Abstract. Ab initio calculations including relativistic effects employing the Breit-Pauli R-matrix (BPRM) method are reported for fine structure energy levels and oscillator strengths up to \( n = 10 \) and \( 0 \leq l \leq 9 \) for 15 Li-like ions: C IV, N V, O VI, F VII, Ne VIII, Na IX, Mg X, Al XI, Si XII, S XIV, Ar XVI, Ca XIII, Ti XX, Cr X XII, and Ni XXVI. About one hundred bound fine structure energy levels of total angular momenta, \( 1/2 \leq J \leq 17/2 \) of even and odd parities, total orbital angular momentum, \( 0 \leq L \leq 9 \) and spin multiplicity \((2S+1) = 2, 4\) are considered for each ion. The levels provide almost 900 dipole allowed and intercombination bound-bound transitions. The BPRM method enables consideration of a large set of transitions with uniform accuracy compared to the best available theoretical methods. The CC eigenfunction expansion for each ion includes the lowest 17 fine structure energy levels of the core configurations \( 1s^2, 1s2s, 1s2p, 1s3s, 1s3p, \) and \( 1s3d \). The calculated energies of the ions agree with the measured values to within 1\% for most levels. The transition probabilities show good agreement with the best available calculated values. The results provide the largest sets of energy levels and transition rates for the ions and are expected to be useful in the analysis of X-ray and EUV spectra from astrophysical sources.

Key words: atomic data - radiative transition probabilities - fine structure transitions - Lithium-like ions - X-ray sources

1. Introduction

A wealth of high resolution astrophysical spectra are being obtained by ground-based telescopes and by space based observatories such as HST, CHANDRA, ISO, FUSE. Accurate spectral analysis provides diagnostic of element abundances, temperatures etc.. However, a major task is the identification of the large number of lines, especially from UV to X-ray region for use in sythetic models, calculating opacities. Ab initio relativistic calculations using the Breit-Pauli R-matrix (BPRM) method, developed under the Iron Project (IP, Hummer et al. 1993), are carried out for extensive and accurate sets of oscillator strengths \((f)\), line strengths \((S)\) and radiative transition probabilities \((A)\) for a number of Li-like ions from carbon to nickel. Results for lithium like Fe XXIV were reported earlier (Nahar and Pradhan 1999). Compared to the very accurate theoretical methods for oscillator strengths for a relatively small number of transitions, the BPRM method allows consideration of a large number of transitions with comparable accuracy for most of the transitions.

Relatively smaller sets of transitions are available for the lithium like ions considered. An evaluated compilation of the results by various investigators obtained using various approximation is available from the web based database of the National Institute for
Standards and Technology (NIST). The previous large sets of non-relativistic data were obtained by Peach et al. (1988) under the Opacity Project (OP 1995, 1996) which are accessible through the OP database, TOPbase (Cunto et al. 1993). Nahar (1998) obtained later a larger set of transitions for O VI using a larger wavefunction expansion. These results consider only the dipole allowed $LS$ multiplets, i.e., no relativistic fine structure splitting were taken into account. The OP datasets for a number of ions have been reprocessed to obtain fine structure oscillator strengths through pure algebraic transformation of the line strengths and utilizing the observed energies for improved accuracy, such as, the recent compilation of transition probabilities by NIST for C, N, O ions (Wiese et al 1996), the transition probabilities for Fe II by Nahar (1995).

2. Theory

Theoretical details are discussed in previous works, such as in the first large scale relativistic calculations using the BPRM method for bound-bound transitions in Fe XXIV and Fe XXV (Nahar and Pradhan 1999). The close coupling (CC) approximation using the R-matrix method as employed under the OP (Seaton 1987, Berrington et al. 1987) was extended to BPRM method under the Iron Project (IP, Hummer et al. 1993) to include the relativistic effects in the Breit-Pauli approximation (Scott and Burke 1980, Scott and Taylor 1982, Berrington et al. 1995). They are derived from atomic collision theory using the coupled channel approximation. The BPRM method has been used for several other ions, such as Fe V (Nahar et al. 2000), Ar XIII and Fe XXI (Nahar 2000), C II and C III (Nahar 2002), C III (Berrington et al. 2001), Na III (Berrington 2001), and Cl-like ions (Berrington et al. 2001).

In the CC approximation the wavefunction expansion, $\Psi(E)$, for a (N+1) electron system with total spin and orbital angular momenta symmetry $SL\pi$ or total angular momentum symmetry $J\pi$, is described in terms of the target ion states as:

$$\Psi_E(e + ion) = A \sum_i \chi_i(ion)\theta_i + \sum_j c_j \Phi_j(e + ion),$$  \hspace{1cm} (1)

where $\chi_i$ is the target ion wavefunction in a specific state $S_iL_i\pi_i$ or level $J_i\pi_i$, and $\theta_i$ is the wavefunction for the interacting (N+1)th electron in a channel labeled as $S_iL_i(J_i)\pi_i$ and $k_i^2 \ell_i^2 (SL\pi \ or \ J\pi)$; $k_i^2$ is the incident kinetic energy. In the second sum the $\Phi_j$’s are correlation wavefunctions of the (N+1) electron system that (a) compensate for the orthogonality conditions between the continuum and the bound orbitals, and (b) represent additional short-range correlation that is often of crucial importance in scattering and radiative CC calculations for each $SL\pi$.

The relativistic (N+1)-electron Hamiltonian for the N-electron target ion and a free electron in the Breit-Pauli approximation, as adopted under the IP, is

$$H_{N+1}^{BP} = H_{N+1} + H_{N+1}^{\text{mass}} + H_{N+1}^{\text{Dar}} + H_{N+1}^{\text{so}},$$  \hspace{1cm} (2)
where $H_{N+1}$ is the non-relativistic Hamiltonian,

$$H_{N+1} = \sum_{i=1}^{N+1} \left\{ -\nabla_i^2 - \frac{2Z}{r_i} + \sum_{j>i}^{N+1} \frac{2}{r_{ij}} \right\}, \tag{3}$$

added by the one-body mass correction term, the Darwin term and the spin-orbit interaction term. The mass-correction and Darwin terms do not break the LS symmetry, while the spin-orbit interaction split the LS terms into fine-structure levels labeled by $J\pi$. The BP Hamiltonian in the present work does not include the full Breit-interaction in that the two-body spin-spin and spin-other-orbit terms are not included.

The set of $S\ell\pi$ are recoupled to obtain $(e + \text{ion})$ states with total $J\pi$, following the diagonalization of the (N+1)-electron Hamiltonian,

$$H^B_{N+1}\Psi = E\Psi. \tag{4}$$

Substitution of the wavefunction expansion introduces set of coupled equations that are solved using the R-matrix approach. The details of the solutions for the wavefunctions and energies can be found in the OP papers (1995) and in Hummer et al. (1993). The channels, characterized by the spin and angular quantum numbers of the $(e + \text{ion})$ system, describe the scattering process with the free electron interacting with the target at positive energies ($E > 0$), while at negative total energies ($E < 0$), the solutions of the close coupling equations occur at discrete eigenvalues of the $(e + \text{ion})$ Hamiltonian that correspond to pure bound states $\Psi_B$.

The oscillator strength ($f$-values) for a bound-bound transition can be obtained from the transition matrix,

$$< \Psi_B | D | \Psi_{B'} >, \tag{5}$$

where $D$ is the dipole operator. The transition matrix can be reduced to the generalised line strength ($S$), in either length or velocity form as

$$S_L = \left| \left\langle \Psi_f \left| \sum_{j=1}^{N+1} r_j | \Psi_i \right\rangle \right. \right|^2, \tag{6}$$

and

$$S_V = \omega^{-2} \left| \left\langle \Psi_f \left| \sum_{j=1}^{N+1} \frac{\partial}{\partial r_j} | \Psi_i \right\rangle \right. \right|^2, \tag{7}$$

where $\omega$ is the incident photon energy in Rydberg units, $\Psi_i$ and $\Psi_f$ are the initial and final state bound wavefunctions respectively.

In terms of the transition energy $E_{ji}$ between states $i$ and $j$, the oscillator strength, $f_{ij}$, is obtained from $S$ as

$$f_{ij} = \frac{E_{ji}}{3g_i} S, \tag{8}$$

and the transition probability or Einstein’s A-coefficient, $A_{ji}$, as

$$A_{ji}(\text{a.u.}) = \frac{1}{2} \alpha^2 \frac{g_i}{g_j} E_{ji}^2 f_{ij}, \tag{9}$$
where \( \alpha \) is the fine structure constant, and \( g_i, g_j \) are the statistical weight factors of the initial and final states, respectively. The lifetime of a level can be obtained from the A-values of the level as,
\[
\tau_k(s) = \frac{1}{A_k},
\]
where \( A_k \) is the total radiative transition probability for the level \( k \), i.e.,
\[
A_k = \sum_i A_{ki}(s^{-1}) , \quad \text{and} \quad A_{ji}(s^{-1}) = A_{ji}(a.u.)/\tau_0, \quad \tau_0 = 2.4191 \times 10^{-17} \text{s is the atomic unit of time.}
\]

3. Atomic calculations

The Breit-Pauli R-matrix calculations for the Li-like ions are carried out using an eigenfunction expansion of 17 fine structure levels of configurations, \( 1s^2, 1s2s, 1s2p, 1s3s, 1s3p \) and \( 1s3d \) of the He-like target or core (Table 1) for each ion.

The orbital wavefunctions of the target are obtained from the atomic structure calculations using the code SUPERSTRUCTURE (Eissner et al. 1974) that employs Thomas-Fermi potential. The wavefunctions of the spectroscopic levels are optimized individually for each ion. \( 4s \) and \( 4p \) are treated as correlation orbitals. The optimization is carried out such that the set of configurations and Thomson Fermi scaling parameters (\( \lambda \)) for the orbitals yield calculated level energies that agree closely with the measured values and the discrepancy between the length and velocity form oscillator strengths is less than 5% for the allowed transitions from the ground level. While the set of spectroscopic configurations remains the same for each ion, the set of correlation configurations and parameters \( \lambda \) for the orbitals vary for some, as seen in Table 1. The level energies given in the table are mainly from the measured values in the database of the NIST. The calculated fine structure energies differ by much less than 1% from the measured values of the levels. However, in the R-matrix calculations the calculated energies are replaced by the observed values whenever available, i.e., calculated energies are used only when the measured values are not available.

For the \((N+1)\)th electron, all partial waves of \( 0 \leq l \leq 9 \) are included. The bound-channel term of the wavefunction, the second term in Eq. (1), includes all possible \((N+1)\)-configurations from a vacant shell to maximum occupancies of \( 1s^2, 2s^2, 2p^2, 3s^2, 3p^2, 3d^2, 4s, \) and \( 4p \).

The BPRM calculations consist of several stages of computation (Berrington et al. 1995). The orbital wavefunctions of SUPERSTRUCTURE are used as the input for the BPRM codes to compute the one- and two-electron radial integrals. The R-matrix basis set consists of 30 continuum functions for each ion. The calculations included all possible bound levels for \( 0.5 \leq J \leq 8.5 \) of even and odd parities, with \( n < 10, \ell \leq 9, 0 \leq L \leq 11 \) or \( 12 \), and \((2S+1) = 2, 4 \). The intermediate coupling calculations are carried out on
recoupling the $LS$ symmetries in a pair-coupling representation in stage RECUPD. The 
(e + core) Hamiltonian matrix is diagonalized for each resulting $J\pi$ in STGH.

