Theoretical energy level spectra and transition data for $4p^64d$, $4p^64f$ and $4p^54d^2$ configurations of W$^{37+}$ ion

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Abstract

The ab initio quasirelativistic Hartree-Fock method developed specifically for the calculation of spectral parameters of heavy atoms and highly charged ions was applied to determine atomic data for tungsten ions. The correlation effects were included by adopting configuration interaction method. The Breit-Pauli approximation for quasirelativistic Hartree-Fock radial orbitals was employed to take into account relativistic effects. The energy level spectra, radiative lifetimes, Lande factors $g$ were calculated for the $4p^64d$, $4p^64f$ and $4p^54d^2$ configurations of W$^{37+}$ ion. The atomic data, namely, the transition wavelengths, spontaneous emission rates and oscillator strengths for the electric dipole, electric quadrupole and magnetic dipole transitions among and within the levels of these configurations are tabulated.

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1. Introduction

Due to its unique features, the metallic tungsten is widely employed in devices which operate at extremely high temperatures. These properties facilitate adoption of tungsten in fusion reactors including internationally developed ITER tokamak [1, 2]. High temperatures within fusion plasma cause tungsten to evaporate. Furthermore, the tungsten atoms in plasma are ionized to very high degrees. This process has a negative consequences on plasma since it makes plasma temperatures to drop significantly.

To perform plasma processes modeling and diagnostics one needs huge amount of spectroscopic data describing various ionization stages of tungsten and other atoms [3, 4]. Atomic spectroscopy can help to determine important properties of plasma [5–7]. Nevertheless, the spectra of the tungsten ions present in fusion plasma devices are still not investigated properly. This conclusion is evident from review [8] where all available experimental wavelengths and energy level spectra for ions from W III to W LXXIV are provided.

It is evident from the analysis of [8] and references within, that only a few data for the spectra of tungsten ions with open 4d-shells are available. In present work we investigate a relatively simple system, namely W 37+. This ion has only one valence 4d-electron in its ground state. It follows from [8] that only 11 excited levels from the possible 48 ones for the configurations under consideration have been determined experimentally. On the other hand, a theoretical study of energy level spectra was presented in [9]. However, this work suffers from the fact that the data are provided just for some fifty percent of existing levels representing the configurations under consideration. Furthermore, the transition data were determined for the highly excited levels only.

In present work we employ the quasirelativistic method [10–12] developed specifically for the ab initio calculation of spectral parameters of heavy atoms and highly charged ions. A preliminary analysis of the suitability of this method for the tungsten ions with open 4d-shell was presented in [13]. It was demonstrated that our quasirelativistic approach is appropriate for the inclusion of the relativistic effects, and the further improvement of accuracy of the calculated data can be achieved with inclusion of the correlation effects.

In Section 2 we provide a short description of our calculation method. The more detailed description of the applied approach and the analysis of the convergence within the configuration interaction (CI) approximation applied for the inclusion of correlation effects is presented in [14]. Obtained results are discussed in Section 3.
2. Calculation method

2.1. Quasirelativistic approximation

We use a quasirelativistic approximation for \textit{ab initio} calculations of ion energy spectra. This approach significantly differs from widely used method described in [15]. In our method, the radial orbitals (RO) are obtained by solving the quasirelativistic equations of the following form:

\[
\begin{align*}
\left\{ \frac{d^2}{dr^2} - & \frac{l(l+1)}{r^2} - \frac{V(nl|r) - \epsilon_{nl}}{r} \right\} P(nl|r) - X(nl|r) \\
+ & \frac{\alpha^2}{4} (\epsilon_{nl} + V(nl|r))^2 P(nl|r) + \frac{\alpha^2}{4} (\epsilon_{nl} + V(nl|r)) X(nl|r) \\
+ & \frac{\alpha^2}{4} \left( 1 - \frac{\alpha^2}{4} (\epsilon_{nl} + V(nl|r)) \right)^{-1} \frac{d}{dr} \left( \frac{\alpha^2 Z^2}{30} \left( -\frac{37}{9n} - \frac{5} {9n^2} + \frac{2}{3n^2} \right) + 1 \right) \\
& = 0.
\end{align*}
\]  

(1)

