

Relativistic fine structure oscillator strengths for Li-like ions: C IV - Si XII, S XIV, Ar XVI, Ca XVIII, Ti XX, Cr XXII, and Ni XXVI

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Abstract. Ab initio calculations including relativistic effects in the Breit-Pauli R -matrix (BPRM) method are reported for fine structure energy levels and oscillator strengths upto $n = 10$ 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 XVIII, Ti XX, Cr XXII, 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 obtained for each ion. The levels provide almost 900 allowed bound-bound transitions. The BPRM method enables consideration of 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

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 & 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 & Pradhan 1999). The close coupling

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** Complete electronic files for energies (e.g. Tables 3a and 3b) and transition probabilities (e.g. Table 7) are available at the CDS via anonymous ftp to cdsarc.u-strasbg.fr (130.79.128.5) or via <http://cdsweb.u-strasbg.fr/cgi-bin/qcat?J/A+A/389/716>

(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 & Burke 1980; Scott & 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:

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

where χ_i is the target ion wavefunction in a specific state $S_i L_i \pi_i$ or level $J_i \pi_i$, and θ_i is the wavefunction for the interacting $(N + 1)$ th electron in a channel labeled as $S_i L_i (J_i) \pi_i$ $k_i^2 \ell_i (SL\pi \text{ or } J\pi)$; k_i^2 is the incident kinetic energy. In the second sum the Φ_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

$$H_{N+1}^{\text{BP}} = H_{N+1} + H_{N+1}^{\text{mass}} + H_{N+1}^{\text{Dar}} + H_{N+1}^{\text{so}}, \quad (2)$$

where H_{N+1} is the non-relativistic Hamiltonian,

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

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

$$H_{N+1}^{\text{BP}} \Psi = E \Psi. \quad (4)$$

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 Ψ_B .

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

$$\langle \Psi_B || \mathbf{D} || \Psi_{B'} \rangle, \quad (5)$$

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

$$S_L = \left| \left\langle \Psi_f \left| \sum_{j=1}^{N+1} r_j \right| \Psi_i \right\rangle \right|^2 \quad (6)$$

and

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

where ω is the incident photon energy in Rydberg units, Ψ_i and Ψ_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

$$f_{ij} = \frac{E_{ji}}{3g_i} S, \quad (8)$$

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

$$A_{ji}(\text{au}) = \frac{1}{2} \alpha^3 \frac{g_i}{g_j} E_{ji}^2 f_{ij}, \quad (9)$$

where α 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,

$$\tau_k(s) = \frac{1}{A_k}, \quad (10)$$

where A_k is the total radiative transition probability for the level k , i.e., $A_k = \sum_i A_{ki}(s^{-1})$, and $A_{ji}(s^{-1}) = A_{ji}(\text{au})/\tau_0$, $\tau_0 = 2.4191 \times 10^{-17}$ 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.

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 ($1s^2$, $1s2s$, $1s2p$, $1s3s$, $1s3p$, $1s3d$) is common to each ion. The common correlation configurations are: $2s^2$, $2p^2$, $3s^2$, $3p^2$, $3d^2$, $2s2p$, $2s3s$, $2s3p$, $2s3d$, $2s4s$, $2s4p$, $2p3s$, $2p3p$, $2p4s$, $2p4p$ while the additional ones are listed below the table alongwith the values of the Thomas-Fermi scaling parameter (λ) for the orbitals.

Level	Energy (Ry)							
	Z = 6	7	8	9	10	11	12	13
$1s2(^1S_0^e)$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$1s2s(^3S_1^e)$	21.9730	30.8550	41.2320	53.1272	66.5220	81.3907	97.8349	115.7588
$1s2p(^3P_0^e)$	22.3731	31.3320	41.7870	53.7702	67.2350	82.1766	98.7083	116.7137
$1s2p(^3P_1^e)$	22.3730	31.3320	41.7880	53.7716	67.2380	82.1896	98.7159	116.7250
$1s2p(^3P_2^e)$	22.3742	31.3350	41.7930	53.7803	67.2520	82.2172	98.7484	116.7717
$1s2s(^1S_0^e)$	22.3718	31.3410	41.8120	53.7930	67.2760	82.2395	98.7702	116.7858
$1s2p(^1P_1^e)$	22.6301	31.6560	42.1840	54.2195	67.7670	82.8055	99.3884	117.4722
$1s3s(^3S_1^e)$	25.8760	36.3770	48.6510	62.7416	78.5790	96.2408	115.6504	136.8765
$1s3p(^3P_0^e)$	25.9840	36.5070	48.8040	62.9008	78.7740	96.4588	115.8901	137.1388
$1s3p(^3P_1^e)$	25.9840	36.5070	48.8040	62.9008	78.7740	96.4626	115.8925	137.1436
$1s3p(^3P_2^e)$	25.9840	36.5070	48.8040	62.9008	78.7790	96.4705	115.9021	137.1562
$1s3s(^1S_0^e)$	25.9819	36.5050	48.8110	62.9072	78.7780	96.4603	115.8977	137.1480
$1s3p(^1P_1^e)$	26.0565	36.6000	48.9220	63.0286	78.9210	96.6379	116.0333	137.3475
$1s3d(^3D_1^e)$	26.0377	36.5730	48.8840	62.9953	78.8880	96.5905	116.0337	137.3005
$1s3d(^3D_2^e)$	26.0377	36.5730	48.8840	62.9953	78.8890	96.5915	116.0371	137.3009
$1s3d(^3D_3^e)$	26.0378	36.5730	48.8840	63.0131	78.8890	96.5941	116.0435	137.3060
$1s3d(^1D_2^e)$	26.0397	36.5760	48.8940	63.0286	78.9380	96.5996	116.0772	137.3131
	Z = 14	16	18	20	22	24	28	
$1s2(^1S_0^e)$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
$1s2s(^3S_1^e)$	135.1951	178.6273	228.1502	283.7881	345.5828	413.5640	568.2566	
$1s2p(^3P_0^e)$	136.2322	179.8323	229.5280	285.3436	347.3211	415.4929	570.5865	
$1s2p(^3P_1^e)$	136.2485	179.8615	229.5746	285.4185	347.4254	415.6301	570.7938	
$1s2p(^3P_2^e)$	136.3136	179.9805	229.7776	285.7403	347.9236	416.3704	572.2873	
$1s2s(^1S_0^e)$	136.3142	179.9340	229.6480	285.4858	347.4809	416.6692	570.7920	
$1s2p(^1P_1^e)$	137.0731	180.8527	230.7528	286.8104	349.0801	417.6073	573.6669	
$1s3s(^3S_1^e)$	159.8976	211.3517	270.0387	335.9927	409.2639	489.8955	673.4568	
$1s3p(^3P_0^e)$	160.1828	211.6834	270.4184	336.4222	409.7447	490.4294	674.1039	
$1s3p(^3P_1^e)$	160.1877	211.6924	270.4327	336.4421	409.7715	490.4622	674.1493	
$1s3p(^3P_2^e)$	160.2070	211.7277	270.4929	336.5386	409.9204	490.6840	674.5945	
$1s3s(^1S_0^e)$	160.1932	211.6973	270.4351	336.4391	409.7630	490.4485	674.1223	
$1s3p(^1P_1^e)$	160.4142	211.9645	270.7570	336.8302	410.2367	491.0240	674.9808	
$1s3d(^3D_1^e)$	160.3648	211.9116	270.7034	337.1180	410.6500	491.6310	676.6240	
$1s3d(^3D_2^e)$	160.3651	211.9119	270.7033	337.1220	410.6550	491.6380	676.6320	
$1s3d(^3D_3^e)$	160.3725	211.9258	270.9580	337.1630	410.7170	491.7270	676.8060	
$1s3d(^1D_2^e)$	160.3794	211.9352	270.7384	337.1730	410.7270	491.7390	676.8190	
C V - λ : 0.991(1s), 0.991(2s), 0.776(2p), 1.16883(3s), 0.91077(3p), 1.00746(3d), -1.59699(4s), -1.61237(4p)								
N VI - λ : 0.991(1s), 0.991(2s), 0.776(2p), 1.16883(3s), 0.91077(3p), 1.00746(3d), -1.59699(4s), -1.61237(4p)								
O VII - λ : 0.991(1s), 0.991(2s), 0.776(2p), 1.16883(3s), 0.91077(3p), 1.00746(3d), -1.59699(4s), -1.61237(4p)								
F VIII - 2p3d; λ : 1.10(1s), 0.99(2s), 1.10(2p), 1.0(3s), 1.0(3p), 1.0(3d), -1.55(4s), -1.7(4p)								
Ne IX - 1s4s,1s4p,2p3d; λ : 0.991(1s), 0.991(2s), 0.776(2p), 1.16883(3s), 0.91077(3p), 1.00746(3d), -1.59699(4s), -1.61237(4p)								
Na X - 1s4s,1s4p,2p3d; λ : 1.10(1s), 0.99(2s), 1.10(2p), 1.0(3s), 1.0(3p), 1.0(3d), -1.55(4s), -1.7(4p)								
Mg XI - 1s4s,1s4p,2p3d; λ : 0.991(1s), 0.991(2s), 1.0(2p), 1.0(3s), 1.0(3p), 1.0(3d), -1.597(4s), -1.61234(4p)								
Al XII - 1s4s,1s4p,2p3d; λ : 1.1(1s), 0.99(2s), 1.1(2p), 1.0(3s), 1.0(3p), 1.0(3d), -1.55(4s), -1.7(4p)								
Si XIII - 1s4s,1s4p,2p3d; λ : 0.991(1s), 0.991(2s), 1.0(2p), 1.0(3s), 1.0(3p), 1.0(3d), -1.597(4s), -1.61237(4p)								
S XV - 1s4s,1s4p,2p3d; λ : 1.1(1s), 0.991(2s), 1.0(2p), 1.0(3s), 1.0(3p), 1.0(3d), -1.597(4s), -1.61237(4p)								
Ar XVII - 1s4s,1s4p,2p3d; λ : 1.1(1s), 0.99(2s), 1.1(2p), 1.0(3s), 1.0(3p), 1.0(3d), -1.55(4s), -1.7(4p)								
Ca XIX - 1s4s,1s4p,2p3d; λ : 1.1(1s), 0.99(2s), 1.1(2p), 1.0(3s), 1.0(3p), 1.0(3d), -1.55(4s), -1.7(4p)								
Ti XXI - 1s4s,1s4p,2p3d; λ : 1.1(1s), 1.10(2s), 1.0(2p), 1.0(3s), 1.0(3p), 1.0(3d), -1.50(4s), -1.44(4p)								
Cr XXIII - 1s4s,1s4p,2p3d; λ : 1.1(1s), 1.10(2s), 1.0(2p), 1.0(3s), 1.0(3p), 1.0(3d), -1.52(4s), -1.40(4p)								
Ni XXVII - 1s4s,1s4p,2p3d; λ : 1.1(1s), 1.10(2s), 1.0(2p), 1.0(3s), 1.0(3p), 1.0(3d), -1.72(4s), -1.39(4p)								