The fine structure bound levels are sorted through the poles in the (e + ion) Hamiltonian with a fine mesh of effective quantum number $\nu$. The mesh ($\Delta \nu = 0.001$) is finer than that typically used for $LS$ energy terms ($\Delta \nu = 0.01$) to avoid any missing levels and to obtain accurate energies for the higher levels.

About a hundred fine structure bound energy levels are obtained for each ion. They are obtained as sets of levels belonging to symmetries $J\pi$ only, complete spectroscopic designations for identifications are not specified. The level identification scheme, based on quantum defect analysis and percentage of channel contributions to the levels, as developed in the code PRCBPID (Nahar and Pradhan 2000) is employed. Hund’s rule is used for positions of the levels such that a level with higher angular orbital momentum $L$ may lie below the low $L$ one. Although level identification of Li-like ions is straightforward, it is more involved for complex ions. The final designation is given by $C_t(S_tL_t\pi_t)J_tnlJ(SL)\pi$ where $C_t$, $S_tL_t\pi_t$, $J_t$ are the configuration, $LS$ term and parity, and total angular momentum of the target, $nl$ are the principal and orbital quantum numbers of the outer or the valence electron, and $J$ and $SL\pi$ are the total angular momentum, $LS$ term and parity of the $(N + 1)$-electron system.

4. Results and Discussions

Extensive sets of fine structure energy levels and oscillator strengths and transition probabilities for the bound-bound transitions are obtained for 15 Li-like ions: C IV, N V, O VI, F VII, Ne VIII, Na IX, Mg X, Al XI, Si XII, S XIV, Ar XVI, Ca XXI, Ti XXII, Cr XXII, and Ni XXVI. The energy levels and bound-bound transitions are discussed separately in the two following sections.

4.1. Fine Structure Energy Levels

A total of about 98 fine structure energy levels are obtained for each 15 Li-like ion (97 or 99 for a few of them). They correspond to levels of $2 \leq n \leq 10$ and $0 \leq l \leq 9$ with total angular momentum, $1/2 \leq J \leq 17/2$ of even and odd parities, total spin multiplicity $2S+1 = 2$, and total orbital angular momentum, $0 \leq L \leq 9$. All levels have been identified. The number of levels obtained far exceed the observed or previously calculated ones.

The calculated energies are compared in Table 2 with the measured values, compiled by the NIST. The table presents comparison of energies of a few ions, such as C IV, O VI, and Ni XXVI, as examples. The calculated energies of each ion agree very well with the measured values, within 1% for almost all levels, and for all the ions. For levels with $L \geq 4$ there is nearly exact agreement, as expected for hydrogenic behavior of the highly
excited states. These are the most detailed close coupling calculations for these ions. The complete energy levels of the 15 ions are available electronically.

The complete set of energies are presented in two formats, as in the case for other ions obtained previously, e.g. for Fe V (Nahar et al. 2000), for consistency. One is in LS term format where the fine structure components of a $LS$ term are grouped together, useful for spectroscopic diagnostics. Table 3a presents sample of the table containing total sets of energies. The table contains partial set of levels of C IV and Ni XXVI. For each set of levels, the columns provide the core information, $C_t(SL\pi J)_t$, the configuration of the outer electron, $nl$, total angular momentum, $J$, energy in Rydberg, the effective quantum number of the valence electron, $\nu$, and the $LS$ term designation of the level. The top line of the set gives the number of fine structure levels expected ($Nlv$), followed by the spin and parity of the set ($2S+1L\pi$), followed by the values of $L$, where values of the total angular momentum $J$, associated with each $L$, are given within parentheses. The last line gives the number of calculated levels ($Nlv(c)$) obtained with a statement of completeness of the calculated set.

In the other format, the fine structure levels are presented in sets belonging to different $J\pi$ symmetries where levels are in energy order as shown in sample table, Table 3b. The format is convenient for easy implementation in astrophysical models requiring large number of energy levels and the corresponding transitions. At the top of each set, the total number of energy levels ($Nlv$) and the symmetry information $J\pi$ are given. For example, there are 9 fine structure levels of C IV with $J\pi = 0^e$. The levels are identified with the configuration and $LS$ term of the core, the outer electron quantum numbers, energy, the effective quantum number ($\nu$), and the $LS$ term designation. $\nu = z/\sqrt{(E - E_t)}$ where $E_t$ is the next immediate target threshold energy.

Table 4 lists the energies of the eight fine structure levels of $n = 2$ and 3 complexes of all ions from C IV to Ni XXVI. These levels are of astrophysical interest as they are often displayed in the spectra. They have been singled out to present the oscillator strengths for transitions among them.

### 4.2. Oscillator strengths

About nine hundred oscillator strengths are obtained for the allowed transitions in each Li-like ion. Astrophysical models, such as for stellar opacity calculations, will require all possible transitions for $n$ going upto 10. However, spectral diagnostics may involve only the lowest transitions.

Table 5 presents the oscillator strengths ($f$) and the transition probabilities ($A$) for transitions among $n = 2$ and 3 levels for each 15 ions from C IV to Ni XXVI. There are 14 such transitions for the 8 fine structure levels as presented in Table 4. Here the
energies are expressed in transition wavelengths rather than individual level energies in Rydberg since wavelengths are often used in astrophysical spectral analysis. However, these transition wavelengths are calculated from the measured level energies, as given in the NIST compiled table, and using the conversion factor, 1 Ry = 911.2671 Å. Hence, the \( f \) and \( A \)-values in this table are slightly different from those in the original calculated set where calculated transition energies are used. The energy independent line strengths \( S \) remain the same in both sets. Since the difference between the calculated and measured energies is typically less than 1\%, the reprocessed set in Table 5 has slight improved accuracy.

The BPRM \( A \)-values are compared with the available data, mainly from the compiled table by the NIST where they rate the accuracy to be less than 10\%. The lifetimes of some levels of Li-like ions have been measured and can be obtained theoretically from the sum of the \( A \) values as mentioned above. Lifetime experiments have been carried out by, for example, Heckmann et al. (1976), Pinnington et al. (1974) for O VI, Traëbert et al. (1977) for Si XII using beam-foil technique. However, present comparison is made mainly with individual \( A \)-values. Table 6 shows that present \( A \)-values are in very good agreement with the highly rated compiled values by NIST indicating that present \( A \)-values can be estimated to be accurate at least within 10\%.

Transition probabilities \( (A) \) for a few ions, such as S XIV, Ar XVI, and Ca XVII are not available in the NIST compilation. \( A \)-values for these ion are compared with those obtained from very accurate relativistic third-order many-body perturbation theory by Johnson et al. (1996). Present values agree almost exactly with those by Johnson et al (1996) for the two transitions \( 2s(2S_{1/2}) - 2p(2P^o_{1/2,3/2}) \), and by less than 5\% for the two transitions, \( 2p(2P^o_{1/2,3/2}) - 3s(2S_{1/2}) \). Yan et al (1998) have calculated the level energies and oscillator strengths for lithium like ions up to \( Z = 20 \) using Hylleras type variational method including finite nuclear mass effects. They present nonrelativistic \( 1s^22s(2S) - 1s^22p(2P^o) \) oscillator strengths for the ions. Present weighted averaged \( f \)-values for S XIV, Ar XVI, and Ca XXVII are compared with those by Yan et al. at the end of Table 6. Present \( f \)-values agree within 10\% with the nonrelativistic values by Yan et al.

The agreement between the present values and those from previous calculations indicates that the higher order relativistic and QED terms omitted from the BP Hamiltonian (Eq. 2) may not affect the transition probabilities of the ions considered herein by more than a few percent.

The complete set of fine structure transitions for the ions are available electronically. The tables contain calculated transition probabilities \( (A) \), oscillator strengths \( (f) \), and line strengths \( (S) \). The calculated level energies are also given in the same table. A
sample set of transitions is presented in Table 7 for O VI. The top of the table specifies the nuclear charge (Z = 8) and number of electrons in the ion, \(N_{elc} (= 3)\). Below this line are the sets of oscillator strengths belonging to pairs of symmetries, \(J_i\pi_i - J_k\pi_k\). The symmetries are expressed in the form of \(2J_i\) and \(\pi_i\) (\(\pi = 0\) for even and \(\pi = 1\) for odd parity), \(2J_k\) and \(\pi_k\), at the top of the set. For example, Table 7 present partial transitions for two pairs of symmetries, \(J = 1/2^e - J = 1/2^o\) and \(J = 1/2^e - J = 3/2^o\) of O VI. The line below the symmetries gives the number of bound levels of the two transitional symmetries, \(N_{Ji}\) and \(N_{Jk}\). The line is followed by \(N_{Ji} \times N_{Jk}\) number of transitions. The first two columns are the energy level indices, \(I_i\) and \(I_k\), whose identification can be found from the energy table, the third and the fourth columns provide the energies, \(E_i\) and \(E_k\), in Rydberg unit. The fifth column is the \(gf_L\) for the allowed transitions (\(\Delta J = 0, \pm 1\)). where \(f_L\) is the oscillator strength in length form, and \(g = 2J + 1\) is the statistical weight factor of the initial or the lower level. A negative value for \(gf\) means that \(i\) is the lower level, while a positive one means that \(k\) is the lower level. Column six is the line strength (S) and the last column is the transition probability, \(A_{ki}(sec^{-1})\).

5. Conclusion

Accurate and large-scale calculations have been carried out for the set of fine structure energy levels and transition probabilities up to \(n = 10\) for 15 Li-like ions from C IV to Ni XXVI. The set of results far exceeds the currently available experimental and theoretical data.

The results are obtained in intermediate coupling including relativistic effects using the Breit Pauli R-matrix method (BPRM) in the close coupling approximation. Both the energies and the transition probabilities show very good agreement, within 1-10%, with almost all accurate calculated and measured values available. This indicates that for these highly charged ions the higher order relativistic and QED effects omitted in the BPRM calculations may lead to an error not exceeding the estimated uncertainty.

The results from the present work should be particularly useful in the analysis of X-ray and Extreme Ultraviolet spectra from astrophysical and laboratory sources where non-local thermodynamic equilibrium (NLTE) atomic models with many excited levels are needed.