The first line of Eq.(1) represents the traditional Hartree-Fock equations, where \(X(nl|r)\) denotes the exchange part of the potential and \(V(nl|r)\) represents the direct part of the potential including the interaction of an electron with nucleus \(U(r)\) and with other electrons. We take into account the finite size of a nucleus within the nucleus potential \(U(r)\) [16]. This allows us to represent the radial orbitals in powers of a radial variable in the nucleus region. Next two terms with the multiplier \((\epsilon_{nl} + V(nl|r))\) describe the relativistic correction of the mass-velocity dependence. The last term of Eq.(1) represents the potential of the electron contact interaction with the nucleus. In our approach we include the contact interaction with the nucleus not only for the s-electrons but also some part of it for the p-electrons:

\[
D(nl|r) = \left( \delta(l,0) + \frac{1}{3} \delta(l,1) \right) \frac{dU(r)}{dr} \left( \frac{d}{dr} - \frac{1}{r} \left( \alpha^2 Z^2 \delta(l,1) \left( \frac{-37}{30} - \frac{5}{9n} + \frac{2}{3n^2} \right) + 1 \right) \right).
\]  

(2)

A detailed discussion of the particular features of Eq.(1) is given in [10, 11], whereas their solution techniques are described in [17, 18].

Concluding the description of applied approximation, we want to articulate the unique features of our quasirelativistic method which significantly differs from widely used approach described in [15]. The main differences arise from our adopted set of Hartree-Fock quasirelativistic equations (QRHF) featuring several distinctive properties, namely:

1. No statistical potentials are used. There are only conventional self-consistent field direct and exchange potentials in QRHF.
2. The finite size of the nucleus is taken into account to determine the potential while solving the quasirelativistic equations [16, 18].
3. The mass-velocity term is divided into two parts - the direct potential and the exchange one.
4. The contact interaction term contains only the nucleus potential derivative in the numerator. There are no two-electron potentials in the numerator.
5. Only the direct part of the potential is included into the denominator of the contact interaction with a nucleus term.
6. The contact interaction with a nucleus is taken into account not only for s-electrons, but also for p-electrons with some additional corrections made [11].

One must look in [10, 11] for the most complete description of the way to determine QRHF equations employed in this work. The methods to calculate the energy level spectra were discussed extensively in [12].

For the energy level spectra calculation, we include all two-electron interactions in the same way as it is done in conventional Breit-Pauli approximation. This similarity makes it possible to apply widely used code MCHF BREIT [19] for the angular integration.
of the Breit-Pauli Hamiltonian matrix elements. We employ the computer program MCHF MLTPOL [20] to determine the matrix elements of transition operators along with the code MCHF LSJTR [21] which has been adopted for use with the quasirelativistic radial orbitals.

2.2. Correlation effects

We use configuration interaction (CI) approximation to include electron correlation effects. In present work, depending on the type of one-electron state, two sorts of radial orbitals are exploited in the CI expansion of wavefunctions. For the configurations under consideration (adjusted configurations), we employ one-electron radial orbitals $P_{QR}(nl|r)$ determined from solutions of Eq.(1). This type of RO was applied for all electrons with $n \leq 4$ and $l \leq 3$. We adopt the transformed radial orbitals (TRO) to describe virtually excited electrons included in CI expansion.

The method of transformed radial orbitals to account for the configuration interaction effects was developed in [22] and successfully applied for the non-relativistic radial orbitals (see, e.g. [23–26]). The comparison of TRO properties with those of the solutions of the multiconfigurational Hartree-Fock-Jucys equations [27] demonstrates their close similarity [28, 29]. Such a way to include correlation effects within our quasirelativistic approach was successfully applied for the studies of the tungsten spectral parameters in [30].

In current work the TRO were employed to describe the admixed configurations, having virtually excited electrons with the principal quantum number $4 < n \leq 7$ and with all allowed values of orbital quantum number $l$. These orbitals are determined from the RO of the configurations under consideration by ensuring the effective inclusion of the correlation effects. For the present calculations, we employ the form of TRO with two free variational parameters $k$ and $B$:

$$P_{TRO}(nl|r) = N \left( j^{l-\frac{1}{2}+k} \exp(-Br)P(n|0|r) - \sum_{n^\prime < n} P(n^\prime|l|r)j^{l-\frac{1}{2}+k} \exp(-Br)P_{QR}(n|^0|0)r dr \right).$$  

(3)

Here the multiplier $N$ ensures the normalization of determined TRO, the first term in parenthesis performs the necessary transformation, and the second term provides the orthogonality of all employed radial orbitals. The parameters $k$ and $B$ are varied in order to ensure the maximum of averaged energy correction $\Delta E$ to the energy of the adjusted configuration in the second order of perturbation theory:

$$\Delta E_{PT}(K_0, K') = \sum_{TLST}(2L+1)(2S+1)|K_0TL||H||K'T'LST|^2$$

$$g(K_0)(E(K')(E(K_0))^{-1}).$$  

(4)

We apply the same set of radial orbitals to describe both the even and odd configurations. This approach enables us to avoid any problems caused by the non-orthogonality of RO in calculation of the electron transition parameters.

