3P
   0.08186357    0.00670164    2s(2).2p(6).3s_2S.3p_1P.3d(2)3P2_3P
   -0.07330494    0.00537361    2s(2).2p(6).3s_2S.3p_3P.3d(2)1D2_3P
   -0.05007114    0.00250712    2s(2).2p(6).3s_2S.3p_3P.3d(2)3P2_3P
-----
.....

4    2  -          -2794.938367562    99.746%
   0.54278368    0.29461412    2s(2).2p(6).3s_2S.3p(3)2P1_3P
   0.61826021    0.38224569    2s(2).2p(6).3s(2).3p_2P.3d_3F
   0.37809496    0.14295580    2s(2).2p(6).3s(2).3p_2P.3d_1D
   0.29469334    0.08684416    2s(2).2p(6).3s_2S.3p(3)2D3_3D
   0.17060037    0.02910449    2s(2).2p(6).3s(2).3p_2P.3d_3P
   -0.16453825    0.02707283    2s(2).2p(6).3s_2S.3p(3)4S3_5S
   0.12507106    0.01564277    2s(2).2p(6).3s_2S.3p(3)2D3_1D
   -0.06574377    0.00432224    2s(2).2p(6).3s(2).3p_2P.3d_3D
   0.06041988    0.00365056    2s(2).2p(6).3p(3)2P1_2P.3d_3F
   0.05069300    0.00256978    2s(2).2p(6).3s_2S.3p_3P.3d(2)1S0_3P
   0.03868154    0.00149626    2s(2).2p(6).3p(3)2P1_2P.3d_3P
   0.03576268    0.00127897    2s(2).2p(6).3p(3)2P1_2P.3d_1D
   -0.03187628    0.00101610    2s(2).2p(6).3s_2S.3p_1P.3d(2)3F2_3F
-----
.....

```

Below is the odd7.uni.lsj.sum file that provides the information – J, position, composition, serial number, and identification – for each ASF, where the serial number is the number of CSFs used in determining the composition. If the serial number of the composition is equal 1 the level is identified with the largest expansion coefficient, if 2, ..., etc., as in example below for levels with J = 2 Pos = 4 and Pos = 8, the levels are relabeled.

Output file odd7.uni.lsj.sum

```
-----
          Composition  Serial No.      Coupling
                   of compos.
J =      0
-----
Pos  1  0.896700420    1  2s(2).2p(6).3s_2S.3p(3)2P1_3P
Pos  2  0.886787690    1  2s(2).2p(6).3s(2).3p_2P.3d_3P
-----
```

.....

```
          Composition  Serial No.      Coupling
                   of compos.
J =      2
-----
Pos  1  0.816598140    1  2s(2).2p(6).3s_2S.3p(3)4S3_5S
Pos  2  0.623434900    1  2s(2).2p(6).3s_2S.3p(3)2D3_3D
Pos  6  0.495079260    1  2s(2).2p(6).3s(2).3p_2P.3d_3P
Pos  5  0.477147080    1  2s(2).2p(6).3s(2).3p_2P.3d_3F
Pos  7  0.400735720    1  2s(2).2p(6).3s(2).3p_2P.3d_3D
Pos  4  0.294614120    2  2s(2).2p(6).3s_2S.3p(3)2P1_3P
Pos  3  0.283483530    1  2s(2).2p(6).3s_2S.3p(3)2D3_1D
Pos  8  0.137996860    3  2s(2).2p(6).3s(2).3p_2P.3d_1D
-----
```

.....

The program can also be used in non-default mode. The typical run proceeds as follows:

```
Default settings? (y/n)
>>n
All levels (Y/N)
>>y
Maximum % of omitted composition
>>0.5
What is the value below which an eigenvector component is to be neglected
in the determination of the LSJ expansion: should be smaller than: 0.00500
>>0.003
What is the value below which an eigenvector composition is to be neglected
for printing?
>>0.0005
Do you need the output file *.lsj.c? (y/n)
>>y
Do you need the output file *.lsj.j? (y/n)
>>y
```

The non-default mode is useful in several cases:

(1) The present code allows the user, through the first parameter (0.5), to select the maximum percentage of the ASF composition that can be omitted. Given this information and with the help of the second parameter (0.003), it is easy to derive the largest small coefficient in the CSF expansion that may be included. However, with many components of about the same size, smaller values may be needed to meet the original objective. In this implementation, the user specifies the CSFs that can be omitted. The remaining CSFs define the basis that is to be transformed. By transforming this basis in decreasing order of importance, the desired percentage of the wave function can be transformed. A third parameter (0.0005) controls the printing of expansion coefficients in the *LSJ* basis and their contribution to the composition of the wave function. The default is to transform at least 99% of the wave function composition and print components in *LSJ* that contribute more than 0.1% to the composition. The cut-off for the *jj*-expansion has the value of 0.005, whereas the cut-off for printing is 0.001.

(2) In particular, the user may request a complete transformation, with a resulting list of CSFs in *LSJ*-coupling in name .1sj . c and their expansion coefficients in name .1sj . j. The two files have the same format as in ATSP2K [14]. Complete expansions are feasible only for small expansions. In this case the first and second parameter should be 0.

(3) The non-default option should be used if we choose a unique labeling option, but the program will not give the unique identification for all levels. In this case we need to transform a larger amount of ASF with larger number of expansion coefficients. It can be done with help of the first and second parameter.