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 Thomal Fermi scaling parameters (λ) 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 λ 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 $(e + \text{core})$ Hamiltonian matrix is diagonalized for each resulting $J\pi$ in STGH.

The fine structure bound levels are sorted through the poles in the $(e + \text{ion})$ Hamiltonian with a fine mesh of effective quantum number ν . 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 & 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 straight forward, it is more

involved for complex ions. The final designation is given by $C_t(S_t L_t \pi_t) J_t n l J(SL)\pi$ where C_t , $S_t L_t \pi_t$, J_t are the configuration, LS term and parity, and total angular momentum of the target, $n l$ 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 XIII, Ti XX, 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, $n l$, total angular momentum, J , energy in Rydberg, the effective quantum number of the valence electron, ν , and the LS term designation of the level. The top line of the set gives the number of fine structure levels expected ($Nl\nu$), followed by the spin and parity of the set ($^{2S+1}L^\pi$), 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

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	$E_o(\text{Ry})$	$E_c(\text{Ry})$
C IV			
1s22s	$^2S^e$	0.5	4.74020
1s22p	$^2P^o$	1.5	4.15160
1s22p	$^2P^o$	0.5	4.15260
1s23s	$^2S^e$	0.5	1.98050
1s23p	$^2P^o$	1.5	1.82340
1s23p	$^2P^o$	0.5	1.82370
1s23d	$^2D^e$	2.5	1.77960
1s23d	$^2D^e$	1.5	1.77970
1s24s	$^2S^e$	0.5	1.08290
1s24p	$^2P^o$	1.5	1.01930
1s24p	$^2P^o$	0.5	1.01940
1s24d	$^2D^e$	2.5	1.00090
1s24d	$^2D^e$	1.5	1.00100
1s24f	$^2F^o$	3.5	1.00010
1s24f	$^2F^o$	2.5	1.00010
1s25s	$^2S^e$	0.5	0.68172
1s25p	$^2P^o$	1.5	0.64987
1s25p	$^2P^o$	0.5	0.64994
1s25d	$^2D^e$	2.5	0.64052
1s25d	$^2D^e$	1.5	0.64053
1s25f	$^2F^o$	3.5	0.64006
1s25f	$^2F^o$	2.5	0.64006
1s25g	$^2G^e$	4.5	0.63998
1s25g	$^2G^e$	3.5	0.63998
O VI			
1s22s	$^2S^e$	0.5	11.01520
1s22p	$^2P^o$	1.5	9.26850
1s22p	$^2P^o$	0.5	9.27340
1s23s	$^2S^e$	0.5	4.31910
1s23p	$^2P^o$	1.5	4.08010
1s23p	$^2P^o$	0.5	4.08150
1s23d	$^2D^e$	2.5	4.00350
1s23d	$^2D^e$	1.5	4.00390
1s24s	$^2S^e$	0.5	2.38130
1s24p	$^2P^o$	1.5	2.28370
1s24p	$^2P^o$	0.5	2.28430
1s24d	$^2D^e$	2.5	2.25180
1s24d	$^2D^e$	1.5	2.25200
1s24f	$^2F^o$	3.5	2.25010
1s24f	$^2F^o$	2.5	2.25020
1s25s	$^2S^e$	0.5	1.50650
1s25p	$^2P^o$	1.5	1.45740
1s25p	$^2P^o$	0.5	1.45740
1s25d	$^2D^e$	2.5	1.44120
1s25d	$^2D^e$	1.5	1.44120
1s25f	$^2F^o$	3.5	1.44010
1s25f	$^2F^o$	2.5	1.44010
1s25g	$^2G^e$	4.5	1.44000
1s25g	$^2G^e$	3.5	1.44000
Ni XXVI			
1s22s	$^2S^e$	0.5	176.3300
1s22p	$^2P^o$	1.5	170.8200
1s22p	$^2P^o$	0.5	172.4400
1s23s	$^2S^e$	0.5	77.1840
1s23p	$^2P^o$	1.5	75.7630
1s23p	$^2P^o$	0.5	76.2460
1s23d	$^2D^e$	2.5	75.2520
1s23d	$^2D^e$	1.5	75.3890

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, ν is the effective quantum number.

$C_t(S_tL_t\pi_t)$	J_t	nl	J	$E(\text{Ry})$	ν	$SL\pi$
C VI						
$Nlv = 1, \ ^2L^e: S(1)/2$						
1s2	(1Se)	0 2s	1	-4.73899E+00	1.84	$^2S^e$
$Nlv(c) = 1: \text{set complete}$						
$Nlv = 2, \ ^2L^o: P(31)/2$						
1s2	(1Se)	0 2p	1	-4.15050E+00	1.96	$^2P^o$
1s2	(1Se)	0 2p	3	-4.14885E+00	1.96	$^2P^o$
$Nlv(c) = 2: \text{set complete}$						
Ni XXVI						
$Nlv = 1, \ ^2L^e: S(1)/2$						
1s2	(1Se)	0 2s	1	-1.76520E+02	1.96	$^2S^e$
$Nlv(c) = 1: \text{set complete}$						
$Nlv = 2, \ ^2L^o: P(31)/2$						
1s2	(1Se)	0 2p	1	-1.72635E+02	1.98	$^2P^o$
1s2	(1Se)	0 2p	3	-1.70819E+02	1.99	$^2P^o$
$Nlv(c) = 2: \text{set complete}$						

Table 3b. Sample table for calculated fine structure energy levels of C IV and Ni XXVI in $J\pi$ order. Nlv is the total number of levels of the symmetry.