As a consequence of adopted TRO, the basis of radial orbitals and the number of possible admixed configurations increases rapidly. Therefore one needs to perform a selection of the admixed configurations by including only those which have the greatest influence on the configurations being adjusted. As a selection criteria we apply the mean weight of the admixed configuration within the CI expansion of the adjusted configuration wavefunction determined in the second order of perturbation theory:

$$W_{PT}(K_0, K') = \sum_{TLST}(2L+1)(2S+1)|K_0TL||H||K'T'LST|^2$$

$$g(K_0)(E(K')(E(K_0))^{-1}).$$  

(5)

We include only those configurations which have $W_{PT}(K_0, K')$ larger than the specified small parameter $S$ in our calculation of energy levels and transition parameters. The methods and computer codes to calculate the mean weight from Eq. (5) have been described in [31, 32]. Such a way to select the interacting configurations in the non-relativistic approximation was successfully exploited (see, e.g., earlier mentioned [23–26] and many others).
The configuration state functions (CSFs) of the selected configurations are used to form the energy operator matrices. By diagonalizing these Hamiltonian matrices, we can determine the energy eigenvalues and eigenfunctions for the investigated configurations and exploit them for calculation of transition parameters. More details of employed approach one can find in [12] and references therein, whereas some examples of application of our method are presented in [30, 33].

In present work we have selected only those admixed configurations which have the mean weights in the wave functions of the configurations under consideration larger than $10^{-6}$. This procedure has allowed us to reduce the number of admixed configurations in the CI expansion of the wavefunctions to 102 for even configurations and to 217 for odd configurations. So here we use an approximation denoted as $\mathbf{F}$ in [14]. It was demonstrated in [14] that any further expansion of the admixed configurations basis does not lead to significant improvement in the calculated energy level spectra accuracy.

We have determined energy eigenvalues and eigenfunctions by diagonalizing Hamiltonian matrices obtained in the LSJ-coupling scheme in Breit-Pauli approximation. Using these results, we have calculated the transition parameters. We have computed data for the electric dipole (E1), electric quadrupole (E2) and magnetic dipole (M1) operators for the transitions both between the configurations under consideration and within these configurations. The emission transition rates of all above mentioned types were used to determine the radiative lifetimes of excited states.

3. Results and discussion

We present the energy level spectra with the percentage contribution of eigenfunctions together with Lande factors $g$ and the radiative lifetimes $\tau$ for the investigated configurations in Table 1. It was demonstrated in [14] that deviations of our theoretical level energy values from the experimental spectra data do not exceed 1% in most cases. Consequently, we can conclude that these discrepancies in transition energies do not affect significantly the accuracy of calculated values of the transition rates or oscillator strengths. In Table A we compare our calculated energy levels with data obtained from the completely relativistic calculations RELAC [9] and with available experimental data [7] presented in compilation [8]. This evaluation favorably demonstrates a better agreement of our data with the experimental level energies, especially for highly-excited states, comparing to the data from relativistic calculations RELAC. This is caused mainly by considerably improved inclusion of correlation effects.

Such a good agreement with experimental data leads to conclusion that our quasirelativistic approach adequately accounts for the relativistic effects even for highly-ionized heavy atoms. It is worth to mention a very good agreement of theoretical fine-structure level splitting for the ground term $4p^5d^2D$ pointing to close spin-orbit interaction values obtained in our work and in fully relativistic calculations [9].

As it was mentioned before, all our calculations were performed in $LS$-coupling scheme. It is well established fact that the spin-orbit interaction induces a very strong mixing of $LS$-terms for highly-charged ions. Therefore in Table A we present only the level numbers (indices) $N$ taken from Table 1 where one can find a corresponding CI wavefunction expansion. It is easy to notice from the CSFs contributions presented in Table 1 that the strong mixing occurs both for the $LS$-terms of the same configuration and for terms of different configurations.

