Transition Probabilities for Hydrogen-Like Atoms

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E1, M1, E2, M2, E3, and M3 transition probabilities for hydrogen-like atoms are calculated with point-nucleus Dirac eigenfunctions for $Z=1-118$ and up to large quantum numbers $\ell=25$ and $n=26$, increasing existing data more than a thousandfold. A critical evaluation of the accuracy shows a higher reliability with respect to previous works. Tables for hydrogen containing a subset of the results are given explicitly, listing the states involved in each transition, wavelength, term energies, statistical weights, transition probabilities, oscillator strengths, and line strengths. The complete results, including 1 863 574 distinct transition probabilities, lifetimes, and branching fractions are available at http://www.fisica.unam.mx/research/tables/spectra/1el [DOI: 10.1063/1.1796671]

Key words: branching fractions; electric dipole; electric octupole; electric quadrupole; hydrogen-like; lifetimes; magnetic dipole; magnetic octupole; magnetic quadrupole; oscillator strengths; transition probabilities; variational principle.

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1. Introduction

Several nonrelativistic electric–dipole transition probabilities A_{ki}^{E1} for the hydrogen atom have been available for a long time.[1,2] The corresponding $A_{ki}^{\mathrm{E1}}(Z)$ values for nuclides of charge Z can be obtained from the $Z=1$ values through the relation:

$$A_{ki}^{\mathrm{E1}}(Z)=Z^4A_{ki}^{\mathrm{E1}}(1)\frac{\mu(Z)^2}{\mu(1)^2}, \tag{1}$$

where $\mu(Z)$ is the electron reduced mass for the given nuclide. With increasing Z values, relativistic effects become noticeable causing the need to correct Eq. (1) by adding higher powers of Z in a complicated way. The first numerical results for relativistic electric dipole transitions[3] in hydrogen-like atoms modeled by the point-nucleus Dirac Hamiltonian cover several Lyman-α transitions and yield correct oscillator strengths. Moreover, the Babushkin formulas[3,4] form the basis for the modern treatment of multipolar electric and magnetic transition probabilities,[5] which allow for interference between various electric and magnetic multipoles.

Magnetic multipole transition probabilities, on the other hand, are different from zero only in a relativistic framework. Recently, Pal'chikov[6] discussed another set of analytical formulas for E1, M1, E2, and M2 transition probabilities in hydrogen-like atoms also modeled by the point-nucleus Dirac Hamiltonian, restricting his results to a subset of all state transitions that may take place between levels $1s$, $2s$, $3s$, $2p$, $3p$, $4p$, and $3d$. The work of Pal'chikov[6] filled a gap in the literature on one-electron systems, since magnetic dipole, electric quadrupole, and magnetic quadrupole transitions for hydrogen-like atoms had barely been mentioned in the early literature.[7,8]

In contrast with nonrelativistic transition probabilities, the Z dependence of the relativistic electric and magnetic multi-

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polar transitions, particularly the magnetic transitions, do not follow a simple power law[6] and thus they must be recalculated explicitly for each Z value. A thorough analysis of Z dependence has been given by the authors.[9]

In this paper, we considerably extend the scope of the relativistic calculations of Pal'chikov:

(a) from $\ell=2$ up to $\ell=25$, and from $n=4$ up to $n=26$, thus embracing most transitions conceivably needed for physical and astrophysical research and
(b) by incorporating E3 and M3 transitions probabilities, so far unreported in the literature.

When more than one multipole is involved, viz., M1+E2 +M3 or M1+E2 or M2+E3, the separated as well as the consolidated results are given, the later for the first time. Also, our tabulation[10] is more explicit than the Pal'chikov tabulation, giving, for each electric and magnetic multipole, the transitions involved, wavelengths, term energies, statistical weights, transition probabilities, oscillator strengths, line strengths and log(gf), the last three only for electric dipole transitions. As an extra bonus, all numbers were produced and printed automatically avoiding possible transcription errors. For completeness, all nuclides with $Z=1-118$ have been considered.

Section 2 gives the basic formulas for transition probabilities. Different from Pal'chikov's analytical approach, ours is a numerical one based on general expressions for multipole transition probabilities,[5] and on a relatively new version of variational relativistic quantum mechanics.[11] Our method of calculation, which is embedded in a general purpose computer program for nonrelativistic and relativistic many-electron atomic calculations[12] is discussed in Sec. 3 together with computational details.

Distinct from previous works that take relativity into account, we give in Sec. 4 a comprehensive critical evaluation of accuracy revealing, among other things, small corrections due to the occurrence of a radiative recoil factor. The standard tabulation of Wiese *et al.*[2] includes all E1 transitions up to $\ell=5$ and $n=6$. Although extension to high ℓ and n values is straightforward,[13] finding reliable numerical results is far from trivial, even in the nonrelativistic regime, as also discussed in Sec. 4. The scope of the tabulation is presented in Sec. 5, and a selection of results for atomic hydrogen is given in Sec. 6. Finally, conclusions are given in Sec. 7.

2. Basic Formulas and Model

The emission transition probability $A_{ki}^{L(\mathrm{E,M})}$ for an electric (E) or magnetic (M) multipole of order L is given in terms of the oscillator strength $f_{ik}^{L(\mathrm{E,M})}$ by Dyall *et al.*[14]

$$A_{ki}^{L(\mathrm{E,M})}=2\frac{(\Delta E)^2}{c^3}\frac{g_i}{g_k}f_{ik}^{L(\mathrm{E,M})}, \tag{2}$$

$$f_{ik}^{L(\mathrm{E,M})}=\frac{\pi c^3}{g_i\cdot(2L+1)\cdot(\Delta E)^2}|\langle\Psi_i\|\mathrm{O}^{L(\mathrm{E,M})}\|\Psi_k\rangle|^2. \tag{3}$$

In general, the reduced matrix element $\langle\Psi_i\|\mathrm{O}^{L(\mathrm{E,M})}\|\Psi_k\rangle$ is expressed in terms of the configuration interaction expansion coefficients, radial integrals and Wigner $3j$ coefficients. In Eq. (3) we have incorporated a factor c^2 which is missing in the original reference. Transition probabilities are evaluated assuming the traditional multipole expansion in terms of E1, E2, E3, etc., for electric multipole radiation, and M1, M2, M3, etc., for magnetic multipole radiation. As in the work of Pal'chikov,[6] H-like atoms are modeled after the point-nucleus Dirac Hamiltonian.

3. Method and Computational Details

In principle, the eigenfunctions of the one-electron Dirac Hamiltonian and its transition matrix elements can be evaluated using analytic closed expressions.[6,16] Using 16-figure arithmetic, however, these well-known exact representations do not provide the most accurate way to carry out calculations even for small principal quantum numbers n. As we shall illustrate in Secs. 3.2. and 4, by using variational calculations and numerical integration of Hamiltonian matrix elements, very accurate results are obtained, reaching almost machine accuracy. Another advantage of using a variational method is that numerical instabilities are better known and understood. This, together with a very general computer program,[12] which has passed through many tests in several contexts, and a large number of specific verifications,[16] guarantees the reliability of millions of results which we could not possibly check individually.

In the following we explain the Drake–Goldman variational principle, which is crucial to obtain very accurate Dirac eigenfunctions and eigenvalues.

