Atomic Data and Nuclear Data Tables 100 (2014) 1322–1336

Contents lists available at ScienceDirect

Atomic Data and Nuclear Data Tables

journal homepage: www.elsevier.com/locate/adt

Oscillator strengths and transition probabilities from the Breit–Pauli R-matrix method: Ne IV

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HIGHLIGHTS

- The first application of BPRM method for accurate E1 transitions in Ne IV is reported.
- Amount of atomic data (n going up to 10) is complete for most practical applications.
- The calculated energies are in very good agreement with most observed levels.
- Very good agreement of A-values and lifetimes with other relativistic calculations.
- The results should provide precise nebular abundances, chemical evolution etc.

ARTICLE INFO

Article history:
Received 13 August 2013
Received in revised form
20 November 2013
Accepted 4 February 2014
Available online 23 May 2014

Keywords:
Fine structure levels
Ne IV
Oscillator strengths
Transition probabilities
Lifetimes
Breit–Pauli R-matrix method

ABSTRACT

The atomic parameters – oscillator strengths, line strengths, radiative decay rates (A), and lifetimes – for fine structure transitions of electric dipole (E1) type for the astrophysically abundant ion Ne IV are presented. The results include 868 fine structure levels with $n \leq 10$, $l \leq 9$, and $1/2 \leq J \leq 19/2$ of even and odd parities, and the corresponding 83,767 E1 transitions. The calculations were carried out using the relativistic Breit–Pauli R-matrix method in the close coupling approximation. The transitions have been identified spectroscopically using an algorithm based on quantum defect analysis and other criteria. The calculated energies agree with the 103 observed and identified energies to within 3% or better for most of the levels. Some larger differences are also noted. The A-values show good to fair agreement with the very limited number of available transitions in the table compiled by NIST, but show very good agreement with the latest published multi-configuration Hartree–Fock calculations. The present transitions should be useful for diagnostics as well as for precise and complete spectral modeling in the soft X-ray to infra-red regions of astrophysical and laboratory plasmas.

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http://dx.doi.org/10.1016/j.adt.2014.02.001
0092-640X/

Contents

1. Introduction

Spectral lines of neon ions have been seen in many astronomical objects (see e.g., Ref. [1]). These provide information regarding the physical conditions and chemical evolution in the astronomical object. Ne V lines have been used for diagnostics in planetary nebulae (see e.g., Ref. [2]) and Ne IV lines have been observed in SN1987 [3] and radio galaxies [4]. Ne V combines to form Ne IV very easily. Radiative-collisional models for diagnostics and synthetic spectra require atomic parameters for both Ne IV and Ne V. The current report is a part of the Iron Project [5] for such studies, particularly for determination of nebular abundances. The present results can be used for diagnostics of optically allowed transitions. The collision strengths for electron-impact excitation of Ne V have been obtained and reported by Dance et al. [6] and for photoionization cross sections by Nahar [7].

The present study reports results for an extensive set of transitions in Ne IV corresponding to the large number of excited levels obtained using the relativistic Breit–Pauli R-matrix method. Such a set is needed for precise astrophysical modeling as well as for accurate diagnostics. The earlier non-relativistic R-matrix calculation in *LS* coupling was carried out under the Opacity Project (OP) [8] by Lennon and Burke [9]. The work and the data were not published. However, the data are available through the OP database TOPbase [10]. Other theoretical work includes two-configuration calculations by Levinsonas et al. [11] and calculations using the Coulomb potential approximation by Wiese et al. [12]. The latest calculations for levels up to the 4*s* orbital were carried out by Froese-Fischer and Tachiev [13]. Several experimental measurements were carried out in the past and have been compiled at the National Institute of Standards and Technology (NIST) [14]. They are from work by Bockasten et al. [15], Goldsmith and Kaufman [16], Lindeberg [17,18], Marling [19], and Kramida et al. [20]. The available values are in *LS* coupling from which the fine structure components are obtained through algebraic transformation.

2. Theory

The present calculations were carried out using the Breit–Pauli R-matrix (BPRM) method developed under the Opacity Project [8] and the Iron Project [5]. A brief outline of the R-matrix method in the close coupling (CC) approximation (see e.g., Refs. [21,22]) is given below. In the CC approximation the atomic system is described as an N-electron target (core) interacting with the $(N+1)$th electron. The total wavefunction expansion, Ψ_E, of the $(N+1)$-electron system is expressed 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/core ion wavefunction of a specific *LS* state $S_iL_i\pi_i$ or fine structure level $J_i\pi_i$, and θ_i is the wavefunction of the interacting $(N+1)$th electron in a channel labeled as $S_iL_i(J_i)\pi_i\, k_i^2\ell_i$ ($SL\pi$ or $J\pi$) where k_i^2 is the incident kinetic energy. The sum includes channels of various excitations of the core ion along with wavefunctions of the interacting electron. Φ_j's are correlation wavefunctions of the $(N+1)$-electron system that (a) compensate the orthogonality conditions between the continuum and the bound orbitals and (b) represent additional short-range correlation.

The Hamiltonian of the $(N+1)$-electron system is given, in the relativistic Breit–Pauli approximation, by (see e.g., Refs. [23,22])

$$H_{N+1}^{\text{BP}} = H_{N+1} + H_{N+1}^{\text{mass}} + H_{N+1}^{\text{Dar}} + H_{N+1}^{\text{so}} + \frac{1}{2}\sum_{i\neq j}^{N}[g_{ij}(so+so') + g_{ij}(ss') + g_{ij}(css') + g_{ij}(d) + g_{ij}(oo')] \quad (2)$$

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

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

H_{N+1}^{mass} is the mass correction, H_{N+1}^{Dar} is the Darwin term, and H_{N+1}^{so} is the spin–orbit interaction term. The two-body interaction terms are with notation *c* for contraction, *d* for Darwin, *o* for orbit, *s* for spin, and a prime indicates 'other'. The Breit–Pauli R-matrix Hamiltonian under the Iron Project [5] includes the first three one-body corrections and the parts of two-body terms that are much weaker.

The wavefunction and energies are obtained by solving

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

using the R-matrix approach. In the BPRM method, the set of states $SL\pi$ are recoupled to obtain $(e+\text{ion})$ states with total $J\pi$, following the diagonalization of the $(N+1)$-electron Hamiltonian. 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 matrix elements for radiative transitions of electric dipole (E1) type are given by $\langle\Psi_B\|\mathbf{D}\|\Psi_{B'}\rangle$ where $\mathbf{D} = \sum_i \mathbf{r}_i$ is the dipole operator and i is the index of the electron. These can be reduced to generalized line strengths as

$$S = \left|\left\langle\Psi_f\left|\sum_{j=1}^{N+1} r_j\right|\Psi_i\right\rangle\right|^2 \quad (5)$$

where Ψ_i and Ψ_f are the initial and final bound wavefunctions, respectively. The line strengths are energy independent quantities

and are related to the oscillator strength, f_{ij}, and the radiative decay rates or Einstein A-coefficients as

$$f_{ij} = \frac{E_{ji}}{3g_i} S, \qquad A_{ji}(a.u.) = \frac{1}{2}\alpha^3 \frac{g_i}{g_j} E_{ji}^2 f_{ij}. \tag{6}$$

E_{ji}, in atomic units ($a.u.$), is the energy difference between the initial and final states, α is the fine structure constant, and g_i and g_j are the statistical weight factors of the initial and final states, respectively.

The lifetime of a level k can be obtained from the sum of A-values of the radiative decays from the level as

$$\tau_k(s) = \frac{1}{\sum_i A_{ki}(s^{-1})}. \tag{7}$$

In units of time, $A_{ji}(s^{-1}) = A_{ji}(a.u.)/\tau_0$, where $\tau_0 = 2.4191 \times 10^{-17}$s is the atomic unit of time.

3. Calculations

The computations have been carried out using the package of Breit–Pauli R-matrix codes that consists of a number of stages, named STG1, STG2, RECUPD, STGH, STGB, STGBB, etc. [24,25]. Stage 1, STG1, of the R-matrix code is initiated with orbital wavefunctions of the core or target levels and these are obtained from an atomic structure code, typically SUPERSTRUCTURE [26,27], that employs the Thomas–Fermi–Dirac approximation and includes relativistic effects in the Breit–Pauli approximation. The wavefunction expansion for the Ne V core was obtained from optimization of 24 configurations as given in Table A. The Thomas–Fermi–Dirac scaling parameters for the orbitals are also listed in Table A. Only the first 20 levels of Ne V were included in the wavefunction for Ne IV since no more bound states of Ne IV with core excitation beyond these levels are expected to form. These levels and comparison of their calculated energies with those of experiment (compiled by NIST [14]) are given in Table A. The observed and calculated energies show good agreement.

The partial wave expansion for the interacting electron includes $0 \le \ell \le 14$, with a R-matrix basis set of 15 continuum functions. The R-matrix boundary was chosen to be large enough, 9 a_o, to accommodate the bound orbitals. The second term of the wavefunction in Eq. (1), which represents the bound state correlation functions, includes 76 $(N+1)$-particle configurations with orbital occupancies from the minimum to a maximum number, as given within parentheses, of the orbitals: $1s$(2-2), $2s$(0-2), $2p$(0-5), $3s$(0-2), $3p$(0-3), $3d$(0-2), $4s$(0-2), and $4p$(0-2). Computations have been carried out for all angular momenta, $0 \le L \le 12$, $1/2 \le J \le 21/2$.

The fine structure energy levels of Ne IV were computed by STGB of the R-matrix package. These energies were sorted by scanning through the poles in the (e + ion) Hamiltonian with a fine energy mesh of effective quantum number $\Delta\nu$ of 0.001. The energies were identified through a theoretical spectroscopy procedure based on quantum defect analysis, percentage of channel contributions, and angular momenta algebra, as described earlier (see e.g., Ref. [28]) and using the code PRCBPID [29]. The oscillator strengths for bound–bound transitions were obtained using the code STGBB of the R-matrix package. The transitions were processed for energies and transition wavelengths using the code PBPRAD (see e.g., Ref. [30]).

All energies from the present BPRM calculations have been identified spectroscopically using a theoretical spectroscopic algorithm (see e.g., Refs. [28,29]). The levels are designated as $C_t(S_tL_t\pi_t)J_t nlJ\ SL\pi$, where C_t, $S_tL_t\pi_t$, J_t are the configuration, LS term, parity, and total angular momentum of the target or the core, 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. The algorithm is different from that of an atomic structure calculation that assigns a spectroscopic designation based on percentage contributions or higher mixing coefficients of the contributing configurations. In contrast, the R-matrix method involves couplings of a large number of channels and percentage contributions are determined from the outer region of the R-matrix boundary. Hence identification requires several considerations such as the quantum defect, percentage of channel contributions, and angular momentum algebra, as explained in detail by Nahar [28]. Hund's rule is used as a guide for levels arising from the same configuration such that a level with higher spin multiplicity $(2S+1)$ and higher orbital angular momentum L lies lower than that one with lower spin multiplicity and lower total orbital angular momentum. Hence, the same level can have two different designations from atomic structure and from BPRM calculations. In principle, both designations should be correct as both are possible designations, but with different percentage contributions.