A well-established case of a strong interaction between the $4p^5dN+1$ and $4p^6dN−1f$ configurations (see [34]) can be confirmed from the analysis of the wave function percentage contributions. For example, a contribution from the $4p^64f$ configuration for the $J = 2.5$ level $N = 32$ in Table 1 is merely 49%. Moreover, the largest contribution for the level $N = 28$ comes from the $4p^64f$ configuration although the level itself clearly must be attributed to the configuration $4p^5d^2$. 
In Table 2 we present the transition wavelengths $\lambda$, the emission transition rates $A$ and the weighted oscillator strength values $gf$. We use only the level indices $N$ and the total angular momentum $J$ from Table 1 to describe both the initial and final levels along with the type of transition operator (E1, E2 or M1) applied to calculate the transition parameters. We present the transitions from the excited level to lower-lying levels in decreasing order of their rates. We limit the number of presented transitions by removing those having the transition rate values by 3 orders of magnitude lower comparing to the strongest transition from the particular energy level. This condition would remove completely the E2 transitions. Nonetheless, we have placed some most important E2 transitions in Table 2.

The magnetic dipole M1 transitions within configuration $4p^64d$ were computed using a completely relativistic approximation in [35]. As one can see from Table 2, their value of transition rate $3.97 \times 10^4$ is very close to the value of $3.94 \times 10^4$ from our calculation.

From analysis of data presented in Table 2, we can notice that the electric dipole transition rates are the most strong ones for all excited configuration levels when the total angular momentum $J \leq 3.5$. Furthermore, the strong E1 transitions define the values of radiative lifetimes $\tau$ for these levels presented in Table 1. The only exemption from this rule demonstrates the level $N = 14$ with total angular momentum $J = 3.5$. Even if the E1 transitions from this level have the largest rates $A$, the values of two M1 transition rates are of the same order of magnitude as for the E1 transitions. This causes the significant decrease of the radiative lifetime value $\tau$ for this energy level.

The electric dipole transitions from the excited levels with $J \geq 4.5$ are forbidden because the largest value of total angular momentum of the ground state $J = 2.5$. Consequently, the radiative lifetimes $\tau$ for these levels are determined by the magnetic dipole transitions since the E2 transition rates are significantly smaller.

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Table A  
Comparison of calculated energy levels (in 100 cm$^{-1}$) of W$^{37+}$ with available experimental data (EXP) from [8] and relativistic calculations RELAC from [9]. Level identifications from both [8] and [9] are used where available, and level numbers $N$ are from Table 1.

| $N$ | Term [8] | Level Name [9] | $J$ | EXP [8] | QRHF | RELAC [9] |
|-----|----------|----------------|-----|---------|------|-----------|
| 1   | 4p$^6$4d$^2$ 2D | (4p)$^6$(4d$^-$)$^1$ | 1.5 | 0       | 0    | 0         |
| 2   | 4p$^6$4d$^2$ 2D | (4p)$^6$(4d$^-$)$^1$ | 2.5 | 1546    | 1538 | 1537      |
| 3   | 4p$^5$4d$^2$ 3F (3/2,2) | (4p$^-$)$^2$(4p$^+$)$^3$(4d$^-$)$^1$ | 0.5 | 12276   | 12311|
| 4   | 4p$^5$4d$^2$ 3F (3/2,2) | (4p$^-$)$^2$(4p$^+$)$^3$(4d$^-$)$^1$ | 1.5 | 12276   | 12312|

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Explanation of Tables

Table 1. Energy levels and radiative lifetimes of \(4p^6 4d, 4p^6 4f\) and \(4p^5 4d^2\) configurations of \(W^{37+}\).

Throughout the table we present all the eigenfunction components which have their percentage contributions higher than 10%.

- \(N\): The energy level number (index)
- \(E\): The level energy in \(10^2 \text{ cm}^{-1}\)
- \(g\): The Lande factor \(g\). The notation \(a(b)\) means \(a \times 10^b\)
- \(\tau\): The radiative lifetime in \(10^{-9} \text{ s}\)
- \(J\): The total angular momentum
- Contribution: The percentage contribution of CSF in level eigenfunction

Table 2. Electron transitions among and within the \(4p^6 4d, 4p^6 4f\) and \(4p^5 4d^2\) configurations of \(W^{37+}\).

The transitions from the upper level to the lower ones are presented in the descending order of the transition rate values \(A\). The number of presented transitions is limited to those having the transition rate values less than 3 orders of magnitude smaller comparing to the strongest transition from the particular energy level.

