

State	T_e	w_e	w_{ex_e}	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e ($\text{\AA}$)	Observed Transitions Design.	References
$^1\text{H}^8\text{Br}$ (continued)									
$c \ ^1\Pi$	$v \ 70578$	2552	Z	52	7.89		1.465	$C \leftarrow X, q$ R	(13)(32)*
$b_0 \ ^3\Pi_0$	$0^+ v \ (68998)$	[2452]			[7.996] ^r		[1.455]	$b_0 \leftarrow X, R$	(13)(32)*
$b_1 \ ^3\Pi_1$	$0^- v \ (68991)$							$b_0 \leftarrow X, R$	(13)(32)*
$b_1 \ ^3\Pi_1$	$v \ (67180)$	[2444.2]	Z		8.148 ^r		1.442	$b_1 \leftarrow X, R$	(13)* (32)*
$b_2 \ ^3\Pi_2$	$v \ [67663.0]$				[7.805] ^r		[1.473]	$b_2 \leftarrow X, R$	(13)(32)*

- ^1HBr : a From $D_0^0(\text{H}_2)$, $D_0^0(\text{Br}_2)$, and $\Delta H_{f0}^0(\text{HBr})$; from gaseous H_2 , Br_2 .
 b Average value from photoionization (10) and photoelectron spectra (23)(29); refers to $X \ ^2\Pi_{3/2}$ of the ion.
 c A more recent paper (39) gives 11.645 eV.
 d Strongly broadened by preionization; estimated lifetime against preionization 9.5×10^{-15} s (46).
 e I, J, K correspond to absorption bands with clear analogues in DBr.
 f From the observed HBr-DBr isotope shift assuming that the observed bands are 0-0 bands.
 g Band [37] of (15).
 h Ω -type doubling, $\Delta v_{ef} = +0.14_2 \times J(J+1) - \dots$; B and D represent average values.
 i Band [28] of (13). Sharp P, Q, R branches; the Q levels appear to be predissociated for $J \geq 14$.
 j From R, P branches. $\Delta v_{ef} = -0.041 \times J(J+1)$.
 k Band [26] of (13).
 l Perturbed at high J.
 m Slightly diffuse lines.
 n Perturbed.
 o Derived from $\text{H}^+ + \text{Br}^-$; configuration $\dots 6^4 \pi^4 6^*$.
 p Heavily perturbed extensive band system. Absorption lines above 75923 cm^{-1} are diffuse. B' varies irregularly between 3.4 and 4.5 cm^{-1} .
 q Average values for the two Ω -type doubling components.
 r Very strong absorption, lines are diffuse.
 s Diffuse rotational structure.
 t Diffuse Q head.
 u Configuration $\dots 6^2 \pi^3 5\pi$.
 v Configuration $\dots 6^2 \pi^3 5p$.
 w Configuration $\dots 6^2 \pi^3 5s$.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e ($\text{\AA}$)	Observed Transitions Design.	References
$^1\text{H}^8\text{Br}$ (continued)									
A ($^1\Pi$) w		Continuous absorption starting at ~ 35000 with maximum at 56400 cm^{-1} .							
X $^1\Sigma^+$	0	2648.975 ^x	Z 45.217 ^y	8.46488 ^x	0.23328 ^z	3.457 ^{a'}	1.41443 ⁵	A ← X Rot.-vibr. sp. b'c' Rotation spectrum d'c' Raman sp. e' Mol. beam el. reson. f'	(1)(2)(4)(5)(26) (21) (8)(17)(31) (45) (42)

 ^1HBr (continued):

^wConfiguration ... $6^2\pi^3\sigma^*$.

^xThese are Y_{10} and Y_{01} values; applying Dunham corrections (21) obtain $w_e = 2649.21_5$, $B_e = 8.46506_5$. Additional corrections (adiabatic, non-adiabatic) are discussed by (38). The microwave B_0 value of (17) was included in the evaluation of B_e . See also b'f'.

^y $w_e y_e = -0.0029$.

^z $+0.000873_5(v+\frac{1}{2})^2 - 0.000120(v+\frac{1}{2})^3$.

