Atoms **2014**, *2*, 215-224; doi:10.3390/atoms2020215

OPEN ACCESS

atoms

ISSN 2218-2004

www.mdpi.com/journal/atoms

Review

Validation and Implementation of Uncertainty Estimates of Calculated Transition Rates

Jörgen Ekman [1,*], **Michel R. Godefroid** [2] **and Henrik Hartman** [1]

[1] Materials Science and Applied Mathematics, Malmö University, Malmö SE-205 06, Sweden; E-Mail: henrik.hartman@mah.se

[2] Chimie Quantique et Photophysique, Université Libre de Bruxelles, Brussels B-1050, Belgium; E-Mail: michel.godefroid@ulb.ac.be

* Author to whom correspondence should be addressed; E-Mail: jorgen.ekman@mah.se; Tel.: +46-709-655-459.

Received: 31 January 2014; in revised form: 29 April 2014 / Accepted: 2 May 2014 / Published: 15 May 2014

Abstract: Uncertainties of calculated transition rates in LS-allowed electric dipole transitions in boron-like O IV and carbon-like Fe XXI are estimated using an approach in which differences in line strengths calculated in length and velocity gauges are utilized. Estimated uncertainties are compared and validated against several high-quality theoretical data sets in O IV, and implemented in large scale calculations in Fe XXI.

Keywords: transition rates; uncertainty; boron-like; carbon-like

1. Introduction

In recent years the field of computational atomic structure has benefited from, as it seems, a never-ending evolution of computer capacity. Together with sophisticated and refined theoretical methods, calculated properties of more complex atomic systems often reveal astonishing accuracy when validated against experimental observations and the term "spectroscopical accuracy" is used and justified [1–3]. This term refers to the high accuracy of experimental transition energies, and the level energies derived from these. Experimental techniques and calibration against frequency standards allow in general for determination of transition energies to an accuracy of 1 part in 10^5–10^{10} [4–6], excluding the spectacular frequency-comb measurements [7]. The knowledge of higher ionization stages

is usually less complete in coverage than for neutral or singly ionized atoms, and for many elements, only the lowest levels and transitions are known. Astrophysical emission line spectra are in a few cases the most accurate sources for transition energies [8]. Measured wavelengths have an accuracy sufficient to bench-mark the quality of the calculations.

Theoretical error bars are rarely reported for transition probabilities although it is in principle possible to calculate rigorous upper and lower bounds to dipole oscillator strengths from non relativistic quantum mechanics principles [9]. These bounds are however usually too distant for providing useful error estimates, even with elaborate electronic wave functions [10,11]. Experimental transition rates are scarce and associated with larger uncertainties than transition energies. Specific transitions can be accurately measured, but the majority of the transitions for higher ionization stages have unknown radiative rates. This is particularly true for the high excitation lines. Only in rare cases the transition rates can be measured directly; a more common method is the combination of radiative lifetimes and relative intensities for lines sharing a common upper or lower level. Although the requirement of detailed knowledge of the physical properties of the emitting plasma is circumvented using this approach, intensity calibration and lifetime measurements can be uncertain or even impossible. The most accurate and complete transition rates are found for low ionization elements, with typical uncertainties of 1%–20%.

The accuracy of calculated transition rates is often not even estimated and in many cases their quality is argued on the basis of comparisons with other theoretical works when available, or through other properties that are experimentally known, such as transition and excitation energies, hyperfine structure, etc., even if the considered observables are probing the quality of the electronic wave functions in rather different regions of the configuration space. This specificity can make the comparison severely misleading. The Atomic Spectra Database [12], on the other hand, is using a ranking based on the "extent of possible errors" which may be useful, but it is important to realize that the data used for the critical evaluation is sometimes not up to date. Altogether it is thus clear that properly validated methods for uncertainty estimates are needed. In this article one method, with variants, is validated against several recent calculations in O IV, and implemented in large scale calculations in Fe XXI.

2. Theoretical Background

To estimate *ab initio* atomic properties, wave functions must be calculated by solving the time-independent wave equation using a suitable Hamiltonian. The resulting wave functions are referred to as atomic state functions (ASFs) and are often expanded in configuration state functions (CSFs). Typically the coefficients of the CSFs are obtained by using a self-consistent procedure such as in the non-relativistic multi-configuration Hartree-Fock (MCHF) approach [13] or in the fully relativistic multi-configuration Dirac-Hartree-Fock (MCDHF) approach [14].

