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Vibration–Rotation Spectrum of Iodine Monobromide

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The high-resolution infrared spectrum of iodine monobromide was recorded in absorption by Fourier transform spectroscopy. About 400 rovibrational transitions were observed near 260 cm^{-1}. The lines were assigned to the $v = 1 \leftarrow 0$ and $v = 2 \leftarrow 1$ bands of the $X\,^1\Sigma^+$ electronic state of $I^{79}Br$ and $I^{81}Br$. The infrared data were combined with millimeter-wave data from the literature to give improved molecular constants.

INTRODUCTION

Iodine monobromide has been the subject of many spectroscopic studies in the past 60 years. The techniques utilized in these studies include visible absorption spectroscopy (*1–7*), emission spectroscopy (*8–11*), resonance Raman spectroscopy (*12–16*), microwave and millimeter spectroscopy (*17–22*), magnetic rotation spectroscopy (*23–25*), laser-induced fluorescence spectroscopy (*26–31*), vacuum ultraviolet spectroscopy (*32–36*), optical–optical double resonance (*37–40*), photoelectron spectroscopy (*41*), and Doppler-free laser spectroscopy (*25, 42*). Information from these spectroscopic studies has played an integral role in the development of theories regarding the potential curves of diatomic interhalogens (*43–51*). Detailed investigations of the potential energy curves have been particularly aided by studies using the techniques of photofragment spectroscopy (*52–56*) and fluorescence excitation spectroscopy (*35, 57–61*). Recent spectroscopic studies have dealt primarily with the determination of the properties of the ion-pair excited electronic states. Ab initio calculations of the electronic states of IBr have been completed (*62, 63*). Considerable interest in diatomic interhalogens has been generated by the observation of laser action (*51, 64–67*). There have also been recent investigations of rare gas–halogen van der Waals molecules (*68*).

In spite of these numerous studies, IBr remains the only diatomic interhalogen for which the infrared rotation–vibration spectrum in its ground electronic state ($X\,^1\Sigma^+$) has not been published. This is a result of the fact that the origin of the fundamental band of IBr is located at 268 cm^{-1}, a region which traditionally is not easily accessible by IR spectrometers. In this paper we present the Fourier transform infrared absorption spectrum of IBr.

EXPERIMENTAL DETAILS

The high-resolution infrared spectrum of IBr was observed with the Bruker IFS 120 HR Fourier transform spectrometer at the University of Waterloo. A liquid-helium-

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TABLE I

Observed Line Positions of $I^{79}Br$ (in cm^{-1})

