Molecular constants describing the $B(^3\Pi_{0u}^+) - X(^1\Sigma_g^+)$ transitions of $^{127,129}I_2$ and $^{129,129}I_2$

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Molecular constants describing the B–X absorption spectra of the radioactive species $^{127,129}I_2$ and $^{129,129}I_2$, are presented. Combined with previous results for the naturally occurring isotopomer $^{127,127}I_2$, they provide the basis for a publicly accessible interactive computer program that automatically yields an ordered and assigned list of all transitions in a specified frequency range, together with the associated (predicted) Franck–Condon and Boltzmann factors.

On présente des constantes moléculaires décrivant les spectres d'absorption B–X des molécules radiatives $^{127,129}I_2$ et $^{129,129}I_2$. Combinées avec des résultats antérieurs pour l'isotopomère $^{127,127}I_2$, ces constantes fournissent la base requise pour l'utilisation d'un programme interactif d'ordinateur, accessible publiquement, qui fournit automatiquement une liste ordonnée et identifiée de toutes les transitions situées dans un intervalle de fréquences spécifié, en même temps que les valeurs associées (prédites) des facteurs de Franck–Condon et de Boltzmann.

[Traduit par la rédaction]

1. Introduction

An extensive compilation of the molecular constants characterizing the $B \leftarrow X$ band system of $^{127,127}I_2$ was published in 1985 (1). When combined with appropriate Franck–Condon factors[2] and with the Boltzmann factors representing the fraction of the molecular population found in each ground-state vibration–rotation level at a given temperature T, they may readily be used to predict the frequencies and intensities of all transitions occurring within a given spectral range (2). In view of the extensive use of this I_2 spectrum as a wavelength standard for the visible region, this is clearly an important capability. Moreover, the accuracy of such predictions is crucial if one wishes to study the hyperfine structure accessible to modern laser spectroscopy (3), since the correct identification of the individual hyperfine components depends critically on the accuracy of the J assignment. In this regard, the availability of reliable predictions will be even more important for the radioactive isotopomers $^{129,129}I_2$ (which, depending on the J parity, has 28 or 36 hyperfine components) and $^{127,129}I_2$ (which has 48 such components).

This communication presents and tests extensive sets of molecular constants for the two radioactive isotopomers $^{127,129}I_2$ and $^{129,129}I_2$. Franck–Condon factors for all thermally accessible bands of these species, for a wide range of rotational quantum numbers, have also been generated. This information, together with analogous results for the naturally occurring isotopomer $^{127,127}I_2$, is incorporated into an interactive computer program that will generate an ordered and assigned listing of the spectral lines in any specified wave-number region, and then combine the associated Franck–Condon factors with the Boltzmann population factors for a chosen temperature to yield

predicted absorption intensities. This program is available to the public through direct access to a guest account at the P.S.I. computer center at the Université de Paris Sud (XI) at Orsay.[3]

In the following, Sect. 2 describes how the molecular constants for the radioactive isotopomers are determined, while Sect. 3 describes tests of their accuracy based on comparisons with some of the (relatively limited) data available for those species. Section 4 then presents an illustrative application of the interactive computer program mentioned above.

2. Molecular constants of the isotopic species $^{127,129}I_2$ and $^{129,129}I_2$

The determination of molecular constants for the radioactive isotopomers of diatomic iodine involves two independent calculations. First of all, the Dunham coefficients $\{Y_{l,0}\}$ and $\{Y_{l,1}\}$, defining the vibrational energies G_v and rotational constants B_v for levels of their X and B states, are generated from the known (1) coefficients for the $^{127,127}I_2$ isotopomer using the usual isotopic relations (4)

$$[1] \quad Y_{l,m}(i) = \rho_i^{l+2m} Y_{l,m}(127, 127)$$

where $\rho_i = [\mu(127, 127)/\mu(i)]^{1/2}$ and $\mu(i)$ is the reduced mass of isotopomer i. In this work, reduced masses of 63.452 2378, 63.948 454, and 64.452 495 u are used for the isotopomers $^{127,127}I_2$, $^{127,129}I_2$, and $^{129,129}I_2$, respectively (5). The resulting values of the $\{Y_{l,m}\}$ expansion coefficients for $^{127,129}I_2$ and $^{129,129}I_2$ are listed in Tables 1 and 2.