- \(J_i\): The total angular momentum \(J\) of the initial level
- \(N_i\): The initial energy level number \(N\)
- \(J_f\): The total angular momentum \(J\) of the final level
- \(N_f\): The final energy level number \(N\)
- Type: The electron transition type
- \(\lambda\) (Å): The transition wavelength \(\lambda\) in Å
- \(A (s^{-1})\): The emission transition rate \(A\) in \(s^{-1}\). The notation \(a(b)\) means \(a \times 10^b\)
- \(gf\): The weighted oscillator strength \(gf\). The notation \(a(b)\) means \(a \times 10^b\)
| N  | E   | g   | τ   | J   | Contribution               |
|----|-----|-----|-----|-----|---------------------------|
| 1  | 0   | 0.80| 1.5 | 98 4d 2D                   |
| 2  | 1538| 1.20| 2.55| +4  | 2.5 98 4d 2D              |
| 3  | 12311| 1.00| 8.44| –1  | 1.5 42 4p 3d(F2) 4D       |
| 4  | 12312| 0.12| 2.44| –1  | 0.5 84 4p 3d(F2) 4D       |
| 5  | 12591| 1.03| 3.83| –1  | 2.5 36 4p 3d(F2) 4F       |
| 6  | 12752| 1.03| 1.75| +1  | 3.5 32 4p 3d(F2) 4G       |
| 7  | 13284| 1.36| 5.37| +0  | 1.5 28 4p 3d(F2) 3P       |
| 8  | 13636| 1.30| 1.95| +1  | 2.5 42 4p 3d(F2) 4D       |
| 9  | 13915| 1.29| 2.88| –1  | 3.5 35 4p 3d(F2) 4F       |
| 10 | 13922| 1.18| 3.04| +4  | 4.5 70 4p 3d(F2) 4G       |
| 11 | 14052| 1.09| 1.29| –1  | 1.5 40 4p 3d(F2) 4D       |
| 12 | 14104| 1.23| 4.29| +1  | 2.5 40 4p 3d(F2) 3P       |
| 13 | 14255| 1.17| 2.68| +6  | 5.5 57 4p 3d(G2) 4H       |
| 14 | 14290| 1.06| 1.15| +4  | 3.5 29 4p 3d(F2) 4G       |
| 15 | 14408| 1.66| 4.37| +2  | 0.5 33 4p 3d(F2) 4P       |
| 16 | 14631| 1.17| 3.20| –1  | 3.5 20 4p 3d(F2) 4D       |
| 17 | 14680| 1.22| 1.60| –1  | 2.5 36 4p 3d(F2) 4D       |
| 18 | 14756| 1.39| 2.77| –1  | 1.5 30 4p 3d(F2) 4S       |
| 19 | 14853| 1.13| 1.47| –5  | 4.5 38 4p 3d(G2) 4G       |
| 20 | 15220| 0.88| 6.50| –3  | 2.5 41 4p 3d(G2) 4F       |
| 21 | 15500| 1.20| 1.70| +4  | 5.5 57 4p 3d(F2) 4G       |
| 22 | 15618| 0.85| 2.16| –3  | 1.5 32 4p 3d(F2) 4P       |
| 23 | 15619| 1.21| 1.60| +0  | 2.5 24 4p 3d(F2) 4D       |
| 24 | 15671| 1.22| 5.32| –2  | 3.5 34 4p 3d(F2) 4D       |
| 25 | 15854| 1.17| 1.20| +4  | 4.5 38 4p 3d(F2) 4F       |
| 26 | 15972| 1.08| 6.58| –3  | 0.5 65 4p 3d(F2) 4P       |
| 27 | 16350| 0.76| 1.49| –3  | 0.5 52 4p 3d(F2) 4P       |
| 28 | 16551| 1.18| 4.48| –2  | 3.5 16 4p 3d(F2) 4F       |
| 29 | 16897| 1.27| 5.82| –1  | 1.5 50 4p 3d(F2) 4S       |
| 30 | 17355| 1.09| 1.03| +3  | 2.5 29 4p 3d(F2) 4D       |
| 31 | 17553| 1.36| 1.58| –3  | 1.5 20 4p 3d(F2) 4S       |
| 32 | 17752| 0.93| 1.21| –3  | 2.5 49 4f 4f             |
| 33 | 17889| 1.12| 1.72| –3  | 3.5 63 4f 4f             |
| 34 | 20319| 0.77| 8.80| –4  | 2.5 39 4p 3d(F2) 4G       |
| 35 | 21314| 1.02| 7.13| –1  | 3.5 46 4p 3d(F2) 4G       |
| 36 | 21387| 1.07| 1.70| –2  | 2.5 18 4p 3d(F2) 4F       |
| 37 | 21478| 1.07| 9.10| –3  | 1.5 37 4p 3d(F2) 4D       |
| 38 | 21547| 1.96| 1.39| –3  | 0.5 41 4p 3d(F2) 4P       |
| 39 | 21555| 0.43| 9.08| –4  | 0.5 56 4p 3d(F2) 4D       |
| 40 | 21754| 1.04| 1.39| –2  | 4.5 45 4p 3d(G2) 4H       |
| 41 | 22069| 0.88| 3.03| –4  | 1.5 43 4p 3d(F2) 4D       |
| 42 | 22794| 1.29| 2.73| –3  | 3.5 45 4p 3d(F2) 4D       |
| 43 | 23116| 1.15| 3.88| –4  | 2.5 34 4p 3d(F2) 4D       |
|     |      |     |     |     |                           |

