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Publication Date
1968-08-01

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NUCLEAR QUADRUPOLE RATIO OF BROMINE ISOTOPES IN MOLECULAR LiBr

A. J. Hebert and K. Street, Jr.

August 7, 1968

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To be submitted to Physical Review

UCRL-18353 Rev.

UNIVERSITY OF CALIFORNIA

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Berkeley, California

AEC Contract No. W-7405-eng-48

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NUCLEAR QUADRUPOLE RATIO OF BROMINE ISOTOPES IN MOLECULAR LiBr*

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(Received 12 August 1968)

The Molecular Beam Electric Resonance method has been used to determine the ^{79}Br to ^{81}Br nuclear quadrupole moment ratio in molecular LiBr. The observed ratio of 1.197056(6) agrees with one obtained elsewhere for atomic bromine, thus indicating no observable nuclear polarizability effect.

generator at a 19 Hz rate across each line in synchronization with the channel advance in a modified Northern multichannel analyzer. The detected "flop-in" transitions were all $J = 1$, $m_J = \pm 1$ to $J = 1$, $m_J = 0$ for the three lowest vibrational levels of each isotope. Peak signal intensities were better than 10^4 transitions per channel above background for all observed lines with no observable baseline slope. Typical run times were from one to three hours (approximatley 70 to 210 thousand sweeps) for each line with signal to noise ratios of 100 or better. Line position reproducibility was better than 1 part in 10^6 of frequency for runs made on different days. This corresponds to an uncertainty of less than 15 Hz at 15 MHz, compared to the previous several hundred Hz. All observed lines occurred between 8 and 20 MHz.

Previous strong field electric dipole moment measurements[1] were checked and found to be accurate. Measurements performed in this laboratory by F. W. Breivogel, Jr. on the ^{7}LiBr isotopes[4] allowed hyperfine corrections for the ^{6}Li quadrupole and spin-rotation interactions. Second order quadrupole, Stark-quadrupole, and magnetic dipole spin-spin interaction effects were included in treating the data. Calculations indicate that a large electron coupled spin-spin interaction, (i.e. much greater than the calculated dipole spin-spin interaction of approximately 90 cps), would have a negligible effect on the values reported here.

Calculated hyperfine interaction constants are given in Table I. The present results for each of the three vibrational states measured are in agreement with our previously reported values. The present bromine nuclear quadrupole moment ratios are lower than those previously reported by almost

3 times the probable error. This discrepancy arises primarily from the manner in which the data were treated. In the previous report the quadrupole coupling constants for each isotopic species were separately extrapolated to $v = -1/2$ and the ratio then taken. The probable error was assigned assuming that the errors would be random. The new measurements indicate that there was a non-random trend in the data, which was accentuated by extrapolation to the equilibrium internuclear distance. In our opinion, this non-random trend was produced by a combination of decreasing signal to noise ratio for higher vibrational states, and a previous lack of knowledge about the magnitude of the ^{6}Li quadrupole interaction.

In looking for a nuclear polarizability effect a much better method of treating the data is to simply interpolate the ^{81}Br coupling constant for each vibrational state the very short distance in v necessary to achieve the same energy as the corresponding ^{79}Br vibrational state. This small correction is much less sensitive to uncertainties in $(eqQ)_I$ and $(eqQ)_{II}$. The bromine nuclear quadrupole moment ratios calculated in this manner are given in Table II. Treating the previous data in the same manner gives an average ^{79}Br to ^{81}Br nuclear quadrupole ratio of 1.19712(8) for the weak field data, and an average of 1.19706(8) for the three states observed at intermediate electric field strength.

The best present ^{79}Br to ^{81}Br nuclear quadrupole ratio of 1.197056(6) for LiBr (calculated from the $v = 0$ vibrational states corrected to a common energy), is in excellent agreement with the value 1.1970568(15) observed by Brown and King for atomic Br, thus indicating no observable nuclear polarizability effect.

Table I. Hyperfine Interaction Constants of LiBr ($\times \frac{1}{h}$ K Hz).*

Vibrational State	$^6Li\ ^{79}Br$ Present	$^6Li\ ^{79}Br$ Previous[a]	$^6Li\ ^{81}Br$ Present	$^6Li\ ^{81}Br$ Previous[a]
		$(eqQ)_{Br}$		
0	38,463.92(30)	38,463(5) 38,464(5)	32,131.06(30)	32,127(5) 32,130(5)
1	41,307.01(40)	41,304(5) 41,306(5)	34,504.11(40)	34,500(5) 34,504(5)
2	44.069.71(50)	44,067(5) 44,070(5)	36,810.41(50)	36,805(5) 36,810(5)
3		46,751(5)		39,046(5)
4		49,355(5)		41,222(5)
5		51,883(5)		
		$(eqQ)_{Li}$[b]		
0	4.3(2)		(4.3(2)	
1	4.3(4)		4.3(4)	
2	4.3(6)		4.3(6)	
		c_{Br}		
0	9.064(70)	9.2(2)	9.793(70)	9.9(2)
1	9.024(80)	9.2(2)	9.727(80)	9.9(2)
2	9.017(90)	9.2(2)	9.690(90)	9.9(2)
		c_{Li}[b]		
0	0.22(13)		0.22(13)	
1	0.22(13)		0.22(13)	
2	0.22(13)		0.22(13)	
	$(eqQ)_v = (eqQ)_e + (eqQ)_I\ (v + \frac{1}{2}) + (eqQ)_{II}\ (v + \frac{1}{2})^2$			
		$(eqQ)_e$		
	37,012.233(850)	37,015(3)	30919.501(850)	30,916(2)
		$(eqQ)_I$		
	2,923.474(900)	2,918(2)	2,439.798(900)	2,438(2)
		$(eqQ)_{II}$		
	-40.194(350)	-39(2)	-33.374(350)	-33(2)

* All values were calculated using h = 6.6253×10^{-27} erg-sec and c = 2.997925×10^{10} cm/sec.

a. Ref. 1. Where two values are given the second is from data taken at intermediate fields.

b. Isotope corrected values calculated from data in Ref. 4.

Table II. Nuclear Quadrupole Moment Ratios Q_{79}/Q_{81}

V	$\frac{(eqQ)_{79}}{(eqQ)_{81}}$ (Uncorrected)	$\frac{(eqQ)_{79}}{(eqQ)_{81}}$ (Corrected to a common vibrational energy)
0	1.197095(6)	1.197056(6)
1	1.197162(9)	1.197055(9)
2	1.197208(12)	1.197046(12)

$[(eqQ)_e]_{79_{Br}} / [(eqQ)_e]_{81_{Br}} = 1.197051(12)$

Atomic Bromine Ratio[3] $\frac{Q_{79}}{Q_{81}} = 1.1970568(15)$

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*This work was supported under the auspices of the U. S. Atomic Energy Commission.

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