Level	$E(\text{Ry})$	ν	$SL\pi$
C IV: $N_b = 98$			
$Nlv = 9, \ J\pi = 1/2^e$			
1	1s2($^1S_0^e$)	2s 1/2	-4.73899E+00
2	1s2($^1S_0^e$)	3s 1/2	-1.98187E+00
3	1s2($^1S_0^e$)	4s 1/2	-1.08239E+00
4	1s2($^1S_0^e$)	5s 1/2	-6.81555E-01
5	1s2($^1S_0^e$)	6s 1/2	-4.68304E-01
6	1s2($^1S_0^e$)	7s 1/2	-3.41472E-01
7	1s2($^1S_0^e$)	8s 1/2	-2.59968E-01
8	1s2($^1S_0^e$)	9s 1/2	-2.04509E-01
9	1s2($^1S_0^e$)	10s 1/2	-1.65074E-01
Ni XXVI: $N_b = 98$			
$Nlv = 9, \ J\pi = 1/2^e$			
1	1s2($^1S_0^e$)	2s 1/2	-1.76520E+02
2	1s2($^1S_0^e$)	3s 1/2	-7.73614E+01
3	1s2($^1S_0^e$)	4s 1/2	-4.39347E+01
4	1s2($^1S_0^e$)	5s 1/2	-2.82478E+01
5	1s2($^1S_0^e$)	6s 1/2	-1.95208E+01
6	1s2($^1S_0^e$)	7s 1/2	-1.42712E+01
7	1s2($^1S_0^e$)	8s 1/2	-1.08829E+01
8	1s2($^1S_0^e$)	9s 1/2	-8.57080E+00
9	1s2($^1S_0^e$)	10s 1/2	-6.92420E+00

($Nlv(c)$) 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 ($Nl\nu$) 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 (ν), 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, $1 \text{ Ry} = 911.2671 \text{ \AA}$. 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 re-processed set in Table 5 has slight improved accuracy.

The BPRM A -values are compared with the available data obtained by various investigators, 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, Traäbert 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

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	$E(\text{Ry})$	$SL\pi$
C IV: $N_b = 97$					
1	$1s2(1S_0^e)$	2s	1/2	-4.73899E+00	^2Se
2	$1s2(1S_0^e)$	3s	1/2	-1.98187E+00	^2Se
1	$1s2(1S_0^e)$	2p	1/2	-4.15050E+00	^2Po
2	$1s2(1S_0^e)$	3p	1/2	-1.82526E+00	^2Po
1	$1s2(1S_0^e)$	3d	3/2	-1.78290E+00	^2De
1	$1s2(1S_0^e)$	2p	3/2	-4.14885E+00	^2Po
2	$1s2(1S_0^e)$	3p	3/2	-1.82478E+00	^2Po
1	$1s2(1S_0^e)$	3d	5/2	-1.78277E+00	^2De
N V: $N_b = 99$					
1	$1s2(1S_0^e)$	2s	1/2	-7.19258E+00	^2Se
2	$1s2(1S_0^e)$	3s	1/2	-3.03900E+00	^2Se
1	$1s2(1S_0^e)$	2p	1/2	-6.45820E+00	^2Po
2	$1s2(1S_0^e)$	3p	1/2	-2.84225E+00	^2Po
1	$1s2(1S_0^e)$	3d	3/2	-2.78368E+00	^2De
1	$1s2(1S_0^e)$	2p	3/2	-6.45458E+00	^2Po
2	$1s2(1S_0^e)$	3p	3/2	-2.84120E+00	^2Po
1	$1s2(1S_0^e)$	3d	5/2	-2.78337E+00	^2De
O VI: $N_b = 98$					
1	$1s2(1S_0^e)$	2s	1/2	-1.01495E+01	^2Se
2	$1s2(1S_0^e)$	3s	1/2	-4.31964E+00	^2Se
1	$1s2(1S_0^e)$	2p	1/2	-9.27097E+00	^2Po
2	$1s2(1S_0^e)$	3p	1/2	-4.08326E+00	^2Po
1	$1s2(1S_0^e)$	3d	3/2	-4.00734E+00	^2De
1	$1s2(1S_0^e)$	2p	3/2	-9.26399E+00	^2Po
2	$1s2(1S_0^e)$	3p	3/2	-4.08121E+00	^2Po
1	$1s2(1S_0^e)$	3d	5/2	-4.00676E+00	^2De
F VII: $N_b = 98$					
1	$1s2(1S_0^e)$	2s	1/2	-1.36088E+01	^2Se
2	$1s2(1S_0^e)$	3s	1/2	-5.82277E+00	^2Se
1	$1s2(1S_0^e)$	2p	1/2	-1.25857E+01	^2Po
2	$1s2(1S_0^e)$	3p	1/2	-5.54675E+00	^2Po
1	$1s2(1S_0^e)$	3d	3/2	-5.45287E+00	^2De
1	$1s2(1S_0^e)$	2p	3/2	-1.25735E+01	^2Po
2	$1s2(1S_0^e)$	3p	3/2	-5.54317E+00	^2Po
1	$1s2(1S_0^e)$	3d	5/2	-5.45184E+00	^2De
Ne VI: $N_b = 98$					
1	$1s2(1S_0^e)$	2s	1/2	-1.75703E+01	^2Se
2	$1s2(1S_0^e)$	3s	1/2	-7.54886E+00	^2Se
1	$1s2(1S_0^e)$	2p	1/2	-1.64042E+01	^2Po
2	$1s2(1S_0^e)$	3p	1/2	-7.23360E+00	^2Po
1	$1s2(1S_0^e)$	3d	3/2	-7.12122E+00	^2De
1	$1s2(1S_0^e)$	2p	3/2	-1.63841E+01	^2Po
2	$1s2(1S_0^e)$	3p	3/2	-7.22771E+00	^2Po
1	$1s2(1S_0^e)$	3d	5/2	-7.11949E+00	^2De
Na IX: $N_b = 98$					
1	$1s2(1S_0^e)$	2s	1/2	-2.20373E+01	^2Se
2	$1s2(1S_0^e)$	3s	1/2	-9.49911E+00	^2Se
1	$1s2(1S_0^e)$	2p	1/2	-2.07270E+01	^2Po
2	$1s2(1S_0^e)$	3p	1/2	-9.14417E+00	^2Po
1	$1s2(1S_0^e)$	3d	3/2	-9.01214E+00	^2De
1	$1s2(1S_0^e)$	2p	3/2	-2.06961E+01	^2Po
2	$1s2(1S_0^e)$	3p	3/2	-9.13518E+00	^2Po
1	$1s2(1S_0^e)$	3d	5/2	-9.00947E+00	^2De

Table 4. continued.