Table A
Levels and energies (E_t) of the target (core ion) Ne V in the wavefunction expansion of Ne IV. They were optimized using a set of 24 spectroscopic configurations: $2s^22p^2(1)$, $2s2p^3(2)$, $2s^22p3s(3)$, $2p^4(4)$, $2s^22p3p(5)$, $2s^22p3d(6)$, $2s^22p4s(7)$, $2s^22p4p(8)$, $2s2p^23s(9)$, $2s2p^23p(10)$, $2s2p^23d(11)$, $2s^23s^2(12)$, $2s^23p^2(13)$, $2s^23d^2(14)$, $2s^24s^2(15)$, $2s^24p^2(16)$, $2s^23s3p(17)$, $2s^23s3d(18)$, $2s^23s4s(19)$, $2s^23s4p(20)$, $2s^23p3d(21)$, $2p^33s(22)$, $2p^33p(23)$, and $2p^33d(24)$ with filled $1s$ orbital. The Thomas–Fermi scaling parameters for the orbitals are 1.476 37($1s$), 1.476 37($2s$), 1.271 84($2p$), 1.476 37($3s$), 1.271 84($3p$), 1.193 06($3d$), 1.476 37($4s$), and 1.271 84($4p$). The present calculated energies (from the code SUPERSTRUCTURE, "SS") are compared with the observed energies in the NIST compilation [14].

	Level	J_t	E_t (Ry) NIST	E_t (Ry) SS
1	$1s^22s^22p^2(^3P)$	0	0.0	0.
2	$1s^22s^22p^2(^3P)$	1	0.003 758	0.003 9556
3	$1s^22s^22p^2(^3P)$	2	0.010 116	0.011 366
4	$1s^22s^22p^2(^1D)$	2	0.276 036	0.303 91
5	$1s^22s^22p^2(^1S)$	2	0.582 424	0.574 13
6	$1s^22s2p^3(^5S^o)$	2	0.8052	0.716 04
7	$1s^22s2p^3(^3D^o)$	3	1.602 32	1.629 57
8	$1s^22s2p^3(^3D^o)$	2	1.602 96	1.629 32
9	$1s^22s2p^3(^3D^o)$	1	1.603 16	1.629 29
10	$1s^22s2p^3(^3P^o)$	2	1.896 87	1.923 63
11	$1s^22s2p^3(^3P^o)$	1	1.896 87	1.923 40
12	$1s^22s2p^3(^3P^o)$	0	1.897 19	1.923 28
13	$1s^22s2p^3(^1D^o)$	2	2.465 56	2.593 26
14	$1s^22s2p^3(^3S^o)$	1	2.545 76	2.649 56
15	$1s^22s2p^3(^1P^o)$	1	2.768 54	2.889 88
16	$1s^22s2p^4(^3P)$	2	3.760 63	3.860 76
17	$1s^22s2p^4(^3P)$	1	3.767 78	3.868 07
18	$1s^22s2p^4(^3P)$	0	3.770 85	3.871 55
19	$1s^22s2p^4(^1D)$	2		4.138 16
20	$1s^22s2p^4(^1S)$	0		4.744 72

4. Results and discussions

Fine structure energy levels, oscillator strengths, line strengths, and radiative decay rates for a large number of allowed E1 transitions, as well as lifetimes, for Ne IV, obtained from the relativistic Breit–Pauli R-matrix method, are presented. The energies, radiative transitions, and lifetimes are discussed below in separate subsections.

4.1. Fine structure energies

An extensive set of fine structure bound levels, 868 in total with $n \le 10$, $0 \le l \le 9$, and $1/2 \le J \le 19/2$ of even and odd parities, of Ne IV is presented. A total of 103 identified energy levels are currently available at the NIST website. The calculated energies from

the Opacity Project [8] are for 340 states (including non-bound *LS* states) available from the TOPbase database [10].

Energies of Ne IV are presented in two formats. In one format, the energy levels are presented in sets representing fine structure components that belong to the same *LS* or a set of *LS* terms of same spin multiplicity of a common configuration. A partial set of identified calculated energy levels in this format is given in Table 1 where the *LS* term is specified in the rightmost column. The format is similar to that used by NIST and is useful for spectroscopic diagnostics. However, these energies are not statistically averaged to get the *LS* term energies since the *LS* designation may not be completely unique. There may be more than one possible designation. This format also helps in checking the completeness of the number of calculated fine structure levels that belong to a *LS* term. The identification program PRCBPID [29] carries out the check and issues a message indicating the completeness. If not all the levels of the fine structure set are found, then the calculated number of levels is not complete, and the program prints the list of missing levels. Very high lying *LS* terms can have incomplete sets because the missing levels typically exceed the limit of J levels included in the calculation.

As stated above, some levels may have more than one designation of L values as seen in Table 1. For example, some levels of the $2s^2 2p^2(^3P^e)3d$ configuration in Table 1 have more than one total possible angular momentum designation. The first level has three possible designations, $^4(PDF)^e$. Using Hund's rule, these levels can be uniquely defined. This particular level can be assigned with the highest angular momentum, $^4F^e$, for being the lowest level. Since $^4F^e$ has four levels, $J = 9/2, 7/2, 5/2, 3/2$ (specified in the line "Nlv" at the top of the set), the top four levels in the set can be grouped for the $^4F^e$ state. The four levels below them may be grouped together for the $^4D^e$ state while the three lowest ones are for the $^4P^e$ state. Another example is the set of levels of the $2s^2 2p^2(^3P^e)3p(^2D^o, ^2P^o, ^2S^o)$ configuration where it is easy to determine the components. $^2D^o$ can have the 2nd and 3rd levels as they are already uniquely designated, 1st and 5th levels can belong to $^2P^o$ and the 4th level to $^2S^o$. For a multi-electron system, Hund's rule may not be necessarily followed, but it provides a guidance for identification.

Table B presents a sample set of fine structure level energies in $J\pi$ order, the other format for energies, of the complete set of 868 levels of Ne IV. This order is convenient for locating transitions with indices and for use in modeling codes. Astrophysical models use observed transition energies, hence the calculated energies, as well as the corresponding level designation, for the 103 observed levels have been replaced by the observed energies in the table. These 868 energies will be available online at NORAD-Atomic-Data [31].

The BPRM energies for Ne IV are compared with the observed values, listed in the NIST-compiled on-line table [14], in Table C. The NIST wavelengths are used later. The values given in the table correspond to dividing the NIST wavelengths by 109 737.3 for Rydberg conversion and then scaled with the ionization energy for absolute values to compare with BPRM energies. Negligible differences may occur due to differences in the number of digits chosen after the decimal point during conversion. The difference is within the uncertainties of the present work and hence should not affect any result. The agreement is within 3% for most of the levels. However, some relatively large differences going up to, for example, 7% for the $2s2p3(5So)3d(^4D^o)$ level, have also been found. It may be noted that all levels have been identified uniquely based on the criteria mentioned above and with correspondence between the fine structure levels and their *LS* terms such that the exact number of fine structure levels is accounted for in each *LS* term. However due to mixing of states and similar quantum defects, spectroscopic designations could be swapped with respect to the atomic structure calculations.

Table B
Partial set of fine structure energy levels of Ne IV in $J\pi$ order. i_k is the energy index for the total set, I_J is the energy index for position of the level in its symmetry. The last column is the encoded identification of the level.

i_e	$J\pi$	I_J	E (Ry)	Config	$^{2S+1}L^\pi$	jjpiiii
1	0.5 e	1	−5.453 90E+00	2s2p4	^{4}Pe	100001
2	0.5 e	2	−4.407 60E+00	2s2p4	^{2}Se	100002
3	0.5 e	3	−4.215 20E+00	2s2p4	^{2}Pe	100003
4	0.5 e	4	−2.775 70E+00	2s22p2(3P)3s	^{4}Pe	100004
5	0.5 e	5	−2.686 40E+00	2s22p2(3P)3s	^{2}Pe	100005
6	0.5 e	6	−2.107 90E+00	2s22p2(1S)3s	^{2}Se	100006
7	0.5 e	7	−1.883 20E+00	2s22p2(3P)3d	^{2}Pe	100007
8	0.5 e	8	−1.877 04E+00	2s22p2(3Pe)3d	^{4} PDe	100008
9	0.5 e	9	−1.855 00E+00	2s22p2(3P)3d	^{4}Pe	100009
10	0.5 e	10	−1.552 30E+00	2s22p2(1D)3d	^{2}Pe	100010
11	0.5 e	11	−1.517 60E+00	2s22p2(1D)3d	^{2}Se	100011
12	0.5 e	12	−1.488 24E+00	2s2p3(5So)3p	^{4} Pe	100012
13	0.5 e	13	−1.365 40E+00	2s22p2(3P)4s	^{4}Pe	100013
14	0.5 e	14	−1.340 90E+00	2s22p2(3P)4s	^{2}Pe	100014
15	0.5 e	15	−1.008 10E+00	2s22p2(3P)4d	^{4}Pe	100015
16	0.5 e	16	−1.036 44E+00	2s22p2(3Pe)4d	^{4} PDe	100016
17	0.5 e	17	−1.026 17E+00	2s22p2(3Pe)4d	^{2} Pe	100017
18	0.5 e	18	−8.219 10E−01	2s22p2(3P)5s	^{4}Pe	100018
19	0.5 e	19	−8.035 04E−01	2s22p2(1Se)4s	^{2} Se	100019
20	0.5 e	20	−7.947 47E−01	2s22p2(3Pe)5s	^{2} Pe	100020
21	0.5 e	21	−7.455 30E−01	2s22p2(1D)4d	^{2}Pe	100021
22	0.5 e	22	−7.474 90E−01	2s22p2(1De)4d	^{2} SPe	100022
23	0.5 e	23	−7.257 07E−01	2s22p2(3Pe)5d	^{4} PDe	100023
24	0.5 e	24	−7.175 89E−01	2s22p2(3Pe)5d	^{4} PDe	100024
25	0.5 e	25	−6.615 98E−01	2s22p2(3Pe)5d	^{2} Pe	100025
26	0.5 e	26	−6.508 77E−01	2s22p2(3Pe)6s	^{4} Pe	100026
27	0.5 e	27	−6.502 35E−01	2s22p2(3Pe)6s	^{2} Pe	100027
28	0.5 e	28	−6.308 38E−01	2s2p3(5So)4p	^{4} Pe	100028
29	0.5 e	29	−5.407 20E−01	2s22p2(3Pe)6d	^{4} PDe	100029
30	0.5 e	30	−5.326 27E−01	2s22p2(3Pe)6d	^{4} PDe	100030
31	0.5 e	31	−4.565 07E−01	2s22p2(1Se)5s	^{2} Se	100031
32	0.5 e	32	−4.487 76E−01	2s22p2(3Pe)6d	^{2} Pe	100032
33	0.5 e	33	−4.477 46E−01	2s22p2(3Pe)7s	^{4} Pe	100033
34	0.5 e	34	−4.348 18E−01	2s22p2(3Pe)7s	^{2} Pe	100034
35	0.5 e	35	−4.316 61E−01	2s22p2(3Pe)7d	^{4} PDe	100035

4.2. Allowed E1 transitions

The complete set of transition parameters, f-, S-, and A-values for E1 transitions in Ne IV obtained using the *ab initio* close-coupling approximation in the relativistic Breit–Pauli R-matrix method is available electronically. The set consists of a total number of 83,767 transitions

Table D presents a sample set of f-, S-, A-values contained in the complete file. The first line of each set of transitions specifies the transition symmetries expressed by their statistical weight factors, $g = 2J + 1$, and parity π (=0 for even and =1 for odd parity). The same line also specifies the number of levels "Ni" and "Nk" belonging to symmetries J_i and J_k, and the total number of transitions "NN" (=Ni × Nk). This line is followed by the f-, S-, and A-values for the number NN of transitions. The indices of the transition levels correspond to I_i and I_k in Table B. The third column provides the calculated transition wavelengths (λ) in Å obtained using E (Å) $= 911.2671/E_{ik}$ (Rydberg). The sixth column gives the oscillator strength, f, in the length form. The sign of f indicates the upper and lower levels in the transition; a negative value means that the level i is lower and a positive value means that the level k is lower. Column seven is the line strength, S, and column eight gives the transition probability or the radiative decay rate $A_{ki}(s^{-1})$. While S is independent, f- and A-values are dependent on the transition energies. For observed lines, f- and A-values have been reevaluated from the calculated S-values but using the observed transition energies. All wavelengths are considered in vacuum.

