C.W. Optical–Optical Double Resonance in I_2: Hyperfine Structure in the $E\,0^+_{-g}$–$B\,0^+_u$ System

J. B. KOFFEND,† R. BACIS,† M. BROYER,† J. P. PIQUE‡
and S. CHURASSY†

† Laboratoire de Spectrométrie Ionique et Moléculaire, Université Lyon I, 43 Boulevard du 11 Novembre 1918, 69622 Villeurbanne, France. ‡ Laboratoire de Spectrométrie Physique, Université Scientifique et Médicale de Grenoble, BP 53X, 38041 Grenoble Cedex, France

Hyperfine structure for several $E(0^+_g) - B(0^+_u)$ rovibrational transitions has been measured for the first time. Two single frequency lasers were used to excite $E(0^+_g)$ $(v^*, J^*) - B(0^+_u)(v', J') - X(^1\Sigma^+_g)(v'', J'')$ transitions which result in Doppler-free $E(0^+_g)(v^*, J^*) - B(0^+_u)(v', J')$ fluorescence excitation spectra. Hyperfine parameters are obtained for $E(0^+_g)v = 11$ $(eQq = +483 \pm 4 \text{ MHz}, C = -210 \pm 3 \text{ kHz})$ and $E(0^+_g)v = 8$ $(eQq = +492.3 \pm 2.5 \text{ MHz}, C = -205 \pm 3 \text{ kHz})$. The non-zero C constant is shown to arise from mixing with a nearby 1g state and the eQq constant shows the $^3P_2(I^+)$ origin of the $E(0^+_g)$ state.

1. INTRODUCTION

In recent years there has been a wealth of spectroscopic studies related to the ion-pair states of molecular iodine. One important question concerns the identification of the 18 case c low-lying ion-pair states predicted by Mulliken.[1] The first two groups correlate to the $I^+(^3P_2) + I^-(^1S)$ and $I^+(^3P_{1,0}) + I^-(^1S)$ ions. Mulliken estimated the first group to have the minimum of the potential at $T_2 \sim 35\,000 \text{ cm}^{-1}$ and the second to have $T_e \sim 41\,000 \text{ cm}^{-1}$. Although a number of multiphoton absorption spectra[2,3,4] seem to confirm these estimates a detailed analysis of the emission spectrum of I_2[5] predicts these two groups at $40\,000 \text{ cm}^{-1}$ and $47\,000 \text{ cm}^{-1}$. A recent analysis[6] has located the

lowest expected $D'(2g)$ state at $T_e = 40\,386.2\,\text{cm}^{-1}$ but further spectroscopic studies are needed in order to assign the atomic origin of these states.

An important tool in the understanding of the structure of an electronic state is its hyperfine structure. In particular, it has been shown[7] that the hyperfine structure of an I_2 molecular state is related to its atomic character. As recent C.W. double resonance studies[6] have shown that the $E(0_g^+)$ state may be easily excited, we have undertaken the study of its hyperfine structure. This state is the best known of the I_2 charge transfer states and has been studied by conventional[8,9] or double resonance techniques.[10,11,12,13,14,15] However, hyperfine structure has not been measured for any of the ion-pair states of I_2.

In this paper we report sub-Doppler C.W. optical optical double resonance in I_2. This has allowed the analysis and interpretation of hyperfine structure of some rovibrational levels of the I_2 $E(0_g^+)$ state.

2. EXPERIMENT

Figure 1 shows a diagram of the experimental set up. The beam of a Spectral Physics model 171 krypton laser oscillating at 413.1 or 406.7 nm was directed into an I_2 cell. The krypton laser was equipped with a temperature stabilized solid intracavity etalon (Spectra Physics model 583) and the end mirror was mounted on a piezo-electric transducer. A portion of the krypton laser beam was directed into a 30 cm confocal reference cavity and onto a photodiode using quartz flats. The krypton laser frequency was stabilized to the external cavity using a feedback loop, which reduced the linewidth to a few MHz. The mirrors of the krypton laser were mounted on holders fixed to the laser table in order to insulate them from vibrations caused by the flow of cooling water circulating in the plasma tube. Typical power densities were $0.24\,\text{W cm}^{-2}$ for 413.1 nm and $0.20\,\text{W cm}^{-2}$ for 406.7 nm in the I_2 cell.