As in the work on $^{127,127}I_2$ (1, 6), the second type of calculation involves use of Hutson's method (7) to compute the centrifugal distortion constants D_v, H_v, L_v, and M_v for levels

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TABLE 1. Dunham coefficients $\{Y_{l,m}\}$ for the X and B states of $^{127,129}I_2$, as determined from the experimental results of ref. 1 for $^{127,127}I_2$ and the isotope relations of [1]

l	$Y_{l,0}$ (cm^{-1})	$Y_{l,1}$ (cm^{-1})
	X state for levels $0 \leqslant v'' \leqslant 19$	
0		0.370 781 605 931 × 10^{-1}
1	0.213 695 264 472 × 10^{+3}	-0.112 492 938 231 × 10^{-3}
2	-0.608 216 680 874	-0.301 430 803 093 × 10^{-6}
3	-0.101 540 547 432 × 10^{-3}	-0.401 432 651 209 × 10^{-8}
4	-0.140 516 504 805 × 10^{-3}	0.932 219 368 224 × 10^{-10}
5	0.859 629 495 603 × 10^{-5}	-0.453 925 690 858 × 10^{-11}
6	-0.296 653 257 309 × 10^{-6}	
7	0.412 757 820 710 × 10^{-8}	
	B state for levels $0 \leqslant v'' \leqslant 80$	
0		0.287 756 905 107 × 10^{-1}
1	0.125 180 170 692 × 10^{+3}	-0.147 701 403 946 × 10^{-3}
2	-0.744 576 967 346	-0.124 091 444 518 × 10^{-5}
3	-0.409 590 043 932 × 10^{-2}	0.353 884 449 161 × 10^{-7}
4	0.221 416 497 989 × 10^{-3}	-0.116 189 457 143 × 10^{-7}
5	-0.316 641 264 942 × 10^{-4}	0.156 510 523 105 × 10^{-8}
6	0.276 209 280 540 × 10^{-5}	-0.135 850 214 304 × 10^{-9}
7	-0.165 194 629 633 × 10^{-6}	0.788 935 849 224 × 10^{-11}
8	0.702 596 492 681 × 10^{-8}	-0.316 937 885 234 × 10^{-12}
9	-0.215 963 533 190 × 10^{-9}	0.897 950 787 181 × 10^{-14}
10	0.483 223 177 923 × 10^{-11}	-0.180 637 693 304 × 10^{-15}
11	-0.783 994 986 871 × 10^{-13}	0.256 550 378 969 × 10^{-17}
12	0.908 582 521 702 × 10^{-15}	-0.251 621 580 763 × 10^{-19}
13	-0.730 440 896 777 × 10^{-17}	0.162 269 203 588 × 10^{-21}
14	0.385 950 216 960 × 10^{-19}	-0.619 457 789 727 × 10^{-24}
15	-0.120 291 353 905 × 10^{-21}	0.106 087 293 998 × 10^{-26}
16	0.167 304 015 786 × 10^{-24}	