2.1. Transition Rates and Line Strengths

Given a set of atomic state functions , $\Psi(\gamma J)$, where J is the total angular momentum and γ is any other quantum number needed to describe the state, the transition rate for an electric dipole (E1) transition between an upper state u and a lower state l is given by

$$A(\gamma_u J_u, \gamma_l J_l) = \frac{4}{3}\alpha \frac{(E_{\gamma_u J_u} - E_{\gamma_l J_l})^3}{\hbar^3 c^2} \frac{S(\gamma_l J_l, \gamma_u J_u)}{2J_u + 1}. \quad (1)$$

In the expression above α is the fine structure constant, $E_{\gamma_u J_u} - E_{\gamma_l J_l}$ is the transition energy and $S(\gamma_l J_l, \gamma_u J_u)$ is the line strength which, in the non-relativistic case and the commonly used length form, can be written

$$S_{len}(\gamma_l J_l, \gamma_u J_u) = \left| \langle \gamma_l J_l || \sum_{i=1}^{N} r(i) \mathbf{C}^{(1)}(i) || \gamma_u J_u \rangle \right|^2 \quad (2)$$

where $\mathbf{C^{(1)}}$ denotes the renormalized spherical harmonics of rank 1. Sometimes the line strength is also expressed in the velocity form [15]:

$$S_{vel}(\gamma_l J_l, \gamma_u J_u) = \left(\frac{\hbar^2}{m_e} \right)^2 \frac{1}{(E_{\gamma_u J_u} - E_{\gamma_l J_l})^2} \left| \langle \gamma_l J_l || \sum_{i=1}^{N} r(i) \boldsymbol{\nabla}^{(1)}(i) || \gamma_u J_u \rangle \right|^2 \quad (3)$$

As shown by Grant [16], the dipole length and velocity expressions, Equations (2) and (3), can be obtained from the nonrelativistic limit of the Babushkin and Coulomb gauges that are used in the fully relativistic calculations.

For allowed E1 transitions we must have $\Delta J = 0, \pm 1$ $(0 \nleftrightarrow 0)$, and to qualify as LS-allowed transitions we also require the more approximate selection rules $\Delta S = 0$ and $\Delta L = 0, \pm 1$ $(0 \nleftrightarrow 0)$. In addition, E1 transitions are always associated with a parity change $\Delta\pi = \pm 1$, with $\pi = (-1)^{\sum_i \ell_i}$.

2.2. Accuracy Estimates

In a work by Froese Fischer [17], the use of calculated line strengths in length and velocity gauges as a measure of a theoretical uncertainty is discussed in detail. It is argued that a plausible estimate of the uncertainty of LS-allowed transition rates, $\delta A'$, is given by

$$\delta A' = (\delta E + \delta S)\, A' \quad (4)$$

where A' is the energy-scaled transition rate computed from the observed transition energy (E_{obs}), $\delta E = |E_{calc} - E_{obs}|/E_{obs}$ is the relative error in the transition energy and $\delta S = |S_{len} - S_{vel}|/\max(S_{len}, S_{vel})$ is the relative discrepancy between the length and velocity forms of the line strengths. Alternatively, one may estimate the transition probability uncertainty from

$$\widetilde{\delta A'} = |A'_{len} - A'_{vel}|/\max(A'_{len}, A'_{vel}) \quad (5)$$

where the energy-scaled length (A'_{len}) and velocity (A'_{vel}) transition rates are estimated according to

$$A'_{len} = A_{len} \left(\frac{E_{obs}}{E_{calc}} \right)^3 \quad (6)$$

$$A'_{vel} = A_{vel} \left(\frac{E_{obs}}{E_{calc}} \right) \quad (7)$$

in which the energy-scaled velocity form of the line strength $S'_{vel} = S_{vel}(E_{calc}/E_{obs})^2$ has been used.

In cases when the observed transition energy is not known, a natural simplification of Equation (4) is to omit the δE term and use the unscaled *ab initio* transition probability A to estimate the uncertainty:

$$\delta A = (\delta S)A \tag{8}$$

A quantity related to $\delta A/A$ above, that is also used for assessing the accuracy of theoretical transition rates [2], is the ratio of obtained transition probabilities in length and velocity gauges, $R = A_{len}/A_{vel}$. By comparing with Equation (8) it is seen that $|R-1| = \delta A/A$ for $A_{vel} > A_{len}$ and $|R-1| > \delta A/A$ otherwise.

