Calculated frequency differences of the hyperfine structure lines of some transitions ($\Delta F = \pm 1$, $\Delta F = 0$) and of cross-over-lines of $^{129}I_2$ and $^{127}I_2$.

PART I :
Transitions R(127)11-5 and R(47)9-2 of $^{127}I_2$ and P(110)10-2 and R(113)14-4 of $^{129}I_2$.

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1. Introduction

In the fields of metrology and spectroscopy very accurate values of wavelengths and frequencies of the hyperfine structure (HFS) components of iodine are desired. There are three HFS components of $^{127}I_2$ whose absolute frequencies have been determined and are recommended by the Comité Consultatif pour la Définition du Mètre (CCDM) [1]. The known frequency differences between other HFS-components and the recommended ones have been assembled in order to be recommended as well [2].

The uncertainties of these values are mainly determined by the reproducibilities of the corresponding measurements. But, even if the corresponding measurements are of high precision, systematic shifts can exceed the reproducibility of the measurements. One of these systematic shifts is caused by superpositions of neighboring lines [3]. Neighboring lines of the same signal amplitude are always known if they are resolved. So their influence is known, at least qualitatively. Smaller lines, however, are often not seen, but they shift the frequency, too, if their distance to the main line has an appropriate value. So it would be useful to know the positions not only of the HFS components of the allowed transitions ($\Delta F = \pm 1$) having the largest signal amplitude, but also those of the forbidden transitions ($\Delta F = 0$) having an estimated relative amplitude of $(2 \cdot J^2)^{-1}$ and those of the cross-over lines with an estimated relative amplitude of $(2 \cdot J^2)^{-\frac{1}{2}}$, both amplitudes estmated at low saturation level ; F and J represent the quantum numbers of the total and the rotational angular momentum, respectively. Equally, it would be useful to know the HFS lines of other rotation-vibrational transitions in the same wavelength region having probably a lower transition probability and so a smaller signal amplitude as the normally used lines. These iodine transitions can be calculated by using the molecular constants given in ref.[4] with an uncertainty of less than 250 MHz for $^{127}I_2$.

In this work the HFS splittings including the $\Delta F = \pm 1$ and $\Delta F = 0$ transitions are calculated by using a computer program developed by H.J. Foth [5, 6].

The frequency shift, caused by the superposition of two or more lines, depends mainly on the unperturbed line shape and on the distance of both lines. Calculations of those shifts of saturated absorption lines, supposing Lorentzian line shapes, are reported in ref.[7, 8].

2. Procedure and Results

On the basis of measured frequency differences between the allowed HFS-components of an iodine transition, the molecular constants, described in ref.[5], are optimized (see Table 1). From these constants, the values of the HFS level frequencies have been calculated, and from the values of the HFS level frequencies, the transition frequencies of the allowed $\Delta F = \pm 1$ and forbidden $\Delta F = 0$ transitions have been calculated (Tables 2-5). The positions of the cross-over lines result from both the allowed transitions and the forbidden ones having one common level. The frequency zero points coincide with the HFS-components whose wavelengths have been recommended by the CCDM [1].

The number of each group of lines depends on the atomic nuclear spin I of the iodine isotope : $I = 5/2$ for ^{127}I and $I = 7/2$ for ^{129}I, as well as on the value of J of the corresponding molecule. The component number of a $\Delta F = \pm 1$ transition is : $N_a = 2I\ (I + \frac{1}{2})$ for even J-values and : $N_a = 2(I + 1)\ (I + \frac{1}{2})$ for uneven J-values. The component number of a $\Delta F = 0$ transition is : $N_f = (2N_a - 2I - 1)/2$, the number of the cross-over lines is : $N_c = 2N_f$. In Tables 2 to 5 the allowed and forbidden lines having a common level, as well as the derived cross-over lines, are arranged in the same or the following writing line. So each forbidden line appears twice according to the two possibilities to produce a cross-over line.

The nomenclature attributed to the lines corresponds to the recommendations of ref.[6, 9], but other used notations are also given in the tables and figures.

Fig. 1 to 24 give the positions of the calculated HFS components as vertical lines above ($\Delta F = \pm 1$), across (cross-over) or below ($\Delta F = 0$) the frequency axis. The diagonal lines connecting the top of a $\Delta F = \pm 1$ line with the bottom of a $\Delta F = 0$ line are given to visualize the position of the respective cross-over lines at the cross-points of the diagonal lines with the frequency axis.

The most remarkable perturbations of the strong allowed HFS-lines by lines of the same transition are given in Table 6. To know all perturbing lines, all rotation-vibrational iodine transitions of the concerned spectral region of the used iodine molecules must be analyzed. In the emission range of a He-Ne laser at a wavelength of $\lambda = 633$ nm, the $^{127}I_2$ transition : R(127)11-5; the $^{129}I_2$ transitions : P(54)8-4, P(69)12-6, R(60)8-4, P(33)6-3; and the $^{127}I^{129}I$ transition : P(33)6-3, have been found experimentally [2]. The calculation using Luc's data [4] gives the further $^{127}I_2$ transition : R(80)1-0, about 300 MHz lower than R(127)11-5. In the emission range of a He-Ne laser at a wavelength of $\lambda = 612$ nm, the $^{127}I_2$ transitions : R(47)9-2, P(48)11-3, R(48)15-5 [10] and the $^{129}I_2$ transitions : P(110)10-2 and R(113)14-4 [6, 11, 12] have been found experimentally [2]. The calculation also gives the $^{127}I_2$ transition : R(34)17-6, about 500 MHz higher than R(47)9-2. So the perturbations given in table 6 have to be completed by lines of the other cited transitions.

An analysis of the remaining transitions at $\lambda = 633$ nm and $\lambda = 612$ nm, as well as those at other wavelengths, is in process.

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Table 1 : Calculated molecular constants of the hyperfine splitting of four iodine transitions

	$^{127}I_2$		$^{129}I_2$	
	R(127)11-5	R(47)9-2	P(110)10-2	R(113)14-4
eQq'(MHz)	-513.95 ± 0.09	-511 ± 29	-448 ± 7	-529 ± 12
eQq"(MHz)	-2458.63 ± 0.09	-2459 ± 29	-1813 ± 7	-1887 ± 12
ΔeQq(MHz)	1944.681 ± 0.004	1948.3 ± 0.6	1365.3 ± 0.2	1358.42 ± 0.15
ΔC (kHz)	28.44 ± 0.001	25.2 ± 0.2	17.6 ± 0.06	21.2 ± 0.04
ΔD (kHz)	-18.93 ± 0.08	-14 ± 8	-34 ± 10	14 ± 9
ΔA (kHz)	-14.38 ± 0.03	-21 ± 3	-7 ± 1	13 ± 0.9

Table 2 : Frequency differences between the hyperfine structure components of the R(127)11-5 transition of $^{127}I_2$ at a wavelength of λ = 633 nm, measured values from ref.[2, 13]. The estimated errors of the calculated values are : for ΔF = + 1 lines : σ = 0.01 MHz, for ΔF = 0 and cross-over lines : σ = 0.1 MHz.

In the same line as the allowed (ΔF = + 1) transition (or in the following line), the forbidden (ΔF = 0) transition, having one common level with the allowed one, is given, along with the appropriate cross-over line.

ΔF = + 1						ΔF = 0			Cross-over	
Component		$\Delta\nu_{meas}$[MHz]	I	F-J	$\Delta\nu_{calc}$[MHz]	Comp	F	$\Delta\nu_{calc}$[MHz]	Comp	$\Delta\nu_{calc}$[MHz]
a_1	u		5	-5	-607.853	f_{6a}	123	-249.38	c_{4a}	-428.62
a_2	t		1	0	-583.086	f_{18a}	128	342.34	c_{19a}	-120.37
						f_{1a}	127	-778.98	c_{1a}	-681.03
a_3	s		5	5	-559.265	f_{2a}	132	-642.16	c_{2a}	-600.71
a_4	r		5	-4	-320.752	f_{11a}	124	52.77	c_{17a}	-133.99
						f_{6a}	123	-249.38	c_{9a}	-285.07
a_5	q		3	-1	-292.791	f_{12a}	127	72.91	c_{21a}	-109.94
						f_{5a}	126	-334.33	c_{7a}	-313.56
a_6	p		3	1	-290.290	f_{9a}	129	-102.23	c_{11a}	-196.26
						f_{3a}	128	-371.74	c_{5a}	-331.01
a_7	o		5	4	-263.192	f_{2a}	132	-642.16	c_{3a}	-452.68
						f_{4a}	131	-343.08	c_{8a}	-303.14
a_8	n	-162.814	3	-3	-162.809	f_{7a}	125	-156.24	c_{14a}	-159.53
a_9	m	-153.801	3	-2	-153.815	f_{5a}	126	-334.33	c_{10a}	-244.07
						f_{7a}	125	-156.24	c_{15a}	-155.03
a_{10}	l	-137.994	3	2	-137.971	f_{8a}	130	-132.43	c_{16a}	-135.20
						f_{9a}	129	-102.23	c_{20a}	-120.10

Table 2 (cont.)

		$\Delta F = +1$				$\Delta F = 0$			Cross-over	
Component		$\Delta\nu_{meas}$ [MHz]	I	F-J	$\Delta\nu_{calc}$ [MHz]	Comp	F	$\Delta\nu_{calc}$ [MHz]	Comp	$\Delta\nu_{calc}$ [MHz]
a_{11}	k	-129.950	3	3	-129.960	f_{8a}	130	-132.43	c_{18a}	-131.19
a_{12}	j	-21.564	5	-3	-21.573	f_{14a}	125	160.13	c_{25a}	69.28
						f_{11a}	124	52.77	c_{23a}	15.60
a_{13}	i	0	3	0	-0.010	f_{3a}	128	-371.74	c_{12a}	-185.87
						f_{12a}	127	72.91	c_{24a}	36.45
a_{14}	h	21.939	5	3	21.943	f_{4a}	131	-343.08	c_{13a}	-160.57
						f_{10a}	130	-20.67	c_{22a}	0.64
a_{15}	g	125.696	5	-2	125.691	f_{17a}	126	319.77	c_{30a}	222.73
						f_{14a}	125	160.13	c_{27a}	142.91
a_{16}	f	138.892	1	-1	138.887	f_{1a}	127	-778.98	c_{6a}	-320.05
a_{17}	e	152.255	1	1	152.254	f_{18a}	128	342.34	c_{31a}	247.30
a_{18}	d	165.114	5	2	165.117	f_{10a}	130	-20.67	c_{26a}	72.22
						f_{13a}	129	124.96	c_{28a}	145.04
a_{19}	c	283.006	5	-1	283.024	f_{15a}	127	288.73	c_{32a}	285.88
						f_{17a}	126	319.77	c_{36a}	301.40
a_{20}	b	291.100	5	0	291.098	f_{16a}	128	297.42	c_{34a}	294.26
						f_{15a}	127	288.74	c_{33a}	289.92
a_{21}	a	299.931	5	1	299.924	f_{13a}	129	124.96	c_{29a}	212.44
						f_{16a}	128	297.42	c_{35a}	298.67

Table 3 : Frequency differences between the hyperfine structure components of the R(47)9-2 transition of $^{127}I_2$ at a wavelength of λ = 612 nm, measured values from ref.[2, 12, 14, 15]. The estimated errors of the calculated values are : for ΔF = + 1 lines : σ = 0.02 MHz, for ΔF = 0 and cross-over lines : σ = 0.2 MHz. For other specifications, see Table 2.

ΔF = + 1						ΔF = 0			Cross-over	
Component		$\Delta\nu_{meas}$[MHz]	I	F-J	$\Delta\nu_{calc}$[MHz]	Comp	F	$\Delta\nu_{calc}$[MHz]	Comp	$\Delta\nu_{calc}$[MHz]
a_1	u	-357.16	5	-5	-357.18	f_{6a}	43	-16.4	c_{4a}	-186.8
a_2	t	-334.04	1	0	-333.98	f_{18a}	48	596.1	c_{20a}	131.1
						f_{1a}	47	-524.7	c_{1a}	-429.3
a_3	s	-312.56	5	5	-312.48	f_{2a}	52	-395.9	c_{2a}	-354.2
a_4	r	-86.17	5	-4	-86.17	f_{9a}	44	123.6	c_{11a}	18.7
						f_{6a}	43	-16.4	c_{8a}	-51.3
a_5	q	-47.32	3	1	-47.26	f_{10a}	49	146.6	c_{12a}	49.6
						f_{3a}	48	-126.7	c_{5a}	-87.0
a_6	p	-36.86	3	-1	-36.75	f_{12a}	47	323.5	c_{22a}	143.4
						f_{5a}	46	-74.3	c_{7a}	-55.5
a_7	o	0	5	4	0.09	f_{2a}	52	-395.9	c_{3a}	-197.9
						f_{4a}	51	-76.0	c_{9a}	-38.0
a_8	n	81.47	5	-3	81.47	f_{14a}	45	429.8	c_{23a}	255.7
						f_{9a}	44	123.6	c_{15a}	102.5
a_9	m	99.18	3	-2	99.14	f_{5a}	46	-74.2	c_{10a}	12.5
						f_{7a}	45	65.5	c_{14a}	82.3
a_{10}	l	107.52	3	2	107.50	f_{8a}	50	120.5	c_{17a}	114.0
						f_{10a}	49	146.6	c_{19a}	127.0

Table 3 (cont.)

		ΔF = + 1					ΔF = 0		Cross-over	
Component		$\Delta\nu_{meas}$ [MHz]	I	F-J	$\Delta\nu_{calc}$ [MHz]	Comp	F	$\Delta\nu_{calc}$ [MHz]	Comp	$\Delta\nu_{calc}$ [MHz]
a_{11}	k	119.11	3	3	119.10	f_{8a}	50	120.5	c_{18a}	119.8
a_{12}	j	219.62	3	-3	219.66	f_{7a}	45	65.5	c_{21a}	142.6
a_{13}	i	249.60	3	0	249.66	f_{3a}	48	-126.7	c_{13a}	61.5
						f_{12a}	47	323.5	c_{25a}	286.6
a_{14}	h	284.37	5	3	284.36	f_{4a}	51	-76.0	c_{16a}	104.2
						f_{11a}	50	244.4	c_{24a}	264.4
a_{15}	g	358.35	5	-2	357.43	f_{17a}	46	568.6	c_{29a}	463.0
						f_{14a}	45	429.8	c_{27a}	393.6
a_{16}	f	384.76	1	-1	384.72	f_{1a}	47	-524.7	c_{6a}	-70.0
a_{17}	e	403.85	1	1	403.84	f_{18a}	48	596.1	c_{31a}	500.0
a_{18}	d	430.04	5	2	430.04	f_{11a}	50	244.4	c_{26a}	337.2
						f_{13a}	49	395.6	c_{28a}	412.8
a_{19}	c	527.20	5	-1	527.25	f_{15a}	47	541.0	c_{32a}	534.1
						f_{17a}	46	568.6	c_{34a}	547.9
a_{20}	b	539.31	5	0	539.28	f_{16a}	48	557.4	c_{35a}	548.4
						f_{15a}	47	541.0	c_{33a}	540.1
a_{21}	a	555.23	5	1	555.19	f_{13a}	49	395.6	c_{30a}	475.4
						f_{16a}	48	557.4	c_{36a}	556.3

Table 4 : Frequency differences between the hyperfine structure components of the P(110)10-2 transition of $^{129}I_2$ at a wavelength of λ = 612 nm, measured values from ref.[6, 11, 12]. The estimated errors of the calculated values are : for ΔF = - 1 lines : σ = 0.03 MHz, for ΔF = 0 and cross-over lines : σ = 0.3 MHz. For other specifications see Table 2.

