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Hyperfine structure near infrared spectrum of atomic iodine



Lun hua Deng*, Xiao yun Li, Yuan yue Zhu, Yang qin Chen

State Key Laboratory of Precision Spectroscopy, East China Normal University, Shanghai 200062, China

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ABSTRACT

The hyperfine structure of spectral lines of neutral iodine (II) in the wavenumber region from $11\,300\text{ cm}^{-1}$ to $13\,000\text{ cm}^{-1}$ was studied using optical heterodyne concentration modulation absorption spectroscopy with a tunable single-mode cw Ti:Sapphire laser. The iodine atoms were produced and excited by a discharge operated in a mixture of helium and iodine vapor. A total of 89 lines were observed and the hyperfine structure of 45 of these lines was studied. For 40 lines, the hyperfine structure was not previously known. The magnetic dipole and the electric quadrupole hyperfine structure constants of 18 even and 28 odd levels were extracted. The constants of one even level and of 16 odd levels are presented for the first time.

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1. Introduction

The fine and hyperfine structures (*hfs*) of atomic iodine (II) have been studied for many years. The early spark spectrum of iodine was observed by Tolansky [1,2] and the nuclear spin of iodine was found to be $\frac{5}{2}$. Eshbach and Fisher [3] measured the infrared spectrum of iodine and reported the wavenumbers and intensities for 31 lines. In 1959, Kiess and Corliss [4] reported a list of more than 900 lines emitted by neutral atoms in the region from 1195 to $23\,070\text{ \AA}$. Later in the 1970s, Humphreys et al. [5,6] expanded the spectral of II to the $4\text{-}\mu\text{m}$ region. Minnhagen [7] recalculated the entire energy level system and presented them in a concise form. Moore [8] summarized the earlier spectral works of II.

Spectral research related to the *hfs* of II was limited. Luc-Koenig et al. [9] observed the spectrum of II in the region from $3\,000$ to $11\,500\text{ cm}^{-1}$ using the Fourier transform spectrometry method and 130 *hfs* were analyzed. They reported the magnetic dipole and the electric quadrupole hyperfine structure constants for 37 even

levels and 42 odd levels. However, the *hfs* constants remained unknown for many levels. This work presents the *hfs* spectrum of II in the region from $11\,300$ to $13\,000\text{ cm}^{-1}$, and the *hfs* constants were obtained by classifying and simulating the *hfs* patterns.

2. Hyperfine structure

For atoms that consist of a nonzero nuclear spin I , the fine structure levels with total angular momentum J greater than zero will split into sub-levels, which form the hyperfine structures of the spectral lines. The interaction between the nuclear moments, magnetic dipole μ_I and electric quadrupole Q , and the magnetic fields due to the electrons leads to the splitting of the fine structure E_J sublevels E_{FJ} .

The hyperfine levels are identified by the quantum number F associated with I and J , and the value of F can be $|J-I|, |J-I+1, \dots, J+I-1, J+I$. The hyperfine transition selection rules are $\Delta F=0, \pm 1$ under the precondition of $\Delta J=0, \pm 1$ between different parities. But the transitions from $F_e=0$ to $F_o=0$ are forbidden, and the subscript letters e and o stand for even and odd parities, respectively.

* Corresponding author. Tel.: +86 6223 3872; fax: +86 6223 2056.
E-mail address: lhdeng@phy.ecnu.edu.cn (L.h. Deng).

Table 1
Spectral lines of II and their classifications.