3. Statistical Analysis of Calculated Transition Rates in O IV

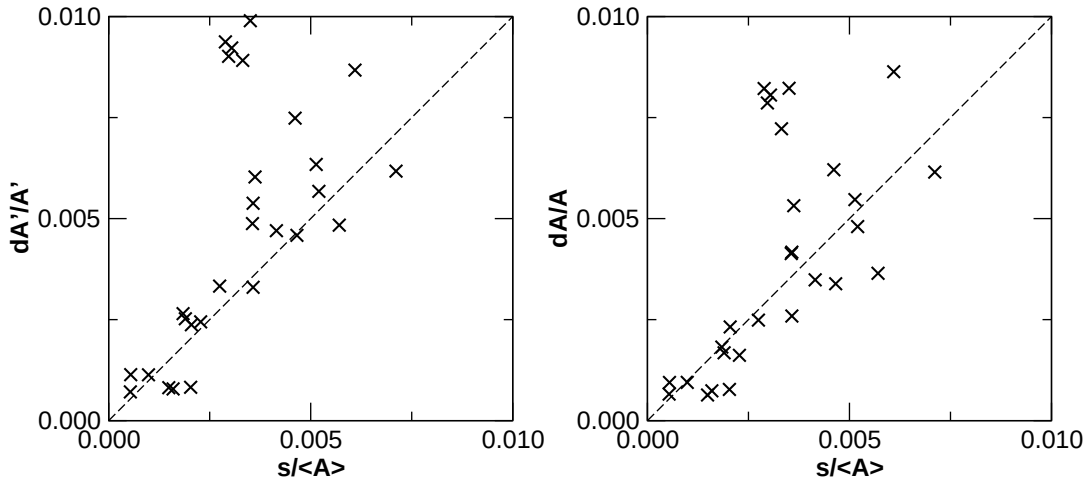
3.1. LS-Allowed Transitions

Boron-like oxygen (O IV) turns out to be a very suitable system for the validation of the uncertainty estimates discussed above. The reason for this is that no less than four recent works have been realized on this ion, leading to four sets of calculated transition rates for LS-allowed electric dipole transitions between states belonging to the odd parity $2s^2 2p$ and $2p^3$ configurations and the even parity $2s2p^2$ configuration [18–21]. These data sets result from different computational strategies and correlation models, consisting in non-relativistic variational calculations, capturing relativistic corrections through the Breit-Pauli approximation [18,19], and fully relativistic [20,21] methods, using either numerical approaches [18,21] or analytic basis sets [19,20]. Other calculations do exist [22–24] but cannot easily be used in our statistical analysis. Altogether, four completely independent sets of transition rates for 28 LS-allowed E1 transitions in O IV are available [18–21] in which the reported transition energies are of similar accuracy and accurate enough, on the per mille level, to support the approximation $A \approx A'$ as a first reasonable indicator of the quality of the wave functions. The full compilation of the calculated transition rates is given in [21] where also length and velocity values are reported. This unique situation allows for a meaningful statistical analysis in which the sample standard deviation s can be used as measure of the uncertainty of the calculated transition rates:

$$s = \sqrt{\frac{1}{M-1}\sum_{j=1}^{M}(A_j - \bar{A})^2} \tag{9}$$

where $\bar{A}$ is the mean value from the sample, $\bar{A} = \langle A \rangle = \frac{1}{M}\sum_{i=1}^{M} A_i$, and $M = 4$ is the number of independent data sets. In the left panel of Figure 1, $\delta A'/A'$ from Equation (4) is plotted against the quantity $s/\bar{A}$ for the LS-allowed electric dipole transitions mentioned above. It is seen that the two quantities are strongly correlated for individual transitions and on average, s is well described by $\delta A'$ (the dashed line represents $\delta A'/A' = s/\bar{A}$). In the right panel of Figure 1, the *ab initio* relative uncertainty $\delta A/A$ calculated from Equation (8) is plotted against $s/\bar{A}$ with a similar result, confirming that the observed and calculated transition energies agree well and that δS is the dominating factor in Equation (4) in this case. On average it is found that $\delta A'/A' = 0.48\%$ and $\delta A/A = 0.40\%$ are slightly overestimating $s/\bar{A} = 0.32\%$, which is preferred instead of an opposite scenario .

Figure 1. Left panel shows $\delta A'/A'$ vs $s/\bar{A}$ and right panel shows $\delta A/A$ vs $s/\bar{A}$ for 28 LS-allowed E1 transitions in O IV. Transition rates are taken from [21]. See text for details.