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Table 1. Fine structure energy levels of the He-like core included in the eigenfunction expansion of the Li-like ions. The spectroscopic set of configurations (1s², 1s2s, 1s2p, 1s3s, 1s3p, 1s3d) is common to each ion. The common correlation configurations are: 2s², 2p², 3s², 3p², 3d², 2s2p, 2s3s, 2s3p, 2s3d, 2s4s, 2s4p, 2p3s, 2p3p, 2p4s, 2p4p while the additional ones are listed below the table along with the values of the Thomas-Fermi scaling parameter (λ) for the orbitals.

| Level | Z= 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 |
|-------|------|---|---|---|----|----|----|----|
| s(1S) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| s(3S) | 21.9730 | 30.8550 | 41.2320 | 53.1272 | 66.5220 | 81.3907 | 97.8349 | 115.7588 |
| p(3P) | 22.3731 | 31.3320 | 41.7870 | 53.7702 | 67.2350 | 82.1766 | 98.7083 | 116.7137 |
| p(3P) | 22.3730 | 31.3320 | 41.7880 | 53.7716 | 67.2380 | 82.1896 | 98.7159 | 116.7250 |
| p(3P) | 22.3742 | 31.3350 | 41.7930 | 53.7803 | 67.2520 | 82.2172 | 98.7484 | 116.7717 |
| s(1S) | 22.3718 | 31.3410 | 41.8120 | 53.7930 | 67.2760 | 82.2395 | 98.7702 | 116.7858 |
| p(1P) | 22.6301 | 31.6560 | 42.1840 | 54.2195 | 67.6760 | 82.8055 | 99.3884 | 117.4722 |
| s(3S) | 25.8760 | 36.3770 | 48.6510 | 62.7416 | 78.5790 | 96.2408 | 115.6504 | 136.8765 |
| p(3P) | 25.9840 | 36.5070 | 48.8040 | 62.9008 | 78.7740 | 96.4588 | 115.8901 | 137.1388 |
| p(3P) | 25.9840 | 36.5070 | 48.8040 | 62.9008 | 78.7740 | 96.4626 | 115.8925 | 137.1436 |
| p(3P) | 25.9840 | 36.5070 | 48.8040 | 62.9008 | 78.7790 | 96.4705 | 115.9021 | 137.1562 |
| s(3S) | 25.9819 | 36.5050 | 48.8110 | 62.9072 | 78.7780 | 96.4603 | 115.8977 | 137.1480 |
| p(1P) | 26.0565 | 36.6000 | 48.9220 | 63.0286 | 78.9210 | 96.6379 | 116.0333 | 137.3475 |
| s(3S) | 26.0377 | 36.5730 | 48.8840 | 62.9953 | 78.8880 | 96.5905 | 116.0337 | 137.3005 |
| d(3P) | 26.0377 | 36.5730 | 48.8840 | 62.9953 | 78.8890 | 96.5915 | 116.0371 | 137.3009 |
| d(3S) | 26.0378 | 36.5730 | 48.8840 | 63.0131 | 78.8890 | 96.5941 | 116.0435 | 137.3060 |
| d(3S) | 26.0397 | 36.5760 | 48.8940 | 63.0286 | 78.9380 | 96.5996 | 116.0772 | 137.3131 |

| Level | Z= 14 | 16 | 18 | 20 | 22 | 24 | 28 |
|-------|------|---|---|---|----|----|----|
| s(1S) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| s(3S) | 135.1951 | 178.6273 | 228.1502 | 283.7881 | 345.5828 | 413.5640 | 568.2566 |
| p(3P) | 136.2322 | 179.8323 | 229.5280 | 285.3436 | 347.3211 | 415.4929 | 570.5865 |
| p(3P) | 136.2485 | 179.8615 | 229.5746 | 285.4185 | 347.4254 | 415.6301 | 570.7938 |
| p(3P) | 136.3136 | 179.9805 | 229.7776 | 285.7403 | 347.9236 | 416.3704 | 572.2873 |
| s(3S) | 136.3142 | 179.9340 | 229.6480 | 285.4858 | 347.4809 | 416.6692 | 570.7920 |
| p(1P) | 137.0731 | 180.8527 | 230.7528 | 286.8104 | 349.0801 | 417.6073 | 573.6669 |
| s(3S) | 159.8976 | 211.3517 | 270.0387 | 335.9927 | 409.2639 | 489.8955 | 673.4568 |
| p(3P) | 160.1828 | 211.6834 | 270.4184 | 336.4222 | 409.7447 | 490.4294 | 674.1039 |
| p(3P) | 160.1877 | 211.6924 | 270.4327 | 336.4421 | 409.7715 | 490.4622 | 674.1493 |
| p(3P) | 160.2070 | 211.7277 | 270.4929 | 336.5386 | 409.9204 | 490.6840 | 674.5945 |
| s(3S) | 160.1932 | 211.6973 | 270.4351 | 336.4391 | 409.7630 | 490.4485 | 674.1223 |
| p(1P) | 160.4142 | 211.9645 | 270.5750 | 336.8302 | 410.2367 | 491.0240 | 674.9808 |
| d(3P) | 160.3643 | 211.9116 | 270.7034 | 337.1180 | 410.6500 | 491.6310 | 676.6240 |
| d(3P) | 160.3648 | 211.9140 | 270.7528 | 337.1428 | 410.8550 | 491.8380 | 676.9223 |
Table 2. Comparison of calculated fine structure energies, $E_c$, with the observed values, $E_o$ (NIST) for C IV, O VI and Ni XXVI.

| Level | J  | $E_c$(Ry) | $E_o$(Ry) |
|-------|----|-----------|-----------|
| **C IV** |     |           |           |
| 1s22s $2S^o$ | 0.5 | 4.74020   | 4.73899   |
| 1s22p $2P^o$ | 1.5 | 4.15160   | 4.14885   |
| 1s22p $2P^o$ | 0.5 | 4.15260   | 4.15050   |
| 1s23s $2S^o$ | 0.5 | 1.98050   | 1.98187   |
| 1s23p $2P^o$ | 1.5 | 1.82340   | 1.82478   |
| 1s23p $2P^o$ | 0.5 | 1.82370   | 1.82526   |
| 1s23d $2D^o$ | 2.5 | 1.77960   | 1.78277   |
| 1s23d $2D^o$ | 1.5 | 1.77970   | 1.78290   |
| 1s24s $2S^o$ | 0.5 | 1.08290   | 1.08239   |
| 1s24p $2P^o$ | 1.5 | 1.01930   | 1.01878   |
| 1s24p $2P^o$ | 0.5 | 1.01940   | 1.01898   |
| 1s24d $2D^o$ | 2.5 | 1.00090   | 1.00100   |
| 1s24d $2D^o$ | 1.5 | 1.00100   | 1.00105   |
| 1s24f $2F^o$ | 3.5 | 1.00010   | 1.00004   |
| 1s24f $2F^o$ | 2.5 | 1.00010   | 1.00007   |
| 1s25s $2S^o$ | 0.5 | 0.68172   | 0.68155   |
| 1s25p $2P^o$ | 1.5 | 0.64987   | 0.64959   |
| 1s25p $2P^o$ | 0.5 | 0.64994   | 0.64969   |
| 1s25d $2D^o$ | 2.5 | 0.64052   | 0.64044   |
| 1s25d $2D^o$ | 1.5 | 0.64053   | 0.64047   |
| 1s25f $2F^o$ | 3.5 | 0.64006   | 0.64004   |
| 1s25f $2F^o$ | 2.5 | 0.64006   | 0.64005   |
| 1s25g $2G^o$ | 4.5 | 0.63998   | 0.63999   |
| 1s25g $2G^o$ | 3.5 | 0.63998   | 0.64000   |
| **O VI** |     |           |           |
| 1s22s $2S^o$ | 0.5 | 11.01520  | 11.01495  |
| 1s22p $2P^o$ | 1.5 | 9.26850   | 9.26399   |
| 1s22p $2P^o$ | 0.5 | 9.27340   | 9.27097   |
| 1s23s $2S^o$ | 0.5 | 4.31910   | 4.31964   |
| 1s23p $2P^o$ | 1.5 | 4.08010   | 4.08121   |
| 1s23p $2P^o$ | 0.5 | 4.08150   | 4.08326   |
| 1s23d $2D^o$ | 2.5 | 4.00350   | 4.00676   |
| 1s23d $2D^o$ | 1.5 | 4.00390   | 4.00734   |
| 1s24s $2S^o$ | 0.5 | 2.38130   | 2.38171   |
| 1s24p $2P^o$ | 1.5 | 2.28370   | 2.28321   |
| 1s24p $2P^o$ | 0.5 | 2.28430   | 2.28406   |
| 1s24d $2D^o$ | 2.5 | 2.25180   | 2.25168   |
| 1s24d $2D^o$ | 1.5 | 2.25200   | 2.25192   |
Table 3a. Sample table of fine structure energy levels of Li-like ions as sets of \( LS \) term components. \( C_t \) is the core configuration, \( \nu \) is the effective quantum number.

| \( C_t(S_t L_t \pi_t) \) | \( J_t \) | \( n \) | \( l \) | \( E(\text{Ry}) \) | \( \nu \) | \( S \pi \) |
|----------------|--------|-----|-----|----------------|-----|-----|
| **C VI** | | | | | | |
| \( \nu:\=1, \; ^2L^+; \; S\; (\; 1\;)/2 \) | \( 1s2 \) | \( (1Se) \) | 0 | 2 | 1 | -4.73899E+00 | 1.84 | 2 S e |
| \( \nu(\nu)\=1: \; \text{set complete} \) | | | | | | |
| \( \nu:\=2, \; ^2L^+; \; P\; (\; 3\; 1\;)/2 \) | \( 1s2 \) | \( (1Se) \) | 0 | 2p | 1 | -4.15050E+00 | 1.96 | 2 P o |
| \( \nu(\nu)\=2: \; \text{set complete} \) | | | | | | |
| **Ni XXVI** | | | | | | |
| \( \nu:\=1, \; ^2L^+; \; S\; (\; 1\;)/2 \) | \( 1s2 \) | \( (1Se) \) | 0 | 2s | 1 | -1.76520E+02 | 1.96 | 2 S e |
| \( \nu(\nu)\=1: \; \text{set complete} \) | | | | | | |
| \( \nu:\=2, \; ^2L^+; \; P\; (\; 3\; 1\;)/2 \) | \( 1s2 \) | \( (1Se) \) | 0 | 2p | 1 | -1.72635E+02 | 1.98 | 2 P o |
| \( \nu(\nu)\=2: \; \text{set complete} \) | | | | | | |
| Level  | E(Ry)              | ν      | SLπ  |
|--------|--------------------|--------|------|
|        | Ni lv = 98         |        |      |
|        | Nlv= 9, J π = 1/2 e|        |      |
| C IV:  |                    |        |      |
| 1      | 1s2(1 S°) 2 s      | 1/2    | -4.73899E+00 1.84 | 2Se |
| 2      | 1s2(1 S°) 3 s      | 1/2    | -1.98187E+00 2.84 | 2Se |
| 3      | 1s2(1 S°) 4 s      | 1/2    | -1.08239E+00 3.84 | 2Se |
| 4      | 1s2(1 S°) 5 s      | 1/2    | -6.81555E-01 4.84 | 2Se |
| 5      | 1s2(1 S°) 6 s      | 1/2    | -4.68304E-01 5.84 | 2Se |
| 6      | 1s2(1 S°) 7 s      | 1/2    | -3.41472E-01 6.84 | 2Se |
| 7      | 1s2(1 S°) 8 s      | 1/2    | -2.59968E-01 7.84 | 2Se |
| 8      | 1s2(1 S°) 9 s      | 1/2    | -2.04509E-01 8.84 | 2Se |
| 9      | 1s2(1 S°) 10 s     | 1/2    | -1.65074E-01 9.85 | 2Se |
| Ni XXVI: |                    |        |      |
|        | Nlv= 9, J π = 1/2 e|        |      |
| 1      | 1s2(1 S°) 2 s      | 1/2    | -1.76520E+02 1.96 | 2Se |
| 2      | 1s2(1 S°) 3 s      | 1/2    | -7.73614E+01 2.96 | 2Se |
| 3      | 1s2(1 S°) 4 s      | 1/2    | -4.39347E+01 3.92 | 2Se |
| 4      | 1s2(1 S°) 5 s      | 1/2    | -2.82478E+01 4.89 | 2Se |
| 5      | 1s2(1 S°) 6 s      | 1/2    | -1.95208E+01 5.88 | 2Se |
| 6      | 1s2(1 S°) 7 s      | 1/2    | -1.42712E+01 6.88 | 2Se |
| 7      | 1s2(1 S°) 8 s      | 1/2    | -1.08829E+01 7.88 | 2Se |
| 8      | 1s2(1 S°) 9 s      | 1/2    | -8.57080E+00 8.88 | 2Se |
| 9      | 1s2(1 S°) 10 s     | 1/2    | -6.92420E+00 9.88 | 2Se |
Table 4. Calculated energies for the fine structure levels of \( n = 2 \) and 3 complexes of Li-like ions. 