A set of transitions, 1787 in total, for the observed fine structure levels listed in the NIST compilation has been reprocessed with complete spectroscopic identification for easy identifications

Table D
Sample set of f-, S- and A-values for allowed E1 transitions, $g_i\pi_i = 2$ even(0) $- g_k\pi_k = 2$ odd(1), in Ne IV. The top line specifies $Z = 10$, $N_e = 7$ number of electrons. "Ni" and "Nk" are the numbers of bound levels.

10		7						
I_i	I_k	λ (Å)	E_i (Ry)	E_k (Ry)	f	S	A_{ki} (s^{-1})	
	2 0	2 1	62 61 3782 = g_i	π_i g_k π_k	Ni Nk	NN(=Ni x Nk)		
1	1	817.21	−5.4539E+00	−6.5690E+00	1.238E−06	6.662E−06	1.237E+04	
1	2	332.15	−5.4539E+00	−2.7104E+00	−2.596E−06	5.677E−06	1.569E+05	
1	3	302.73	−5.4539E+00	−2.4438E+00	−1.606E−06	3.201E−06	1.169E+05	
1	4	297.43	−5.4539E+00	−2.3901E+00	−2.371E−04	4.644E−04	1.788E+07	
1	5	294.39	−5.4539E+00	−2.3585E+00	−9.247E−04	1.792E−03	7.118E+07	
1	6	283.54	−5.4539E+00	−2.2401E+00	−4.014E−08	7.495E−08	3.330E+03	
1	7	259.37	−5.4539E+00	−1.9405E+00	−9.890E−08	1.689E−07	9.806E+03	
1	8	245.83	−5.4539E+00	−1.7469E+00	−4.307E−08	6.972E−08	4.755E+03	
1	9	218.77	−5.4539E+00	−1.2885E+00	−6.656E−04	9.588E−04	9.275E+07	
1	10	218.13	−5.4539E+00	−1.2763E+00	−4.253E−03	6.109E−03	5.962E+08	
1	11	215.03	−5.4539E+00	−1.2161E+00	−5.674E−04	8.033E−04	8.184E+07	
1	12	213.47	−5.4539E+00	−1.1851E+00	−4.248E−08	5.971E−08	6.218E+03	
1	13	211.91	−5.4539E+00	−1.1536E+00	−4.191E−05	5.847E−05	6.225E+06	
1	14	209.70	−5.4539E+00	−1.1084E+00	−4.343E−02	5.996E−02	6.587E+09	
1	15	204.92	−5.4539E+00	−1.0070E+00	−1.488E−01	2.007E−01	2.364E+10	
1	16	204.58	−5.4539E+00	−9.9958E−01	−5.944E−04	8.007E−04	9.476E+07	
1	17	199.86	−5.4539E+00	−8.9426E−01	−6.968E−07	9.169E−07	1.163E+05	
1	18	197.31	−5.4539E+00	−8.3554E−01	−8.910E−03	1.158E−02	1.527E+09	
1	19	194.05	−5.4539E+00	−7.5797E−01	−7.262E−06	9.279E−06	1.286E+06	
1	20	193.76	−5.4539E+00	−7.5084E−01	−2.374E−04	3.029E−04	4.218E+07	
1	21	193.18	−5.4539E+00	−7.3661E−01	−8.335E−04	1.060E−03	1.489E+08	
1	22	192.59	−5.4539E+00	−7.2215E−01	−7.668E−06	9.723E−06	1.379E+06	
1	23	192.46	−5.4539E+00	−7.1912E−01	−2.277E−08	2.886E−08	4.101E+03	
1	24	192.25	−5.4539E+00	−7.1379E−01	−2.013E−08	2.548E−08	3.633E+03	
1	25	189.13	−5.4539E+00	−6.3581E−01	−1.286E−03	1.602E−03	2.398E+08	
1	26	188.12	−5.4539E+00	−6.0973E−01	−7.566E−08	9.372E−08	1.426E+04	
1	27	184.17	−5.4539E+00	−5.0586E−01	−1.262E−06	1.530E−06	2.481E+05	
1	28	184.05	−5.4539E+00	−5.0276E−01	−9.264E−06	1.123E−05	1.824E+06	
1	29	183.82	−5.4539E+00	−4.9660E−01	−6.792E−05	8.221E−05	1.341E+07	
1	30	183.47	−5.4539E+00	−4.8709E−01	−1.661E−06	2.007E−06	3.293E+05	
1	31	182.20	−5.4539E+00	−4.5240E−01	−5.448E−08	6.536E−08	1.095E+04	
1	32	181.69	−5.4539E+00	−4.3827E−01	−1.426E−03	1.706E−03	2.882E+08	
1	33	179.03	−5.4539E+00	−3.6376E−01	−4.270E−05	5.034E−05	8.888E+06	

and diagnostics. Table 2 presents a partial set of these transitions. The transitions have been grouped together as fine structure components of *LS* multiplets. Dipole allowed fine structure transitions with same-spin multiplicity can be added with the statistical weight factor to obtain the f-, S-, and A-values of the *LS* multiplets.

The present A-values are compared with those from NIST in Table E. The compiled table from the NIST website reports 644 lines of Ne IV. However, it contains radiative decay rates for only a limited number of transitions. As mentioned above, the earlier measured lines for transition wavelengths at NIST are from Bockasten et al. [15], Lindeberg [17,18], Goldsmith and Kaufman [16], and recently from Kramida et al. [20]. The earlier theoretical work for A-values that NIST includes were obtained with consideration of two configurations by Levinsonas et al. [11] and using the Coulomb potential approximation by Wiese et al. [12]. NIST also includes transitions obtained by Weiss [32]. R-matrix calculations, but in non-relativistic *LS* coupling, were carried out by Lennon and Burke [9].

Most of the transitions in the NIST compilation were obtained in *LS* coupling, designated with "*LS*" in Table E, which were split in to fine structure components by algebraic transformation of the *LS* multiplets. The most recent work was carried out in the multi-configuration Hartree–Fock approximation where the relativistic effects were included in the Breit–Pauli approximation by Froese-Fischer and Tachiev [13]. BPRM A-values for transitions in Ne IV are compared with those obtained experimentally and theoretically in Table E. The comparison shows that the present BPRM A-values have good to fair agreement with those listed by NIST calculated with simpler approximations, and have very good agreement with those from relativistic multi-configuration calculations by Froese-Fischer and Tachiev [13]. This indicates higher accuracy in general of the present BPRM transition parameters. However, the agreement within 10% found for these transitions can differ significantly for very weak transitions, particularly intercombination transitions, and individual differences could be 50% or more depending on the sensitivity of the wavefunctions in transition matrix.

4.3. Lifetimes

Lifetimes of all 867 excited fine structure levels of Ne IV were obtained from the BPRM A-values for E1 transitions. The complete table is available electronically. A sample set of lifetimes is given in Table F. The last column in the table lists the number of transitions of the level to lower levels and the A-values of these transitions that were included in determination of the lifetimes.

The present lifetimes are compared with those obtained by Froese-Fischer and Tachiev [13] in Table G. The comparison shows that the present lifetimes agree well with their calculated values.

5. Conclusions

A large set of transition probabilities and oscillator strengths for E1 transitions in Ne IV was obtained from use of the relativistic BPRM method. The atomic data contains 868 fine structure levels with $n \leq 10$ and comprises 83,767 E1 transitions among these levels. The fine structure levels have been identified spectroscopically. However, due to mixing of levels with different weights and similar quantum defects, the present identifications of the levels may not necessarily match those from other atomic structure calculations, especially for the high-lying levels. Although all designations from various calculations are theoretically correct, the difference arises from individual percentage contributions to the final state.

Table E
Comparison of the present *A*-values for E1 transitions in Ne IV with those in references [18](*a*), [20](*b*), [32](*c*), [12](*d*), [17](*e*), [19](*f*), [13](*g*). Alphabetic letters are the accuracy ratings from NIST. LS notation on the right indicates that NIST obtained the A-value from the LS multiplet.

