ATOMIC DATA FOR PERMITTED RESONANCE LINES OF ATOMS AND IONS FROM H TO Si, AND S, Ar, Ca AND Fe

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We list vacuum wavelengths, energy levels, statistical weights, transition probabilities and oscillator strengths for permitted resonance spectral lines of all ions of 18 astrophysically important elements (H through Si, S, Ar, Ca, Fe). Using a compilation of experimental energy levels, we derived accurate wavelengths for 5599 lines of 1828 ground-term multiplets which have gf-values calculated in the Opacity Project. We recalculated the Opacity Project multiplet gf-values to oscillator strengths and transition probabilities of individual lines. For completeness, we added 372 resonance lines of Ne I, Ar I, Fe I and Fe II ions which are not covered by the Opacity Project. Intercombination and forbidden lines are not included in the present compilation.

INTRODUCTION

Recently, a large international collaboration known as the Opacity Project (hereafter OP; Seaton et al.[1]) produced a complete set of accurate atomic data for all stages of ionization of astrophysically important elements: $1 \leq Z \leq 14$ and $Z = 16, 18, 20, 26$, where Z is the atomic number. In particular, the OP data include oscillator strengths for all optically allowed transitions between states with $n \leq 10$ and $l \leq 4$, where n and l are the active-electron principal and orbital quantum numbers respectively. The OP data do not include intercombination and forbidden transitions. The OP calculations are based on high level methods such as the R-matrix method (Burke, Hibbert, and Robb[2]) and the new asymptotic techniques developed by Seaton[3]. Extensive comparisons of the OP data with experiment and theory (Seaton et al.[1], Mendoza[4], Verner, Barthel, and Tytler[5], Verner and Yakovlev[6]) have confirmed the high accuracy of the OP calculations. The OP data are available through the TOPbase database (Cunto et al.[7]).

However, the OP transition probabilities and oscillator strengths cannot be directly used for spectroscopic applications because the OP gives all the data for multiplets only, not for individual lines. Moreover, the OP theoretical multiplet wavelengths are accurate to a few angstroms, which is not good enough for spectroscopy.

In an earlier paper (Verner et al.[5]) we assigned accurate experimental wavelengths to 1086 OP lines from the ground (zero energy) level at wavelengths greater than 228 Å. In the present paper, we extend this analysis for all the OP permitted resonance lines, i.e. lines connecting the ground level and excited fine-structure levels of the ground term to excited levels via optically allowed transitions (transitions between levels of opposite parity with $|\Delta L| \leq 1$, $|\Delta S| = 0$, $|\Delta J| \leq 1$, where L is the orbital, S the spin, and J the total angular momentum quantum number).

We retrieved from the TOPbase 0.7 database the gf-values for all multiplets which involve the ground term. These 6018 resonance multiplets include 23505 lines. In the OP calculations, relativistic effects are neglected, and LS-coupling is assumed throughout. We calculated the f-values of all individual lines in multiplets based on LS-coupling rules (Russell[8]). To assign accurate wavelengths to these lines, we made a compilation of experimental energy levels (complete to October 1995; references are given in Table A). Vacuum wavelengths calculated from experimental energy levels should be more reliable than measurements of individual resonance lines, because the experimental energy levels are based on the analysis of the whole experimental spectrum in each case. The number of digits we keep in the tabulated wavelengths is determined by accuracy of the experimental energy levels quoted in the corresponding papers. For some hydrogenic ions, Erikson[9] lists energy levels for various isotopes. In such cases, we used the values of energy levels of the most naturally abundant isotopes.

By this method, we assign accurate wavelengths to 5599 optically allowed LS-type lines in 1828 multiplets (references to the OP data are given in Table B). Beyond that, some gaps in the data still remain. Firstly, atomic data for Fe I and Fe II ions are not included in the TOPbase database. In the framework of the OP extension known as the Iron Project (Hummer et al.[10]), Nahar[11] calculated transition probabilities for 21,589 allowed transitions of Fe II which have experimentally determined wavelengths. We included in our compilation all resonance lines of Fe II from Nahar's paper. Multiplet tables for Fe I, which include 9759 lines, have been recently published by Nave et al.[12]. For our list, we selected the resonance lines of Fe I which have gf-values in the Nave et al. tables, and added the complete resonance multiplets of Fe I from the compilation by Morton[13]. Secondly, the OP calculations are based on LS-coupling, and only allowed LS-type lines are covered by our procedure. In particular, no data for lines of Ne I or Ar I can be obtained from the Opacity Project. To fill this gap, we included the resonance non-LS-type lines of Ne I and Ar I from the compilation by Verner et al.[5].

In the whole, we list accurate wavelengths, energy levels, statistical weights, transition probabilities and oscillator strengths for 5971 resonance lines. Intercombination (i.e. $|\Delta S| > 1$) and forbidden lines are not included in our compilation.

We calculated also the multiplet energy levels by averaging the weighted energy level values. The multiplet averaged wavelengths are calculated by use of the averaged energy levels. For multiplets where not all levels of the upper term are known, the averaged values are obtained from the available levels. For these cases, the averaged multiplet upper level and wavelength are not the "true" averaged values.