#### 4. Results

In the recent calculations of energy spectra for Sr XXV [4] two pairs of odd levels with  $J = 2$  had the same label and were separated by adding subscripts ‘a’ and ‘b’. In the NIST database [15] for two ( $3s\ 3p^3\ ({}^2P) {}^3P_2^o$  and the  $3s^2\ 3p\ 3d\ {}^3F_2^o$ ) of these levels there is no data and the  $3s^2\ 3p\ 3d\ {}^1D_2^o$  level is not identified.

Running the JJ2LSJ program for Sr XXV levels 13 and 25 are relabeled in the Table 1. Table 1 gives also the labels from [4]. As we see level 13 had the same label as level 14, and 25 was labeled as 17. In Table 1 also the compositions in *LSJ*- coupling are given. In the Table 2 transition data of E1, M1, M2 transitions for relabeled levels are presented.

**Table 1.** Energy levels in  $\text{cm}^{-1}$  and *LSJ*-composition for Si-like Sr. In the original data levels 13 and 14 had the same label and subscripts ‘a’ and ‘b’ were introduced to separate the levels. Using the JJ2LSJ program levels 13 and 14 are now assigned unique labels.

| No. | Level [4]                     | Level (Relabeled)             | <i>LSJ</i> -Composition  | $n = 7$   |
|-----|-------------------------------|-------------------------------|--|-----------|
| 1   | $3s^2\ 3p^2\ ({}^3P) {}^3P_0$ | $3s^2\ 3p^2\ ({}^3P) {}^3P_0$ | $0.82 + 0.16\ 3s^2\ 3p^2\ ({}^1S) {}^1S$                                   | 0         |
| 2   | $3s^2\ 3p^2\ ({}^3P) {}^3P_1$ | $3s^2\ 3p^2\ ({}^3P) {}^3P_1$ | 0.98   | 92 950    |
| 3   | $3s^2\ 3p^2\ ({}^3P) {}^3P_2$ | $3s^2\ 3p^2\ ({}^3P) {}^3P_2$ | $0.54 + 0.44\ 3s^2\ 3p^2\ ({}^1D) {}^1D$                                   | 122 240   |
| 4   | $3s^2\ 3p^2\ ({}^1D) {}^1D_2$ | $3s^2\ 3p^2\ ({}^1D) {}^1D_2$ | $0.54 + 0.44\ 3s^2\ 3p^2\ ({}^3P) {}^3P$                                   | 239 120   |
| 5   | $3s^2\ 3p^2\ ({}^1S) {}^1S_0$ | $3s^2\ 3p^2\ ({}^1S) {}^1S_0$ | $0.81 + 0.16\ 3s^2\ 3p^2\ ({}^3P) {}^3P$                                   | 313 384   |
| 6   | $3s\ 3p^3\ ({}^4S) {}^5S_2^o$ | $3s\ 3p^3\ ({}^4S) {}^5S_2^o$ | $0.82 + 0.14\ 3s\ 3p^3\ ({}^2P) {}^3P^o + 0.02\ 3s\ 3p^3\ ({}^3D) {}^3D^o$ | 537 112   |
| 7   | $3s\ 3p^3\ ({}^2D) {}^3D_1^o$ | $3s\ 3p^3\ ({}^2D) {}^3D_1^o$ | $0.64 + 0.17\ 3s\ 3p^3\ ({}^1P) {}^3P^o + 0.09\ 3s^2\ 3p\ 3d\ {}^3D^o$     | 648 560   |
| 8   | $3s\ 3p^3\ ({}^2D) {}^3D_2^o$ | $3s\ 3p^3\ ({}^2D) {}^3D_2^o$ | $0.62 + 0.14\ 3s\ 3p^3\ ({}^1P) {}^3P^o + 0.11\ 3s\ 3p^3\ ({}^4S) {}^5S^o$ | 665 804   |
| 9   | $3s\ 3p^3\ ({}^2D) {}^3D_3^o$ | $3s\ 3p^3\ ({}^2D) {}^3D_3^o$ | $0.88 + 0.10\ 3s^2\ 3p\ 3d\ {}^3D^o$                                       | 700 704   |
| 10  | $3s\ 3p^3\ ({}^2P) {}^3P_0^o$ | $3s\ 3p^3\ ({}^2P) {}^3P_0^o$ | $0.90 + 0.09\ 3s^2\ 3p\ 3d\ {}^3P^o$                                       | 767 747   |