A (s^{-1}):NIST	Present	Transition: C_i–C_f	
2.5E+09:E[a], 1.79E+09[g]	1.76E+09	$2s22p3\ ^4S^o_{3/2}$	$2s2p4\ ^4P_{3/2}$:*LS*
2.5E+09:E[a], 1.77E+09[g]	1.74E+09	$2s22p3\ ^4S^o_{3/2}$	$2s2p4\ ^4P_{5/2}$:*LS*
2.5E+09:E[a], 1.80E+09[g]	1.78E+09	$2s22p3\ ^4S^o_{3/2}$	$2s2p4\ ^4P_{1/2}$:*LS*
4.8E+09:E[b], 6.720E+09[g]	6.63E+09	$2s22p3\ ^4S^o_{3/2}$	$2s22p2(3P)3s\ ^4P_{5/2}$:*LS*
4.8E+09:E[b], 6.745E+09[g]	6.62E+09	$2s22p3\ ^4S^o_{3/2}$	$2s22p2(3P)3s\ ^4P_{3/2}$:*LS*
4.8E+09:E[b], 6.782E+09[g]	6.62E+09	$2s22p3\ ^4S^o_{3/2}$	$2s22p2(3P)3s\ ^4P_{1/2}$:*LS*
4.6E+09:E[a], 3.864E+09[g]	3.78E+09	$2s22p3\ ^2D^o_{3/2}$	$2s2p4\ ^2D_{3/2}$:*LS*
4.9E+08:E[a], 4.013E+08[g]	3.92E+08	$2s22p3\ ^2D^o_{5/2}$	$2s2p4\ ^2D_{3/2}$:*LS*
4.9E+09:E[a], 3.935E+09[g]	3.85E+09	$2s22p3\ ^2D^o_{5/2}$	$2s2p4\ ^2D_{5/2}$:*LS*
3.3E+08:E[a], 2.482E+08[g]	2.45E+08	$2s22p3\ ^2D^o_{3/2}$	$2s2p4\ ^2D_{5/2}$:*LS*
7.4E+08:E[a], 7.585E+08[g]	7.65E+08	$2s22p3\ ^2D^o_{5/2}$	$2s22p2(1D)3s\ ^2D_{3/2}$
7.0E+09:E[b], 8.310E+09[g]	8.15E+09	$2s22p3\ ^2D^o_{5/2}$	$2s22p2(1D)3s\ ^2D_{5/2}$
6.9E+09:E[b], 7.949E+09[g]	7.81E+09	$2s22p3\ ^2D^o_{3/2}$	$2s22p2(1D)3s\ ^2D_{3/2}$
4.9E+08:E[c], 6.917E+08[g]	6.71E+08	$2s22p3\ ^2D^o_{3/2}$	$2s22p2(1D)3s\ ^2D_{5/2}$
1.50E+10:E[b], 1.791E+10[g]	1.77E+10	$2s22p3\ ^2D^o_{3/2}$	$2s2p4\ ^2P_{1/2}$:*LS*
1.40E+10:E[b], 1.648E+10[g]	1.63E+10	$2s22p3\ ^2D^o_{5/2}$	$2s2p4\ ^2P_{3/2}$:*LS*
1.5E+09:E[b], 1.990E+9[g]	1.94E+09	$2s22p3\ ^2D^o_{3/2}$	$2s2p4\ ^2P_{3/2}$:*LS*
5.1E+09:E[a], 2.803E+09[g]	2.60E+09	$2s22p3\ ^2P^o_{1/2}$	$2s2p4\ ^2P_{1/2}$:*LS*
2.4E+09:E[a], 2.027E+09[g]	1.95E+09	$2s22p3\ ^2P^o_{3/2}$	$2s2p4\ ^2P_{1/2}$:*LS*
1.2E+09:E[a], 7.510E+08[g]	7.10E+08	$2s22p3\ ^2P^o_{1/2}$	$2s2p4\ ^2P_{3/2}$:*LS*
6.2E+09:E[a], 3.514E+09[g]	3.33E+09	$2s22p3\ ^2P^o_{3/2}$	$2s2p4\ ^2P_{3/2}$:*LS*
4.1E+09:E[a], 3.384E+09[g]	3.37E+09	$2s22p3\ ^2P^o_{1/2}$	$2s2p4\ ^2S_{1/2}$
8.0E+09:E[a], 6.349E+09[g]	6.22E+09	$2s22p3\ ^2P^o_{3/2}$	$2s2p4\ ^2S_{1/2}$
6.4E+08:E[a], 4.736E+08[g]	4.56E+08	$2s22p3\ ^2P^o_{1/2}$	$2s2p4\ ^2D_{3/2}$
1.3E+08:E[a], 6.612E+07[g]	6.70E+07	$2s22p32P^o_{3/2}$	$2s2p4\ ^2D_{3/2}$
7.6E+08:E[a], 5.968E+08[g]	5.73E+08	$2s22p3\ ^2P^o_{3/2}$	$2s2p4\ ^2D_{5/2}$
4.0E+07:D[d], 4.569E+07[g]	4.70E+07	$2s22p2(1D)3s\ ^2D_{5/2}$	$2s22p2(1D)3p\ ^2D^o_{3/2}$:*LS*
3.7E+08:D[e], 2.990E+08[g]	3.03E+08	$2s22p2(1D)3s\ ^2D_{3/2}$	$2s22p2(1D)3p\ ^2D^o_{3/2}$:*LS*
3.8E+08:D[f], 3.217E+08[g]	3.27E+08	$2s22p2(1D)3s\ ^2D_{5/2}$	$2s22p2(1D)3p\ ^2D^o_{5/2}$:*LS*
2.7E+07:D[d], 1.739E+07[g]	1.78E+07	$2s22p2(1D)3s\ ^2D_{3/2}$	$2s22p2(1D)3p\ ^2D^o_{5/2}$:*LS*
1.3E+08:D[e], 1.107E+08[g]	1.09E+08	$2s22p2(3P)3s\ ^4P_{1/2}$	$2s22p2(3P)3p\ ^4P^o_{3/2}$:*LS*
9.5E+07:D[d], 6.95-E+07[g]	6.55E+07	$2s22p2(3P)3s\ ^4P_{3/2}$	$2s22p2(3P)3p\ ^4P^o_{5/2}$
5.2E+07:D[e], 4.003E+07[g]	3.89E+07	$2s22p2(3P)3s\ ^4P_{1/2}$	$2s22p2(3P)3p\ ^4P^o_{1/2}$
4.2E+07:D[e], 5.223E+07[g]	5.44E+07	$2s22p2(3P)3s\ ^4P_{3/2}$	$2s22p2(3P)3p\ ^4P^o_{3/2}$

Table F
Sample set of lifetimes of Ne IV levels obtained from E1 transitions.

	Level		J	Ij	E (Ry)	Lifetime (s)	#transitions
1	2*s*2*p*4	4Pe	0.5	1	−5.4539E+00	5.631E−10	4
2	2*s*2*p*4	2Se	0.5	2	−4.4076E+00	1.038E−10	4
3	2*s*2*p*4	2Pe	0.5	3	−4.2152E+00	4.491E−11	4
4	2*s*22*p*2(3*P*)3*s*	4Pe	0.5	4	−2.7757E+00	1.510E−10	4
5	2*s*22*p*2(3*P*)3*s*	2Pe	0.5	5	−2.6864E+00	5.477E−11	6
6	2*s*22*p*2(1*S*)3*s*	2Se	0.5	6	−2.1079E+00	8.532E−11	15
7	2*s*22*p*2(3*P*)3*d*	2Pe	0.5	7	−1.8832E+00	8.403E−11	18
8	2*s*22*p*2 3Pe 3*d*	4 PDe	0.5	8	−1.8770E+00	5.092E−11	18
9	2*s*22*p*2(3*P*)3*d*	4Pe	0.5	9	−1.8550E+00	1.392E−11	18
10	2*s*22*p*2(1*D*)3*d*	2Pe	0.5	10	−1.5523E+00	2.542E−11	21
11	2*s*22*p*2(1*D*)3*d*	2Se	0.5	11	−1.5176E+00	1.114E−10	21
12	2*s*2*p*3 5So 3*p*	4 Pe	0.5	12	−1.4882E+00	2.868E−11	21
13	2*s*22*p*2(3*P*)4*s*	4Pe	0.5	13	−1.3654E+00	1.761E−10	21
14	2*s*22*p*2(3*P*)4*s*	2Pe	0.5	14	−1.3409E+00	1.114E−10	21
15	2*s*22*p*2(3*P*)4*d*	4Pe	0.5	15	−1.0081E+00	3.432E−10	35
16	2*s*22*p*2 3Pe 4*d*	4 PDe	0.5	16	−1.0364E+00	6.726E−11	34
17	2*s*22*p*2 3Pe 4*d*	2 Pe	0.5	17	−1.0262E+00	3.261E−11	34
18	2*s*22*p*2(3*P*)5*s*	4Pe	0.5	18	−8.2191E−01	3.399E−10	46
19	2*s*22*p*2 1Se 4*s*	2 Se	0.5	19	−8.0350E−01	1.616E−10	46
20	2*s*22*p*2 3Pe 5*s*	2 Pe	0.5	20	−7.9475E−01	8.632E−11	46
21	2*s*22*p*2(1*P*)4*d*	2Pe	0.5	21	−7.4553E−01	6.180E−11	49
22	2*s*22*p*2 1De 4*d*	2 SPe	0.5	22	−7.4749E−01	2.454E−10	49
23	2*s*22*p*2 3Pe 5*d*	4 PDe	0.5	23	−7.2571E−01	8.225E−11	54
24	2*s*22*p*2 3Pe 5*d*	4 PDe	0.5	24	−7.1759E−01	6.708E−11	58
25	2*s*22*p*2 3Pe 5*d*	2 Pe	0.5	25	−6.6160E−01	6.117E−10	60

Comparisons with existing energies show very good agreement with the measured values for most levels. *A*-values and lifetimes show very good agreement, particularly for stronger transition, with the latest calculations by Froese-Fischer and Tachiev [13].

Table C
Comparison of calculated BPRM energies for Ne IV with observed values [14]. I_J is the calculated level index for its position in its $J\pi$ symmetry. Negative sign for energies is omitted for convenience.

Level		J: I_J	E (Ry, BPRM)	E (Ry, NIST)
$2s^22p3$	$^4S^o$	1.5:1	7.228 46E+00	7.1380E+00
$2s^22p3$	$^2D^o$	2.5:1	6.832 43E+00	6.7622E+00
$2s^22p3$	$^2D^o$	1.5:2	6.832 75E+00	6.7618E+00
$2s^22p3$	$^2P^o$	1.5:3	6.614 72E+00	6.5690E+00
$2s^22p3$	$^2P^o$	0.5:1	6.614 85E+00	6.5690E+00
$2s2p4$	$^4P^e$	2.5:1	5.518 70E+00	5.4625E+00
$2s2p4$	$^4P^e$	1.5:1	5.513 70E+00	5.4569E+00
$2s2p4$	$^4P^e$	0.5:1	5.510 75E+00	5.4539E+00
$2s2p4$	$^2D^e$	2.5:2	4.855 23E+00	4.8226E+00
$2s2p4$	$^2D^e$	1.5:2	4.855 14E+00	4.8224E+00
$2s2p4$	$^2S^e$	0.5:2	4.392 62E+00	4.4076E+00
$2s2p4$	$^2P^e$	1.5:3	4.235 01E+00	4.2216E+00
$2s2p4$	$^2P^e$	0.5:3	4.228 90E+00	4.2152E+00
$2s^22p^2(^3P)3s$	$^4P^e$	2.5:3	2.769 34E+00	2.7670E+00
$2s^22p^2(^3P)3s$	$^4P^e$	1.5:4	2.775 49E+00	2.7722E+00
$2s^22p^2(^3P)3s$	$^4P^e$	0.5:4	2.779 23E+00	2.7757E+00
$2p5$	$^2P^o$	1.5:4	2.706 14E+00	2.7192E+00
$2p5$	$^2P^o$	0.5:2	2.697 07E+00	2.7104E+00
$2s^22p^2(^3P)3s$	$^2P^e$	1.5:5	2.677 17E+00	2.6800E+00
$2s^22p^2(^3P)3s$	$^2P^e$	0.5:5	2.684 50E+00	2.6864E+00
$2s^22p^2(^1D)3s$	$^2D^e$	2.5:4	2.446 77E+00	2.4751E+00
$2s^22p^2(^1D)3s$	$^2D^e$	1.5:6	2.446 72E+00	2.4749E+00
$2s^22p^2(^3P)3p$	$^4D^o$	3.5:1	2.382 40E+00	2.3806E+00
$2s^22p^2(^3P)3p$	$^4D^o$	2.5:2	2.387 46E+00	2.3850E+00
$2s^22p^2(^3P)3p$	$^4D^o$	1.5:5	2.390 99E+00	2.3882E+00
$2s^22p^2(^3P)3p$	$^4D^o$	0.5:4	2.393 07E+00	2.3901E+00
$2s^22p^2(^3P)3p$	$^4P^o$	2.5:3	2.355 50E+00	2.3536E+00
$2s^22p^2(^3P)3p$	$^4P^o$	1.5:6	2.359 10E+00	2.3568E+00
$2s^22p^2(^3P)3p$	$^4P^o$	0.5:5	2.360 94E+00	2.3585E+00
$2s^22p^2(^3P)3p$	$^2D^o$	2.5:4	2.288 88E+00	2.2946E+00
$2s^22p^2(^3P)3p$	$^2D^o$	1.5:7	2.296 32E+00	2.3013E+00
$2s^22p^2(^3P)3p$	$^4S^o$	1.5:8	2.286 27E+00	2.2811E+00
$2s2p3(5So)3s$	$^6S^o$	2.5:5	2.050 64E+00	2.2308E+00
$2s^22p^2(1S)3s$	$^2S^e$	0.5:6	2.165 55E+00	2.1079E+00
$2s^22p^2(^1D)3p$	$^2F^o$	3.5:2	2.046 98E+00	2.0766E+00

Table G
Comparison of the present lifetimes, τ, of Ne IV in s with those in Ref. [13].

Level		Present	Ref. [13]
$2s2p^4$	$^4P^e_{1/2}$	5.631e−10	5.556e−10
$2s2p^4$	$^2S^e_{1/2}$	1.038e−11	1.023e−11
$2s2p^4$	$^2S^e_{1/2}$	4.401e−11	4.399e−11
$2p^5$	$^2P^o_{3/2}$	9.123e−11	8.724e−11
$2p^2(^1D)3s$	$^2D^e_{3/2}$	8.475e−11	8.344e−11
$2s^22p^2(^3P)3s$	$^4P^e_{3/2}$	1.508e−10	1.481e−10
$2s^22p^2(^3P)3d$	$^4F^e_{5/2}$	1.804e−09	1.823e−09

Based on the comparison with experimental energies and other theoretical work, and the high accuracy of the *ab initio* BPRM method itself, the present set of transitions is of comparable or higher accuracy than the existing limited number of published transitions referred to in the Results Section. The present set of transitions is more complete for any practical purpose, and hence is expected to provide a more complete and precise basis for astrophysical modeling.