TABLE 2. Dunham coefficients $\{Y_{l,m}\}$ for the X and B states of $^{129,129}I_2$, as determined from the experimental results of ref. 1 for $^{127,127}I_2$ and the isotope relations of [1]

l	$Y_{l,0}$ (cm^{-1})	$Y_{l,1}$ (cm^{-1})
	X state for levels $0 \leqslant v'' \leqslant 19$	
0		0.367 881 985 892 × 10^{-1}
1	0.212 858 044 863 × 10^{+3}	-0.111 175 930 240 × 10^{-3}
2	-0.603 460 249 467	-0.296 734 684 517 × 10^{-6}
3	-0.100 351 764 256 × 10^{-3}	-0.393 630 322 820 × 10^{-8}
4	-0.138 327 338 463 × 10^{-3}	0.910 519 277 382 × 10^{-10}
5	0.842 921 558 177 × 10^{-5}	-0.441 622 261 126 × 10^{-11}
6	-0.289 747 798 303 × 10^{-6}	
7	0.401 570 225 591 × 10^{-8}	
	B state for levels $0 \leqslant v'' \leqslant 80$	
0		0.285 506 562 385 × 10^{-1}
1	0.124 689 737 299 × 10^{+3}	-0.145 972 193 807 × 10^{-3}
2	-0.738 754 158 824	-0.122 158 171 170 × 10^{-5}
3	-0.404 794 779 718 × 10^{-2}	0.347 006 277 503 × 10^{-7}
4	0.217 966 956 275 × 10^{-3}	-0.113 484 812 871 × 10^{-7}
5	-0.310 486 959 549 × 10^{-4}	0.152 268 383 341 × 10^{-8}
6	0.269 779 713 977 × 10^{-5}	-0.131 650 251 224 × 10^{-9}
7	-0.160 717 111 487 × 10^{-6}	0.761 549 655 006 × 10^{-11}
8	0.680 874 927 171 × 10^{-8}	-0.304 737 472 511 × 10^{-12}
9	-0.208 466 828 268 × 10^{-9}	0.860 001 901 468 × 10^{-14}
10	0.464 621 671 184 × 10^{-11}	-0.172 325 848 397 × 10^{-15}
11	-0.750 862 061 792 × 10^{-13}	0.243 786 626 443 × 10^{-17}
12	0.866 775 095 646 × 10^{-15}	-0.238 166 280 362 × 10^{-19}
13	-0.694 100 405 373 × 10^{-17}	0.152 990 217 763 × 10^{-21}
14	0.365 311 780 093 × 10^{-19}	-0.581 747 395 047 × 10^{-24}
15	-0.113 412 773 478 × 10^{-21}	0.992 387 467 486 × 10^{-27}
16	0.157 119 140 284 × 10^{-24}	

of the X and B states of the two radioactive isotopomers from the corresponding RKR potentials. The requisite potential energy curves were generated from the Dunham expansions for G_v and B_v using the method of Tellinghuisen (8).[2] The resulting centrifugal distortion constants were then incorporated into the program for predicting segments of the $B \leftarrow X$ spectrum, mentioned above (see footnote 3). Tabulations of the vibrational energies (G_v) and the rotational (B_v) and centrifugal distortion constants $(D_v, H_v, L_v, \text{and } M_v)$ for X-state levels $v'' = 0$–19 and B-state levels $v' = 0$–80 of the two radioactive isotopomers may be obtained from the program IODINE IDENTIFICATION described in footnote 3.

Within the first-order semiclassical or WKB approximation, on which both the RKR method and [1] are based, the RKR potentials for the three isotopomers are identical, and it is only higher order contributions and Born–Oppenheimer breakdown effects that lead to differences among them. Fortunately, these differences are quite small for a species with a reduced mass as large as that of I_2, and to the accuracy of a few millikayser (mk) (1 mk $= 10^{-3}$ cm^{-1}) typically associated with Fourier transform spectroscopy, these high-order corrections can be neglected (9). In particular, the well depths $D_e' = 4381.249(1)$ cm^{-1} (10) and $D_e'' = 12\ 547.340(6)$ cm^{-1}, the B-state electronic term value $T_e = 15\ 769.068(2)$ cm^{-1} (1), and the distance between the potential asymptotes (the $^2P_{3/2} - {}^2P_{1/2}$ atomic spin-orbit splitting (11)) 7602.977(2) cm^{-1} are assumed to be the same for all three species. Note that these D_e values include the second-order WKB or Kramer corrections

