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ABSORPTION LINE SERIES AND
AUTOIONIZATION RESONANCE
STRUCTURE ANALYSIS
IN THE ULTRAVIOLET SPECTRUM
OF Sr I

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PREFACE

This report, on long series and autoionization resonance structures in Sr I, is given in two parts. Furnace absorption spectra, extending from the middle quartz-ultraviolet through the Schumann region, were obtained by two of us (WRS; KC) about 1960 with the three-meter vacuum spectrograph at Imperial College, London. This work also embraced the absorption spectra of Ca I and Ba I, on which papers have been already published (Garton and Codling, 1960, 1965). Because of the greater complexity of the configuration-mixing effects, including autoionization, in Sr I, publication on this spectrum has been delayed. In the meantime, notable advance in the theoretical interpretation of the profiles of autoionization "resonances" has occurred, especially through the contributions of U. Fano (1961), Fano and Cooper (1965), Shore (1967), -- which provide a general phenomenological interpretive framework, -- and through several ab initio calculations of positions, widths and transition probabilities of resonances for simpler systems, like He I (C.F. Burke, 1965). These theoretical developments have emphasized to the experimental spectroscopist the necessity for specification, in as much detail as possible, of the course of intensity, -- whether in absorption or emission, -- in any portion of spectrum showing autoionization effects. In the past, the little that has been done in this respect has almost invariably come a good deal later than observation of the spectrum itself, and as the result of investigations aimed at the determination of photoionization cross sections.

The second part of the present report provides scientific recognition of the need explained. A detailed photometric study

has been made of the structures of the first 22 autoionization resonances, counting from the long wavelength member, by means of the one-meter vacuume spectrophotometer at Harvard Observatory. By means of a computer program, to be described elsewhere by G.L. Grasdalen and L. Toy, this portion of the Sr I Schumann region absorption spectrum has been unfolded in terms of the prescription given by Fano (loc. cit.).

Ultraviolet Extensions of the Arc Spectra of the Alkaline Earths:
The Absorption Spectrum of Strontium Vapour

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Abstract

A photoelectric spectrometer has been used to measure relative absorption cross-sections in the Sr I spectrum, over the region comprising about 22 of the autoionization resonances described in the preceding paper. The results are unfolded by a computer program into Fano-type or dispersion profiles, and values of "line-profile-indices" and autoionization damping constants are derived. One additional resonance, not recognizable from the photographic spectrum, is reported.

1. Introduction

Our present description of the absorption spectrum of Strontium vapour connects with previous papers on Ca I and Ba I (Garton and Codling, 1960; 1965), which contain explanations of objectives and general experimental details. As before, the work has led to considerable extension of the singlet resonance series, and consequent improvement of the value for the ionization potential, the location of the perturbing level, - in this case $4d5p\ ^1P_1^o$, - and discovery of a large number of lines due to simultaneous excitation of both electrons, classifiable chiefly into six series, with marked configuration mixing and autoionization effects. Curiously, the two-electron spectrum of Sr I has a more complicated appearance and structure than the corresponding cases of Ca I and Ba I. Consequently, of the six series expected, only two can be considered to be certainly established and two are very tentative. The Schumann region absorption spectrum has also led to a reassignment of an autoionized multiplet early recognized by White (1931).

Until recently, reports on autoionization effects have often appeared as by-products of general structural analyses of individual spectra or from investigations deliberately aimed at observation and term analysis - into series where possible - of absorption spectra, expected to exhibit such effects. In both cases, the aim has been to give a reasonable classification of lines observed, with only rough qualitative indications of intensities and line widths. During the last few years, considerable theoretical efforts have been mounted towards description and interpretation of "auto-ionization resonances", especially in the hands of Fano and collaborators (Fano, 1961; Fano and Cooper, 1965), Burke (1965,

Smith (1966), Shore (1967) and others, and the experimenters increasingly realize that, in addition to specifying rough wavelengths of heavily broadened spectral features, and classification if possible, it is essential to report full details in emission or absorption respectively, of the profiles of the observed resonances. This dual task has been performed in one or two notable cases, such as that of He I (Madden and Codling, 1965), though more often up to the present, the profile work has been done much later than the observation of the spectrum, by investigators interested in determination of photoionization cross-sections. The work reported in the present paper was started by the present writers just before the surge of theoretical papers mentioned, and was followed more recently by a "Fano-type" analysis of the main portion of the spectrum discovered. Since two overlapping groups of workers have been concerned, we confine this paper to a description of the spectrum, with analysis into series, and the Fano-type break-down of the portion studied photometrically appears in the paper immediately following.