σ_{cal} (cm ⁻¹)	σ_{cg} (cm ⁻¹)	E_e (cm ⁻¹)	J_e	E_o (cm ⁻¹)	J_o	σ_{cal} (cm ⁻¹)	σ_{cg} (cm ⁻¹)	E_e (cm ⁻¹)	J_e	E_o (cm ⁻¹)	J_o
11 339.116 ^a	11 339.598(3) ^b	66 020.469	2.5	77 359.585	2.5	12 410.139	u	70 151.201	2.5	82 561.34	2.5
11 386.315	11 386.328(6)	66 020.469	2.5	77 406.784	1.5	12 417.599	u	70 151.201	2.5	82 568.80	2.5
11 427.789	11 427.802(6)	76 417.783	0.5	64 989.994	1.5	12 425.014	12 425.006(5)	66 355.093	1.5	78 780.107	0.5
11 451.920	11 451.967(4)	68 587.859	2.5	80 039.779	1.5	12 428.670	12 428.680(3)	54 633.460	2.5	67 062.130	1.5
11 490.036	11 490.082(4)	68 549.743	1.5	80 039.779	1.5	12 434.669	12 434.686(6)	63 186.758	0.5	75 621.427	1.5
11 517.112	11 517.119(6)	67 298.328	0.5	78 815.44	1.5	12 460.347	u	66 355.093	1.5	78 815.44	1.5
11 537.591	11 537.601(5)	68 587.859	2.5	80 125.45	2.5	12 460.715	u	77 450.709	2.5	64 989.994	1.5
11 567.405	11 567.396(7)	61 819.779	1.5	73 387.184	0.5	12 490.941	12 490.951(7)	60 896.243	0.5	73 387.184	0.5
11 575.707	u ^c	68 549.743	1.5	80 125.45	2.5	12 499.654	u	66 355.093	1.5	78 854.747	2.5
11 673.096	u	70 354.834	1.5	82 027.93	2.5	12 536.582	12 536.593(6)	67 298.328	0.5	79 834.91	1.5
11 678.706	u	70 354.834	1.5	82 033.54	1.5	12 544.419	u	77 450.709	2.5	64 906.290	2.5
11 690.556	11 690.536(6)	70 354.834	1.5	82 045.39	1.5	12 558.710	12 558.732(7)	78 415.670	0.5	65 856.960	0.5
11 698.864	11 698.871(6)	77 555.824	1.5	65 856.960	0.5	12 565.830	12 565.825(8)	77 555.824	1.5	64 989.994	1.5
11 881.211	u	78 943.341	2.5	67 062.130	1.5	12 571.716	u	70 354.834	1.5	82 926.55	2.5
11 968.862	11 968.890(6)	79 030.992	1.5	67 062.130	1.5	12 572.103	12 572.101(9)	66 020.469	2.5	78 592.572	2.5
11 996.979	11 996.979(4)	76 903.269	2.5	64 906.290	2.5	12 575.576	u	70 354.834	1.5	82 930.41	1.5
12 036.461	12 036.513(3)	68 587.859	2.5	80 624.32	2.5	12 583.055	12 583.221(5)	67 298.328	0.5	79 881.383	1.5
12 060.154	12 060.174(4)	66 355.093	1.5	78 415.247	1.5	12 583.405	12 583.610(7)	67 298.328	0.5	79 881.733	0.5
12 064.780	u	68 559.540	3.5	80 624.32	2.5	12 600.926	u	68 615.734	0.5	81 216.66	1.5
12 066.387	12 066.423(4)	68 549.743	1.5	80 616.13	1.5	12 610.156	12 610.211(7)	68 615.734	0.5	81 225.89	0.5
12 069.316	u	70 354.834	1.5	82 424.15	1.5	12 611.506	12 611.543(6)	68 615.734	0.5	81 227.24	1.5
12 074.577	12 074.624(5)	68 549.743	1.5	80 624.32	2.5	12 613.801	12 613.863(6)	68 587.859	2.5	81 201.66	3.5
12 099.490	u	68 559.540	3.5	80 659.03	2.5	12 617.531	u	68 587.859	2.5	81 205.39	2.5
12 101.720	u	68 559.540	3.5	80 661.26	3.5	12 619.281	12 619.382(4)	68 587.859	2.5	81 207.14	3.5
12 103.185	u	67 726.415	4.5	79 829.600	4.5	12 631.291	u	68 587.859	2.5	81 219.15	2.5
12 105.116	12 105.166(7)	68 615.734	0.5	80 720.85	0.5	12 642.120	u	68 559.540	3.5	81 201.66	3.5
12 106.540	u	67 726.415	4.5	79 832.955	3.5	12 645.850	u	68 559.540	3.5	81 205.39	2.5
12 116.307	u	63 186.758	0.5	75 303.065	0.5	12 647.600	u	68 559.540	3.5	81 207.14	3.5
12 121.268	u	67 726.415	4.5	79 847.683	3.5	12 655.647	u	68 549.743	1.5	81 205.39	2.5
12 132.595	u	67 726.415	4.5	79 859.01	5.5	12 657.960	u	68 559.540	3.5	81 217.50	4.5
12 133.155	u	67 726.415	4.5	79 859.570	4.5	12 666.917	u	68 549.743	1.5	81 216.66	1.5
12 158.355	12 158.361(6)	60 896.243	0.5	73 054.598	1.5	12 669.407	u	68 549.743	1.5	81 219.15	2.5
12 171.107	12 171.159(6)	68 549.743	1.5	80 720.85	0.5	12 676.147	12 676.209(5)	68 549.743	1.5	81 225.89	0.5
12 206.506	u	70 354.834	1.5	82 561.34	2.5	12 677.497	12 677.530(4)	68 549.743	1.5	81 227.24	1.5
12 209.921	12 209.945(4)	68 587.859	2.5	80 797.78	1.5	12 717.208	u	66 015.023	3.5	78 732.231	2.5
12 213.966	u	70 354.834	1.5	82 568.80	2.5	12 741.451	12 741.502(6)	67 298.328	0.5	80 039.779	1.5
12 223.143	12 223.156(6)	79 285.273	0.5	67 062.130	1.5	12 794.971	12 794.974(6)	66 020.469	2.5	78 815.44	1.5
12 237.479	12 237.500(5)	66 355.093	1.5	78 592.572	2.5	12 829.280	u	66 015.023	3.5	78 844.303	3.5
12 260.916	u	70 354.834	1.5	82 615.75	0.5	12 834.278	u	66 020.469	2.5	78 854.747	2.5
12 272.949	u	70 151.201	2.5	82 424.15	1.5	12 852.552	u	79 914.682	2.5	67 062.130	1.5
12 333.767	12 333.801(7)	79 395.897	1.5	67 062.130	1.5	12 869.563	u	66 355.093	1.5	79 224.656	1.5
12 356.359	12 356.371(9)	79 418.489	2.5	67 062.130	1.5	12 884.993	u	79 947.123	1.5	67 062.130	1.5
12 394.778	12 394.796(6)	66 020.469	2.5	78 415.247	1.5	12 934.845	u	67 726.415	4.5	80 661.26	3.5
12 403.263	12 403.263(7)	67 298.328	0.5	79 701.591	0.5	12 957.057	12 957.084(6)	68 549.743	1.5	81 506.80	0.5
12 408.879	u	70 151.201	2.5	82 560.08	3.5						