ΔF = - 1						ΔF = 0			Cross-over	
Component		$\Delta\nu_{meas}$[MHz]	I	F-J	$\Delta\nu_{calc}$[MHz]	Comp	F	$\Delta\nu_{calc}$[MHz]	Comp	$\Delta\nu_{calc}$[MHz]
a_1	b'	-376.30	0	0	-376.29					
a_2	a'	-244.80	6	-6	-244.76	f_{2a}	104	-273.6	c_{1a}	-259.2
a_3	z	-230.77	4	1	-230.92	f_{13a}	110	-33.2	c_{11a}	-132.0
						f_{3a}	111	-261.3	c_{3a}	-246.1
a_4	y	-229.43	4	-1	-229.42	f_{8a}	108	-100.9	c_{7a}	-165.2
						f_{1a}	109	-274.7	c_{2a}	-252.1
a_5	x	-216.10	6	6	-216.07	f_{9a}	115	-81.3	c_{9a}	-148.7
a_6	w	-149.40	6	-5	-149.39	f_{2a}	104	-273.6	c_{4a}	-211.5
						f_{4a}	105	-164.3	c_{8a}	-156.9
a_7	v	-134.70	4	-2	-134.71	f_{10a}	107	-73.7	c_{16a}	-104.2
						f_{8a}	108	-100.9	c_{14a}	-117.8
a_8	u	-131.00	4	2	-131.01	f_{3a}	111	-261.3	c_{5a}	-196.2
						f_{5a}	112	-146.0	c_{10a}	-138.5
a_9	t	-116.67	6	5	-116.66	f_{11a}	114	-55.8	c_{19a}	-86.2
						f_{9a}	115	-81.3	c_{17a}	-99.0
a_{10}	s	-96.30	6	-4	-96.29	f_{4a}	105	-164.3	c_{12a}	-130.3
						f_{6a}	106	-141.6	c_{13a}	-118.9

Table 4 (cont.)

$\Delta F = -1$						$\Delta F = 0$			Cross-over	
Component		$\Delta\nu_{meas}$ [MHz]	I	F-J	$\Delta\nu_{calc}$ [MHz]	Comp	F	$\Delta\nu_{calc}$ [MHz]	Comp	$\Delta\nu_{calc}$ [MHz]
a_{11}	r	-90.70	4	-3	-90.80	f_{16a}	106	34.6	c_{25a}	-28.1
						f_{10a}	107	-73.7	c_{20a}	-82.2
a_{12}	q	-84.20	4	0	-84.08	f_{1a}	109	-274.7	c_{6a}	-179.4
						f_{13a}	110	-33.2	c_{22a}	-58.6
a_{13}	p	-77.80	4	3	-77.85	f_{5a}	112	-146.0	c_{15a}	-112.0
						f_{7a}	113	-109.1	c_{18a}	-93.5
a_{14}	o	-72.70	6	4	-72.77	f_{20a}	113	125.3	c_{29a}	26.3
						f_{11a}	114	-55.8	c_{21a}	-64.3
a_{15}	n	1.50	4	-4	1.64	f_{16a}	106	34.5	c_{28a}	18.1
a_{16}	m	10.60	2	-1	10.62	f_{23a}	108	202.3	c_{40a}	106.5
						f_{12a}	109	-51.6	c_{26a}	-20.5
a_{17}	l	15.90	2	1	15.83	f_{24a}	110	274.0	c_{44a}	144.9
						f_{14a}	111	-30.9	c_{27a}	-7.5
a_{18}	k	25.30	4	4	25.31	f_{7a}	113	-109.1	c_{24a}	-41.9
a_{19}	j	49.40	6	-3	49.47	f_{6a}	106	-141.6	c_{23a}	-46.0
						f_{17a}	107	50.4	c_{31a}	49.9
a_{20}	i	54.70	6	-2	54.57	f_{17a}	107	50.4	c_{32a}	52.5
						f_{15a}	108	24.3	c_{30a}	39.4
a_{21}	h	69.00	6	2	69.02	f_{22a}	111	197.7	c_{42a}	133.4
						f_{18a}	112	69.8	c_{34a}	69.4

Table 4 (cont.)

	ΔF = − 1					ΔF = 0			Cross-over	
Component		$\Delta\nu_{meas}$ [MHz]	I	F-J	$\Delta\nu_{calc}$ [MHz]	Comp	F	$\Delta\nu_{calc}$ [MHz]	Comp	$\Delta\nu_{calc}$ [MHz]
a_{22}	g	74.50	6	3	74.46	f_{18a}	112	69.8	c_{35a}	72.1
						f_{20a}	113	125.3	c_{38a}	99.9
a_{23}	f	110.60	6	0	110.59	f_{21a}	109	171.8	c_{43a}	141.2
						f_{19a}	110	95.6	c_{39a}	103.1
a_{24}	e	153.07	2	-2	153.07	f_{23a}	108	202.3	c_{46a}	177.7
a_{25}	d	154.73	6	-1	154.75	f_{15a}	108	24.3	c_{37a}	89.5
						f_{21a}	109	171.8	c_{45a}	163.3
a_{26}	c	164.03	6	1	163.97	f_{19a}	110	95.6	c_{41a}	129.8
						f_{22a}	111	197.7	c_{47a}	180.8
a_{27}	b	166.17	2	2	166.26	f_{14a}	111	-30.9	c_{33a}	67.7
a_{28}	a	208.30	2	0	208.34	f_{12a}	109	-51.6	c_{36a}	78.4
						f_{24a}	110	274.0	c_{48a}	241.2

Table 5 : Frequency differences between the hyperfine structure components of the R(113)14-4 transition of $^{129}I_2$ at a wavelength of λ = 612 nm, measured values from ref.[2, 6]. The estimated errors of the calculated values are : for ΔF = + 1 lines : σ = 0.2 MHz, for ΔF = 0 and cross-over lines : σ = 2 MHz. For other specifications, see Table 2.

ΔF = + 1					ΔF = 0			Cross-over	
Component	$\Delta\nu_{meas}$[MHz]	I	F-J	$\Delta\nu_{calc}$[MHz]	Comp	F	$\Delta\nu_{calc}$[MHz]	Comp	$\Delta\nu_{calc}$[MHz]
b_1	-	7	-7	-796.0	f_{6b}	107	-603.7	c_{4b}	-699.8
b_2	-	1	0	-774.7	f_{32b}	114	-30.3	c_{37b}	-402.5
					f_{1b}	113	-983.7	c_{1b}	-879.2
b_3	-	7	7	-752.8	f_{2b}	120	-814.7	c_{2b}	-783.7
b_4	-	7	-6	-655.3	f_{11b}	108	-514.9	c_{10b}	-585.1
					f_{6b}	107	-603.7	c_{8b}	-629.5
b_5	-	3	1	-629.3	f_{27b}	115	-217.1	c_{35b}	-423.2
					f_{3b}	114	-764.9	c_{5b}	-697.1
b_6	-	3	-1	-629.0	f_{31b}	113	-161.1	c_{38b}	-395.0
					f_{4b}	112	-742.3	c_{6b}	-685.6
b_7	-	7	6	-602.7	f_{2b}	120	-814.7	c_{3b}	-708.7
					f_{5b}	119	-661.5	c_{7b}	-632.1
b_8	-	7	-5	-551.8	f_{19b}	109	-358.8	c_{32b}	-455.3
					f_{11b}	108	-514.9	c_{15b}	-533.3
b_9	-	5	-2	-535.0	f_{21b}	112	-336.6	c_{33b}	-435.8
					f_{8b}	111	-555.3	c_{13b}	-545.2
b_{10}	-	5	2	-529.3	f_{16b}	116	-458.4	c_{24b}	-493.8
					f_{7b}	115	-589.3	c_{12b}	-559.3

Table 5 (cont.)

ΔF = + 1						ΔF = 0			Cross-over	
Component		$\Delta\nu_{meas}$[MHz]	I	F-J	$\Delta\nu_{calc}$[MHz]	Comp	F	$\Delta\nu_{calc}$[MHz]	Comp	$\Delta\nu_{calc}$[MHz]
b_{11}		-	5	5	-514.2	f_{9b}	118	-534.9	c_{17b}	-524.5
b_{12}		-	5	-5	-504.4	f_{13b}	109	-498.0	c_{21b}	-501.2
b_{13}		-	5	-4	-497.4	f_{14b}	110	-492.7	c_{23b}	-495.1
						f_{13b}	109	-498.0	c_{22b}	-497.7
b_{14}		-	5	-3	-491.6	f_{8b}	111	-555.3	c_{18b}	-523.4
						f_{14b}	110	-492.7	c_{25b}	-492.2
b_{15}		-	5	0	-483.7	f_{20b}	114	-348.1	c_{36b}	-415.9
						f_{10b}	113	-523.6	c_{19b}	-503.6
b_{16}		-	5	3	-475.7	f_{15b}	117	-471.4	c_{28b}	-473.6
						f_{16b}	116	-458.4	c_{30b}	-467.0
b_{17}		-	5	4	-470.1	f_{9b}	118	-534.9	c_{20b}	-502.5
						f_{15b}	117	-471.4	c_{29b}	-470.7
b_{18}		-	7	5	-460.7	f_{5b}	119	-661.5	c_{11b}	-561.1
						f_{12b}	118	-502.4	c_{27b}	-481.5
b_{19}	r	-410.4	7	-4	-410.6	f_{22b}	110	-333.8	c_{41b}	-372.2
						f_{19b}	109	-358.8	c_{39b}	-384.7
b_{20}	q	-390.0	5	-1	-389.8	f_{10b}	113	-523.6	c_{31b}	-456.7
						f_{21b}	112	-336.6	c_{43b}	-363.2
b_{21}	p	-383.9	5	1	-383.6	f_{7b}	115	-589.3	c_{26b}	-486.5
						f_{20b}	114	-348.1	c_{42b}	-365.9

Table 5 (cont.)

ΔF = + 1						ΔF = 0			Cross-over	
Component		$\Delta\nu_{meas}$ [MHz]	I	F-J	$\Delta\nu_{calc}$ [MHz]	Comp	F	$\Delta\nu_{calc}$ [MHz]	Comp	$\Delta\nu_{calc}$ [MHz]
b_{22}	o	-362.8	7	4	-362.6	f_{12b}	118	-502.4	c_{34b}	-432.5
						f_{17b}	117	-400.8	c_{40b}	-381.7
b_{23}	n	-352.9	7	-3	-352.9	f_{26b}	111	-220.8	c_{50b}	-286.8
						f_{22b}	110	-333.8	c_{45b}	-343.3
b_{24}	m	-346.4	3	-2	-346.4	f_{4b}	112	-742.3	c_{14b}	-544.4
						f_{18b}	111	-366.0	c_{44b}	-356.2
b_{25}	l	-330.0	3	2	-330.1	f_{23b}	116	-326.5	c_{48b}	-328.3
						f_{27b}	115	-217.1	c_{52b}	-273.6
b_{26}	k	-324.9	3	3	-325.0	f_{23b}	116	-326.5	c_{49b}	-325.7
b_{27}	j	-304.7	3	-3	-304.7	f_{18b}	111	-366.0	c_{47b}	-335.4
b_{28}	i	-289.4	3	0	-289.8	f_{3b}	114	-764.9	c_{16b}	-527.3
						f_{31b}	113	-161.1	c_{56b}	-225.4
b_{29}	h	-273.1	7	3	-273.3	f_{17b}	117	-400.8	c_{46b}	-337.1
						f_{24b}	116	-294.6	c_{51b}	-284.0
b_{30}	g	-255.7	7	-2	-255.5	f_{30b}	112	-179.7	c_{57b}	-217.6
						f_{26b}	111	-220.8	c_{54b}	-238.1
b_{31}	f	-	1	-1	-246.6	f_{1b}	113	-983.7	c_{9b}	-615.1
b_{32}	e	-236.7	1	1	-236.4	f_{32b}	114	-30.3	c_{64b}	-133.3
b_{33}	d	-	7	2	-227.5	f_{24b}	116	-294.6	c_{53b}	-261.1
						f_{25b}	115	-246.4	c_{55b}	-237.0

Table 5 (cont.)

	$\Delta F = +1$					$\Delta F = 0$			Cross-over	
Component		$\Delta\nu_{meas}$ [MHz]	I	T-J	$\Delta\nu_{calc}$ [MHz]	Comp	F	$\Delta\nu_{calc}$ [MHz]	Comp	$\Delta\nu_{calc}$ [MHz]
b_{34}	c	-198.7	7	-1	-198.4	f_{28b}	113	-194.4	c_{59b}	-196.4
						f_{30b}	112	-179.7	c_{62b}	-189.1
b_{35}	b	-193.1	7	0	-193.2	f_{29b}	114	-188.2	c_{61b}	-190.7
						f_{28b}	113	-194.4	c_{60b}	-193.8
b_{36}	a	-187.0	7	1	-186.9	f_{25b}	115	-246.4	c_{58b}	-216.6
						f_{29b}	114	-188.2	c_{63b}	-187.5

Table 6 : Main perturbing neighbours of the strong allowed HFS-lines consisting of lines having the same rotation-vibrational transition.