Level		J	$E(\text{Ry})$	$SL\pi$
Mg X: $N_b = 98$				
1	1s2($^1S_0^e$)	2s 1/2	-2.70076E+01	^2Se
2	1s2($^1S_0^e$)	3s 1/2	-1.16722E+01	^2Se
1	1s2($^1S_0^e$)	2p 1/2	-2.55546E+01	^2Po
2	1s2($^1S_0^e$)	3p 1/2	-1.12786E+01	^2Po
1	1s2($^1S_0^e$)	3d 3/2	-1.11259E+01	^2De
1	1s2($^1S_0^e$)	2p 3/2	-2.55087E+01	^2Po
2	1s2($^1S_0^e$)	3p 3/2	-1.12652E+01	^2Po
1	1s2($^1S_0^e$)	3d 5/2	-1.11219E+01	^2De
Al XI: $N_b = 98$				
1	1s2($^1S_0^e$)	2s 1/2	-3.24858E+01	^2Se
2	1s2($^1S_0^e$)	3s 1/2	-1.40702E+01	^2Se
1	1s2($^1S_0^e$)	2p 1/2	-3.08882E+01	^2Po
2	1s2($^1S_0^e$)	3p 1/2	-1.36372E+01	^2Po
1	1s2($^1S_0^e$)	3d 3/2	-1.34623E+01	^2De
1	1s2($^1S_0^e$)	2p 3/2	-3.08226E+01	^2Po
2	1s2($^1S_0^e$)	3p 3/2	-1.36179E+01	^2Po
1	1s2($^1S_0^e$)	3d 5/2	-1.34565E+01	^2De
Si XII: $N_b = 98$				
1	1s2($^1S_0^e$)	2s 1/2	-3.84689E+01	^2Se
2	1s2($^1S_0^e$)	3s 1/2	-1.66918E+01	^2Se
1	1s2($^1S_0^e$)	2p 1/2	-3.67286E+01	^2Po
2	1s2($^1S_0^e$)	3p 1/2	-1.62212E+01	^2Po
1	1s2($^1S_0^e$)	3d 3/2	-1.60220E+01	^2De
1	1s2($^1S_0^e$)	2p 3/2	-3.66376E+01	^2Po
2	1s2($^1S_0^e$)	3p 3/2	-1.61945E+01	^2Po
1	1s2($^1S_0^e$)	3d 5/2	-1.60141E+01	^2De
S XIV: $N_b = 98$				
1	1s2($^1S_0^e$)	2s 1/2	-5.19635E+01	^2Se
2	1s2($^1S_0^e$)	3s 1/2	-2.26108E+01	^2Se
1	1s2($^1S_0^e$)	2p 1/2	-4.99351E+01	^2Po
2	1s2($^1S_0^e$)	3p 1/2	-2.20622E+01	^2Po
1	1s2($^1S_0^e$)	3d 3/2	-2.18103E+01	^2De
1	1s2($^1S_0^e$)	2p 3/2	-4.97717E+01	^2Po
2	1s2($^1S_0^e$)	3p 3/2	-2.20141E+01	^2Po
1	1s2($^1S_0^e$)	3d 5/2	-2.17958E+01	^2De
Ar XVI: $N_b = 98$				
1	1s2($^1S_0^e$)	2s 1/2	-6.75077E+01	^2Se
2	1s2($^1S_0^e$)	3s 1/2	-2.94364E+01	^2Se
1	1s2($^1S_0^e$)	2p 1/2	-6.51866E+01	^2Po
2	1s2($^1S_0^e$)	3p 1/2	-2.88090E+01	^2Po
1	1s2($^1S_0^e$)	3d 3/2	-2.84933E+01	^2De
1	1s2($^1S_0^e$)	2p 3/2	-6.49139E+01	^2Po
2	1s2($^1S_0^e$)	3p 3/2	-2.87286E+01	^2Po
1	1s2($^1S_0^e$)	3d 5/2	-2.84690E+01	^2De
Ca XVIII: $N_b = 98$				
1	1s2($^1S_0^e$)	2s 1/2	-8.51083E+01	^2Se
2	1s2($^1S_0^e$)	3s 1/2	-3.71706E+01	^2Se
1	1s2($^1S_0^e$)	2p 1/2	-8.24956E+01	^2Po
2	1s2($^1S_0^e$)	3p 1/2	-3.64652E+01	^2Po
1	1s2($^1S_0^e$)	3d 3/2	-3.60722E+01	^2De
1	1s2($^1S_0^e$)	2p 3/2	-8.20656E+01	^2Po
2	1s2($^1S_0^e$)	3p 3/2	-3.63385E+01	^2Po
1	1s2($^1S_0^e$)	3d 5/2	-3.60333E+01	^2De

Table 4. continued.

Level		J	$E(\text{Ry})$	$SL\pi$
Ti XX: $N_b = 98$				
1	1s2($^1S_0^e$)	2s 1/2	-1.04794E+02	^2Se
2	1s2($^1S_0^e$)	3s 1/2	-4.58280E+01	^2Se
1	1s2($^1S_0^e$)	2p 1/2	-1.01885E+02	^2Po
2	1s2($^1S_0^e$)	3p 1/2	-4.50420E+01	^2Po
1	1s2($^1S_0^e$)	3d 3/2	-4.45516E+01	^2De
1	1s2($^1S_0^e$)	2p 3/2	-1.01238E+02	^2Po
2	1s2($^1S_0^e$)	3p 3/2	-4.48512E+01	^2Po
1	1s2($^1S_0^e$)	3d 5/2	-4.44928E+01	^2De
Cr XXII: 98				
1	1s2($^1S_0^e$)	2s 1/2	-1.26565E+02	^2Se
2	1s2($^1S_0^e$)	3s 1/2	-5.54020E+01	^2Se
1	1s2($^1S_0^e$)	2p 1/2	-1.23360E+02	^2Po
2	1s2($^1S_0^e$)	3p 1/2	-5.45381E+01	^2Po
1	1s2($^1S_0^e$)	3d 3/2	-5.39292E+01	^2De
1	1s2($^1S_0^e$)	2p 3/2	-1.22422E+02	^2Po
2	1s2($^1S_0^e$)	3p 3/2	-5.42612E+01	^2Po
1	1s2($^1S_0^e$)	3d 5/2	-5.38440E+01	^2De
Ni XXVI: 98				
1	1s2($^1S_0^e$)	2s 1/2	-1.76520E+02	^2Se
2	1s2($^1S_0^e$)	3s 1/2	-7.73614E+01	^2Se
1	1s2($^1S_0^e$)	2p 1/2	-1.72635E+02	^2Po
2	1s2($^1S_0^e$)	3p 1/2	-7.63001E+01	^2Po
1	1s2($^1S_0^e$)	3d 3/2	-7.53740E+01	^2De
1	1s2($^1S_0^e$)	2p 3/2	-1.70819E+02	^2Po
2	1s2($^1S_0^e$)	3p 3/2	-7.57620E+01	^2Po
1	1s2($^1S_0^e$)	3d 5/2	-7.52097E+01	^2De

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 $1s^2 2s(^2S) - 1s^2 2p(^2P^o)$ 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.

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}	f	A
						(Å)	(s ⁻¹)	
C IV								
2s	2p	² S ^e	² P ^o	2	2	1550.8	9.501(-2)	2.63(8)
2s	2p	² S ^e	² P ^o	2	4	1548.2	1.904(-1)	2.65(8)
LS		² S ^e	² P ^o	2	6		2.854(-1)	2.64(8)
2s	3p	² S ^e	² P ^o	2	2	312.5	6.810(-2)	4.65(9)
2s	3p	² S ^e	² P ^o	2	4	312.4	1.358(-1)	4.64(9)
LS		² S ^e	² P ^o	2	6		2.039(-1)	4.64(9)
2p	3s	² P ^o	² S ^e	2	2	419.5	3.769(-2)	1.43(9)
2p	3s	² P ^o	² S ^e	4	2	419.7	3.781(-2)	2.86(9)
LS		² P ^o	² S ^e	6	2		3.777(-2)	4.29(9)
3s	3p	² S ^e	² P ^o	2	2	5811.7	1.595(-1)	3.15(7)
3s	3p	² S ^e	² P ^o	2	4	5800.6	3.197(-1)	3.17(7)
LS		² S ^e	² P ^o	2	6		4.792(-1)	3.16(7)
2p	3d	² P ^o	² D ^e	2	4	384.0	6.486(-1)	1.47(10)
2p	3d	² P ^o	² D ^e	4	4	384.2	6.489(-2)	2.93(9)
2p	3d	² P ^o	² D ^e	4	6	384.2	5.839(-1)	1.76(10)
LS		² P ^o	² D ^e	6	10		6.487(-1)	1.76(10)
3p	3d	² P ^o	² D ^e	2	4	20710.6	6.247(-2)	4.86(5)
3p	3d	² P ^o	² D ^e	4	4	20852.8	6.205(-3)	9.52(4)
3p	3d	² P ^o	² D ^e	4	6	20805.2	5.599(-2)	5.75(5)
LS		² P ^o	² D ^e	6	10		6.221(-2)	5.75(5)
N V								
2s	2p	² S ^e	² P ^o	2	2	1242.9	7.783(-2)	3.36(8)
2s	2p	² S ^e	² P ^o	2	4	1238.8	1.563(-1)	3.40(8)
LS		² S ^e	² P ^o	2	6		2.341(-1)	3.38(8)
2s	3p	² S ^e	² P ^o	2	2	209.3	8.004(-2)	1.22(10)
2s	3p	² S ^e	² P ^o	2	4	209.3	1.594(-1)	1.21(10)
LS		² S ^e	² P ^o	2	6		2.394(-1)	1.22(10)
2p	3s	² P ^o	² S ^e	2	2	266.2	3.240(-2)	3.05(9)
2p	3s	² P ^o	² S ^e	4	2	266.4	3.256(-2)	6.12(9)
LS		² P ^o	² S ^e	6	2		3.251(-2)	9.17(9)
3s	3p	² S ^e	² P ^o	2	2	4621.0	1.309(-1)	4.09(7)
3s	3p	² S ^e	² P ^o	2	4	4604.7	2.630(-1)	4.14(7)
LS		² S ^e	² P ^o	2	6		3.939(-1)	4.12(7)
2p	3d	² P ^o	² D ^e	2	4	247.6	6.534(-1)	3.56(10)
2p	3d	² P ^o	² D ^e	4	4	247.7	6.539(-2)	7.11(9)
2p	3d	² P ^o	² D ^e	4	6	247.7	5.883(-1)	4.26(10)
LS		² P ^o	² D ^e	6	10		6.535(-1)	4.26(10)
3p	3d	² P ^o	² D ^e	2	4	15062.3	5.499(-2)	8.08(5)
3p	3d	² P ^o	² D ^e	4	4	15238.6	5.432(-3)	1.56(5)
3p	3d	² P ^o	² D ^e	4	6	15187.8	4.909(-2)	9.46(5)
LS		² P ^o	² D ^e	6	10		5.456(-2)	9.47(5)
O VI								
2s	2p	² S ^e	² P ^o	2	2	1037.2	6.591(-2)	4.09(8)
2s	2p	² S ^e	² P ^o	2	4	1031.4	1.327(-1)	4.16(8)
LS		² S ^e	² P ^o	2	6		1.986(-1)	4.14(8)
2s	3p	² S ^e	² P ^o	2	2	150.1	8.896(-2)	2.63(10)
2s	3p	² S ^e	² P ^o	2	4	150.1	1.771(-1)	2.62(10)
LS		² S ^e	² P ^o	2	6		2.661(-1)	2.63(10)
2p	3s	² P ^o	² S ^e	2	2	183.9	2.892(-2)	5.70(9)
2p	3s	² P ^o	² S ^e	4	2	184.1	2.913(-2)	1.15(10)
LS		² P ^o	² S ^e	6	2		2.906(-2)	1.72(10)
3s	3p	² S ^e	² P ^o	2	2	3835.3	1.110(-1)	5.03(7)
3s	3p	² S ^e	² P ^o	2	4	3812.8	2.234(-1)	5.12(7)
LS		² S ^e	² P ^o	2	6		3.344(-1)	5.09(7)
2p	3d	² P ^o	² D ^e	2	4	172.9	6.568(-1)	7.32(10)
2p	3d	² P ^o	² D ^e	4	4	173.1	6.576(-2)	1.46(10)
2p	3d	² P ^o	² D ^e	4	6	173.1	5.919(-1)	8.79(10)
LS		² P ^o	² D ^e	6	10		6.573(-1)	8.78(10)
3p	3d	² P ^o	² D ^e	2	4	11743.1	4.893(-2)	1.18(6)
3p	3d	² P ^o	² D ^e	4	4	11958.9	4.804(-3)	2.24(5)
3p	3d	² P ^o	² D ^e	4	6	11896.4	4.348(-2)	1.37(6)
LS		² P ^o	² D ^e	6	10		4.834(-2)	1.37(6)