Table 1

Energy levels and radiative lifetimes of 4p^64d, 4p^64f and 4p^54d^2 configurations of W^{37+}. See page 9 for Explanation of Table.
Table 1 (continued)

| N  |   E    |   g   |  τ  |     J     | Contribution |
|----|--------|-------|-----|-----------|--------------|
| 44 | 23159  | 1.20  | 1.5 | 33 4p⁵ 4d²⁵²d⁴D²P | +26 4p⁵ 4d²⁵²d⁴D²D +12 4p⁵ 4d²⁵²p⁴D³P |
| 45 | 23221  | 1.11  | 4.5 | 31 4p⁵ 4d²⁵²d²²F²G | +23 4p⁵ 4d²⁵²d²²G²H +17 4p⁵ 4d²⁵²F²²G²F |
| 46 | 23274  | 1.06  | 3.5 | 53 4p⁵ 4d²⁵²d²²G²G | +29 4p⁵ 4d²⁵²d²²G²F |
| 47 | 23309  | 1.48  | 1.5 | 52 4p⁵ 4d²⁵²F²²P²P | +20 4p⁵ 4d²⁵²F²²P²S +11 4p⁵ 4d²⁵²F²²P³P |
| 48 | 23369  | 1.11  | 2.5 | 35 4p⁵ 4d²⁵²d²²D²P | +24 4p⁵ 4d²⁵²d²²P²D +17 4p⁵ 4d²⁵²d²²P³D |
| 49 | 24058  | 0.67  | 3.13 | 75 4p⁵ 4d²⁵²s⁰²²P | +13 4p⁵ 4d²⁵²P²D |


Table 2

Electron transitions among and within the 4p^64d, 4p^64f and 4p^64d^2 configurations of W^{37+}. See page 9 for Explanation of Table.