3.1. The Drake–Goldman Variational Principle

In relativistic calculations of electronic bound states one starts from a set of g Dirac bispinors

$$\Psi_{ilj m_j}^{(i)}=\frac{1}{r}\begin{pmatrix}P_{ilj}(r)Y_{\kappa m_j}\\ iQ_{il'j}(r)Y_{-\kappa m_j}\end{pmatrix},\quad i=1,2,...,g, \tag{4}$$

$$g=\sum_{(lj)=1}^{n_{\mathrm{irr}}} i_x(lj). \tag{5}$$

The full set is obtained after incorporation of g complementary Dirac bispinors

$$\Psi_{ilj m_j}^{(i+g)}=\frac{1}{r}\begin{pmatrix}P_{ilj}(r)Y_{\kappa m_j}\\ -iQ_{il'j}(r)Y_{-\kappa m_j}\end{pmatrix},\quad i=1,2,...,g, \tag{6}$$

differing from the first set in the minus sign preceding the lower component Q.[11] The P and Q functions in Eqs. (4) and (6) are general radial functions in Hilbert space with appropriate boundary conditions at the origin. If one is concerned just with positive-energy orbitals, an extensive account of their mathematical requirements can be found in the review of Grant.[15]

In the following we resort to the Drake–Goldman variational principle. Drake and Goldman[17] found that the matrix

representation of the Dirac Hamiltonian h_D in certain $2g$-dimensional bases, Eqs. (4) and (6), for $j=\ell+1/2$, $\ell \leqslant 2$, $Z \leqslant 92$

$$h_D \Phi_k = \varepsilon_k \Phi_k , \tag{7}$$

has eigenvalues ε_k satisfying

$$\varepsilon_{i+g} \geqslant E_i , \tag{8}$$

where E_i is the exact ith order eigenvalue of Dirac's equation. When g is increased, convergence towards the exact Dirac's bound eigenvalues is achieved *from above*, as in nonrelativistic calculations sustained by the variational theorem. The validity of the Drake–Goldman variational principle, previously verified up to $\ell \leqslant 10$, $j=\ell \pm 1/2$, $Z \leqslant 118$ and with more general Slater-type bases,[18] has presently been extended up to $\ell \leqslant 25$.

3.2. Computational Details

To generate all reported data we developed a systematic way to handle arbitrary sets of states and corresponding transition probabilities throughout the isoelectronic series. A general purpose computer program to evaluate energy levels, wave functions and transition probabilities[12] was enriched with several program modules, allowing us to carry out all calculations in a single run. The mechanics of the entire procedure is as follows:

(i) analytic self-consistent-field wave functions and energies are computed for each of the states considered;
(ii) the results are sent to proper files;
(iii) all nonzero transition probabilities are calculated and placed in definitive tables;
(iv) intermediate files are removed while the tables are transmitted to a final directory; and
(v) in the input files in (i)–(iii) the nuclear charge is updated to the next value.

Steps (i)–(v) are repeated 117 times to cover the 118 nuclides, $Z=1-118$.

The pertinent one-electron integrals are evaluated numerically using 32-point Gauss-Legendre quadratures in each of 30 Z-dependent intervals in $[0, \infty]$. The normal diagonalization routines from the literature[19,20] are not sufficiently accurate for our purposes. Thus a Jacobi routine[12] was used to obtain highly accurate eigenvalues and eigenvectors.

4. Critical Evaluation of Accuracy

We shall discuss, in succession, the physical and numerical issues involved in the evaluation of accuracy. The point-nucleus Dirac Hamiltonian is quite appropriate for low nuclear charge. For large nuclear charge, however, there are other significant effects which are neglected in this model; they consist mainly of finite nuclear size[21] and quantum electrodynamic[22–24] corrections, both propagating their influence mainly through transition energies. In a more rigorous treatment, the corresponding corrections to the wave functions should also be incorporated. Since these departures from the chosen model have not been fully investigated in the literature, accuracy will only be evaluated with respect to the given model itself.

As pointed out in Sec. 2, transition probabilities are evaluated assuming traditional multipole expansions, viz., a complete multipole expansion including toroidal moments[25,26] is not considered.

Nuclear motion is taken into account only through the standard replacement, in the infinite nuclear mass Hamiltonian, of the electron mass by its reduced mass and the consequent change from a.u. to a.u. (atom). Thus the absolute atomic unit of time[27] $\tau = 2.4188843265 \times 10^{-17}$ has been multiplied by a factor $[1+(m/M)]$, so we actually report

$$A_{ki}[s^{-1}] = A_{ki}[\text{a.u.(atom)}] \Big/ \left(\tau \cdot \left(1 + \frac{m}{M} \right) \right),$$

as it should be.

Extra terms arising from an exact representation of the interaction of the particles with the field are neglected. For E1 transitions in the nonrelativistic regime, the largest of these terms[28,29] can be accounted for by the introduction of a *radiative recoil* factor Z_r given, for nuclear mass M, by

$$Z_r = \frac{(1+Zm/M)}{(1+m/M)}, \tag{9}$$

which enters as a factor Z_r^2 in the transition probabilities. Since its dependence is only through Z and M, Z_r is given separately in each table for a given species. However, it is not considered in the reported values of A_{ki} to facilitate comparison with previous work. Its maximum value occurs for $Z=20$, amounting to an effect of 0.05%. Analogous considerations for other multipoles give similar factors, which for M1 and E2 differ from unity as the fourth power of the ratio of electron and nuclear masses. These factors affect at most the seventh figure and therefore they were neglected altogether.

Since, in general, isotopic effects do not alter the transition probabilities to the reported accuracy, we just considered a single isotope per element. The mass of the most abundant isotope was used when available.[30] Hypothetical masses were used for unknown nuclides of charges 113, 115, 117, and 118. All needed fundamental constants are taken from the 1998 CODATA recommended values.[31,32]

The first numerical issue concerns loss of accuracy in the energies. Setting the zero of energy at the ionization threshold, the Dirac energy eigenvalues $E(n,j)$ are given by Mizushima[33]

$$E(n,j)=c^2\cdot\left[\frac{1}{\sqrt{1+\left(\dfrac{\alpha Z}{n-j-\dfrac{1}{2}+\sqrt{\left(j+\dfrac{1}{2}\right)^2-(\alpha Z)^2}}\right)^2}}-1\right]. \tag{10}$$

For small nuclear charge Z, $E(n,j)$ is equal to a number of order one resulting from the difference of two large numbers of order $\alpha^{-2}\approx 10^4$ (α is the fine structure constant) thus incurring in loss of four decimal figures; accuracy decreases in a complicated way with principal quantum number n as $E(n,j)$ approaches zero. Therefore, 30-figure arithmetic is used to evaluate Eq. (10).

As to the exact eigenfunctions,[33] they were approximated to numerical accuracy as self-consistent-field (SCF) wave functions[34] in order to avoid numerical instabilities inherent to their exact analytic representations. The accuracy of the SCF wave functions is in turn conditioned by the exactness of the energy eigenvalues provided by the Drake–Goldman variational results rather than Eq. (10). Using 16-figure arithmetic, for example, for $Z=1$, $E(2,1/2)=-0.1250020801891714$ a.u. is obtained, to be compared with the 30-figure arithmetic exact result from Eq. (10) of -0.1250020801891716. Thus our 16-figure numerical approach is almost coincident with the exact result.

In extending the range of previous results[2,6] to large principal quantum number, even in a nonrelativistic regime, our method (Sec. 3) overcomes severe loss of accuracy not present in transitions with small principal quantum number. For example, for the nonrelativistic transition $10s\rightarrow 25p$, working with 16-figure arithmetic and analytical expressions[13] we get $A_{ki}^{E1}=600.68\ s^{-1}$ while the correct result is $607.63\ s^{-1}$. The latter can be obtained either by using the analytical expressions together with 30-figure arithmetic or through our numerical approach with only 16-figure arithmetic. (The relativistic result for either $10s\rightarrow 25p_{1/2}$ or $10s\rightarrow 25p_{3/2}$ is $607.62\ s^{-1}$.)

We have tested the nonrelativistic transition probabilities in the tabulation of Wiese *et al.*[2] and found them to agree with ours to all reported figures both using nonrelativistic or relativistic calculations, as expected due to the rather small relativistic effects in atomic hydrogen.

