

## Quartet system of C IV

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Theoretical and experimental investigations of the quartet system of C IV are reported. Twenty-seven quartet-state energies are calculated. Based on this work, several lines observed for the first time in the extreme-ultraviolet beam-foil spectra of carbon (10–200 nm) are classified as  $1s2pnl^4L-1s2pn'l'^4L'$  and  $1s2snl^4L-1s2sn'l'^4L'$  ( $n=2,3$ ;  $n'=4,5$ ) transitions. The calculated fine structures for the quartet states are also reported. In addition, a list of new observed lines classified in C III and C IV is given.

### I. INTRODUCTION

Recently, the quartet states of the lithiumlike ions have received a fair amount of attention. For light ions such as Li I,<sup>1,2</sup> Be II,<sup>3–6</sup> and B III (Ref. 6) detailed studies have been made both theoretically and experimentally. However, for systems with nuclear charge  $Z \geq 6$ , only limited data are available.

Most of the theoretical results on quartet states of C IV are limited to low-lying states and to a few angular symmetry states such as  $^4S$ ,  $^4P^o$ , and  $^4P$ .<sup>7–12</sup> With the exception of  $2s2p^4P^o$  and  $2p2p^4P$  states, all theoretical calculations in the literature are nonrelativistic. Since relativistic effects contribute substantially to the energy of C IV, they should be included if reliable results are to be obtained. Very recently, the energies of the C IV  $2s2p^4P^o$  and  $2p2p^4P$  states have been calculated to high accuracy with configuration-interaction wave functions.<sup>13</sup>

In the present work, the method used in Ref. 13, which is not limited to low-lying states,<sup>14</sup> is applied for calculating higher excited quartet states:  $^4S$ ,  $^4S^o$ ,  $^4P^o$ ,  $^4P$ ,  $^4D^o$ ,  $^4D$ ,  $^4F^o$ , and  $^4F$ . A nonrelativistic Hamiltonian and variational method are used as a first step. The relativistic corrections and mass polarization effect are calculated using first-order perturbation theory. The wave function and the computational procedure used are similar to those of Chung and Davis.<sup>5</sup>

Experimental studies of the quartet system of C IV have been made previously using the beam-foil technique<sup>15–18</sup> and transitions occurring nearly exclusively in the wavelength region  $\lambda < 40$  nm were classified in this system.

In this work, beam-foil spectra of carbon are recorded using a grazing incidence spectrometer ( $\lambda=10-40$  nm) and a Seya-Namioka-type spectrometer ( $\lambda=30-200$  nm). Transitions between quartet states are searched in these spectra on the basis of theoretical predictions.

### II. THEORETICAL RESULTS

#### A. Center-of-gravity energy

The nonrelativistic energies ( $E_{nr}$ ) obtained in this work are given in Table I. For comparison purposes, the results

for the  $^4S$  and  $^4P^o$  states of Larsson *et al.*<sup>7</sup> are also given. These are the most accurate theoretical calculations in which a large wave function and  $r_{ij}$  coordinates are explicitly employed. Their  $2s2p^4P^o$  and  $2s3s^4S$  energies are only slightly higher than those of the present work. However, for higher excited states, the deviation is much more substantial. Our results are lower than those of Lunell and Beebe<sup>8</sup> and Holøien and Geltman.<sup>9</sup>

In Table I the sum of the expectation values for the mass correction term and Darwin term<sup>19</sup> denoted as  $\langle(H_1+H_2)\rangle$  is reported. The explicit forms for these operators are given in Ref. 13. For the C IV quartets, the energy contribution from this correction ranges from 0.25 to 0.30 eV, depending on whether the system has a  $1s2s^3S$  or  $1s2p^3P^o$  core. The contribution from the  $^3S$  core is substantially larger than that of the  $^3P^o$  core. This makes a term classification very straightforward: The  $\langle(H_1+H_2)\rangle$  for states with a  $^3P^o$  core is about  $-0.0093$  a.u. whereas that of the  $^3S$  is about  $-0.0104$  a.u.

