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# New Critical Compilations of Atomic Transition Probabilities

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**Abstract**

At the National Institute of Standards and Technology (NIST), we are continuing our critical evaluation and compilation work on atomic transition probabilities. We have recently concentrated our efforts on the spectra of Na, Mg, Al, Si and S – for all stages of ionization – and on Fe I and Fe II. These new compilations represent a drastic improvement in both quantity and quality over earlier NIST publications. We present a number of graphical comparisons in support of our data selections.

**Keywords:**

atomic transition probability, atomic ion, oscillator strength, line strength, sodium, magnesium, aluminum, silicon, sulfur, iron

The Atomic Spectroscopy Data Center at NIST has been involved in publishing critically evaluated atomic transition probabilities since the early 1960s. Our present work involves tabulating data for the elements sodium, magnesium, aluminum, silicon, sulfur and iron. These species were already compiled by us quite some time ago, but in the meantime, much new work has been done which enlarges and improves the database, mostly by sophisticated calculations. Thus, our new compilations contain about 5 – 10 times more transitions than the earlier NIST data volumes, and the uncertainties are generally significantly smaller. Often, we have compiled up to 1000 lines per spectrum.

In our evaluation procedure, we start by considering all published results. By applying certain general assessment criteria, we then narrow our considerations to the sources with the most accurate results. Our final numerical value for each line strength is obtained by averaging among these best data sources (sometimes there is only one clearly superior source), and an accuracy is assigned. NIST compilations are intended to be sources of standard reference data, so that data with large uncertainties are not included.

As a part of the NIST project of critically evaluating transition probabilities of elements from sodium to calcium, we have produced compilations for Na, Mg, Al, Si and S. For allowed transitions lying in the 20 – 170 Å spectral range, which is of special interest for the Chandra X-ray observatory, tables of transition probabilities for 24 ions of neon (Ne V – Ne VIII), magnesium (Mg V – Mg X), silicon (Si VI – Si XII) and sulfur (S VIII – XIV) have already been presented in [1]. In this new work, we consider all transitions (allowed and forbidden) for which experimental energies are known for both lower and upper energy levels. In general we list only lines for which the line strengths have estimated uncertainties of ±50% or less. Because of the very small amount of experimental results available for highly-charged ions, we had to use theoretical data for most transitions.

A large source of data for Na, Mg, Al, Si and S is the "Opacity Project" [2]. The Opacity Project R-matrix computations, which generally span quantum numbers up to $n = 10$ and $l = 4$, were performed in *LS* coupling. For the stronger transitions of many spectra, good agreement exists between the OP data and data from more detailed calculations which consider spin-orbit interactions. However, the agreement among the OP calculations and various relativistic calculations becomes worse for transitions between levels where one or both are appreciably mixed due to the breakdown of *LS* coupling. In general, the accuracy of computed line strengths decreases as the spectra become more complex. The calculations of Froese Fischer and co-workers [3] remain quite accurate, though they only span levels up to $n = 3$ (recently, some $n = 4$ levels have been included for Mg). These calculations were performed by the multiconfiguration Hartree-Fock (MCHF) method, including Breit-Pauli corrections, and some of those spectra were also performed by the multiconfiguration Dirac-Hartree-Fock (MCDHF) method. Another important source of reliable data is the configuration interaction code-version 3 (CIV3) method of Hibbert [4]. Transition probabilities computed using the many-body

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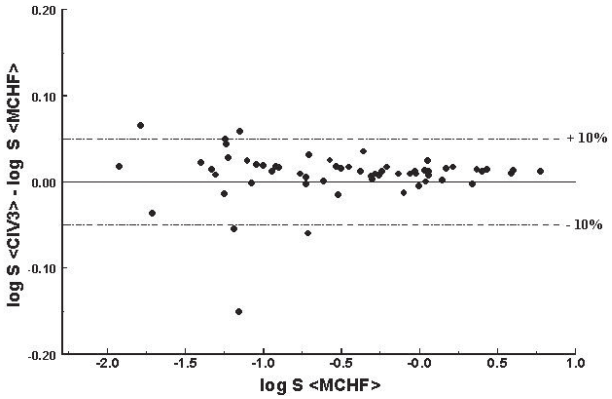


Fig. 1 Comparison of line strengths from the CIV3 [5] calculation with the MCHF [3] calculation for the Ne-like ion S VII. Allowed transitions.

perturbation theory with Breit-Pauli corrections are also quite accurate. Results from many other authors have been used as well.

