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New Critical Compilations of Atomic Transition Probabilities for Neutral and Singly Ionized Carbon, Nitrogen, and Iron

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ABSTRACT

We have undertaken new critical assessments and tabulations of the transition probabilities of important lines of these spectra. For Fe I and Fe II, we have carried out a complete re-assessment and update, and we have relied almost exclusively on the literature of the last 15 years. Our updates for C I, C II and N I, N II primarily address the persistent lower transitions as well as a greatly expanded number of forbidden lines (M1, M2, and E2). For these transitions, sophisticated multiconfiguration Hartree-Fock (MCHF) calculations have been recently carried out, which have yielded data considerably improved and often appreciably different from our 1996 NIST compilation.

1. Introduction

Our new compilations of the atomic transition probabilities for neutral and singly ionized carbon, nitrogen, and iron have been mainly done in response to strong continuing interests and needs of the astrophysical community.

Those needs have also been responsible for significant experimental and theoretical activity on these spectra during the last ten-to-fifteen years that produced a large amount of new material after the publication of our earlier 1988 and 1996 tables [Fuhr (1988); Wiese (1996)]. Thus our earlier compilations are superseded by this new, enlarged edition which is produced in the same format.

2. Fe I and Fe II

For the allowed or electric dipole (E1) lines of Fe I, we have compiled data for 2425 transitions, an expansion of about 25%. All material originates from experimental sources.

For Fe II, the great majority of the data again comes from recent experiments, but this material is supplemented by some results of a new semi-empirical calculation. We compiled a total of 926 transitions, which is an increase of 42% from our earlier tables.

For the forbidden lines, specifically magnetic dipole (M1) and electric quadrupole (E2) transitions, the data situation is greatly improved for Fe II due to new comprehensive calculations as well as a few experimental checks. However, for Fe I, no activity has taken place in recent years, and consequently our earlier data tables remain unchanged.

Most of the new data are of significantly better quality than those listed in our earlier compilation. For example, 1050 allowed (E1) lines of Fe I are now estimated to have uncertainties less than ±10%, while only 199 lines were estimated to be this accurate in our 1988 compilation. Figure 1 shows the overall improvement graphically for the allowed lines of Fe I and Fe II.

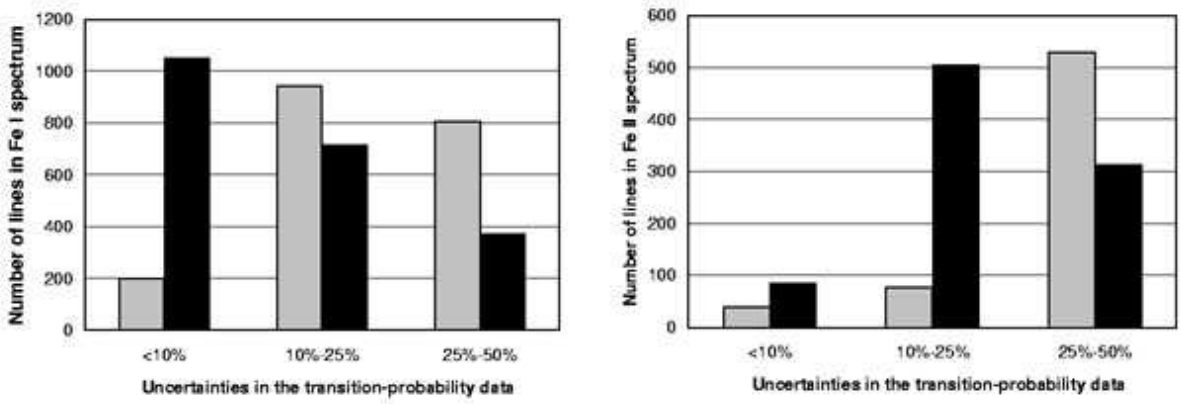

Fig. 1.— Improvement of the data quality for Fe I (left) and Fe II (right). The columns in gray show the number of lines for the three indicated uncertainty ranges compiled in 1988, the black columns show them for the new tables.

We provided detailed explanations of our data evaluation method and our error assessment in earlier transition probability compilations [Wiese (1996)] and will not discuss this here, in view of the very limited space. Our estimated uncertainties are again indicated by letter symbols from A to E as in our earlier data volumes [Fuhr (1988); Wiese (1996)].

3. C I and II, and N I and II

This compilation is a partial update of the NIST transition probability tables for these spectra. Data were previously compiled by us as part of a comprehensive tabulation for the three elements C, N, and O, that was published in 1996 [Wiese (1996)]. We have carried out this new compilation not only because of continuing strong user interest in these four spectra,

especially from astronomers, but also because data of significantly better quality have become available for the persistent transitions in these spectra. For numerous transitions, the new results have produced many significant changes in our tables. Also, data available for the electric-dipole-forbidden lines of the types M1, M2, and E2 were very limited at the time of the publication of our previous tables in 1996, but have now greatly increased. Thus, an update of the principal transition probability data for the four above-cited spectra appears to be timely.