The beam from a Spectra Physics model 380-D dye laser operating with Rhodamine 6-G was directed into the I_2 cell in a direction opposite to the krypton laser. A beam splitter was inserted in the beam to direct 50% of the dye laser intensity into a supersonic molecular beam of I_2. The molecular beam is described in detail
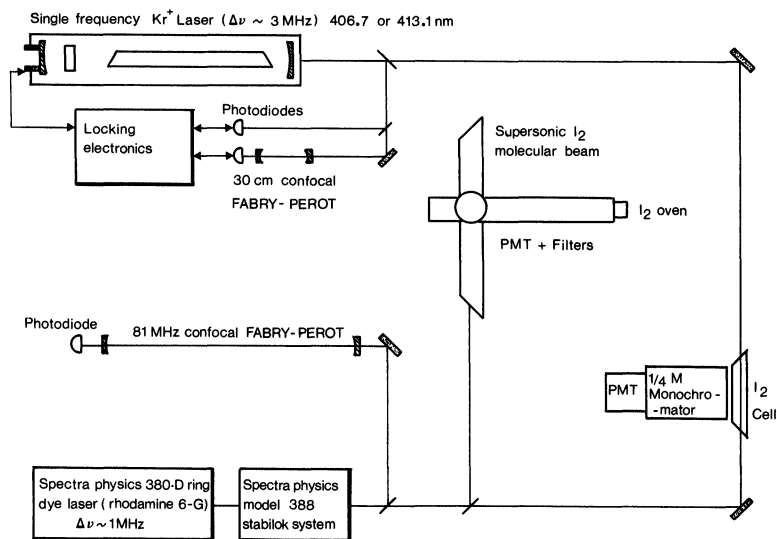
FIGURE 1   Experimental set-up.

elsewhere.[16] The dye laser frequency was actively stabilized using a Spectra Physics model 388 stabilok system resulting in a 1 MHz linewidth. Typical dye laser power densities were 3 W cm^{-2} in the I_2 cell.

$E\ 0_g^+ - B\ 0_u^+$ double resonance excitation spectra were recorded in the following manner. The krypton laser frequency was held fixed at a value that excited an $E\ 0_g^+(v^*, J^*) - B\ 0_u^+(v', J')$ transition and the dye laser was scanned over the corresponding $B\ 0_u^+(v', J') - X\ ^1\Sigma_g^+(v'', J'')$ line. The resulting $E-B$ fluorescence from the I_2 cell along with the $B-X$ fluorescence from the molecular beam (crossing angle $\pi/2 \pm \Delta\theta$, with $\Delta\theta < 0.01$ rd) were simultaneously recorded on a chart recorder. A portion of the dye laser was directed into an 81 MHz confocal Fabry–Perot and the resulting fringes were also recorded. These fringes give a relative frequency scale of good linearity, at least between two successive peaks, due to pressure scanning of the Fabry-Perot cavity of the stabilok system in the ring laser. The E–B fluorescence was detected using a 0.20 meter mono-chromator (Jobin–Yvon model H-20) and an RCA IP-28 photomulti-

plier. For Kr^{++} wavelengths of 406.7 and 413.1 nm the mono-chromator was set a 427 and 430 nm, respectively (Bandwidth ~10 nm). The sidearm of the cell was immersed in an ice bath resulting in an I_2 pressure of 37×10^{-3} torr.