J'	v'	J"	v"	observed	J'	v'	J"	v"	observed	J'	v'	J"	v"	observed
82	1	83	0	256.3019 (18)[a]	27	1	28	0	263.7176 (-01)	28	1	27	0	270.0605 (14)
79	1	80	0	256.7395 (50)	26	1	27	0	263.8436 (18)	29	1	28	0	270.1652 (42)
78	1	79	0	256.8822 (36)	25	1	26	0	263.9649 (-06)	31	1	30	0	270.3624 (-11)
73	1	74	0	257.5942 (10)	24	1	25	0	264.0900 (12)	32	1	31	0	270.4654 (13)
72	1	73	0	257.7359 (10)	23	1	24	0	264.2109 (-08)	33	1	32	0	270.5659 (15)
71	1	72	0	257.8749 (-14)	22	1	23	0	264.3340 (-01)	34	1	33	0	270.6651 (08)
70	1	71	0	258.0191 (18)	21	1	22	0	264.4564 (02)	35	1	34	0	270.7655 (17)
67	1	68	0	258.4394 (14)	20	1	21	0	264.5778 (-01)	36	1	35	0	270.8646 (18)
64	1	65	0	258.8578 (25)	19	1	20	0	264.6991 (-02)	37	1	36	0	270.9591 (-24)
63	1	64	0	258.9949 (12)	18	1	19	0	264.8225 (22)	38	1	37	0	271.0603 (05)
62	1	63	0	259.1310 (-06)	16	1	17	0	265.0611 (01)	39	1	38	0	271.1578 (02)
61	1	62	0	259.2657 (-35)	15	1	16	0	265.1793 (-14)	41	1	40	0	271.3525 (04)
60	1	61	0	259.4058 (-06)	14	1	15	0	265.3022 (21)	42	1	41	0	271.4449 (-38)
59	1	60	0	259.5439 (07)	13	1	14	0	265.4207 (16)	43	1	42	0	271.5447 (-02)
57	1	58	0	259.8158 (01)	12	1	13	0	265.5396 (19)	44	1	43	0	271.6406 (-01)
56	1	57	0	259.9514 (00)	11	1	12	0	265.6541 (-18)	46	1	45	0	271.8329 (18)
55	1	56	0	260.0868 (02)	10	1	11	0	265.7717 (-20)	47	1	46	0	271.9296 (40)
54	1	55	0	260.2213 (-02)	9	1	10	0	265.8886 (-25)	49	1	48	0	272.1193 (56)
53	1	54	0	260.3549 (-11)	8	1	9	0	266.0131 (50)	50	1	49	0	272.2067 (–03)
52	1	53	0	260.4913 (12)	6	1	7	0	266.2403 (-07)	51	1	50	0	272.2979 (–20)
51	1	52	0	260.6223 (-15)	5	1	6	0	266.3558 (-10)	52	1	51	0	272.3920 (–05)
50	1	51	0	260.7529 (-43)	3	1	4	0	266.5823 (-50)	53	1	52	0	272.4845 (-01)
49	1	50	0	260.8894 (-08)	2	1	1	0	267.2731 (38)	54	1	53	0	272.5782 (19)
48	1	49	0	261.0247 (20)	3	1	2	0	267.3787 (-29)	55	1	54	0	272.6659 (-17)
47	1	48	0	261.1558 (09)	6	1	5	0	267.7147 (-13)	56	1	55	0	272.7589 (04)
46	1	47	0	261.2872 (05)	8	1	7	0	267.9373 (02)	58	1	57	0	272.9401 (11)
45	1	46	0	261.4168 (-14)	9	1	8	0	268.0467 (-02)	60	1	59	0	273.1206 (26)
44	1	45	0	261.5477 (-16)	10	1	9	0	268.1583 (19)	61	1	60	0	273.2068 (00)
43	1	44	0	261.6805 (06)	12	1	11	0	268.3767 (24)	62	1	61	0	273.2938 (-14)
42	1	43	0	261.8078 (-24)	13	1	12	0	268.4833 (07)	68	1	67	0	273.8213 (42)
41	1	42	0	261.9392 (-09)	14	1	13	0	268.5841 (-63)	71	1	70	0	274.0766 (42)
40	1	41	0	262.0675 (-21)	15	1	14	0	268.7038 (58)	73	1	72	0	274.2416 (11)
39	1	40	0	262.2011 (24)	16	1	15	0	268.8090 (40)	74	1	73	0	274.3299 (59)
38	1	39	0	262.3272 (-02)	17	1	16	0	268.9120 (03	77	1	76	0	274.5713 (-05)
37	1	38	0	262.4539 (-18)	18	1	17	0	269.0191 (11)	78	1	77	0	274.6539 (03)
36	1	37	0	262.5863 (26)	19	1	18	0	269.1233 (-07)	66	2	67	1	256.9583 (44)
35	1	36	0	262.7061 (-52)	20	1	19	0	269.2287 (-08)	60	2	61	1	257.7801 (-11)
34	1	35	0	262.8405 (21)	21	1	20	0	269.3332 (-14)	57	2	58	1	258.1909 (13)
33	1	34	0	262.9638 (-14)	22	1	21	0	269.4425 (32)	56	2	57	1	258.3266 (16)
32	1	33	0	263.0900 (-16)	23	1	22	0	269.5454 (18)	55	2	56	1	258.4589 (-10)
31	1	32	0	263.2180 (04)	24	1	23	0	269.6478 (03)	51	2	52	1	258.9949 (-11)
30	1	31	0	263.3434 (02)	25	1	24	0	269.7521 (11)	50	2	51	1	259.1310 (20)
29	1	30	0	263.4649 (-35)	26	1	25	0	269.8532 (-09)	49	2	50	1	259.2657 (40)
28	1	29	0	263.5941 (08)	27	1	26	0	269.9559 (-09)	48	2	49	1	259.3932 (-08)

[a] Observed - calculated line positions using the constants of Table VI.

cooled Si bolometer detector and a 3.5-μm mylar beamsplitter were used. The spectrum was recorded with a resolution of 0.003 cm^{-1} in the region of 30 to 400 cm^{-1}. The spectral band pass was limited by a cold filter for the upper limit and by the detector response for the lower limit.