The mass polarization effect  $\langle H_3 \rangle$  is also tabulated in Table I. Although this effect is very small, nevertheless, it can be experimentally observed by measuring the isotope shift of  $^{12}\text{C}$  and  $^{14}\text{C}$ . The calculated result given in this table is obtained by approximating the  $^{12}\text{C}$  nucleus with six protons and six neutrons. The retardation effect  $\langle H_4 \rangle$  is somewhat larger than  $\langle H_3 \rangle$  for C IV. In general,  $\langle H_3 \rangle$  and  $\langle H_4 \rangle$  are opposite in sign except for those states where both effects are very small.

The center-of-gravity energies given by

$$E_{CG} = E_{nr} + \langle(H_1+H_2)\rangle + \langle H_3 \rangle + \langle H_4 \rangle$$

are quoted in Table I. The wavelengths calculated from the  $E_{CG}$  energies are given in Table II. The conversion factor used is 45.5656 nm/a.u.

#### B. Fine structure

Recent spectroscopic measurements of the fine-structure wavelengths of the  $1s2s2p^4P^o-1s2p2p^4P$  transition in the Li I sequence<sup>17,20–23</sup> have stimulated considerable amount of theoretical interest.<sup>10–13</sup> However, to our knowledge, the only fine-structure data available for

TABLE I. The energies of quartet system of CIV (in a.u.).  $E_{nr}$ , nonrelativistic energy;  $\langle(H_1+H_2)\rangle$  mass correction term and Darwin term;  $\langle H_3\rangle$ , mass polarization term;  $\langle H_4\rangle$ , retardation term.  $E_{CG}$  center-of-gravity energy ( $E_{CG}=E_{nr}+\langle(H_1+H_2)\rangle+\langle H_3\rangle+\langle H_4\rangle$ ).

Term	$-E_{nr}$				$-E_{CG}$		$-E_{nr}$	$-E_{exp}$
	This work	$-10^2\langle(H_1+H_2)\rangle$	$-10^5\langle H_3\rangle$	$-10^4\langle H_4\rangle$	This work	Other works	This work	
$1s2s3s^4S$	22.520631	1.0924	-0.166	-0.069	22.531546	22.51993 <sup>a</sup>	22.531996	
$1s2p3p^4S$	22.194079	0.9533	+9.654	-2.125	22.203496	22.18851 <sup>a</sup>	22.203596	
$1s2s4s^4S$	21.997711	1.0657	+0.074	-0.034	22.008366	21.99678 <sup>a</sup>	22.008402	
$1s2s5s^4S$	21.784968	1.0405	+1.037	-0.287	21.795354	21.78177 <sup>a</sup>		
$1s2p4p^4S$	21.748218	0.9394	+7.805	-1.664	21.757524	21.73375 <sup>a</sup>		
$1s2s6s^4S$	21.663938	1.0550	-0.031	-0.015	21.674486			
$1s2s2p^4P^o$	23.969309	1.0821	+7.609	-1.693	23.980037	23.96919 <sup>a</sup>		
$1s2s3p^4P^o$	22.422499	1.0604	+2.597	-0.486	22.433081	22.42098 <sup>a</sup>	22.433260	
$1s2p3s^4P^o$	22.279031	0.9670	+8.613	-1.850	22.288602	22.27751 <sup>a</sup>	22.288885	
$1s2p3d^4P^o$	22.112594	0.9374	+8.823	-1.912	22.121865	22.05467 <sup>a</sup>	22.122129	
$1s2p4d^4P^o$	21.722642	0.9405	+8.408	-1.794	21.731951		21.731309	
$1s2p2p^4P$	23.631579	0.9619	+14.80	-3.408	23.641006	23.62843 <sup>b</sup>		
$1s2p3p^4P$	22.182004	0.9366	+10.21	-2.273	22.191245		22.191612	
$1s2p4p^4P$	21.751345	0.9294	+9.448	-2.041	21.760529		21.760598	
$1s2p5p^4P$	21.556585	0.9272	+9.213	-1.966	21.565753		21.565969	
$1s2p6p^4P$	21.451948	0.9264	+9.115	-1.934	21.461110			
$1s2s3d^4D$	22.364027	1.0440	-0.528	-0.110	22.374451		22.374539	
$1s2p3p^4D$	22.220369	0.9498	+10.63	-2.097	22.229763		22.230903	
$1s2s4d^4D$	21.939651	1.0511	-0.300	+0.005	21.950160		21.950424	
$1s2p4p^4D$	21.765503	0.9393	+8.883	-1.895	21.774796		21.775512	
$1s2s5d^4D$	21.748642	1.0410	+0.737	-0.148	21.759045		21.759614	
$1s2p3d^4D^o$	22.132368	0.9278	+7.130	-1.834	22.141534		22.141640	
$1s2p4d^4D^o$	21.730712	0.9264	+8.360	-1.866	21.739873		21.739433	
$1s2p5d^4D^o$	21.546101	0.9247	+8.686	-1.877	21.555246		21.554961	
$1s2p4f^4F$	21.727519	0.9267	+8.951	-1.885	21.736687		21.736717	
$1s2p3d^4F^o$	22.171137	0.9292	+12.22	-1.889	22.180362		22.180954	
$1s2s4f^4F^o$	21.921072	1.0509	-0.137	-0.011	21.931579		21.931683	