With a reduction of laser power density and I_2 pressure we obtained a minimum linewidth (FWHM) of 8.5 MHz. Radiative lifetime measurements have been performed for the $E(0_g^+)$ state by Rousseau[17] ($v \sim 46$, $\tau = 27 \pm 2$ ns) and by Chevaleyre *et al.*[14] ($v = 0-40$, $\tau = 28 \pm 1$ ns). A lifetime of 28 ns corresponds with a FWHM of 5.7 MHz. However, in our experiments the extra 3 MHz are due to the combined frequency jitter of the Kr^{++} and ring dye lasers. We have noted that the cell must be very carefully prepared in order to obtain this 8.5 MHz linewidth.[30]. If sufficient care is not taken in cell preparation typical linewidths of the order of 18–20 MHz are observed (apparent lifetimes ~10 ns). Very efficient collisional transfer occurs in this case as discussed in Ref. 6. Such effects could explain disagreement of the previous lifetime measurements[14,17] with the recent results of King *et al.* ($\tau \sim 11$ ns).[18]

The *E–B* double resonance excitation spectra (Figure 2) were obtained by fixing the Kr^{++} laser frequency and scanning the frequency of the dye laser over the corresponding *B–X* line. This figure displays a spectrum recorded for the $E\ 0_g^+(v^* = 8,\ J^* = 98) - B\ 0_u^+(v' = 20,\ J' = 99) - X\ ^1\Sigma_g^+(v'' = 1, J'' = 100)$ double resonance. Also visible in Figure 2 are the fringes from the 81 MHz free spectral range interferometer.

3. RESULTS

The *E–B* spectra involve molecules having non-zero velocities along the direction defined by the two lasers. In order to obtain rest frequency separations of the *E–B* hyperfine lines, the experimental spectra must be deconvoluted. It may be easily shown that:

$$\nu_{EB} = (\nu_{Kr}^{++}) + (\nu' - \nu_{BX})\frac{\nu_{EB}}{\nu_{BX}} \qquad (1)$$

where ν_{EB} is the rest frequency of an $E(v^*, J^*, I^*, F^*) - B(v', J', I', F')$ transition, ν_{BX} is the rest frequency of the corresponding $B(v', J', I', F') - X(v'', J'', I'', F'')$ line, $\nu_{Kr^{++}}$ is the Kr^{++} laser
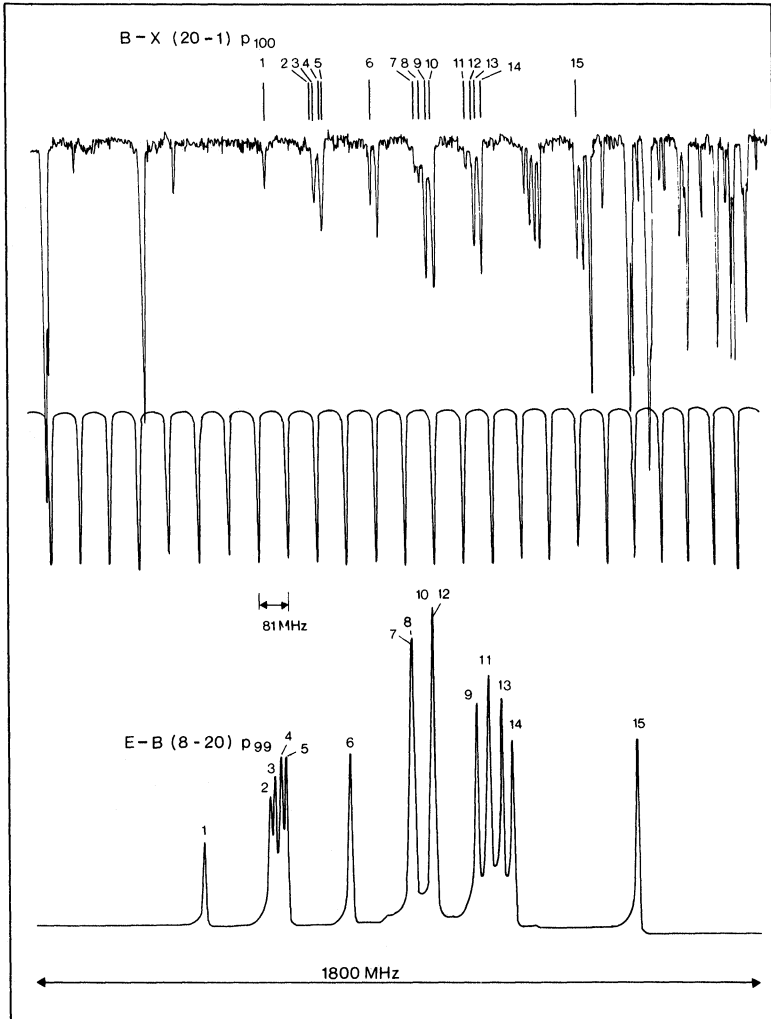
FIGURE 2 A typical double resonance excitation spectrum. The upper part shows the B–X excitation spectrum from the supersonic molecular beam. The P (100) line is rather weak with respect to low J lines appearing on the right or left part of the scan due to the low rotational temperature of the molecular beam.