| 11  | $3s\ 3p^3\ ({}^1D) {}^1D_2^o$ | $3s\ 3p^3\ ({}^1D) {}^1D_2^o$ | $0.28 + 0.23\ 3s^2\ 3p\ 3d\ {}^1D^o + 0.17\ 3s\ 3p^3\ ({}^1P) {}^3P^o$     | 772 281   |
| 12  | $3s\ 3p^3\ ({}^1P) {}^3P_1^o$ | $3s\ 3p^3\ ({}^1P) {}^3P_1^o$ | $0.66 + 0.16\ 3s\ 3p^3\ ({}^2D) {}^3D^o + 0.07\ 3s^2\ 3p\ 3d\ {}^3P^o$     | 779 904   |
| 13  | $3s^2\ 3p\ 3d\ {}^3F_{2a}^o$  | $3s\ 3p^3\ ({}^2P) {}^3P_2^o$ | $0.29 + 0.38\ 3s^2\ 3p\ 3d\ {}^3F^o + 0.14\ 3s^2\ 3p\ 3d\ {}^1D^o$         | 845 815   |
| 14  | $3s^2\ 3p\ 3d\ {}^3F_{2b}^o$  | $3s^2\ 3p\ 3d\ {}^3F_2^o$     | $0.48 + 0.21\ 3s\ 3p^3\ ({}^2D) {}^1D^o + 0.13\ 3s\ 3p^3\ ({}^2P) {}^3P^o$ | 882 783   |
| 15  | $3s\ 3p^3\ ({}^4S) {}^3S_1^o$ | $3s\ 3p^3\ ({}^4S) {}^3S_1^o$ | $0.55 + 0.32\ 3s\ 3p^3\ ({}^1P) {}^1P^o + 0.04\ 3s\ 3p^3\ ({}^2P) {}^3P^o$ | 884 118   |
| 16  | $3s^2\ 3p\ 3d\ {}^3F_3^o$     | $3s^2\ 3p\ 3d\ {}^3F_3^o$     | $0.89 + 0.04\ 3s^2\ 3p\ 3d\ {}^3D^o + 0.03\ 3s^2\ 3p\ 3d\ {}^1F^o$         | 906 676   |
| 17  | $3s^2\ 3p\ 3d\ {}^3P_{2a}^o$  | $3s^2\ 3p\ 3d\ {}^3P_2^o$     | $0.50 + 0.20\ 3s^2\ 3p\ 3d\ {}^3D^o + 0.16\ 3s\ 3p^3\ ({}^2D) {}^1D^o$     | 967 289   |
| 18  | $3s^2\ 3p\ 3d\ {}^3D_1^o$     | $3s^2\ 3p\ 3d\ {}^3D_1^o$     | $0.42 + 0.26\ 3s^2\ 3p\ 3d\ {}^3P^o + 0.16\ 3s^2\ 3p\ 3d\ {}^1P^o$         | 971 435   |
| 19  | $3s^2\ 3p\ 3d\ {}^3F_4^o$     | $3s^2\ 3p\ 3d\ {}^3F_4^o$     | 0.98   | 989 440   |
| 20  | $3s\ 3p^3\ ({}^2P) {}^1P_1^o$ | $3s\ 3p^3\ ({}^2P) {}^1P_1^o$ | $0.42 + 0.31\ 3s\ 3p^3\ ({}^4S) {}^3S^o + 0.17\ 3s^2\ 3p\ 3d\ {}^3D^o$     | 1 007 850 |
| 21  | $3s^2\ 3p\ 3d\ {}^3D_2^o$     | $3s^2\ 3p\ 3d\ {}^3D_2^o$     | $0.40 + 0.28\ 3s^2\ 3p\ 3d\ {}^1D^o + 0.19\ 3s\ 3p^3\ ({}^2D) {}^1D^o$     | 1 052 275 |
| 22  | $3s^2\ 3p\ 3d\ {}^3P_0^o$     | $3s^2\ 3p\ 3d\ {}^3P_0^o$     | $0.89 + 0.09\ 3s\ 3p^3\ ({}^1P) {}^3P^o$                                   | 1 060 646 |
| 23  | $3s^2\ 3p\ 3d\ {}^3D_3^o$     | $3s^2\ 3p\ 3d\ {}^3D_3^o$     | $0.72 + 0.10\ 3s^2\ 3p\ 3d\ {}^1F^o + 0.08\ 3s\ 3p^3\ ({}^2D) {}^3D^o$     | 1 064 175 |
| 24  | $3s^2\ 3p\ 3d\ {}^3P_1^o$     | $3s^2\ 3p\ 3d\ {}^3P_1^o$     | $0.58 + 0.18\ 3s^2\ 3p\ 3d\ {}^3D^o + 0.09\ 3s\ 3p^3\ ({}^1P) {}^3P^o$     | 1 075 683 |
| 25  | $3s^2\ 3p\ 3d\ {}^3P_{2b}^o$  | $3s^2\ 3p\ 3d\ {}^1D_2^o$     | $0.14 + 0.37\ 3s^2\ 3p\ 3d\ {}^3P^o + 0.23\ 3s^2\ 3p\ 3d\ {}^3D^o$         | 1 091 772 |
| 26  | $3s^2\ 3p\ 3d\ {}^1F_3^o$     | $3s^2\ 3p\ 3d\ {}^1F_3^o$     | $0.84 + 0.11\ 3s^2\ 3p\ 3d\ {}^3D^o$                                       | 1 147 847 |
| 27  | $3s^2\ 3p\ 3d\ {}^1P_1^o$     | $3s^2\ 3p\ 3d\ {}^1P_1^o$     | $0.73 + 0.12\ 3s\ 3p^3\ ({}^1P) {}^1P^o + 0.07\ 3s^2\ 3p\ 3d\ {}^3D^o$     | 1 184 571 |