| J_i | N_i | J_f | N_f | Type | λ (Å) | A (s⁻¹) | gf |
|-----|-----|-----|-----|------|-------|---------|----|
| 2.5 | 2   | 1.5 | 1   | M1   | 650.2 | 3.93E+04| 1.49E-05 |
| 1.5 | 1   | 1   | E2  |      | 650.2 | 1.89E+01| 7.19E-09 |
| 1.5 | 3   | 1   | E1  |      | 81.23 | 1.15E+09| 4.56E-03 |
| 2.5 | 2   | E1  |     |      | 92.83 | 3.38E+07| 1.75E-04 |
| 0.5 | 4   | 1   | E1  |      | 81.22 | 4.09E+09| 8.09E-03 |
| 2.5 | 5   | 1   | E1  |      | 79.42 | 2.37E+09| 1.34E-02 |
| 2.5 | 2   | E1  |     |      | 90.47 | 2.47E+08| 1.82E-03 |
| 3.5 | 6   | 2   | E1  |      | 89.18 | 5.72E+07| 5.45E-04 |
| 1.5 | 7   | 2   | E1  |      | 85.14 | 1.78E+08| 7.74E-04 |
| 1.5 | 1   | E1  |     |      | 75.28 | 8.25E+06| 2.80E-05 |
| 2.5 | 8   | 1   | E1  |      | 73.34 | 5.13E+07| 2.48E-04 |
| 2.5 | 2   | E1  |     |      | 82.66 | 3.11E+04| 1.91E-07 |
| 3.5 | 9   | 2   | E1  |      | 80.80 | 3.47E+09| 2.72E-02 |
| 4.5 | 10  | 3.5 | M1  |      | 854.6 | 3.29E+04| 3.60E-05 |
| 4.5 | 6   | 6   | M1  |      | 854.6 | 2.13E+04| 2.33E-09 |
| 1.5 | 11  | 1   | E1  |      | 71.17 | 5.76E+09| 1.75E-02 |
| 2.5 | 2   | E1  |     |      | 79.91 | 1.97E+09| 7.56E-03 |
| 2.5 | 5   | 1   | E1  |      | 70.90 | 2.44E+07| 1.11E-04 |
| 5.5 | 13  | 4.5 | M1  |      | 2999  | 3.68E+02| 5.95E-06 |
| 3.5 | 14  | 2   | E1  |      | 78.42 | 4.94E+04| 3.65E-07 |
| 2.5 | 5   | M1  |      |      | 588.5 | 2.32E+04| 9.64E-06 |
| 3.5 | 6   | M1  |      |      | 650.0 | 1.42E+04| 7.21E-06 |
| 2.5 | 8   | M1  |      |      | 1528  | 2.66E+02| 7.44E-07 |
| 0.5 | 15  | 1   | E1  |      | 69.41 | 2.25E+06| 3.25E-06 |
| 3.5 | 16  | 2.5 | E1  |      | 76.38 | 3.12E+07| 2.18E-04 |
| 2.5 | 17  | 1.5 | E1  |      | 68.12 | 6.25E+09| 2.61E-02 |
| 2.5 | 2   | E1  |     |      | 76.09 | 2.40E+04| 1.25E-07 |
| 1.5 | 18  | 2.5 | E1  |      | 75.65 | 2.47E+08| 8.49E-04 |
| 1.5 | 1   | E1  |     |      | 67.77 | 1.13E+08| 3.12E-04 |
| 4.5 | 19  | 3.5 | M1  |      | 475.9 | 3.48E+03| 1.18E-06 |
| 3.5 | 9   | M1  |      |      | 1066  | 2.55E+03| 4.34E-06 |
| 4.5 | 10  | M1  |      |      | 1074  | 4.18E+02| 7.23E-07 |
| 3.5 | 14  | M1  |      |      | 1777  | 1.63E+02| 7.72E-07 |
| 5.5 | 13  | M1  |      |      | 1673  | 1.07E+02| 4.49E-07 |
| 3.5 | 16  | M1  |      |      | 4510  | 4.65E+01| 1.42E-06 |
| 2.5 | 20  | 1.5 | E1  |      | 65.70 | 1.54E+11| 5.96E-01 |
| 2.5 | 2   | E1  |     |      | 73.09 | 1.94E+08| 9.32E-04 |
| 5.5 | 21  | 4.5 | M1  |      | 633.7 | 4.30E+04| 3.11E-05 |
| 5.5 | 13  | M1  |      |      | 803.5 | 1.50E+04| 1.74E-05 |
| 4.5 | 19  | M1  |      |      | 1546  | 5.80E+02| 2.49E-06 |
| 1.5 | 22  | 1.5 | E1  |      | 64.03 | 4.61E+11| 1.13E+00 |
| $J_i$ | $N_i$ | $J_f$ | $N_f$ | Type | $\lambda$ (Å) | $A$ (s$^{-1}$) | $gf$ |
|------|------|------|------|------|--------------|-------------|------|
| 2.5  | 23   | 2.5  | 2    | E1   | 71.02        | 1.64E+09    | 4.97E−03 |
| 1.5  | 2    | E1   | 64.02| 1.66E+08 | 6.13E−04 |
| 3.5  | 24   | 2.5  | 2    | E1   | 70.76        | 1.88E+10    | 1.13E−01 |
| 4.5  | 25   | 3.5  | 14   | M1   | 639.4        | 3.06E+04    | 1.87E−05 |