The lover trace shows the E–B double resonance excitation spectrum.

frequency and ν' is the dye laser frequency when the E–B hyperfine line is excited in the I_2 cell.

Hyperfine constants for the E state were determined using a two-step process. B–X excitation spectra obtained from the I_2 molecular beam provide values of ν_{BX}. To obtain homogeneous data sets, the measured values of ν_{BX} were least squares fit using a Hamiltonian that included nuclear electric quadrupole and spin–rotation hyperfine coupling constants. The hyperfine constant for the X $^1\Sigma_g^+$ state have been measured accurately.[19,20,21] They were held fixed in the fits at their value taken from Ref. 21, namely $eQq'' = -2452.6$ MHz and $C'' = 3$ kHz. The calculated values of ν_{BX} from the fits were used along with the measured values of ν' from the E–B double resonance excitation spectra to determine ν_{EB} using Eq. (1). The ratio ν_{EB}/ν_{BX} appearing in Eq. (1) was treated as a constant† for each B–X rotational line used as the first step in the double resonance. The Kr^{++} laser frequencies were taken from Ref. 22 ($\nu_{Kr^{++}}$ (413.1 nm) = 24 198.46 cm^{-1} and $\nu_{Kr^{++}}$ (406.7 nm) = 24 578.97 cm^{-1}) while the frequencies of the various B–X lines were calculated using the constants of Gerstenkorn and Luc.[23,24]

The experimentally determined values of ν_{EB} from Eq. 1 were then least squares fit using the same Hamiltonian as in the treatment of the B–X data to obtain the E 0_g^+ state hyperfine constants. In these fits the hyperfine constants for the B state were held fixed at their values determined in the first step. It should be mentioned that the hyperfine coupling constants depend only upon the line separations and not the absolute frequencies. In our measurements the origin was chosen to coincide with the highest frequency component in the $B(v', J') - X(v'', J'')$ rotational line.

Figure 3 shows the rest frequency $E\,0_g^+(v^* = 8, J^* = 98) - B\,0_u^+(v' = 20, J' = 99)$ stick spectrum. This spectrum was calculated using the hyperfine constants of the B and E states determined from the least squares fits. Since the E–B double resonance spectra recorded involve molecules having non-zero velocities there is little

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† The ratio ν_{EB}/ν_{BX} is not really constant for each hyperfine component in a particular E–B line since ν_{EB} changes slightly for each B–X component pumped in the first step. However, the change is at the maximum of the order of 0.03 cm^{-1} (the splitting of the B–X rotational line due to hyperfine structure) whereas ν_{BX} is of the order of 17 500 cm^{-1}. With the same precision $\nu_{EB} = \nu_{Kr^{++}}$. Thus ν_{EB}/ν_{BX} may be treated as a constant with no loss in precision for each B–X rotational line.