<sup>a</sup>Larsson *et al.*, Ref. 7.

<sup>b</sup>Lunell and Beebe, Ref. 8.

quartets in the literature are those of the  $2p2p^4P$  and  $2s2p^4P^o$  states. In the present work, the fine-structure splittings for several quartet states are calculated. The results are quoted in Table III together with the energy for

the  $J_1=L+1.5$  state. It is apparent from this table that states with a  $2p$  electron have a considerably larger splitting as compared with other states. A very illustrative example is the  $^4D$  states. The  $1s2snd^4D$  states have very

TABLE II. Wavelengths (in nm) associated with quartet states in CIV.

Experiment <sup>a</sup>	$I^b$	This work		Assignments	Other experiments
		Theory			
		18.089		$2s2p^4P^o-2p6p^4P$	
		18.873		$2s2p^4P^o-2p5p^4P$	
		19.763		$2s2p^4P^o-2s6s^4S$	
		20.502		$2s2p^4P^o-2p4p^4S$	
		20.516		$2s2p^4P^o-2s5d^4D$	
20.529±0.005	w	20.529		$2s2p^4P^o-2p4p^4P$	20.521 <sup>g</sup>
20.67 ±0.01	(b1)	20.662		$2s2p^4P^o-2p4p^4D$	20.66 <sup>d</sup> ,20.62(b1) <sup>c</sup>
		20.857		$2s2p^4P^o-2s5s^4S$	
21.843±0.005	vw	21.846		$2p2p^4P-2p5d^4D^o$	21.8 <sup>d</sup> ,21.83 <sup>c</sup> ,21.843 <sup>g</sup>
22.451±0.005	m	22.447		$2s2p^4P^o-2s4d^4D$	22.44 <sup>d,e</sup> ,22.45 <sup>g</sup>
23.110±0.005	vw	23.110		$2s2p^4P^o-2s4s^4S$	23.08 <sup>e</sup> ,23.14 <sup>g</sup>
23.860±0.015	vw	23.868		$2p2p^4P-2p4d^4P^o$	
23.962±0.005	m	23.967		$2p2p^4P-2p4d^4D^o$	24.05 <sup>d</sup> ,24.00 <sup>c</sup> ,23.972 <sup>g</sup>
25.478±0.005	m	25.473		$2s2p^4P^o-2p3p^4P$	25.43 <sup>d,h</sup> ,25.46 <sup>e</sup> ,25.475 <sup>g</sup>
25.650±0.005	vw	25.648		$2s2p^4P^o-2p3p^4S$	25.656 <sup>g</sup> ,25.66 <sup>h</sup>
		26.033		$2s2p^4P^o-2p3p^4D$	

TABLE II. (Continued).