All data files for energies and transition parameters will also be available online at the NORAD-Atomic-Data website (NaharOSURadiativeAtomicData): www.astronomy.ohio-state.edu/~nahar/nahar_radiativeatomicdata.

Acknowledgments

This work was partially supported by NSF (AST-1312441) and DOE (DE-FG52-09NA29580). The computational work was carried out using the high performance computing resources at the Ohio Supercomputer Center in Columbus, Ohio.

Appendix A. Supplementary data

Supplementary material related to this article can be found online at http://dx.doi.org/10.1016/j.adt.2014.02.001.

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Explanation of Tables

Table 1. Fine structure levels of Ne IV

The table presents a partial set of 868 energy levels of Ne IV. The levels are grouped as fine structure components of the *LS* terms. They are designated as $C_t(S_tL_t\pi_t)J_t\,nlJ\;SL\pi$.

The top line of each set provides the expected number of fine structure levels ($Nl\upsilon$) for the possible $^{(2S+1)}L^{\pi}$ terms with the given configuration. In the set, the spin multiplicity $(2S+1)$ and parity π are fixed, but L varies. Within parenthesis next to each L, all possible J-values associated with the given LS term are specified. This line is followed by the set of energy levels of same configuration. "Nlv(c)" at the end specifies the total number of calculated J-levels found for the set. If Nlv = Nlv(c), the calculated energy set for the given terms is complete. The levels are designated as $C_t(S_tL_t\pi_t)J_t\,nlJ(SL)\pi$.

C_t	Rarget configuration
$S_tL_t\pi_t$	$SL\pi$ symmetry of the target
J_t	Total angular momentum of the target state
nl	Configuration of the valence electron
J	Total angular momentum of the level
E (Ry)	Level energy in Rydbergs
υ	Effective quantum number
$SL\pi$	Symmetry of the level

Table 2. Transitions for observed levels of Ne IV.

The table presents E1 transition probabilities for observed levels of Ne IV. The transitions are grouped as fine structure components of *LS* multiplets.

$C_{i,k}$	Configurations of transition levels
T_i	*LS* term designation of the level
g_i	Statistical weight factor $(2J+1)$ of the level
I	Position index of the level in its $SL\pi$ symmetry
E_{ik}	Transition wavelength λ
f, S, A	Oscillator strength, line strength, radiative decay rate

Table 1
Fine structure levels of Ne IV.

$C_t(S_tL_t\pi_t)$		J_t	nl	$2J$	E (cal)	ν	$SL\pi$
Eqv electron/unidentified levels, parity: o							
$2s^22p3$				3	−7.22846E+00	1.49	4So
Nlv(c) = 1 : set complete							
Eqv electron/unidentified levels, parity: o							
$2s^22p3$				3	−6.83275E+00	1.53	2Do
$2s^22p3$				5	−6.83243E+00	1.53	2Do
Nlv(c) = 2 : set complete							
Eqv electron/unidentified levels, parity: o							
$2s^22p3$				1	−6.61485E+00	1.56	2Po
$2s^22p3$				3	−6.61472E+00	1.56	2Po
Nlv(c) = 2 : set complete							
Eqv electron/unidentified levels, parity: e							
$2s2p^4$				5	−5.51870E+00	1.70	4Pe
$2s2p^4$				3	−5.51370E+00	1.70	4Pe
$2s2p^4$				1	−5.51075E+00	1.70	4Pe
Nlv(c) = 3 : set complete							
Eqv electron/unidentified levels, parity: e							
$2s2p^4$				5	−4.85523E+00	1.82	2De
$2s2p^4$				3	−4.85514E+00	1.82	2De
Nlv(c) = 2 : set complete							
Eqv electron/unidentified levels, parity: e							
$2s2p^4$				1	−4.39262E+00	1.91	2Se
Nlv(c) = 1 : set complete							
Eqv electron/unidentified levels, parity: e							
$2s2p^4$				3	−4.23501E+00	1.94	2Pe
$2s2p^4$				1	−4.22890E+00	1.95	2Pe
Nlv(c) = 2 : set complete							
Nlv = 3, $^4L^e$: $P(531)/2$							
$2s^22p2$	(3Pe)	1	3s	1	−2.77923E+00	2.40	4Pe
$2s^22p2$	(3Pe)	1	3s	3	−2.77549E+00	2.40	4Pe
$2s^22p2$	(3Pe)	2	3s	5	−2.76934E+00	2.40	4Pe
Nlv(c) = 3 : set complete							
Eqv electron/unidentified levels, parity: o							
$2p5$				3	−2.70614E+00	2.43	2Po
$2p5$				1	−2.69707E+00	2.44	2Po
Nlv(c) = 2 : set complete							
Nlv = 2, $^2L^e$: $P(31)/2$							
$2s^22p2$	(3Pe)	1	3s	1	−2.68450E+00	2.44	2Pe
$2s^22p2$	(3Pe)	2	3s	3	−2.67717E+00	2.44	2Pe
Nlv(c) = 2 : set complete							
Nlv = 2, $^2L^e$: $D(53)/2$							
$2s^22p2$	(1De)	2	3s	5	−2.44677E+00	2.42	2De
$2s^22p2$	(1De)	2	3s	3	−2.44672E+00	2.42	2De
Nlv(c) = 2 : set complete							
Nlv = 5, $^2L^o$: $S(1)/2P(31)/2D(53)/2$							
$2s^22p2$	(3Pe)	2	3p	1	−2.44376E+00	2.55	2SPo
$2s^22p2$	(3Pe)	1	3p	3	−2.29632E+00	2.64	2Do
$2s^22p2$	(3Pe)	2	3p	5	−2.28888E+00	2.64	2Do
$2s^22p2$	(3Pe)	1	3p	1	−2.24005E+00	2.67	2SPo
$2s^22p2$	(3Pe)	2	3p	3	−2.23822E+00	2.67	2PDo
Nlv(c) = 5 : set complete							
Nlv = 8, $^4L^o$: $S(3)/2P(531)/2D(7531)/2$							
$2s^22p2$	(3Pe)	0	3p	1	−2.39307E+00	2.59	4Do
$2s^22p2$	(3Pe)	1	3p	3	−2.39099E+00	2.59	4Do
$2s^22p2$	(3Pe)	1	3p	5	−2.38746E+00	2.59	4Do
$2s^22p2$	(3Pe)	2	3p	7	−2.38240E+00	2.59	4Do
$2s^22p2$	(3Pe)	1	3p	1	−2.36094E+00	2.60	4Po
$2s^22p2$	(3Pe)	2	3p	3	−2.35910E+00	2.60	4Po
$2s^22p2$	(3Pe)	2	3p	5	−2.35550E+00	2.60	4Po
$2s^22p2$	(3Pe)	2	3p	3	−2.28627E+00	2.64	4So
Nlv(c) = 8 : set complete							
Nlv = 1, $^2L^e$: $S(1)/2$							
$2s^22p2$	(1Se)	0	3s	1	−2.16555E+00	2.41	2Se
Nlv(c) = 1 : set complete							
Nlv = 1, $^6L^o$: $S(5)/2$							
$2s2p3$	(5So)	2	3s	5	−2.05064E+00	2.37	6So
Nlv(c) = 1 : set complete							
Nlv = 6, $^2L^o$: $P(31)/2D(53)/2F(75)/2$							
$2s^22p2$	(1De)	2	3p	5	−2.04827E+00	2.62	2Fo
$2s^22p2$	(1De)	2	3p	7	−2.04698E+00	2.62	2Fo
$2s^22p2$	(1De)	2	3p	5	−1.99568E+00	2.65	2Do

(*continued on next page*)

Table 1 (*continued*)

$C_t(S_tL_t\pi_t)$		J_t	nl	$2J$	E (cal)	ν	$SL\pi$
2s22p2	(1De)	2	3p	3	−1.99469E+00	2.65	2Do
2s22p2	(1De)	2	3p	1	−1.94054E+00	2.69	2Po
2s22p2	(1De)	2	3p	3	−1.93776E+00	2.69	2PDo
Nlv(c) = 6 : set complete							
Nlv = 11, $^4L^e$: P(531)/2D(7531)/2F(9753)/2							
2s22p2	(3Pe)	0	3d	3	−1.92107E+00	2.89	4PDFe
2s22p2	(3Pe)	1	3d	5	−1.91904E+00	2.89	4PDFe
2s22p2	(3Pe)	1	3d	7	−1.91608E+00	2.89	4DFe
2s22p2	(3Pe)	2	3d	9	−1.91206E+00	2.89	4Fe
2s22p2	(3Pe)	2	3d	5	−1.87963E+00	2.92	4De
2s22p2	(3Pe)	2	3d	3	−1.87949E+00	2.92	4De
2s22p2	(3Pe)	2	3d	7	−1.87754E+00	2.91	4DFe
2s22p2	(3Pe)	2	3d	1	−1.87704E+00	2.91	4PDe
2s22p2	(3Pe)	2	3d	5	−1.85891E+00	2.93	4Pe
2s22p2	(3Pe)	1	3d	3	−1.85619E+00	2.93	4Pe
2s22p2	(3Pe)	2	3d	1	−1.85478E+00	2.93	4Pe
Nlv(c) = 11 : set complete							
Nlv = 6, $^2L^e$: P(31)/2D(53)/2F(75)/2							
2s22p2	(3Pe)	1	3d	3	−1.88528E+00	2.91	2Pe
2s22p2	(3Pe)	1	3d	1	−1.88309E+00	2.91	2Pe
2s22p2	(3Pe)	1	3d	5	−1.85467E+00	2.93	2Fe
2s22p2	(3Pe)	2	3d	7	−1.84757E+00	2.94	2Fe
2s22p2	(3Pe)	1	3d	3	−1.78678E+00	2.99	2De
2s22p2	(3Pe)	2	3d	5	−1.78445E+00	2.99	2De
Nlv(c) = 6 : set complete							
Nlv = 1, $^4L^o$: S(3)/2							
2s2p3	(5So)	2	3s	3	−1.84258E+00	2.46	4So
Nlv(c) = 1 : set complete							
Nlv = 2, $^2L^o$: P(31)/2							
2s22p2	(1Se)	0	3p	3	−1.74709E+00	2.62	2Po
2s22p2	(1Se)	0	3p	1	−1.74694E+00	2.62	2Po
Nlv(c) = 2 : set complete							
Nlv = 3, $^6L^e$: P(753)/2							
2s2p3	(5So)	2	3p	3	−1.64728E+00	2.55	6Pe
2s2p3	(5So)	2	3p	5	−1.64677E+00	2.55	6Pe
2s2p3	(5So)	2	3p	7	−1.64606E+00	2.56	6Pe
Nlv(c) = 3 : set complete							
Nlv = 9, $^2L^e$: S(1)/2P(31)/2D(53)/2F(75)/2G(97)/2							
2s22p2	(1De)	2	3d	7	−1.59511E+00	2.92	2Fe
2s22p2	(1De)	2	3d	5	−1.59400E+00	2.93	2Fe
2s22p2	(1De)	2	3d	7	−1.58021E+00	2.94	2Fe
2s22p2	(1De)	2	3d	9	−1.58019E+00	2.94	2Ge
2s22p2	(1De)	2	3d	3	−1.55810E+00	2.95	2De
2s22p2	(1De)	2	3d	5	−1.55756E+00	2.95	2De
2s22p2	(1De)	2	3d	1	−1.52414E+00	2.98	2Pe
2s22p2	(1De)	2	3d	3	−1.52297E+00	2.98	2Pe
2s22p2	(1De)	2	3d	1	−1.50756E+00	2.63	2Se
Nlv(c) = 9 : set complete							
Nlv = 3, $^4L^e$: P(531)/2							
2s2p3	(5So)	2	3p	5	−1.50808E+00	2.63	4Pe
2s2p3	(5So)	2	3p	3	−1.50775E+00	2.63	4Pe
2s2p3	(5So)	2	3p	1	−1.48824E+00	3.01	4Pe
Nlv(c) = 3 : set complete							
Nlv = 3, $^4L^e$: P(531)/2							
2s22p2	(3Pe)	0	4s	1	−1.36968E+00	3.42	4Pe
2s22p2	(3Pe)	1	4s	3	−1.36630E+00	3.42	4Pe
2s22p2	(3Pe)	2	4s	5	−1.36060E+00	3.42	4Pe
Nlv(c) = 3 : set complete							
Nlv = 2, $^2L^e$: P(31)/2							
2s22p2	(3Pe)	1	4s	1	−1.33908E+00	3.45	2Pe
2s22p2	(3Pe)	2	4s	3	−1.33245E+00	3.45	2Pe
Nlv(c) = 2 : set complete							
Nlv = 2, $^2L^e$: D(53)/2							
2s22p2	(1Se)	0	3d	5	−1.29416E+00	2.80	2De
2s22p2	(1Se)	0	3d	3	−1.29355E+00	2.81	2De
Nlv(c) = 2 : set complete							
Nlv = 8, $^4L^o$: S(3)/2P(531)/2D(7531)/2							
2s22p2	(3Pe)	0	4p	1	−1.23960E+00	3.59	4Do
2s22p2	(3Pe)	1	4p	1	−1.23867E+00	3.59	4Po
2s22p2	(3Pe)	1	4p	3	−1.23726E+00	3.59	4Do
2s22p2	(3Pe)	1	4p	5	−1.23447E+00	3.60	4Do
2s22p2	(3Pe)	2	4p	7	−1.23022E+00	3.59	4Do