^a The frequencies were calculated using levels given in the NIST atomic spectra database [14].

^b The fitted c.g. frequencies. Numbers in parentheses denote one standard deviation in units of the last quoted digit.

^c The letter u means observed but the *hfs* was not resolved for these lines.

The energy of the hyperfine structure multiplet is given by

$$E_F = E_J + \frac{K}{2}A + \frac{3K(K+1) - 4J(J+1)(J+1)}{8J(2I-1)(2J-1)}B \quad (1)$$

$$K = F(F+1) - I(I+1) - J(J+1) \quad (2)$$

where E_J is the energy of the fine structure level with quantum number J ; A is the magnetic dipole coupling constant, and B is the electric quadrupole hyperfine interaction constant.

3. Experimental setup

The experimental setup is the same as that of I_2^+ [10]. The solid iodine was heated and its vapor was discharged together with Helium at a total pressure of 100 Pa. A tunable Ti:sapphire laser (Coherent 899-29) operating in the region from 11 300 to 13 000 cm⁻¹ was used as the laser source. The wave number was initially recorded using an attached wavemeter and was further calibrated using the absorption spectrum of molecular iodine [11], which has a frequency accuracy of 0.007 cm⁻¹.

Concentration modulation spectroscopy (CMS) was used to acquire the spectrum of II. The CMS is specialized in picking out the spectrum of neutral atoms or molecules

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