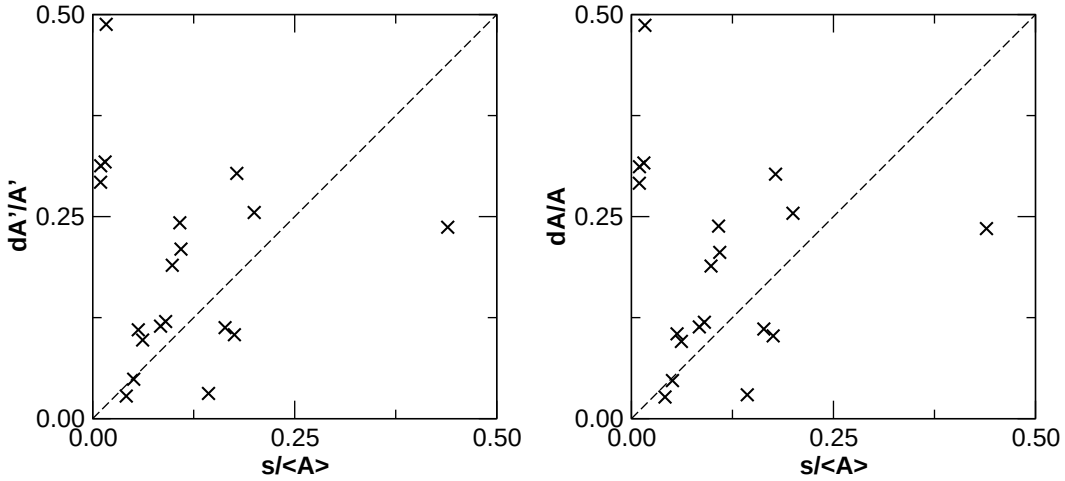


The same transitions in the NIST Atomic Spectra Database [12] are all labeled with accuracy ranking "B", which means that the estimated accuracy of the transition probabilities is $\leq$10%. Comparing the NIST recommended transition rates with $\bar{A}$, a mean relative difference of 1.9% is obtained and the largest deviation for any transition amounts to 6.7%, indicating that the ASD accuracy ranking largely overestimates the uncertainty.

3.2. Intercombination Transitions

LS-forbidden transitions in the non-relativistic framework may become allowed in the relativistic case due to small admixtures of different LS components in the wave functions. This is, for example, the case in intercombination transitions for which $\Delta S \neq 0$. In the work by Froese Fischer [17], it was argued that the discrepancy in the length and velocity form of the line strength is no longer a reliable indicator of the uncertainty and instead the accuracy of the energy separation between levels of the same J and parity should be used. Although these observations are based on the rigorous demonstration that the uncorrected velocity gauge transition operator does not hold in Breit-Pauli calculations [25,26], we adopt here a more pragmatic approach consisting in using the same approach as for the LS-allowed transitions for testing the reliability of the uncertainty estimate of the spin-forbidden transition rates. For intercombination lines in O IV however, only three datasets are available [18,19,21] and therefore $M = 3$ is used for the sample standard deviation and mean value. The results are shown in Figure 2, illustrating that $\delta A'/A'$ and $\delta A/A$ are correlated with $s/\bar{A}$, but to a less extent than for the LS-allowed transitions. It is also seen that the estimated uncertainties are more than an order of magnitude larger (on average $\delta A'/A' = 19.0\%$, $\delta A/A = 18.8\%$ and $s/\bar{A} = 10.8\%$) and that δS is even more dominating (the left and right panels of Figure 2 are virtually identical). In this case $\delta A'/A'$ and $\delta A/A$ can no longer be used as an uncertainty estimate for each individual transition rate. However, for the sample as a whole they are still reasonable indicators of the average uncertainty.

Figure 2. Left panel shows $\delta A'/A'$ vs $s/\bar{A}$ and right panel shows $\delta A/A$ vs $s/\bar{A}$ for 20 intercombination E1 transitions in O IV. Transition rates are taken from [21]. See text for details.