E (0_g^+) – B (0_u^+) (v_E = 8 , v_B = 20) P(99) Hyperfine structure

eQq (B) = – 525.7 MHz C_I (B) = 48 kHz

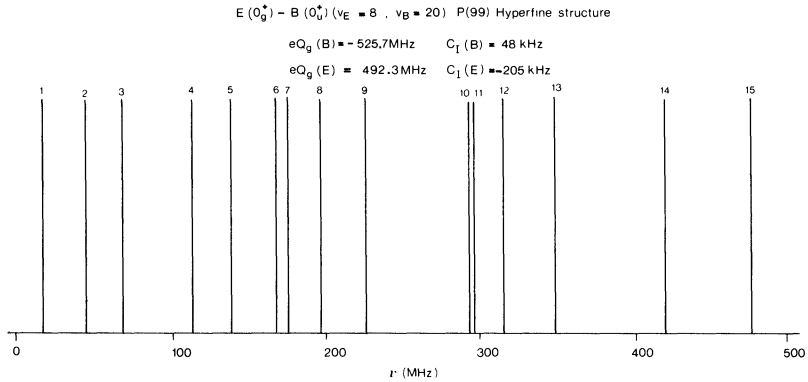eQq (E) = 492.3 MHz C_I (E) = –205 kHz

r (MHz)

FIGURE 3   Calculated relative positions of the hyperfine components in the E'–B ($v^* = 8$, $v' = 20$) $P(99)$ transition (rest frequencies). They correspond to the last column (ν_{EB} (calc)) in Table II except for a change in origin.

Since J is large the relative intensities of the 15 lines are nearly the same and have not been indicated in the figure.

resemblance with the rest frequency spectrum, as can be seen by comparing Figures 2 and 3. Furthermore, the assignment of the E–B spectra recorded is not obvious. In Figure 2, for example, the lines 2, 3, 4 and 5 in the B–X spectrum correspond respectively with the lines 5, 4, 3 and 2 in the E–B spectrum. Other correspondences can be obtained upon examination of Tables I and II.

In this work, three E state levels were studied, having $v^* = 8$, $J^* = 98$, $v^* = 8$, $J^* = 105$, and $v^* = 11$, $J^* = 104$. Each E–B–X double resonance was recorded four times, each time with a slightly different Kr^{++} laser frequency, obtained by tilting the intracavity etalon. Thus a total of 12 spectra were measured for the three E state levels studied. The results of the least squares fits for a typical spectrum are listed in Table I and II. Table III displays the hyperfine constants obtained in this work. The results given are the weighted average of four determinations for each level studied.

4. INTERPRETATION OF THE $E(0_g^+)$ HYPERFINE STRUCTURE

The hyperfine quadrupole constant eQq

To theoretically calculate $eQq(E)$, we must know the eigen function of the E state. As this state has a strong ionic character, it seems

TABLE I

Hyperfine structure of the $B\, 0_u^+(v' = 20, J' = 99) \leftarrow X\, {}^1\Sigma_g^+(v'' = 1, J'' = 100)$ line

Line No.	I'	F'	I''	F''	$\nu_{BX}{}^a$ (obs)	$\nu_{BX}{}^b$ (calc)
1	0	99	0	100	0.0	0.0
2	2	101	2	102	−131.2	−131.8
3	4	100	4	101	−136.7	−136.7
4	4	98	4	99	−153.1	−153.0
5	2	97	2	98	−157.8	−157.2
6	4	99	4	100	−289.1	−289.4
7	4	102	4	103	−414.2	−413.7
8	4	101	4	102	−424.3	−424.1
9	4	97	4	98	−444.2	−443.9
10	4	96	4	97	−454.4	−454.1
11	4	103	4	104	−556.5	−557.1
12	2	100	2	101	−577.0	−576.7
13	2	98	2	99	−580 2	−580.1
14	4	95	4	96	−598.5	−599.5
15	2	99	2	100	−867.8	−867.5

All frequencies given in MHz.

[a] Estimated relative experimental uncertainties are ±2 MHz for unblended lines.