**Table 2.** Transition data for Si-like Sr where each level has been assigned a unique label.

| Upper  | Lower   | EM | $\Delta E$ (cm <sup>-1</sup> ) | $\lambda$ (Å) | $A$ (s <sup>-1</sup> ) | $gf$      | $dT$  |
|--|---|----|--------------------------------|---------------|------------------------|-----------|-------|
| 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3s <sup>2</sup> 3p <sup>2</sup> ( <sup>3</sup> P) <sup>3</sup> P <sub>0</sub> | M2 | 845815                         | 118.23        | 9.680E+00              | 1.014E-10 |       |
| 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3s <sup>2</sup> 3p <sup>2</sup> ( <sup>3</sup> P) <sup>3</sup> P <sub>1</sub> | E1 | 752864                         | 132.83        | 1.712E+07              | 2.264E-04 | 0.014 |
| 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3s <sup>2</sup> 3p <sup>2</sup> ( <sup>3</sup> P) <sup>3</sup> P <sub>1</sub> | M2 | 752864                         | 132.83        | 4.646E+00              | 6.144E-11 |       |
| 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3s <sup>2</sup> 3p <sup>2</sup> ( <sup>3</sup> P) <sup>3</sup> P <sub>2</sub> | M2 | 723575                         | 138.20        | 1.952E+01              | 2.795E-10 |       |
| 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3s <sup>2</sup> 3p <sup>2</sup> ( <sup>3</sup> P) <sup>3</sup> P <sub>2</sub> | E1 | 723575                         | 138.20        | 4.775E+09              | 6.837E-02 | 0.015 |
| 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3s <sup>2</sup> 3p <sup>2</sup> ( <sup>1</sup> D) <sup>1</sup> D <sub>2</sub> | E1 | 606694                         | 164.83        | 1.828E+09              | 3.723E-02 | 0.021 |
| 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3s <sup>2</sup> 3p <sup>2</sup> ( <sup>1</sup> D) <sup>1</sup> D <sub>2</sub> | M2 | 606694                         | 164.83        | 1.179E+02              | 2.402E-09 |       |
| 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3s <sup>2</sup> 3p <sup>2</sup> ( <sup>1</sup> S) <sup>1</sup> S <sub>0</sub> | M2 | 532430                         | 187.82        | 3.162E+01              | 8.361E-10 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> P <sub>1</sub> <sup>o</sup>                | 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup>  | M1 | 338756                         | 295.20        | 2.315E+03              | 9.072E-08 |       |
| 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3s3p <sup>3</sup> ( <sup>4</sup> S) <sup>5</sup> S <sub>2</sub> <sup>o</sup>  | M1 | 308702                         | 323.94        | 1.150E+04              | 9.043E-07 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> F <sub>3</sub> <sup>o</sup>                | 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup>  | M1 | 302032                         | 331.09        | 2.777E+03              | 3.195E-07 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup>  | M1 | 245957                         | 406.57        | 3.507E+03              | 4.346E-07 |       |
| 3s <sup>2</sup> 3p3d <sup>3</sup> P <sub>1</sub> <sup>o</sup>                | 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup>  | M1 | 229868                         | 435.03        | 1.962E+03              | 1.670E-07 |       |
| 3s <sup>2</sup> 3p3d <sup>3</sup> D <sub>3</sub> <sup>o</sup>                | 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup>  | M1 | 218360                         | 457.96        | 6.377E+03              | 1.403E-06 |       |
| 3s <sup>2</sup> 3p3d <sup>3</sup> D <sub>2</sub> <sup>o</sup>                | 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup>  | M1 | 206460                         | 484.35        | 2.293E+03              | 4.032E-07 |       |
| 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3s3p <sup>3</sup> ( <sup>2</sup> D) <sup>3</sup> D <sub>1</sub> <sup>o</sup>  | M1 | 197254                         | 506.96        | 1.069E+03              | 2.060E-07 |       |
| 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3s3p <sup>3</sup> ( <sup>3</sup> D) <sup>3</sup> D <sub>2</sub> <sup>o</sup>  | M1 | 180010                         | 555.52        | 1.380E+04              | 3.193E-06 |       |
| 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup>  | M1 | 162035                         | 617.15        | 1.312E+03              | 2.248E-07 |       |
| 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3s3p <sup>3</sup> ( <sup>2</sup> D) <sup>3</sup> D <sub>3</sub> <sup>o</sup>  | M1 | 145110                         | 689.13        | 5.267E+03              | 1.875E-06 |       |
| 3s <sup>2</sup> 3p3d <sup>3</sup> D <sub>1</sub> <sup>o</sup>                | 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup>  | M1 | 125620                         | 796.05        | 3.721E+02              | 1.061E-07 |       |
| 3s <sup>2</sup> 3p3d <sup>3</sup> P <sub>2</sub> <sup>o</sup>                | 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup>  | M1 | 121474                         | 823.22        | 1.112E+02              | 5.648E-08 |       |
| 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3s3p <sup>3</sup> ( <sup>3</sup> D) <sup>1</sup> D <sub>2</sub> <sup>o</sup>  | M1 | 73533                          | 1359.92       | 3.568E+03              | 4.947E-06 |       |
| 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>1</sub> <sup>o</sup>  | M1 | 65910                          | 1517.20       | 1.725E+03              | 2.976E-06 |       |
| 3s <sup>2</sup> 3p3d <sup>3</sup> F <sub>3</sub> <sup>o</sup>                | 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup>  | M1 | 60861                          | 1643.09       | 2.184E+03              | 6.189E-06 |       |
| 3s3p <sup>3</sup> ( <sup>4</sup> S) <sup>3</sup> S <sub>1</sub> <sup>o</sup> | 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup>  | M1 | 38303                          | 2610.71       | 6.515E+00              | 1.997E-08 |       |