Table 5. continued.

C_i	C_j	T_i	T_j	g_i	g_j	E_{ij}	f	A
						(Å)	(s ⁻¹)	
F VII								
2s	2p	² S ^e	² P ^o	2	2	890.8	5.710(-2)	4.80(8)
2s	2p	² S ^e	² P ^o	2	4	883.0	1.154(-1)	4.93(8)
LS		² S ^e	² P ^o	2	6		1.725(-1)	4.89(8)
2s	3p	² S ^e	² P ^o	2	2	113.0	9.585(-2)	5.01(10)
2s	3p	² S ^e	² P ^o	2	4	112.9	1.906(-1)	4.98(10)
LS		² S ^e	² P ^o	2	6		2.865(-1)	4.99(10)
2p	3s	² P ^o	² S ^e	2	2	134.7	2.652(-2)	9.75(9)
2p	3s	² P ^o	² S ^e	4	2	134.9	2.677(-2)	1.96(10)
LS		² P ^o	² S ^e	6	2		2.669(-2)	2.94(10)
3s	3p	² S ^e	² P ^o	2	2	3277.9	9.619(-2)	5.97(7)
3s	3p	² S ^e	² P ^o	2	4	3247.6	1.944(-1)	6.15(7)
LS		² S ^e	² P ^o	2	6		2.906(-1)	6.09(7)
2p	3d	² P ^o	² D ^e	2	4	127.7	6.601(-1)	1.35(11)
2p	3d	² P ^o	² D ^e	4	4	127.8	6.613(-2)	2.70(10)
2p	3d	² P ^o	² D ^e	4	6	127.8	5.948(-1)	1.62(11)
LS		² P ^o	² D ^e	6	10		6.605(-1)	1.62(11)
3p	3d	² P ^o	² D ^e	2	4	9532.1	4.426(-2)	1.62(6)
3p	3d	² P ^o	² D ^e	4	4	9798.6	4.303(-3)	2.99(5)
3p	3d	² P ^o	² D ^e	4	6	9715.0	3.909(-2)	1.84(6)
LS		² P ^o	² D ^e	6	10		4.346(-2)	1.85(6)
Ne VIII								
2s	2p	² S ^e	² P ^o	2	2	780.2	5.038(-2)	5.52(8)
2s	2p	² S ^e	² P ^o	2	4	770.3	1.023(-1)	5.75(8)
LS		² S ^e	² P ^o	2	6		1.527(-1)	5.67(8)
2s	3p	² S ^e	² P ^o	2	2	88.1	1.013(-1)	8.70(10)
2s	3p	² S ^e	² P ^o	2	4	88.1	2.012(-1)	8.65(10)
LS		² S ^e	² P ^o	2	6		3.025(-1)	8.67(10)
2p	3s	² P ^o	² S ^e	2	2	102.9	2.479(-2)	1.56(10)
2p	3s	² P ^o	² S ^e	4	2	103.1	2.506(-2)	3.15(10)
LS		² P ^o	² S ^e	6	2		2.497(-2)	4.71(10)
3s	3p	² S ^e	² P ^o	2	2	2861.1	8.493(-2)	6.92(7)
3s	3p	² S ^e	² P ^o	2	4	2822.1	1.724(-1)	7.22(7)
LS		² S ^e	² P ^o	2	6		2.573(-1)	7.12(7)
2p	3d	² P ^o	² D ^e	2	4	98.1	6.624(-1)	2.29(11)
2p	3d	² P ^o	² D ^e	4	4	98.3	6.645(-2)	4.59(10)
2p	3d	² P ^o	² D ^e	4	6	98.3	5.976(-1)	2.75(11)
LS		² P ^o	² D ^e	6	10		6.633(-1)	2.75(11)
3p	3d	² P ^o	² D ^e	2	4	7979.6	4.045(-2)	2.12(6)
3p	3d	² P ^o	² D ^e	4	4	8299.3	3.888(-3)	3.76(5)
3p	3d	² P ^o	² D ^e	4	6	8194.8	3.544(-2)	2.35(6)
LS		² P ^o	² D ^e	6	10		3.941(-2)	2.35(6)
Na IX								
2s	2p	² S ^e	² P ^o	2	2	694.0	4.506(-2)	6.24(8)
2s	2p	² S ^e	² P ^o	2	4	681.6	9.201(-2)	6.61(8)
LS		² S ^e	² P ^o	2	6		1.371(-1)	6.48(8)
2s	3p	² S ^e	² P ^o	2	2	70.7	1.057(-1)	1.41(11)
2s	3p	² S ^e	² P ^o	2	4	70.6	2.096(-1)	1.40(11)
LS		² S ^e	² P ^o	2	6		3.153(-1)	1.41(11)
2p	3s	² P ^o	² S ^e	2	2	81.2	2.346(-2)	2.37(10)
2p	3s	² P ^o	² S ^e	4	2	81.3	2.379(-2)	4.80(10)
LS		² P ^o	² S ^e	6	2		2.368(-2)	7.17(10)
3s	3p	² S ^e	² P ^o	2	2	2536.9	7.603(-2)	7.88(7)
3s	3p	² S ^e	² P ^o	2	4	2489.1	1.552(-1)	8.36(7)
LS		² S ^e	² P ^o	2	6		2.312(-1)	8.19(7)
2p	3d	² P ^o	² D ^e	2	4	77.8	6.646(-1)	3.67(11)
2p	3d	² P ^o	² D ^e	4	4	77.9	6.669(-2)	7.33(10)
2p	3d	² P ^o	² D ^e	4	6	77.9	6.000(-1)	4.40(11)
LS		² P ^o	² D ^e	6	10		6.658(-1)	4.39(11)
3p	3d	² P ^o	² D ^e	2	4	6836.2	3.728(-2)	2.66(6)
3p	3d	² P ^o	² D ^e	4	4	7209.4	3.534(-3)	4.53(5)
3p	3d	² P ^o	² D ^e	4	6	7108.2	3.227(-2)	2.84(6)
LS		² P ^o	² D ^e	6	10		3.595(-2)	2.86(6)

Table 5. continued.