2. The Sr I Spectrum

The main references of relevance, cited in AEL (Moore, 1952) are to the work of Saunders (1922), Russell and Saunders (1925), and unpublished data of H.N. Russell. From this work the following levels, which combine with the $5s^2 \ ^1S_0$ ground state, have long been known: $5snp \ ^1P_1^o$ ($n = 5-14$), $^3P_1^o$ ($n = 5-7$), $4d5p \ ^3P_1^o$, $^3D_1^o$. Thus, in contrast to Ca I and Ba I, the doubly-excited level $4d5p \ ^1P_1^o$ has not previously been identified, though a suggestion was made by Shenstone and Russell (1932) in their well-known paper on series perturbations.

The ionization potential quoted in Moore (1952), viz., 45925.6 cm^{-1} , is evidently taken from the Saunders and Russell and Saunders' papers cited; the value was, in fact, obtained from the $5 \text{ }^1\text{S}_0 - n \text{ }^1\text{P}_1^{\circ}$ observations extending to $n = 14$.

A paper by White (1931) treats of autoionization-broadened emission lines observed from arc spectra. He identified five lines in the 3200\AA region as belonging to $5s4d \text{ }^3\text{D} - 4d6p \text{ }^3\text{F}^{\circ}$ with one component missing.

3. Experimental

Practically all details of experimental arrangements have been given previously (Garton and Codling, 1965 and earlier). In brief, absorption spectra of Sr vapour were obtained over a range of temperatures from about 650°C to 1000°C by use of a King furnace and a three-meter normal incidence grating, with a flash-tube or a hydrogen continuum discharge tube as background. In addition, a few emission spectra from carbon-arcs fed with Sr metal were obtained around the 3200\AA region, in order to clarify questions concerning the $\text{ }^3\text{D} - \text{ }^3\text{F}$ multiplet described by White (1931).

4. Results and Interpretation

a. The $5s^2 \text{ }^1\text{S}_0 - 5snp \text{ }^1\text{P}_1^{\circ}, \text{ }^3\text{P}_1^{\circ}$ Series

The singlets, previously followed to $n = 14$, have been extended on our absorption spectra to $n = 33$, with more accurate wavelengths for some of the previously listed lines.

Perturbation of $5snp \text{ }^1\text{P}_1^{\circ}$ by $4d5p \text{ }^1\text{P}_1^{\circ}$ was recognized by Shenstone and Russell (1932), who suggested, - allowing for a slightly different limit, - that the listed $5s9p \text{ }^1\text{P}_1^{\circ}$ at 42462.36 cm^{-1} should be identified as the perturber; Moore's

(1952) tabulation does not include this tentative assignment. As shown below, the autoionizing $5s^2 \ ^1S_0 - 4dnp \ ^1P_1^{\circ}$ series, of which the first member ($n = 5$) should appear as a perturbation in the one-electron series, extrapolates so that the $n = 8$ level is to be removed from Moore's (1952) listing and reclassified, the principal quantum numbers of the levels listed in AEL from $n = 9$ onwards now being reduced by unity. The series intensity peculiarity mentioned by Shenstone and Russell (1932), and quantitatively reported in f-value measurements by Penkin and Shabanova (1965) is consistent with this assignment, the transition $5s^2 \ ^1S_0 - 4d5p \ ^1P_1^{\circ}$ producing a strong line, with some sharing of intensity with the series members immediately adjacent from $n = 8$. Such intensity "anomalies" in spectral series are frequent, and can be understood by reference to the appendix to Fano's (1961) paper, in the sense that the maximum, minimum, or both of the Fano resonance curve may lie within a converging series of discrete transitions.

Measurements of the long $snp \ ^1P_1^{\circ}$ series are given in table 1, and the comparison of the quantum defect curves versus term value in Fig. 1, against the limit given in Moore (1952), and an adjustment of this by 6.4 cm^{-1} , yields an improved ionization potential of $45932.0 \pm 0.2 \text{ cm}^{-1}$. Incidentally, a plotting of the $5snf \ ^1F_3^{\circ}$ terms from Moore (1952) looks much better against this altered limit.

At high vapour densities, our spectra show satellites to the long wavelength sides of the singlet principal series lines from $n = 22-33$. These are listed in table 2, and are identified as the intercombinations $5s^2 \ ^1S_0 - 5snp \ ^3P_1^{\circ}$.

b. The Schumann Ultraviolet Series

As in Ca I and Ba I, the absorption spectrum in the

Schumann region is of striking aspect, as illustrated in plates 1 and 2. A total of 94 absorption lines is recorded in Tables 3-9, of which 88 are classified amongst 6 series due to the transitions $5s^2 \ ^1S_0 - [4dnp]_{J=1}, [4dnf]_{J=1}$, converging in two groups of three series on the metastable $4 \ ^2D_{\frac{3}{2}, \frac{5}{2}}$ term of Sr II. Though the LS-designations have been employed in the tables, their significance is only partial and, for most of the absorption lines, the J1-designation also shown is of more likely utility. The LS-symbols are probably justified for the lower members of the dp series, as evidenced by the relatively sharp character of the lines of the series in Table 5; on this basis the dp $^3D_1^0$ terms are expected to autoionize weakly. However, all the series are expected to move towards Jj or J1 coupling with rising n, and this tendency is complicated by mutual and severe perturbations between members of the individual series. Accordingly, some limitation has to be expressed about the reality of the assignments in the tables.