\( N_b \) is the total number of levels obtained. The number in the first column specifies the energy order of the level in the \( J\pi \) symmetry.

| Level | J  | E(Ry)     | \( SL\pi \) |
|-------|----|-----------|-------------|
|       |    |           |             |
| \( \text{C IV: } N_b = 97 \) |    |           |             |
| 1     | 1s\(^2\)S\(_0\) | 2s | 1/2       | -4.73899E+00 | \(^2\)Se  |
| 2     | 1s\(^2\)S\(_0\) | 3s | 1/2       | -1.98187E+00 | \(^2\)Se  |
| 1     | 1s\(^2\)S\(_0\) | 2p | 1/2       | -4.15050E+00 | \(^2\)Po  |
| 2     | 1s\(^2\)S\(_0\) | 3p | 1/2       | -1.82526E+00 | \(^2\)Po  |
| 1     | 1s\(^2\)S\(_0\) | 3d | 3/2       | -1.78290E+00 | \(^2\)De  |
| 1     | 1s\(^2\)S\(_0\) | 2p | 3/2       | -4.14885E+00 | \(^2\)Po  |
| 2     | 1s\(^2\)S\(_0\) | 3p | 3/2       | -1.82478E+00 | \(^2\)Po  |
| 1     | 1s\(^2\)S\(_0\) | 3d | 5/2       | -1.78277E+00 | \(^2\)De  |
| \( \text{N V: } N_b = 99 \) |    |           |             |
| 1     | 1s\(^2\)S\(_0\) | 2s | 1/2       | -7.19258E+00 | \(^2\)Se  |
| 2     | 1s\(^2\)S\(_0\) | 3s | 1/2       | -3.03900E+00 | \(^2\)Se  |
| 1     | 1s\(^2\)S\(_0\) | 2p | 1/2       | -6.45820E+00 | \(^2\)Po  |
| 2     | 1s\(^2\)S\(_0\) | 3p | 1/2       | -2.84225E+00 | \(^2\)Po  |
| 1     | 1s\(^2\)S\(_0\) | 3d | 3/2       | -2.78368E+00 | \(^2\)De  |
| 1     | 1s\(^2\)S\(_0\) | 2p | 3/2       | -6.45458E+00 | \(^2\)Po  |
| 2     | 1s\(^2\)S\(_0\) | 3p | 3/2       | -2.84120E+00 | \(^2\)Po  |
| 1     | 1s\(^2\)S\(_0\) | 3d | 5/2       | -2.78337E+00 | \(^2\)De  |
| \( \text{O VI: } N_b = 98 \) |    |           |             |
| 1     | 1s\(^2\)S\(_0\) | 2s | 1/2       | -1.01495E+01 | \(^2\)Se  |
| 2     | 1s\(^2\)S\(_0\) | 3s | 1/2       | -4.31964E+00 | \(^2\)Se  |
| 1     | 1s\(^2\)S\(_0\) | 2p | 1/2       | -9.27097E+00 | \(^2\)Po  |
| 2     | 1s\(^2\)S\(_0\) | 3p | 1/2       | -4.08326E+00 | \(^2\)Po  |
| 1     | 1s\(^2\)S\(_0\) | 3d | 3/2       | -4.00734E+00 | \(^2\)De  |
| 1     | 1s\(^2\)S\(_0\) | 2p | 3/2       | -9.26399E+00 | \(^2\)Po  |
| 2     | 1s\(^2\)S\(_0\) | 3p | 3/2       | -4.08121E+00 | \(^2\)Po  |
| 1     | 1s\(^2\)S\(_0\) | 3d | 5/2       | -4.00676E+00 | \(^2\)De  |
| \( \text{F VII: } N_b = 98 \) |    |           |             |
| 1     | 1s\(^2\)S\(_0\) | 2s | 1/2       | -1.36088E+01 | \(^2\)Se  |
| 2     | 1s\(^2\)S\(_0\) | 3s | 1/2       | -5.82277E+00 | \(^2\)Se  |
| 1     | 1s\(^2\)S\(_0\) | 2p | 1/2       | -1.25857E+01 | \(^2\)Po  |
| 2     | 1s\(^2\)S\(_0\) | 3p | 1/2       | -5.54675E+00 | \(^2\)Po  |
| 1     | 1s\(^2\)S\(_0\) | 3d | 3/2       | -5.45287E+00 | \(^2\)De  |
| 1     | 1s\(^2\)S\(_0\) | 2p | 3/2       | -1.25735E+01 | \(^2\)Po  |
| 2     | 1s\(^2\)S\(_0\) | 3p | 3/2       | -5.54317E+00 | \(^2\)Po  |
| 1     | 1s\(^2\)S\(_0\) | 3d | 5/2       | -5.45184E+00 | \(^2\)De  |
Table 4 continues,

| Level | J  | E(Ry)         | $SL\pi$ |
|-------|----|---------------|---------|
| Mg X: $N_b = 98$ | 1 | 1s$^2$($S_0^0$) 2s 1/2 | -2.70076E+01 | $^2S_e$ |
|       | 2 | 1s$^2$($S_0^0$) 3s 1/2 | -1.16722E+01 | $^2S_e$ |
|       | 1 | 1s$^2$($S_0^0$) 2p 1/2 | -2.55546E+01 | $^2P_o$ |
|       | 2 | 1s$^2$($S_0^0$) 3p 1/2 | -1.12786E+01 | $^2P_o$ |
|       | 1 | 1s$^2$($S_0^0$) 3d 3/2 | -1.11259E+01 | $^2D_c$ |
|       | 1 | 1s$^2$($S_0^0$) 2p 3/2 | -2.55087E+01 | $^2P_o$ |
|       | 2 | 1s$^2$($S_0^0$) 3p 3/2 | -1.12652E+01 | $^2P_o$ |
|       | 1 | 1s$^2$($S_0^0$) 3d 5/2 | -1.11219E+01 | $^2D_c$ |
| Al XI: $N_b = 98$ | 1 | 1s$^2$($S_0^0$) 2s 1/2 | -3.24858E+01 | $^2S_e$ |
|       | 2 | 1s$^2$($S_0^0$) 3s 1/2 | -1.40702E+01 | $^2S_e$ |
|       | 1 | 1s$^2$($S_0^0$) 2p 1/2 | -3.08882E+01 | $^2P_o$ |
|       | 2 | 1s$^2$($S_0^0$) 3p 1/2 | -1.36372E+01 | $^2P_o$ |
|       | 1 | 1s$^2$($S_0^0$) 3d 3/2 | -1.34623E+01 | $^2D_c$ |
|       | 1 | 1s$^2$($S_0^0$) 2p 3/2 | -3.08226E+01 | $^2P_o$ |
|       | 2 | 1s$^2$($S_0^0$) 3p 3/2 | -1.36179E+01 | $^2P_o$ |
|       | 1 | 1s$^2$($S_0^0$) 3d 5/2 | -1.34565E+01 | $^2D_c$ |
| Si XII: $N_b = 98$ | 1 | 1s$^2$($S_0^0$) 2s 1/2 | -3.84689E+01 | $^2S_e$ |
|       | 2 | 1s$^2$($S_0^0$) 3s 1/2 | -1.66918E+01 | $^2S_e$ |
|       | 1 | 1s$^2$($S_0^0$) 2p 1/2 | -3.67286E+01 | $^2P_o$ |
|       | 2 | 1s$^2$($S_0^0$) 3p 1/2 | -1.62212E+01 | $^2P_o$ |
|       | 1 | 1s$^2$($S_0^0$) 3d 3/2 | -1.60220E+01 | $^2D_c$ |
|       | 1 | 1s$^2$($S_0^0$) 2p 3/2 | -3.66376E+01 | $^2P_o$ |
|       | 2 | 1s$^2$($S_0^0$) 3p 3/2 | -1.61945E+01 | $^2P_o$ |
|       | 1 | 1s$^2$($S_0^0$) 3d 5/2 | -1.60141E+01 | $^2D_c$ |
| S XIV: $N_b = 98$  | 1 | 1s$^2$($S_0^0$) 2s 1/2 | -5.19635E+01 | $^2S_e$ |
|       | 2 | 1s$^2$($S_0^0$) 3s 1/2 | -2.26108E+01 | $^2S_e$ |
|       | 1 | 1s$^2$($S_0^0$) 2p 1/2 | -4.99351E+01 | $^2P_o$ |
|       | 2 | 1s$^2$($S_0^0$) 3p 1/2 | -2.20622E+01 | $^2P_o$ |
|       | 1 | 1s$^2$($S_0^0$) 3d 3/2 | -2.18103E+01 | $^2D_c$ |
|       | 1 | 1s$^2$($S_0^0$) 2p 3/2 | -4.97717E+01 | $^2P_o$ |
|       | 2 | 1s$^2$($S_0^0$) 3p 3/2 | -2.20141E+01 | $^2P_o$ |
|       | 1 | 1s$^2$($S_0^0$) 3d 5/2 | -2.17958E+01 | $^2D_c$ |
| Ar XVI: $N_b = 98$ | 1 | 1s$^2$($S_0^0$) 2s 1/2 | -5.19635E+01 | $^2S_e$ |
|       | 2 | 1s$^2$($S_0^0$) 3s 1/2 | -2.26108E+01 | $^2S_e$ |
|       | 1 | 1s$^2$($S_0^0$) 2p 1/2 | -4.99351E+01 | $^2P_o$ |
|       | 2 | 1s$^2$($S_0^0$) 3p 1/2 | -2.20622E+01 | $^2P_o$ |
|       | 1 | 1s$^2$($S_0^0$) 3d 3/2 | -2.18103E+01 | $^2D_c$ |
|       | 1 | 1s$^2$($S_0^0$) 2p 3/2 | -4.97717E+01 | $^2P_o$ |
|       | 2 | 1s$^2$($S_0^0$) 3p 3/2 | -2.20141E+01 | $^2P_o$ |
|       | 1 | 1s$^2$($S_0^0$) 3d 5/2 | -2.17958E+01 | $^2D_c$ |
Table 4 continues,

| Level | J   | E(Ry)      | SLπ |
|-------|-----|------------|-----|
| Ti XX: \(N_0 = 98\) |     |            |     |
| 1     | 1s2\((1 \, S_0)\)  | 2s   | 1/2   | -1.04794E+02 | 2Se |
| 2     | 1s2\((1 \, S_0)\)  | 3s   | 1/2   | -4.58280E+01 | 2Se |
| 1     | 1s2\((1 \, S_0)\)  | 2p   | 1/2   | -1.01885E+02 | 2Po |
| 2     | 1s2\((1 \, S_0)\)  | 3p   | 1/2   | -4.50420E+01 | 2Po |
| 1     | 1s2\((1 \, S_0)\)  | 3d   | 3/2   | -4.45516E+01 | 2De |
| Cr XXII: 98 |     |            |     |
| 1     | 1s2\((1 \, S_0)\)  | 2s   | 1/2   | -1.26565E+02 | 2Se |
| 2     | 1s2\((1 \, S_0)\)  | 3s   | 1/2   | -5.54020E+01 | 2Se |
| 1     | 1s2\((1 \, S_0)\)  | 2p   | 1/2   | -1.23360E+02 | 2Po |
| 2     | 1s2\((1 \, S_0)\)  | 3p   | 1/2   | -5.45381E+01 | 2Po |
| 1     | 1s2\((1 \, S_0)\)  | 3d   | 3/2   | -5.39292E+01 | 2De |
| 1     | 1s2\((1 \, S_0)\)  | 3d   | 3/2   | -5.42612E+01 | 2Po |
| 1     | 1s2\((1 \, S_0)\)  | 3d   | 5/2   | -5.38440E+01 | 2De |
| Ni XXVI: 98 |     |            |     |
| 1     | 1s2\((1 \, S_0)\)  | 2s   | 1/2   | -1.76520E+02 | 2Se |
| 2     | 1s2\((1 \, S_0)\)  | 3s   | 1/2   | -7.73614E+01 | 2Se |
| 1     | 1s2\((1 \, S_0)\)  | 2p   | 1/2   | -1.72635E+02 | 2Po |
| 2     | 1s2\((1 \, S_0)\)  | 3p   | 1/2   | -7.63001E+01 | 2Po |
| 1     | 1s2\((1 \, S_0)\)  | 3d   | 3/2   | -7.53740E+01 | 2De |
| 1     | 1s2\((1 \, S_0)\)  | 2p   | 3/2   | -1.70819E+02 | 2Po |
| 2     | 1s2\((1 \, S_0)\)  | 3p   | 3/2   | -7.57620E+01 | 2Po |
| 1     | 1s2\((1 \, S_0)\)  | 3d   | 5/2   | -7.52097E+01 | 2De |
energies are replaced by the observed energies. The notation \(a(b)\) means \(a \times 10^b\).

