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New levels of Ta II with energies higher than 72,000 cm^{-1}

Zaheer Uddin [b], Laurentius Windholz [a,*]

[a] Institute of Experimental Physics, Graz University of Technology, Petersgasse 16, Graz 8010, Austria
[b] Department of Physics, University of Karachi, Karachi 75270, Pakistan

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ABSTRACT

We studied the hyperfine structure of Tantalum lines appearing in a high-resolution Fourier transform spectrum. Hundreds of lines of Ta in this spectrum are still unclassified; most of them, especially in the UV region, belong to Ta II. When investigating such lines we found 14 new levels of Ta II. These new levels are the highest-lying known Ta II levels and do not belong to the already known configurations.

1. Introduction

The key work concerning the classification of Ta II spectral lines is the monograph of Kiess [1]. He not only summarized older results (most of them from himself) of known energy levels, but also introduced a huge number of levels. The Ta II results in the famous tables of Moore [2], even published earlier in 1958, are based mainly on results of Kiess. The first measurements on the hyperfine (hf) structure of Ta I and II lines were published by Brown and Tomboulian [3], who were able to determine the magnetic moment and the electric quadrupole moment of the Ta^{181} nucleus. Wyart and Blaize later introduced further energy levels [4,5]. M. Eriksson et al. analyzed the Ta II spectrum in 2002 taken by a Fourier transform (FT) spectrometer with respect to astrophysical applications. They determined the hf constants of many levels and gave improved center of gravity (cg) wavenumbers of Ta II levels [6]. Messnarz discovered in his PhD work some new Ta II levels and corrected some classifications by means of laser spectroscopy. He also determined the hf constants of several Ta II levels with high accuracy [7,8]. Zilio and Pickering analyzed a FT spectrum and could give a number of hf constants for levels, for which these numbers were not known before [9]. Later on, improved FT spectra from the Kitt Peak observatory and the spectra of the group of J.C. Pickering at Imperial College became available to our group in Graz and did lead to a remarkable improvement of our investigations concerning Ta I and Ta II [10]. The first results on Ta II were reported already in Refs. [11,12]. Accompanying theoretical investigations were made by the group of Dembczynski, but are still published only partly as conference contributions [13–15].

Despite all these efforts, it is still not possible to give a complete picture of the electronic structure of Ta II since a number of energy levels is missing. The levels found during this study belong to new configurations of Ta II. All results presented here are derived from an analysis of the FT spectrum; no laser excitations of the classified lines could be performed since all are in the violet or ultraviolet regions.

2. Hyperfine structure

Atoms, whose nuclei have an even number of nucleons, in most cases have a nuclear spin quantum number $I=0$

* Corresponding author.
E-mail address: windholz@tugraz.at (L. Windholz).

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and show no hf structure. For nuclei with I > 0, there exist two important hf interactions, namely (i) magnetic dipole interaction, and (ii) electric quadrupole interaction.

The magnetic dipole interaction is the interaction of the nuclear magnetic moment $\vec{\mu}$ with the averaged magnetic field $\vec{B}$ produced by the electrons at the site of the nucleus, and the electric quadrupole interaction is caused by the quadrupole moment $\vec{Q}$ of the nucleus and the average gradient of the electric field produced by the electrons at the site of the nucleus. Both the interactions remove the degeneracy of the fine structure levels. The manifold of quantum numbers *F*, which characterize the hyperfine structure levels, spans from $|J-I|$ to $J+I$ (step 1). For the angular momenta, $\vec{F}=\vec{J}+\vec{I}$ is valid.

The energy shift of a hyperfine level having quantum number *F*, with respect to the fine-structure cg energy, is given by

$$\Delta E(F) = A\frac{C}{2} + B\frac{3C(C+1)/2 - 2IJ(I+1)(J+1)}{4IJ(2I-1)(2J-1)}$$

$$C = F(F+1) - I(I+1) - J(J+1)$$

where *I* is the nuclear spin quantum number, *J* is the total angular quantum number of the electronic shell, and *F* is the total angular momentum quantum number of the atom. *A* is the magnetic dipole hyperfine constant and *B* is the electric quadrupole hyperfine constant.

The two terms show the contributions of magnetic dipole interaction and electric quadrupole interaction, respectively. The investigated Ta isotope with mass number 181 (natural abundance 99.988%) has a nuclear spin quantum number $I=7/2$, $\mu=+2.3705(7)\vec{\mu}_N$, $Q=+3.28(6)\times 10^{-28}\ \mathrm{m}^2$ [16].

