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Second spectrum of Manganese (Mn II), Part I: Fine and hyperfine structure analysis of even-parity levels

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ABSTRACT

We have taken advantage of the existence of some experimental Mn II hyperfine magnetic dipole constant (A) values given in literature with low uncertainties to achieve for a first time an accurate hyperfine structure (hfs) parametric study. The monoelectronic hfs parameter values were extracted in their entirety for the alone stable ^{55}Mn II. For example for $3d^4 4s$ configuration we obtain: $a^{10}_{4s} = 198.08$ mk and $a^{01}_{3d} = 17.14$ mk. These semi-empirically extracted single-electron parameters were analyzed and compared with ab-initio calculations. In this first part of a global work, devoted particularly to even-parity levels we have at beginning studied a fine structure of two hundred levels, giving their leading eigenvector percentages and their calculated Landé-factor g_J. We present also predicted singlet, triplet and quintet positions of missing experimental levels up to 120 000 cm^{-1}, not far from Mn II ionization energy of 126 000 cm^{-1}. We close this work by giving predicted values of magnetic dipole hfs constants of all known levels of the most relevant Mn II even-parity configuration: $3d^4 4s$, whose splitting is not yet measured.

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Contents

1. Introduction

Manganese is a chemical element with symbol Mn and atomic number 25. *Manganese*, sometimes *confused with* magnesium (Mg), is often found in minerals in combination with iron. It is a metal with important industrial metal alloy uses, particularly in stainless steels. Naturally occurring manganese is composed of only one stable isotope, ^{55}Mn. Manganese is part of the iron group of elements, which are thought to be synthesized in large stars shortly before the supernova explosion. ^{53}Mn decays to ^{53}Cr with a half-life of 3.7 million years. Since Manganese has a nuclear spin of 5/2 and a nuclear moment of 3.4687 μ_N, Mn II spectral lines exhibit fortunately hyperfine structure (hfs) splitting, whose measured level constants can be of use in a severe test when checking the validity of eigenvectors obtained thanks to fine structure (fs) analysis. Furthermore comprehensive hfs constants for Mn II are needed for the interpretation of stellar spectra, otherwise erroneous abundances may be obtained when hfs is omitted since hfs splittings broaden the lines observed in stellar spectra (see for instance figure 3 in [1]). The first Mn fs studies started earlier, at the beginning of 1920 decade [2,3] but it is only in 1952 [4] that the analysis of the Mn II spectrum has been clearly extended by the classification of approximately 600 additional lines. Most of the newly identified terms belong to the triplet system, for which no levels have previously been located. Intersystem lines have been found which fixed the relative positions of the septet, quintet, and triplet systems and all terms of these systems to be expected within a huge amount of wave numbers of the ground state have been established. No singlet levels have as yet been located. Fortunately few years later, with the exception of one ^{1}S term, the whole number of singlet terms which theory predicts for Mn II in the $3d^6$,$3d^5$4s, and $3d^5$4p configurations, have been discovered by Iglesias team [5–8]; the latter gave 41 atomic energy levels: 16 even and 25 odd. It has been possible to classify a total of 167 lines, 113 being combinations among these singlet terms, and 54 intercombination lines with quintet and triplet terms, already known. Let us add that Johansson et al. [9] and Holt et al. [10] have measured respectively the wavelengths of 9 and 73 lines with high accuracy. Recently the Atomic Spectroscopy Groups at the National Institute of Standards and Technology (NIST) and Imperial College London (ICL) have investigated abundant atomic data of astronomical interest, for instance [11] and [12]. Their spectrometers include Fourier transform (FT) spectrometers at NIST and ICL covering the region 1350 Å to 5.5 μm and a 10.7-m grating spectrometer at NIST covering wavelengths from 300 to 5000Å. Sources for these spectra include high-current continuous and pulsed hollow cathode (HCL) lamps, Penning discharges, and sliding spark discharges. Some of these Mn II measurements, particularly for lines concentrated in the 2380–2700 Å, were analyzed successfully by Kurucz team in order to assign their energy levels and log gf values [13]. We want to take advantage of these recent excellent works to get level eigenvectors in order to transform into actual intermediate coupling the transition matrix beforehand obtained in pure LS coupling with help of Racah algebra. Our final aim is to obtain oscillator strength data recurring to semi-empirical oscillator strength parameterization (OSP) method, described in detail in Ref. [14].

2. Fine structure analysis

The method applied here for fine structure analysis was successfully used previously for the model space: $[nd + (n+1)s]^{N+2}$ in Zr and Hf atoms [15,16] with $N = 2$ (IVB group) and in Zr, Hf ions [17,18] with $N = 1$. The procedure of fs analysis includes electrostatic and spin dependent interactions which are represented by the Slater integrals F^k, G^k and R^k. The spin–orbit integrals ζnd effects also the interactions with distant configurations. The interaction effects with distant configurations influencing the term structure have been taken into account by the three body parameters T(d^2s), T2(22) and T3(42) and two body parameters α and β representing the one- and two-electron excitations on the spin–orbit splitting of the term (electrostatically correlated spin–orbit interaction) were considered in the way reported in Refs. [19,20].

The fs least square fitting procedure has been carried out over two hundred experimental levels, obtained at the beginning by Iglesias [6] and in the course of the time, observed in many astrophysical objects including the sun and nebulae, gathered particularly by the Kurucz team [13]. We have limited our analysis only to 9 configuration levels, not taking into account configurations with open g-shells since our first aim is to study oscillator strength values of lines involving lowest levels of $3d^6$ and $3d^5$4s, whose centers of gravity are very far from those with open g-shells. With 352 parameters (when taking into account second-order of perturbation theory including the effects of closed shell-open shell excitations), 16 of which were treated as free, a good fit has been achieved, resulting in a mean deviation for the energy level values of $\sigma(E)$: 89 cm^{-1}. Most of the fs parameters were fixed to weighted ab-initio values obtained using the Cowan code [21]. In Table 1, are given: the observed energy levels, calculated eigenvalues, percentages of first and second components of the wave functions and the corresponding LS term designations. In this table, the calculated Landé g_J-factor values, deduced from the eigenvector compositions, are compared with experimental ones when available. Tables 2 and 3 contain the derived values of fs radial parameters obtained with help of the least-square fitting procedure. In the present study where close coupling between the experimental work and the

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