### Table 5. \(f\)- and \(A\)-values for \(n = 2\) and 3 transitions in Li-like ions. The calculated transition energies are replaced by the observed energies. The notation \(a(b)\) means \(a \times 10^b\).

| \(C_i\) | \(C_j\) | \(T_i\) | \(T_j\) | \(g_i\) | \(g_j\) | \(E_{ij}\) (\(A\)) | \(f\) | \(A\) (\(s^{-1}\)) |
|-------|-------|-------|-------|-------|-------|----------------|-------|---------|
| \(2s\) | \(2p\) | \(2S^o\) | \(2P^o\) | 2 | 2 | 1550.8 | 9.501(-2) | 2.63(8) |
| \(2s\) | \(2p\) | \(2S^o\) | \(2P^o\) | 2 | 4 | 1548.2 | 1.904(-1) | 2.65(8) |
| \(LS\) | \(2S^o\) | \(2P^o\) | 2 | 6 | 2.854(-1) | 2.64(8) |
| \(2s\) | \(3p\) | \(2S^o\) | \(2P^o\) | 2 | 2 | 312.5 | 6.810(-2) | 4.65(9) |
| \(2s\) | \(3p\) | \(2S^o\) | \(2P^o\) | 2 | 4 | 312.4 | 1.358(-1) | 4.64(9) |
| \(LS\) | \(2S^o\) | \(2P^o\) | 2 | 6 | 2.039(-1) | 4.64(9) |
| \(2p\) | \(3s\) | \(2P^o\) | \(2S^o\) | 2 | 2 | 419.5 | 3.769(-2) | 1.43(9) |
| \(2p\) | \(3s\) | \(2P^o\) | \(2S^o\) | 4 | 2 | 419.7 | 3.781(-2) | 2.86(9) |
| \(LS\) | \(2P^o\) | \(2S^o\) | 6 | 2 | 3.777(-2) | 4.29(9) |
| \(3s\) | \(3p\) | \(2S^o\) | \(2P^o\) | 2 | 2 | 5811.7 | 1.595(-1) | 3.15(7) |
| \(3s\) | \(3p\) | \(2S^o\) | \(2P^o\) | 2 | 4 | 5800.6 | 3.197(-1) | 3.17(7) |
| \(LS\) | \(2S^o\) | \(2P^o\) | 2 | 6 | 4.792(-1) | 3.16(7) |
| \(2p\) | \(3d\) | \(2P^o\) | \(2D^o\) | 2 | 4 | 384.0 | 6.486(-1) | 1.47(10) |
| \(2p\) | \(3d\) | \(2P^o\) | \(2D^o\) | 4 | 4 | 384.2 | 6.489(-2) | 2.93(9) |
| \(2p\) | \(3d\) | \(2P^o\) | \(2D^o\) | 4 | 6 | 384.2 | 5.839(-1) | 1.76(10) |
| \(LS\) | \(2P^o\) | \(2D^o\) | 6 | 10 | 6.487(-1) | 1.76(10) |
| \(3p\) | \(3d\) | \(2P^o\) | \(2D^o\) | 2 | 4 | 20710.6 | 6.247(-2) | 4.86(5) |
| \(3p\) | \(3d\) | \(2P^o\) | \(2D^o\) | 4 | 4 | 20852.8 | 6.205(-3) | 9.52(4) |
| \(3p\) | \(3d\) | \(2P^o\) | \(2D^o\) | 4 | 6 | 20805.2 | 5.599(-2) | 5.75(5) |
| \(LS\) | \(2P^o\) | \(2D^o\) | 6 | 10 | 6.221(-2) | 5.75(5) |

### N V

| \(C_i\) | \(C_j\) | \(T_i\) | \(T_j\) | \(g_i\) | \(g_j\) | \(E_{ij}\) (\(A\)) | \(f\) | \(A\) (\(s^{-1}\)) |
|-------|-------|-------|-------|-------|-------|----------------|-------|---------|
| \(2s\) | \(2p\) | \(2S^o\) | \(2P^o\) | 2 | 2 | 1242.9 | 7.783(-2) | 3.36(8) |
| \(2s\) | \(2p\) | \(2S^o\) | \(2P^o\) | 2 | 4 | 1238.8 | 1.563(-1) | 3.40(8) |
| \(LS\) | \(2S^o\) | \(2P^o\) | 2 | 6 | 2.341(-1) | 3.38(8) |
| \(2s\) | \(3p\) | \(2S^o\) | \(2P^o\) | 2 | 2 | 209.3 | 8.004(-2) | 1.22(10) |
| \(2s\) | \(3p\) | \(2S^o\) | \(2P^o\) | 2 | 4 | 209.3 | 1.594(-1) | 1.21(10) |
| \(LS\) | \(2S^o\) | \(2P^o\) | 2 | 6 | 2.394(-1) | 1.22(10) |
| \(2p\) | \(3s\) | \(2P^o\) | \(2S^o\) | 2 | 2 | 266.2 | 3.240(-2) | 3.05(9) |
| \(2p\) | \(3s\) | \(2P^o\) | \(2S^o\) | 4 | 2 | 266.4 | 3.256(-2) | 6.12(9) |
| \(LS\) | \(2P^o\) | \(2S^o\) | 6 | 2 | 3.251(-2) | 9.17(9) |
| \(3s\) | \(3p\) | \(2S^o\) | \(2P^o\) | 2 | 2 | 4621.0 | 1.309(-1) | 4.09(7) |
| \(3s\) | \(3p\) | \(2S^o\) | \(2P^o\) | 2 | 4 | 4604.7 | 2.630(-1) | 4.14(7) |
| \(LS\) | \(2S^o\) | \(2P^o\) | 2 | 6 | 3.939(-1) | 4.12(7) |
| \(2p\) | \(3d\) | \(2P^o\) | \(2D^o\) | 2 | 4 | 247.6 | 6.534(-1) | 3.56(10) |
| \(2p\) | \(3d\) | \(2P^o\) | \(2D^o\) | 4 | 4 | 247.7 | 6.539(-2) | 7.11(9) |
| \(2p\) | \(3d\) | \(2P^o\) | \(2D^o\) | 4 | 6 | 247.7 | 5.883(-1) | 4.26(10) |
| \(LS\) | \(2P^o\) | \(2D^o\) | 6 | 10 | 6.535(-1) | 4.26(10) |
| \(3p\) | \(3d\) | \(2P^o\) | \(2D^o\) | 2 | 4 | 15062.3 | 5.499(-2) | 8.08(5) |
| \(3p\) | \(3d\) | \(2P^o\) | \(2D^o\) | 4 | 4 | 15238.6 | 5.432(-3) | 1.56(5) |
| \(3p\) | \(3d\) | \(2P^o\) | \(2D^o\) | 4 | 6 | 15187.8 | 4.909(-2) | 9.46(5) |
| \(LS\) | \(2P^o\) | \(2D^o\) | 6 | 10 | 5.456(-2) | 9.47(5) |
| $C_i$ | $C_j$ | $T_i$ | $T_j$ | $g_i$ | $g_j$ | $E_{ij}$ (Å) | $f$ | $A$ ($s^{-1}$) |
|-------|-------|-------|-------|-------|-------|-------------|-----|-------------|
| **F VII** |
| 2s 2p | $^2S^o$ | $^2p^o$ | 2 | 2 | 890.8 | 5.710(-2) | 4.80(8) |
| 2s 2p | $^2S^o$ | $^2p^o$ | 2 | 4 | 883.0 | 1.154(-1) | 4.93(8) |
| LS | $^2S^o$ | $^2p^o$ | 2 | 6 | 1.725(-1) | 4.89(8) |
| 2s 3p | $^2S^o$ | $^2p^o$ | 2 | 2 | 113.0 | 9.585(-2) | 5.01(10) |
| 2s 3p | $^2S^o$ | $^2p^o$ | 2 | 4 | 112.9 | 1.906(-1) | 4.98(10) |
| LS | $^2S^o$ | $^2p^o$ | 2 | 6 | 2.865(-1) | 4.99(10) |
| 2p 3s | $^2p^o$ | $^2S^o$ | 2 | 2 | 134.7 | 2.652(-2) | 9.75(9) |
| 2p 3s | $^2p^o$ | $^2S^o$ | 4 | 2 | 134.9 | 2.677(-2) | 1.96(10) |
| LS | $^2p^o$ | $^2S^o$ | 6 | 2 | 2.669(-2) | 2.94(10) |
| 3s 3p | $^2S^o$ | $^2p^o$ | 2 | 2 | 3277.9 | 9.619(-2) | 5.97(7) |
| 3s 3p | $^2S^o$ | $^2p^o$ | 2 | 4 | 3247.6 | 1.944(-1) | 6.15(7) |
| LS | $^2S^o$ | $^2p^o$ | 2 | 6 | 2.906(-1) | 6.09(7) |
| 2p 3d | $^2p^o$ | $^2D^o$ | 2 | 4 | 127.7 | 6.601(-1) | 1.35(11) |
| 2p 3d | $^2p^o$ | $^2D^o$ | 4 | 4 | 127.8 | 6.613(-1) | 2.70(10) |
| 2p 3d | $^2p^o$ | $^2D^o$ | 4 | 6 | 127.8 | 5.948(-1) | 1.62(11) |
| LS | $^2p^o$ | $^2D^o$ | 6 | 10 | 6.605(-1) | 1.62(11) |
| 3p 3d | $^2p^o$ | $^2D^o$ | 2 | 4 | 9532.1 | 4.426(-2) | 1.62(6) |
| 3p 3d | $^2p^o$ | $^2D^o$ | 4 | 4 | 9798.6 | 4.303(-3) | 2.99(5) |
| 3p 3d | $^2p^o$ | $^2D^o$ | 4 | 6 | 9715.0 | 3.909(-2) | 1.84(6) |
| LS | $^2p^o$ | $^2D^o$ | 6 | 10 | 4.346(-2) | 1.85(6) |
| **Ne VIII** |
| 2s 2p | $^2S^o$ | $^2p^o$ | 2 | 2 | 780.2 | 5.038(-2) | 5.52(8) |
| 2s 2p | $^2S^o$ | $^2p^o$ | 2 | 4 | 770.3 | 1.023(-1) | 5.75(8) |
| LS | $^2S^o$ | $^2p^o$ | 2 | 6 | 1.527(-1) | 5.67(8) |
| 2s 3p | $^2S^o$ | $^2p^o$ | 2 | 2 | 88.1 | 1.013(-1) | 8.70(10) |
| 2s 3p | $^2S^o$ | $^2p^o$ | 2 | 4 | 88.1 | 2.012(-1) | 8.65(10) |
| LS | $^2S^o$ | $^2p^o$ | 2 | 6 | 3.025(-1) | 8.67(10) |
| 2p 3s | $^2p^o$ | $^2S^o$ | 2 | 2 | 102.9 | 2.479(-2) | 1.56(10) |
| 2p 3s | $^2p^o$ | $^2S^o$ | 4 | 2 | 103.1 | 2.506(-2) | 3.15(10) |
| LS | $^2p^o$ | $^2S^o$ | 6 | 2 | 2.497(-2) | 4.71(10) |
| 3s 3p | $^2S^o$ | $^2p^o$ | 2 | 2 | 2861.1 | 8.493(-2) | 6.92(7) |
| 3s 3p | $^2S^o$ | $^2p^o$ | 2 | 4 | 2822.1 | 1.724(-1) | 7.22(7) |
| LS | $^2S^o$ | $^2p^o$ | 2 | 6 | 2.573(-1) | 7.12(7) |
| 2p 3d | $^2p^o$ | $^2D^o$ | 2 | 4 | 98.1 | 6.624(-1) | 2.29(11) |
| 2p 3d | $^2p^o$ | $^2D^o$ | 4 | 4 | 98.3 | 6.645(-2) | 4.59(10) |
| 2p 3d | $^2p^o$ | $^2D^o$ | 4 | 6 | 98.3 | 5.976(-1) | 2.75(11) |
| LS | $^2p^o$ | $^2D^o$ | 6 | 10 | 6.633(-1) | 2.75(11) |
| 3p 3d | $^2p^o$ | $^2D^o$ | 2 | 4 | 7979.6 | 4.045(-2) | 2.12(6) |
| 3p 3d | $^2p^o$ | $^2D^o$ | 4 | 4 | 8299.3 | 3.888(-3) | 3.76(5) |
| 3p 3d | $^2p^o$ | $^2D^o$ | 4 | 6 | 8194.8 | 3.544(-2) | 2.35(6) |
| LS | $^2p^o$ | $^2D^o$ | 6 | 10 | 3.941(-2) | 2.35(6) |
| **Na IX** |
### Table 5 continues.