(*continued on next page*)

Table 1 (*continued*)

$C_t(S_tL_t\pi_t)$		J_t	nl	$2J$	E (cal)	ν	$SL\pi$
2*s*22*p*2	(3Pe)	1	4*p*	3	−1.21470E+00	3.62	4Po
2*s*22*p*2	(3Pe)	2	4*p*	5	−1.21122E+00	3.62	4Po
2*s*22*p*2	(3Pe)	1	4*p*	3	−1.17915E+00	3.68	4So
Nlv(c) = 8 : set complete							
Nlv = 5, $^2L^o$: *S*(1)/2*P*(31)/2*D*(53)/2							
2*s*22*p*2	(3Pe)	1	4*p*	1	−1.21612E+00	3.62	2SPo
2*s*22*p*2	(3Pe)	2	4*p*	5	−1.17237E+00	3.68	2Do
2*s*22*p*2	(3Pe)	2	4*p*	3	−1.16606E+00	3.69	2PDo
2*s*22*p*2	(3Pe)	1	4*p*	1	−1.15358E+00	3.72	2SPo
2*s*22*p*2	(3Pe)	2	4*p*	3	−1.15053E+00	3.71	2PDo
Nlv(c) = 5 : set complete							

Table 2
Transitions for observed levels of Ne IV.

$C_i - C_k$	$T_i - T_k$	g_i:I–g_j:K	E_{ik} (Å)	f	S	A (s^{-1})
2*s*22*p*3–2*s*2*p*4	2Po–4Pe	2: 1–2: 1	817.21	1.24E−06	6.66E−06	1.24E+04
2*s*22*p*3–2*s*2*p*4	2Po–4Pe	4: 3–2: 1	817.21	3.70E−08	3.98E−07	7.38E+02
2*s*22*p*3–2*s*2*p*4	2Po–4Pe	2: 1–4: 1	819.41	4.64E−08	2.50E−07	2.30E+02
2*s*22*p*3–2*s*2*p*4	2Po–4Pe	4: 3–4: 1	819.41	3.26E−06	3.51E−05	3.24E+04
2*s*22*p*3–2*s*2*p*4	2Po–4Pe	4: 3–6: 1	823.56	3.05E−06	3.30E−05	2.00E+04
2*s*2*p*4–2*p*5	4Pe–2Po	2: 1–2: 2	332.15	2.60E−06	5.68E−06	1.57E+05
2*s*2*p*4–2*p*5	4Pe–2Po	2: 1–4: 4	333.22	9.54E−07	2.09E−06	2.86E+04
2*s*2*p*4–2*p*5	4Pe–2Po	4: 1–2: 2	331.79	3.18E−07	1.39E−06	3.85E+04
2*s*2*p*4–2*p*5	4Pe–2Po	4: 1–4: 4	332.86	2.53E−06	1.11E−05	1.52E+05
2*s*2*p*4–2*p*5	4Pe–2Po	6: 1–4: 4	332.18	7.98E−06	5.23E−05	7.23E+05
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	4Pe–4Do	2: 1–2: 4	297.43	2.37E−04	4.64E−04	1.79E+07
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	4Pe–4Do	2: 1–4: 5	297.25	3.52E−04	6.89E−04	1.33E+07
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	4Pe–4Do	4: 1–2: 4	297.14	6.96E−06	2.72E−05	1.05E+06
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	4Pe–4Do	4: 1–4: 5	296.96	9.29E−05	3.63E−04	7.02E+06
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	4Pe–4Do	4: 1–6: 2	296.65	3.94E−04	1.54E−03	1.99E+07
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	4Pe–4Do	6: 1–4: 5	296.41	4.30E−08	2.52E−07	4.89E+03
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	4Pe–4Do	6: 1–6: 2	296.11	1.28E−05	7.49E−05	9.75E+05
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	4Pe–4Do	6: 1–8: 1	295.68	3.22E−04	1.88E−03	1.84E+07
LS	4Pe–4Do	12–20		4.30E−04	5.04E−03	1.96E+07
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	4Pe–4Po	2: 1–2: 5	294.39	9.25E−04	1.79E−03	7.12E+07
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	4Pe–4Po	2: 1–4: 6	294.23	4.16E−03	8.07E−03	1.60E+08
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	4Pe–4Po	4: 1–2: 5	294.11	2.42E−03	9.37E−03	3.73E+08
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	4Pe–4Po	4: 1–4: 6	293.95	6.22E−04	2.41E−03	4.80E+07
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	4Pe–4Po	4: 1–6: 3	293.64	2.45E−03	9.46E−03	1.26E+08
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	4Pe–4Po	6: 1–4: 6	293.42	2.05E−03	1.19E−02	2.38E+08
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	4Pe–4Po	6: 1–6: 3	293.12	4.11E−03	2.38E−02	3.19E+08
LS	4Pe–4Po	12–12		5.76E−03	6.68E−02	4.45E+08
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	4Pe–4Do	2: 1–2: 9	218.77	6.66E−04	9.59E−04	9.28E+07
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	4Pe–4Do	2: 1–4: 14	218.63	4.41E−03	6.35E−03	3.08E+08
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	4Pe–4Do	4: 1–2: 9	218.61	1.70E−04	4.91E−04	4.76E+07
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	4Pe–4Do	4: 1–4: 14	218.48	3.57E−03	1.03E−02	4.99E+08
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	4Pe–4Do	4: 1–6: 8	218.34	6.09E−03	1.75E−02	5.68E+08
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	4Pe–4Do	6: 1–4: 14	218.18	3.11E−04	1.34E−03	6.54E+07
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	4Pe–4Do	6: 1–6: 8	218.05	2.48E−03	1.07E−02	3.48E+08
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	4Pe–4Do	6: 1–8: 3	217.83	9.40E−03	4.04E−02	9.91E+08
LS	4Pe–4Do	12–20		1.02E−02	8.80E−02	8.60E+08
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	4Pe–4Po	2: 1–2: 10	218.13	4.25E−03	6.11E−03	5.96E+08
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	4Pe–4Po	2: 1–4: 15	217.93	2.67E−03	3.84E−03	1.88E+08
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	4Pe–4Po	4: 1–2: 10	217.98	4.51E−04	1.30E−03	1.27E+08
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	4Pe–4Po	4: 1–4: 15	217.77	1.21E−04	3.46E−04	1.70E+07
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	4Pe–4Po	4: 1–6: 9	217.63	1.81E−03	5.20E−03	1.70E+08
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	4Pe–4Po	6: 1–4: 15	217.48	5.79E−04	2.49E−03	1.22E+08
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	4Pe–4Po	6: 1–6: 9	217.34	1.17E−03	5.02E−03	1.65E+08
LS	4Pe–4Po	12–12		2.82E−03	2.43E−02	3.96E+08
2*s*2*p*4–2*s*2*p*3(5So)3*d*	4Pe–4Do	2: 1–2: 15	204.92	1.49E−01	2.01E−01	2.36E+10
2*s*2*p*4–2*s*2*p*3(5So)3*d*	4Pe–4Do	2: 1–4: 21	204.92	1.49E−01	2.01E−01	1.18E+10
2*s*2*p*4–2*s*2*p*3(5So)3*d*	4Pe–4Do	4: 1–2: 15	204.78	1.49E−02	4.02E−02	4.75E+09
2*s*2*p*4–2*s*2*p*3(5So)3*d*	4Pe–4Do	4: 1–4: 21	204.78	9.54E−02	2.57E−01	1.52E+10
2*s*2*p*4–2*s*2*p*3(5So)3*d*	4Pe–4Do	4: 1–6: 13	204.78	1.88E−01	5.06E−01	1.99E+10
2*s*2*p*4–2*s*2*p*3(5So)3*d*	4Pe–4Do	6: 1–4: 21	204.53	6.00E−03	2.42E−02	1.43E+09
2*s*2*p*4–2*s*2*p*3(5So)3*d*	4Pe–4Do	6: 1–6: 13	204.53	5.39E−02	2.18E−01	8.60E+09
2*s*2*p*4–2*s*2*p*3(5So)3*d*	4Pe–4Do	6: 1–8: 6	204.53	2.39E−01	9.67E−01	2.86E+10
LS	4Pe–4Do	12–20		2.99E−01	2.41E+00	2.85E+10
2*s*22*p*3–2*s*2*p*4	2Po–2Se	2: 1–2: 2	421.61	8.98E−02	2.49E−01	3.37E+09
2*s*22*p*3–2*s*2*p*4	2Po–2Se	4: 3–2: 2	421.61	8.29E−02	4.60E−01	6.22E+09
LS	2Po–2Se	6–2		8.52E−02	7.09E−01	9.61E+09
2*s*2*p*4–2*p*5	2Se–2Po	2: 2–2: 2	536.92	8.32E−03	2.94E−02	1.92E+08
2*s*2*p*4–2*p*5	2Se–2Po	2: 2–4: 4	539.72	2.43E−02	8.65E−02	2.79E+08
LS	2Se–2Po	2–6		3.26E−02	1.16E−01	2.49E+08
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	2Se–4Do	2: 2–2: 4	451.68	4.01E−07	1.19E−06	1.31E+04
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	2Se–4Do	2: 2–4: 5	451.26	3.42E−07	1.02E−06	5.61E+03
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	2Se–4Po	2: 2–2: 5	444.72	1.66E−07	4.86E−07	5.60E+03
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	2Se–4Po	2: 2–4: 6	444.35	1.04E−06	3.03E−06	1.75E+04
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	2Se–4Do	2: 2–2: 9	292.16	1.64E−06	3.15E−06	1.28E+05
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	2Se–4Do	2: 2–4: 14	291.91	4.19E−07	8.05E−07	1.64E+04
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	2Se–4Po	2: 2–2: 10	291.02	4.75E−09	9.11E−09	3.74E+02
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	2Se–4Po	2: 2–4: 15	290.66	5.66E−08	1.08E−07	2.23E+03
2*s*2*p*4–2*s*2*p*3(5So)3*d*	2Se–4Do	2: 2–2: 15	267.97	1.71E−07	3.02E−07	1.59E+04
2*s*2*p*4–2*s*2*p*3(5So)3*d*	2Se–4Do	2: 2–4: 21	267.97	1.78E−07	3.14E−07	8.27E+03
2*s*22*p*3–2*s*2*p*4	2Po–2Pe	2: 1–2: 3	387.15	5.84E−02	1.49E−01	2.60E+09

