Hyperfine structure investigations in atomic iodine

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ABSTRACT

Experimental results of the hyperfine structure (*hfs*) constants of levels of the iodine atom are reported. The absorption spectra of 50 transitions in the near infrared spectral region were observed using concentration modulation technique with a tunable single-mode cw Ti:Sapphire laser. Magnetic dipole *hfs* constants *A* and electric quadrupole *hfs* constants *B* for 54 levels were determined, out of which for 10 levels were examined for the first time, the constants were confirmed for 44 levels.

1. Introduction

Spectra and *hfs* of atomic iodine have been studied during many years. Tolansky [1,2] determined the nuclear spin of the iodine atom to be 5/2 from spark and arc spectra of iodine. Eshbach and Fisher observed the spectrum of iodine in the region between 0.8 and 2.2 μm in 1954 [3] and found several energy levels. An extensive study of neutral iodine was finished by Kiess and Corliss in 1959 [4]. They obtained the spectra of atomic iodine in the wide region from 23,070 Å to 1195 Å. Spectra of iodine in the infrared region (1.8–4.0 μm) were observed and analyzed by Humphreys et al. in 1971 and 1972 [5,6]. In 1975, Luc-Koenig et al. analyzed the *hfs* structure of 130 lines of the iodine atom [7]. In 2017, Chilukoti et al. added new *hfs* constants for 9 levels [9].

In a previous study, we investigated the spectral lines between $11300\,cm^{-1}$ and $13000\,cm^{-1}$ and determined the magnetic dipole constants and the electric quadrupole hyperfine structure constants (*A* and *B*) of 18 even levels and 28 odd levels [8]. In the present work, the spectra were re-measured with absorption line-shape and 50 transitions were analyzed. The hyperfine structure constants of 54 levels were determined and the constants of 10 levels were examined for the first time.

2. Experimental setup

The apparatus is the same as used in the previous studies [8,10] of atomic iodine. A tunable Ti:sapphire ring laser (Coherent 899-29) working around 800 nm was used as the laser source. A glass tube with ring electrodes at both ends was filled with flowing helium at a dynamic pressure of 140 pa. The iodine vapor was derived from the heating of solid iodine inside. The electrodes were connected to an AC power supply working at 23 kHz, which produces the excited atomic iodine. The concentration modulation spectroscopy (CMS) was used to enhance the signal to noise ratio of the absorption spectrum of neutral atomic iodine. The CMS is an accompanying technique of the velocity modulation spectroscopy [11,12]. When the mixed gases were discharged at 23 kHz, the concentration of the excited atomic iodine would be modulated by the magnitude of the discharging electric field at 2×23 kHz. When demodulating the output signal of a detector (ET-2030A) at 2×23 kHz, the concentration modulation absorption spectra of the excited atomic iodine would be observed. The laser wavenumber was recorded by an attached wavemeter and was further calibrated according to the absorption spectra of iodine molecules with a frequency calibration error of $0.007\,cm^{-1}$.

3. Results and discussion

There is only one stable isotope, ^{127}I, in the natural abundance of iodine. The nuclear spin quantum number is $I = 5/2$. The coupling of the electron (**J**) and nuclear (**I**) angular momentum induced by the hyperfine interaction forms the total angular momentum, i.e., **F** = **J**+**I**. Due to $I = 5/2$, there are up to 16 hyperfine components for each transition (if $J \geq I$ and $\triangle J=0$). Both the magnetic dipole coupling constant (*A*) and the electric quadrupole coupling constants (*B*) can be obtained by fitting the *hfs* patterns of the recorded spectra [13–15].

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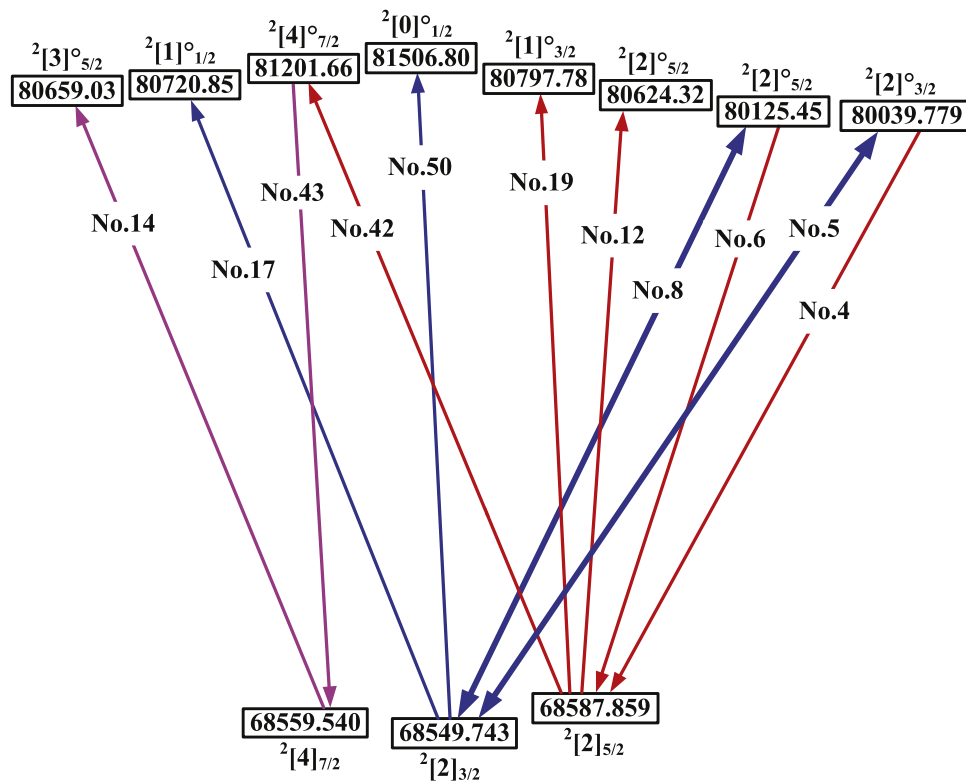*E-mail addresses:* lhdeng@phy.ecnu.edu.cn, denglunhua@126.com (L. Deng), hlwang@phy.ecnu.edu.cn (H. Wang).