I_2 Transition	$\Delta F = \pm 1$ HFS-comp.		Perturbing Neighbour	Frequency Difference (MHz)
R(127)11-5	a_4	r	c_{6a}	0.7
	a_5	q	a_6	2.5
	a_6	p	a_5	2.5
	a_9	m	c_{15a}	1.2
	a_{10}	l	c_{16a}	1.5
	a_{11}	k	c_{18a}	1.2
	a_{13}	i	c_{22a}	0.6
	a_{20}	b	c_{33a}	1.1
	a_{21}	a	c_{35a}	1.3
			c_{36a}	1.5
R(47)9-2	a_4	r	c_{5a}	0.8
	a_6	p	c_{9a}	1.1
	a_8	n	c_{14a}	0.8
	a_{11}	k	c_{18a}	0.7
	a_{20}	b	c_{33a}	0.8
	a_{21}	a	c_{36a}	0.9
P(110)10-2	a_2	a'	c_{3a}	1.3
	a_3	z	a_4	1.3
	a_4	y	a_3	1.3
	a_6	w	c_{9a}	0.7
	a_8	u	c_{12a}	0.7
	a_9	t	c_{14a}	1.1
	a_{18}	k	c_{29a}	1.0
	a_{19}	j	c_{31a}	0.5
	a_{21}	h	c_{34a}	0.4
	a_{24}	e	a_{25}	1.7
	a_{25}	d	a_{24}	1.7
	a_{26}	c	a_{27}	2.1
			c_{45a}	0.7
	a_{27}	b	a_{26}	2.1

Figure Captions

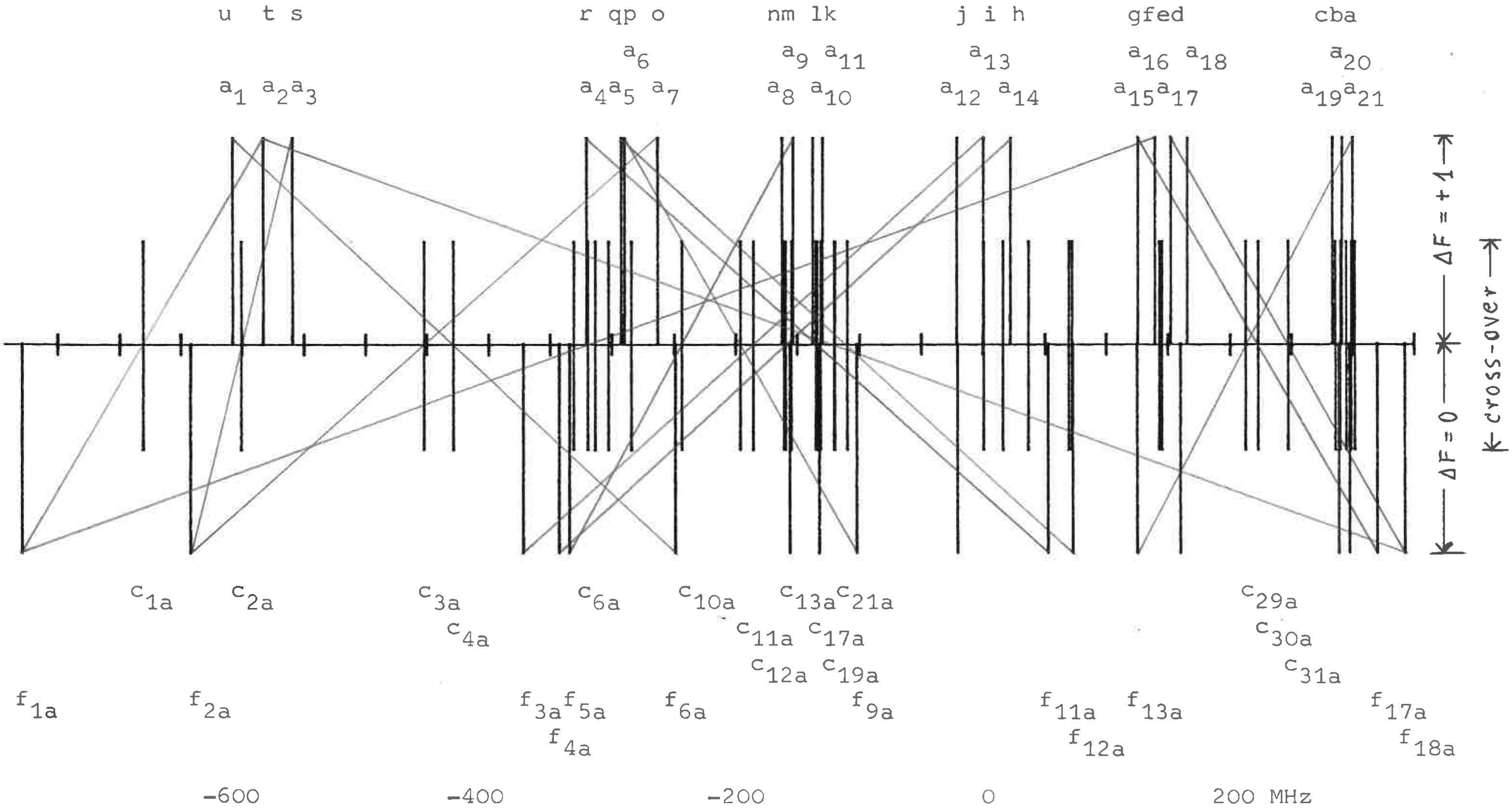
Fig. 1- 5 : Positions of the calculated hyperfine structure componets of R(127)11-5 of $^{127}I_2$ at λ = 633 nm on a frequency scale. The vertical lines represent : the $\Delta F = \pm 1$ transitions above, the cross-over lines, across, and the $\Delta F = 0$ transitions below the frequency axis.

Fig. 6-10 : Hyperfine structure components of R(47)9-2 of $^{127}I_2$ at λ = 612 nm. Further conditions as in Fig. 1-5.

Fig. 11-16 : Hyperfine structure components of P(110)10-2 of $^{129}I_2$ at λ = 612 nm. Further conditions as in Fig. 1-5.

Fig. 17-24 : Hyperfine structure components of R(113)14-4 of $^{129}I_2$ at λ = 612 nm. Further conditions as in Fig. 1-5.