Our 1996 data volume [Wiese (1996)] for C, N, and O was primarily based on the very extensive calculational results of the OPACITY Project [Opacity (1995)], a coordinated undertaking by an international group of about 20 atomic structure theoreticians. But we found from new, very detailed multiconfiguration-Hartree-Fock (MCHF) calculations and from recent lifetime and emission experiments that the OPACITY data are often not as accurate as we had estimated on the basis of limited available comparison data at the time of our previous compilation, that is, pre-1996. This statement applies especially to neutral and singly-ionized carbon and nitrogen.

We have thus carried out a partial update for the transition probabilities of C I, C II, N I and N II, especially utilizing the results of sophisticated MCHF calculations that were performed by Froese Fischer and coworkers in the last six years [Froese Fischer (2004); Zasarinny (2002); Frose Fischer (web site)]. Their multiconfiguration treatment has been very extensive, with wavefunction expansions containing up to 20 000 configuration state functions (CSFs). Also, they included relativistic effects of the Breit-Pauli type, i.e., spin-orbit, spin-spin and spin-other-orbit interactions as well as mass correction and Darwin terms. Thus, they obtained transition probabilities for individual lines including many intersystem and forbidden lines (E2, M1, and M2). The latter were completely missing in the OPACITY results for C and N.

Froese Fischer and coworkers presented their results in the "dipole length" form of the line strength, but they also calculated the "dipole velocity" form. Ideally, these two different formulations of the same quantity should of course agree, so that the differences remaining between the two are good indicators of the achieved accuracy. For each transition, they have listed the difference between the length and velocity results in percent. Indeed, in the best cases, the differences are quite small, of the order of 1–2%.

These new MCHF calculations [Froese Fischer (2004); Zasarinny (2002); Frose Fischer (web site)] are significantly more sophisticated and have been done in a more detailed manner than earlier calculations that were similar in spirit. Froese Fischer et al. also made use of the strong increase in computer power that is now available. Only a few high-accuracy experimental and theoretical results are available to closely test these calculations, especially the results for weaker transitions. Nevertheless, several meaningful comparisons are possible, and we have selected here a comparison with the recent calculations of Corrégé and Hibbert for C II [Corrégé (2002)]. They used the CIV3 code, which is also a sophisticated

multiconfiguration atomic structure code, and they applied it in a similarly detailed manner, with up to 6000 configuration state functions (CSFs). They calculated the line strengths in both the dipole-length as well as the dipole-velocity form, too, as in the work of Froese Fischer and coworkers. The agreement they achieved between these two formulations is nearly as good as Tachiev and Froese Fischer's results. It is thus useful to compare these two sophisticated calculations, which is done in Fig. 2. It is seen that over a wide range of oscillator strengths (gf-values), the agreement between the two calculations is excellent, with the differences never larger than 6%, even for the very weak transitions. To put this into perspective, graphical comparisons of earlier atomic structure calculations, including the Opacity Project calculations [Yan (1987)] always showed large scatter, of factors of two or more, for the weaker transitions.

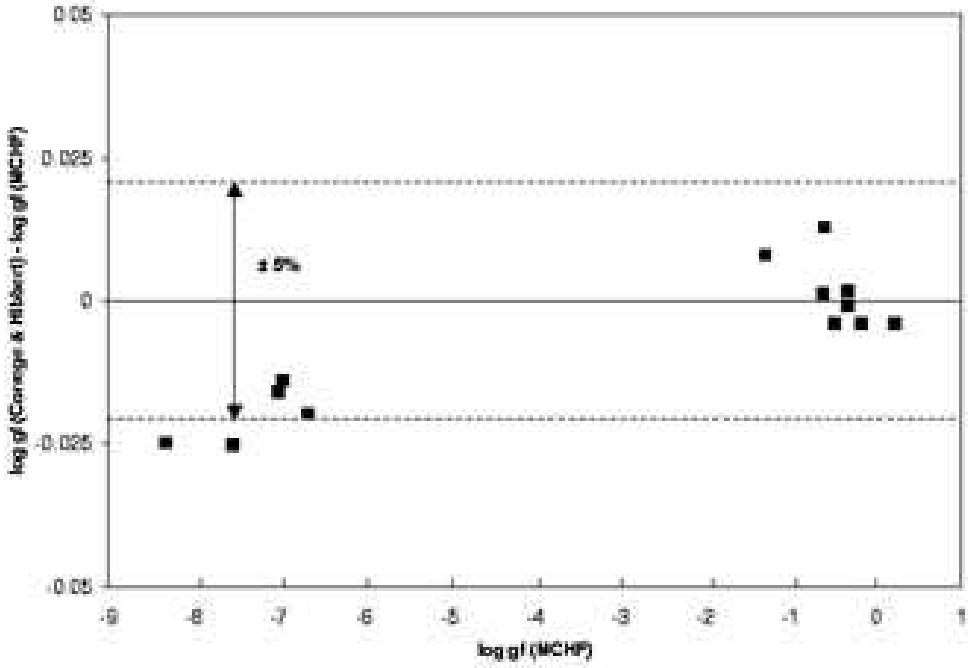

Fig. 2.— Comparison of results from the MCHF and CIV3 calculations, on a logarithmic scale, for C II.

4. Conclusion

We intend to enter all this new material into our comprehensive NIST Atomic Spectra Database (ASD) and publish it in the Journal of Physical and Chemical Reference Data.

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