The work of Pal'chikov[6] provided the first systematic relativistic transition probabilities for hydrogen-like systems. Our results for transitions probabilities agree with those of Pal'chikov to all reported figures. For wavelengths, however, there are noticeable differences. For example, for the $1s_{1/2}\rightarrow 2p_{1/2}$ transition in hydrogen, we get $\lambda=1215.66962039$ Å against 1215.6736456 Å of Pal'chikov. We have traced this disagreement to the use by Pal'chikov of a proton mass $m_p=1.000$ instead of $m_p=1.00727646689$. Also, the oscillator strengths of Pal'chikov are usually in error: they are correct only for Lyman-α transitions when the ratio of statistical weights, g_k and g_I, is equal to one. [There is also a typographical error in his Eq. (4) where the said statistical weights are interchanged relative to the correct expression.]

A necessary, albeit not sufficient, test for the accuracy of the computed transition is the fulfillment of gauge invariance of the electric multipole matrix elements. This amounts to comparing results obtained by using the Coulomb[5] and the Babushkin[35] gauges. For transitions with $\Delta n\neq 0$ the Coulomb and the Babushkin results agree to within 6–14 significant figures (maximum agreement for small values of n). For $\Delta n=0$ transitions, five or more good figures are achieved up to $n=15$. For still larger n values, these $\Delta n=0$ transitions have transition probabilities smaller than 10^{-10}; thus they are irrelevant for all practical purposes.

In our tabulations, five figures are shown for transition probabilities and related quantities, always within the estimated margins of error. Energies and wavelengths are given up to 14 figures; since these are obtained using Eq. (10) in 30-figure arithmetic, all reported data can be considered to be exact within the limitations of the model employed.

If and when a more exact theory is warranted, after incorporation of the new effects, the rest of the calculation can follow the same sequence of steps, all to be performed in a single computer run.

5. Scope and Arrangement of the Tables

We have adhered to the time honored style introduced by Wiese *et al.*[2] in the National Standard Reference Data Series. States are entirely characterized by their orbital designations. In the tables, upper case letters are used for $j=\ell+1/2$ orbitals, while $j=\ell 1/2$ orbitals are denoted by lower case letters. Up to $\ell=25$ we have the following 51 orbitals:

SpPdDfFgGhHiIkKlLmMnNoOqQrRtTuUvVw

WxXyYzZaAbBcCeEjJ,

using all the letters of the alphabet. In a first set of tabulations (Set 1),[10] for $\ell\leqslant 4$ we include states up to $n=7$, and for $\ell\geqslant 5$ we keep orbitals up to $n=\ell+3$ not exceeding $n=26$, thus, only two orbitals for $\ell=24$ and just one orbital for $\ell=25$, totaling 163 states. This selection incorporates large ℓ values in a way allowing to study their decay modes, however it leaves out an important set of states: very large principal quantum number together with small azimuthal number 3. In order to partially fill this gap we have considered, in a second set of tabulations (Set 2),[10] states up to $n=25$, ℓ

TABLE 1. Electric dipole E1 transitions, $Z=1$

No.	Transition	λ (*in vacuo*)	E_i (cm^{-1})	E_k (cm^{-1})	g_i	g_k	A_{ki} (10^8 s^{-1})	f_{ik}
1	$1S-2p$	1 215.669 620	0.000 00	82 259.1914	2	2	6.2649	0.13873
2	$1S-3p$	1 025.720 104	0.000 00	97 492.4832	2	2	1.6725	0.26366E−01
3	$1S-4p$	972.534 456	0.000 00	102 824.1205	2	2	0.68186	0.96633E−02
4	$1S-5p$	949.740 669	0.000 00	105 291.9005	2	2	0.34375	0.46459E−02
5	$1S-6p$	937.801 090	0.000 00	106 632.4204	2	2	0.19728	0.25997E−02
6	$1S-7p$	930.745 894	0.000 00	107 440.7103	2	2	0.12362	0.16046E−02
7	$1S-2P$	1 215.664 226	0.000 00	82 259.5565	2	4	6.2648*	0.27745
8	$1S-3P$	1 025.718 966	0.000 00	97 492.5913	2	4	1.6725*	0.52733E−01
9	$1S-4P$	972.534 024	0.000 00	102 824.1661	2	4	0.68186*	0.19327E−01
10	$1S-5P$	949.740 458	0.000 00	105 291.9239	2	4	0.34375*	0.92919E−02
11	$1S-6P$	937.800 971	0.000 00	106 632.4339	2	4	0.19728*	0.51995E−02
12	$1S-7P$	930.745 820	0.000 00	107 440.7189	2	4	0.12362*	0.32092E−02
13	$2S-3p$	6 564.569 339	82 259.191 41	97 492.4832	2	2	0.22449	0.14495
14	$2S-4p$	4 862.647 462	82 259.191 41	102 824.1205	2	2	0.96683E−01	0.34255E−01
15	$2S-5p$	4 341.651 674	82 259.191 41	105 291.9005	2	2	0.49484E−01	0.13977E−01
16	$2S-6p$	4 102.862 210	82 259.191 41	106 632.4204	2	2	0.28584E−01	0.72097E−02
17	$2S-7p$	3 971.166 327	82 259.191 41	107 440.7103	2	2	0.17972E−01	0.42467E−02
18	$2S-2P$	273 940 977.116	82 259.191 41	82 259.5565	2	4	0.88798E−14*	0.19970E−04
19	$2S-3P$	6 564.522 729	82 259.191 41	97 492.5913	2	4	0.22448*	0.28989
20	$2S-4P$	4 862.636 672	82 259.191 41	102 824.1661	2	4	0.96680E−01*	0.68507E−01
21	$2S-5P$	4 341.647 269	82 259.191 41	105 291.9239	2	4	0.49483E−01*	0.27952E−01
22	$2S-6P$	4 102.859 934	82 259.191 41	106 632.4339	2	4	0.28583E−01*	0.14419E−01
23	$2S-7P$	3 971.164 984	82 259.191 41	107 440.7189	2	4	0.17972E−01*	0.84933E−02
741	$25e-26j$	7 553 333.195 88	109 503.559 43	109 516.7986	48	50	0.93597E−05*	8.3347
744	$25E-26J$	7 553 333.259 64	109 503.559 43	109 516.7986	50	52	0.93673E−05*	8.3281