TABLE 3. The B-state electronic term value $T_0(B)$, and the zero-point energies G_0 and dissociation energies D_0, for the X states (double-prime values) and B states (single-prime values) of the three isotopomers of diatomic I_2

Species	G_0'' (cm^{-1})	G_0' (cm^{-1})	T_0 (cm^{-1})	D_0'' (cm^{-1})	D_0' (cm^{-1})
$^{127,127}I_2$	107.101	62.620	15 724.587	12 440.239	4318.629
$^{127,129}I_2$	106.686	62.378	15 724.759	12 440.654	4318.872
$^{129,129}I_2$	106.268	62.134	15 724.934	12 441.072	4319.115

$Y_{0,0}' = -0.026$ cm^{-1} and $Y_{0,0}'' = -0.010$ cm^{-1}, which are identical (to this accuracy) for these three isotopomers. Table 3 presents values of the zero-point energies G_0' and G_0'', as well as of T_0, and of the X- and B-state dissociation energies D_0' and D_0'' expressed relative to the corresponding zero-point level.

3. Tests of the isotopic relations

As mentioned above, our determination of the constants for $^{127,129}I_2$ and $^{129,129}I_2$ is based on both the Born–Oppenheimer approximation assumption that the electronic potential-energy curves are exactly the same for all three isotopomers, as well as the first-order WKB approximation underlying the isotope relations [1]. These assumptions are quite reliable for a heavy (large reduced mass) molecule such as I_2. One demonstration of this is provided in Table 4, which compares our predicted frequencies for six transitions of $^{129,129}I_2$ with values obtained

TABLE 4. Comparisons between measured (see ref. 3) and calculated energies (σ) for six transitions of $^{129,129}I_2$

Transition	σ(meas.) (cm^{-1})	σ(calc.) (cm^{-1})	Δ (mk)
R(60), 8-4	15 797.9826	15 797.9850	+2.4
R(54), 8-4	15 797.9980	15 798.0003	+2.3
P(69), 12-6	15 798.0213	15 798.0242	+2.9
P(33), 6-3	15 798.0473	15 798.0487	+1.4
R(113), 14-4	16 340.6352	16 340.6378	+2.6
P(110), 10-2	16 340.6486	16 340.6492	+0.6

TABLE 5. Comparison between measured (ref. 3 and footnote 4) and calculated energies (σ), of the P(33), 6-3 transition in the B-X spectrum for the three I_2 isotopomers

Species	σ(meas.) (cm^{-1})	σ(calc.) (cm^{-1})	Δ (mk)
$^{127,127}I_2$	15 797.9763	15 797.9756	-0.7
$^{127,129}I_2$	15 798.0123	15 798.0111	-1.2
$^{129,129}I_2$	15 798.0473	15 798.0487	+1.4

using laser spectroscopy (3). The resulting root-mean-square discrepancy of only 0.0022 cm^{-1} is well within the range of uncertainties associated with the input $^{127,127}I_2$ molecular constants (1), which confirms the validity of the constants determined here.

A second such comparison is presented in Table 5, which compares the laser spectroscopy measurements of the transitions P(33) of the (B-X) 6-3 band for $^{127,127}I_2$, $^{127,129}I_2$ and $^{129,129}I_2$ (3),[4] with predictions generated from the present molecular constants (see footnote 3). The resulting differences Δ are again comparable with the uncertainties in the $^{127,127}I_2$ Fourier transform wave-number measurements, which are the source of all of our molecular constants (see Table 8, p. 19 of ref. 2).