| 3s <sup>2</sup> 3p3d <sup>3</sup> F <sub>2</sub> <sup>o</sup>                | 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>2</sub> <sup>o</sup>  | M1 | 36968                          | 2705.00       | 5.987E+02              | 3.284E-06 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s <sup>2</sup> 3p <sup>2</sup> ( <sup>3</sup> P) <sup>3</sup> P <sub>0</sub> | M2 | 1091772                        | 91.59         | 9.719E+00              | 6.112E-11 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s <sup>2</sup> 3p <sup>2</sup> ( <sup>3</sup> P) <sup>3</sup> P <sub>1</sub> | M2 | 998822                         | 100.12        | 2.608E+00              | 1.960E-11 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s <sup>2</sup> 3p <sup>2</sup> ( <sup>3</sup> P) <sup>3</sup> P <sub>1</sub> | E1 | 998822                         | 100.12        | 5.171E+09              | 3.886E-02 | 0.002 |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s <sup>2</sup> 3p <sup>2</sup> ( <sup>3</sup> P) <sup>3</sup> P <sub>2</sub> | E1 | 969532                         | 103.14        | 8.118E+09              | 6.474E-02 | 0.012 |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s <sup>2</sup> 3p <sup>2</sup> ( <sup>3</sup> P) <sup>3</sup> P <sub>2</sub> | M2 | 969532                         | 103.14        | 1.596E+02              | 1.273E-09 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s <sup>2</sup> 3p <sup>2</sup> ( <sup>1</sup> D) <sup>1</sup> D <sub>2</sub> | M2 | 852652                         | 117.28        | 5.942E+01              | 6.127E-10 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s <sup>2</sup> 3p <sup>2</sup> ( <sup>1</sup> D) <sup>1</sup> D <sub>2</sub> | E1 | 852652                         | 117.28        | 1.036E+11              | 1.068E+00 | 0.003 |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s <sup>2</sup> 3p <sup>2</sup> ( <sup>1</sup> S) <sup>1</sup> S <sub>0</sub> | M2 | 778388                         | 128.47        | 6.258E+01              | 7.742E-10 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s3p <sup>3</sup> ( <sup>4</sup> S) <sup>5</sup> S <sub>2</sub> <sup>o</sup>  | M1 | 554660                         | 180.29        | 4.087E+03              | 9.957E-08 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s3p <sup>3</sup> ( <sup>3</sup> D) <sup>3</sup> D <sub>1</sub> <sup>o</sup>  | M1 | 443212                         | 225.63        | 1.341E+02              | 5.116E-09 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s3p <sup>3</sup> ( <sup>3</sup> D) <sup>3</sup> D <sub>2</sub> <sup>o</sup>  | M1 | 425968                         | 234.76        | 6.591E+03              | 2.723E-07 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s3p <sup>3</sup> ( <sup>3</sup> D) <sup>3</sup> D <sub>3</sub> <sup>o</sup>  | M1 | 391068                         | 255.71        | 2.693E+03              | 1.320E-07 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s3p <sup>3</sup> ( <sup>3</sup> D) <sup>1</sup> D <sub>2</sub> <sup>o</sup>  | M1 | 319491                         | 313.00        | 4.115E+01              | 3.022E-09 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>3</sup> P <sub>1</sub> <sup>o</sup>  | M1 | 311868                         | 320.65        | 2.231E+03              | 1.719E-07 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s <sup>2</sup> 3p3d <sup>3</sup> F <sub>2</sub> <sup>o</sup>                 | M1 | 208989                         | 478.49        | 1.141E+03              | 1.958E-07 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s3p <sup>3</sup> ( <sup>4</sup> S) <sup>3</sup> S <sub>1</sub> <sup>o</sup>  | M1 | 207654                         | 481.57        | 1.285E+02              | 2.234E-08 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s <sup>2</sup> 3p3d <sup>3</sup> F <sub>3</sub> <sup>o</sup>                 | M1 | 185096                         | 540.26        | 3.272E+03              | 7.160E-07 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s <sup>2</sup> 3p3d <sup>3</sup> P <sub>2</sub> <sup>o</sup>                 | M1 | 124483                         | 803.32        | 1.272E+04              | 6.151E-06 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s <sup>2</sup> 3p3d <sup>3</sup> P <sub>2</sub> <sup>o</sup>                 | M1 | 124483                         | 803.32        | 1.272E+04              | 6.151E-06 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s <sup>2</sup> 3p3d <sup>3</sup> D <sub>1</sub> <sup>o</sup>                 | M1 | 120337                         | 831.00        | 5.753E+02              | 2.978E-07 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> P <sub>1</sub> <sup>o</sup>                | 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                 | M1 | 92798                          | 1077.60       | 2.314E+02              | 1.208E-07 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s3p <sup>3</sup> ( <sup>2</sup> P) <sup>1</sup> P <sub>1</sub> <sup>o</sup>  | M1 | 83922                          | 1191.58       | 7.850E+02              | 8.355E-07 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> F <sub>3</sub> <sup>o</sup>                | 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                 | M1 | 56074                          | 1783.34       | 1.104E+02              | 3.686E-07 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s <sup>2</sup> 3p3d <sup>3</sup> D <sub>2</sub> <sup>o</sup>                 | M1 | 39497                          | 2531.81       | 3.077E+01              | 1.478E-07 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s <sup>2</sup> 3p3d <sup>3</sup> D <sub>3</sub> <sup>o</sup>                 | M1 | 27597                          | 3623.57       | 1.171E+02              | 1.153E-06 |       |
| 3s <sup>2</sup> 3p3d <sup>1</sup> D <sub>2</sub> <sup>o</sup>                | 3s <sup>2</sup> 3p3d <sup>3</sup> P <sub>1</sub> <sup>o</sup>                 | M1 | 16089                          | 6215.18       | 4.670E+01              | 1.352E-06 |       |

Another example for which problems with unique labels occur is P-like W. Calculations using the MCDHF and RCI methods show that there are many levels with the same labels [16].

