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Semi-empirical calculations of oscillator strengths and hyperfine constants for Ti II

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ABSTRACT

As the result of our studies on the atomic structure of complex atoms we produced high quality wave functions for both the even and odd systems of configurations. The quality of wave functions was proved via comparison of the expected and experimental hyperfine structure constants and g_J-factors. These wave functions were used for the parametrization of the oscillator strengths for electromagnetic transitions in Ti II, where reliable experimental data were available. The least squares fit to experimental values for some transitions, published in the NIST Atomic Spectra Database, allowed us to obtain the values of transition integrals and parametrize the oscillator strengths.

1. Introduction

Accurate oscillator strengths (*gf*-values) are among the most important kinds of atomic data. They are of particular importance in astronomy, for reliable determinations of chemical abundances in stellar atmospheres, in plasma physics, and for comparison with theoretical works. A powerful method for obtaining absolute oscillator strengths (or, equivalently, *f*-values and transition probabilities) is to combine measurements of normalized relative line intensities from a given energy level (branching fractions) with an absolute measurement of the level lifetime [1].

There are available several reasonably accurate experimental studies of oscillator strengths of Ti II, including those of Wobig [2], Wolnik and Berthel [3], Roberts et al. [4,5], Danzmann and Kock [6], Blackwell et al. [7], Pickering et al. [8], Wiese et al. [9] and Wood et al. [10].

In 1941, King published the results of relative *gf*-values measurements for 63 Ti II lines by means of the absorption technique [11]. The *gf*-values of 108 lines determined by the emission method from a vortex-stabilized arc were published by Tatum in 1961 [12]. The results presented in both papers had to be corrected for a significant error in the temperature of the source, as well as self-absorption. In 1962, Wobig measured the oscillator strengths for 33 Ti II lines using the emission method [2]. The shock-tube measurements of absolute *gf*-values for neutral and singly ionized titanium were carried out by Boni in 1968 [13] and Wolnik and Berthel in 1973 [3].

A comprehensive experiment of Roberts, Andersen and Sørensen [4] (hereafter RAS) combining the techniques of beam-foil atomic lifetimes and branching ratios by use of a gas flow-stabilized arc reported the absolute oscillator strengths for approximately 300 Ti II transitions and the relative oscillator strengths for 75 more. In 1975, Roberts et al. made emission measurements of 149 relative oscillator strengths for Ti II lines, converted to the absolute scale using RAS data [5]. In the same year, a critical data

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compilation of transition probabilities for allowed lines for scandium and titanium was published by Wiese and Fuhr [14]. Danzmann and Kock in 1980 determined the oscillator strengths from a combination of hook and emission measurements [6]. In 1982, relative oscillator strengths were precisely determined for 18 lines of Ti II by Blackwell, Menon and Petford, using the Oxford furnace technique [7]. The relative values were put on an absolute scale by use of lifetime measurements. The subsequent data compilation of transition probabilities for elements from scandium through manganese was published by Martin et al. in 1988 [15].

In 1990, Savanov et al. [16] published a catalog of oscillator strengths incorporating weighted measurements from 10 sources, with lifetimes rescaled where relevant to the beam foil measurements of Roberts et al. [4]. This catalog contains 419 lines from 244 to 542 nm and includes the results of Danzmann and Kock [6] by a combination of emission and hook methods for 67 lines in the range 305–542 nm. In 1994, Ryabchikova [17] renormalized existing data for the visible region to absolute astrophysical values and obtained good agreement with Danzman and Kock. The astrophysical oscillator strengths were determined by Kostyk and Orlova [18] from the Liege solar atlas. The measurements of radiative lifetimes for 42 levels of Ti II were carried out by Bizzarri et al. [19] by using the time-resolved laser fluorescence on slow ionic beams. Transition probabilities for 100 lines between 305 and 993 nm, originating from seven of these levels were obtained from branching fractions measured by high resolution Fourier transform spectroscopy (FTS) at the US National Solar Observatory. The measurements of the oscillator strengths for the Ti II vacuum ultraviolet resonance transitions at $\lambda_{vac} = 191.0938$ nm and 191.0609 nm using the High Sensitivity Absorption Spectroscopy Experiment at the Synchrotron Radiation Center in Stoughton were reported by Wiese et al. in 2001 [9]. In the same year, Pickering, Thorne and Perez published the relative intensities of 694 emission lines of Ti II between 187 nm and 602 nm from 89 levels measured by high-resolution Fourier transform spectrometry, using a hollow cathode lamp as light source [8]. Recently, Wood, Lawler, Sneden and Cowan reported transition probability measurements for 364 lines in the UV through near-IR spectral region [10].