For levels near a dissociation limit, the only data available for the radioactive isotopomers are those obtained by King et al. (12). In Table 6, their results are compared with predictions yielded by the constants presented herein. Although the agreement with experiment in this case is relatively poor, the root-mean-square discrepancy being 0.032 cm^{-1}, this value is significantly smaller than that (0.046 cm^{-1}) associated with the smoothed predictions reported by King et al. (see last columns of Table 6). Moreover, our differences are still of the order of the experimental uncertainties, which were estimated to be ca. 0.01 cm^{-1} (12). Thus, these discrepancies are not unreasonable, especially in view of the suggestion that the Born–Oppenheimer approximation may tend to break down close to this dissociation limit (13). In any case, we have shown elsewhere (13) that more accurate measurements are necessary for providing definitive tests of the accuracy of our molecular constants (1) in this region.

4. Illustrative application of the new molecular constants

Let us assume that we wish to study transitions in the B-X system of $^{129,129}I_2$ near the argon ion laser line at 5020 Å (597 366 GHz) (1 Å = 10^{-10} m). The molecular constants of Table 2 and the associated calculated centrifugal distortion constants (see Sect. 2) may readily be used to calculate the energies of levels associated with any specified lines. However, it would be a very tedious procedure to calculate exhaustively all possible transition energies, to order them to determine which ones lie in the chosen energy range, and to calculate their intensities and Boltzman weighting in order to ascertain their importance. This procedure has been automated by our publicly accessible computer program, IODINE IDENTIFICATION (see footnote 3).

A sample of the output provided by IODINE IDENTIFICATION for the wave-number range 19 925.5–19 926.8 cm^{-1} bracketing the 5020 Å argon ion-laser line is presented in Table 7. The transitions are listed in order of increasing energy σ (column 2), with the corresponding assignment being given in column 1; as usual (4), $J' - J'' = +1$ and -1 for R- and P-lines, respectively. Transitions marked with with an asterisk correspond to high-J values for which our calculated molecular constants are no longer valid.[5] Columns 3 and 4 give the energies of the lower and upper state levels for the specified transition, expressed relative to the ground-state zero-point level, while column 5 lists the fractional Boltzmann population factor for the initial-state level at the specified temperature (here 293 K).

Column 6 of Table 7 presents the relevant Franck–Condon factors (FCF). For $v' \leq 40$, values of these factors were computed for $J = 0, 25, 50, 75, 100, 125, 150, 175,$ and 200, and stored inside the program; for higher v', values were generated on this same mesh up to the highest J within the range for which the present molecular constants are valid.[5] For J's up to the highest value stored in the grid for that value of v', a FCF is obtained by linear interpolation with respect to the variable $[J(J + 1)]$ between adjacent stored values; for J above this highest value, the FCF for the $J = 0$ case is given instead (see notation in the last column). For example, the Franck–Condon factor printed for P(45), 66-0 is determined by interpolating between the stored values for $J = 25$ and 50. Note that rather than storing separate sets of P- and R-branch results, these FCF values were actually calculated for (fictitious) Q-branch ($\Delta J = 0$) transitions. However, for a heavy molecule such as I_2, errors introduced by this approximation will be quite small (14).

Column 7 then lists the product Int. = (Boltz. × FCF), which indicates the relative intensity of that particular absorption line; the suffix " + + " is attached to values for high-J transitions approximately by $J = 0$ matrix elements. Finally, column 8 lists the value of the "r-centroid" (RC) for each transition, which is defined in terms of a ratio of radial wave-function matrix elements:

$$[2] \quad RC = \frac{<v'', J'' \,|r|\, v', J'>}{<v'', J''|v', J'>}$$

where r is the internuclear distance (in ångstrom).

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[4]See also Table 14 of ref. 2, and J. M. Chartier (private communication).

[5]The range of J for which these calculated molecular constants are valid is discussed in detail in ref. 2. For $v' \leq 40$ it is $J \leq 200$, while for $v' > 40$ it is given by the expression $J \leq 375 - 4.375v'$, except when this exceeds the range of J associated with that band in the $^{127,127}I_2$ spectrum.