| $C_i$ | $C_j$ | $T_i$ | $T_j$ | $g_i$ | $g_j$ | $E_{ij}$ (Å) | $f$ (s$^{-1}$) | $A$ (s$^{-1}$) |
|-------|-------|-------|-------|-------|-------|---------------|---------------|---------------|
|       |       |       |       |       |       |               |               |               |
| **Mg X** |
| 2s    | 2p    | $^2S^e$ | $^2P^o$ | 2  | 2  | 624.6        | 4.078(2)      | 6.97(8)       |
| 2s    | 2p    | $^2S^e$ | $^2P^o$ | 2  | 4  | 609.5        | 8.384(2)      | 7.53(8)       |
| LS    |       | $^2S^e$ | $^2P^o$ | 2  | 6  | 1.246(-1)    | 7.34(8)       |               |
| 2s    | 3p    | $^2S^e$ | $^2P^o$ | 2  | 2  | 57.9         | 1.094(-1)     | 2.18(11)      |
| 2s    | 3p    | $^2S^e$ | $^2P^o$ | 2  | 4  | 57.9         | 2.167(-1)     | 2.16(11)      |
| LS    |       | $^2S^e$ | $^2P^o$ | 2  | 6  | 3.261(-1)    | 2.16(11)      |               |
| 2p    | 3s    | $^2P^o$ | $^2S^e$ | 2  | 2  | 65.7         | 2.242(-2)     | 3.47(10)      |
| 2p    | 3s    | $^2P^o$ | $^2S^e$ | 4  | 2  | 65.8         | 2.282(-2)     | 7.02(10)      |
| LS    |       | $^2P^o$ | $^2S^e$ | 6  | 2  | 2.269(-2)    | 1.05(11)      |               |
| 3s    | 3p    | $^2S^e$ | $^2P^o$ | 2  | 2  | 2278.2       | 6.880(-2)     | 8.84(7)       |
| 3s    | 3p    | $^2S^e$ | $^2P^o$ | 2  | 4  | 2211.8       | 1.420(-1)     | 9.68(7)       |
| LS    |       | $^2S^e$ | $^2P^o$ | 2  | 6  | 2.108(-1)    | 9.39(7)       |               |
| 2p    | 3d    | $^2P^o$ | $^2D^e$ | 2  | 4  | 63.2         | 6.666(-1)     | 5.57(11)      |
| 2p    | 3d    | $^2P^o$ | $^2D^e$ | 4  | 4  | 63.3         | 6.689(-2)     | 1.11(11)      |
| 2p    | 3d    | $^2P^o$ | $^2D^e$ | 4  | 6  | 63.3         | 6.019(-1)     | 6.68(11)      |
| LS    |       | $^2P^o$ | $^2D^e$ | 6  | 10 | 6.678(-1)    | 6.68(11)      |               |
| 3p    | 3d    | $^2P^o$ | $^2D^e$ | 2  | 4  | 5917.3       | 3.486(-2)     | 3.32(6)       |
| 3p    | 3d    | $^2P^o$ | $^2D^e$ | 4  | 4  | 6417.4       | 3.210(-3)     | 5.20(5)       |
| 3p    | 3d    | $^2P^o$ | $^2D^e$ | 4  | 6  | 6241.6       | 2.975(-2)     | 3.40(6)       |
| LS    |       | $^2P^o$ | $^2D^e$ | 6  | 10 | 3.308(-2)    | 3.40(6)       |               |
| **Al XI** |
| 2s    | 2p    | $^2S^e$ | $^2P^o$ | 2  | 2  | 568.1        | 3.721(-2)     | 7.69(8)       |
| 2s    | 2p    | $^2S^e$ | $^2P^o$ | 2  | 4  | 550.3        | 7.717(-2)     | 8.50(8)       |
| LS    |       | $^2S^e$ | $^2P^o$ | 2  | 6  | 1.144(-1)    | 8.22(8)       |               |
| 2s    | 3p    | $^2S^e$ | $^2P^o$ | 2  | 2  | 48.3         | 1.125(-1)     | 3.21(11)      |
| 2s    | 3p    | $^2S^e$ | $^2P^o$ | 2  | 4  | 48.3         | 2.224(-1)     | 3.18(11)      |
| LS    |       | $^2S^e$ | $^2P^o$ | 2  | 6  | 3.349(-1)    | 3.19(11)      |               |
| 2p    | 3s    | $^2P^o$ | $^2S^e$ | 2  | 2  | 54.2         | 2.159(-2)     | 4.90(10)      |
| 2p    | 3s    | $^2P^o$ | $^2S^e$ | 4  | 2  | 54.4         | 2.205(-2)     | 9.94(10)      |
| LS    |       | $^2P^o$ | $^2S^e$ | 6  | 2  | 2.190(-2)    | 1.48(11)      |               |
| 3s    | 3p    | $^2S^e$ | $^2P^o$ | 2  | 2  | 2066.4       | 6.287(-2)     | 9.82(7)       |
| 3s    | 3p    | $^2S^e$ | $^2P^o$ | 2  | 4  | 1994.0       | 1.305(-1)     | 1.09(8)       |
| LS    |       | $^2S^e$ | $^2P^o$ | 2  | 6  | 1.934(-1)    | 1.06(8)       |               |
| 2p    | 3d    | $^2P^o$ | $^2D^e$ | 2  | 4  | 52.3         | 6.679(-1)     | 8.14(11)      |
| 2p    | 3d    | $^2P^o$ | $^2D^e$ | 4  | 4  | 52.5         | 6.710(-2)     | 1.63(11)      |
| 2p    | 3d    | $^2P^o$ | $^2D^e$ | 4  | 6  | 52.4         | 6.034(-1)     | 9.75(11)      |
| LS    |       | $^2P^o$ | $^2D^e$ | 6  | 10 | 6.693(-1)    | 9.75(11)      |               |
| 3p    | 3d    | $^2P^o$ | $^2D^e$ | 2  | 4  | 5177.7       | 3.291(-2)     | 4.09(6)       |
| 3p    | 3d    | $^2P^o$ | $^2D^e$ | 4  | 4  | 5695.4       | 2.988(-3)     | 6.14(5)       |
| 3p    | 3d    | $^2P^o$ | $^2D^e$ | 4  | 6  | 5556.5       | 2.761(-2)     | 3.98(6)       |
| LS    |       | $^2P^o$ | $^2D^e$ | 6  | 10 | 3.084(-2)    | 4.04(6)       |               |