Table 3 presents the part of energy spectra with unique labels and *LSJ*-composition. The levels which were relabeled are marked with grey color.

**Table 3.** *LSJ*-composition and energy levels in  $\text{cm}^{-1}$  for P-like W from relativistic configuration interaction (RCI) calculations. Levels that are assigned new labels using the JJ2LSJ program are marked with grey background.

| No. | Level                                   | <i>LSJ</i> -Composition  | <i>E</i> (RCI) |
|-----|---|--|----------------|
| 1   | $3s^2 3p^3 ({}^2D) 2D_{3/2}^\circ$      | 0.27 + 0.48 $3s^2 3p^3 ({}^2P) 2P^\circ$ + 0.25 $3s^2 3p^3 ({}^4S) 4S^\circ$             | 0              |
| 2   | $3s^2 3p^2 ({}^3P) 3P 3d^4 F_{3/2}$     | 0.34 + 0.31 $3s^2 3p^2 ({}^1S) 1S 3d^2 D$ + 0.11 $3s^2 3p^2 ({}^3P) 3P 3d^4 D$           | 1 853 012      |
| 3   | $3s^2 3p^2 ({}^1D) 1D 3d^2 F_{5/2}$     | 0.002 + 0.30 $3s^2 3p^2 ({}^1S) 1S 3d^2 D$ + 0.20 $3s^2 3p^2 ({}^3P) 3P 3d^4 D$          | 2 613 799      |
| 4   | $3s^2 3p^3 ({}^4S) 4S_{3/2}^\circ$      | 0.55 + 0.44 $3s^2 3p^3 ({}^3D) 2D^\circ$   | 2 752 643      |
| 5   | $3s^2 3p^3 ({}^2D) 2D_{5/2}^\circ$      | 0.99   | 2 847 490      |
| 6   | $3s^2 3p^3 ({}^2P) 2P_{1/2}^\circ$      | 0.99   | 2 971 667      |
| 7   | $3s 3p^4 ({}^3P) 4P_{5/2}$              | 0.66 + 0.27 $3s 3p^4 ({}^1D) 2D$ + 0.02 $3s^2 3p^2 ({}^1D) 1D 3d^2 D$                    | 4 157 536      |
| 8   | $3s 3p^4 ({}^1D) 2D_{3/2}$              | 0.24 + 0.33 $3s 3p^4 ({}^3P) 2P$ + 0.11 $3s 3p^4 ({}^3P) 4P$                             | 4 398 405      |
| 9   | $3s 3p^4 ({}^1S) 2S_{1/2}$              | 0.54 + 0.24 $3s 3p^4 ({}^3P) 4P$ + 0.07 $3s 3p^4 ({}^3P) 2P$                             | 4 413 592      |
| 10  | $3s^2 3p^2 ({}^3P) 3P 3d^4 F_{5/2}$     | 0.47 + 0.29 $3s^2 3p^2 ({}^1D) 1D 3d^2 F$ + 0.16 $3s^2 3p^2 ({}^3P) 3P 3d^2 F$           | 4 584 963      |
| 11  | $3s^2 3p^2 ({}^3P) 3P 3d^4 D_{1/2}$     | 0.80 + 0.13 $3s^2 3p^2 ({}^3P) 3P 3d^2 P$ + 0.04 $3s^2 3p^2 ({}^3P) 3P 3d^4 P$           | 4 611 635      |
| 12  | $3s^2 3p^2 ({}^3P) 3P 3d^4 D_{3/2}$     | 0.28 + 0.33 $3s^2 3p^2 ({}^3P) 3P 3d^4 F$ + 0.12 $3s^2 3p^2 ({}^3P) 3P 3d^2 P$           | 4 613 253      |
| 13  | $3s^2 3p^2 ({}^1D) 1D 3d^2 G_{7/2}$     | 0.52 + 0.18 $3s^2 3p^2 ({}^3P) 3P 3d^4 F$ + 0.14 $3s^2 3p^2 ({}^3P) 3P 3d^2 F$           | 4 683 926      |
| 14  | $3s^2 3p^2 ({}^3P) 3P 3d^2 D_{5/2}$     | 0.30 + 0.24 $3s^2 3p^2 ({}^1D) 1D 3d^2 F$ + 0.12 $3s^2 3p^2 ({}^3P) 3P 3d^4 P$           | 4 922 718      |
| 15  | $3s^2 3p^2 ({}^1D) 1D 3d^2 P_{1/2}$     | 0.35 + 0.31 $3s^2 3p^2 ({}^3P) 3P 3d^4 P$ + 0.18 $3s^2 3p^2 ({}^1D) 1D 3d^2 S$           | 5 004 842      |