Experiment <sup>a</sup>	<i>I</i> <sup>b</sup>	This work		Assignments	Other experiments
		Theory			
28.381±0.005	s	28.379		$2s\ 2p\ ^4P^o-2s\ 3d\ ^4D$	28.4 <sup>d</sup> ,28.40 <sup>e</sup> ,28.38 <sup>g</sup>
30.000±0.005	m	29.994		$2p\ 2p\ ^4P^o-2p\ 3d\ ^4P^o$	30.00 <sup>e</sup> ,30.002 <sup>g</sup>
30.390±0.005	m	30.388		$2p\ 2p\ ^4P-2p\ 3d\ ^4D^o$	30.34 <sup>d</sup> ,30.35 <sup>e</sup> ,30.382 <sup>g</sup>
31.467±0.005	m	31.457		$2s\ 2p\ ^4P^o-2s\ 3s\ ^4S$	31.46 <sup>d</sup> ,31.45 <sup>e</sup> ,31.456 <sup>g</sup>
33.700±0.005	w	33.692		$2p\ 2p\ ^4P-2p\ 3s\ ^4P^o$	33.72 <sup>e</sup> ,33.695 <sup>g</sup>
		55.064		$2p\ 3s\ ^4P^o-2p\ 6p\ ^4P$	
		60.065		$2s\ 3p\ ^4P^o-2s\ 6s\ ^4S$	
63.03 ±0.02	w	63.036		$2p\ 3s\ ^4P^o-2p\ 5p\ ^4P$	
		66.966		$2p\ 3d\ ^4D^o-2p\ 6p\ ^4P$	
67.41 ±0.02	vw	67.553		$2p\ 3p\ ^4D-2p\ 5d\ ^4D^o$	
67.64 ±0.02	vw	67.601		$2s\ 3p\ ^4P^o-2s\ 5d\ ^4D$	
		68.960		$2p\ 3d\ ^4P^o-2p\ 6p\ ^4P$	
		71.450		$2s\ 3p\ ^4P^o-2s\ 5s\ ^4S$	
		71.644		$2p\ 3p\ ^4P-2p\ 5d\ ^4D^o$	
		79.136		$2p\ 3d\ ^4D^o-2p\ 5p\ ^4P$	
		81.936		$2p\ 3d\ ^4P^o-2p\ 5p\ ^4P$	
		85.798		$2p\ 3s\ ^4P^o-2p\ 4p\ ^4S$	
86.27 ±0.03	vw	86.286		$2p\ 3s\ ^4P^o-2p\ 4p\ ^4P$	
88.74 ±0.02	w	88.682		$2p\ 3s\ ^4P^o-2p\ 4p\ ^4D$	88.75 <sup>g,h</sup>
		91.531		$2p\ 3p\ ^4D-2p\ 4d\ ^4P^o$	
		93.011		$2p\ 3p\ ^4D-2p\ 4d\ ^4D^o$	
94.36 ±0.02	m	94.354		$2s\ 3p\ ^4P^o-2s\ 4d\ ^4D$	
96.48 ±0.02	w	96.630		$2p\ 3p\ ^4S-2p\ 4d\ ^4P^o$	
		99.208		$2p\ 3p\ ^4P-2p\ 4d\ ^4P^o$	
		100.949		$2p\ 3p\ ^4P-2p\ 4d\ ^4D^o$	
102.57 ±0.02	m	102.700		$2p\ 3d\ ^4F^o-2p\ 4f\ ^4F$	
102.89 ±0.02	m	102.886		$2s\ 3d\ ^4D-2s\ 4f\ ^4F^o$	102.88 <sup>g,h</sup>
107.26 ±0.02	vw	107.285		$2s\ 3p\ ^4P^o-2s\ 4s\ ^4S$	
		112.351		$2p\ 3d\ ^4F^o-2p\ 4p\ ^4D$	
112.53 ±0.02	m	112.549		$2p\ 3d\ ^4D^o-2p\ 4f\ ^4F$	
		119.593		$2p\ 3d\ ^4D^o-2p\ 4p\ ^4P$	
		124.245		$2p\ 3d\ ^4D^o-2p\ 4p\ ^4D$	
		125.062		$2p\ 3d\ ^4P^o-2p\ 4p\ ^4S$	
126.04 ±0.02	w	126.103		$2p\ 3d\ ^4P^o-2p\ 4p\ ^4P$	
		131.287		$2p\ 3d\ ^4P^o-2p\ 4p\ ^4D$	
134.42 ±0.02	vs	134.422 <sup>c</sup>		$2s\ 2p\ ^4P^o-2p\ 2p\ ^4P$	134.6 <sup>d</sup> ,134.59 <sup>e</sup> ,134.42 <sup>f,g</sup>
		163.457		$2p\ 4d\ ^4D^o-2p\ 6p\ ^4P$	
		168.237		$2p\ 4d\ ^4P^o-2p\ 6p\ ^4P$	
		180.395		$2s\ 3d\ ^4D-2p\ 3d\ ^4P^o$	
		187.557		$2s\ 3s\ ^4S-2p\ 3s\ ^4P^o$	
		188.413		$2s\ 3p\ ^4P^o-2p\ 3p\ ^4P$	
		195.630		$2s\ 3d\ ^4D-2p\ 3d\ ^4D^o$	
		198.468		$2s\ 3p\ ^4P^o-2p\ 3p\ ^4S$	
		207.542		$2p\ 4p\ ^4D-2p\ 5d\ ^4D^o$	
		208.816		$2s\ 4d\ ^4D-2p\ 4d\ ^4P^o$	
		216.680		$2s\ 4d\ ^4D-2p\ 4d\ ^4D^o$	
		221.966		$2p\ 4p\ ^4P-2p\ 5d\ ^4D^o$	
		223.583		$2s\ 5d\ ^4D-2p\ 5d\ ^4D^o$	
		224.110		$2s\ 3p\ ^4P^o-2p\ 3p\ ^4D$	
		233.798		$2s\ 4f\ ^4F^o-2p\ 4f\ ^4F$	
		234.764		$2s\ 3d\ ^4D-2p\ 3d\ ^4F^o$	