[b] Calculated using $eQq' = -521.7$ MHz, $eQq'' = -2452.6$ MHz, $C' = 48$ kHz and $C'' = 3.0$ KHz. RMS deviation of the fit 0.47 MHz.

reasonable to consider a symmetrized product of the eigenfunctions of the two ions I^+ and I^-. If we assume that the $E(0_g^+)$ state is correlated to the $I^+({}^3P_2) + I^-({}^1S)$ ions, its eigenfunction may be written as:

$$\psi_E = \frac{1}{\sqrt{2}}[|{}^3P_2M_J = 0\rangle_a|{}^1S\rangle_b - |{}^1S\rangle_a|{}^3P_2M_J = 0\rangle_b] \qquad (2)$$

where a and b represent the two iodine atoms.

Following the method and notations used in Ref. 7, we obtain:

$$q_E = \langle_a{}^3P_2M_J = 0|V_0^2(e, a)|{}^3P_2M_J = 0\rangle_a$$

$$= (-1)^2\begin{pmatrix} 2 & 2 & 2 \\ 0 & 0 & 0 \end{pmatrix}\langle_a{}^3P_2\|V^2(e, a)\|{}^3P_2\rangle_a \qquad (3)$$

The reduced matrix element $\langle_a{}^2P_2\|V^2(e, a)\|{}^3P_2\rangle_a$ can be related by standard methods to the q values in the ${}^3P_2$ level of the I^+ ion. Unfortunately the hyperfine structure of this ion is not known. To avoid this difficulty, we consider the $5p^4$ electronic configuration of

TABLE II

Hyperfine structure of the EO_g^+ $(v^* = 8, J^* = 98) \leftarrow BO_u^+ (v' = 20, J' = 99)$ line

Line No.	I^*	F^*	I'	F'	ν' [a] (obs)	ν' [c] (calc)	ν_{EB} [b] (obs)	ν_{EB} [d] (calc)
1	0	98	0	99	66.7	66.7	92.0	92.0
2	2	96	2	97	−112.7	−111.0	61.4	63.7
3	4	97	4	98	−125.8	−124.1	37.5	39.8
4	4	99	4	100	−143.5	−141.0	−9.4	−6.0
5	2	100	2	101	−157.7	−154.7	−35.7	−31.7
6	4	98	4	99	−333.2	−332.3	−60.4	−59.2
7	4	95	4	96	−500.0	−500.8	−63.3	−64.3
8	4	96	4	97	−507.1	−506.3	−87.1	−86.1
9	4	94	4	95	−681.0	−682.5	−112.3	−114.3
10	4	100	4	101	−556.1	−558.1	−181.9	−184.7
11	2	97	2	98	−714.2	−714.4	−184.8	−185.1
12	4	101	4	102	−562.5	−563.4	−205.1	−206.4
13	2	99	2	100	−749.6	−749.3	−238.3	−237.9
14	4	102	4	103	−780.9	−782.0	−308.5	−310.0
15	2	98	2	99	−1133.2	−1131.4	−366.2	−363.8

All frequencies given in MHz.

[a] Estimated relative experimental uncertainties are ±2 MHz for unblended lines. ν' defined in Eq. 1.

[b] Calculated with equation 1 using observed values of ν' and calculated values of ν_{BX} from Table I. Then these relative frequencies corresponds to the rest frequencies. Value of ν_{EB}/ν_{BX} used is 1.3785.

[c] Calculated using Eq. 1 with fitted values of ν_{EB} and ν_{BX} from Table I.

[d] Calculated values from the least squares fit of ν_{EB} (obs) with $eQq(B) = -525.7$ MHz, $eQq^*(E) = 488.1$ MHz, $C'(B) = -48$ kHz, and $C^*(E) = -204$ kHz. RMS deviation of the fit 2.5 MHz.