C_i	C_j	T_i	T_j	g_i	g_j	E_{ij}	f	A
						(Å)		(s ⁻¹)
Mg X								
2s	2p	² S ^e	² P ^o	2	2	624.6	4.078(-2)	6.97(8)
2s	2p	² S ^e	² P ^o	2	4	609.5	8.384(-2)	7.53(8)
LS		² S ^e	² P ^o	2	6		1.246(-1)	7.34(8)
2s	3p	² S ^e	² P ^o	2	2	57.9	1.094(-1)	2.18(11)
2s	3p	² S ^e	² P ^o	2	4	57.9	2.167(-1)	2.16(11)
LS		² S ^e	² P ^o	2	6		3.261(-1)	2.16(11)
2p	3s	² P ^o	² S ^e	2	2	65.7	2.242(-2)	3.47(10)
2p	3s	² P ^o	² S ^e	4	2	65.8	2.282(-2)	7.02(10)
LS		² P ^o	² S ^e	6	2		2.269(-2)	1.05(11)
3s	3p	² S ^e	² P ^o	2	2	2278.2	6.880(-2)	8.84(7)
3s	3p	² S ^e	² P ^o	2	4	2211.8	1.420(-1)	9.68(7)
LS		² S ^e	² P ^o	2	6		2.108(-1)	9.39(7)
2p	3d	² P ^o	² D ^e	2	4	63.2	6.666(-1)	5.57(11)
2p	3d	² P ^o	² D ^e	4	4	63.3	6.689(-2)	1.11(11)
2p	3d	² P ^o	² D ^e	4	6	63.3	6.019(-1)	6.68(11)
LS		² P ^o	² D ^e	6	10		6.678(-1)	6.68(11)
3p	3d	² P ^o	² D ^e	2	4	5917.3	3.486(-2)	3.32(6)
3p	3d	² P ^o	² D ^e	4	4	6417.4	3.210(-3)	5.20(5)
3p	3d	² P ^o	² D ^e	4	6	6241.6	2.975(-2)	3.40(6)
LS		² P ^o	² D ^e	6	10		3.308(-2)	3.40(6)
Al XI								
2s	2p	² S ^e	² P ^o	2	2	568.1	3.721(-2)	7.69(8)
2s	2p	² S ^e	² P ^o	2	4	550.3	7.717(-2)	8.50(8)
LS		² S ^e	² P ^o	2	6		1.144(-1)	8.22(8)
2s	3p	² S ^e	² P ^o	2	2	48.3	1.125(-1)	3.21(11)
2s	3p	² S ^e	² P ^o	2	4	48.3	2.224(-1)	3.18(11)
LS		² S ^e	² P ^o	2	6		3.349(-1)	3.19(11)
2p	3s	² P ^o	² S ^e	2	2	54.2	2.159(-2)	4.90(10)
2p	3s	² P ^o	² S ^e	4	2	54.4	2.205(-2)	9.94(10)
LS		² P ^o	² S ^e	6	2		2.190(-2)	1.48(11)
3s	3p	² S ^e	² P ^o	2	2	2066.4	6.287(-2)	9.82(7)
3s	3p	² S ^e	² P ^o	2	4	1994.0	1.305(-1)	1.09(8)
LS		² S ^e	² P ^o	2	6		1.934(-1)	1.06(8)
2p	3d	² P ^o	² D ^e	2	4	52.3	6.679(-1)	8.14(11)
2p	3d	² P ^o	² D ^e	4	4	52.5	6.710(-2)	1.63(11)
2p	3d	² P ^o	² D ^e	4	6	52.4	6.034(-1)	9.75(11)
LS		² P ^o	² D ^e	6	10		6.693(-1)	9.75(11)
3p	3d	² P ^o	² D ^e	2	4	5177.7	3.291(-2)	4.09(6)
3p	3d	² P ^o	² D ^e	4	4	5695.4	2.988(-3)	6.14(5)
3p	3d	² P ^o	² D ^e	4	6	5556.5	2.761(-2)	3.98(6)
LS		² P ^o	² D ^e	6	10		3.084(-2)	4.04(6)
Si XII								
2s	2p	² S ^e	² P ^o	2	2	520.4	3.426(-2)	8.44(8)
2s	2p	² S ^e	² P ^o	2	4	499.3	7.172(-2)	9.59(8)
LS		² S ^e	² P ^o	2	6		1.060(-1)	9.20(8)
2s	3p	² S ^e	² P ^o	2	2	41.0	1.153(-1)	4.59(11)
2s	3p	² S ^e	² P ^o	2	4	40.9	2.275(-1)	4.53(11)
LS		² S ^e	² P ^o	2	6		3.428(-1)	4.55(11)
2p	3s	² P ^o	² S ^e	2	2	45.5	2.092(-2)	6.73(10)
2p	3s	² P ^o	² S ^e	4	2	45.7	2.144(-2)	1.37(11)
LS		² P ^o	² S ^e	6	2		2.127(-2)	2.04(11)
3s	3p	² S ^e	² P ^o	2	2	1882.8	5.806(-2)	1.09(8)
3s	3p	² S ^e	² P ^o	2	4	1800.9	1.218(-1)	1.25(8)
LS		² S ^e	² P ^o	2	6		1.799(-1)	1.20(8)
2p	3d	² P ^o	² D ^e	2	4	44.0	6.693(-1)	1.15(12)
2p	3d	² P ^o	² D ^e	4	4	44.2	6.726(-2)	2.30(11)
2p	3d	² P ^o	² D ^e	4	6	44.2	6.051(-1)	1.38(12)
LS		² P ^o	² D ^e	6	10		6.710(-1)	1.38(12)
3p	3d	² P ^o	² D ^e	2	4	4579.2	3.124(-2)	4.97(6)
3p	3d	² P ^o	² D ^e	4	4	5148.4	2.776(-3)	6.99(5)
3p	3d	² P ^o	² D ^e	4	6	4979.6	2.586(-2)	4.64(6)
LS		² P ^o	² D ^e	6	10		2.888(-2)	4.71(6)

Table 5. continued.