In order to obtain reliable uncertainty estimates for the transition probabilities, we made graphical and numerical comparisons of the results of the various advanced calculations for as many transitions as possible. We present such a comparison for the Ne-like sulfur spectrum, S VII. Because of the important relativistic effects in this spectrum, we only considered calculations that include spin-orbit effects. A comparison for the allowed transitions between the CIV3 results of Hibbert *et al.* [5] and the MCHF data of Fischer [2] is given in Fig. 1. There is good agreement (within 10%) for most of these transitions.

For the spectra of Fe I and Fe II, we have mainly utilized recent experimental data obtained by a combination of accurate lifetime and emission branching-ratio measurements. These new compilations have been expanded to about 2400 lines for Fe I and 900 lines for Fe II. As shown below in Fig. 2, the improvement in both the quality and quantity of the data can be clearly seen. For Fe I, our data choices relied heavily on the accurate absorption data of Blackwell *et al.* [6] and the comprehensive emission/branching-ratio/lifetime data O'Brian *et al.* [7]. A comparison between these two data sources is shown in Fig. 3. In the case of Fe II, we also utilized data sources that combined lifetime measurements with branching fraction determinations. Such references include a series of experiments done at the University of Wisconsin [8] and a very recent paper by Schnabel *et al.* [9]. Figure 4 shows a comparison between these groups and supports our choice of data selections for this spectrum.

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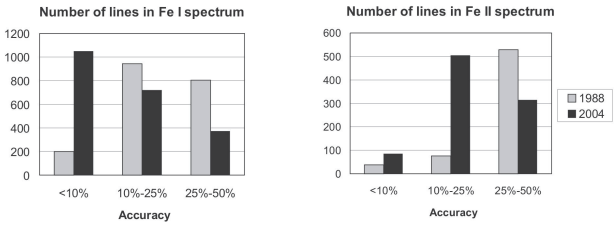


Fig. 2 Improvement in the f-value situation for Fe I and Fe II from 1988 to 2004

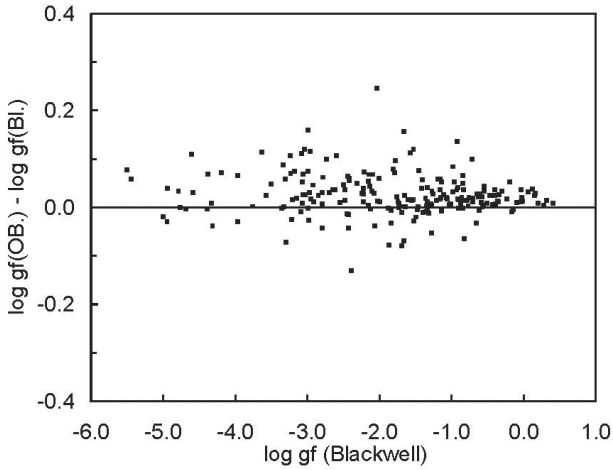


Fig. 3 Comparison between the emission/branching-ratio/lifetime data of O'Brian *et al.* [7] and the absorption data of Blackwell and co-workers [6].

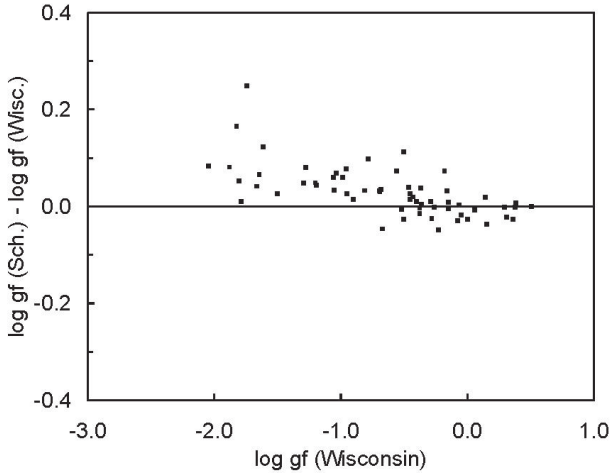


Fig. 4 Comparison between the emission experiments by Schnabel *et al.* [9] and the University of Wisconsin group [8].

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