4. Uncertainty Analysis of Calculated Transition Rates for Increasing Orbital Sets in O IV

From the small sample variance indicated in Figure 1, it makes sense to assume that $\bar{A}$ is close to the actual value. This in turn makes it possible to monitor the relative error in the transition rates as a function of successively increased orbital sets. For this reason the calculations described in [21] were reproduced using the latest version of the GRASP2K package [27] and in the following a brief summary of the computational method will be given. As a starting point a multireference consisting of 8 CSFs in the even parity $2s2p^2$ configuration and 7 CFSs in the odd parity $2s^22p$ and $2p^3$ configurations were chosen, including the $J = 1, 2, 3, 4, 5$ symmetries for both parities. Initially Dirac-Fock (DF) calculations in the extended optimum level (EOL) scheme [14] were performed for each parity, followed by multiconfiguration calculations allowing for single and double (SD) excitations within the $n = 2$ orbital set. The active orbital sets were then gradually increased to $n = 3, 4, 5..., 9$ including angular momentum up to $l = 5$ (restricted to $l = 4$ for $n = 9$) and using SD excitations within each orbital set. In addition an extended multireference was used for $n = 9$. Finally, relativistic configuration interaction (RCI) calculations [27] were performed taking into account the Breit interaction and leading QED effects and within rounding errors, the published level energies and transition rates in [21] were reproduced. For each orbital set n, the transition rates $\{A^n\}$ were obtained and compared with $\bar{A}$ and a relative error represented by the root mean square (rms) of the relative deviation for all $N = 28$ LS-allowed E1 transitions was calculated:

$$|A^n - \bar{A}|/\bar{A} = \sqrt{\frac{1}{N}\sum_{k=1}^{N}\left(\frac{A_k^n - \bar{A}_k}{\bar{A}_k}\right)^2} \tag{10}$$

In Figure 3, the relative errors calculated from Equation (10), $|A^n - \bar{A}|/\bar{A}$, are compared, for the different active orbital sets n, with the ratios

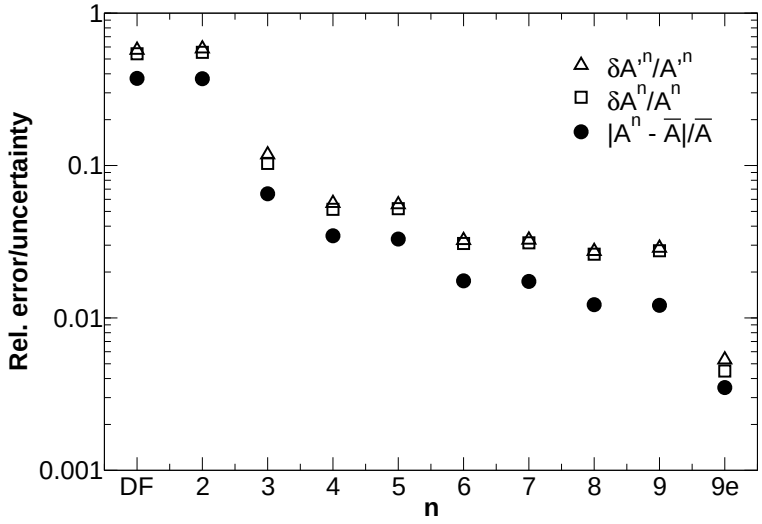
$$\delta A'^{\,n}/A'^{\,n} = \sqrt{\frac{1}{N}\sum_{k=1}^{N}(\delta A_k'^{\,n}/A_k'^{\,n})^2} \tag{11}$$

and

$$\delta A^n/A^n = \sqrt{\frac{1}{N}\sum_{k=1}^{N}\left(\delta A_k^n/A_k^n\right)^2} \tag{12}$$

estimated from Equations (4) and (8), respectively. From the figure it is seen that, although $\delta A'^n/A'^n$ and $\delta A^n/A^n$ are slightly larger than $|A^n-\bar{A}|/\bar{A}$, the uncertainty estimates are strongly correlated with the actual errors, which indeed is encouraging and again fully justifies the use of the uncertainty estimates.

Figure 3. Relative error (solid dots) compared with uncertainty estimates (open symbols) against active orbital set expansion in calculations. DF and 9e stands for Dirac-Fock and $n = 9$ with an extended multireference, respectively. See text for details.