C_i	C_j	T_i	T_j	g_i	g_j	E_{ij}	f	A
						(Å)		(s ⁻¹)
S XIV								
2s	2p	² S ^e	² P ^o	2	2	445.8	2.951(-2)	9.90(8)
2s	2p	² S ^e	² P ^o	2	4	417.6	6.335(-2)	1.21(9)
LS		² S ^e	² P ^o	2	6		9.285(-2)	1.13(9)
2s	3p	² S ^e	² P ^o	2	2	30.5	1.198(-1)	8.61(11)
2s	3p	² S ^e	² P ^o	2	4	30.4	2.354(-1)	8.48(11)
LS		² S ^e	² P ^o	2	6		3.552(-1)	8.52(11)
2p	3s	² P ^o	² S ^e	2	2	33.4	1.989(-2)	1.19(11)
2p	3s	² P ^o	² S ^e	4	2	33.5	2.056(-2)	2.44(11)
LS		² P ^o	² S ^e	6	2		2.034(-2)	3.63(11)
3s	3p	² S ^e	² P ^o	2	2	1615.7	4.980(-2)	1.27(8)
3s	3p	² S ^e	² P ^o	2	4	1506.2	1.072(-1)	1.58(8)
LS		² S ^e	² P ^o	2	6		1.570(-1)	1.47(8)
2p	3d	² P ^o	² D ^e	2	4	32.4	6.705(-1)	2.13(12)
2p	3d	² P ^o	² D ^e	4	4	32.6	6.753(-2)	4.24(11)
2p	3d	² P ^o	² D ^e	4	6	32.6	6.073(-1)	2.55(12)
LS		² P ^o	² D ^e	6	10		6.729(-1)	2.54(12)
3p	3d	² P ^o	² D ^e	2	4	3674.5	2.857(-2)	7.06(6)
3p	3d	² P ^o	² D ^e	4	4	4402.3	2.382(-3)	8.20(5)
3p	3d	² P ^o	² D ^e	4	6	4142.1	2.283(-2)	5.92(6)
LS		² P ^o	² D ^e	6	10		2.544(-2)	5.98(6)
Ar XVI								
2s	2p	² S ^e	² P ^o	2	2	389.1	2.594(-2)	1.14(9)
2s	2p	² S ^e	² P ^o	2	4	353.9	5.747(-2)	1.53(9)
LS		² S ^e	² P ^o	2	6		8.340(-2)	1.39(9)
2s	3p	² S ^e	² P ^o	2	2	23.5	1.232(-1)	1.48(12)
2s	3p	² S ^e	² P ^o	2	4	23.5	2.410(-1)	1.45(12)
LS		² S ^e	² P ^o	2	6		3.642(-1)	1.46(12)
2p	3s	² P ^o	² S ^e	2	2	25.5	1.915(-2)	1.96(11)
2p	3s	² P ^o	² S ^e	4	2	25.7	2.000(-2)	4.04(11)
LS		² P ^o	² S ^e	6	2		1.972(-2)	6.01(11)
3s	3p	² S ^e	² P ^o	2	2	1421.6	4.334(-2)	1.43(8)
3s	3p	² S ^e	² P ^o	2	4	1281.7	9.659(-2)	1.96(8)
LS		² S ^e	² P ^o	2	6		1.399(-1)	1.77(8)
2p	3d	² P ^o	² D ^e	2	4	24.8	6.723(-1)	3.63(12)
2p	3d	² P ^o	² D ^e	4	4	25.0	6.774(-2)	7.22(11)
2p	3d	² P ^o	² D ^e	4	6	25.0	6.089(-1)	4.33(12)
LS		² P ^o	² D ^e	6	10		6.746(-1)	4.33(12)
3p	3d	² P ^o	² D ^e	2	4	2874.7	2.792(-2)	1.13(7)
3p	3d	² P ^o	² D ^e	4	4	3689.3	2.172(-3)	1.06(6)
3p	3d	² P ^o	² D ^e	4	6	3387.6	2.135(-2)	8.27(6)
LS		² P ^o	² D ^e	6	10		2.383(-2)	8.40(6)
Ca XVIII								
2s	2p	² S ^e	² P ^o	2	2	344.8	2.315(-2)	1.30(9)
2s	2p	² S ^e	² P ^o	2	4	302.2	5.332(-2)	1.95(9)
LS		² S ^e	² P ^o	2	6		7.645(-2)	1.71(9)
2s	3p	² S ^e	² P ^o	2	2	18.7	1.262(-1)	2.40(12)
2s	3p	² S ^e	² P ^o	2	4	18.7	2.455(-1)	2.34(12)
LS		² S ^e	² P ^o	2	6		3.717(-1)	2.36(12)
2p	3s	² P ^o	² S ^e	2	2	20.1	1.870(-2)	3.10(11)
2p	3s	² P ^o	² S ^e	4	2	20.2	1.973(-2)	6.44(11)
LS		² P ^o	² S ^e	6	2		1.939(-2)	9.54(11)
3s	3p	² S ^e	² P ^o	2	2	1621.5	2.999(-2)	7.61(7)
3s	3p	² S ^e	² P ^o	2	4	1364.2	7.	

Table 5. continued.

C_i	C_j	T_i	T_j	g_i	g_j	E_{ij}	f	A
						(Å)		(s^{-1})
Ti XX								
2s	2p	$^2S^e$	$^2P^o$	2	2	308.9	2.093(-2)	1.46(9)
2s	2p	$^2S^e$	$^2P^o$	2	4	259.6	5.040(-2)	2.49(9)
LS		$^2S^e$	$^2P^o$	2	6		7.130(-2)	2.11(9)
2s	3p	$^2S^e$	$^2P^o$	2	2	15.3	1.281(-1)	3.67(12)
2s	3p	$^2S^e$	$^2P^o$	2	4	15.2	2.481(-1)	3.58(12)
LS		$^2S^e$	$^2P^o$	2	6		3.762(-1)	3.61(12)
2p	3s	$^2P^o$	$^2S^e$	2	2	16.3	1.811(-2)	4.56(11)
2p	3s	$^2P^o$	$^2S^e$	4	2	16.4	1.935(-2)	9.54(11)
LS		$^2P^o$	$^2S^e$	6	2		1.894(-2)	1.41(12)
3s	3p	$^2S^e$	$^2P^o$	2	2	1111.3	3.541(-2)	1.91(8)
3s	3p	$^2S^e$	$^2P^o$	2	4	926.1	8.561(-2)	3.33(8)
LS		$^2S^e$	$^2P^o$	2	6		1.210(-1)	2.80(8)
2p	3d	$^2P^o$	$^2D^e$	2	4	15.9	6.720(-1)	8.86(12)
2p	3d	$^2P^o$	$^2D^e$	4	4	16.1	6.802(-2)	1.76(12)
2p	3d	$^2P^o$	$^2D^e$	4	6	16.0	6.113(-1)	1.06(13)
LS		$^2P^o$	$^2D^e$	6	10		6.759(-1)	1.05(13)
3p	3d	$^2P^o$	$^2D^e$	2	4	1852.2	2.768(-2)	2.69(7)
3p	3d	$^2P^o$	$^2D^e$	4	4	2778.3	1.840(-3)	1.59(6)
3p	3d	$^2P^o$	$^2D^e$	4	6	2385.5	1.936(-2)	1.51(7)
LS		$^2P^o$	$^2D^e$	6	10		2.161(-2)	1.54(7)
Cr XXII								
2s	2p	$^2S^e$	$^2P^o$	2	2	279.5	1.909(-2)	1.63(9)
2s	2p	$^2S^e$	$^2P^o$	2	4	223.3	4.847(-2)	3.24(9)
LS		$^2S^e$	$^2P^o$	2	6		6.751(-2)	2.62(9)
2s	3p	$^2S^e$	$^2P^o$	2	2	12.7	1.302(-1)	5.42(12)
2s	3p	$^2S^e$	$^2P^o$	2	4	12.6	2.506(-1)	5.24(12)
LS		$^2S^e$	$^2P^o$	2	6		3.808(-1)	5.30(12)
2p	3s	$^2P^o$	$^2S^e$	2	2	13.4	1.783(-2)	6.63(11)
2p	3s	$^2P^o$	$^2S^e$	4	2	13.6	1.931(-2)	1.40(12)
LS		$^2P^o$	$^2S^e$	6	2		1.882(-2)	2.07(12)
3s	3p	$^2S^e$	$^2P^o$	2	2	1428.3	2.270(-2)	7.42(7)
3s	3p	$^2S^e$	$^2P^o$	2	4	1042.6	6.275(-2)	1.93(8)
LS		$^2S^e$	$^2P^o$	2	6		8.540(-2)	1.45(8)
2p	3d	$^2P^o$	$^2D^e$	2	4	13.1	6.707(-1)	1.29(13)
2p	3d	$^2P^o$	$^2D^e$	4	4	13.3	6.808(-2)	2.56(12)
2p	3d	$^2P^o$	$^2D^e$	4	6	13.3	6.114(-1)	1.54(13)
LS		$^2P^o$	$^2D^e$	6	10		6.754(-1)	1.54(13)
3p	3d	$^2P^o$	$^3D^e$	2	4	1493.9	2.833(-2)	4.23(7)
3p	3d	$^2P^o$	$^2D^e$	4	4	2436.5	1.732(-3)	1.95(6)
3p	3d	$^2P^o$	$^2D^e$	4	6	1998.4	1.909(-2)	2.13(7)
LS		$^2P^o$	$^2D^e$	6	10		2.121(-2)	2.13(7)
Ni XXVI								
2s	2p	$^2S^e$	$^2P^o$	2	2	234.3	1.618(-2)	1.97(9)
2s	2p	$^2S^e$	$^2P^o$	2	4	165.4	4.677(-2)	5.70(9)
LS		$^2S^e$	$^2P^o$	2	6		6.286(-2)	4.16(9)
2s	3p	$^2S^e$	$^2P^o$	2	2	9.1	1.339(-1)	1.08(13)
2s	3p	$^2S^e$	$^2P^o$	2	4	9.1	2.541(-1)	1.03(13)
LS		$^2S^e$	$^2P^o$	2	6		3.880(-1)	1.05(13)
2p	3s	$^2P^o$	$^2S^e$	2	2	9.6	1.759(-2)	1.28(12)
2p	3s	$^2P^o$	$^2S^e$	4	2	9.7	1.965(-2)	2.77(12)
LS		$^2P^o$	$^2S^e$	6	2		1.897(-2)	4.05(12)
3s	3p	$^2S^e$	$^2P^o$	2	2	971.5	2.372(-2)	1.68(8)
3s	3p	$^2S^e$	$^2P^o$	2	4	641.3	7.273(-2)	5.90(8)
LS		$^2S^e$	$^2P^o$	2	6		9.635(-2)	4.10(8)
2p	3d	$^2P^o$	$^2D^e$	2	4	9.4	6.690(-1)	2.53(13)
2p	3d	$^2P^o$	$^2D^e$	4	4	9.5	6.826(-2)	4.99(12)
2p	3d	$^2P^o$	$^2D^e$	4	6	9.5	6.125(-1)	3.00(13)
LS		$^2P^o$	$^2D^e$	6	10		6.752(-1)	2.99(13)
3p	3d	$^2P^o$	$^2D^e$	2	4	1063.3	2.842(-2)	8.38(7)
3p	3d	$^2P^o$	$^2D^e$	4	4	2436.5	1.235(-3)	1.39(6)
3p	3d	$^2P^o$	$^2D^e$	4	6	1783.3	1.529(-2)	2.14(7)
LS		$^2P^o$	$^2D^e$	6	10		1.757(-2)	2.37(7)