TABLE 2. Magnetic quadrupole M2 transitions, $Z=1$

No.	Transition	λ (*in vacuo*)	E_i (cm^{-1})	E_k (cm^{-1})	G_i	g_k	A_{ki} (10^8 s^{-1})
1	$1S-2P$	1 215.664 225 63	0.000 00	82 259.556 46	2	4	0.46843E−01*
2	$1S-3P$	1 025.718 966 28	0.000 00	97 492.591 33	2	4	0.17566E−01*
3	$1S-4P$	972.534 023 93	0.000 00	102 824.166 09	2	4	0.79661E−02*
4	$1S-5P$	949.740 457 94	0.000 00	105 291.923 88	2	4	0.42111E−02*
5	$1S-6P$	937.800 970 63	0.000 00	106 632.433 89	2	4	0.24787E−02*
6	$1S-7P$	930.745 820 32	0.000 00	107 440.718 85	2	4	0.15768E−02*
7	$1S-4f$	972.533 880 07	0.000 00	102 824.181 29	2	6	0.16268E−14*
8	$1S-5f$	949.740 387 70	0.000 00	105 291.931 66	2	6	0.14216E−14*
9	$1S-6f$	937.800 930 99	0.000 00	106 632.438 39	2	6	0.10426E−14*
10	$1S-7f$	930.745 795 74	0.000 00	107 440.721 69	2	6	0.74795E−15*
11	$2S-2P$	273 940 977.115 62	82 259.191 41	82 259.556 46	2	4	0.13075E−26*
12	$2S-3P$	6 564.522 729 41	82 259.191 41	97 492.591 33	2	4	0.57562E−04*
13	$2S-4P$	4 862.636 672 30	82 259.191 41	102 824.166 09	2	4	0.45182E−04*
14	$2S-5P$	4 341.64 7269 32	82 259.191 41	105 291.923 88	2	4	0.29008E−04*
15	$2S-6P$	4 102.859 933 80	82 259.191 41	106 632.433 89	2	4	0.18763E−04*
16	$2S-7P$	3 971.164 984 43	82 259.191 41	107 440.718 85	2	4	0.12593E−04*
17	$2S-4f$	4 862.633 075 93	82 259.191 41	102 824.181 29	2	6	0.83043E−16*
18	$2S-5f$	4 341.645 801 40	82 259.191 41	105 291.931 66	2	6	0.71866E−16*
19	$2S-6f$	4 102.859 175 18	82 259.191 41	106 632.438 39	2	6	0.52196E−16*
20	$2S-7f$	3 971.164 536 88	82 259.191 41	107 440.721 69	2	6	0.37177E−16*
21	$2p-3d$	6 564.522 729 41	82 259.191 41	97 492.591 33	2	4	0.55261E−05*
22	$2p-4d$	4 862.636 672 30	82 259.191 41	102 824.166 09	2	4	0.32130E−05*
23	$2p-5d$	4 341.647 269 32	82 259.191 41	105 291.923 88	2	4	0.18418E−05*
990	$25e-26j$	7 553 333.195 883 9	109 503.559 43	109 516.798 62	48	50	0.89137E−13*
994	$25E-26J$	7 553 333.259 643 8	109 503.559 43	109 516.798 62	50	52	0.11343E−12*

TABLE 3. Electric octupole E3 transitions, $Z=1$

No.	Transition	λ (*in vacuo*)	E_i (cm^{-1})	E_k (cm^{-1})	g_i	g_k	A_{ki} (s^{-1})
1	$1S-4f$	972.533 880 07	0.000 00	102 824.181 29	2	6	0.31074E−03*
2	$1S-5f$	949.740 387 70	0.000 00	105 291.931 66	2	6	0.25666E−03*
3	$1S-6f$	937.800 930 99	0.000 00	106 632.438 39	2	6	0.18267E−03*
4	$1S-7f$	930.745 795 74	0.000 00	107 440.721 69	2	6	0.12871E−03*
5	$1S-4F$	972.533 808 15	0.000 00	102 824.188 90	2	8	0.31073E−03
6	$1S-5F$	949.740 352 58	0.000 00	105 291.935 56	2	8	0.25666E−03
7	$1S-6F$	937.800 911 18	0.000 00	106 632.440 65	2	8	0.18266E−03
8	$1S-7F$	930.745 783 44	0.000 00	107 440.723 10	2	8	0.12871E−03
9	$2S-4f$	4 862.633 075 93	82 259.191 41	102 824.181 29	2	6	0.12240E−03*
10	$2S-5f$	4 341.645 801 40	82 259.191 41	105 291.931 66	2	6	0.70464E−04*
11	$2S-6f$	4 102.859 175 18	82 259.191 41	106 632.438 39	2	6	0.41356E−04*
12	$2S-7f$	3 971.164 536 88	82 259.191 41	107 440.721 69	2	6	0.25959E−04*
13	$2S-4F$	4 862.631 277 75	82 259.191 41	102 824.188 90	2	8	0.12240E−03
14	$2S-5F$	4 341.645 067 45	82 259.191 41	105 291.935 56	2	8	0.70464E−04
15	$2S-6F$	4 102.858 795 88	82 259.191 41	106 632.440 65	2	8	0.41356E−04
16	$2S-7F$	3 971.164 313 11	82 259.191 41	107 440.723 10	2	8	0.25959E−04
17	$2p-3D$	6 564.507 193 28	82 259.191 41	97 492.627 38	2	6	0.12575E−04*
18	$2p-4D$	4 862.633 075 93	82 259.191 41	102 824.181 29	2	6	0.17554E−13*
19	$2p-5D$	4 341.645 801 40	82 259.191 41	105 291.931 66	2	6	0.39261E−06*
20	$2p-6D$	4 102.859 175 18	82 259.191 41	106 632.438 39	2	6	0.51044E−06*
21	$2p-7D$	3 971.164 536 88	82 259.191 41	107 440.721 69	2	6	0.45651E−06*
22	$2p-5g$	4 341.645 067 45	82 259.191 41	105 291.935 56	2	8	0.25134E−04
23	$2p-6g$	4 102.858 795 88	82 259.191 41	106 632.440 65	2	8	0.24812E−04
1547	$25e-26j$	7 553 333.195 883 9	109 503.559 43	109 516.798 62	48	50	0.36168E−14*
1552	$25E-26J$	7 553 333.259 643 8	109 503.559 43	109 516.798 62	50	52	0.36204E−14*

TABLE 4. E1 + M2 consolidated transitions, $Z=1$

No.	Transition	λ (*in vacuo*)	E_i (cm^{-1})	E_k (cm^{-1})	g_i	g_k	A_{ki} (s^{-1})
1	$1S-2P$	1 215.664 225 63	0.000 00	82 259.556 46	2	4	6.2648
2	$1S-3P$	1 025.718 966 28	0.000 00	97 492.591 33	2	4	1.6725
3	$1S-4P$	972.534 023 93	0.000 00	102 824.166 09	2	4	0.68186
4	$1S-5P$	949.740 457 94	0.000 00	105 291.923 88	2	4	0.34375
5	$1S-6P$	937.800 970 63	0.000 00	106 632.433 89	2	4	0.19728
6	$1S-7P$	930.745 820 32	0.000 00	107 440.718 85	2	4	0.12362
7	$2S-2P$	273 940 977.115 62	82 259.191 41	82 259.556 46	2	4	0.88798E−14
8	$2S-3P$	6 564.522 729 41	82 259.191 41	97 492.591 33	2	4	0.22448
9	$2S-4P$	4 862.636 672 30	82 259.191 41	102 824.166 09	2	4	0.96680E−01
10	$2S-5P$	4 341.647 269 32	82 259.191 41	105 291.923 88	2	4	0.49483E−01
11	$2S-6P$	4 102.859 933 80	82 259.191 41	106 632.433 89	2	4	0.28583E−01
12	$2S-7P$	3 971.164 984 43	82 259.191 41	107 440.718 85	2	4	0.17972E−01
13	$2p-3d$	6 564.522 729 41	82 259.191 41	97 492.591 33	2	4	0.53877
14	$2p-4d$	4 862.636 672 30	82 259.191 41	102 824.166 09	2	4	0.17188
15	$2p-5d$	4 341.647 269 32	82 259.191 41	105 291.923 88	2	4	0.78548E−01
16	$2p-6d$	4 102.859 933 80	82 259.191 41	106 632.433 89	2	4	0.42877E−01
17	$2p-7d$	3 971.164 984 43	82 259.191 41	107 440.718 85	2	4	0.26093E−01
18	$2P-3S$	6 564.726 652 87	82 259.556 46	97 492.483 17	4	2	0.42097E−01
19	$2P-4S$	4 862.733 778 70	82 259.556 46	102 824.120 45	4	2	0.17190E−01
20	$2P-5S$	4 341.720 484 47	82 259.556 46	105 291.900 51	4	2	0.85920E−02
21	$2P-6S$	4 102.923 659 90	82 259.556 46	106 632.420 37	4	2	0.49006E−02
22	$2P-7S$	3 971.223 895 69	82 259.556 46	107 440.710 33	4	2	0.30581E−02
23	$3S-3P$	924 549 772.088 00	97 492.483 17	97 492.591 33	2	4	0.13859E−14
69	$6P-7S$	123 720.047 044 76	106 632.433 89	107 440.710 33	4	2	0.84350E−03
70	$6d-7p$	123 720.047 044 76	106 632.433 89	107 440.710 33	4	2	0.51050E−03