| 16  | $3s^2 3p^2 ({}^1D) 1D 3d^2 D_{3/2}$     | 0.27 + 0.22 $3s^2 3p^2 ({}^3P) 3P 3d^4 P$ + 0.15 $3s^2 3p^2 ({}^1D) 1D 3d^2 P$           | 5 009 796      |
| 17  | $3s^2 3p^2 ({}^3P) 3P 3d^4 D_{7/2}$     | 0.47 + 0.37 $3s^2 3p^2 ({}^3P) 3P 3d^4 F$ + 0.07 $3s^2 3p^2 ({}^3P) 3P 3d^2 F$           | 5 242 340      |
| 18  | $3s^2 3p^2 ({}^3P) 3P 3d^2 P_{3/2}$     | 0.25 + 0.23 $3s^2 3p^2 ({}^3P) 3P 3d^4 P$ + 0.20 $3s^2 3p^2 ({}^1D) 1D 3d^2 P$           | 5 342 886      |
| 19  | $3s^2 3p^2 ({}^1D) 1D 3d^2 G_{9/2}$     | 0.62 + 0.37 $3s^2 3p^2 ({}^3P) 3P 3d^4 F$  | 5 346 296      |
| 20  | $3s^2 3p^2 ({}^3P) 3P 3d^2 F_{5/2}$     | 0.33 + 0.25 $3s^2 3p^2 ({}^1D) 1D 3d^2 D$ + 0.22 $3s^2 3p^2 ({}^3P) 3P 3d^4 D$           | 5 371 289      |
| 21  | $3s^2 3p^2 ({}^3P) 3P 3d^4 P_{5/2}$     | 0.35 + 0.27 $3s^2 3p^2 ({}^1D) 1D 3d^2 D$ + 0.14 $3s^2 3p^2 ({}^3P) 3P 3d^2 D$           | 5 534 143      |
| 22  | $3s^2 3p^2 ({}^1D) 1D 3d^2 F_{7/2}$     | 0.44 + 0.18 $3s^2 3p^2 ({}^3P) 3P 3d^2 F$ + 0.17 $3s^2 3p^2 ({}^3P) 3P 3d^4 F$           | 5 544 364      |
| 23  | $3s^2 3p^2 ({}^3P) 3P 3d^2 D_{3/2}$     | 0.46 + 0.22 $3s^2 3p^2 ({}^1D) 1D 3d^2 P$ + 0.14 $3s^2 3p^2 ({}^1D) 1D 3d^2 D$           | 5 614 260      |
| 24  | $3s^2 3p^2 ({}^1D) 1D 3d^2 S_{1/2}$     | 0.36 + 0.31 $3s^2 3p^2 ({}^3P) 3P 3d^2 P$ + 0.23 $3s^2 3p^2 ({}^1D) 1D 3d^2 P$           | 5 645 215      |
| 25  | $3s^2 3p^3 ({}^2P) 2P_{3/2}^\circ$      | 0.51 + 0.28 $3s^2 3p^3 ({}^3D) 2D^\circ$ + 0.20 $3s^2 3p^3 ({}^4S) 4S^\circ$             | 5 738 961      |
| 26  | $3s 3p^3 ({}^4S) 5S 3d^6 D_{5/2}^\circ$ | 0.19 + 0.20 $3s^2 3p^2 ({}^3P) 3P 3d^4 F^\circ$ + 0.11 $3s 3p^3 ({}^2P) 3P 3d^4 F^\circ$ | 5 975 676      |
| 27  | $3s 3p^3 ({}^2P) 3P 3d^4 D_{3/2}^\circ$ | 0.20 + 0.23 $3s 3p^3 ({}^4S) 5S 3d^6 D^\circ$ + 0.14 $3s 3p^3 ({}^2P) 3P 3d^4 P^\circ$   | 5 993 157      |
| 28  | $3s 3p^3 ({}^2D) 3D 3d^4 P_{1/2}^\circ$ | 0.06 + 0.39 $3s 3p^3 ({}^2P) 3P 3d^4 P^\circ$ + 0.29 $3s 3p^3 ({}^4S) 5S 3d^6 D^\circ$   | 6 011 091      |
| 29  | $3s 3p^3 ({}^2P) 3P 3d^4 F_{7/2}^\circ$ | 0.23 + 0.17 $3s 3p^3 ({}^2P) 3P 3d^2 F^\circ$ + 0.16 $3s 3p^3 ({}^4S) 5S 3d^6 D^\circ$   | 6 061 088      |
| 30  | $3s 3p^3 ({}^2D) 3D 3d^4 F_{3/2}^\circ$ | 0.12 + 0.20 $3s 3p^3 ({}^2P) 1P 3d^2 D^\circ$ + 0.11 $3s 3p^3 ({}^2P) 3P 3d^4 P^\circ$   | 6 210 048      |
| 31  | $3s 3p^3 ({}^2D) 3D 3d^4 G_{5/2}^\circ$ | 0.20 + 0.21 $3s 3p^3 ({}^2P) 1P 3d^2 F^\circ$ + 0.11 $3s^2 3p 3d^2 ({}^3F) 4G^\circ$     | 6 299 645      |
| 32  | $3s 3p^3 ({}^2D) 3D 3d^4 D_{1/2}^\circ$ | 0.11 + 0.25 $3s 3p^3 ({}^2P) 1P 3d^2 P^\circ$ + 0.17 $3s 3p^3 ({}^4S) 3S 3d^4 D^\circ$   | 6 335 321      |
| 33  | $3s^2 3p 3d^2 ({}^3F) 4G_{5/2}^\circ$   | 0.42 + 0.15 $3s^2 3p 3d^2 ({}^1D) 2F^\circ$ + 0.13 $3s^2 3p 3d^2 ({}^3F) 2F^\circ$       | 6 551 091      |