<sup>a</sup>The quoted uncertainties represent the error on the position of the line maximum (except for the 134.42-nm transition—see text).

<sup>b</sup>Observed intensity. vw, very weak; w, weak; m, mean; s, strong; vs, very strong; bl, blended line.

<sup>c</sup>Value obtained by taking into account the radiative correction of Ref. 12 (see Ref. 13).

<sup>d</sup>Berry *et al.*, Ref. 15.

<sup>e</sup>Buchet-Poulizac, Ref. 16.

<sup>f</sup>Livingston and Berry, Ref. 17.

<sup>g</sup>To *et al.*, Ref. 18.

<sup>h</sup>Jacques *et al.*, Ref. 26.

TABLE III. The fine structure of quartet system of CIV.  $J_1=L+1.5$ ;  $J_2=L+0.5$ ;  $J_3=L-0.5$ ;  $J_4=L-1.5$  (in  $\text{cm}^{-1}$ ).

Term	$-E_{J_1}$ (a.u.)	$E_{J_1}-E_{J_2}$	$E_{J_2}-E_{J_3}$	$E_{J_3}-E_{J_4}$
$1s2s2p^4P^o$	23.979 819	94.27	3.778	
$1s2s3p^4P^o$	22.433 026	23.50	1.523	
$1s2p3s^4P^o$	22.288 355	104.82	11.41	
$1s2p3d^4P^o$	22.121 974	-37.09	-32.08	
$1s2p4d^4P^o$	21.732 083	-46.22	-35.38	
$1s2p2p^4P$	23.640 857	39.91	76.01	
$1s2p3p^4P$	22.191 127	34.09	53.50	
$1s2p4p^4P$	21.760 414	33.94	49.44	
$1s2p5p^4P$	21.565 639	33.82	48.09	
$1s2p6p^4P$	21.460 998	33.57	47.38	
$1s2s3d^4D$	22.374 421	9.522	2.706	-0.014
$1s2p3p^4D$	22.229 472	86.17	36.81	12.19
$1s2s4d^4D$	21.950 155	1.917	0.246	-0.301
$1s2p4p^4D$	21.774 528	78.90	33.93	11.38
$1s2s5d^4D$	21.759 024	6.496	2.371	0.515
$1s2p3d^4D^o$	22.141 468	6.979	26.51	24.52
$1s2p4d^4D^o$	21.739 809	6.198	26.25	24.48
$1s2p4f^4F$	21.736 650	-2.807	18.07	23.75
$1s2p3d^4F^o$	22.180 110	64.64	32.82	14.09
$1s2s4f^4F^o$	21.931 575	1.156	0.309	-0.096

small splittings whereas those of the  $1s2pnp^4D$  states are much larger.