The IBr was contained in an 80-cm-long stainless steel tube with polyethylene windows (1 mm thick). The absorption cell was filled with 630 mTorr of IBr and 224 scans were coadded. The recording time was limited by the coating of IBr on the polyethylene windows.

RESULTS

A portion of the recorded spectrum is given in Fig. 1. As is evident from Fig. 1, the quality of the spectrum was poor but usable. The observed spectrum exhibits approximately 400 lines corresponding to bands with $v = 1 \leftarrow 0$ and $v = 2 \leftarrow 1$ for both the $I^{79}Br$ and $I^{81}Br$ isotopic species. The observed line positions are given in Tables I and II. No lines for the $v = 3 \leftarrow 2$ transition were observed for either isotopomer.

TABLE I—*Continued*

J'	v'	J"	v"	observed	J'	v'	J"	v"	observed	J'	v'	J"	v"	observed
47	2	48	1	259.5208 (-51)	26	2	27	1	262.2011 (-48)	34	2	33	1	269.0053 (15)
45	2	46	1	259.7887 (02)	25	2	26	1	262.3272 (-20)	40	2	39	1	269.5914 (-02)
44	2	45	1	259.9222 (30)	23	2	24	1	262.5801 (54)	41	2	40	1	269.6858 (-24)
43	2	44	1	260.0516 (20)	15	2	14	1	267.0457 (-01)	42	2	41	1	269.7882 (39)
42	2	43	1	260.1790 (-05)	17	2	16	1	267.2543 (-44)	43	2	42	1	269.8805 (04)
41	2	42	1	260.3084 (-07)	18	2	17	1	267.3705 (59)	44	2	43	1	269.9769 (15)
40	2	41	1	260.4376 (-06)	20	2	19	1	267.5794 (42)	45	2	44	1	270.0716 (13)
39	2	40	1	260.5650 (-20)	21	2	20	1	267.6805 (06)	46	2	45	1	270.1652 (03)
38	2	39	1	260.6930 (-24)	22	2	21	1	267.7851 (09)	47	2	46	1	270.2622 (32)
36	2	37	1	260.9482 (-29)	24	2	23	1	267.9874 (-41)	50	2	49	1	270.5398 (11)
35	2	36	1	261.0793 (10)	25	2	24	1	268.0994 (49)	51	2	50	1	270.6267 (-45)
34	2	35	1	261.2082 (30)	26	2	25	1	268.1917 (-55)	52	2	51	1	270.7237 (05)
33	2	34	1	261.3309 (-07)	27	2	26	1	268.2962 (-32)	56	2	55	1	271.0904 (31)
32	2	33	1	261.4592 (15)	28	2	27	1	268.4048 (35)	57	2	56	1	271.1780 (07)
31	2	32	1	261.5826 (-07)	29	2	28	1	268.5017 (-10)	60	2	59	1	271.4449 (02)
30	2	31	1	261.7056 (-30)	30	2	29	1	268.6076 (39)	63	2	62	1	271.7112 (28)
29	2	30	1	261.8341 (06)	31	2	30	1	268.7038 (-06)	65	2	64	1	271.8816 (−60)
28	2	29	1	261.9572 (-09)	32	2	31	1	268.8090 (45)	67	2	66	1	272.0536 (−67)
27	2	28	1	262.0806 (-15)	33	2	32	1	268.9064 (20)					

The line positions were measured by PC-DECOMP, a program developed by J. W. Brault, which fits the peaks with Voigt lineshape functions. The precision of the lines was limited by the poor signal-to-noise ratio, which ranged from 2 to 10. The strongest lines in the spectrum are determined only to ± 0.001 cm^{-1}, while the precision of the weakest lines is as poor as 0.008 cm^{-1}. Absolute calibration of the spectrum was carried out using the impurity H_2O lines (*69*) in the spectrum.