Fig.1: $^{127}I_2$; R(127)11-5; λ=633 nm



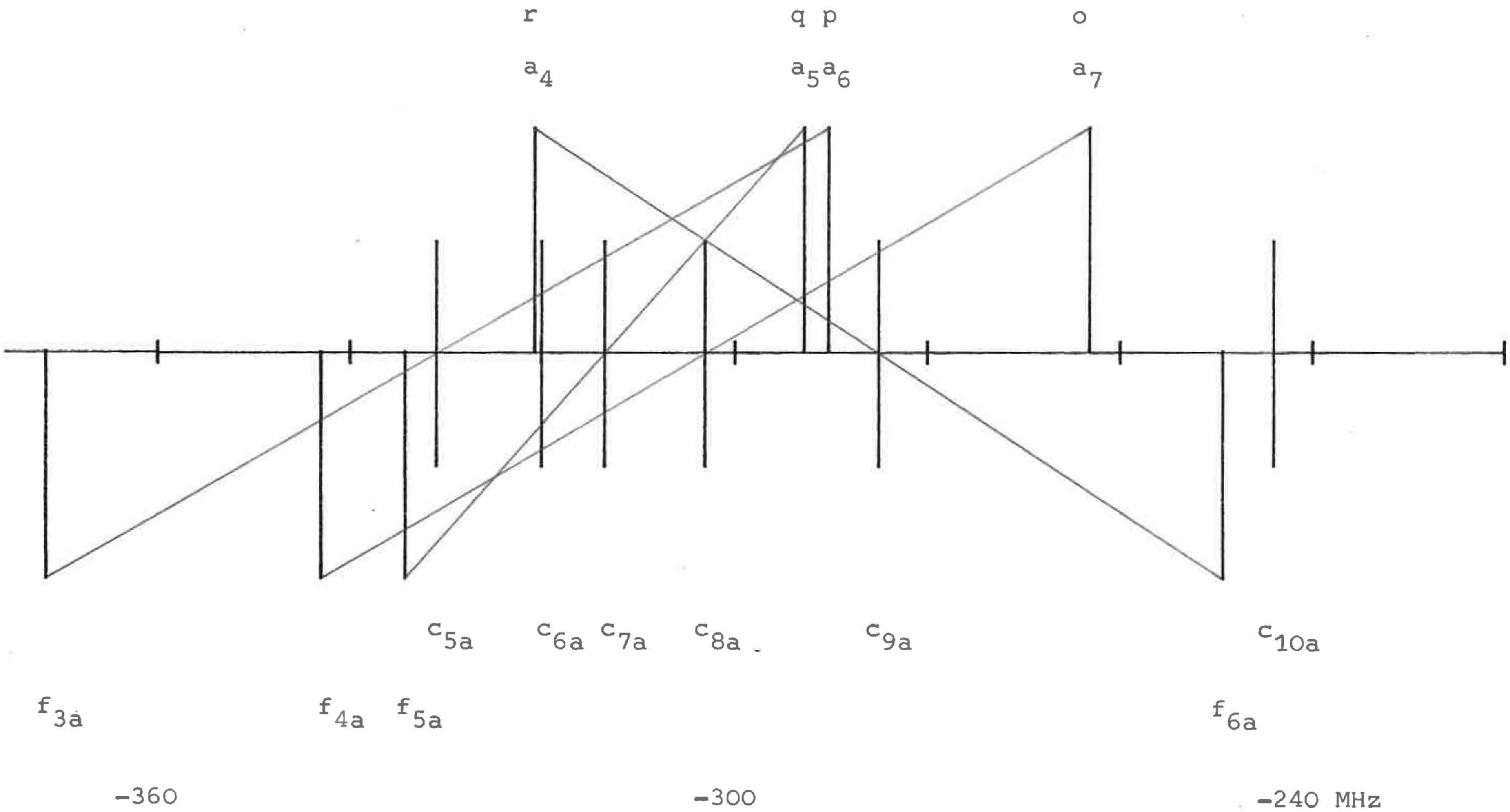


Fig.2: $^{127}I_2$; R(127)11-5; λ=633 nm

Fig.3: $^{127}I_2$; R(127)11-5; λ=633 nm

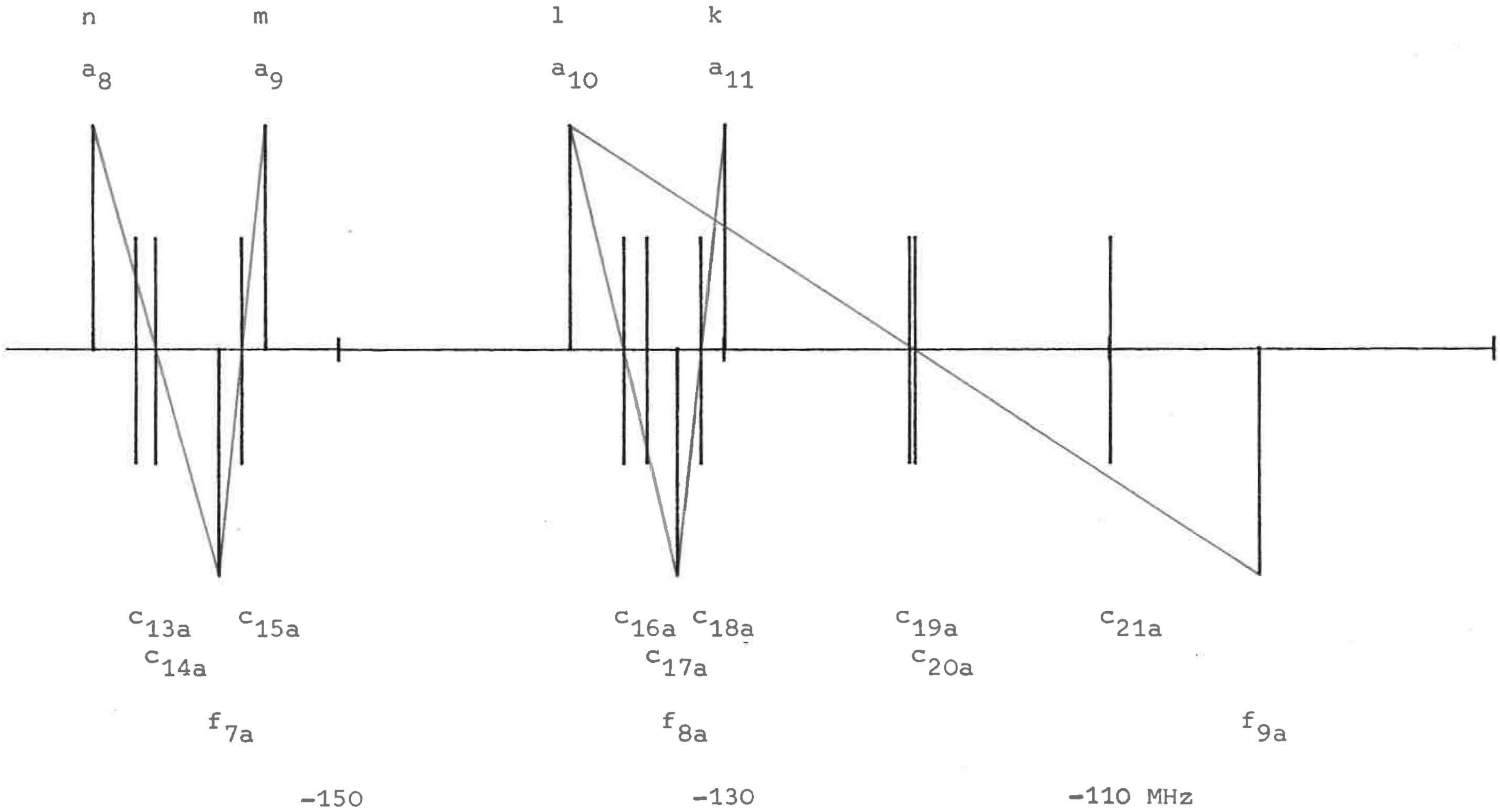


Fig.4: $^{127}I_2$; R(127)11-5; λ=633 nm

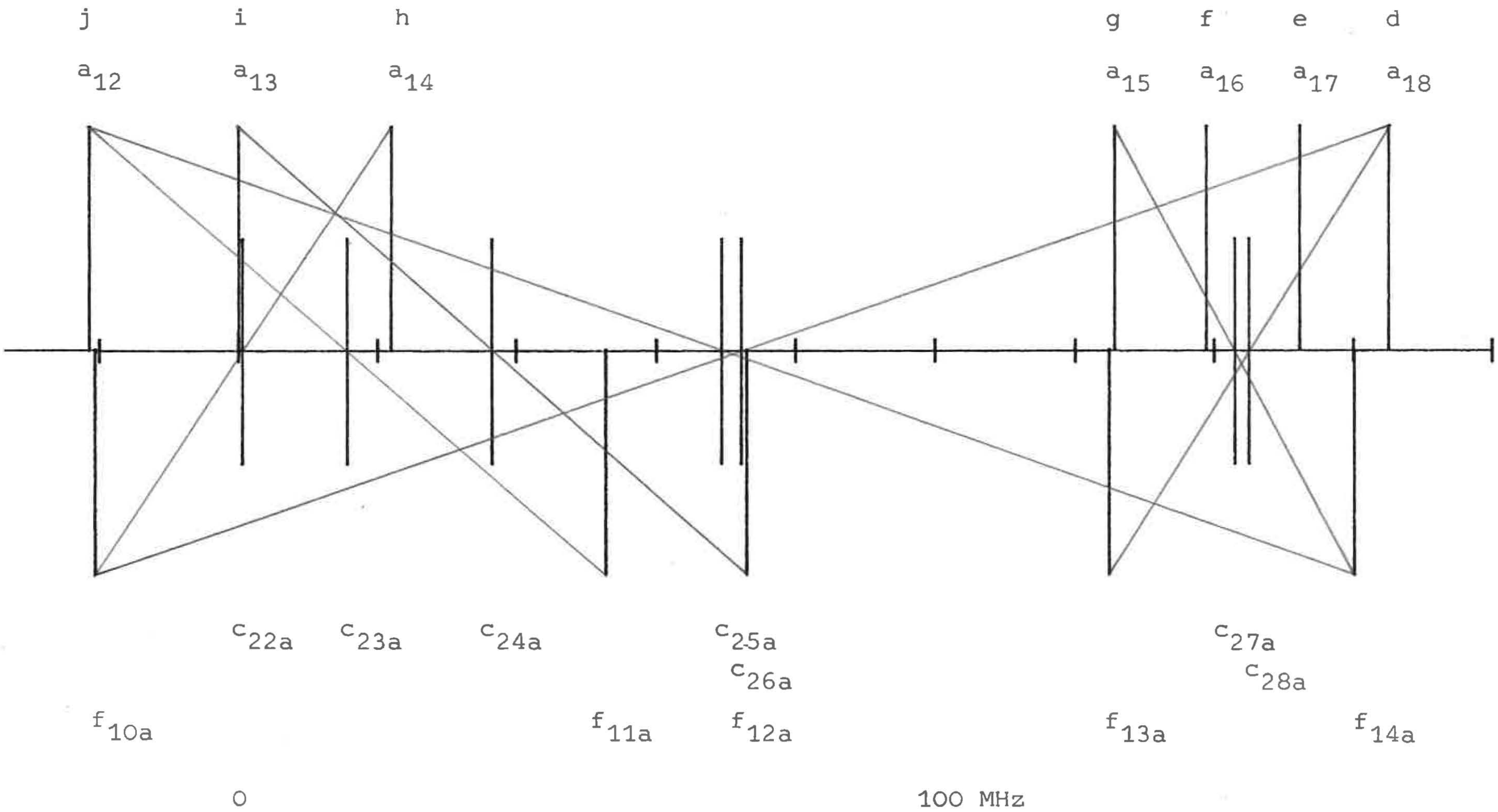


Fig.5: $^{127}I_2$; R(127)11-5; λ=633 nm

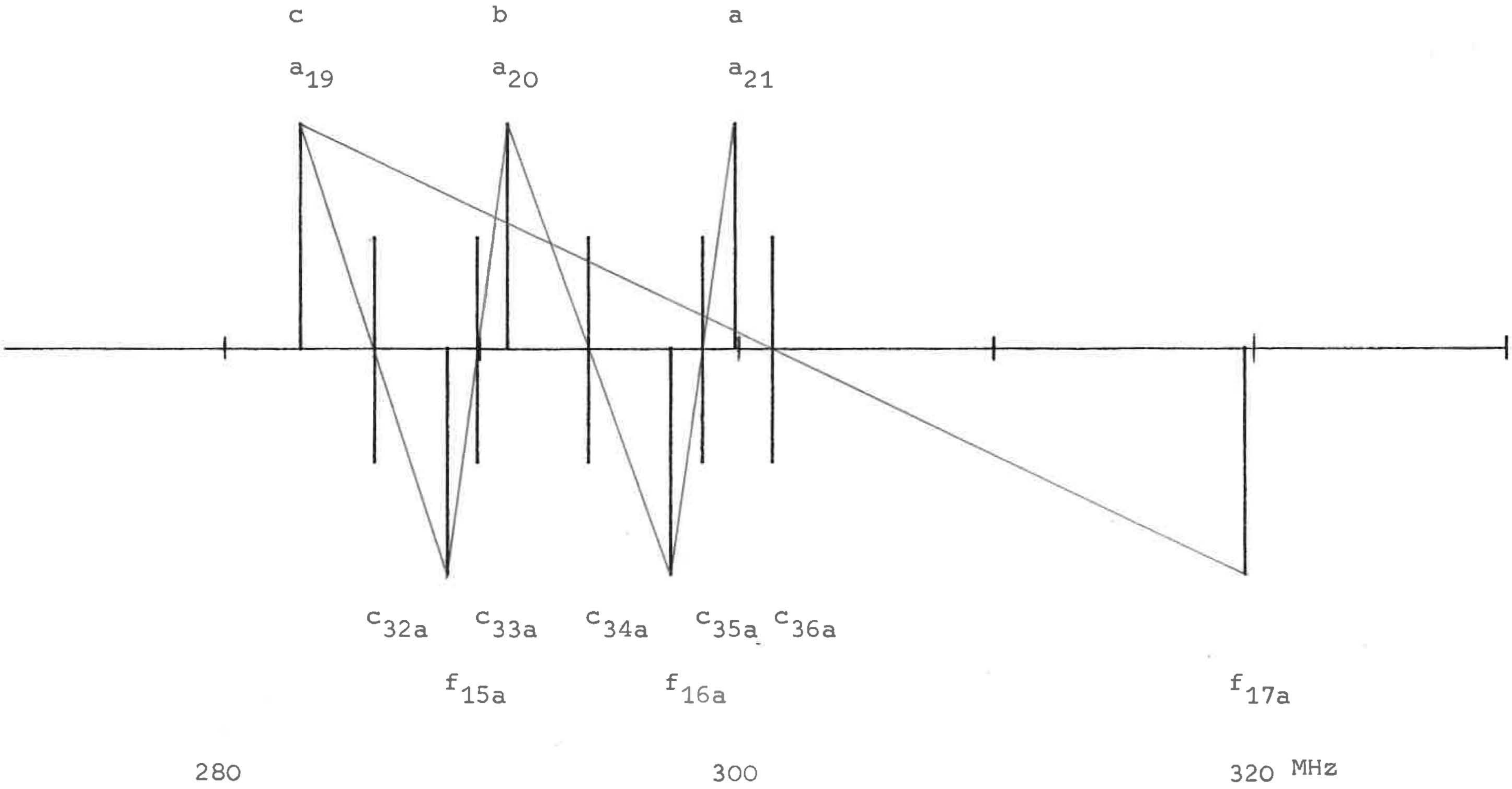