The series of tables 3 and 6 seem secure as judged from the run of quantum defects, the intensities and widths. Thus, the $4dnp \ ^1P_1^0$ assignments extrapolate to confirm the placing of $4d5p \ ^1P_1^0$ mentioned above, and the quantum defects in the series, viz., ~ 2.7 , agree with those in the principal series of Sr II and Y II. Likewise, the strongest series arising from $4dnf$, given in Table 6, appears convincing, with reasonably well-behaved quantum defects less than 0.2; in fact, the levels of Table 6 check consistently by raising the $5snf \ ^1F_3^0$ terms (Moore 1952) by the wave number difference of the Sr II $5 \ ^2S_{\frac{1}{2}} - 4 \ ^2D_{\frac{5}{2}}$ interval. We note also that all three members of each line group identified with presence of an f-electron are markedly more diffuse than the adjacent dp $^3D_1^0$ transition. This conforms with the coupling tending more strongly to J1 or Jj rather than LS in the df series, another pointer in the same sense being the smaller separations, for low n, of the two df levels converging on $^2D_{\frac{5}{2}}$.

The series of Tables 4 and 5 seem fairly convincing, again as judged from run of quantum defects, the intensities and widths. The other two series, tables 7 and 8, are very tentative beyond $n = 8$, though no doubts exist of the reality of the absorption lines. Moreover, a few weak lines, shown in table 9, could not be plausibly fitted.

The spectra of plates 1 and 2, together with the tabulations, contain the following notable features. As in Ca I and Ba I, the first member of the series $4dnp \ ^1P_1^0$ above the ionization potential, in this case $n = 6$ member, - has a very large width and, as in Ca I, the next two members ($n=7$ and 8) exhibit pronounced intensity and width perturbations. These are ascribable to the occurrence of the structure $6s5p \ ^1,^3P_1^0$, identified in the present spectrum as the weak diffuse feature Y and the "Fano-window" resonance shown at X in plate 1, respectively.*

In the paper on Ca I (Garton and Codling 1965) mention was made of a perturbation effect, recognized as an alternation of intensities amongst the higher lines of two series converging on the separate $^2D_{3/2, 5/2}$ limits. The same effect is present amongst the higher lines of tables 3 and 4, and elsewhere also, amongst the rather crowded structure towards the series limits. Full examination of this effect requires use of higher dispersion than has so far been applied.

At Z marked on plate 2, in the region 1640\AA , an interesting near coincidence of 2 diffuse lines occurs. In the first plates obtained by us, by use of a flash tube working in a helium atmosphere, this feature was assumed to be one wide line with the strong 1640\AA

* Note: For a description of the analogous situation in Ca I see Newsom (1966).

line of helium, present in the spectrum of the background source, showing through near the line center. This interpretation was subsequently corrected, when the same structure was found to occur when a hydrogen tube background was employed. The spectrum reproduced here was obtained with a flash-tube.

The energy level responsible for the first line of the 2-electron spectrum (towards longer wavelengths), namely, that shown as $5\ ^1S_0 - 4d6p\ ^3D_1^{\circ}$, is very close to the level listed by Moore (1952) as $4d6p\ ^3F_2^{\circ}$, which was based on White's (1931) assignment of a group 5 diffuse lines in the 3200\AA region as $4d5s\ ^3D - 4d6p\ ^3F^{\circ}$. White made no comment on the absence of an expected 6th line of the multiplet. Our marked absorption line at 2023.86\AA suggested that the upper term of White's multiplet should be $^3D^{\circ}$, which should have 7 components. This led us to examine the spectrum of a carbon arc fed with strontium metal, in the region of 3200\AA . We observed White's five components and two weaker components at vacuum wavelength 3184.95 and 3180.21\AA . Accordingly, White's multiplet, with these additions is reclassified as shown in Fig. 2. The two new components, though somewhat broadened by autoionization, have on our scale the relatively sharp appearance of the $4d6p\ ^3D_1^{\circ}$ combination with the ground state recognized from the absorption spectrum. On the arc plates also, we have found two, much broader, weak emission lines at 3183.50 and 3173.20 (vacuum values) which have the separation of $5s4d\ (^3D_2 - ^3D_3)$ very closely. These lines have been further studied by Mr. G. Newsom of Harvard Observatory (unpublished), who has recently found a number of new autoionized lines in shock tube and arc emission spectra, and identifies the pair as representing the combinations of $5s4d\ ^3D_{2,3}$ with the strongly autoionizing level $4d6p\ ^3P_2^{\circ}$ at 49731 cm^{-1} .