### III. EXPERIMENTAL TECHNIQUE AND RESULTS

$\text{C}^+$  beams of about  $1 \mu\text{A}$  (diameter 5 or 10 mm) are supplied by a 2- or a 3-MV Van de Graaff accelerator equipped with an rf source into which CO gas was admitted. Beam light emitted after the carbon foil ( $\approx 10 \mu\text{g}/\text{cm}^2$ ) is observed with a grazing-incidence spectrometer ( $\lambda=10-40 \text{ nm}$ ) or with a Seya-Namioka-type spectrometer ( $\lambda=30-200 \text{ nm}$ ). The grazing-incidence spectrometer is equipped with a curved exit slit and five channeltron detectors; the Seya-Namioka with three channeltron detectors ( $\lambda < 125 \text{ nm}$ ) or with an EMR542G

photomultiplier tube ( $\lambda > 105 \text{ nm}$ ). These two beam-foil spectroscopy arrangements are described in detail in Refs. 24 and 25, respectively.

Typical spectra of carbon between 22 and 26 nm and between 119 and 137 nm are shown in Figs. 1 and 2, respectively. The experimental linewidths [full width at half-maximum (FWHM)] are about 0.04 nm with the grazing-incidence spectrometer and 0.07 nm with the Seya-Namioka spectrometer.

The wavelengths of the lines appearing in our spectra and assigned to transitions between quartet states in CIV on the basis of theoretical predictions are reported in Table II together with rough estimations of the observed line intensities. This table shows that an excellent agreement exists between our theoretical and experimental wavelengths.

TABLE IV. Newly observed lines in C III.

$\lambda$ (nm)	Intensity <sup>a</sup>	Assignment
172.54	w	$2p3p^3P_2-2p4d^3D_3^o$
170.33	m	$2s4p^1P_1^o-2p4p^1P_1$
162.32	w	$2s4d^1D_2-2p4d^1D_2^o$
154.58	m	$2s5p^3P_{1,2}^o-2p5p^3P_2$
150.16	s	$2s4p^3P_{0,1,2}^o-2p4p^3P_{1,2}$
149.37	s	$2s4s^3S_1-2p4s^3P_2^o$
149.14	vw	$2s4d^3D_{1,2,3}-2p4d^3P_2^o$
140.36	vw	$2p3d^3D_{1,2,3}^o-2p5p^3P_2$
135.66	s	$2p3s^3P_{1,2}^o-2p4p^3D_{2,3}$
131.43	(b1)	$2p3s^3P_2^o-2p4p^3P_{1,2}$
131.33	(b1)	$2p3s^3P_{0,1}^o-2p4p^3P_{1,2}$
130.18	vw	$2p3d^1D_2^o-2p5p^1D_2$
129.15	vw	$2p3d^3F_{3,4}^o-2p5f^3F_4$
114.35	vw	$2p3p^3D_{2,3}-2p5d^3D_3^o$

<sup>a</sup>vw, very weak; w, weak; m, mean; s, strong; bl, blended line.

TABLE V. Newly observed lines in CIV.

$\lambda$ (nm)	Intensity <sup>a</sup>	Assignment
165.44	m	$4d^2D-6p^2P^o$
165.39	m	$4p^2P^o-6s^2S$
163.77	vs	$4d^2D-6f^2F^o$
144.01	m	$4s^2S-6p^2P^o$
135.30 <sup>b</sup>	m	$4f^2F^o-7g^2G$
135.14	m	$4d^2D-7f^2F^o$
131.56	m	$4p^2P^o-7d^2D$
121.38	w	$4d^2D-8f^2F^o$
121.06	w	$4s^2S-7p^2P^o$
118.44	vw	$4p^2P^o-8d^2D$

<sup>a</sup>vw, very weak; w, weak; m, mean; vs, very strong.

<sup>b</sup>Previously observed in Ref. 26 but at 135.20 nm.