| 34  | $3s 3p^3 ({}^2D) 3D 3d^4 G_{9/2}^\circ$ | 0.10 + 0.47 $3s 3p^3 ({}^2P) 3P 3d^4 F^\circ$ + 0.30 $3s 3p^3 ({}^4S) 5S 3d^6 D^\circ$   | 6 636 519      |
| 35  | $3s 3p^3 ({}^2D) 1D 3d^2 D_{5/2}^\circ$ | 0.05 + 0.20 $3s 3p^3 ({}^2P) 3P 3d^4 P^\circ$ + 0.16 $3s 3p^3 ({}^2P) 3P 3d^2 D^\circ$   | 6 771 988      |
| 36  | $3s 3p^3 ({}^4S) 5S 3d^6 D_{7/2}^\circ$ | 0.14 + 0.23 $3s 3p^3 ({}^2P) 3P 3d^2 F^\circ$ + 0.19 $3s 3p^3 ({}^2P) 3P 3d^4 D^\circ$   | 6 832 810      |
| 37  | $3s 3p^3 ({}^2D) 3D 3d^2 D_{3/2}^\circ$ | 0.07 + 0.19 $3s 3p^3 ({}^2P) 3P 3d^2 D^\circ$ + 0.17 $3s 3p^3 ({}^4S) 5S 3d^4 D^\circ$   | 6 845 169      |
| 38  | $3s^2 3p 3d^2 ({}^3P) 4D_{1/2}^\circ$   | 0.36 + 0.26 $3s^2 3p 3d^2 ({}^1S) 2P^\circ$ + 0.12 $3s^2 3p 3d^2 ({}^3P) 2P^\circ$       | 6 891 509      |
| 39  | $3s^2 3p 3d^2 ({}^3F) 4F_{3/2}^\circ$   | 0.30 + 0.25 $3s^2 3p 3d^2 ({}^3F) 2D^\circ$ + 0.07 $3s^2 3p 3d^2 ({}^3F) 4D^\circ$       | 6 929 835      |
| 40  | $3s 3p^3 ({}^2P) 1P 3d^2 F_{7/2}^\circ$ | 0.25 + 0.16 $3s 3p^3 ({}^4S) 3S 3d^4 D^\circ$ + 0.11 $3s 3p^3 ({}^2D) 3D 3d^4 G^\circ$   | 6 971 178      |
| 41  | $3s 3p^4 ({}^3P) 4P_{3/2}$              | 0.70 + 0.16 $3s 3p^4 ({}^1D) 2D$ + 0.03 $3s^2 3p^2 ({}^3P) 3P 3d^4 D$                    | 6 998 090      |
| 42  | $3s 3p^3 ({}^2P) 3P 3d^2 P_{1/2}^\circ$ | 0.36 + 0.27 $3s 3p^3 ({}^4S) 5S 3d^4 D^\circ$ + 0.07 $3s 3p^3 ({}^2P) 3P 3d^4 D^\circ$   | 7 042 278      |
| 43  | $3s 3p^3 ({}^2P) 1P 3d^2 D_{5/2}^\circ$ | 0.17 + 0.12 $3s 3p^3 ({}^2P) 3P 3d^2 F^\circ$ + 0.09 $3s 3p^3 ({}^2D) 3D 3d^4 F^\circ$   | 7 084 012      |
| 44  | $3s 3p^3 ({}^2P) 1P 3d^2 P_{3/2}^\circ$ | 0.18 + 0.13 $3s 3p^3 ({}^2D) 3D 3d^4 P^\circ$ + 0.11 $3s 3p^3 ({}^4S) 3S 3d^2 D^\circ$   | 7 100 823      |
| 45  | $3s 3p^4 ({}^1D) 2D_{5/2}$              | 0.63 + 0.24 $3s 3p^4 ({}^3P) 4P$ + 0.04 $3s^2 3p^2 ({}^3P) 3P 3d^4 D$                    | 7 144 999      |
| 46  | $3s^2 3p 3d^2 ({}^3F) 4G_{7/2}^\circ$   | 0.55 + 0.14 $3s^2 3p 3d^2 ({}^3F) 2G^\circ$ + 0.13 $3s^2 3p 3d^2 ({}^3F) 4F^\circ$       | 7 224 945      |

## 5. Conclusions

In this paper, a new version of the JJ2LSJ program, consistent with the approach described in [7–10], is presented. The program performs the transformation of ASFs from a *jj*-to *LSJ*-coupling and provides the option to assign all level unique labels. Examples of the program use and explanations of possible options are given. In the paper, a few cases (Si-like Sr and P-like W) where the problem with unique labeling in energy spectra occur, are discussed and new labels are assigned.

The program is freely distributed. It may be obtained from the corresponding author.

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