Fig. 1. A group of transitions used to determine the *hfs* constants of the involved levels (energy given in units of cm^{-1}). The transitions are colored and numbered for clarity (numbers correspond to Table 1). The double arrow lines show the beginning of the fits. One can follow the arrows to obtain the sequences of the fit procedure.

The observed lines were classified as transitions between the known levels given in the NIST atomic spectra database [18]. The 50 investigated transitions are listed in Table 1. Each transition is numbered in the table to allow an easier discussion.

A program named Elements [13,14] was used to simulate the observed *hfs* patterns and to estimate rough constants. These constants, *A* and *B*, as well as the ones determined in the previous studies [4,8] were used as initial values in another program named Fitter [15] to obtain the accurate constants.

Totally, the *hfs* constants for 54 levels were obtained from the 50 transitions. These transitions were grouped according to the relationships between the involved levels. Fig. 1 shows the first investigated group. The levels relate with each other using the observed transitions together with their numbers (as listed in Table 1).

Since in laser spectroscopic measurements quite often saturation effects are observable. Components with low transition probability show up enhanced in intensity compared to the main hyperfine structure components. An example of such situation one can find in ref. [17]. Thus the fit result may be influenced by assumptions concerning the intensity ratios of not completely resolved components. We tried to base our data evaluation on lines where most of the components are well separated from each other. The intensities of such components can then be assumed as free parameters in the fit procedure.

Firstly, we fitted the spectra of line No.5 and line No.8 independently to determine the *hfs* constants of the level 68549.743 cm^{-1}. These two transitions are drawn using double arrows lines in Fig. 1 to illustrate the beginning of the fit procedure. These fits gave 1820.5 and 1819 MHz for *A*(68549.743 cm^{-1}) and 1086 and 1097 MHz, respectively, for *B*(68549.743 cm^{-1}). The average values of *A*(68549.743 cm^{-1}) and *B*(68549.743 cm^{-1}) are 1820(2) and 1091(10) MHz, respectively, and we report as so for them.

Secondly, we re-fitted line No.5 with *A*(68549.743 cm^{-1}) fixed at 1820 MHz and *B*(68549.743 cm^{-1}) fixed at 1091 MHz. This fit reported 2263(5) and 888(15) MHz for *A*(80039.779 cm^{-1}) and *B*(80039.779 cm^{-1}), respectively. Fig. 2 displays the fit of line No.5 with a calculated center-of-gravity (*c.g.*) wavenumber of 11490.036 cm^{-1}. The *hfs* spectral line shapes were well modeled using the sum of a Gaussian (75%) and a Lorentzian (25%) profiles. Similarly, *A*(80125.45 cm^{-1}) = 1575(3) MHz and *B*(80125.45 cm^{-1}) = 984(15) MHz were obtained by re-fitting line No.8.

When the constants of the level 80039.779 cm^{-1} and 80125.45 cm^{-1} were obtained and fixed, the fit of line No.4 and line No.6 gave *A*(68587.859 cm^{-1}) = 2494(3) MHz and *B*(68587.859 cm^{-1}) = 2096(15) MHz. Sequentially, fixing the constants of level 68587.859 cm^{-1} to those values, line No.12, line No.19 and line No.42 were fitted to get constants of levels 80624.32 cm^{-1}, 80797.78 cm^{-1} and 81201.66 cm^{-1}. The above transitions are labeled using arrow lines and one can follow them to get the sequences of the fit procedure. In this way, the constants of the rest four levels were determined by fixing the known constants.

Shown in Fig. 3(a)–(c) are the other well related transitions. The *hfs* constants for the involved levels were determined as same method as those performed for levels in Fig. 1.

Fig. 3(d) contains the remaining transitions and levels without good relationship. Transition line No.36 was directly fitted to get the constants for the involved levels since no other transitions were related. Line No.7 and line No.34 gave the averaged constants for level 73387.184 cm^{-1}; line No.3 and line No.39 gave the averaged constants for level 64989.994 cm^{-1}; and the constants for other related levels were sequentially determined.

Limited by the small splitting (comparing to the line width) of level 63186.758 cm^{-1}, line No.15 and line No.32 were both fitted well and they gave 107(2) MHz and −119(2) MHz for *A*(63186.758 cm^{-1}), respectively. If *A*(63186.758 cm^{-1}) =