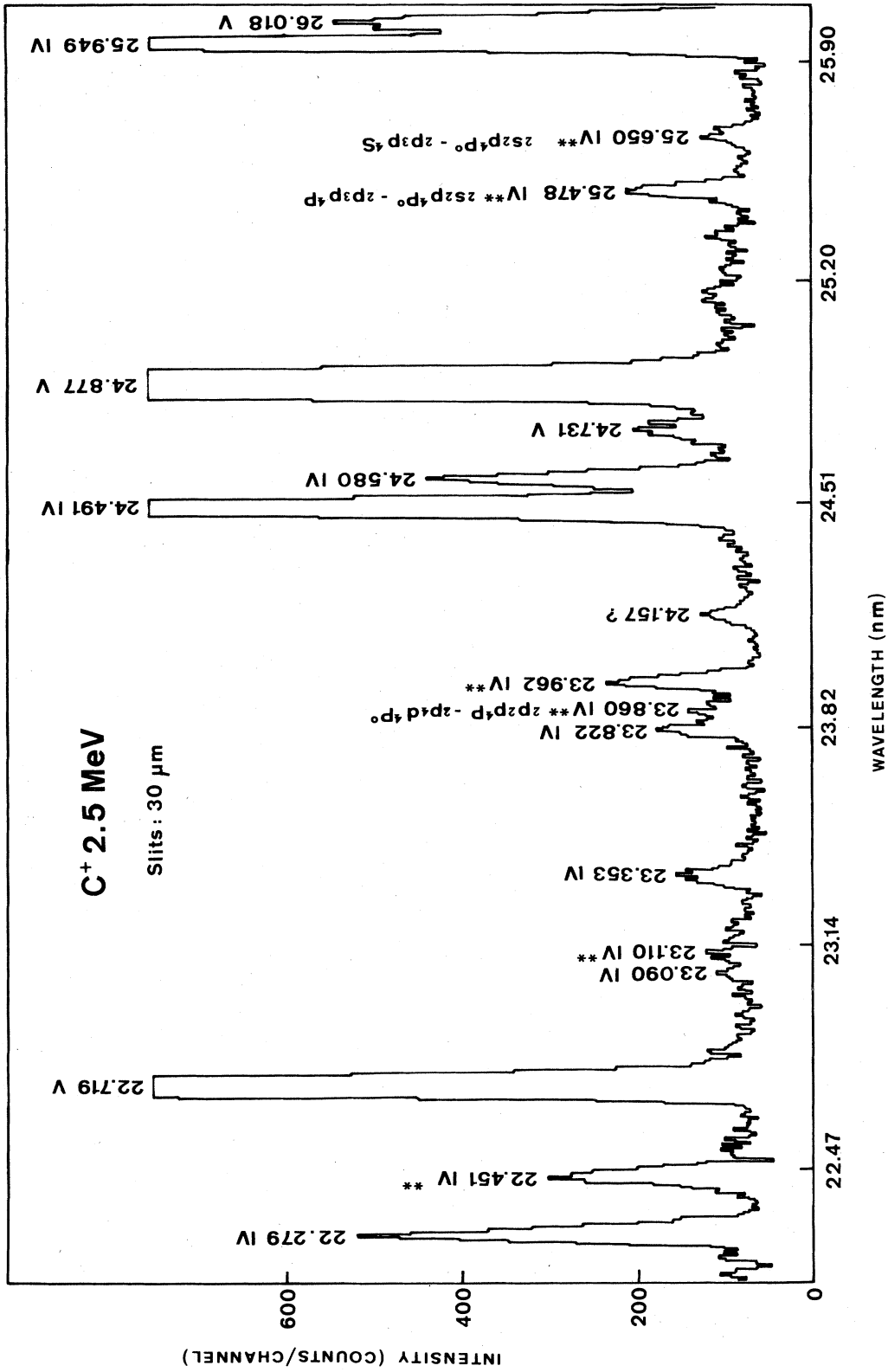


FIG. 1. A section of the beam-foil spectrum of carbon between 22 and 26 nm (grazing-incidence spectrometer). Assignments of newly classified lines are indicated.