TABLE 6. Comparisons between measured and calculated energies $G_{v'}$ (relative to the ground-state zero-point level) for levels lying near the dissociation limits of B-state $^{127,129}I_2$ and $^{129,129}I_2$; the numbers in parentheses are the reported uncertainties in the last digits quoted for the experimental values

| | | Measured | | Predicted | | |
| | | Ref. 12 | This work | | Ref. 12 | |
Species	v'	$G_{v'}$ (cm^{-1})	$G_{v'}$ (cm^{-1})	Δ (mk)	$G_{v'}$ (cm^{-1})	Δ (mk)
$^{129,129}I_2$	71	20 018.295(7)	20 018.286	+9	20 018.243	+52
	72	20 023.002(7)	20 022.994	+8	20 022.972	+30
	73	20 027.110(5)	20 027.061	+49	20 027.055	+55
	74	20 030.574(6)	20 030.540	+34	20 030.544	+30
	75	20 033.487(6)	20 033.482	+5	20 033.493	−6
	76	20 035.919(5)	20 035.941	−22	20 035.952	−33
	77	20 037.994(5)	20 037.965	+29	20 037.973	+21
	78	20 039.633(10)	20 039.603	+30	20 039.603	+30
	79	20 040.885(29)	20 040.903	−18	20 040.890	−5
$^{127,129}I_2$	70	20 014.075(23)	20 014.035	+40	20 013.976	+99
	73	20 027.766(10)	20 027.705	+61	20 027.705	+61

TABLE 7. Sample output yielded by the program IODINE IDENTIFICATION for transitions of $^{129,129}I_2$ in the energy range 19 925.5–19 926.8 cm^{-1}, assuming a temperature of $T = 293$ K

Assignment	σ (cm^{-1})	$E_{v''J''}$ (cm^{-1})	$E_{v'J'}$ (cm^{-1})	Boltz.	FCF	Int. (= Boltz. × FCF)	RC (Å)	
$P(57)$, 74-0*	19 925.5098	121.3896	20 046.8994	0.7497-002	0.659-003	0.494-005 + +	2.630	$J = 0$
$P(45)$, 66-0	19 925.5357	76.0175	20 001.5531	0.7412-002	0.195-002	0.145-004	2.634	
$R(42)$, 65-0	19 925.6046	66.3246	19 991.9292	0.7261-002	0.224-002	0.163-004	2.634	
$R(22)$, 62-0	19 925.7351	18.5855	19 944.3207	0.4859-002	0.324-002	0.158-004	2.634	
$P(21)$, 62-0	19 925.8823	16.9695	19 942.8518	0.4680-002	0.324-002	0.152-004	2.634	
$R(31)$, 63-0	19 925.9022	36.4343	19 962.3365	0.6232-002	0.289-002	0.180-004	2.634	
$R(57)$, 78-0*	19 925.9160	121.3896	20 047.3056	0.7497-002	0.288-003	0.216-005 + +	2.630	$J = 0$
$R(54)$, 70-0	19 926.0583	109.0568	20 035.1151	0.7549-002	0.124-002	0.936-005 + +	2.631	$J = 0$
$P(57)$, 78-0*	19 926.1072	121.3896	20 047.4968	0.7497-002	0.288-003	0.216-005 + +	2.630	$J = 0$
$P(52)$, 69-0	19 926.1236	101.2014	20 027.3250	0.7558-002	0.121-002	0.915-005	2.634	
$R(56)$, 72-0*	19 926.1751	117.2053	20 043.3804	0.7519-002	0.921-003	0.692-005 + +	2.630	$J = 0$
$P(30)$, 63-0	19 926.2038	34.1575	19 960.3612	0.6102-002	0.289-002	0.176-004	2.634	
$P(57)$, 80-0*	19 926.2350	121.3896	20 047.6246	0.7497-002	0.164-003	0.123-005 + +	2.630	$J = 0$
$P(41)$, 65-0	19 926.2750	63.2404	19 989.5154	0.7198-002	0.224-002	0.161-004	2.634	
$R(37)$, 64-0	19 926.3186	51.6372	19 977.9559	0.6886-002	0.255-002	0.176-004	2.634	
$P(50)$, 68-0	19 926.3934	93.6393	20 020.0327	0.7545-002	0.143-002	0.108-004	2.634	
$R(57)$, 74-0*	19 926.4727	121.3896	20 047.8622	0.7497-002	0.659-003	0.494-005 + +	2.630	$J = 0$
$R(55)$, 71-0	19 926.5775	113.0944	20.039.6719	0.7537-002	0.107-002	0.806-005 + +	2.631	$J = 0$
$R(57)$, 80-0*	19 926.6159	121.3896	20 048.0055	0.7497-002	0.164-003	0.123-005 + +	2.630	$J = 0$
$P(57)$, 75-0*	19 926.6506	121.3896	20 048.0401	0.7497-002	0.549-003	0.412-005 + +	2.630	$J = 0$
$R(56)$, 79-0*	19 926.6850	117.2053	20 043.8903	0.7519-002	0.222-003	0.167-005 + +	2.630	$J = 0$
$P(36)$, 64-0	19 926.7923	48.9199	19 975.7122	0.6792-002	0.256-002	0.174-004	2.634	