(*continued on next page*)

Table 2 (*continued*)

$C_i - C_k$	$T_i - T_k$	g_i:I–g_j:K	E_{ik} (Å)	f	S	A (s^{-1})
2*s*22*p*3–2*s*2*p*4	2Po–2Pe	4: 3–2: 3	387.15	2.19E−02	1.12E−01	1.95E+09
2*s*22*p*3–2*s*2*p*4	2Po–2Pe	2: 1–4: 3	388.20	3.21E−02	8.20E−02	7.10E+08
2*s*22*p*3–2*s*2*p*4	2Po–2Pe	4: 3–4: 3	388.20	7.53E−02	3.85E−01	3.33E+09
LS	2Po–2Pe	6–6		9.50E−02	7.28E−01	4.21E+09
2*s*2*p*4–2*p*5	2Pe–2Po	2: 3–2: 2	605.57	1.48E−01	5.90E−01	2.69E+09
2*s*2*p*4–2*p*5	2Pe–2Po	2: 3–4: 4	609.14	7.00E−02	2.81E−01	6.30E+08
2*s*2*p*4–2*p*5	2Pe–2Po	4: 3–2: 2	603.01	3.73E−02	2.96E−01	1.37E+09
2*s*2*p*4–2*p*5	2Pe–2Po	4: 3–4: 4	606.54	1.81E−01	1.45E+00	3.29E+09
LS	2Pe–2Po	6–6		2.18E−01	2.62E+00	3.95E+09
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	2Pe–4Do	2: 3–2: 4	499.30	3.80E−06	1.25E−05	1.02E+05
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	2Pe–4Do	2: 3–4: 5	498.78	1.77E−07	5.82E−07	2.38E+03
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	2Pe–4Do	4: 3–2: 4	497.55	6.96E−07	4.56E−06	3.75E+04
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	2Pe–4Do	4: 3–4: 5	497.04	2.40E−06	1.57E−05	6.47E+04
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	2Pe–4Do	4: 3–6: 2	496.17	3.35E−07	2.19E−06	6.05E+03
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	2Pe–4Po	2: 3–2: 5	490.80	9.83E−09	3.18E−08	2.72E+02
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	2Pe–4Po	2: 3–4: 6	490.35	4.21E−06	1.36E−05	5.84E+04
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	2Pe–4Po	4: 3–2: 5	489.11	1.09E−06	7.04E−06	6.09E+04
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	2Pe–4Po	4: 3–4: 6	488.67	4.95E−07	3.19E−06	1.38E+04
2*s*2*p*4–2*s*22*p*2(3*P*)3*p*	2Pe–4Po	4: 3–6: 3	487.83	8.60E−06	5.52E−05	1.61E+05
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	2Pe–4Do	2: 3–2: 9	311.36	2.69E−04	5.52E−04	1.85E+07
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	2Pe–4Do	2: 3–4: 14	311.09	5.10E−07	1.04E−06	1.76E+04
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	2Pe–4Do	4: 3–2: 9	310.68	3.55E−04	1.45E−03	4.91E+07
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	2Pe–4Do	4: 3–4: 14	310.41	1.24E−07	5.07E−07	8.58E+03
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	2Pe–4Do	4: 3–6: 8	310.13	2.47E−07	1.01E−06	1.14E+04
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	2Pe–4Po	2: 3–2: 10	310.07	6.58E−05	1.34E−04	4.56E+06
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	2Pe–4Po	2: 3–4: 15	309.66	6.59E−07	1.34E−06	2.29E+04
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	2Pe–4Po	4: 3–2: 10	309.40	6.21E−05	2.53E−04	8.65E+06
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	2Pe–4Po	4: 3–4: 15	308.99	1.01E−06	4.12E−06	7.08E+04
2*s*2*p*4–2*s*22*p*2(3*P*)4*p*	2Pe–4Po	4: 3–6: 9	308.69	1.42E−07	5.79E−07	6.64E+03
2*s*2*p*4–2*s*2*p*3(5So)3*d*	2Pe–4Do	2: 3–2: 15	284.04	2.16E−07	4.04E−07	1.79E+04
2*s*2*p*4–2*s*2*p*3(5So)3*d*	2Pe–4Do	2: 3–4: 21	284.04	2.05E−08	3.84E−08	8.48E+02
2*s*2*p*4–2*s*2*p*3(5So)3*d*	2Pe–4Do	4: 3–2: 15	283.48	5.28E−08	1.97E−07	8.76E+03
2*s*2*p*4–2*s*2*p*3(5So)3*d*	2Pe–4Do	4: 3–4: 21	283.48	2.27E−07	8.47E−07	1.88E+04
2*s*2*p*4–2*s*2*p*3(5So)3*d*	2Pe–4Do	4: 3–6: 13	283.48	1.80E−07	6.72E−07	9.96E+03
2*s*22*p*3–2*s*22*p*2(3*P*)3*s*	2Po–4Pe	2: 1–2: 4	240.23	3.83E−06	6.06E−06	4.43E+05
2*s*22*p*3–2*s*22*p*2(3*P*)3*s*	2Po–4Pe	4: 3–2: 4	240.23	7.43E−06	2.35E−05	1.72E+06
2*s*22*p*3–2*s*22*p*2(3*P*)3*s*	2Po–4Pe	2: 1–4: 4	240.01	9.68E−06	1.53E−05	5.60E+05
2*s*22*p*3–2*s*22*p*2(3*P*)3*s*	2Po–4Pe	4: 3–4: 4	240.01	2.59E−05	8.20E−05	3.00E+06
2*s*22*p*3–2*s*22*p*2(3*P*)3*s*	2Po–4Pe	4: 3–6: 3	239.68	6.87E−08	2.17E−07	5.31E+03
2*s*22*p*2(3*P*)3*s*–2*p*5	4Pe–2Po	2: 4–2: 2	13955.09	3.33E−09	3.06E−07	1.14E−01
2*s*22*p*2(3*P*)3*s*–2*p*5	4Pe–2Po	2: 4–4: 4	16128.57	1.47E−09	1.56E−07	1.88E−02
2*s*22*p*2(3*P*)3*s*–2*p*5	4Pe–2Po	4: 4–2: 2	14745.42	5.56E−10	1.08E−07	3.41E−02
2*s*22*p*2(3*P*)3*s*–2*p*5	4Pe–2Po	4: 4–4: 4	17193.65	5.07E−10	1.15E−07	1.14E−02
2*s*22*p*2(3*P*)3*s*–2*p*5	4Pe–2Po	6: 3–4: 4	19064.14	6.87E−10	2.59E−07	1.89E−02
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	4Pe–4Do	2: 4–2: 4	2363.24	1.68E−01	2.61E+00	2.00E+08
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	4Pe–4Do	2: 4–4: 5	2351.66	1.85E−01	2.87E+00	1.12E+08
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	4Pe–4Do	4: 4–2: 4	2384.89	1.35E−02	4.25E−01	3.17E+07
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	4Pe–4Do	4: 4–4: 5	2373.09	9.58E−02	2.99E+00	1.13E+08
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	4Pe–4Do	4: 4–6: 2	2353.48	2.25E−01	6.97E+00	1.81E+08
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	4Pe–4Do	6: 3–4: 5	2405.67	4.13E−03	1.96E−01	7.14E+06
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	4Pe–4Do	6: 3–6: 2	2385.52	4.50E−02	2.12E+00	5.27E+07
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	4Pe–4Do	6: 3–8: 1	2358.35	2.60E−01	1.21E+01	2.34E+08
LS	4Pe–4Do	12–20		3.25E−01	3.03E+01	2.33E+08
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	4Pe–4Po	2: 4–2: 5	2184.24	2.78E−02	4.00E−01	3.89E+07
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	4Pe–4Po	2: 4–4: 6	2175.38	1.54E−01	2.21E+00	1.09E+08
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	4Pe–4Po	4: 4–2: 5	2202.72	8.56E−02	2.48E+00	2.35E+08
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	4Pe–4Po	4: 4–4: 6	2193.71	3.93E−02	1.13E+00	5.44E+07
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	4Pe–4Po	4: 4–6: 3	2176.94	6.98E−02	2.00E+00	6.55E+07
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	4Pe–4Po	6: 3–4: 6	2221.52	5.58E−02	2.45E+00	1.13E+08
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	4Pe–4Po	6: 3–6: 3	2204.32	1.53E−01	6.68E+00	2.11E+08
LS	4Pe–4Po	12–12		2.00E−01	1.74E+01	2.75E+08
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	4Pe–4Do	2: 4–2: 9	612.74	1.21E−02	4.89E−02	2.15E+08
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	4Pe–4Do	2: 4–4: 14	611.67	6.86E−02	2.76E−01	6.11E+08
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	4Pe–4Do	4: 4–2: 9	614.19	8.28E−05	6.70E−04	2.93E+06
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	4Pe–4Do	4: 4–4: 14	613.11	3.36E−02	2.71E−01	5.97E+08
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	4Pe–4Do	4: 4–6: 8	612.04	8.30E−02	6.69E−01	9.85E+08
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	4Pe–4Do	6: 3–4: 14	615.26	1.27E−03	1.54E−02	3.35E+07
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	4Pe–4Do	6: 3–6: 8	614.19	1.51E−02	1.83E−01	2.67E+08
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	4Pe–4Do	6: 3–8: 3	612.45	9.59E−02	1.16E+00	1.28E+09
LS	4Pe–4Do	12–20		1.08E−01	2.62E+00	1.16E+09
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	4Pe–4Po	2: 4–2: 10	607.75	4.91E−02	1.96E−01	8.86E+08

(*continued on next page*)

Table 2 (*continued*)