A final point worth mention is the possible existence of the $J = 1$ levels of $5p5d$ multiplets within the spectral range studied.

Rough calculation gives the expectation that the levels will lie between 55500 and 57700 cm^{-1} , so that any attempt at quantitative description of the perturbations in this part of the absorption spectrum should include the possibility of interference from such levels.

5. Acknowledgments

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Table 1: Sr I: Principal Series $5s^2 \ ^1S_0 - 5snp \ ^1P_1^o$

n	$\lambda_{\text{vac}} \text{ \AA}$	$\nu \text{ cm}^{-1}$	n^*
8	2355.029	42462.32	5.624
9	2307.974	43328.04	6.492
10	2276.007	43936.60	7.417
11	2253.954	44366.48	8.372
12	2238.350	44675.77	9.346
13	2226.996	44903.52	10.330
14	2218.507	45075.36	11.319
15	2211.999	45207.98	12.311
16	2206.927	45311.87	13.302
17	2202.863	45395.47	14.302
18	2199.579	45463.25	15.301
19	2196.900	45518.69	16.294
20	2194.663	45565.08	17.292
21	2192.788	45604.04	18.290
22	2191.196	45637.18	19.293
23	2189.841	45665.42	20.288
24	2188.673	45689.79	21.286
25	2187.652	45711.11	22.288
26	2186.776	45729.42	23.273
27	2185.982	45746.03	24.281
28	2185.304	45760.22	25.273
29	2184.681	45773.27	26.296
30	2184.138	45784.65	27.286
31	2183.644	45795.01	28.300
32	2183.212	45804.07	29.291
33	2182.810	45812.51	30.304

Limit: 45932.0 cm^{-1}

Table 2: Sr I: $5s^2 \ ^1S_0 - 5snp \ ^3P_1^0$ Series

n	$\lambda_{\text{vac}} \text{ \AA}$	$\nu \text{ cm}^{-1}$	n^*
22	2193.80	45583.0	17.75
23	2192.04	45619.6	18.74
24	2190.53	45651.1	19.76
25	2189.32	45676.3	20.72
26	2188.22	45699.2	21.71
27	2187.28	45718.9	22.69
28	2186.43	45736.7	23.70
29	2185.67	45752.1	24.70
30	2185.04	45765.8	25.70
31	2184.45	45778.1	26.70
32	2183.92	45789.2	27.72
33	2183.45	45799.1	28.73

Limit: 45932.0 cm^{-1}

Table 3: Sr I $5s^2 \ ^1S_0 - 4d \ (^2D_{5/2})np[~~3~~]₁^{\circ}; \ (^1P_1^{\circ})$ Series

n	$\lambda_{\text{vac}} \text{ \AA}$	$\nu \text{ cm}^{-1}$	n*
5	2428.828	41172.12	2.3664
6	1957.0	51090	3.368
7	1810.8	55223	4.449
8	1755.9	56950	5.361
9	1721.97	58073.0	6.381
10	1703.20	58713.2	7.307
11	1689.62	59184.8	8.325
12	1680.60	59502.4	9.311
13	1673.95	59739.0	10.326
14	1669.28	59906.1	11.282
15	1665.52	60041.2	12.286
16	1662.50	60150.3	13.327
17	1660.31	60229.9	14.279
18	1658.36	60300.5	15.318
19	1656.95	60352.0	16.238
20	1655.57	60402.1	17.313
21	1654.48	60441.8	18.335
22	1653.60	60474.1	19.316
23	1652.82	60502.7	20.330
24	1652.17	60526.3	21.299
25	1651.61	60547.0	22.273

Limit: 60768.2 cm^{-1}

Table 4: Sr I $5s^2 \ ^1S_0 - 4d \ (^2D_{3/2}) \ np \ \left[\frac{s}{p}\right]_1^o; \ (^3P_1^o)$ Series

n	$\lambda_{\text{vac}} \text{ \AA}$	$\nu \text{ cm}^{-1}$	n*
6	2018.3	49547	3.167
7	1827.19	54728.7	4.365
8	1766.47	56610.1	5.320
9	1731.81	57743.2	6.323
10	1710.58	58459.8	7.356
11	1698.21	58885.5	8.275
12	1688.63	59219.5	9.301
13	1681.60	59467.3	10.369
14	1677.29(d)	59619.9	11.244
15	1673.35	59760.5	12.283
16	1670.26	59871.0	13.337
17	1668.12	59947.9	14.255
18	1666.15	60018.7	15.293
19	1664.66	60072.2	16.248
20	1663.29	60121.7	17.311
21	1662.24	60159.7	18.285