Fig.6: $^{127}I_2$; R(47)9-2; λ=612 nm

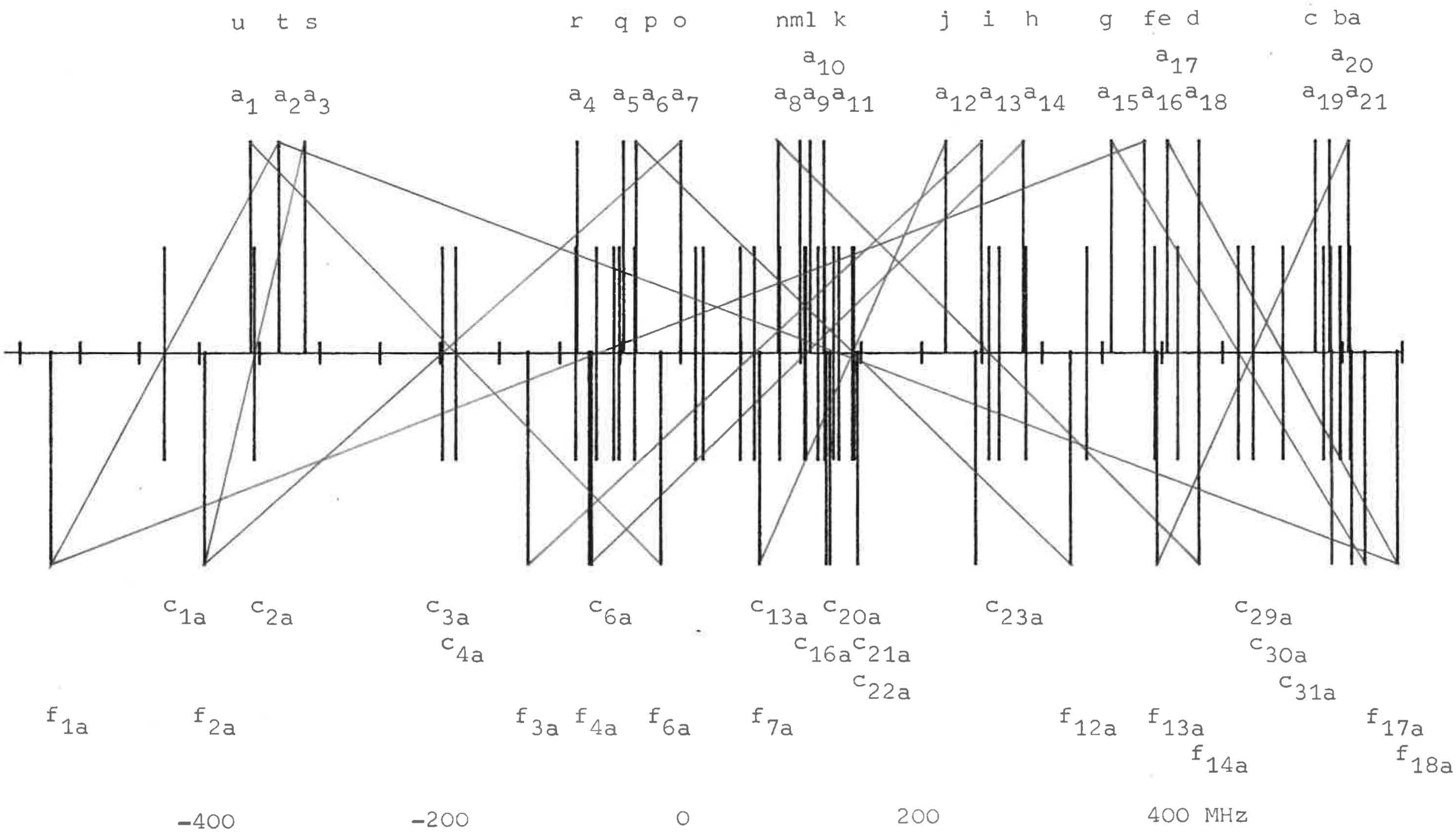


Fig.7: $^{127}I_2$; R(47)9-2; λ=612 nm

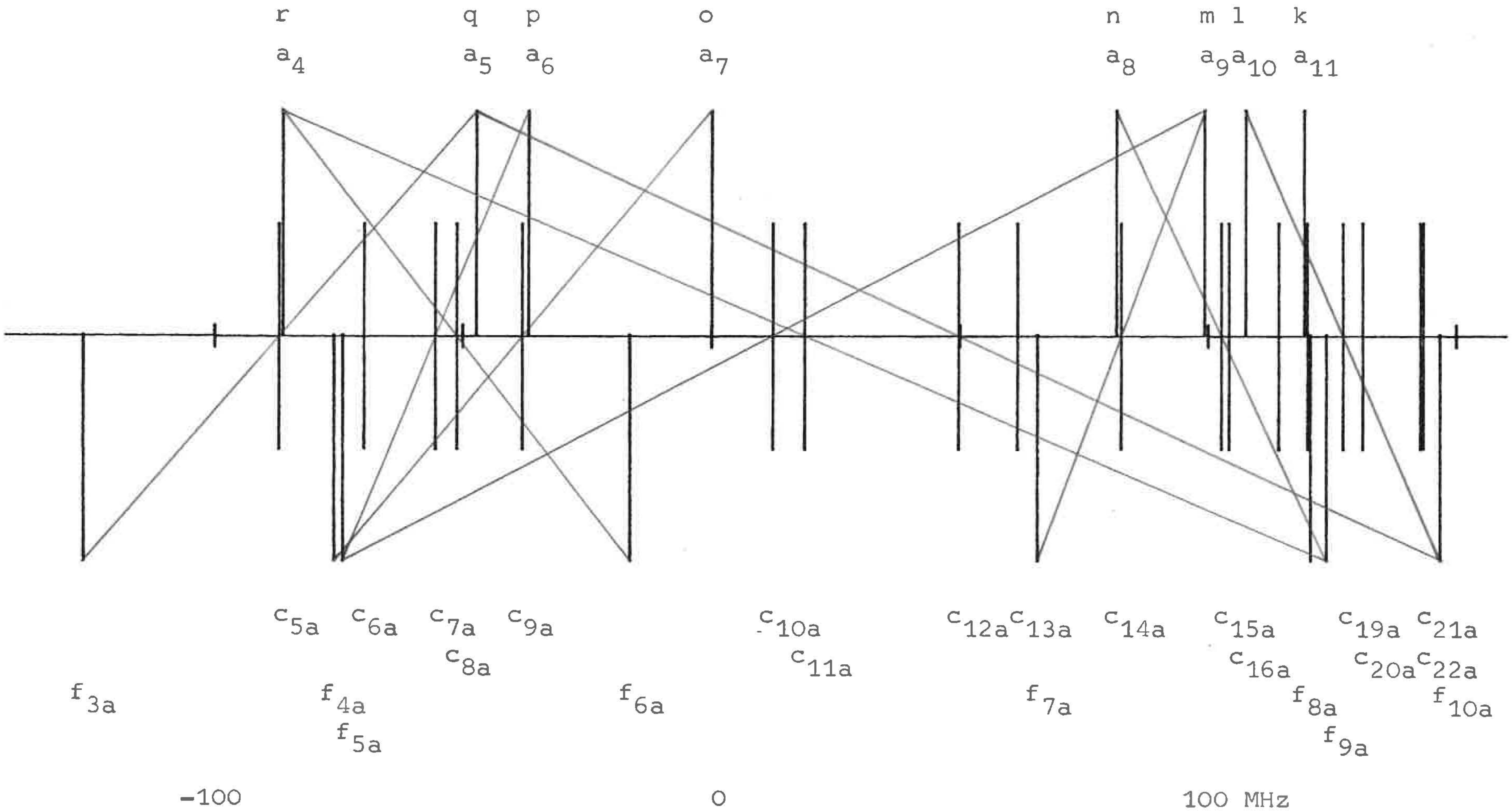


Fig.8: $^{127}I_2$; R(47)9-2; λ=612 nm

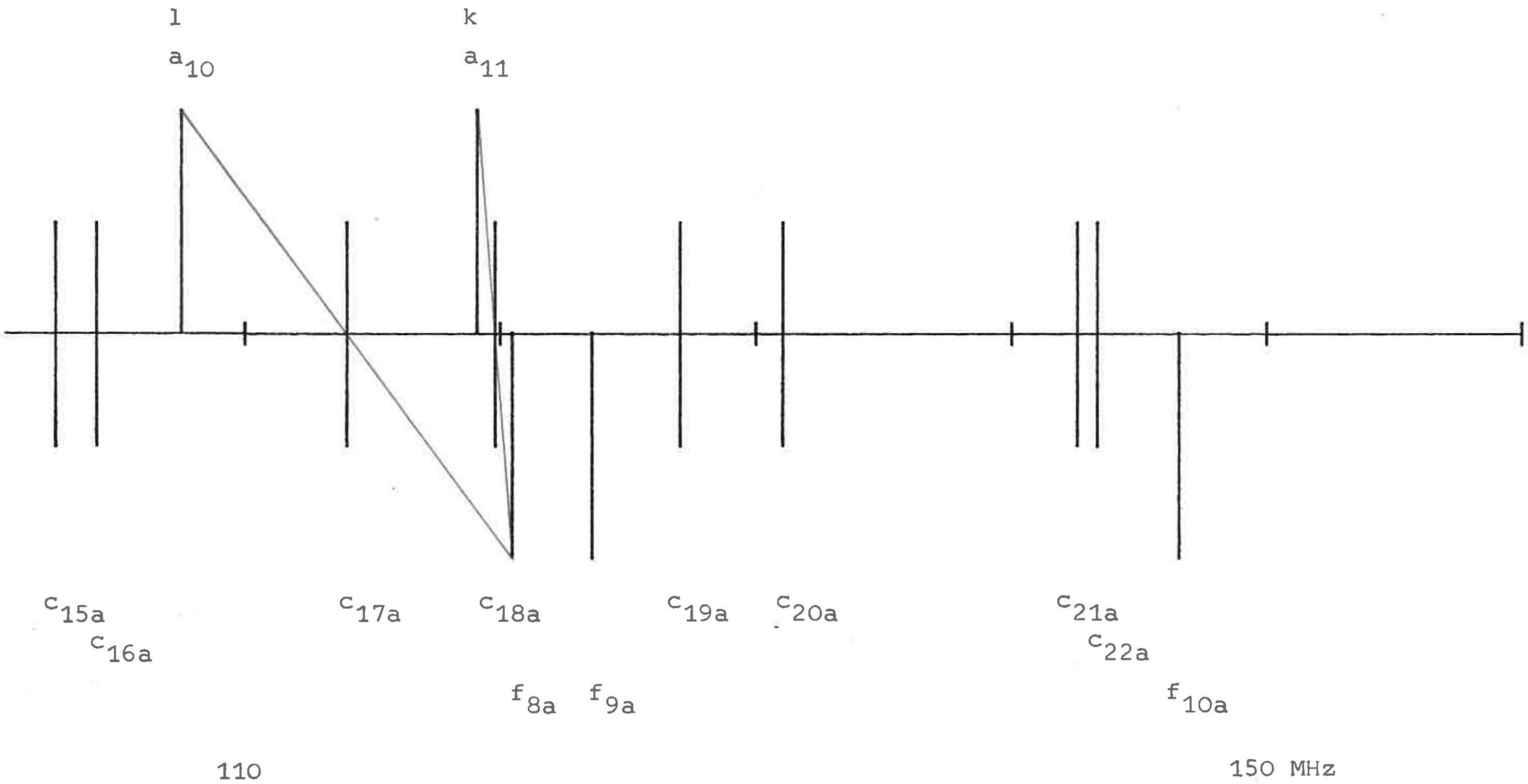


Fig.9: $^{127}I_2$; R(47)9-2; λ=612 nm

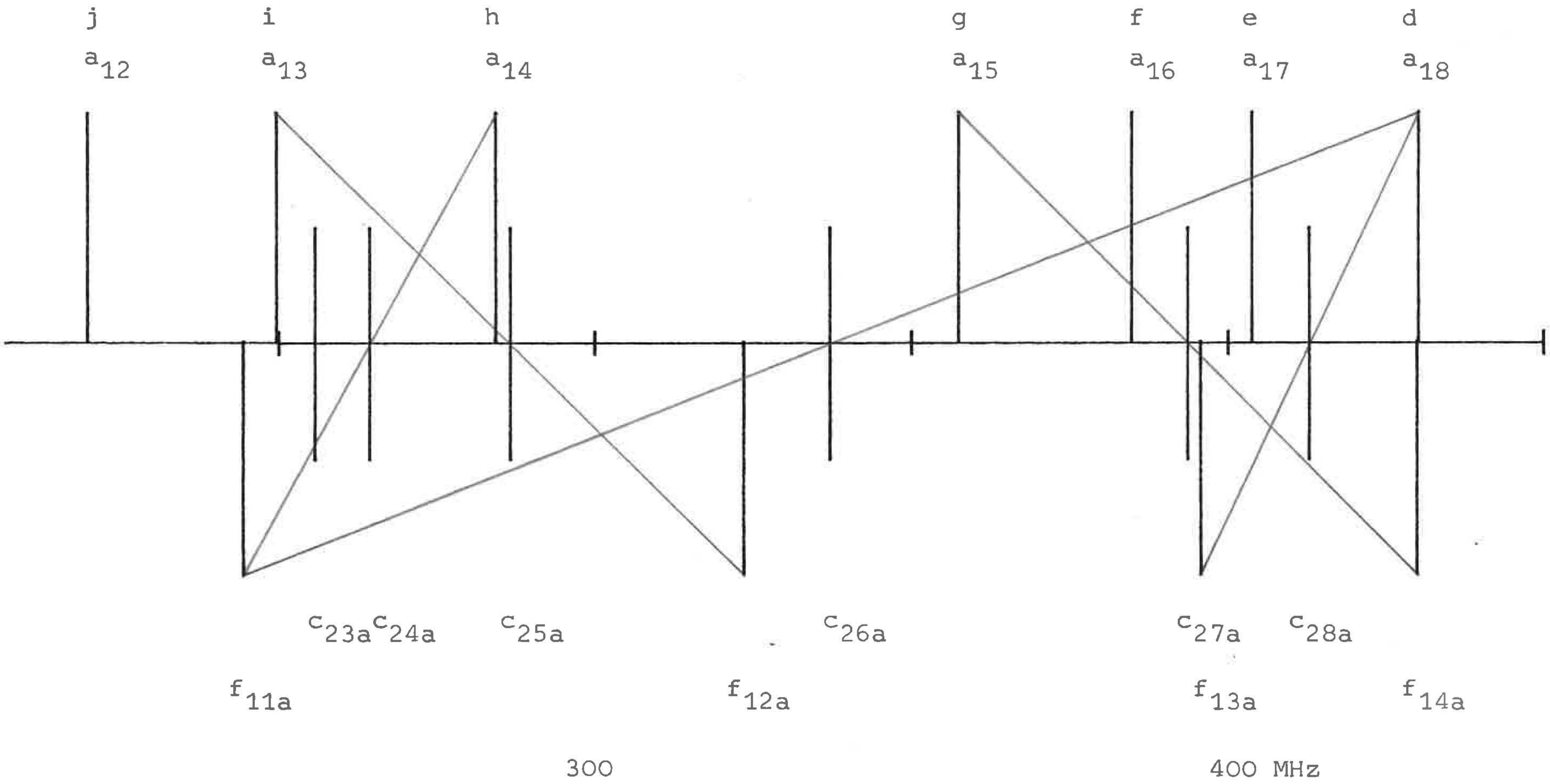


Fig.10: $^{127}I_2$; R(47)9-2; λ=612 nm