NOTE: Transitions marked * correspond to high-J values for which our calculated molecular constants are no longer valid.
The suffix " + + " is attached to values for high-J transitions approximated by $J = 0$ matrix elements.

As an illustration of the importance of an accurate tabulation of this type, Table 8 compares the present predictions for lines in the subinterval from 19 925.70 to 19 926.66 cm^{-1} with those given in ref. 15. In particular, columns 1–3 show the assignments and energies taken from the IODINE IDENTIFICATION output of Table 7, column 4 lists the predictions for these transitions given in ref. 15, and column 5 shows the discrepancies (Δ) between the two. It is clear that the predictions implied by the less-accurate molecular constants used in the earlier work would have led to incorrect assignments for at least half of these transitions! This should not be too surprising, since

the work of ref. 15 was based on molecular constants taken from various sources (16, 17) whose predictions differ with those generated here by as much as ten times the line width due to the hyperfine structure, which is known to be of the order of 0.030 cm^{-1} (18, 19). However, it dramatically illustrates how readily small discrepancies in molecular constants can give rise to misleading assignments.

5. Concluding remarks

The above examples clearly illustrate the reliability and usefulness of the molecular constants for the radioactive

TABLE 8. Comparison of predicted transition frequencies yielded by the program IODINE IDENTIFICATION (see Table 7) with those reported in ref. 15

Present predictions			Ref. 15	Diff.
Assignment	σ (cm^{-1})	σ (GHz)	σ (GHz)	Δ (GHz)
$R(22)$, 62-0	19 925.735	59 7358.512	59 7358.26	0.25
$P(21)$, 62-0	19 925.882	59 7362.923	59 7362.68	0.24
$R(31)$, 63-0	19 925.902	59 7363.520	59 7363.40	0.12
$P(30)$, 63-0	19 926.204	59 7372.561	59 7372.36	0.20
$P(41)$, 65-0	19 926.275	59 7374.697	59 7361.36	13.34
$R(37)$, 64-0	19 926.319	59 7376.004	59 7375.64	0.36
$P(50)$, 68-0	19 926.393	59 7378.245	59 7361.10	17.14
$R(57)$, 74-0	19 926.473	59 7380.622	59 7369.20	11.42
$R(55)$, 71-0	19 926.578	59 7383.766	59 7366.30	17.47
$P(57)$, 75-0	19 926.651	59 7385.955	59 7375.53	10.43

isotopomers of I_2 determined here. They also demonstrate the importance and practical utility of a program such as IODINE IDENTIFICATION (see footnote 3) for one attempting to make assignments in dense spectra such as those of the radioactive isotopomers of diatomic iodine.

Acknowledgements

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