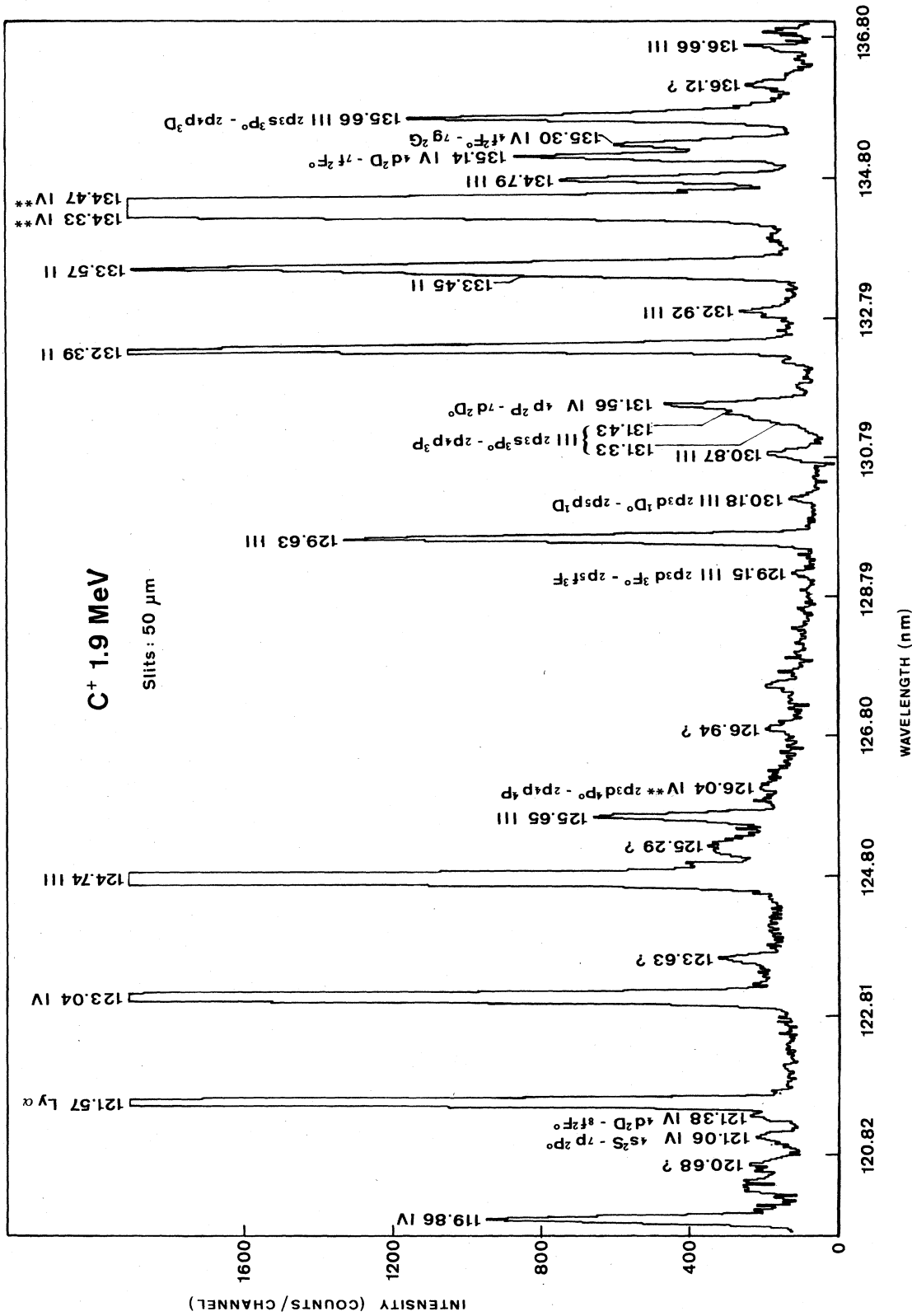


FIG. 2. A section of the beam-foil spectrum of carbon between 119 and 137 nm (Seya-Namioka-type spectrometer). Assignments of newly classified lines are indicated.



more reliable and complete than those previously reported. Twenty-seven quartet states have been calculated together with 20 fine-structure splittings which are significant for many of these quartets. Twenty-seven lines appearing in the beam-foil spectra of carbon (11 observed for the first time) have been classified in the quartet system of C IV. The wavelengths observed for these transitions are in very good agreement with our theoretical predictions and with the other experimental data available.

Twenty-four new lines appearing in our spectra have also been identified as transitions between known energy levels in C III and C IV.

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