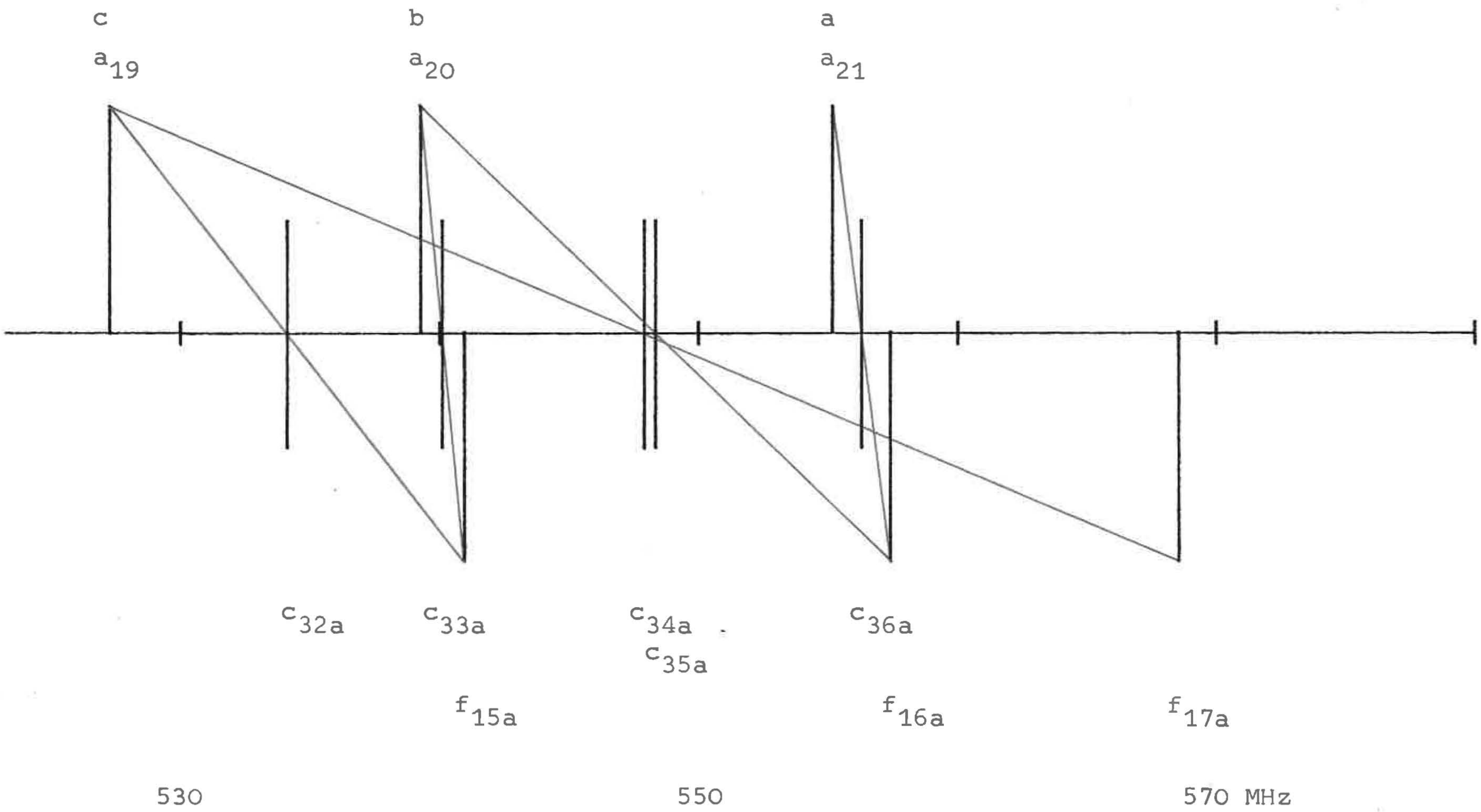


Fig.11: $^{129}I_2$; P(110)10-2; λ=612 nm

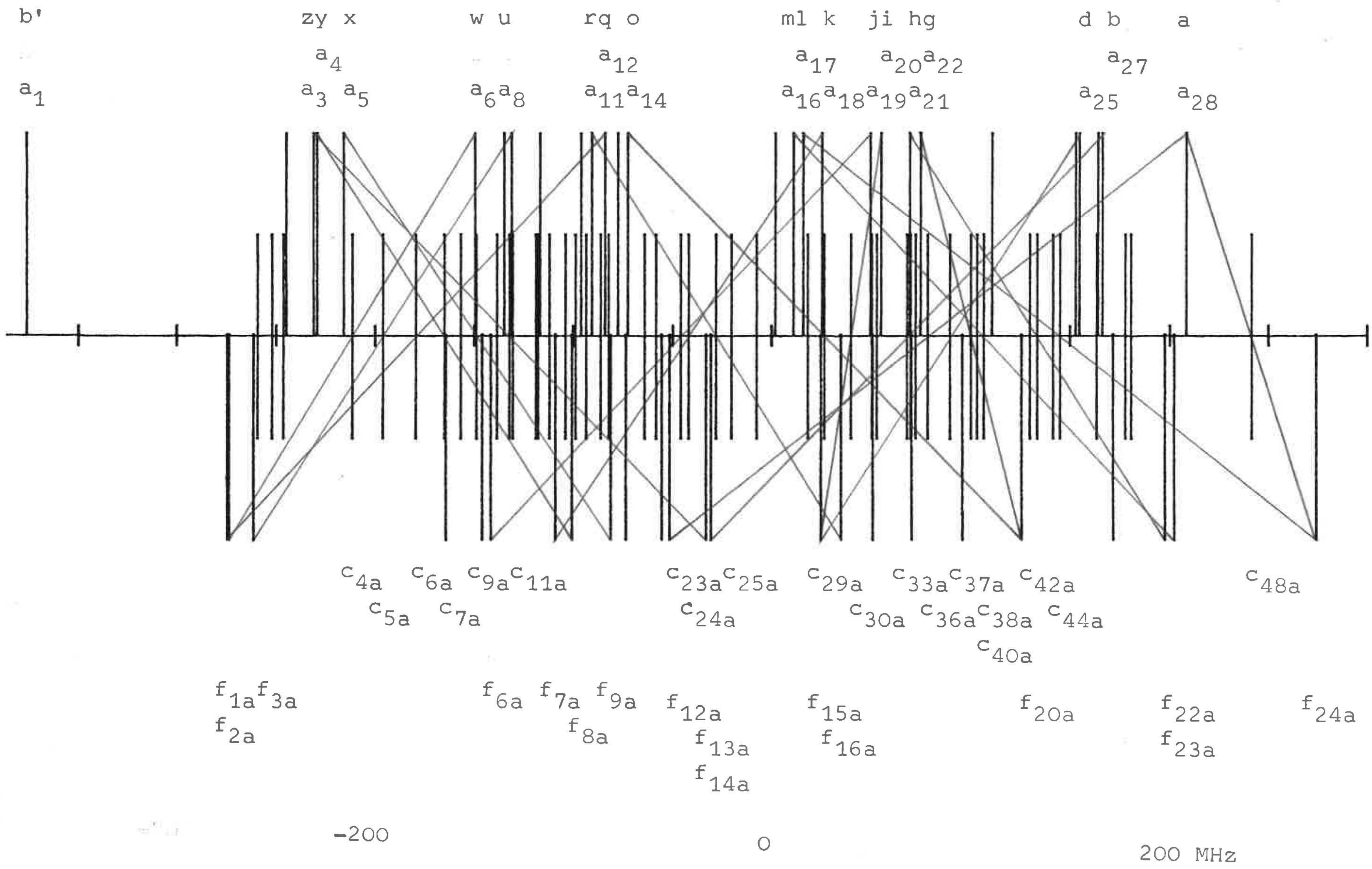


Fig.12: $^{129}I_2$; p(110)10-2; λ=612 nm

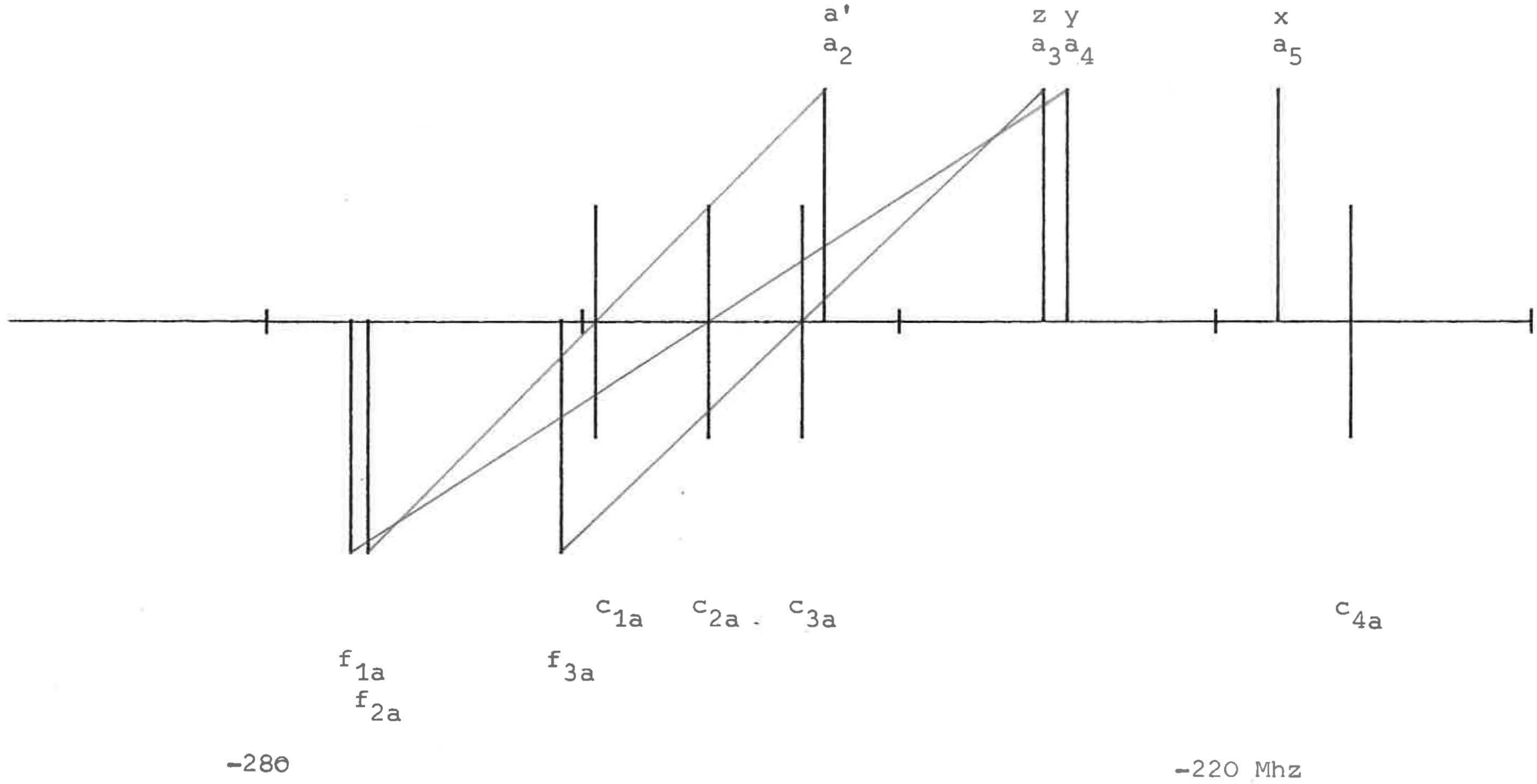


Fig.13: $^{129}I_2$; P(110)10-2; λ=612 nm

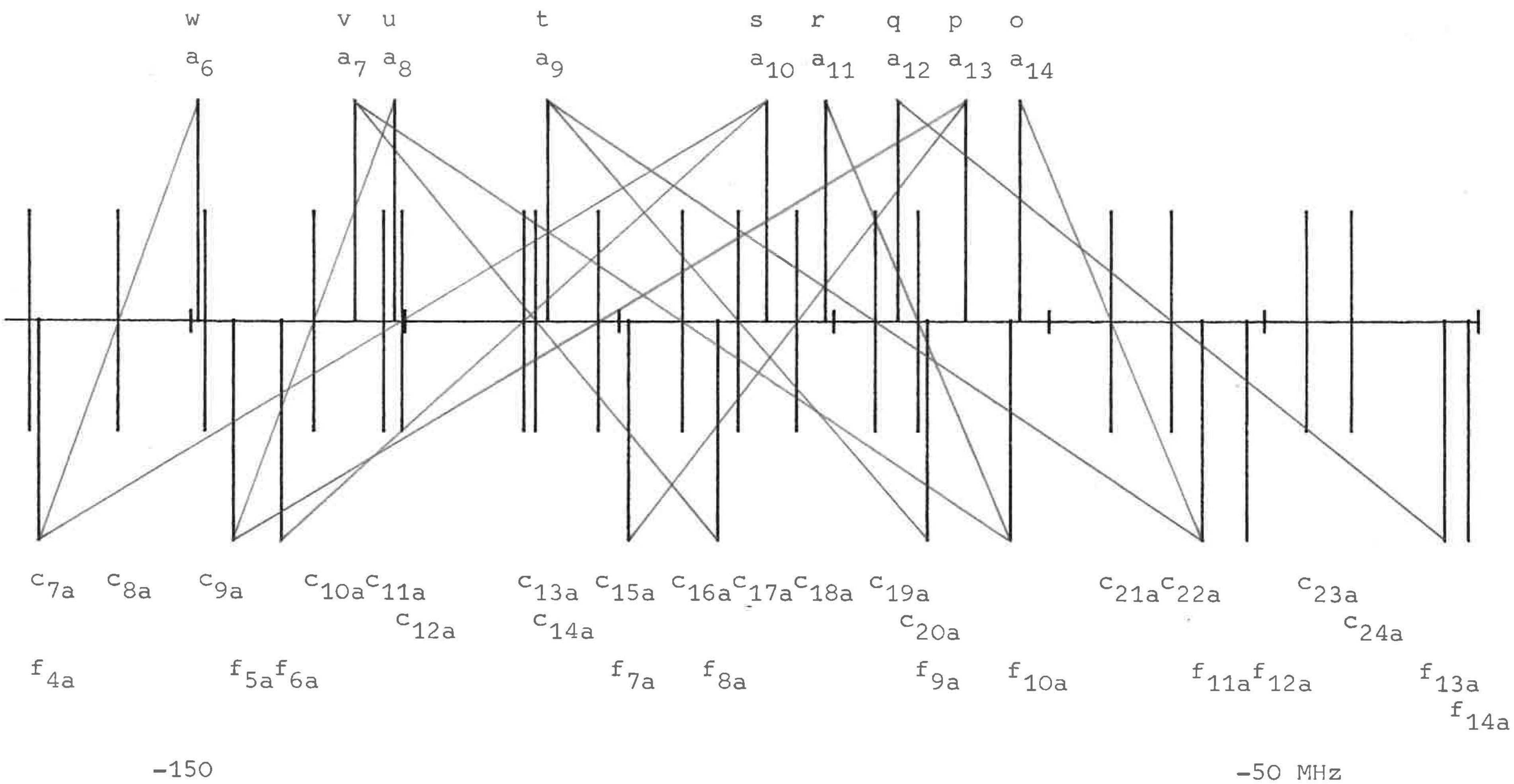


Fig.14: $^{129}I_2$; P(110)10-2; λ=612 nm

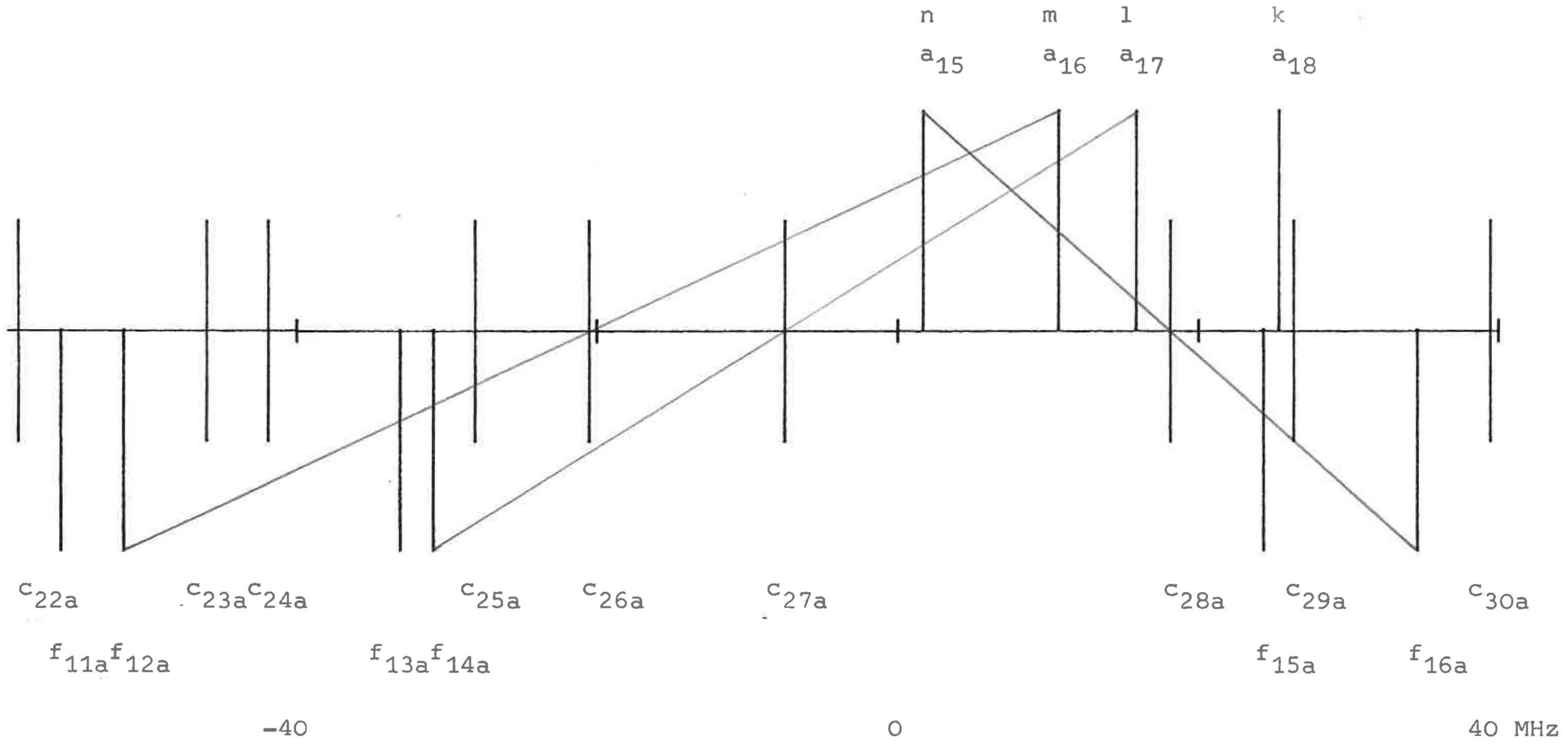


Fig.15: $^{129}I_2$: P(110)10-2; λ=612 nm