TABLE 5. M2+E3 consolidated transitions, $Z=1$

No.	Transition	λ (*in vacuo*)	E_i (cm^{-1})	E_k (cm^{-1})	g_i	g_k	A_{ki} (s^{-1})
1	$1S-4f$	972.533 880 07	0.000 00	102 824.181 29	2	6	0.31074E−03
2	$1S-5f$	949.740 387 70	0.000 00	105 291.931 66	2	6	0.25666E−03
3	$1S-6f$	937.800 930 99	0.000 00	106 632.438 39	2	6	0.18267E−03
4	$1S-7f$	930.745 795 74	0.000 00	107 440.721 69	2	6	0.12871E−03
5	$2S-4f$	4 862.633 075 93	82 259.191 41	102 824.181 29	2	6	0.12240E−03
6	$2S-5f$	4 341.645 801 40	82 259.191 41	105 291.931 66	2	6	0.70464E−04
7	$2S-6f$	4 102.859 175 18	82 259.191 41	106 632.438 39	2	6	0.41356E−04
8	$2S-7f$	3 971.164 536 88	82 259.191 41	107 440.721 69	2	6	0.25959E−04
9	$2p-3D$	6 564.507 193 28	82 259.191 41	97 492.627 38	2	6	0.51873E−04
10	$2p-4D$	4 862.633 075 93	82 259.191 41	102 824.181 29	2	6	0.22848E−04
11	$2p-5D$	4 341.645 801 40	82 259.191 41	105 291.931 66	2	6	0.13490E−04
12	$2p-6D$	4 102.859 175 18	82 259.191 41	106 632.438 39	2	6	0.85164E−05
13	$2p-7D$	3 971.164 536 88	82 259.191 41	107 440.721 69	2	6	0.56572E−05
14	$2P-5g$	4 341.713 878 55	82 259.556 46	105 291.935 56	4	8	0.83782E−05
15	$2P-6g$	4 102.920 245 98	82 259.556 46	106 632.440 65	4	8	0.82707E−05
16	$2P-7g$	3 971.221 881 62	82 259.556 46	107 440.723 10	4	8	0.66411E−05
17	$3S-4f$	18 755.750 543 68	97 492.483 17	102 824.181 29	2	6	0.11182E−05
18	$3S-5f$	12 821.419 371 01	97 492.483 17	105 291.931 66	2	6	0.10644E−05
19	$3S-6f$	10 940.972 636 30	97 492.483 17	106 632.438 39	2	6	0.15765E−05
20	$3S-7f$	10 052.030 803 35	97 492.483 17	107 440.721 69	2	6	0.13737E−05
21	$3p-3D$	693 416 688.359 22	97 492.483 17	97 492.627 38	2	6	0.13422E−28
22	$3p-4D$	18 755.750 543 68	97 492.483 17	102 824.181 29	2	6	0.12224E−05
23	$3p-5D$	12 821.419 371 01	97 492.483 17	105 291.931 66	2	6	0.58210E−06
441	$22A-26e$	1 553 720.667 578 5	109 452.436 98	109 516.798 62	44	48	0.35458E−13
456	$23B-26j$	2 218 028.620 788 4	109 471.713 54	109 516.798 62	46	50	0.26000E−13

TABLE 6. E1+M2+E3 consolidated transitions, $Z=1$

No.	Transition	λ (*in vacuo*)	E_i (cm^{-1})	E_k (cm^{-1})	g_i	g_k	A_{ki} (10^8 s^{-1})
1	$2P-3d$	6 564.680 040 63	82 259.556 46	97 492.591 33	4	4	0.10775
2	$2P-4d$	4 862.722 988 91	82 259.556 46	102 824.166 09	4	4	0.34375E−01
3	$2P-5d$	4 341.716 080 49	82 259.556 46	105 291.923 88	4	4	0.15709E−01
4	$2P-6d$	4 102.921 383 94	82 259.556 46	106 632.433 89	4	4	0.85748E−02
5	$2P-7d$	3 971.222 552 96	82 259.556 46	107 440.718 85	4	4	0.52183E−02
6	$2P-3D$	6 564.664 503 76	82 259.556 46	97 492.627 38	4	6	0.64651
7	$2P-4D$	4 862.719 392 41	82 259.556 46	102 824.181 29	4	6	0.20625
8	$2P-5D$	4 341.714 612 53	82 259.556 46	105 291.931 66	4	6	0.94254E−01
9	$2P-6D$	4 102.920 625 30	82 259.556 46	106 632.438 39	4	6	0.51450E−01
10	$2P-7D$	3 971.222 105 40	82 259.556 46	107 440.721 69	4	6	0.31311E−01
11	$3P-4d$	18 756.184 544 19	97 492.591 33	102 824.166 09	4	4	0.11729E−01
12	$3P-5d$	12 821.609 979 60	97 492.591 33	105 291.923 88	4	4	0.56525E−02
13	$3P-6d$	10 941.107 506 28	97 492.591 33	106 632.433 89	4	4	0.31296E−02
14	$3P-7d$	10 052.142 961 40	97 492.591 33	107 440.718 85	4	4	0.19159E−02
15	$3P-3D$	2 773 719 066.271 1	97 492.591 33	97 492.627 38	4	6	0.38495E−16
16	$3P-4D$	18 756.131 037 32	97 492.591 33	102 824.181 29	4	6	0.70376E−01
17	$3P-5D$	12 821.597 177 64	97 492.591 33	105 291.931 66	4	6	0.33915E−01
18	$3P-6D$	10 941.102 111 54	97 492.591 33	106 632.438 39	4	6	0.18778E−01
19	$3P-7D$	10 052.140 093 76	97 492.591 33	107 440.721 69	4	6	0.11496E−01
20	$3d-4P$	18 756.184 544 19	97 492.591 33	102 824.166 09	4	4	0.34754E−03
21	$3d-5P$	12 821.609 979 60	97 492.591 33	105 291.923 88	4	4	0.14954E−03
22	$3d-6P$	10 941.107 506 28	97 492.591 33	106 632.433 89	4	4	0.78242E−04
23	$3d-7P$	10 052.142 961 40	97 492.591 33	107 440.718 85	4	4	0.46362E−04
627	$25c-26e$	7 553 333.125 522 8	109 503.559 43	109 516.798 62	46	48	0.86425E−05
633	$25e-26j$	7 553 333.195 883 9	109 503.559 43	109 516.798 62	48	50	0.93597E−05