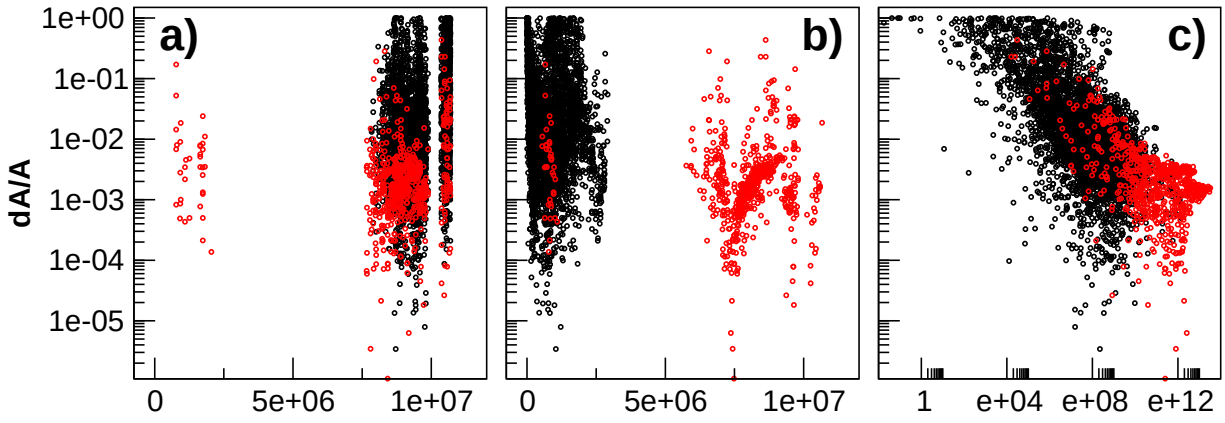
5. Implementation of Uncertainty Estimates in Carbon-Like Fe XXI

Very recently, large-scale calculations in C-like systems using the GRASP2K package have been performed including 130 even parity and 132 odd parity states [1]. Transition rates for all possible electric dipole transitions between the states were derived and the quality of the obtained transition rates was indicated with the ratio R, as defined above. In this work we estimate the uncertainties in the calculated transition rates by using Equation (8) and in Figure 4, $\delta A/A$ is plotted against calculated excitation energies of upper levels, calculated transition energies and calculated transition rates in the length gauge for 4637 LS-allowed E1 transitions in carbon-like Fe XXI.

In panel (a) it is seen that the energy levels in Fe XXI are clearly divided into two parts, where the lower part consists of levels belonging to the even parity $2s^22p^2$ and $2p^4$ configurations and the odd parity $2s2p^3$ configuration whereas the upper part (divided into two sub blocks) consists of configurations of both parities that include one electron in either the $n = 3$ and $n = 4$ shells. We conclude from panels (a) and (b) that most of the transitions (3914) occur between levels in the upper part and that these transitions on average have a lower transition energy and a larger relative uncertainty (0.074) than transitions where the lower levels belong to the lower part (relative uncertainty of 0.007). Panel (c) shows the uncertainty estimate $\delta A/A$ as a function of transition probabilities, which span over approximately 15 orders of magnitude. It is evident that there is, on average, a strong correlation between the transition probability

and the estimated uncertainty, which is not surprising. For smaller transition rates cancellation effects are often present which increase the uncertainty. For the entire sample the average estimated uncertainty is 0.064.

Figure 4. Uncertainty estimate $\delta A/A$ plotted against calculated excitation energies of upper levels (**a**); calculated transition energies (**b**) and calculated transition rates (**c**) for 4637 LS-allowed E1 transitions in carbon-like Fe XXI. Data points in red indicate transitions where the lower level belongs to the lower energy structure of Fe XXI. See text for details.



6. Conclusions

A suggested method for estimating uncertainties of calculated transition rates for LS-allowed E1 transitions has been investigated and validated against a statistical analysis of several recent calculations in boron-like O IV. Together with an analysis of the evolution of transition rates as a function of the size of the active orbital set, it is seen that the estimated errors are correlated with and very close to the presumed actual errors. A validation of the method extended to intercombination lines in O IV reveals a smaller correlation in the statistical analysis and suggests that the uncertainty estimate in this case should only be used if averaging over a larger sample. In addition, estimated uncertainties of transition rates are calculated for 4637 LS-allowed transitions in carbon-like Fe XXI. The results emphasize the strong correlation between the magnitude of the transition rates and their estimated uncertainties. Altogether , we conclude that, at least for lighter systems where relativistic effects are small, the discrepancy between the length and velocity form in transitions rates is a reliable indicator of uncertainties of transition rates. This is especially the case for LS-allowed transitions but also, to a less extent, for intercombination lines if the average uncertainty for the sample as a whole is considered. Further validation is needed for heavier systems. Until then, it is recommended to report transition probabilities for LS-allowed E1 transitions with the uncertainties estimated by using the proposed procedure.

Acknowledgments

This work was partially supported by the IUAP Belgian State Science Policy (Brix network P7/12) and the Swedish Research Council (621-2011-4206).

Author Contributions

Each author contributed to all aspects of this work.

Conflicts of Interest

The authors declare no conflicts of interest.

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