$C_i - C_k$	$T_i - T_k$	g_i:I–g_j:K	E_{ik} (Å)	f	S	A (s^{-1})
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	4Pe–4Po	2: 4–4: 15	606.18	2.61E−02	1.04E−01	2.37E+08
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	4Pe–4Po	4: 4–2: 10	609.18	4.97E−03	3.99E−02	1.79E+08
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	4Pe–4Po	4: 4–4: 15	607.59	9.83E−03	7.87E−02	1.78E+08
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	4Pe–4Po	4: 4–6: 9	606.46	1.03E−02	8.25E−02	1.25E+08
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	4Pe–4Po	6: 3–4: 15	609.71	1.24E−02	1.50E−01	3.35E+08
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	4Pe–4Po	6: 3–6: 9	608.57	3.49E−02	4.20E−01	6.29E+08
LS	4Pe–4Po	12–12		4.46E−02	1.07E+00	8.02E+08
2*s*22*p*2(3*P*)3*s*–2*s*2*p*3(5So)3*d*	4Pe–4Do	2: 4–2: 15	515.22	1.08E−03	3.65E−03	2.70E+07
2*s*22*p*2(3*P*)3*s*–2*s*2*p*3(5So)3*d*	4Pe–4Do	2: 4–4: 21	515.22	1.07E−03	3.63E−03	1.35E+07
2*s*22*p*2(3*P*)3*s*–2*s*2*p*3(5So)3*d*	4Pe–4Do	4: 4–2: 15	516.24	1.07E−04	7.30E−04	5.38E+06
2*s*22*p*2(3*P*)3*s*–2*s*2*p*3(5So)3*d*	4Pe–4Do	4: 4–4: 21	516.24	6.86E−04	4.66E−03	1.72E+07
2*s*22*p*2(3*P*)3*s*–2*s*2*p*3(5So)3*d*	4Pe–4Do	4: 4–6: 13	516.24	1.34E−03	9.12E−03	2.24E+07
2*s*22*p*2(3*P*)3*s*–2*s*2*p*3(5So)3*d*	4Pe–4Do	6: 3–4: 21	517.77	4.29E−05	4.38E−04	1.60E+06
2*s*22*p*2(3*P*)3*s*–2*s*2*p*3(5So)3*d*	4Pe–4Do	6: 3–6: 13	517.77	3.84E−04	3.93E−03	9.56E+06
2*s*22*p*2(3*P*)3*s*–2*s*2*p*3(5So)3*d*	4Pe–4Do	6: 3–8: 6	517.77	1.69E−03	1.73E−02	3.16E+07
LS	4Pe–4Do	12–20		2.13E−03	4.35E−02	3.19E+07
2*s*22*p*3–2*s*22*p*2(3*P*)3*s*	2Po–2Pe	2: 1–2: 5	234.71	4.74E−02	7.33E−02	5.74E+09
2*s*22*p*3–2*s*22*p*2(3*P*)3*s*	2Po–2Pe	4: 3–2: 5	234.71	1.11E−02	3.42E−02	2.68E+09
2*s*22*p*3–2*s*22*p*2(3*P*)3*s*	2Po–2Pe	2: 1–4: 5	234.32	2.53E−02	3.91E−02	1.54E+09
2*s*22*p*3–2*s*22*p*2(3*P*)3*s*	2Po–2Pe	4: 3–4: 5	234.32	6.06E−02	1.87E−01	7.37E+09
LS	2Po–2Pe	6–6		7.20E−02	3.34E−01	8.74E+09
2*p*5–2*s*22*p*2(3*P*)3*s*	2Po–2Pe	2: 2–2: 5	37969.20	2.83E−07	7.07E−05	1.31E+00
2*p*5–2*s*22*p*2(3*P*)3*s*	2Po–2Pe	4: 4–2: 5	27782.57	9.26E−08	3.39E−05	1.60E+00
2*p*5–2*s*22*p*2(3*P*)3*s*	2Po–2Pe	2: 2–4: 5	29975.85	1.38E−07	2.73E−05	5.13E−01
2*p*5–2*s*22*p*2(3*P*)3*s*	2Po–2Pe	4: 4–4: 5	23246.71	5.30E−07	1.62E−04	6.54E+00
LS	2Po–2Pe	6–6		5.55E−07	2.94E−04	5.16E+00
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	2Pe–4Do	2: 5–2: 4	3075.49	2.62E−06	5.31E−05	1.85E+03
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	2Pe–4Do	2: 5–4: 5	3055.89	3.08E−05	6.19E−04	1.10E+04
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	2Pe–4Do	4: 5–2: 4	3143.38	3.05E−06	1.26E−04	4.12E+03
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	2Pe–4Do	4: 5–4: 5	3122.92	1.07E−06	4.39E−05	7.31E+02
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	2Pe–4Do	4: 5–6: 2	3089.04	3.22E−05	1.31E−03	1.50E+04
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	2Pe–4Po	2: 5–2: 5	2779.10	2.21E−04	4.04E−03	1.91E+05
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	2Pe–4Po	2: 5–4: 6	2764.77	4.09E−05	7.45E−04	1.79E+04
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	2Pe–4Po	4: 5–2: 5	2834.42	2.29E−04	8.54E−03	3.80E+05
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	2Pe–4Po	4: 5–4: 6	2819.51	1.80E−05	6.69E−04	1.51E+04
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)3*p*	2Pe–4Po	4: 5–6: 3	2791.87	2.55E−04	9.39E−03	1.46E+05
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	2Pe–4Do	2: 5–2: 9	651.88	2.35E−02	1.01E−01	3.68E+08
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	2Pe–4Do	2: 5–4: 14	650.67	1.32E−05	5.67E−05	1.04E+05
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	2Pe–4Do	4: 5–2: 9	654.88	2.14E−02	1.84E−01	6.65E+08
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	2Pe–4Do	4: 5–4: 14	653.66	1.02E−06	8.78E−06	1.59E+04
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	2Pe–4Do	4: 5–6: 8	652.44	1.66E−05	1.43E−04	1.74E+05
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	2Pe–4Po	2: 5–2: 10	646.24	4.67E−03	1.99E−02	7.46E+07
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	2Pe–4Po	2: 5–4: 15	644.46	1.49E−05	6.30E−05	1.19E+05
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	2Pe–4Po	4: 5–2: 10	649.19	4.18E−03	3.58E−02	1.32E+08
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	2Pe–4Po	4: 5–4: 15	647.39	3.66E−06	3.12E−05	5.82E+04
2*s*22*p*2(3*P*)3*s*–2*s*22*p*2(3*P*)4*p*	2Pe–4Po	4: 5–6: 9	646.11	6.87E−05	5.84E−04	7.32E+05
2*s*22*p*2(3*P*)3*s*–2*s*2*p*3(5So)3*d*	2Pe–4Do	2: 5–2: 15	542.61	4.31E−07	1.54E−06	9.77E+03
2*s*22*p*2(3*P*)3*s*–2*s*2*p*3(5So)3*d*	2Pe–4Do	2: 5–4: 21	542.61	2.27E−06	8.11E−06	2.57E+04
2*s*22*p*2(3*P*)3*s*–2*s*2*p*3(5So)3*d*	2Pe–4Do	4: 5–2: 15	544.69	9.05E−08	6.49E−07	4.07E+03
2*s*22*p*2(3*P*)3*s*–2*s*2*p*3(5So)3*d*	2Pe–4Do	4: 5–4: 21	544.69	1.04E−06	7.48E−06	2.34E+04
2*s*22*p*2(3*P*)3*s*–2*s*2*p*3(5So)3*d*	2Pe–4Do	4: 5–6: 13	544.69	4.15E−06	2.98E−05	6.23E+04
2*s*22*p*3–2*s*22*p*2(1*S*)3*s*	2Po–2Se	2: 1–2: 6	204.27	2.52E−02	3.38E−02	4.02E+09
2*s*22*p*3–2*s*22*p*2(1*S*)3*s*	2Po–2Se	4: 3–2: 6	204.27	2.41E−02	6.47E−02	7.69E+09
LS	2Po–2Se	6–2		2.45E−02	9.85E−02	1.18E+10
2*p*5–2*s*22*p*2(1*S*)3*s*	2Po–2Se	2: 2–2: 6	1512.48	9.46E−06	9.42E−05	2.76E+04
2*p*5–2*s*22*p*2(1*S*)3*s*	2Po–2Se	4: 4–2: 6	1490.70	1.06E−05	2.09E−04	6.38E+04
LS	2Po–2Se	6–2		1.02E−05	3.03E−04	9.07E+04
2*s*22*p*2(3*P*)3*p*–2*s*22*p*2(1*S*)3*s*	4Do–2Se	2: 4–2: 6	3229.15	1.43E−06	3.03E−05	9.13E+02
2*s*22*p*2(3*P*)3*p*–2*s*22*p*2(1*S*)3*s*	4Do–2Se	4: 5–2: 6	3251.04	6.67E−07	2.85E−05	8.42E+02
2*s*22*p*2(3*P*)3*p*–2*s*22*p*2(1*S*)3*s*	4Po–2Se	2: 5–2: 6	3636.34	1.13E−07	2.71E−06	5.70E+01
2*s*22*p*2(3*P*)3*p*–2*s*22*p*2(1*S*)3*s*	4Po–2Se	4: 6–2: 6	3661.18	1.99E−07	9.60E−06	1.98E+02
2*s*22*p*2(1*S*)3*s*–2*s*22*p*2(3*P*)4*p*	2Se–4Do	2: 6–2: 9	1112.12	9.59E−06	7.02E−05	5.17E+04
2*s*22*p*2(1*S*)3*s*–2*s*22*p*2(3*P*)4*p*	2Se–4Do	2: 6–4: 14	1108.60	2.52E−06	1.84E−05	6.83E+03
2*s*22*p*2(1*S*)3*s*–2*s*22*p*2(3*P*)4*p*	2Se–4Po	2: 6–2: 10	1095.80	4.18E−07	3.01E−06	2.32E+03
2*s*22*p*2(1*S*)3*s*–2*s*22*p*2(3*P*)4*p*	2Se–4Po	2: 6–4: 15	1090.68	3.82E−06	2.74E−05	1.07E+04
2*s*22*p*2(1*S*)3*s*–2*s*2*p*3(5So)3*d*	2Se–4Do	2: 6–2: 15	827.75	1.64E−08	8.93E−08	1.60E+02
2*s*22*p*2(1*S*)3*s*–2*s*2*p*3(5So)3*d*	2Se–4Do	2: 6–4: 21	827.75	1.39E−08	7.58E−08	6.77E+01
2*s*22*p*3–2*s*22*p*2(3*P*)3*d*	2Po–2Pe	2: 1–2: 7	194.47	3.34E−02	4.27E−02	5.89E+09
2*s*22*p*3–2*s*22*p*2(3*P*)3*d*	2Po–2Pe	4: 3–2: 7	194.47	8.49E−03	2.18E−02	3.00E+09

(*continued on next page*)

Table 2 (*continued*)

$C_i - C_k$	$T_i - T_k$	g_i:I–g_j:K	E_{ik} (Å)	f	S	A (s^{-1})
2*s*22*p*3–2*s*22*p*2(3*P*)3*d*	2Po–2Pe	2: 1–4: 8	194.62	4.09E−02	5.24E−02	3.60E+09
2*s*22*p*3–2*s*22*p*2(3*P*)3*d*	2Po–2Pe	4: 3–4: 8	194.62	8.79E−02	2.25E−01	1.55E+10
LS	2Po–2Pe	6–6		8.90E−02	3.42E−01	1.57E+10
2*p*5–2*s*22*p*2(3*P*)3*d*	2Po–2Pe	2: 2–2: 7	1101.63	8.82E−08	6.39E−07	4.85E+02
2*p*5–2*s*22*p*2(3*P*)3*d*	2Po–2Pe	4: 4–2: 7	1090.03	3.78E−08	5.42E−07	4.24E+02
2*p*5–2*s*22*p*2(3*P*)3*d*	2Po–2Pe	2: 2–4: 8	1106.44	1.54E−07	1.12E−06	4.20E+02
2*p*5–2*s*22*p*2(3*P*)3*d*	2Po–2Pe	4: 4–4: 8	1094.75	3.70E−07	5.34E−06	2.06E+03
LS	2Po–2Pe	6–6		3.53E−07	7.64E−06	1.95E+03