the $^3P_2$ I^+ ion as equivalent to the $5p^2$ configuration through the Racah theorem. With this hypothesis, the reduced matrix element $\langle_a Sl_1 l_2 LJ \| V^2(e, a) \| Sl_1 l_2 LJ \rangle_a$ may be calculated using standard Racah algebra and the fact that:

$$V_q^2(e, a) = V_q^2(e_1, a) + V_q^2(e_2, a) \tag{4}$$

the symbols e_1 and e_2 representing the two electrons. We obtain:

$$\langle_a Sl_1 l_2 LJ \| V^2(e_1, a) \| Sl_1 l_2 LJ \rangle_a$$

$$= (-1)^{L+S+J+2}(2J+1)\begin{pmatrix} L & J & S \\ J & L & 2 \end{pmatrix}$$

$$\times (-1)^{l_1+l_2+L+2}(2L+1)\begin{pmatrix} l_1 & L & l_2 \\ L & l_1 & 2 \end{pmatrix}$$

$$\langle_a l_1 \| V^2(e_1, a) \| l_1 \rangle_a \tag{5}$$

TABLE III
$E0_g^+$ and $B0_u^+$ hyperfine constants

J_B	v_B	eQq (B)	C (B)	J_E	v_E	$eQq(E)$	$C(E)$
(a) 99	20	−525.7 (10)	48 (2)	98	8	492.3 (25)	−205 (3)
(b) 106	20	−523.7 (13)	48 (2)	105	8	490.1 (46)	−204 (3)
(c) 105	19	−522.7 (10)	46 (2)	106	11	483.1 (40)	−210 (3)

eQq is given in MHz while units of C are kHz. Estimated values of two standard deviations are given in parentheses. Ground state hyperfine constants were fixed at their values from Ref. 19 $[eQq(X\ ^1\Sigma_g^+) = -2452.6$ MHz and $C(X\ ^1\Sigma_g^+) = 3.0$ kHz$]$.

(a) Excitation scheme: $P(100)$ or $R(98)$ (20, 1) B–X (dye laser) followed by $P(99)$ (8, 20) E–B (Kr^{++} $\lambda = 413.1$ nm).

(b) Excitation scheme: $P(107)$ or $R(105)$ (20, 1) B–X (dye laser) followed by $P(106)$ (8, 20) E–B (Kr^{++} $\lambda = 413.1$ nm).

(c) Excitation scheme: $P(106)$ or $R(104)$ (19, 1) B–X (dye laser) followed by R(105) (11, 19) E–B (Kr^{++} $\lambda = 406.7$ nm).

The reduced matrix element $\langle_a l_1 \| V^2(e_1, a) \| l_1 \rangle_a$ may be easily related to the q_{510} constant in the $5p$ orbital of the iodine atom

$$q_{510} = 2\langle m = 51_1 = 1 m_{1_1} = 0 | V_0^2 (a, e) | m = 51_1 = 1 m_{1_1} = 0 \rangle \qquad (6)$$

the constant eQq_{510} is for example given in Refs. 25 or 26.

Taking into account the minus sign arising from the Racah theorem, we finally obtain:

$$eQq_{(E)} = \frac{eQq_{510}}{4} = +573 \text{ MHz} \qquad (7)$$

This result is in rather good agreement with the experimental one $(eQq_{(E)} \simeq 490$ MHz$)$.

TABLE IV
eQq estimations in $E(0_g^+)$ states

Configuration	State	eQq
2242	$^3\Sigma_g^-(0^+)$ or $^1\Sigma_g^+$	+1150 MHg
1432	$^3\Pi(0_g^+)$	−575 MHz
0442	$^1\Sigma_g^+$	−2300 MHz

eQq estimation in $E(0_g^+)$ state were calculated from LCAO eigenfunctions of Ref. 1 using $eQq_{510} = 2300$ MHz for the ^{127}I atom.

The same calculation can be performed if we assume a correlation of the $E(0_g^+)$ state with the $^3P_1$ state of I^+, the result is $eQq = -573$ MHz, in total disagreement with the experimental value.

It is also possible to use the usual LCAO eigenfunctions[1] as in Refs. 25 or 7. The results are given in Table IV, they show that no eQq value obtained by this method is in agreement with the experimental values.

