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Short Tabulation of Hyperfine Structure in $^{129}I_2$

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Abstract

Hyperfine constants are presented for different ro-vibrational transitions in the B-X system in $^{129}I_2$ calculated from experimental results obtained from different groups. Constants are listed for radiation of wavelength 612 nm and 633 nm.

In connection with the present definition of the Metre, adopted in 1983 [1], a list of recommended radiations is given by the Comité International des Poids et Mesures (CIPM) as one of the means of the practical realization of the Metre [2]. The list, which is a part of the *Mise en Pratique* of the Definition of the Metre [3], was revised by the CIPM in 1992 and now contains eight recommended radiations of which six are obtained using iodine [3]. In the *Mise en Pratique* recommended frequency tables are listed, containing hyperfine components originating from 20 different ro-vibrational transitions in $^{127}I_2$ and $^{129}I_2$.

Recently, a tabulation was presented [4] of calculations, made by different groups, on the hyperfine structure and hyperfine constants of different ro-vibrational transitions in the B-X system in $^{127}I_2$. We present here five complementary tables of hyperfine constants on transitions in $^{129}I_2$: 14-4 R(113), 10-2 P(110), 8-4 P(54), 12-6 P(69) and 6-3 P(33) of the B-X system.[1] The experimental data used to calculate the presented constants are listed in [3].

Four hyperfine constants are usually needed in the theoretical expression to describe the relative energy levels of the hyperfine structure of molecular iodine with the same precision as those obtained by experiment. The Hamiltonian of hyperfine interaction, H_{hfs}, can be written

$$H_{hfs} = eQq \cdot H_{eQq} + C \cdot H_{SR} + d \cdot H_{TSS} + \delta \cdot H_{SSS} \tag{1}$$

where H_{eQq}, H_{SR}, H_{TSS} *and* H_{SSS} represent the electric quadrupole, spin-rotation, tensorial spin-spin, and scalar spin-spin interactions, respectively, and where *eQq, C, d* and δ represent the corresponding constants for each of those interactions.

To calculate the hyperfine constants of $^{129}I_2$, we have modified a computer programme usually used to calculate the hyperfine structure for $^{127}I_2$ [6,7]. First, we consider the interaction from rotational levels with rotational quantum number $J \pm 2$ in the quadrupole

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[1] Constants of these transitions have earlier been listed by Gläser [5]. We have discovered an error in the computer programme used by Gläser; H_{TSS} was calculated for a total nuclear spin of 5 instead of 7.

interaction term [8]. We have calculated the rotational energies for $^{129}I_2$ by correcting the rotational constants given by Luc and Gerstenkorn, for $^{127}I_2$ [9], by the square root of the ratio between the reduced masses, ρ, for the two isotopic molecules: $\rho = 0{,}992210$. Second, the nuclear spin is incremented by 1 for ^{129}I compared to ^{127}I. This gives 36 or 28 hyperfine components depending on whether the quantum number of the total spin is an odd or even number, respectively. Third, we have empirically deduced a lower state electric quadrupole hyperfine constant, eQq'', by correcting the eQq'' for $^{127}I_2$ found by Yokozeki and Muenter [10] by the ratio of the quadrupolar moments, Q, of the nuclei: $^{129}Q/^{127}Q = 0{,}699$ [11]. This results in $eQq''= -1714{,}4$ MHz. We have kept the other lower state hyperfine constants at zero during the calculations. The experimental values vary considerably in uncertainty. This is the reason why we have weighted the calculations proportionally to the inverse of the square of the experimental uncertainties.

The results are listed in Tables 1 and 2. The reference of the measurement is given at the top of each column and the fitted constants ΔeQq, ΔC, Δd and $\Delta \delta$ are listed. The symbol Δ indicates the difference between the upper and the lower state constants. The calculated standard deviation of the fit is represented by *s*. The calculated uncertainties in the last digit(s) are shown in parantheses. The constant has been fixed in the calculation when no parantheses are indicated.

Table 1.

$\lambda = 612$ nm, $^{129}I_2$		
trans.	10-2 P(110)	14-4 R(113)
meas.	[3,12-14]	[3,11,12]
ΔeQq/MHz	1364,86(6)	1357(1)
ΔC/kHz	17,67(2)	20,9(2)
$\Delta\delta$/kHz	0	0
Δd/kHz	-16,3(9)	0
s/kHz	42	270

Table 2.

$\lambda = 633$ nm, $^{129}I_2$			
trans.	8-4 P(54)	12-6 P(69)	6-3 P(33)
meas.	[3,15-20]	[3,15,18,20]	[3,15,20-22]
ΔeQq/MHz	1368,0(1)	1362,3(2)	1369,5(6)
ΔC/kHz	15,79(9)	18,9(1)	14,70(8)
$\Delta\delta$/kHz	0	0	0
Δd/kHz	-9(3)	-13(7)	-8,5(9)
s/kHz	47	160	68

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