TABLE 7. Magnetic dipole M1 transitions, $Z=1$

No.	Transition	λ (*in vacuo*)	E_i (cm^{-1})	E_k (cm^{-1})	g_i	g_k	A_{ki} (s^{-1})	
1	$1S-2S$	1 215.669 620 39	0.000 00	82 259.191 41	2	2	0.24946E−05	
2	$1S-3S$	1 025.720 104 24	0.000 00	97 492.483 17	2	2	0.11087E−05	
3	$1S-4S$	972.534 455 51	0.000 00	102 824.120 45	2	2	0.53028E−06	
4	$1S-5S$	949.740 668 67	0.000 00	105 291.900 51	2	2	0.28705E−06	
5	$1S-6S$	937.801 089 53	0.000 00	106 632.420 37	2	2	0.17111E−06	
6	$1S-7S$	930.745 894 08	0.000 00	107 440.710 33	2	2	0.10968E−06	
7	$1S-3d$	1 025.718 966 28	0.000 00	97 492.591 33	2	4	0.69290E−08	*
8	$1S-4d$	972.534 023 93	0.000 00	102 824.166 09	2	4	0.43210E−08	*
9	$1S-5d$	949.740 457 94	0.000 00	105 291.923 88	2	4	0.25793E−08	*
10	$1S-6d$	937.800 970 63	0.000 00	106 632.433 89	2	4	0.16136E−08	*
11	$1S-7d$	930.745 820 32	0.000 00	107 440.718 85	2	4	0.10633E−08	*
12	$2S-3S$	6 564.569 339 41	82 259.191 41	97 492.483 17	2	2	0.18769E−08	
13	$2S-4S$	4 862.647 461 71	82 259.191 41	102 824.120 45	2	2	0.16174E−08	
14	$2S-5S$	4 341.651 673 16	82 259.191 41	105 291.900 51	2	2	0.10815E−08	
15	$2S-6S$	4 102.862 209 69	82 259.191 41	106 632.420 37	2	2	0.71477E−09	
16	$2S-7S$	3 971.166 327 12	82 259.191 41	107 440.710 33	2	2	0.48587E−09	
17	$2S-3d$	6 564.522 729 41	82 259.191 41	97 492.591 33	2	4	0.10496E−09	*
18	$2S-4d$	4 862.636 672 30	82 259.191 41	102 824.166 09	2	4	0.60319E−10	*
19	$2S-5d$	4 341.647 269 32	82 259.191 41	105 291.923 88	2	4	0.33608E−10	*
20	$2S-6d$	4 102.859 933 80	82 259.191 41	106 632.433 89	2	4	0.20124E−10	*
21	$2S-7d$	3 971.164 984 43	82 259.191 41	107 440.718 85	2	4	0.12889E−10	*
22	$2p-3p$	6 564.569 339 41	82 259.191 41	97 492.483 17	2	2	0.49047E−09	
23	$2p-4p$	4 862.647 461 71	82 259.191 41	102 824.120 45	2	2	0.38497E−09	
688	$24A-25c$	6 698 669.019 887 5	109 488.631 09	109 503.559 43	44	46	0.10833E−17	*
689	$24A-26c$	3 550 187.487 340 4	109 488.631 09	109 516.798 62	44	46	0.70012E−18	*

TABLE 8. Electric quadrupole E2 transitions, $Z=1$

No.	Transition	λ (*in vacuo*)	E_i (cm^{-1})	E_k (cm^{-1})	g_i	g_k	A_{ki} (s^{-1})
1	$1S-3d$	1 025.718 966 28	0.000 00	97 492.591 33	2	4	593.75
2	$1S-4d$	972.534 023 93	0.000 00	102 824.166 09	2	4	326.79
3	$1S-5d$	949.740 457 94	0.000 00	105 291.923 88	2	4	184.51
4	$1S-6d$	937.800 970 63	0.000 00	106 632.433 89	2	4	112.06
5	$1S-7d$	930.745 820 32	0.000 00	107 440.718 85	2	4	72.545
6	$1S-3D$	1 025.718 586 97	0.000 00	97 492.627 38	2	6	593.74
7	$1S-4D$	972.533 880 07	0.000 00	102 824.181 29	2	6	326.78
8	$1S-5D$	949.740 387 70	0.000 00	105 291.931 66	2	6	184.51
9	$1S-6D$	937.800 930 99	0.000 00	106 632.438 39	2	6	112.06
10	$1S-7D$	930.745 795 74	0.000 00	107 440.721 69	2	6	72.543
11	$2S-3d$	6 564.522 729 41	82 259.191 41	97 492.591 33	2	4	51.007
12	$2S-4d$	4 862.636 672 30	82 259.191 41	102 824.166 09	2	4	5.1491
13	$2S-5d$	4 341.647 269 32	82 259.191 41	105 291.923 88	2	4	0.96388
14	$2S-6d$	4 102.859 933 80	82 259.191 41	106 632.433 89	2	4	0.25376
15	$2S-7d$	3 971.164 984 43	82 259.191 41	107 440.718 85	2	4	0.83368E−01
16	$2S-3D$	6 564.507 193 28	82 259.191 41	97 492.627 38	2	6	51.007
17	$2S-4D$	4 862.633 075 93	82 259.191 41	102 824.181 29	2	6	5.1493
18	$2S-5D$	4 341.645 801 40	82 259.191 41	105 291.931 66	2	6	0.96398
19	$2S-6D$	4 102.859 175 18	82 259.191 41	106 632.438 39	2	6	0.25380
20	$2S-7D$	3 971.164 536 88	82 259.191 41	107 440.721 69	2	6	0.83387E−01
21	$2p-2P$	273 940 977.115 62	82 259.191 41	82 259.556 46	2	4	0.13095E−21
22	$2p-3P$	6 564.522 729 41	82 259.191 41	97 492.591 33	2	4	11.954
23	$2p-4P$	4 862.636 672 30	82 259.191 41	102 824.166 09	2	4	5.1485
1156	$25C-26J$	7 553 332.904 213 5	109 503.559 43	109 516.798 62	48	52	0.18636E−05
1157	$25e-26e$	7 553 333.511 860 3	109 503.559 43	109 516.798 62	48	48	0.15334E−06

TABLE 9. Magnetic octupole M3 transitions, $Z=1$

No.	Transition	λ (*in vacuo*)	E_i (cm^{-1})	E_k (cm^{-1})	g_i	g_k	A_{ki} (s^{-1})
1	$1S-3D$	1 025.718 586 97	0.000 00	97 492.627 38	2	6	0.73908E−07*
2	$1S-4D$	972.533 880 07	0.000 00	102 824.181 29	2	6	0.45248E−07*
3	$1S-5D$	949.740 387 70	0.000 00	105 291.931 66	2	6	0.26790E−07*
4	$1S-6D$	937.800 930 99	0.000 00	106 632.438 39	2	6	0.16687E−07*
5	$1S-7D$	930.745 795 74	0.000 00	107 440.721 69	2	6	0.10967E−07*
6	$1S-5g$	949.740 352 58	0.000 00	105 291.935 56	2	8	0.29315E−21
7	$1S-6g$	937.800 911 18	0.000 00	106 632.440 65	2	8	0.33161E−21
8	$1S-7g$	930.745 783 44	0.000 00	107 440.723 10	2	8	0.28850E−21
9	$2S-3D$	6 564.507 193 28	82 259.191 41	97 492.627 38	2	6	0.15502E−09*
10	$2S-4D$	4 862.633 075 93	82 259.191 41	102 824.181 29	2	6	0.28520E−10*
11	$2S-5D$	4 341.645 801 40	82 259.191 41	105 291.931 66	2	6	0.66974E−11*
12	$2S-6D$	4 102.859 175 18	82 259.191 41	106 632.438 39	2	6	0.19745E−11*
13	$2S-7D$	3 971.164 536 88	82 259.191 41	107 440.721 69	2	6	0.69246E−12*
14	$2S-5g$	4 341.645 067 45	82 259.191 41	105 291.935 56	2	8	0.30242E−22
15	$2S-6g$	4 102.858 795 88	82 259.191 41	106 632.440 65	2	8	0.34047E−22
16	$2S-7g$	3 971.164 313 11	82 259.191 41	107 440.723 10	2	8	0.29488E−22
17	$2p-4f$	4 862.633 075 93	82 259.191 41	102 824.181 29	2	6	0.54315E−11*
18	$2p-5f$	4 341.645 801 40	82 259.191 41	105 291.931 66	2	6	0.45547E−11*
19	$2p-6f$	4 102.859 175 18	82 259.191 41	106 632.438 39	2	6	0.32626E−11*
20	$2p-7f$	3 971.164 536 88	82 259.191 41	107 440.721 69	2	6	0.23068E−11*
21	$2p-4F$	4 862.631 277 75	82 259.191 41	102 824.188 90	2	8	0.10999E−09
22	$2p-5F$	4 341.645 067 45	82 259.191 41	105 291.935 56	2	8	0.92232E−10
23	$2p-6F$	4 102.858 795 88	82 259.191 41	106 632.440 65	2	8	0.66067E−10
24	$2p-7F$	3 971.164 313 11	82 259.191 41	107 440.723 10	2	8	0.46713E−10
1500	$24c-26j$	3 550 187.446 899 2	109 488.631 09	109 516.798 62	46	50	0.16704E−19*