For data analysis the lines of the rotation–vibration transitions recorded in the infrared were combined with the lines of the pure rotational transitions from the

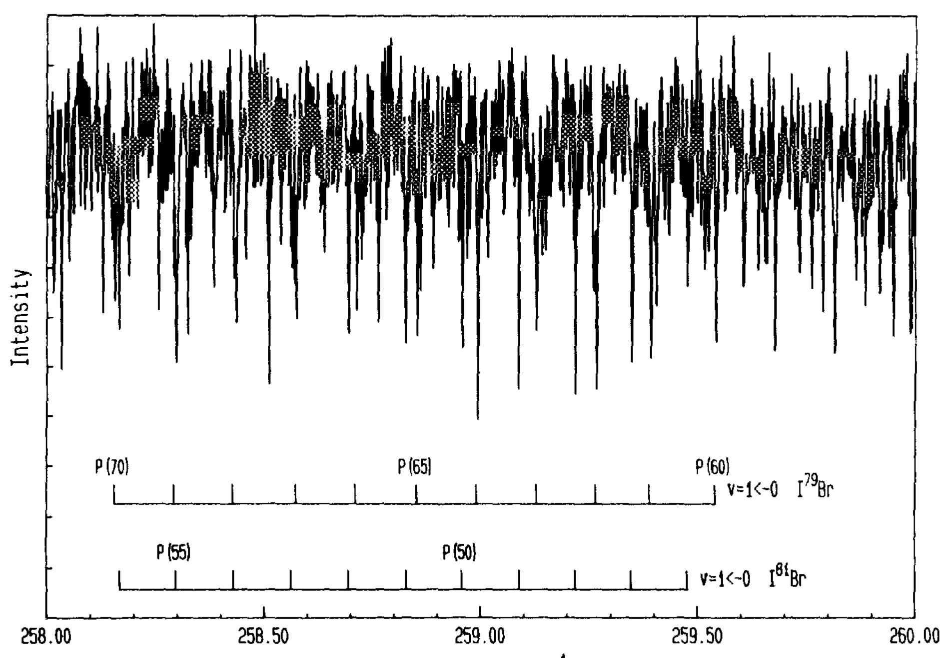

FIG. 1. Portion of the high-resolution infrared spectrum of IBr between 258 and 260 cm^{-1}. The $v = 1 \leftarrow 0$ band of both $I^{79}Br$ and $I^{81}Br$ are indicated on the spectrum.

TABLE II

Observed Line Positions of $I^{81}Br$ (in cm^{-1})