The extensive calculations of energy levels and *gf*-values for astrophysically important atoms and ions provided by Kurucz [20–23] also include Ti II. His *gf*-values for strong lines are well known to agree rather well with experimental values, but for weak lines they are inevitably more uncertain.

Recently, we have performed a method for determining oscillator strengths that is an alternative to the commonly used, purely theoretical calculations, or to the semi-empirical approach combined with theoretically calculated transition integrals [24]. The angular coefficients of the transition matrix in pure *SL* coupling were found from straightforward Racah algebra. The transition matrix was transformed into the actual intermediate coupling by the fine structure eigenvectors obtained from the semi-empirical approach. The transition integrals were treated as free parameters in the least squares fit to experimental *gf* values. As an example, the results of the calculation for the electric dipole transitions for Sc II were presented. The system under consideration contains configurations with two electrons on open shells. In the present paper, we applied our method for configuration with three electrons on open shells, using numerous data available for the titanium ion.

2. Fine structure eigenvectors

For the purpose of this study we used the parametrization method, taking into account both the first-order effects of perturbation theory (electrostatic, spin–orbit and mixed magnetic interactions) and its the second-order effects (effective electrostatic interactions and electrostatically correlated spin–orbit interactions) [25–28].

The fine structure angular coefficient matrices for the multiconfiguration system, necessary for the least-squares fitting program can be constructed with the use of our own computer code. Having constructed the energy matrix, it is necessary to determine the magnitudes of radial integrals occurring there, so that the matrix elements may be put into numerical form ready for diagonalization. The radial integrals can be evaluated in semi-empirical calculations, based on the least-squares fitting procedure of the calculated eigenvalues to the observed energy levels (*fs* LSQ-fit), where radial integrals are considered as adjustable parameters.

We have performed calculations on many-configuration approximations, which means that the extended basis system used in this work consists of 61 configurations, both even and odd.

Even configuration system:

$$\begin{aligned}
&3d^3 + \sum_{n'=4}^{10} 3d^2 n's + \sum_{n''=4}^{10} 3d^2 n''d + \sum_{n'''=5}^{9} 3d^2 n'''g + 3d4s^2 \\
&+ \sum_{n'=5}^{10} 3d4sn's + \sum_{n''=4}^{10} 3d4sn''d + \sum_{n'''=5}^{9} 3d4sn'''g + 3d4p^2 \\
&+ 3d4d^2 \quad + 3d4p4f + 4s4p^2 + \sum_{n'=5}^{10} 4s^2 n's \\
&+ \sum_{n''=4}^{10} 4s^2 n''d + \sum_{n'''=5}^{9} 4s^2 n'''g.
\end{aligned}$$

Odd configuration system:

$$\begin{aligned}
&\sum_{n'=4}^{10} 3d^2 n'p + \sum_{n''=4}^{10} 3d^2 n''f + \sum_{n'''=6}^{10} 3d^2 n'''h + \sum_{n'=4}^{10} 3d4sn'p \\
&+ \sum_{n''=4}^{10} 3d4sn''f + \sum_{n'''=6}^{10} 3d4sn'''h \\
&+ 3d4p4d + 3d4p5s \\
&+ 3d4d4f + 3d4p4f + 4p^3 + \sum_{n'=5}^{10} 4s^2 n'p \\
&+ \sum_{n''=4}^{10} 4s^2 n''f + \sum_{n'''=6}^{10} 4s^2 n'''h.
\end{aligned}$$

For the systems composed of many Rydberg configurations, in our earlier works [29,30], we showed how to reduce the number of free parameters by the relation between radial parameters differing only by the principal