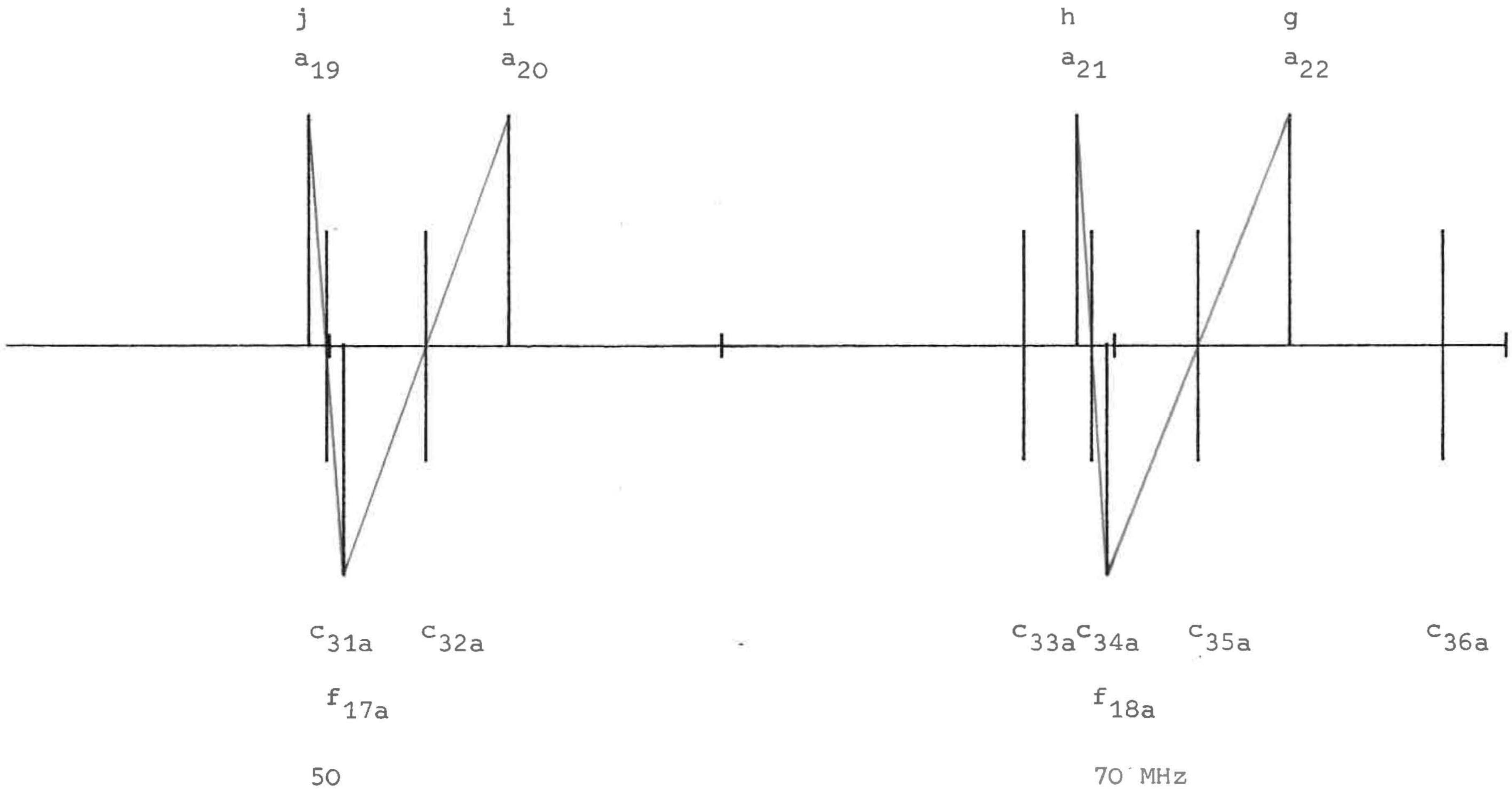


Fig.16: $^{129}I_2$; P(110)10-2; λ=612 nm

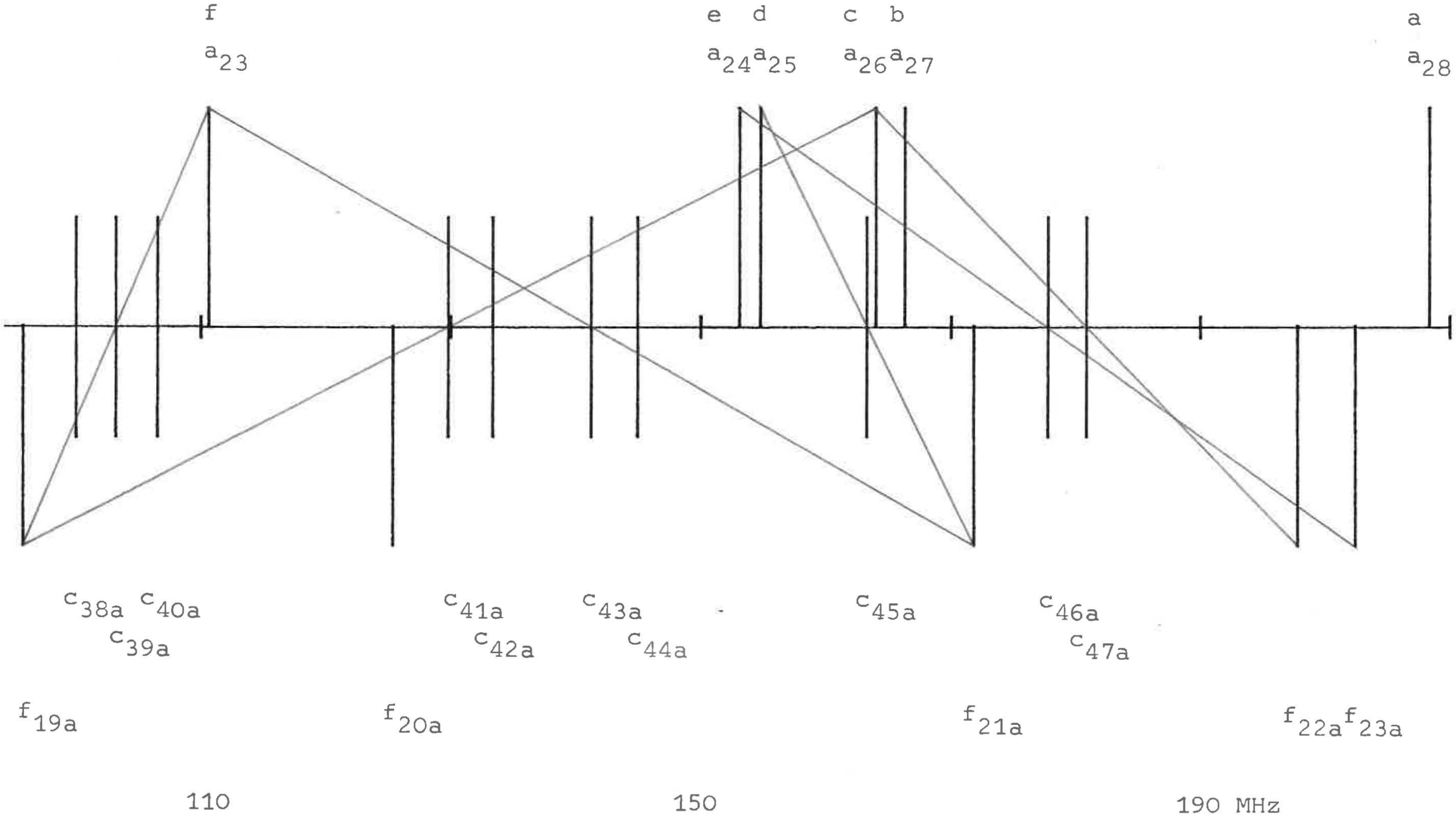


Fig.17: $^{129}I_2$; R(113)14-4; λ=612 nm

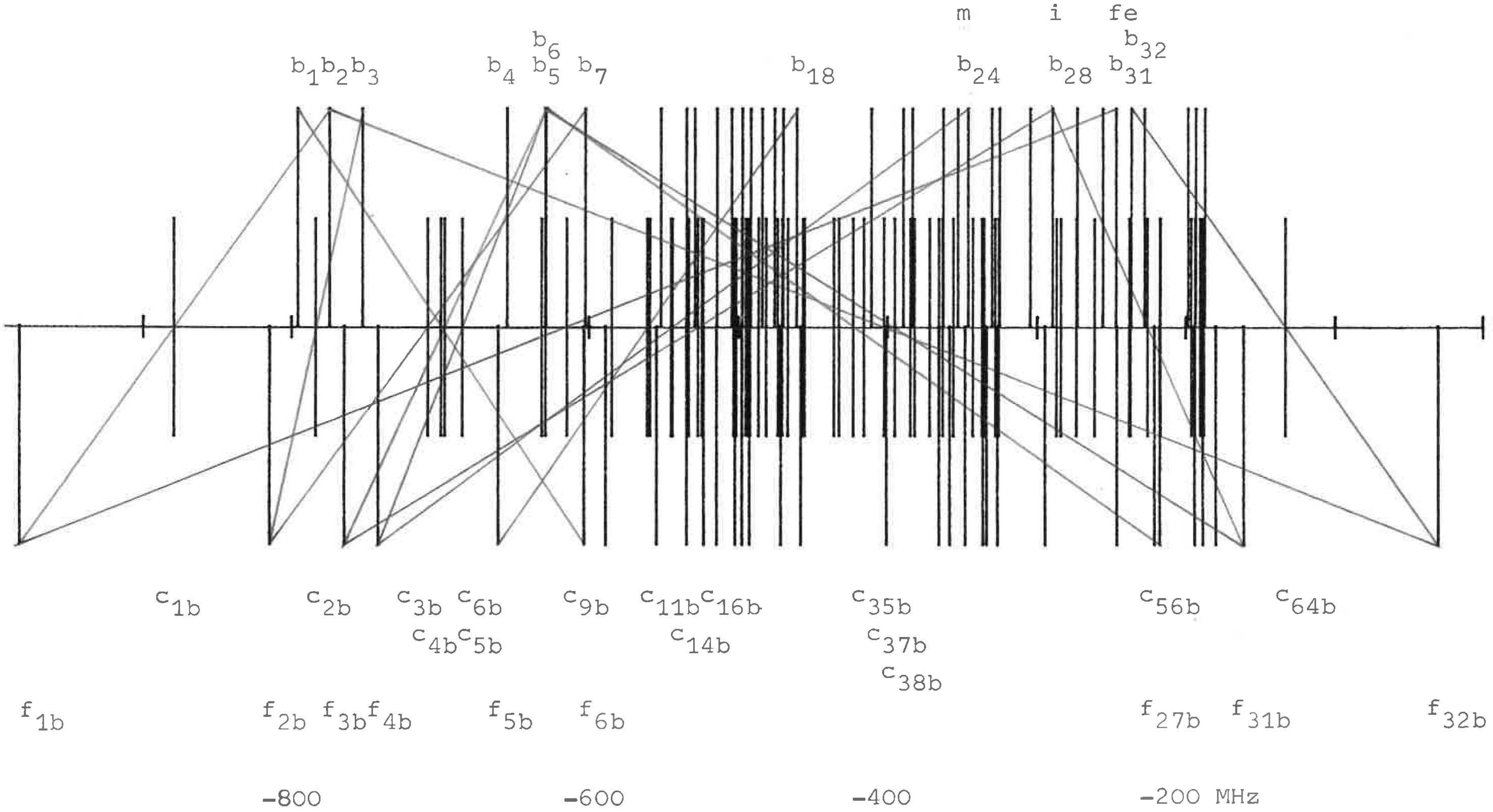


Fig.18: $^{129}I_2$; R(113)14-4; λ=612 nm

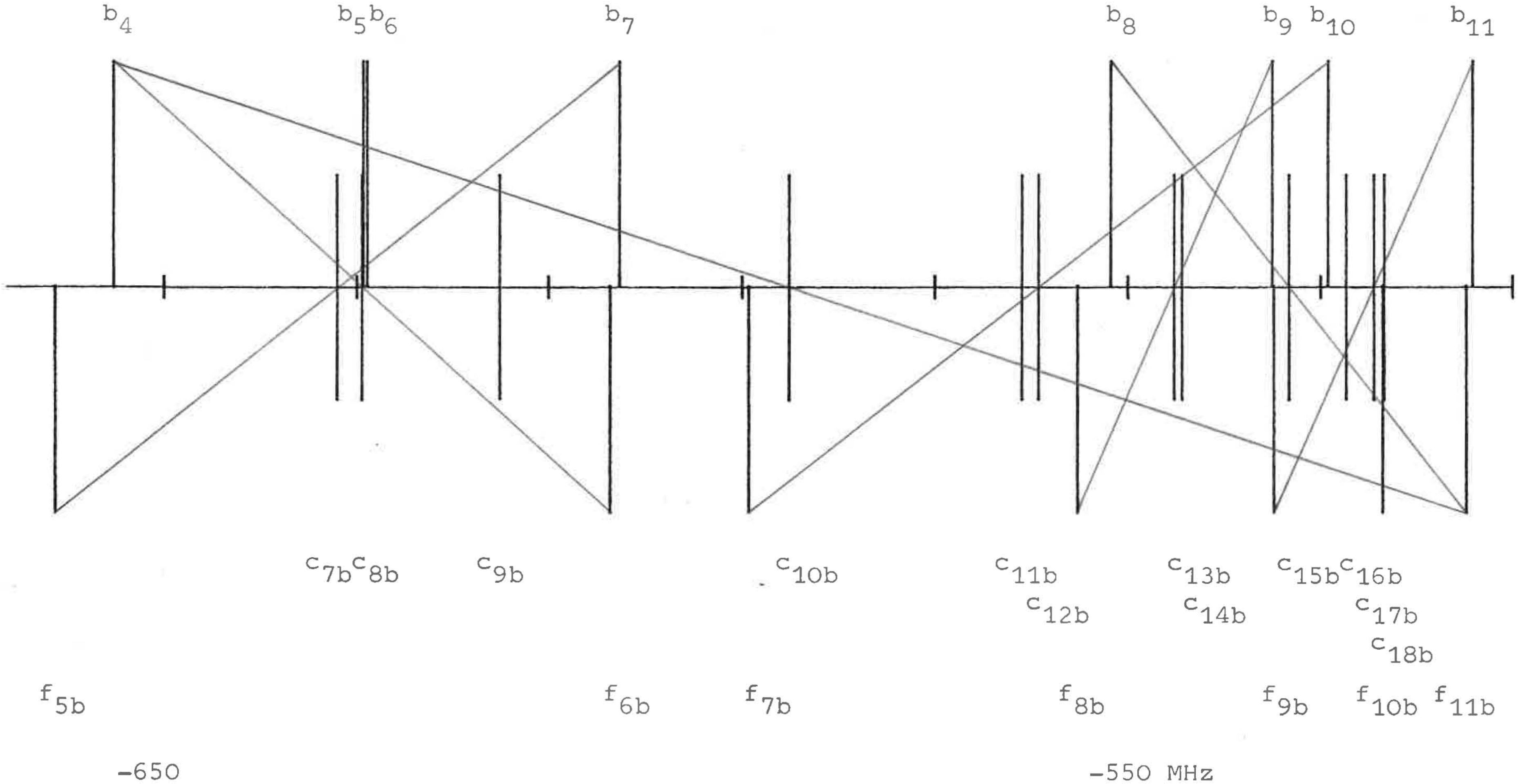


Fig.19: $^{129}I_2$; R(113)14-4; λ=612 nm

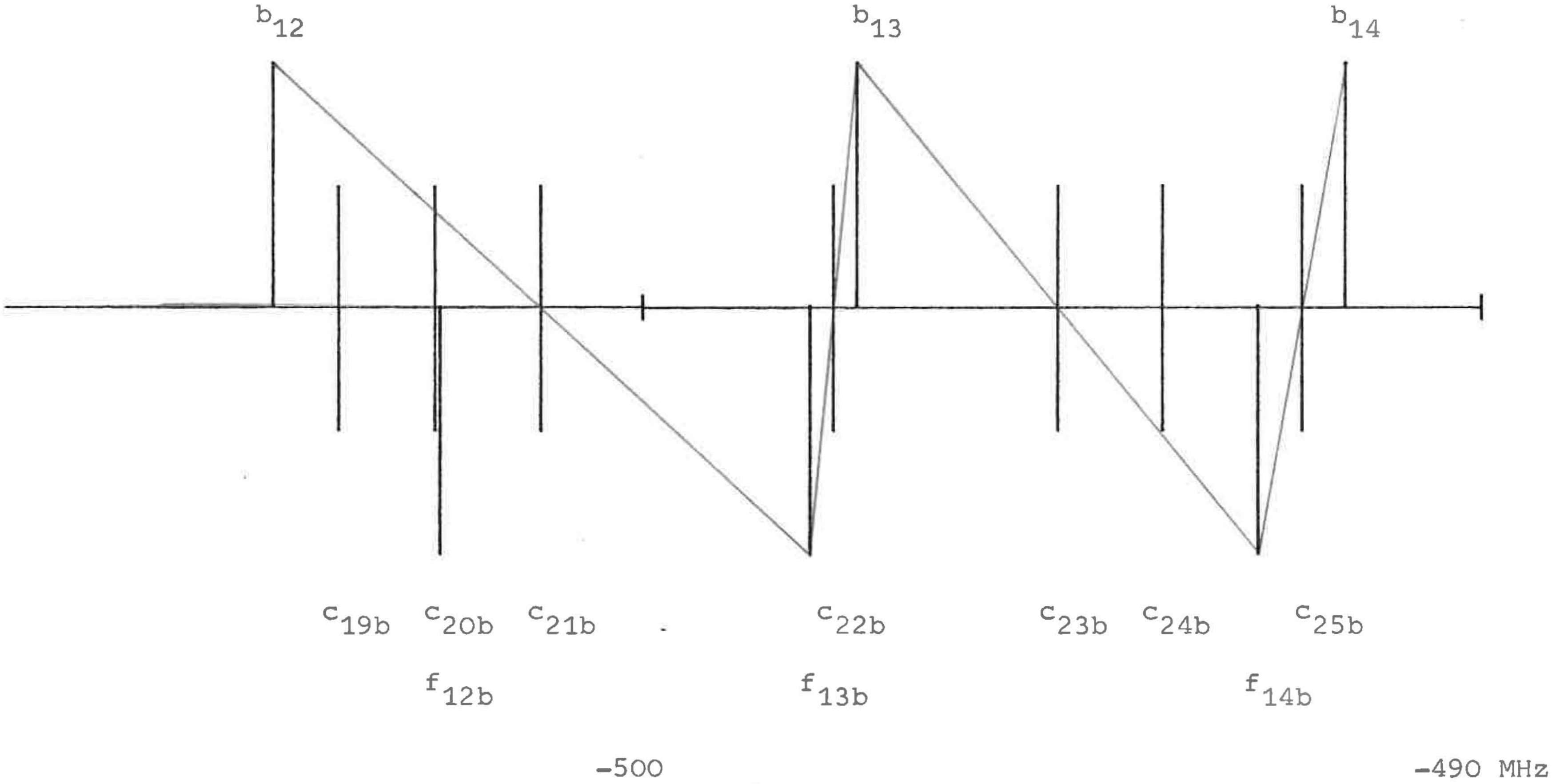