J'	v'	J"	v"	observed	J'	v'	J"	v"	observed	J'	v'	J"	v"	observed
80	1	81	0	254.7286 (-19)[a]	24	1	25	0	262.1074 (09)	31	1	30	0	268.2887 (23)
74	1	75	0	255.5760 (-10)	23	1	24	0	262.2274 (-01)	32	1	31	0	268.3821 (-36)
73	1	74	0	255.7167 (00)	22	1	23	0	262.3497 (17)	33	1	32	0	268.4836 (-09)
71	1	72	0	255.9972 (21)	21	1	22	0	262.4681 (-01)	34	1	33	0	268.5864 (34)
70	1	71	0	256.1353 (15)	20	1	21	0	262.5863 (-18)	35	1	34	0	268.6770 (-40)
69	1	70	0	256.2713 (-08)	19	1	20	0	262.7061 (-14)	36	1	35	0	268.7764 (-23)
68	1	69	0	256.4099 (-01)	18	1	19	0	262.8248 (-17)	37	1	36	0	268.8745 (-14)
67	1	68	0	256.5481 (05)	17	1	18	0	262.9439 (-13)	38	1	37	0	268.9777 (48)
65	1	66	0	256.8258 (43)	16	1	17	0	263.0635 (00)	39	1	38	0	269.0649 (-44)
64	1	65	0	256.9597 (18)	15	1	16	0	263.1795 (-18)	40	1	39	0	269.1651 (-03)
63	1	64	0	257.0920 (-19)	14	1	15	0	263.3003 (14)	41	1	40	0	269.2590 (-20)
62	1	63	0	257.2298 (02)	13	1	14	0	263.4157 (-04)	42	1	41	0	269.3559 (-05)
61	1	62	0	257.3631 (-18)	12	1	13	0	263.5299 (-29)	44	1	43	0	269.5454 (-03)
60	1	61	0	257.4937 (-62)	11	1	12	0	263.6509 (18)	45	1	44	0	269.6434 (38)
59	1	60	0	257.6352 (08)	10	1	11	0	263.7677 (26)	46	1	45	0	269.7372 (37)
58	1	59	0	257.7724 (38)	9	1	10	0	263.8776 (-31)	47	1	46	0	269.8255 (-13)
57	1	58	0	257.9039 (15)	8	1	9	0	263.9958 (-01)	48	1	47	0	269.9184 (–13)
56	1	57	0	258.0369 (10)	7	1	8	0	264.1090 (-17)	49	1	48	0	270.0121 (–01)
55	1	56	0	258.1698 (09)	5	1	6	0	264.3366 (-26)	50	1	49	0	270.1077 (34)
54	1	55	0	258.3003 (-13)	4	1	5	0	264.4595 (66)	52	1	51	0	270.2874 (01)
53	1	54	0	258.4316 (-23)	2	1	3	0	264.6745 (-46)	53	1	52	0	270.3797 (15)
51	1	52	0	258.6958 (-15)	1	1	2	0	264.7983 (67)	54	1	53	0	270.4640 (–46)
50	1	51	0	258.8289 (04)	2	1	1	0	265.2373 (-05)	55	1	54	0	270.5553 (–34)
49	1	50	0	258.9610 (17)	3	1	2	0	265.3470 (-14)	56	1	55	0	270.6476 (–09)
48	1	49	0	259.0895 (-03)	4	1	3	0	265.4590 (04)	57	1	56	0	270.7372 (–05)
47	1	48	0	259.2204 (06)	5	1	4	0	265.5671 (-13)	58	1	57	0	270.8227 (–38)
46	1	47	0	259.3496 (01)	6	1	5	0	265.6776 (-02)	59	1	58	0	270.9125 (–25)
44	1	45	0	259.9086 (01)	7	1	6	0	265.7846 (-22)	60	1	59	0	270.9994 (–37)
45	1	46	0	259.4788 (00)	8	1	7	0	265.8915 (-40)	61	1	60	0	271.0904 (–05)
43	1	44	0	259.7349 (-13)	9	1	8	0	266.0029 (-08)	62	1	61	0	271.1780 (–01)
42	1	43	0	259.8663 (19)	10	1	9	0	266.1115 (-01)	63	1	62	0	271.2635 (–14)
41	1	42	0	259.9939 (17)	11	1	10	0	266.2193 (03)	64	1	63	0	271.3528 (14)
40	1	41	0	260.1195 (-00)	12	1	11	0	266.3295 (33)	66	1	65	0	271.5252 (21)
39	1	40	0	260.2481 (15)	13	1	12	0	266.4312 (-17)	67	1	66	0	271.6058 (–26)
38	1	39	0	260.3768 (36)	14	1	13	0	266.5371 (-21)	69	1	68	0	271.7781 (05)
37	1	38	0	260.4978 (-17)	15	1	14	0	266.6469 (19)	70	1	69	0	271.8627 (11)
36	1	37	0	260.6223 (-31)	16	1	15	0	266.7504 (-02)	71	1	70	0	271.9452 (–01)
35	1	36	0	260.7529 (20)	17	1	16	0	266.8551 (06)	74	1	73	0	272.1921 (–16)
34	1	35	0	260.8748 (-13)	19	1	18	0	267.0657 (09)	75	1	74	0	272.2749 (–09)
33	1	34	0	261.0000 (-08)	20	1	19	0	267.1698 (10)	76	1	75	0	272.3575 (02)
32	1	33	0	261.1263 (11)	22	1	21	0	267.3733 (-22)	77	1	76	0	272.4387 (02)
31	1	32	0	261.2490 (-02)	23	1	22	0	267.4764 (-19)	78	1	77	0	272.5180 (-13)
30	1	31	0	261.3729 (01)	24	1	23	0	267.5794 (-13)	79	1	78	0	272.5971 (–25)
29	1	30	0	261.4938 (-22)	25	1	24	0	267.6805 (-22)	81	1	80	0	272.7589 (–02)
28	1	29	0	261.6194 (05)	26	1	25	0	267.7851 (07)	83	1	82	0	272.9175 (05)
27	1	28	0	261.7457 (44)	27	1	26	0	267.8863 (07)	85	1	84	0	273.0742 (09)
26	1	27	0	261.8629 (-05)	28	1	27	0	267.9874 (11)	93	1	92	0	273.6818 (02)
25	1	26	0	261.9844 (-08)	29	1	28	0	268.0879 (11)	71	2	72	1	254.3963 (-01)

[a] Observed - calculated line positions using the constants of Table VI.

millimeter-wave data of Willis and Clarke (*20, 21*). The millimeter-wave data were corrected for the effect of hyperfine structure by R. E. Willis (*20*). The millimeter-wave data for $I^{79}Br$ and $I^{81}Br$ used in our fits are listed in the Ph.D. thesis of R. E. Willis (*20*) and are shown in Table III.