Limit: 60487.9 cm^{-1}

(d) signifies double line

Table 5: Sr I $5s^2 \ ^1S_0 - 4d \ (^2D_{3/2}) \ np \ [^1P_1^o], \ (^3D_1^o)$ Series

n	$\lambda_{\text{vac}} \text{ \AA}$	$\nu \text{ cm}^{-1}$	n*
6	2023.86	49410.6	3.147
7	-	-	-
8	1772.79	56408.2	5.186
9	1734.71	57646.7	6.215
10	1712.44	58396.2	7.243
11	1700.44	58808.5	8.083
12	1690.69	59147.4	9.048
13	1682.12	59448.9	10.227
14	1677.29(d)	59619.9	11.244

Limit: 60487.9 cm^{-1}

Table 6: Sr I $5s^2 \ ^1S_0 - 4d \ (^2D_{5/2}) \ nf \ [^2P_{1/2}]_1^{\circ}; \ (^1P_1^{\circ})$ Series

n	$\lambda_{\text{vac}} \text{ \AA}$	$\nu \text{ cm}^{-1}$	n*
4	1867.55	53546.2	3.898
5	1780.32	56169.6	4.885
6	1737.03	57569.5	5.857
7	1711.67	58422.3	6.840
8	1695.76	58970.7	7.813
9	1684.62 (d)	59360.5	8.830
10	1676.13	59661.2	9.956
11	1671.48 (d)	59827.3	10.799
12	1667.12 (d)	59983.6	11.826
13	1663.94 (d)	60098.3	12.799
14	1661.15	60199.3	13.889
15	1659.16	60271.5	14.864
16	1657.59	60328.4	15.798
17	1656.23	60378.3	16.776
18	1655.06	60420.7	17.770
19	1654.08	60456.5	18.763
20	1653.23	60487.5	19.772
21	1652.50	60514.3	20.790
22	1651.89	60536.9	21.781
23	1651.34	60556.8	22.783

Limit: 60768.2 cm^{-1}

Table 7: Sr I $5s^2 \ ^1S_0 - 4d \ (^2D_{5/2}) \ nf \ [^1_2]_1^0$ Series ?

n	$\lambda_{\text{vac}} \text{ \AA}$	$\nu \text{ cm}^{-1}$	n*
4	-	-	-
5	1782.29	56107.7	4.852
6	1739.82	57477.1	5.774
7	1715.65	58287.0	6.650
8	1697.03	58926.5	7.719
9	1688.09	59238.5	8.470

Limit: 60768.2 cm^{-1}

Table 8: Sr I $5s^2 \ ^1S_0 - 4d \ (^2D_{3/2}) \ nf \ [^3_2]_1^{\circ}$ Series ?

n	$\lambda_{\text{vac}} \text{ \AA}$	$\nu \text{ cm}^{-1}$	n*
4	1877.83	53253.0	3.896
5	1790.60	55847.3	4.863
6	1747.17	57235.5	5.809
7	1723.50	58021.5	6.670
8	1705.95	58618.3	7.661
9	1693.97	59032.9	8.684
10	1684.62 (d)	59360.5	9.866
11	1678.76	59567.8	10.921
12	1674.48	59720.0	11.954
13	1671.48 (d)	59827.3	12.889
14	1668.75	59925.2	13.965
15	1667.12 (d)	59983.6	14.751
16	1665.12	60055.7	15.934
17	1663.94 (d)	60098.3	16.782
18	1662.71	60142.9	17.835
19	1661.55	60184.8	19.027

Limit: 60487.9 cm^{-1}

Table 9: Sr I Miscellaneous

Transition	$\lambda_{\text{vac}} \text{ \AA}$	$\nu \text{ cm}^{-1}$
† $5s^2 \ ^1S_0 - 6s5p \ ^3P_1^{\circ}$	1890.8	52359
†† - $6s5p \ ^1P_1^{\circ}$	1862	53706
Unidentified	1660.58	60220.1
"	1660.10	60237.2
"	1659.88	60245.4
"	1659.46	60260.6
"	1658.79	60285.1
"	1657.71	60324.3

† "window resonance" X in Plate 1.

†† Feature Y in Plate 1.