We subsequently used accurate wavelengths to improve the f-values calculated by the OP. The OP calculations give line strength S and transition energy E, where S is given by an integral over the atomic wave functions and does not involve E. Then gf-values are calculated from S and E since gf = const $\times S \times E$ (or gf = const $\times S/\lambda$). The OP used their theoretical values of E to calculate gf-values. To improve the gf-values we now use the more accurate experimental wavelengths instead of the theoretical E values. We recalculated the OP f-values as

$$f_{\mathrm{improved}} = f_{\mathrm{OP}} \times (\lambda_{\mathrm{OP}}/\lambda_{\mathrm{exp}}). \tag{1}$$

Transition probabilities are calculated from oscillator strengths in accordance with the standard formula:

$$A_{ki} = 6.670 \times 10^{15} g_i f_{ik}/(g_k \lambda^2) \ \ \mathrm{s}^{-1}, \tag{2}$$

where λ is in Å.

To estimate the accuracy of the calculated oscillator strengths and transition probabilities, we have compared the improved OP f-values for iron ions with the f-values taken from the National Institute of Standards and Technology (NIST) evaluated compilation of atomic transition probabilities (Fuhr, Martin, and Wiese[14]). Figure 1 shows this comparison for all the NIST resonance iron lines with estimated accuracy better than 10%. All these lines are strong transitions of the highly ionized (Fe XV and higher) ions. The agreement is remarkably good. The rms deviation of the improved OP f-values from the NIST f-values is 8.4%, and no values deviate by more than 15%. Note that all the NIST values are obtained by relativistic calculations, and relativistic effects should be more important for iron than for other OP elements. Generally, for the strong lines which can be classified as LS-type allowed transitions, the improved OP data are fairly accurate. The obtained oscillator strengths and transition probabilities are less accurate for weaker lines and for lines that are not pure LS-type, in particularly, for high l ($p-d$ and higher) transitions. We do not list here branching ratios which indicate the purity of LS coupling, since such data are available for a smaller portion of the lines only. However, special caution should be taken when using the listed oscillator strengths and transition probabilities for the lines of neutrals and first ions of the third row elements (Mg, Al, Si, S, Ar), especially for the weak lines.

The main incompleteness of our compilation comes from the fact that all lines which cannot be classified as allowed LS-type lines are not covered here (except Ne I and Ar I lines). However, the present compilation is accurate and complete for the permitted LS-type lines of all ionization states of 18 elements. This compilation is supplementary to the compilation of the resonance absorption lines above 912 Åby Morton[13], the compilation of ground level absorption lines above 228 Åby Verner et al.[5], and the NIST evaluated compilations of the atomic transition probabilities by Martin et al.[15], Fuhr et al.[14], Wiese et al.[16]).

Tables I and II in electronic form are available through anonymous ftp at asta.pa.uky.edu, directory dima/lines, or through the World Wide Web page “Atomic Data for Astrophysics”, http://www.pa.uky.edu/~verner/atom.html.

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EXPLANATION OF TABLES

Table I. Wavelengths and Oscillator Strengths of Permitted Resonance Absorption Lines
The data are sorted by element from H to Fe, ionization state (starting with neutral state), multiplet (starting with the largest averaged multiplet wavelength), and wavelength (decreasing wavelength within the multiplet). Theoretical energy levels are given in square brackets. The averaged multiplet data values of the listed levels and wavelengths are given in *italic*.

Species	Atom or ion
Transition	Electronic configurations of lower (ground term) and upper levels. If an upper level has an uncertain identification in the Opacity Project (OP), the relevant configuration is marked by semicolon (:) If the order of levels within a spectroscopic series in the OP does not coincide with the order of levels within the spectroscopic series stated in the corresponding source of experimental energy levels, the OP identifications are used, and the relevant configurations are marked by asterisk (*)
Multiplet	Terms of lower and upper levels
λ	Vacuum wavelength in Å
E_i, E_k	Energies of lower and upper levels in cm^{-1} If an upper level energy has a question mark in the source of experimental energy levels, we also indicate it and the corresponding wavelength by question mark (?) If experimental spectroscopy of the upper term is not complete, and the experimental energy of an upper level is unknown, we leave the upper level energy and the corresponding wavelength entries blank
g_i, g_k	Statistical weights of lower and upper levels
A_{ki}	Atomic transition probability in s^{-1}
f_{ik}	Absorption oscillator strength

Table II. Finding List of Lines
The lines are sorted by increasing wavelength.

λ	Vacuum wavelength in Å
Species	Atom or ion
g_i, g_k	Statistical weights of lower and upper levels
f_{ik}	Absorption oscillator strength

FIGURE CAPTION

Figure 1. Improved Opacity Project oscillator strengths (Eq. 1) vs. the oscillator strengths from Fuhr et al.[14] for iron lines which are classified by Fuhr et al.[14] as accurate to within 10%.