^{a'} $-0.0397 \times 10^{-4}(v+\frac{1}{2}) + 0.0038(v+\frac{1}{2})^2$;

^{b'} $H_v = 7.63 \times 10^{-9} - 0.55 \times 10^{-9}(v+\frac{1}{2})$.

In absorption the 1-0, 2-0, 3-0, 3-1, 4-0, 5-0, 6-0 bands have been studied (6)(7)(12)(21)(41); in emission 1-0, 2-1, 3-2, 4-3 (11)(20). The constants in the table are from (21), those of (20)(41) are very similar and of comparable accuracy. See also (47). Absolute intensities have been measured (16)(18)(30)(33) and the dipole moment function has been

calculated; (40) give for H^{79}Br [$D, \text{\AA}$], $\mu_{ef}(r) = +0.788 + 0.315(r-r_e) + 0.575(r-r_e)^2$; see also (24)(34)(37).

^{c'}For observations and measurements of pressure-induced bands and pure rotation lines ($\Delta J=2$) see (22)(27). The pressure broadening of the lines has been studied by (16)(25).

^{d'}Absolute intensities have been measured by (19).

^{e'}Raman cross sections in gaseous HBr.

^{f'}The following constants (as well as corresponding values for H^{79}Br) are given in (42):

- $\mu_{ef}(v=0, J=1) = 0.8265 \text{ D}$ [in a later paper (44) derive 0.8282 D from Stark effect of rotation spectrum];
- quadrupole and other hyperfine coupling constants;
- $\epsilon_J = 0.3712$.

These constants supersede earlier values of (9)(17)(26)(31)(35).

State	T _e	w _e	w _e x _e	B _e	α _e	D _e (10 ⁻⁴ cm ⁻¹)	r _e (Å)	Observed Transitions Design. ν ₀₀	References
2H ⁸¹ Br									
μ = 1.96518641 D ₀ ⁰ = 3.804 eV ^a I.P. = 11.67 ₃ eV ^b Numerous absorption bands above 114000 cm ⁻¹ ; see ¹ HBr.									
M (1 ¹ Σ ⁺) (109374)		[1000]	v=0...5 observed.	} See ¹ HBr.				M←X, 108937	(13)*
L (1 ¹ Σ ⁺ , 1Π) (104141)		[971]	v=0...4 observed.					L←X, (103690)	(13)*
Further absorption bands of doubtful assignment between 72000 and 83800 cm ⁻¹ .									
K ^c 1 (83908)		(1792) ^d		[4.121] ^e		[0.80]	[1.442 ₈]	K←X, R 83867.1 ^f	Z (6)
J ^c 1 (81248)		(1781) ^d		[4.083] ^g		[1.36]	[1.449 ₅]	J←X, R 81202.2 ^f	Z (6)*
I ^c 1 (80442)		(1797) ^d		[4.107]		[1.38]	[1.445 ₂]	I←X, R 80403.8 ^f	Z (6)
G (3 ² Σ ⁻) ⁰⁺ (78125)		[1440.6]	Z	[3.79]	(0.40) ^h	[14]	[1.50 ₄]	G←X, R 77908.8	Z (6)(10)
F 1 _Δ [77989.0]				[4.095]			[1.447 ₃]	F←X, R 77052.3	Z (6)(10)
f ₁ 3 _Δ ₁ (76787)				4.06 ₄	0.07 ₆		1.453	f ₁ ←X, R 76679.2	Z (6)(10)
D 1 _Π (76280)				4.128 ⁱ	0.07 ₆		1.441 ₅	D←X, R 76209.1	Z (6)(10)*
d ₀ 3 _Π ₀ [77027.4]				[3.993] ^j			[1.466]	d ₀ ←X, R 76090.7	Z (10)*
E (1 ¹ Σ ⁺) ⁰⁺ (75682)				[3.953]	(0.78) ^h		[1.472 ₉]	E←X, R 75428.1	Z (6)(10)
V 1 _Σ ⁺		Extensive absorption system above 75700 cm ⁻¹ , incompletely analysed because of strong perturbations. B _v values range from 1.68 to 2.12.							
f ₂ 3 _Δ ₂ (74370)		[1660.3]	Z	4.29 ₄	0.097	[2.4]	1.413	f ₂ ←X, R 74263.1	Z (6)(10)*
f ₃ 3 _Δ ₃ [75088.6]				[3.83]		[-2.1]	[1.49 ₇]	f ₃ ←X, R 74151.9	Z (10)*
e 3 _Σ ⁺ [74677]				Weak transition.				e←X, 73740	(10)
d ₁ 3 _Π ₁ [74499]				Very diffuse, unresolved band.				d ₁ ←X, R 73562	(6)(10)
d ₂ 3 _Π ₂ [74391.5]				Diffuse band, rotational structure unresolved.				d ₂ ←X, R 73454.8	Z (6)(10)*
C 1 _Π 70563		1811.2	Z 25.5	4.02 ^k	0.10 ₅	[0.36]	[1.482]	C←X, R (70501)	H ^Q (6)(8)*