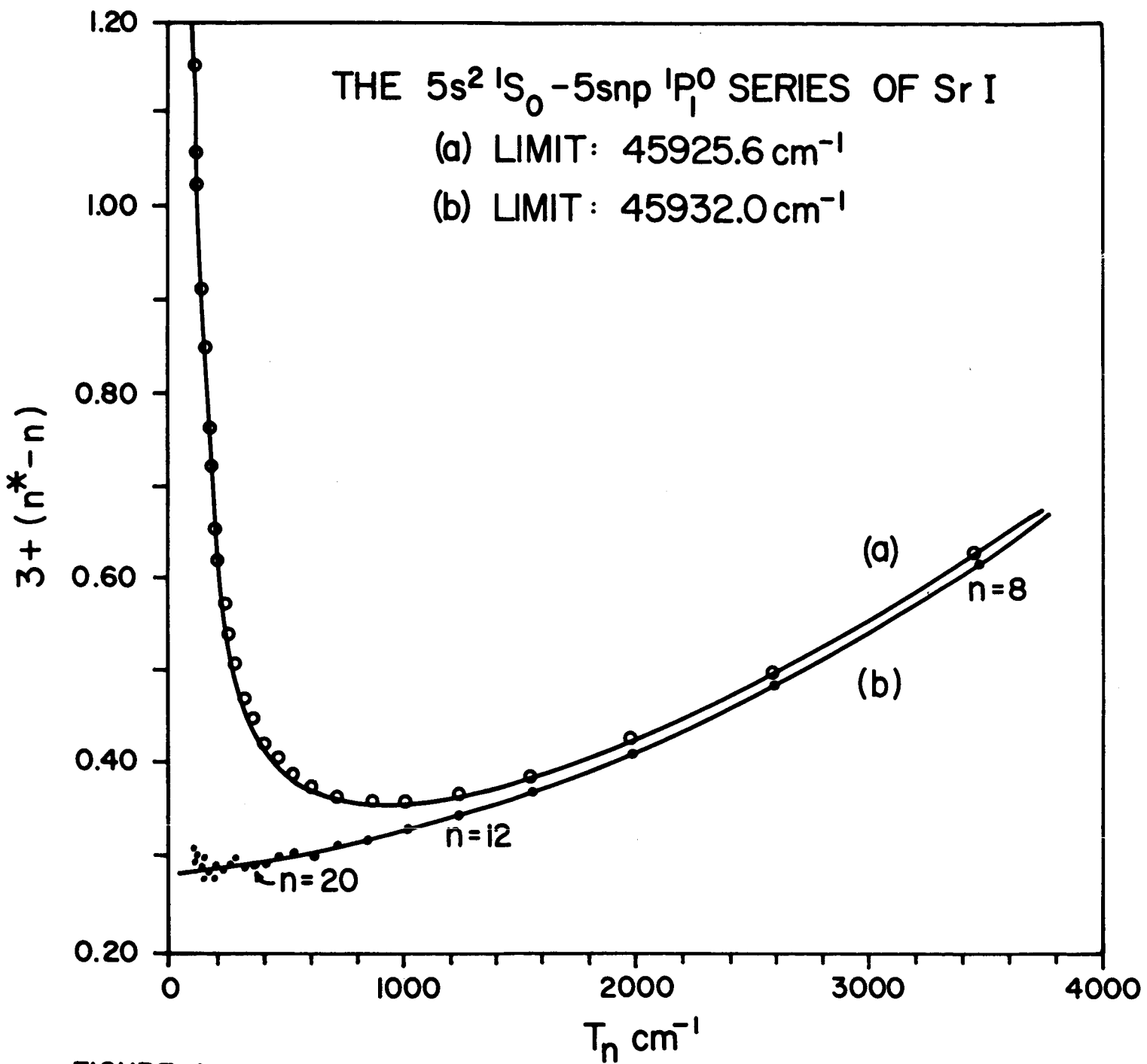


FIGURE 1