Initially the lines for each isotopomer were fit to the usual energy level expression (*70*)

$$F_v(J) = T_v + B_vJ(J+1) - D_v[J(J+1)]^2 + H_v[J(J+1)]^3. \qquad (1)$$

The results of the final band-by-band fit are shown in Table IV. The combined millimeter-wave and infrared lines were also fit to the Dunham expression (*71*) for energy levels:

$$T(v, J) = \sum Y_{ij}(v + 1/2)^i[J(J+1)]^j. \qquad (2)$$

TABLE II—*Continued*

J'	v'	J"	v"	observed	J'	v'	J"	v"	observed	J'	v'	J"	v"	observed
70	2	71	1	254.5362 (04)	28	2	29	1	260.0090 (05)	28	2	27	1	266.3558 (19)
68	2	69	1	254.8139 (24)	26	2	27	1	260.2484 (-39)	29	2	28	1	266.4523 (-15)
67	2	68	1	254.9487 (-01)	25	2	26	1	260.3738 (01)	30	2	29	1	266.5536 (01)
63	2	64	1	255.4963 (22)	24	2	25	1	260.4913 (-35)	31	2	30	1	266.6469 (-57)
61	2	62	1	255.7610 (-36)	19	2	20	1	261.0945 (05)	32	2	31	1	266.7504 (-11)
60	2	61	1	255.8999 (07)	18	2	19	1	261.2074 (-53)	33	2	32	1	266.8436 (-62)
59	2	60	1	256.0337 (02)	17	2	18	1	261.3315 (06)	34	2	33	1	266.9472 (-07)
57	2	58	1	256.3006 (-03)	14	2	15	1	261.6813 (-23)	34	2	33	1	266.9474 (05)
55	2	56	1	256.5701 (33)	11	2	12	1	262.0296 (-31)	35	2	34	1	267.0484 (29)
54	2	55	1	256.7022 (30)	6	2	5	1	264.0488 (-58)	36	2	35	1	267.1424 (-02)
52	2	53	1	256.9587 (-41)	7	2	6	1	264.1623 (-09)	37	2	36	1	267.2400 (06)
51	2	52	1	257.0958 (16)	8	2	7	1	264.2741 (27)	38	2	37	1	267.3362 (03)
50	2	51	1	257.2292 (46)	9	2	8	1	264.3786 (-06)	39	2	38	1	267.4344 (26)
45	2	46	1	257.8750 (13)	11	2	10	1	264.5958 (20)	40	2	39	1	267.5285 (10)
43	2	44	1	258.1291 (-15)	12	2	11	1	264.6972 (-33)	41	2	40	1	267.6252 (23)
42	2	43	1	258.2584 (00)	14	2	13	1	264.9108 (-18)	42	2	41	1	267.7147 (-28)
40	2	41	1	258.5133 (02)	16	2	15	1	265.1309 (77)	43	2	42	1	267.8133 (13)
39	2	40	1	258.6397 (00)	17	2	16	1	265.2222 (-58)	44	2	43	1	267.9045 (-15)
38	2	39	1	258.7643 (-17)	18	2	17	1	265.3329 (07)	45	2	44	1	268.0027 (31)
37	2	38	1	258.8904 (-16)	19	2	18	1	265.4363 (00)	47	2	46	1	268.1912 (61)
35	2	36	1	259.1462 (34)	21	2	20	1	265.6430 (01)	48	2	47	1	268.2783 (02)
34	2	35	1	259.2656 (-20)	22	2	21	1	265.7430 (-27)	49	2	48	1	268.3767 (66)
33	2	34	1	259.3948 (27)	23	2	22	1	265.8458 (-22)	50	2	49	1	268.4626 (10)
31	2	32	1	259.6378 (-19)	24	2	23	1	265.9509 (09)	55	2	54	1	268.9120 (-17)
30	2	31	1	259.7640 (10)	25	2	24	1	266.0542 (27)	58	2	57	1	269.1831 (31)
29	2	30	1	259.8846 (-14)	26	2	25	1	266.1524 (03)					

The Dunham coefficients are listed in Table V.