TABLE 10. M1 + E2 consolidated transitions, $Z=1$

No.	Transition	λ (*in vacuo*)	E_i (cm^{-1})	E_k (cm^{-1})	g_i	g_k	A_{ki} (s^{-1})
1	$1S-3d$	1 025.718 966 28	0.000 00	97 492.591 33	2	4	593.75
2	$1S-4d$	972.534 023 93	0.000 00	102 824.166 09	2	4	326.79
3	$1S-5d$	949.740 457 94	0.000 00	105 291.923 88	2	4	184.51
4	$1S-6d$	937.800 970 63	0.000 00	106 632.433 89	2	4	112.06
5	$1S-7d$	930.745 820 32	0.000 00	107 440.718 85	2	4	72.545
6	$2S-3d$	6 564.522 729 41	82 259.191 41	97 492.591 33	2	4	51.007
7	$2S-4d$	4 862.636 672 30	82 259.191 41	102 824.166 09	2	4	5.1491
8	$2S-5d$	4 341.647 269 32	82 259.191 41	105 291.923 88	2	4	0.96388
9	$2S-6d$	4 102.859 933 80	82 259.191 41	106 632.433 89	2	4	0.25376
10	$2S-7d$	3 971.164 984 43	82 259.191 41	107 440.718 85	2	4	0.83368E−01
11	$2p-2P$	273 940 977.115 62	82 259.191 41	82 259.556 46	2	4	0.43784E−12
12	$2p-3P$	6 564.522 729 41	82 259.191 41	97 492.591 33	2	4	11.954
13	$2p-4P$	4 862.636 672 30	82 259.191 41	102 824.166 09	2	4	5.1485
14	$2p-5P$	4 341.647 269 32	82 259.191 41	105 291.923 88	2	4	2.6351
15	$2p-6P$	4 102.859 933 80	82 259.191 41	106 632.433 89	2	4	1.5222
16	$2p-7P$	3 971.164 984 43	82 259.191 41	107 440.718 85	2	4	0.95705
17	$2P-3p$	6 564.726 652 87	82 259.556 46	97 492.483 17	4	2	23.908
18	$2P-4p$	4 862.733 778 70	82 259.556 46	102 824.120 45	4	2	10.297
19	$2P-5p$	4 341.720 484 47	82 259.556 46	105 291.900 51	4	2	5.2699
20	$2P-6p$	4 102.923 659 90	82 259.556 46	106 632.420 37	4	2	3.0441
21	$2P-7p$	3 971.223 895 69	82 259.556 46	107 440.710 33	4	2	1.9139
22	$3S-3d$	924 549 772.088 00	97 492.483 17	97 492.591 33	2	4	0.67313E−23
23	$3S-4d$	18 755.804 048 38	97 492.483 17	102 824.166 09	2	4	3.7596
68	$6P-7p$	123 720.047 044 76	106 632.433 89	107 440.710 33	4	2	0.35399E−01
69	$6d-7S$	123 720.047 044 76	106 632.433 89	107 440.710 33	4	2	0.16100E−01

TABLE 11. E2+M3 consolidated transitions, $Z=1$

No.	Transition	λ (*in vacuo*)	E_i (cm^{-1})	E_k (cm^{-1})	g_i	g_k	A_{ki} (s^{-1})
1	$1S-3D$	1 025.718 586 97	0.000 00	97 492.627 38	2	6	593.74
2	$1S-4D$	972.533 880 07	0.000 00	102 824.181 29	2	6	326.78
3	$1S-5D$	949.740 387 70	0.000 00	105 291.931 66	2	6	184.51
4	$1S-6D$	937.800 930 99	0.000 00	106 632.438 39	2	6	112.06
5	$1S-7D$	930.745 795 74	0.000 00	107 440.721 69	2	6	72.543
6	$2S-3D$	6 564.507 193 28	82 259.191 41	97 492.627 38	2	6	51.007
7	$2S-4D$	4 862.633 075 93	82 259.191 41	102 824.181 29	2	6	5.1493
8	$2S-5D$	4 341.645 801 40	82 259.191 41	105 291.931 66	2	6	0.96398
9	$2S-6D$	4 102.859 175 18	82 259.191 41	106 632.438 39	2	6	0.25380
10	$2S-7D$	3 971.164 536 88	82 259.191 41	107 440.721 69	2	6	0.83387E−01
11	$2p-4f$	4 862.633 075 93	82 259.191 41	102 824.181 29	2	6	48.051
12	$2p-5f$	4 341.645 801 40	82 259.191 41	105 291.931 66	2	6	32.123
13	$2p-6f$	4 102.859 175 18	82 259.191 41	106 632.438 39	2	6	20.548
14	$2p-7f$	3 971.164 536 88	82 259.191 41	107 440.721 69	2	6	13.611
15	$2P-4F$	4 862.717 594 17	82 259.556 46	102 824.188 90	4	8	61.780
16	$2P-5F$	4 341.713 878 55	82 259.556 46	105 291.935 56	4	8	41.300
17	$2P-6F$	4 102.920 245 98	82 259.556 46	106 632.440 65	4	8	26.419
18	$2P-7F$	3 971.221 881 62	82 259.556 46	107 440.723 10	4	8	17.500
19	$3S-3D$	693 416 688.359 22	97 492.483 17	97 492.627 38	2	6	0.28354E−22
20	$3S-4D$	18 755.750 543 68	97 492.483 17	102 824.181 29	2	6	3.7596
21	$3S-5D$	12 821.419 371 01	97 492.483 17	105 291.931 66	2	6	1.0853
22	$3S-6D$	10 940.972 636 30	97 492.483 17	106 632.438 39	2	6	0.42539
23	$3S-7D$	10 052.030 803 35	97 492.483 17	107 440.721 69	2	6	0.20458
470	$24c-26j$	3 550 187.446 899 2	109 488.631 09	109 516.798 62	46	50	0.88563E−04
471	$24C-26J$	3 550 187.478 931 7	109 488.631 09	109 516.798 62	48	52	0.88714E−04

TABLE 12. M1+E2+M3 consolidated transitions, $Z=1$

No.	Transition	λ (*in vacuo*)	E_i (cm^{-1})	E_k (cm^{-1})	g_i	g_k	A_{ki} (s^{-1})
1	$2P-3P$	6 564.680 040 63	82 259.556 46	97 492.591 33	4	4	11.954
2	$2P-4P$	4 862.722 988 91	82 259.556 46	102 824.166 09	4	4	5.1483
3	$2P-5P$	4 341.716 080 49	82 259.556 46	105 291.923 88	4	4	2.6350
4	$2P-6P$	4 102.921 383 94	82 259.556 46	106 632.433 89	4	4	1.5221
5	$2P-7P$	3 971.222 552 96	82 259.556 46	107 440.718 85	4	4	0.95700
6	$2P-4f$	4 862.719 392 41	82 259.556 46	102 824.181 29	4	6	13.729
7	$2P-5f$	4 341.714 612 53	82 259.556 46	105 291.931 66	4	6	9.1778
8	$2P-6f$	4 102.920 625 30	82 259.556 46	106 632.438 39	4	6	5.8709
9	$2P-7f$	3 971.222 105 40	82 259.556 46	107 440.721 69	4	6	3.8888
10	$3P-4P$	18 756.184 544 19	97 492.591 33	102 824.166 09	4	4	1.2748
11	$3P-5P$	12 821.609 979 60	97 492.591 33	105 291.923 88	4	4	0.71391
12	$3P-6P$	10 941.107 506 28	97 492.591 33	106 632.433 89	4	4	0.42532
13	$3P-7P$	10 052.142 961 40	97 492.591 33	107 440.718 85	4	4	0.27149
14	$3P-4f$	18 756.131 037 32	97 492.591 33	102 824.181 29	4	6	1.2853
15	$3P-5f$	12 821.597 177 64	97 492.591 33	105 291.931 66	4	6	0.57343E−02
16	$3P-6f$	10 941.102 111 54	97 492.591 33	106 632.438 39	4	6	0.26452E−01
17	$3P-7f$	10 052.140 093 76	97 492.591 33	107 440.721 69	4	6	0.47988E−01
18	$3d-4d$	18 756.184 544 19	97 492.591 33	102 824.166 09	4	4	0.83281
19	$3d-5d$	12 821.609 979 60	97 492.591 33	105 291.923 88	4	4	0.40133
20	$3d-6d$	10 941.107 506 28	97 492.591 33	106 632.433 89	4	4	0.22221
21	$3d-7d$	10 052.142 961 40	97 492.591 33	107 440.718 85	4	4	0.13603
22	$3d-3D$	2 773 719 066.271 1	97 492.591 33	97 492.627 38	4	6	0.50615E−15
23	$3d-4D$	18 756.131 037 32	97 492.591 33	102 824.181 29	4	6	0.23795
607	$25C-26C$	7 553 333.511 860 3	109 503.559 43	109 516.798 62	48	48	0.29499E−06
613	$25E-26E$	7 553 333.551 314 3	109 503.559 43	109 516.798 62	50	50	0.15336E−06