**Si XII**
Table 5 continues.

|   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|
| $C_i$ | $C_j$ | $T_i$ | $T_j$ | $g_i$ | $g_j$ | $E_{ij}$ (Å) | $f$ | $A$ (s$^{-1}$) |
| S XIV |
| 2s | 2p | $^2S^e$ | $^2P^o$ | 2 | 2 | 445.8 | 2.951(-2) | 9.90(8) |
| 2s | 2p | $^2S^e$ | $^2P^o$ | 2 | 4 | 417.6 | 6.335(-2) | 1.21(9) |
| LS | $^2S^e$ | $^2P^o$ | 2 | 6 | 9.285(-2) | 1.13(9) |
| 2s | 3p | $^2S^e$ | $^2P^o$ | 2 | 2 | 30.5 | 1.198(-1) | 8.61(11) |
| 2s | 3p | $^2S^e$ | $^2P^o$ | 2 | 4 | 30.4 | 2.354(-1) | 8.48(11) |
| LS | $^2S^e$ | $^2P^o$ | 2 | 6 | 3.552(-1) | 8.52(11) |
| 2p | 3s | $^2P^o$ | $^2S^e$ | 2 | 2 | 33.4 | 1.989(-2) | 1.19(11) |
| 2p | 3s | $^2P^o$ | $^2S^e$ | 4 | 2 | 33.5 | 2.056(-2) | 2.44(11) |
| LS | $^2P^o$ | $^2S^e$ | 6 | 2 | 2.034(-2) | 3.63(11) |
| 3s | 3p | $^2S^e$ | $^2P^o$ | 2 | 2 | 1615.7 | 4.980(-2) | 1.27(8) |
| 3s | 3p | $^2S^e$ | $^2P^o$ | 2 | 4 | 1506.2 | 1.072(-1) | 1.58(8) |
| LS | $^2S^e$ | $^2P^o$ | 2 | 6 | 1.570(-1) | 1.47(8) |
| 2p | 3d | $^2P^o$ | $^2D^e$ | 2 | 4 | 32.4 | 6.705(-1) | 2.13(12) |
| 2p | 3d | $^2P^o$ | $^2D^e$ | 4 | 4 | 32.6 | 6.753(-2) | 4.24(11) |
| 2p | 3d | $^2P^o$ | $^2D^e$ | 4 | 6 | 32.6 | 6.073(-1) | 2.55(12) |
| LS | $^2P^o$ | $^2D^e$ | 6 | 10 | 6.729(-1) | 2.54(12) |
| 3p | 3d | $^2P^o$ | $^2D^e$ | 2 | 4 | 3674.5 | 2.857(-2) | 7.06(6) |
| 3p | 3d | $^2P^o$ | $^2D^e$ | 4 | 4 | 4402.3 | 2.382(-3) | 8.20(5) |
| 3p | 3d | $^2P^o$ | $^2D^e$ | 4 | 6 | 4142.1 | 2.283(-2) | 5.92(6) |
| LS | $^2P^o$ | $^2D^e$ | 6 | 10 | 2.544(-2) | 5.98(6) |
| Ar XVI |
| 2s | 2p | $^2S^e$ | $^2P^o$ | 2 | 2 | 389.1 | 2.594(-2) | 1.14(9) |
| 2s | 2p | $^2S^e$ | $^2P^o$ | 2 | 4 | 353.9 | 5.747(-2) | 1.53(9) |
| LS | $^2S^e$ | $^2P^o$ | 2 | 6 | 8.340(-2) | 1.39(9) |
| 2s | 3p | $^2S^e$ | $^2P^o$ | 2 | 2 | 23.5 | 1.232(-1) | 1.48(12) |
| 2s | 3p | $^2S^e$ | $^2P^o$ | 2 | 4 | 23.5 | 2.410(-1) | 1.45(12) |
| LS | $^2S^e$ | $^2P^o$ | 2 | 6 | 3.642(-1) | 1.46(12) |
| 2p | 3s | $^2P^o$ | $^2S^e$ | 2 | 2 | 25.5 | 1.915(-2) | 1.96(11) |
| 2p | 3s | $^2P^o$ | $^2S^e$ | 4 | 2 | 25.7 | 2.000(-2) | 4.04(11) |
| LS | $^2P^o$ | $^2S^e$ | 6 | 2 | 1.972(-2) | 6.01(11) |
| 3s | 3p | $^2S^e$ | $^2P^o$ | 2 | 2 | 1421.6 | 4.334(-2) | 1.43(8) |
| 3s | 3p | $^2S^e$ | $^2P^o$ | 2 | 4 | 1281.7 | 9.659(-2) | 1.96(8) |
| LS | $^2S^e$ | $^2P^o$ | 2 | 6 | 1.399(-1) | 1.77(8) |
| 2p | 3d | $^2P^o$ | $^2D^e$ | 2 | 4 | 24.8 | 6.723(-1) | 3.63(12) |
| 2p | 3d | $^2P^o$ | $^2D^e$ | 4 | 4 | 25.0 | 6.774(-2) | 7.22(11) |
| 2p | 3d | $^2P^o$ | $^2D^e$ | 4 | 6 | 25.0 | 6.089(-1) | 4.33(12) |
| LS | $^2P^o$ | $^2D^e$ | 6 | 10 | 6.746(-1) | 4.33(12) |
| 3p | 3d | $^2P^o$ | $^2D^e$ | 2 | 4 | 2874.7 | 2.792(-2) | 1.13(7) |
| 3p | 3d | $^2P^o$ | $^2D^e$ | 4 | 4 | 3689.3 | 2.172(-3) | 1.06(6) |
| 3p | 3d | $^2P^o$ | $^2D^e$ | 4 | 6 | 3387.6 | 2.135(-2) | 8.27(6) |
| LS | $^2P^o$ | $^2D^e$ | 6 | 10 | 2.383(-2) | 8.40(6) |
| Ca XVIII |
Table 5 continues.

|  $C_i$ |  $C_j$ |  $T_i$ |  $T_j$ |  $g_i$ |  $g_j$ |  $E_{ij}$ |  $f$ |  $A$ |
|-------|-------|-------|-------|-------|-------|---------|-----|-----|
|       |       |       |       |       |       | (Å)     |     | (s⁻¹) |
|       |       |       |       |       |       |         |     |      |
| Ti XX |       |       |       |       |       |         |     |      |
| 2s 2p | 2s 2p | 2p² | 2p² | 2 | 2 | 308.9 | 2.093(-2) | 1.46(9) |
| 2s 2p | 2s 2p | 2p² | 2p² | 2 | 4 | 259.6 | 5.040(-2) | 2.49(9) |
| LS    | LS    | 2p² | 2p² | 2 | 6 | 7.130(-2) | 2.11(9) |
| 2s 3p | 2s 3p | 2p² | 2p² | 2 | 2 | 15.3 | 1.281(-1) | 3.67(12) |
| 2s 3p | 2s 3p | 2p² | 2p² | 2 | 4 | 15.2 | 2.481(-1) | 3.58(12) |
| LS    | LS    | 2p² | 2p² | 2 | 6 | 3.762(-1) | 3.61(12) |
| 2p 3s | 2p 3s | 2p² | 2p² | 2 | 2 | 16.3 | 1.811(-2) | 4.56(11) |
| 2p 3s | 2p 3s | 2p² | 2p² | 2 | 4 | 16.4 | 1.935(-2) | 9.54(11) |
| LS    | LS    | 2p² | 2p² | 2 | 6 | 1.894(-2) | 1.41(12) |
| 3s 3p | 3s 3p | 2p² | 2p² | 2 | 2 | 1111.3 | 3.541(-2) | 1.91(8) |
| 3s 3p | 3s 3p | 2p² | 2p² | 2 | 4 | 926.1 | 8.561(-2) | 3.33(8) |
| LS    | LS    | 2p² | 2p² | 2 | 6 | 1.210(-1) | 2.80(8) |
| 2p 3d | 2p 3d | 2p² | 2p² | 2 | 4 | 15.9 | 6.720(-1) | 8.86(12) |
| 2p 3d | 2p 3d | 2p² | 2p² | 2 | 4 | 16.1 | 6.802(-2) | 1.76(12) |
| 2p 3d | 2p 3d | 2p² | 2p² | 2 | 6 | 16.0 | 6.113(-1) | 1.06(13) |
| LS    | LS    | 2p² | 2p² | 2 | 6 | 6.759(-1) | 1.05(13) |
| 3p 3d | 3p 3d | 2p² | 2p² | 2 | 4 | 1852.2 | 2.768(-2) | 2.69(7) |
| 3p 3d | 3p 3d | 2p² | 2p² | 2 | 4 | 2778.3 | 1.840(-3) | 1.59(6) |
| 3p 3d | 3p 3d | 2p² | 2p² | 2 | 6 | 2385.5 | 1.936(-2) | 1.51(7) |
| LS    | LS    | 2p² | 2p² | 2 | 6 | 2.161(-2) | 1.54(7) |
| Cr XXII |       |       |       |       |       |         |     |      |
| 2s 2p | 2s 2p | 2p² | 2p² | 2 | 2 | 279.5 | 1.909(-2) | 1.63(9) |
| 2s 2p | 2s 2p | 2p² | 2p² | 2 | 4 | 223.3 | 4.847(-2) | 3.24(9) |
| LS    | LS    | 2p² | 2p² | 2 | 6 | 6.751(-2) | 2.62(9) |
| 2s 3p | 2s 3p | 2p² | 2p² | 2 | 2 | 12.7 | 1.302(-1) | 5.42(12) |
| 2s 3p | 2s 3p | 2p² | 2p² | 2 | 4 | 12.6 | 2.506(-1) | 5.24(12) |
| LS    | LS    | 2p² | 2p² | 2 | 6 | 3.808(-1) | 5.30(12) |
| 2p 3s | 2p 3s | 2p² | 2p² | 2 | 2 | 13.4 | 1.783(-2) | 6.63(11) |
| 2p 3s | 2p 3s | 2p² | 2p² | 2 | 4 | 13.6 | 1.931(-2) | 1.40(12) |
| LS    | LS    | 2p² | 2p² | 2 | 6 | 1.882(-2) | 2.07(12) |
| 3s 3p | 3s 3p | 2p² | 2p² | 2 | 2 | 1428.3 | 2.270(-2) | 7.42(7) |
| 3s 3p | 3s 3p | 2p² | 2p² | 2 | 4 | 1042.6 | 6.275(-2) | 1.93(8) |
| LS    | LS    | 2p² | 2p² | 2 | 6 | 8.540(-2) | 1.45(8) |
| 2p 3d | 2p 3d | 2p² | 2p² | 2 | 4 | 13.1 | 6.707(-1) | 1.29(13) |
| 2p 3d | 2p 3d | 2p² | 2p² | 2 | 4 | 13.3 | 6.808(-2) | 2.56(12) |
| 2p 3d | 2p 3d | 2p² | 2p² | 2 | 6 | 13.3 | 6.114(-1) | 1.54(13) |
| LS    | LS    | 2p² | 2p² | 2 | 6 | 6.754(-1) | 1.54(13) |
| Ni XXVI |       |       |       |       |       |         |     |      |
| 2s 2s | 2s 2s | 2p² | 2p² | 2 | 2 | 314.3 | 1.618(-2) | 1.97(9) |
Table 6. Comparison of BPRM A-values with those in the NIST compilation, Refs: a-Johnson et al (1996), b-Yan et al. (1998).