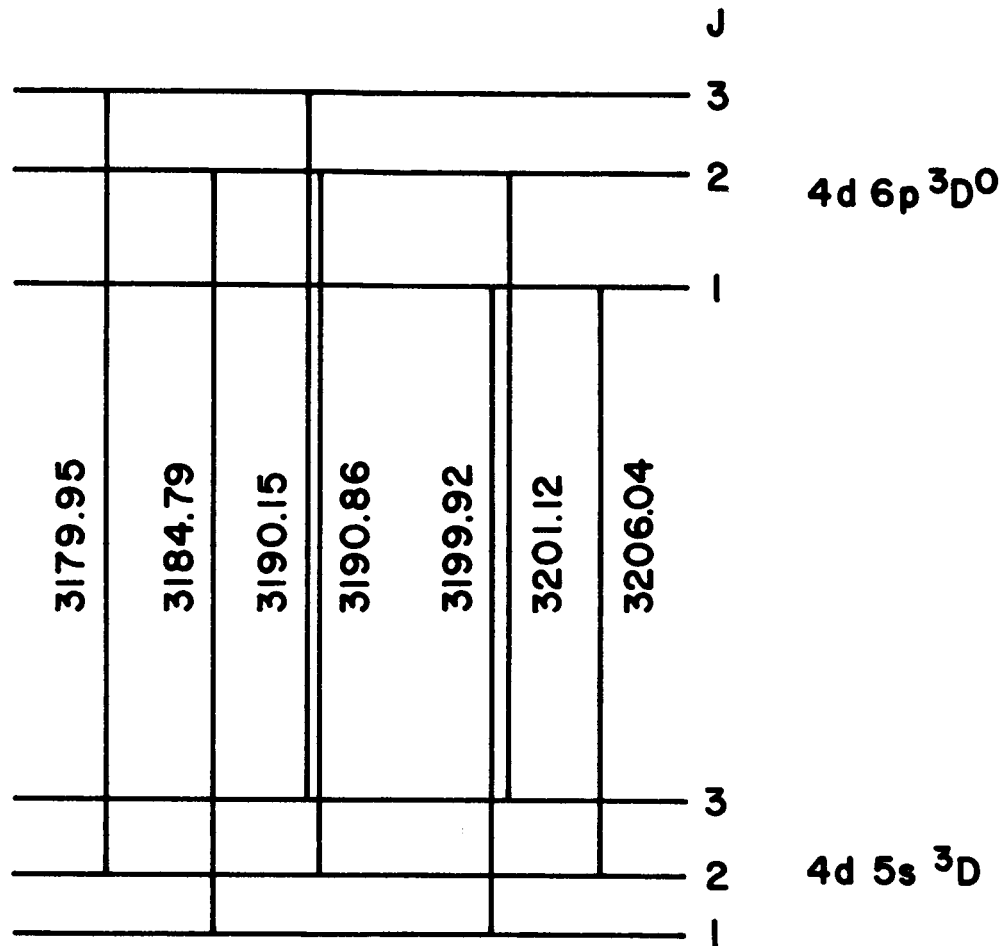
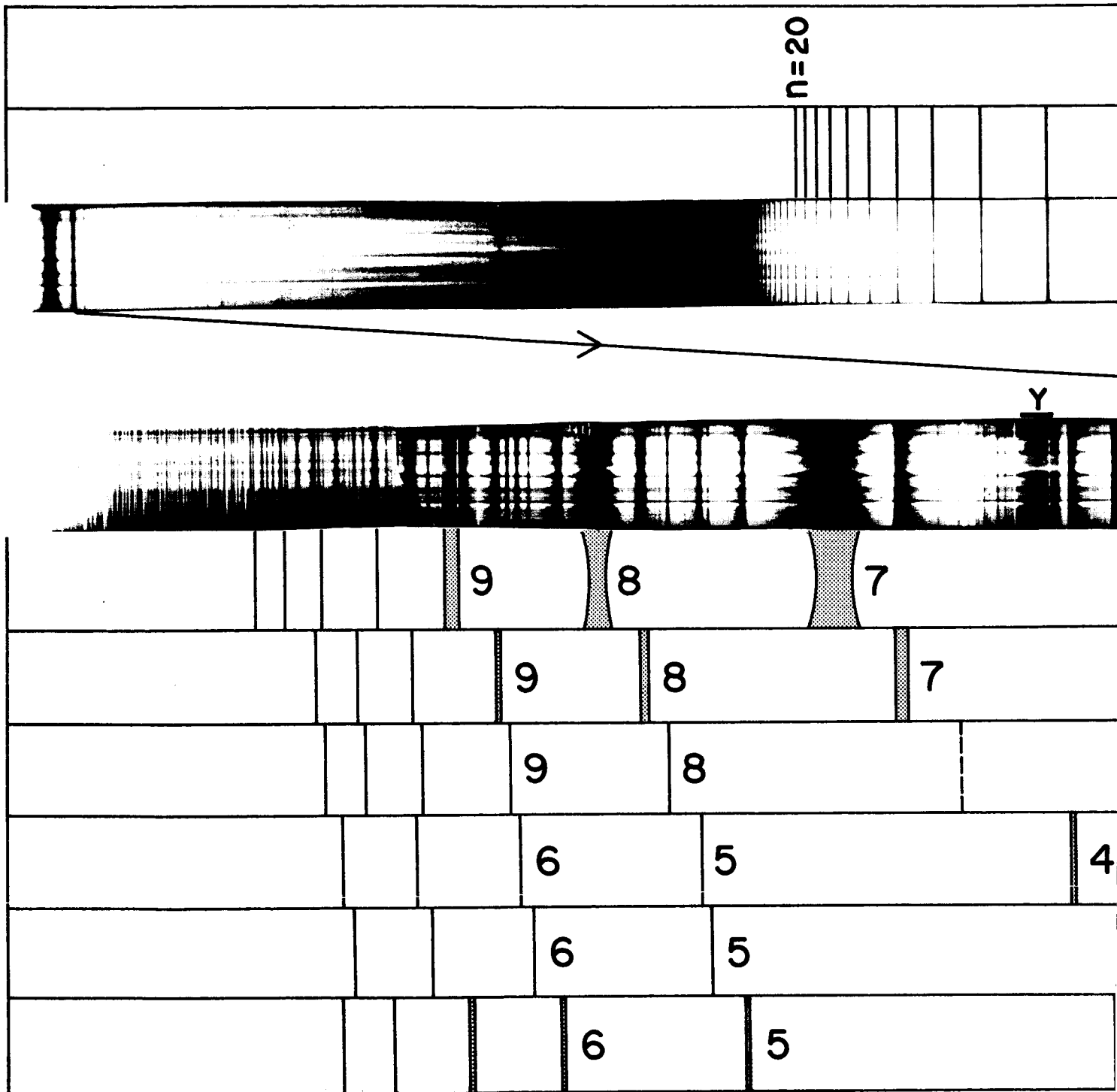