$\leqslant 3$, coincidentally also totaling 163 states. Together, both sets give rise to 1 863 574 distinct transitions.

Selection rules call for the construction of 12 tables consisting of E1, E2, E3, M1, M2, M3, E1+M2, M2+E3, E1+M2+E3, M1+E2, E2+M3, and M1+E2+M3 transitions, respectively, giving $12\times 118=1416$ tables of transition probabilities for all nuclides, for each set of calculations. Transitions are presented as absorptions starting from the lowest state. Wavelengths are given in Å, the energies of the initial and final states are in cm^{-1}. There follow initial and final level statistical weights, the actual A_{ki} values in either s^{-1} or 10^8 s^{-1} (the latter only when E1 transitions are involved), the f_{ik} values, and finally line strengths S (in a.u.) and log(gf).

Entries marked with an asterisk after the A_{ki} column occur in another table without the asterisk, the latter meaning that the final result has been consolidated between all allowed multipoles for the given transition. E2 and M2 transitions always need to be consolidated with other multipoles, thus all their entries carry asterisks. A few E1, E3, M1, and M3 entries do not carry asterisks, while the six tables involving consolidated transitions carry no asterisks. For example, both transitions $2p_{1/2}\rightarrow 3d_{3/2}$ and $2p_{3/2}\rightarrow 3d_{3/2}$ occur in the E1 table with an asterisk, anticipating their occurrence elsewhere, the first one in the E1+M2 table, the second one in the E1+M2+E3 table. Had we included E4 and M4 multipoles, E3 and M3 would be consolidated with other multipoles, and so on.

Two-photon transitions from the $2s_{1/2}$ states are taken from the literature.[36] Because of the Lamb shift, the $2s_{1/2}$ states will also decay to $2p_{1/2}$ states, but this cannot be considered unless QED energy corrections are taken into account. Other two-photon transitions from higher-excited states compete too unfavorably with E1 transitions and can then be discarded.

5.1. E1, M2, and E3 Transitions

E1, M2, and E3 transitions require change of parity between initial and final states. The physically significant quantities are the sums E1+M2+E3, if all are allowed, or any partial sums of allowed transitions: E1+M2, M2+E3, and also E1, M2 and E3. E1+M2+E3, E1+M2 and M2+E3 are mutually exclusive. Most of E1 and E3 transitions and all M2 transitions need to be consolidated with one or two multipole partners, in which case they are tabulated with an asterisk as mentioned above. Only E1 $ns_{1/2}\rightarrow mp_{1/2}$ transitions and E3 transitions with $\Delta j=3$ do not have to be consolidated with other multipole partners, and thus represent bonafide final results. The first six tables of Sec. 6 show parity-changing transition probabilities for hydrogen.

5.2. M1, E2, and M3 Transitions

M1, E2, and M3 transitions require no change of parity between initial and final states. The physically significant quantities are the sums M1+E2+M3, if all are allowed, or any partial sums of allowed transitions: M1+E2, E2+M3, and also M1, E2 and M3. M1+E2+M3, M1+E2 and E2+M3 are mutually exclusive. All M1 transitions (except $mS\rightarrow nS$ and $mp\rightarrow np$), all E2, and all M3 (except those with $\Delta j=3$) need to be consolidated with one or two multipole partners. Analogously as before, they are given in the last six tables of Sec. 6.

6. Tables of Transition Probabilities for Hydrogen

Here we present, for $Z=1$, a subset of results of the Set 1 specified in Sec. 5. The data are arranged in the 12 tables previously described (see Tables 1–12), each corresponding to a given multipole or to any allowed combination of them. Only the first few transitions and the last three most significant ones are exhibited, so as to give a flavor of the extent of the tabulation. The data in the complete tables for $Z=1-118$ may be considered benchmarks for future reference since they were produced using well-tested numerical procedures and tabulated in a fully automatic way, guaranteeing a high degree of reliability. They are available at a recognized web site.[10]

7. Conclusions

We have presented E1, M1, E2, M2, E3, and M3 transition probabilities for hydrogen-like atoms calculated with point-nucleus Dirac eigenfunctions for $Z=1-118$ and up to large quantum numbers $\ell=25$, $n=26$, increasing existing data more than a thousandfold. A critical evaluation of the accuracy, together with automatic generation of millions of results in a single computer run, has been crucial to achieve high reliability. Our tabulation serves three useful purposes:

(1) provides a substantial check of previous work;
(2) furnishes a clear and self-contained source of basic data not available in the literature; and
(3) can be used for estimating transition probabilities in N-electron systems behaving as one-electron systems, particularly in the study of inner shell transitions.[9,37]

Consolidated results are provided for the first time: E1+M2, M2+E3, E1+M2+E3, M1+E2, E2+M3, and M1+E2+M3 when selection rules so require. For one-electron systems, the possibility of interference among E1, M2, and E3, or among M1, E2, and M3, or between any selection-allowed pair of them is precluded in the absence of a magnetic field.[38] As expected, the E1+M2 and E1+M2+E3 transitions are widely dominated by E1. This fact is reflected in the coincidence, to all significant figures, in the corresponding results for $Z=1$. For $Z=92$, however, already a one percent contribution of M2 is observed for large transition probabilities such as $1s_{1/2}\rightarrow 2p_{3/2}$.

Surprisingly, M2+E3 results are significantly different than M2 or E3 alone. For example, in the transition $2p_{1/2}$

$\rightarrow 3d_{5/2}$ (through all Z values) M2 never contributes more than 76% to M2+E3 (for hydrogen, see the corresponding tables).

M1+E2 and M1+E2+M3 are entirely dominated by E2, except for $\Delta\ell=0$ transitions. In the M1+E2 transition $2p_{1/2}\rightarrow 3p_{3/2}$, the M1 contribution, negligible for $Z=1$, increases from 0.1% ($Z=47$) to 50% for $Z=92$. In the M1+E2+M3 transition $2p_{3/2}\rightarrow 3p_{3/2}$, the M1 contribution reaches 2% for $Z=92$. The (E2, M3) pair behaves similarly as (E1, M2): when existing, E2+M3 coincides with E2 for low Z. For $Z=92$, a 1% contribution of M3 is attained for the $1s_{1/2}\rightarrow 3d_{5/2}$ transition probability.

A comprehensive picture of transition probabilities, emission and absorption patterns in H-like systems is given elsewhere.[9] Tables of lifetimes, branching fractions and Z-dependent branching fractions are also available.[10]

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