Table 6. Comparison of BPRM A-values with those in the NIST compilation, Refs: a-Johnson et al. (1996), b-Yan et al. (1998).

C_i	C_j	T_i	T_j	g_i	g_j	E_{ij}	$A(s^{-1})$	$A(s^{-1})$
						(Ry)	present	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)
2s	2p	$^2S^e$	$^2P^o$	2	4	681.6	6.61(8)	6.63(8)
2p	3s	$^2P^o$	$^2S^e$	2	2	81.2	2.37(10)	2.36(10)
2p	3s	$^2P^o$	$^2S^e$	4	2	81.3	4.80(10)	4.70(10)
Mg X								
2s	2p	$^2S^e$	$^2P^o$	2	2	624.6	6.97(8)	7.00(8)
2s	2p	$^2S^e$	$^2P^o$	2	4	609.5	7.53(8)	7.53(8)
2s	3p	$^2S^e$	$^2P^o$	2	2	57.9	2.18(11)	2.09(11)
2s	3p	$^2S^e$	$^2P^o$	2	4	57.9	2.16(11)	2.09(11)
2p	3d	$^2P^o$	$^2D^e$	2	4	63.2	5.57(11)	5.60(11)
2p	3d	$^2P^o$	$^2D^e$	4	4	63.3	1.11(11)	1.12(11)
2p	3d	$^2P^o$	$^2D^e$	4	6	63.3	6.68(11)	6.70(11)
Al XI								
2s	2p	$^2S^e$	$^2P^o$	2	2	568.1	7.69(8)	7.83(8)
2s	2p	$^2S^e$	$^2P^o$	2	4	550.3	8.50(8)	8.62(8)
2p	3s	$^2P^o$	$^2S^e$	2	2	54.2	4.90(10)	4.80(10)
2p	3s	$^2P^o$	$^2S^e$	4	2	54.4	9.94(10)	9.60(10)
3s	3p	$^2S^e$	$^2P^o$	2	4	1994.0	1.09(8)	1.09(8)

Table 6. continued.

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	45.5	6.73(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	1.21(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								
2s	2p	$^2S^e$	$^2P^o$	2	2	234.3	1.97(9)	1.99(9)
2s	2p	$^2S^e$	$^2P^o$	2	4	165.4	5.70(9)	5.75(9)
2s	3p	$^2S^e$	$^2P^o$	2	2	9.1	1.08(13)	1.04(13)
2s	3p	$^2S^e$	$^2P^o$	2	4	9.1	1.03(13)	9.99(12)
2p	3s	$^2P^o$	$^2S^e$	2	2	9.6	1.28(12)	1.30(12)
2p	3s	$^2P^o$	$^2S^e$	4	2	9.7	2.77(12)	2.50(12)
2p	3d	$^2P^o$	$^2D^e$	2	4	9.4	2.53(13)	2.59(13)
2p	3d	$^2P^o$	$^2D^e$	4	4	9.5	4.99(12)	5.00(12)
C_i	C_j	T_i	T_j	g_i	g_j		f present	f others
S XIV								
2s	2p	$^2S^e$	$^2P^o$	2	6		9.285(-2)	8.823(-2) ^b
Ar XVI								
2s	2p	$^2S^e$	$^2P^o$	2	6		8.340(-2)	7.750(-2) ^b
Ca XVII								
2s	2p	$^2S^e$	$^2P^o$	2	6		7.645(-2)	6.909(-2) ^b

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, $N_{\text{elc}} (= 3)$. 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 π_i ($\pi = 0$ for even and $=1$ for odd parity), $2J_k$ and π_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_{J_i} and N_{J_k} . The line is followed by $N_{J_i} \times N_{J_k}$ 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, $A_{ki}(s^{-1})$.

5. Conclusion

Accurate and large-scale calculations have been carried out for the set of fine structure energy levels and transition probabilities upto $n = 10$ 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 7. Sample set of f - and A -values of O VI in $J\pi$ order as obtained from BPRM calculations.

8		3			E_j (Ry)	gf_L	S	$A_{ji}(s^{-1})$
1	0	1	1					
9	9	E_i (Ry)						
1	1	-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	-4.300E-03	1.346E-03	1.586E+09		
1	8	-1.01495E+01	-4.47461E-01	-2.951E-03	9.125E-04	1.116E+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	5.782E-02	3.503E-02	5.693E+09		
2	2	-4.31964E+00	-4.08326E+00	-2.208E-01	2.802E+00	4.955E+07		
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		
...		
1		3			E_j (Ry)	gf_L	S	$A_{ji}(s^{-1})$
9	9	E_i (Ry)						
1	1	-1.01495E+01	-9.26399E+00	-2.660E-01	9.012E-01	4.189E+08		
1	2	-1.01495E+01	-4.08122E+00	-3.540E-01	1.750E-01	2.618E+10		
1	3	-1.01495E+01	-2.28321E+00	-9.838E-02	3.752E-02	1.222E+10		
1	4	-1.01495E+01	-1.45698E+00	-4.197E-02	1.448E-02	6.369E+09		
1	5	-1.01495E+01	-1.00983E+00	-2.216E-02	7.274E-03	3.718E+09		
1	6	-1.01495E+01	-7.40903E-01	-1.325E-02	4.225E-03	2.355E+09		
1	7	-1.01495E+01	-5.66676E-01	-8.582E-03	2.687E-03	1.582E+09		
1	8	-1.01495E+01	-4.47387E-01	-5.891E-03	1.822E-03	1.113E+09		
1	9	-1.01495E+01	-3.62149E-01	-4.224E-03	1.295E-03	8.125E+08		
2	1	-4.31964E+00	-9.26399E+00	1.164E-01	7.063E-02	1.143E+10		
2	2	-4.31964E+00	-4.08122E+00	-4.457E-01	5.608E+00	5.087E+07		
2	3	-4.31964E+00	-2.28321E+00	-3.679E-01	5.420E-01	3.064E+09		
2	4	-4.31964E+00	-1.45698E+00	-1.101E-01	1.154E-01	1.811E+09		
2	5	-4.31964E+00	-1.00983E+00	-4.898E-02	4.440E-02	1.077E+09		
2	6	-4.31964E+00	-7.40903E-01	-2.673E-02	2.241E-02	6.875E+08		
2	7	-4.31964E+00	-5.66676E-01	-1.642E-02	1.313E-02	4.643E+08		
2	8	-4.31964E+00	-4.47387E-01	-1.089E-02	8.437E-03	3.278E+08		
2	9	-4.31964E+00	-3.62149E-01	-7.626E-03	5.781E-03	2.398E+08		
3	1	-2.38171E+00	-9.26399E+00	2.310E-02	1.007E-02	4.395E+09		
3	2	-2.38171E+00	-4.08122E+00	2.570E-01	4.537E-01	2.981E+09		
3	3	-2.38171E+00	-2.28321E+00	-6.222E-01	1.895E+01	1.212E+07		
3	4	-2.38171E+00	-1.45698E+00	-3.938E-01	1.278E+00	6.762E+08		
3	5	-2.38171E+00	-1.00983E+00	-1.192E-01	2.607E-01	4.503E+08		
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