Fig.20: $^{129}I_2$; R(113)14-4; λ=612 nm

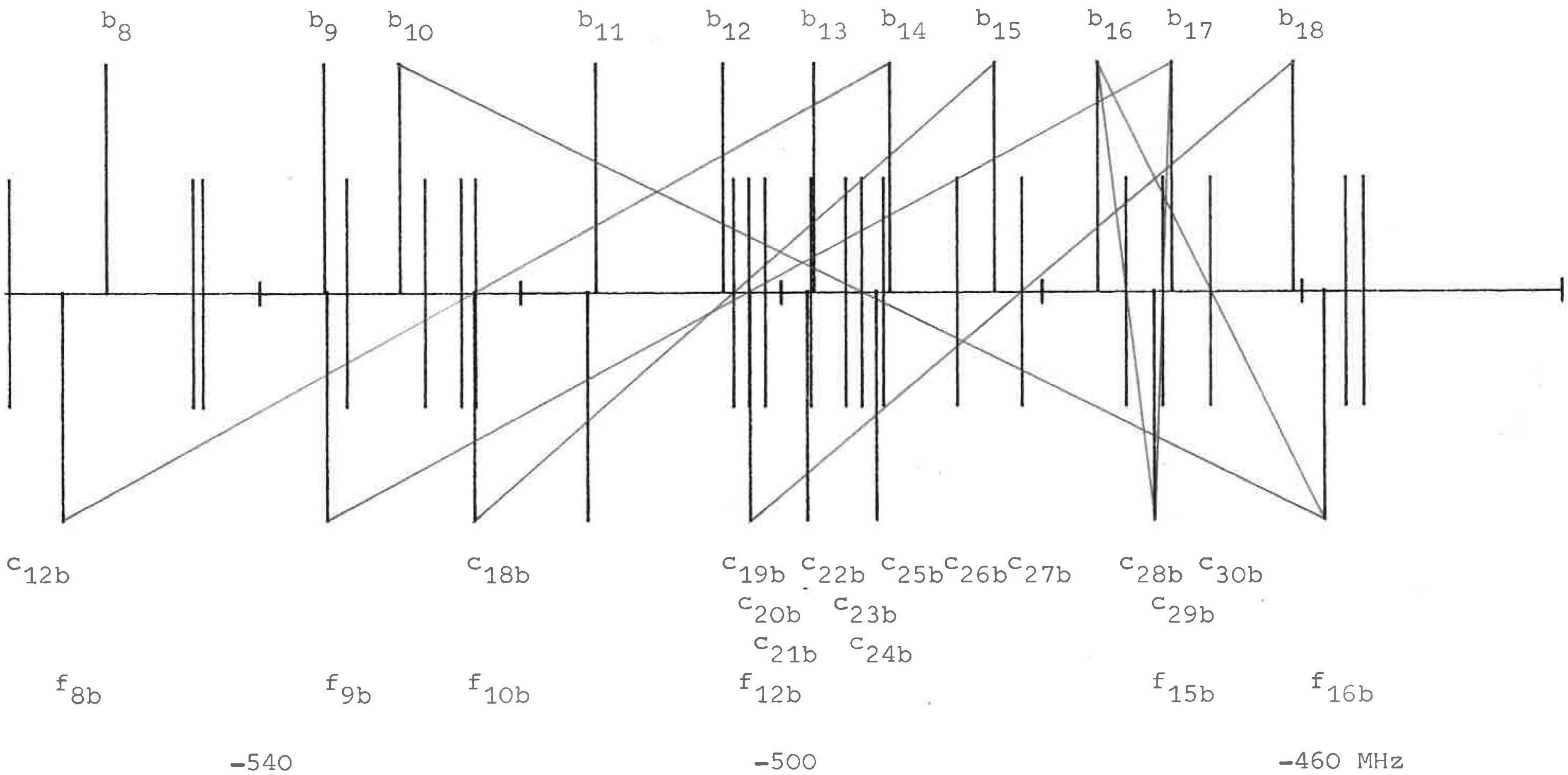


Fig.21: $^{129}I_2$; R(113)14-4; λ=612 nm

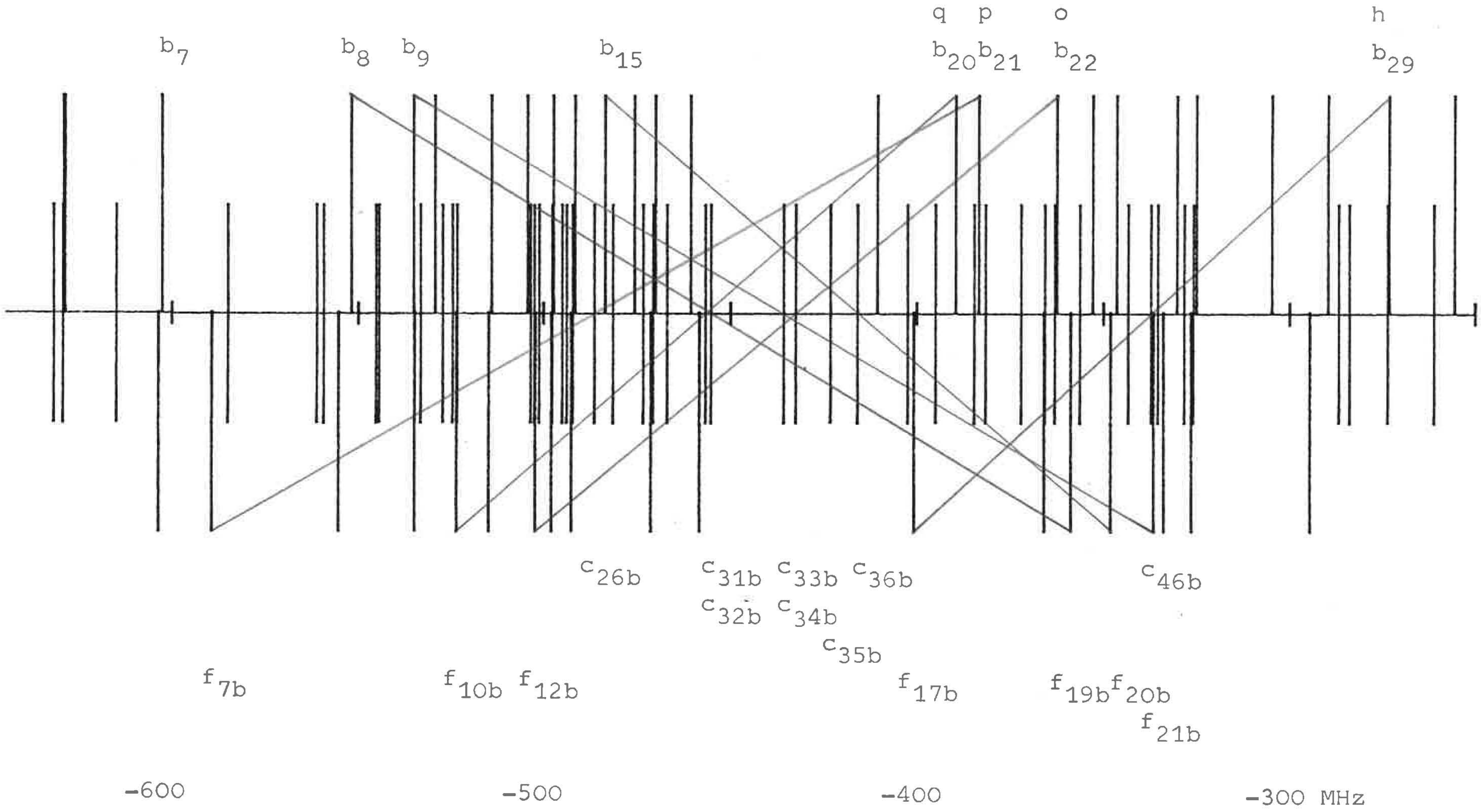


Fig.22: R(113)14-4; λ=612 nm

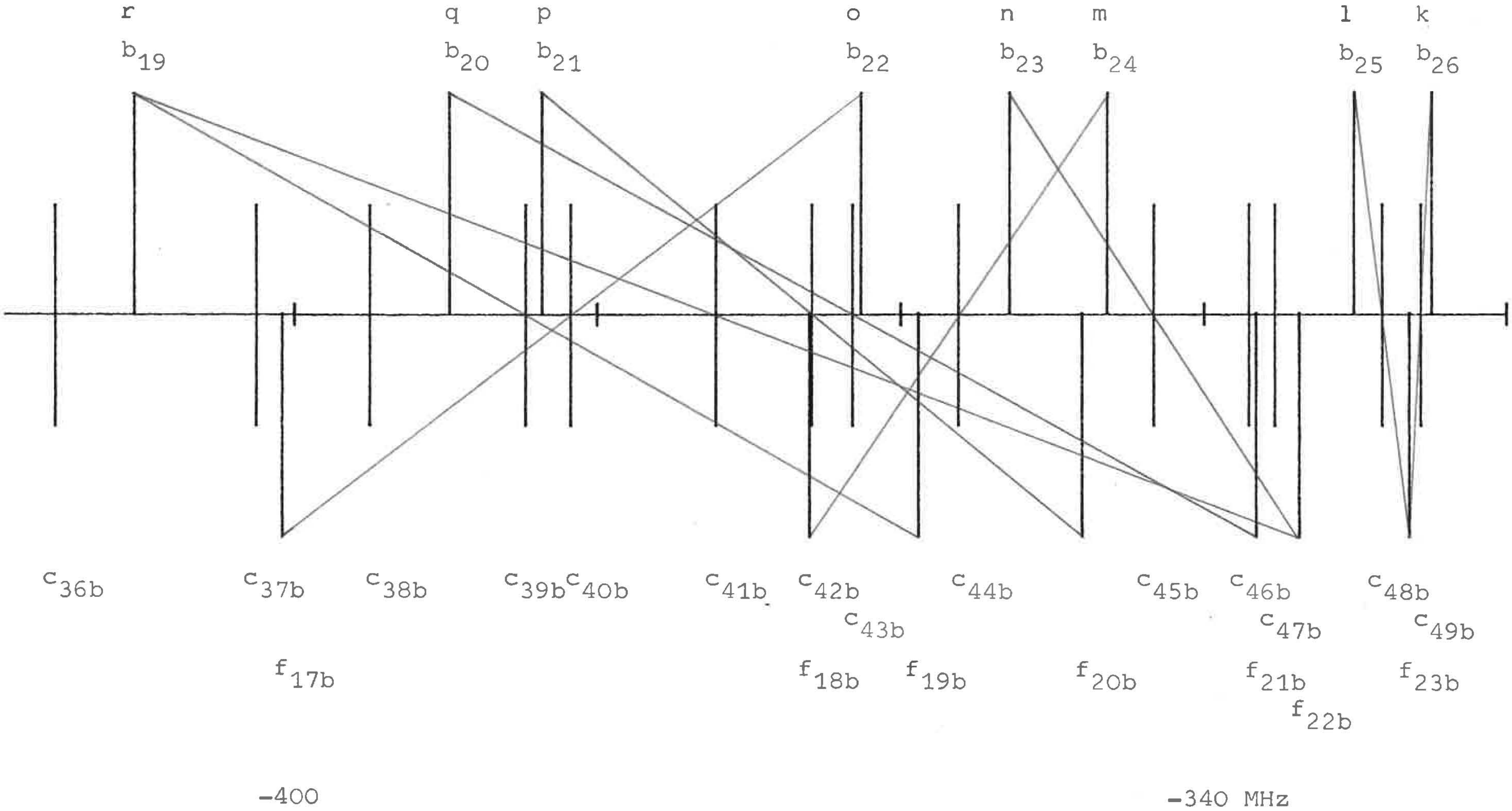


Fig.23: $^{129}I_2$; R(113)14-4; λ=612 nm

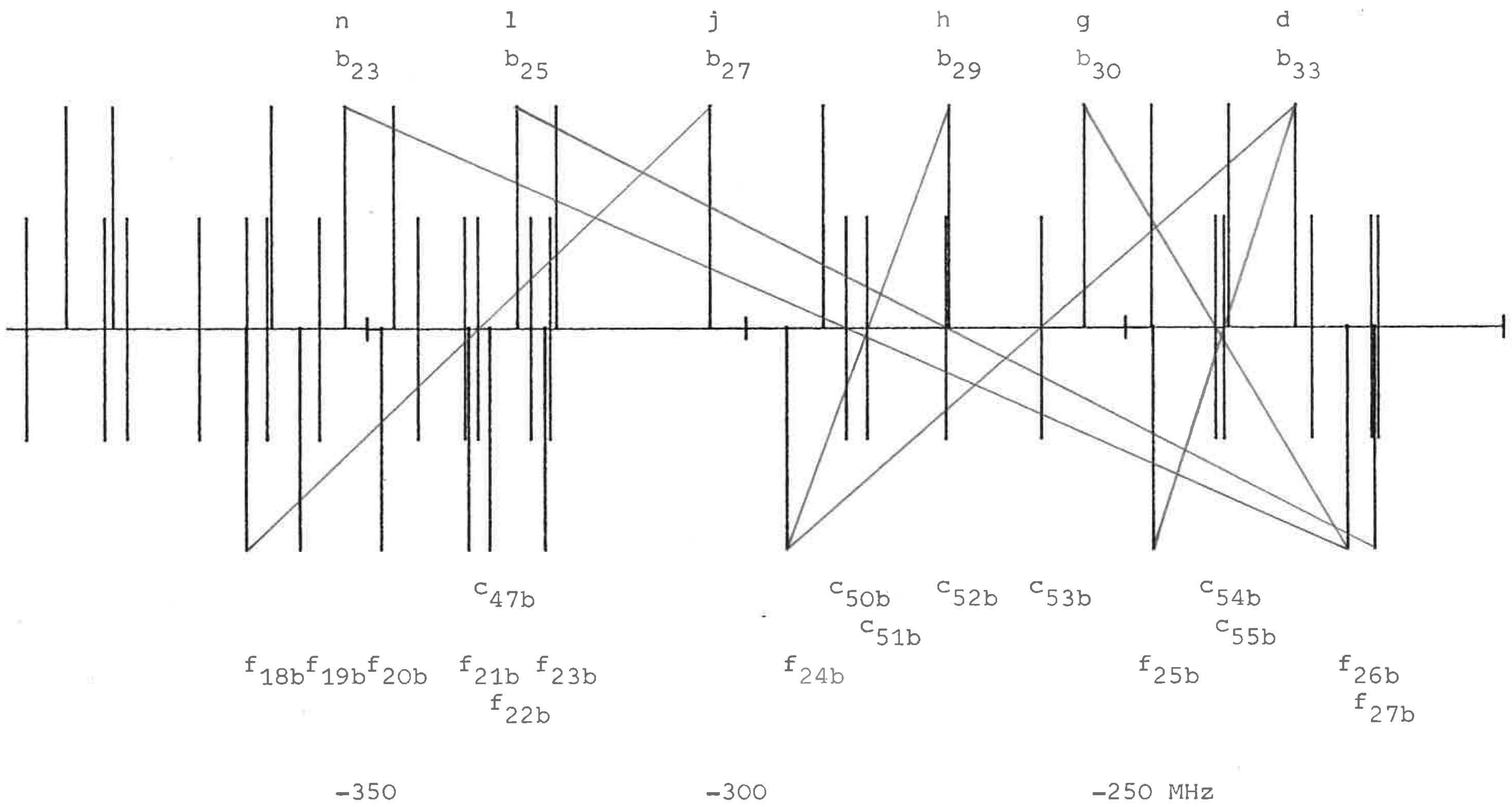


Fig.24: $^{129}I_2$; R(113)14-4; λ=612 nm