| 3.5  | 9    | 2    | E1   | 615.6| 7.63E−02    | 1.05E−05    |
| 4.5  | 10   | 22   | 2.5  | E1   | 4.59E+08    | 2.08E−03    |
| 1.5  | 1    | E1   | 61.16| 6.71E+01 | 7.53E−01 |
| 2.5  | 29   | 2.5  | 2    | E1   | 65.11        | 1.23E+09    | 3.13E−03 |
| 1.5  | 1    | E1   | 59.18| 4.87E+01 | 1.19E−01 |
| 2.5  | 30   | 1.5  | 1    | E1   | 57.03        | 5.33E+11    | 1.56E+00 |
| 2.5  | 2    | E1   | 62.51| 4.46E+11 | 1.57E+00 |
| 3.5  | 31   | 2.5  | 2    | E1   | 62.44        | 6.34E+11    | 1.48E+00 |
| 1.5  | 1    | E1   | 56.97| 4.87E+01 | 2.21E+04 |
| 3.5  | 32   | 1.5  | 1    | E1   | 56.33        | 5.39E+11    | 1.54E+00 |
| 2.5  | 33   | 2.5  | 2    | E1   | 61.16        | 5.81E+11    | 2.61E+00 |
| 2.5  | 34   | 1.5  | 1    | E1   | 49.22        | 1.14E+12    | 2.47E+00 |
| 3.5  | 35   | 2.5  | 2    | E1   | 53.25        | 7.48E+08    | 1.91E−03 |
| 2.5  | 36   | 2.5  | 2    | E1   | 50.57        | 1.40E+09    | 4.28E−03 |
| 1.5  | 1    | E1   | 46.76| 6.11E+09 | 1.20E−02 |
| 2.5  | 37   | 1.5  | 1    | E1   | 46.56        | 9.49E+10    | 1.23E−01 |
| 2.5  | 38   | 2    | E1   | 50.15| 1.50E+10    | 2.26E−02    |
| 0.5  | 39   | 1.5  | 1    | E1   | 46.41        | 7.20E+11    | 4.65E−01 |
| 0.5  | 40   | 5.5  | 13   | M1   | 133.4        | 4.27E+06    | 1.14E−04 |
| 4.5  | 19   | M1   | 144.9| 1.81E+06 | 5.68E−05 |
| 3.5  | 16   | M1   | 140.4| 3.26E+05 | 9.63E−06 |
| 3.5  | 14   | M1   | 134.0| 3.09E+05 | 8.32E−06 |
| 3.5  | 9    | M1   | 127.6| 8.37E+04 | 2.04E−06 |
| 4.5  | 10   | M1   | 127.7| 8.22E+04 | 2.01E−06 |
| 5.5  | 13   | M1   | 123.4| 6.84E+04 | 1.82E−06 |
| 4.5  | 19   | E2   | 144.9| 6.03E+04 | 1.90E−06 |
| 1.5  | 41   | 1.5  | 1    | E1   | 45.31        | 3.29E+12    | 4.06E+00 |
| 2.5  | 2    | E1   | 48.71| 1.15E+10 | 1.63E−02 |
| 3.5  | 42   | 2.5  | 2    | E1   | 47.05        | 3.67E+11    | 9.74E−01 |
| $J_i$ | $N_i$ | $J_f$ | $N_f$ | Type | $\lambda$ (Å) | $A$ (s$^{-1}$) | $gf$ |
|------|------|------|------|------|-------------|-------------|-----|
| 2.5  | 43   | 2.5  | 2    | E1   | 46.34       | 2.58E+12    | 4.98E+00 |
| 1.5  | 1    | E1   | 43.26 | 6.71E+08 | 1.13E+03 |
| 1.5  | 44   | 2.5  | 2    | E1   | 46.25       | 2.17E+11    | 2.78E+01 |
| 1.5  | 1    | E1   | 43.18 | 1.57E+10 | 1.76E+02 |
| 4.5  | 45   | 5.5  | 21   | M1   | 129.5       | 4.47E+00    | 1.13E+04 |
| 4.5  | 25   | M1   | 135.7 | 2.10E+06 | 5.81E+05 |
| 3.5  | 28   | M1   | 149.9 | 3.53E+05 | 1.19E+05 |
| 3.5  | 33   | M1   | 187.5 | 1.57E+05 | 8.29E+06 |
| 3.5  | 24   | M1   | 132.5 | 1.34E+05 | 3.52E+06 |
| 4.5  | 25   | E2   | 135.7 | 8.96E+04 | 2.48E+06 |
| 5.5  | 21   | E2   | 129.5 | 8.02E+04 | 2.02E+06 |
| 3.5  | 35   | M1   | 524.5 | 7.74E+04 | 3.19E+05 |
| 3.5  | 46   | 2.5  | 2    | E1   | 46.01       | 1.94E+12    | 4.91E+00 |
| 1.5  | 47   | 2.5  | 2    | E1   | 45.93       | 2.13E+12    | 2.70E+00 |
| 1.5  | 1    | E1   | 42.90 | 2.80E+09 | 3.09E+03 |
| 2.5  | 48   | 2.5  | 2    | E1   | 45.81       | 2.12E+09    | 4.00E+03 |
| 1.5  | 1    | E1   | 42.79 | 9.56E+06 | 1.57E+05 |
| 0.5  | 49   | 1.5  | 1    | E1   | 41.57       | 3.20E+10    | 1.66E+02 |