In conclusion it seems that the $E(0_g^+)$ state has a strong ionic character. Moreover, our hyperfine structure measurements are greatly in favour of a correlation of the $E(0_g^+)$ state with the $^3P_2$ state of I^+, in agreement with the observation of the $2g(^2P_2)$ ionic state at 40 386.2 cm^{-1} [6] and with Tellinghuisen's hypothesis.[5]

The nuclear spin-rotation hyperfine constant C

In a $\Omega = 0$ state the C constant may be written as the summation of two terms[27,28] $C = C_D + C_E$. C_D is the direct interaction between the magnetic moment of one nucleus and the orbital angular momentum of the other nucleus. C_E results from second order interaction with $\Omega \neq 0$ electronic states through the rotational hamiltonian. In molecular iodine C_D is very small (≈ 0.15 kHz) and the measured value of C in the E state ($C \approx -200$ kHz) is therefore mainly due to second order effects.

A $1g$ ion pair is known[14,15] to lie very close to the $E(0_g^+)$ state, and it seems reasonable to consider that C in the E state arises mainly from the interaction with this $1g$ state. With this hypothesis, C may be calculated.[29] We obtain:

$$C \approx C_E = \sum_{v'} - \frac{\langle 0_g^+, v | V_{-1}^1(a) | 1_g, v' \rangle \langle 1_g, v' | \frac{\hbar^2}{\sqrt{2}\,\mu r^2}(L_+ + S_+) | 0_g^+, v \rangle}{E_{0_g^+, v, J} - E_{1_g, v', J}}$$

(8)

If we assume that the electronic matrix elements are independent of the internuclear distance, formula (8) becomes:

$$C \approx \langle 0_g^+ | V_{-1}^1(a) 1g \rangle \langle 1g | L_+ + S_+ | 0_g^+ \rangle f(v)$$

(9)

where

$$f(v) = \sum_{v'} \frac{\langle v|v'\rangle \left\langle \dfrac{v'\hbar^2}{\sqrt{2}\,\mu r^2}\Big|v\right\rangle}{E_{0_g^+ vJ} - E_{1gv'J}} \tag{10}$$

As the RKR potential curve of the $1g$ state is known,[15] $f(v)$ may be calculated. The result is given in Table V. The slight variation with v of C is well represented by the theory. Moreover the order of magnitude of $\langle 0_g^+|V_{-1}^1(a)|1g\rangle\langle 1g|L_+ + S_+|0_g^+\rangle$ may be estimated. Indeed if $\psi_E(0_g^+)$ is given by (2) and $\psi(1g)$ by the same formula with $M_J = 1$,

$$\langle 1g|L_+ + S_+|0_g^+\rangle = \sqrt{6} \times \sqrt{2}.$$

but $\langle 0_g^+|V_{-1}^1(a)|1g\rangle$ is more difficult to evaluate.

It is in principle possible to perform the calculation of this matrix element by the method used for calculating eQq value. The magnetic dipole matrix element inside the $^2P_{1/2}$ I atom ($a_{1/2} = 6.6$ GHz) is involved in this calculation. This permits to estimate $\langle 0_g^+|V_{-1}^1(a)|1g\rangle$ of the order of a few GHz (<6.6 GHz) in rough agreement with the value which can be inferred from the experimental value of C through this interpretation.

CONCLUSION

The high resolution of a C.W. optical–optical double resonance in iodine has allowed for the first time the determination of the hyperfine structure in some levels of an ion-pair state in iodine ($E(0_g^+)$). The

TABLE V
$f(v)$ value (Expression (10) in text] for two vibrational levels of the $E(0_g^+)$ state

$v(E\,(0_g^+)$ state)	$f(v)$	C (kHz)	C/f(v) (GHz)
8	-4.790×10^{-5}	-205	4.28
11	-4.893×10^{-5}	-210	4.29

The summation on vibrational levels of the $1g$ state extends from 0 to 29. The main contribution is due to $1g$ v levels under the $E\,(0_g^+)$ ($v = 8$ or 11) states. The RKR curve needed for the calculation of $f(v)$ were calculated for $J_E = 100$ and $J_{1g} = 100$.

theoretical estimates of the hyperfine parameters confirm the $^3P_2$ (I^+) origin of the $E(0_g^+)$ state and shows that the high value of the nuclear spin rotation parameter is due to the nearby $1g$ ion-pair state.

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