|       | Ci   | Cj   | Ti   | Tj   | gi  | gj  | Eij  | \(A(s^{-1})\) present | \(A(s^{-1})\) NIST |
|-------|------|------|------|------|-----|-----|------|-----------------------|-------------------|
|       |      |      |      |      |     |     |      |                       |                   |
| C IV  |      |      |      |      |     |     |      |                       |                   |
| 2s    | 2p   | \(2S^e\) | \(2P^o\) | 2   | 2   |     | 1550.8 | 2.63(8)                | 2.64(8)           |
| 2s    | 2p   | \(2S^e\) | \(2P^o\) | 2   | 4   |     | 1548.2 | 2.65(8)                | 2.65(8)           |
| 2s    | 3p   | \(2S^e\) | \(2P^o\) | 2   | 2   |     | 312.5  | 4.65(9)                | 4.63(9)           |
| 2s    | 3p   | \(2S^e\) | \(2P^o\) | 2   | 4   |     | 312.4  | 4.64(9)                | 4.63(9)           |
| 2p    | 3s   | \(2P^o\) | \(2S^e\) | 2   | 2   |     | 419.5  | 1.43(9)                | 1.42(9)           |
| 2p    | 3s   | \(2P^o\) | \(2S^e\) | 4   | 2   |     | 419.7  | 2.86(9)                | 2.85(9)           |
| N V   |      |      |      |      |     |     |      |                       |                   |
| 2s    | 2p   | \(2S^e\) | \(2P^o\) | 2   | 2   |     | 1242.9 | 3.36(8)                | 3.37(8)           |
| 2s    | 2p   | \(2S^e\) | \(2P^o\) | 2   | 4   |     | 1238.8 | 3.40(8)                | 3.40(8)           |
| 2s    | 3p   | \(2S^e\) | \(2P^o\) | 2   | 2   |     | 209.3  | 1.22(10)               | 1.21(10)          |
| 2s    | 3p   | \(2S^e\) | \(2P^o\) | 2   | 4   |     | 209.3  | 1.21(10)               | 1.21(10)          |
| 2p    | 3s   | \(2P^o\) | \(2S^e\) | 2   | 2   |     | 266.2  | 3.05(9)                | 3.04(9)           |
| 2p    | 3s   | \(2P^o\) | \(2S^e\) | 4   | 2   |     | 266.4  | 6.12(9)                | 6.07(9)           |
| O VI  |      |      |      |      |     |     |      |                       |                   |
| 2s    | 2p   | \(2S^e\) | \(2P^o\) | 2   | 2   |     | 1037.2 | 4.09(8)                | 4.09(8)           |
| 2s    | 2p   | \(2S^e\) | \(2P^o\) | 2   | 4   |     | 1031.4 | 4.16(8)                | 4.16(8)           |
| 2s    | 3p   | \(2S^e\) | \(2P^o\) | 2   | 2   |     | 150.1  | 2.63(10)               | 2.62(10)          |
| 2s    | 3p   | \(2S^e\) | \(2P^o\) | 2   | 4   |     | 150.1  | 2.62(10)               | 2.62(10)          |
| 2p    | 3d   | \(2P^o\) | \(2D^e\) | 2   | 4   |     | 172.9  | 7.32(10)               | 7.33(10)          |
| 2p    | 3d   | \(2P^o\) | \(2D^e\) | 4   | 4   |     | 173.1  | 1.46(10)               | 1.46(10)          |
| 2p    | 3d   | \(2P^o\) | \(2D^e\) | 4   | 6   |     | 173.1  | 8.79(10)               | 8.78(10)          |
| F VII |      |      |      |      |     |     |      |                       |                   |
| 2s    | 2p   | \(2S^e\) | \(2P^o\) | 2   | 2   |     | 890.8  | 4.80(8)                | 4.69(8)           |
| 2s    | 2p   | \(2S^e\) | \(2P^o\) | 2   | 4   |     | 883.0  | 4.93(8)                | 4.81(8)           |
| 2s    | 3p   | \(2S^e\) | \(2P^o\) | 2   | 2   |     | 113.0  | 5.01(10)               | 4.99(10)          |
| 2s    | 3p   | \(2S^e\) | \(2P^o\) | 2   | 4   |     | 112.9  | 4.98(10)               | 4.99(10)          |
| 2p    | 3s   | \(2P^o\) | \(2S^e\) | 2   | 2   |     | 134.7  | 9.75(9)                | 8.83(9)           |
| 2p    | 3s   | \(2P^o\) | \(2S^e\) | 4   | 2   |     | 134.9  | 1.96(10)               | 1.75(10)          |
| Ne VIII |  | | | | | | | |
| 2s    | 2p   | \(2S^e\) | \(2P^o\) | 2   | 2   |     | 780.2  | 5.52(8)                | 5.50(8)           |
| 2s    | 2p   | \(2S^e\) | \(2P^o\) | 2   | 4   |     | 770.3  | 5.75(8)                | 5.72(8)           |
| 2s    | 3p   | \(2S^e\) | \(2P^o\) | 2   | 2   |     | 88.1   | 8.70(10)               | 8.53(10)          |
| 2s    | 3p   | \(2S^e\) | \(2P^o\) | 2   | 4   |     | 88.1   | 8.65(10)               | 8.53(10)          |
| 2p    | 3s   | \(2P^o\) | \(2S^e\) | 2   | 2   |     | 102.9  | 1.56(10)               | 1.53(10)          |
| 2p    | 3s   | \(2P^o\) | \(2S^e\) | 4   | 2   |     | 103.1  | 3.15(10)               | 3.07(10)          |
| Na IX |      |      |      |      |     |     |      |                       |                   |
| 2s    | 2p   | \(2S^e\) | \(2P^o\) | 2   | 2   |     | 694.0  | 6.24(8)                | 6.30(8)           |
Table 6 continues.

| $C_i$ | $C_j$ | $T_i$ | $T_j$ | $g_i$ | $g_j$ | $E_{ij}$ (Ry) | $A(s^{-1})$ present | $A(s^{-1})$ NIST |
|------|------|------|------|------|------|----------------|---------------------|------------------|
| Si XII |
| 2s 2p $^2S^e$ $^2P^o$ 2 2 520.4 8.44(8) 8.59(8) |
| 2s 2p $^2S^e$ $^2P^o$ 2 4 499.3 9.59(8) 9.56(8) |
| 2p 3s $^2P^o$ $^2S^e$ 2 2 45.4 6.78(10) 6.68(10) |
| 2p 3s $^2P^o$ $^2S^e$ 4 2 45.7 1.37(11) 1.32(11) |
| 2p 3d $^2P^o$ $^2D^e$ 2 4 44.0 1.15(12) 1.16(12) |
| 2p 3d $^2P^o$ $^2D^e$ 4 4 44.2 2.30(11) 2.30(11) |
| 2p 3d $^2P^o$ $^2D^e$ 4 6 44.2 1.38(12) 1.38(12) |
| S XIV |
| 2s 2p $^2S^e$ $^2P^o$ 2 2 445.8 9.90(8) 9.92(8)a |
| 2s 2p $^2S^e$ $^2P^o$ 2 4 417.6 1.31(9) 1.21(9)a |
| 2p 3s $^2P^o$ $^2S^e$ 2 2 33.4 1.19(11) 1.18(11)a |
| 2p 3s $^2P^o$ $^2S^e$ 4 2 33.5 2.44(11) 2.40(11)a |
| Ar XVI |
| 2s 2p $^2S^e$ $^2P^o$ 2 2 389.1 1.14(9) 1.15(9)a |
| 2s 2p $^2S^e$ $^2P^o$ 2 4 353.9 1.53(9) 1.53(9)a |
| 2p 3s $^2P^o$ $^2S^e$ 2 2 25.5 1.96(11) 1.94(11)a |
| 2p 3s $^2P^o$ $^2S^e$ 4 2 25.7 4.04(11) 3.97(11)a |
| Ca XVIII |
| 2s 2p $^2S^e$ $^2P^o$ 2 2 389.1 1.14(9) 1.15(9)a |
| 2s 2p $^2S^e$ $^2P^o$ 2 4 353.9 1.53(9) 1.53(9)a |
| 2p 3s $^2P^o$ $^2S^e$ 2 2 25.5 1.96(11) 1.94(11)a |
| 2p 3s $^2P^o$ $^2S^e$ 4 2 25.7 4.04(11) 3.97(11)a |
| Ti XX |
| 2s 2p $^2S^e$ $^2P^o$ 2 2 308.9 1.46(9) 1.48(9) |
| 2s 2p $^2S^e$ $^2P^o$ 2 4 259.6 2.49(9) 2.52(9) |
| 2s 3p $^2S^e$ $^2P^o$ 2 2 15.3 3.67(12) 3.58(12) |
| 2s 3p $^2S^e$ $^2P^o$ 2 4 15.2 3.58(12) 3.50(12) |
| Cr XXII |
| 2s 2p $^2S^e$ $^2P^o$ 2 2 279.5 1.63(9) 1.65(9) |
| 2s 2p $^2S^e$ $^2P^o$ 2 4 223.3 3.24(9) 3.29(9) |
| 2s 3p $^2S^e$ $^2P^o$ 2 2 12.7 5.42(12) 5.28(12) |
| 2s 3p $^2S^e$ $^2P^o$ 2 4 12.6 5.24(12) 5.13(12) |
| 2p 3s $^2P^o$ $^2S^e$ 2 2 13.4 6.63(11) 6.00(9) |
| 2p 3s $^2P^o$ $^2S^e$ 4 2 13.6 1.40(12) 1.30(9) |
| 2p 3d $^2P^o$ $^2D^e$ 2 4 13.1 1.29(13) 1.29(13) |
| 2p 3d $^2P^o$ $^2D^e$ 4 4 13.3 2.56(12) 2.60(12) |
| 2p 3d $^2P^o$ $^2D^e$ 4 6 13.3 1.54(13) 1.54(13) |
| Ni XXVI |

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$a$ denotes additional references.
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Table 7. Sample set of $f$- and $A$-values of O VI in $J\pi$ order as obtained from BPRM calculations.

| $f$  | $A$  | $E_i$ (Ry) | $E_j$ (Ry) | $gf_L$ | S     | $A_{ji}$ (sec$^{-1}$) |
|------|------|-------------|-------------|--------|-------|---------------------|
| 1    | 0    | -1.01495E+01| -9.27099E+00| -1.318E-01| 4.501E-01| 4.085E+08          |
| 1    | 2    | -1.01495E+01| -4.08326E+00| -1.778E-01| 8.793E-02| 2.628E+10          |
| 1    | 3    | -1.01495E+01| -2.28406E+00| -4.934E-02| 1.882E-02| 1.226E+10          |
| 1    | 4    | -1.01495E+01| -1.45741E+00| -2.104E-02| 7.262E-03| 6.385E+09          |
| 1    | 5    | -1.01495E+01| -1.01008E+00| -1.111E-02| 3.647E-03| 3.726E+09          |
| 1    | 6    | -1.01495E+01| -7.41061E-01| -6.638E-03| 2.117E-03| 2.360E+09          |
| 1    | 7    | -1.01495E+01| -5.66782E-01| -4.347E-03| 1.346E-03| 1.586E+09          |
| 1    | 8    | -1.01495E+01| -4.47461E-01| -2.951E-03| 9.125E-04| 1.126E+09          |
| 1    | 9    | -1.01495E+01| -3.62203E-01| -2.116E-03| 6.486E-04| 8.141E+08          |
| 2    | 1    | -4.31964E+00| -9.27099E+00| -2.660E-01| 2.802E+00| 4.955E+07          |
| 2    | 2    | -4.31964E+00| -4.08326E+00| -3.540E-01| 1.750E-01| 2.618E+10          |
| 2    | 3    | -4.31964E+00| -2.28406E+00| -1.850E-01| 2.726E+01| 3.079E+09          |
| 2    | 4    | -4.31964E+00| -1.45741E+00| -5.526E-02| 5.792E-02| 1.818E+09          |
| 2    | 5    | -4.31964E+00| -1.01008E+00| -2.457E-02| 2.227E-02| 1.081E+09          |
| 2    | 6    | -4.31964E+00| -7.41061E-01| -1.341E-02| 1.124E-02| 6.896E+08          |
| 2    | 7    | -4.31964E+00| -5.66782E-01| -8.232E-03| 6.581E-03| 4.656E+08          |
| 2    | 8    | -4.31964E+00| -4.47461E-01| -5.459E-03| 4.229E-03| 3.287E+08          |
| 2    | 9    | -4.31964E+00| -3.62203E-01| -3.824E-03| 2.899E-03| 2.405E+08          |
| 3    | 1    | -2.38171E+00| -9.27099E+00| -1.149E-02| 5.003E-03| 2.191E+09          |
| 3    | 2    | -2.38171E+00| -4.08326E+00| -1.278E-01| 2.253E-01| 1.485E+09          |
| 3    | 3    | -2.38171E+00| -2.28406E+00| -3.083E-01| 9.471E+00| 1.181E+07          |
| 3    | 4    | -2.38171E+00| -1.45741E+00| -1.981E-01| 6.430E-01| 6.798E+08          |
| 3    | 5    | -2.38171E+00| -1.01008E+00| -5.985E-02| 1.309E-01| 4.522E+08          |
| 4    | 1    | -2.38171E+00| -9.27099E+00| -2.310E-01| 1.822E-03| 1.113E+09          |
| 4    | 2    | -2.38171E+00| -4.08326E+00| -6.455E-01| 7.274E-03| 3.718E+09          |
| 4    | 3    | -2.38171E+00| -2.28406E+00| -3.893E-01| 1.278E+00| 6.762E+08          |
| 4    | 4    | -2.38171E+00| -1.45741E+00| -1.192E-01| 6.807E-02| 4.503E+08          |
| 5    | 1    | -2.38171E+00| -9.27099E+00| -2.820E-01| 1.624E-03| 1.136E+09          |
| 5    | 2    | -2.38171E+00| -4.08326E+00| -4.470E-01| 7.274E-03| 3.718E+09          |
| 5    | 3    | -2.38171E+00| -2.28406E+00| -3.893E-01| 1.278E+00| 6.762E+08          |
| 5    | 4    | -2.38171E+00| -1.45741E+00| -1.192E-01| 6.807E-02| 4.503E+08          |