For the final analysis the infrared and millimeter-wave data for both isotopes were combined and fit to the mass-reduced Dunham expression, including Watson's correction due to the breakdown of the Born–Oppenheimer approximation (*72, 73*),

TABLE III

Pure Rotational Transitions of IBr (*20*) (in cm^{-1})

$^{127}I^{79}Br$				$^{127}I^{81}Br$			
v	J' ← J"	observed	o.–c. /10^{-8}	v	J'←J"	observed	o.–c. /10^{-8}
0	44 ← 43	4.989 117 17	20	0	45 ← 44	5.024 786 85	-11
0	53 ← 52	6.007 730 85	138	0	54 ← 53	6.027 839 96	38
0	62 ← 61	7.025 289 47	-12	0	63 ← 62	7.029 852 30	-15
0	79 ← 78	8.943 842 70	180	0	72 ← 71	8.030 650 89	-35
0	80 ← 79	9.056 534 63	55	0	81 ← 80	9.030 063 06	158
0	88 ← 87	9.957 350 62	-16	1	45 ← 44	5.007 367 46	23
1	44 ← 43	4.971 688 11	25	1	54 ← 53	6.006 926 63	-47
1	53 ← 52	5.986 725 32	-73	1	63 ← 62	7.005 441 08	-22
1	62 ← 61	7.000 706 80	17	1	72 ← 71	8.002 737 85	187
1	80 ← 79	9.024 773 70	66	2	45 ← 44	4.989 864 36	9
2	53 ← 52	5.965 622 06	77	2	54 ← 53	5.985 914 43	47
2	62 ← 61	6.976 004 38	-85	2	63 ← 62	6.980 912 21	-132
				2	72 ← 71	7.974 687 24	-7

TABLE IV

Rotational Constants of $I^{79}Br$ and $I^{81}Br$ (in cm^{-1})

$I^{79}Br$

Constant	v = 0	v = 1	v = 2
T_v	-	267.043 68(11)	532.441 28(19)
B_v	0.056 734 005 3(93)[a]	0.056 536 196 1(41)	0.056 337 408 4(289)
$10^9 D_v$	10.195 64(210)	10.261 85(53)	10.315 93(446)
$10^{15} H_v$	-1.33(13)	-	-

$I^{81}Br$

Constant	v = 0	v = 1	v = 2
T_v	-	265.015 306 (90)	528.409 83(15)
B_v	0.055 871 032 1(114)	0.055 677 704 5(69)	0.055 483 438 0(82)
$10^9 D_v$	9.890 0(31)	9.947 8(12)	9.998 5(10)
$10^{15} H_v$	-0.98(26)	-	-

[a] One standard deviation error in the last digits in parentheses.

$$Y_{ij} = \mu^{-(i+2j)/2} U_{ij}\left[1 + \left(\frac{m_e}{m_{Br}}\right)\Delta_{ij}^{Br}\right], \qquad (3)$$

where μ is the reduced mass, U_{ij} are the mass-independent parameters, m_{Br} is the atomic mass of Br, m_e is the electron mass, and Δ_{ij} are the mass scaling factors. The mass-independent Dunham coefficients are listed in Table VI.

TABLE V

Dunham Coefficients for $I^{79}Br$ and $I^{81}Br$ (in cm^{-1})

Coefficient	$I^{79}Br$	$I^{81}Br$
Y_{10}	268.689 79(25)[a]	266.636 17(22)
Y_{20}	−0.823 030(89)	−0.810 422(77)
Y_{01}	0.056 832 583(10)	0.055 967 363(12)
$10^3 Y_{11}$	−0.196 918 0(92)	−0.192 426 2(87)
$10^6 Y_{21}$	−4.757(28)	−4.632(29)
$10^6 Y_{02}$	−0.010 170 9(19)	−0.009 866 4(12)
$10^9 Y_{12}$	−0.049 59(64)	−0.048 65(59)
$10^{15} Y_{03}$	−1.33(11)	−0.92(23)

[a] One standard deviation error in the last digits in parentheses.

TABLE VI

Mass-Reduced Dunham Coefficients for IBr (in cm^{-1})

Coefficient	Value
U_{10}	1874.266 7(12)[a]
U_{20}	−40.045 2(29)
U_{01}	2.765 414 8(30)
U_{11}	−0.066 836 0(19)
10^3U_{21}	−1.130 3(43)
10^3U_{02}	−0.024 081 6(31)
10^6U_{12}	-0.826 7(71)
10^9U_{03}	−0.149 1(88)
Δ_{01}^{Br}	−0.52(16)

[a] One standard deviation error in the last digits in parentheses.

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