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e ($\text{\AA}$)	Observed Transitions Design. v_{00}	References
$2\text{H}^{81}\text{Br}$ (continued)									
b_0 $3\pi_0$ 0^+ 0^-	[69837.1] [69832]	Unresolved Q branch, assignment uncertain.		[4.082] ^m			[1.450]	$b_0 \leftarrow X$, R (68900.4 Z R (68895)	(6)* (8)*
b_1 $3\pi_1$	67113.9	1814	Z 27	4.10 ⁿ	0.09		1.44 ₆	$b_1 \leftarrow X$, R (67077.5 Z	(6)(8)
b_2 $3\pi_2$	[67290.7]	Continuous absorption beginning at $\sim 39000 \text{ cm}^{-1}$.		[4.018] ^m			[1.461]	$b_2 \leftarrow X$, R (66354.0 Z	(6)(8)
A (1π)								$A \leftarrow X$,	(1)
X $1\Sigma^+$	0	1884.75	Z 22.71 ₈ ^o	[4.245596] ^p	0.083 ₈	[0.8832] ^p	1.414 ₅	Rot.-vibr. sp. ^q Rotation spectrum ^r	(2)(5) (3)(4)(9)(12)
		1837.33 = 1884.75 - 2(22.71)							

2HBr : ^aFrom $D_0(^1\text{HBr})$.

^bFrom the photoelectron sp. (11) of the isotopic mixture.

^cSee d of ^1HBr .

^dSee e of ^1HBr .

^e Ω -type doubling, $\Delta v_{ef} \approx + 0.0371 J(J+1)$.

^fBands {35}, {27}, {26} of (6).

^g Ω -type doubling, $\Delta v_{ef} = + 0.0314 J(J+1)$.

^h $v=0$ and 1 only; $v=1$ is perturbed.

ⁱFrom P, R branches. $B_0(Q) = 4.109$.

^jFrom P, R branches. $B_0(Q) = 3.926$.

^kBranches are slightly diffuse.

^lDiffuse rotational structure; $v=0\dots 4$.

^mSlightly diffuse lines.

ⁿ $v=2$, 3 diffuse. Slightly diffuse lines for $v=0$, 1.

^o $w_e v_e = - 0.0106$.

^pMicrowave value (9)(12).

^q1-0, 2-0, 3-0 bands in absorption (2), $\Delta v=1$ sequence in

emission (5).

$r_{\mu_{e2}}$ ($v=0$) = 0.8233 D from Stark effect of 1-0 line (12).
Quadrupole and other hyperfine coupling const. (7)(9)(12).

(1) See ref. (1) of ^1HBr .

(2) Keller, Nielsen, JCP 22, 294 (1954).

(3) Palik, JCP 23, 217 (1955).

(4) Cowan, Gordy, PR 111, 209 (1958)

(5) See ref. (11) of ^1HBr .

(6) See ref. (15) of ^1HBr .

(7) See ref. (26) of ^1HBr .

(8) See ref. (32) of ^1HBr .

(9) De Lucia, Helminger, Gordy, PR A 3, 1849 (1971).

(10) See ref. (36) of ^1HBr .

(11) See ref. (39) of ^1HBr .

(12) See ref. (44) of ^1HBr .

(13) See ref. (43) of ^1HBr .