A spectral line, treated as a transition between two combining energy levels, shows a hf pattern composed by the hf structure of both upper and lower levels. Thus the hf structure of a transition contains a “finger print” of the combining levels, and the levels can be identified through their hf constants.

For the relative intensities of the hf components of a spectral line we used

$$I_{rel}(F \to F') = \frac{(2F+1)(2F'+1)}{2I+1}\begin{Bmatrix} J & F & I \\ F' & J' & 1 \end{Bmatrix}^2$$

where the prime notes the lower level, and {..} is a 6*j*-symbol [17].

3. Hyperfine resolved lines of the Fourier transform spectrum

The FT spectra available to us were recorded at the Imperial College London and the Kitt Peak observatory and cover the range from 2120 Å up to 47,000 Å [9,10]. The resolution of the FT spectra were chosen between 0.03 and 0.05 cm^{-1} in order to obtain high sensitivity and to resolve the Doppler width of the lines as good as possible. The observed line profiles of a single hf component of a Ta line could be best approximated by using a Gaussian profile (width ca. 2700 MHz or 0.09 cm^{-1} at wavelengths between 3800 and 3000 Å). In some cases the hf structure pattern is smaller than this Gaussian width, and the hf components could not be individually resolved. In other cases, if the hf splitting of the lines is large enough, it is possible to fit the hyperfine structure and obtain the angular momenta *J* and the hyperfine constants of the levels involved in the transitions. In order to illustrate this, the hyperfine structure of the Ta I line 3484.618 Å is shown in Fig. 1. Assuming a Gaussian width of 800 MHz, as can be obtained in laser spectroscopic recordings, the position of the highest components of the structure can be seen clearly, and the hf pattern is fairly well resolved. For a Gaussian width of 2700 MHz (as in our spectrum), the whole hyperfine structure is completely masked. In such cases it is very difficult or even impossible to extract the hyperfine constants of the involved levels from the line profile. To the contrary, if the hf splitting is large enough, as in the example shown in Fig. 2, it is possible to

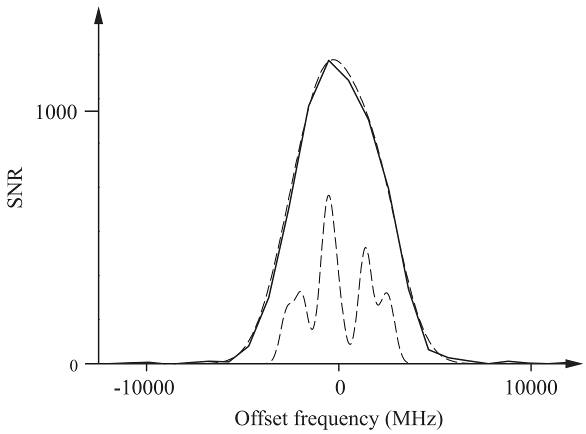

Fig. 1. Hyperfine structure of the Ta I line at 3484.618 Å. The Gaussian widths are (i) 800 MHz, as may be observed by laser spectroscopy, (ii) 2700 MHz. The hyperfine structure is completely masked if the Gaussian width is high (dashed line). The solid line shows the line profile observed in the FT spectrum. A small asymmetry of the FT line profile can be noticed.

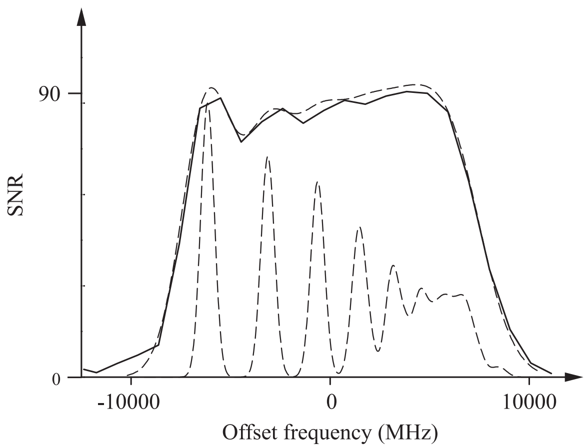

Fig. 2. Hyperfine structure of the Ta II line at 3235.130 Å. The Gaussian widths are (i) 800 MHz and (ii) 3000 MHz. The hyperfine structure is partially masked. It is easy to determine the position of the highest peak, but the position of small hyperfine components cannot be found. However, a fit of the structure is possible. The solid line shows the profile as observed in the FT spectrum.