FIGURE 2
 $4d\ 5s\ ^3D - 4d\ 6p\ ^3D^0$ MULTIPLET OF Sr I
(WAVELENGTHS INDICATED ARE VACUUM VALUES)

Plate 1

Ultraviolet Absorption Spectrum
of Strontium Vapour, and
Series Classifications



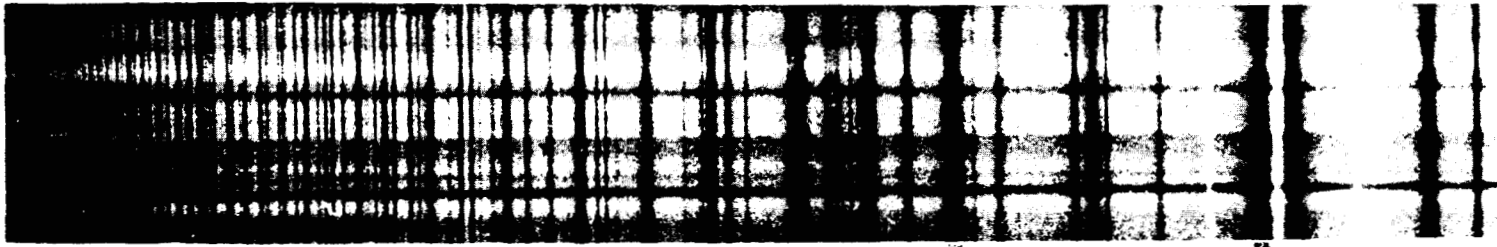
ULTRAVIOLET ABS
OF STRONT
AND SERIES CL

	$n=8$	$\leftarrow 5s^2 {}^1S_0 - 4d5p {}^1P_1^0$
		$5s^2 {}^1S_0 - 5snp {}^1P_1^0$
\times		
	6	$5s^2 {}^1S_0 - 4dnp {}^1P_1^0$
	6	$-4dnp {}^3P_1^0$
	6	$-4dnp {}^3D_1^0$
		$-4d({}^2D_{5/2})nf \left[\begin{smallmatrix} 3 \\ 2 \end{smallmatrix} \right]_1^0$
		$-4d({}^2D_{5/2})nf \left[\begin{smallmatrix} 1 \\ 2 \end{smallmatrix} \right]_1^0$
4		$-4d({}^2D_{3/2})nf \left[\begin{smallmatrix} 3 \\ 2 \end{smallmatrix} \right]_1^0$

ORPTION SPECTRUM
 UM VAPOUR,
 ASSIFICATIONS

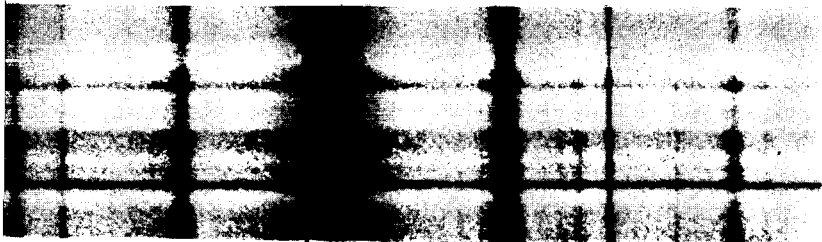
Plate 2

Ultraviolet Absorption Spectrum
of Strontium Vapour



				12			
					12		
					12		
				10			
					9		
				10			

ULTRAVIOLET ABSORPTION SPECTRUM OF STRONTIUM



	8			$5s^2\ ^1S_0 - 4dnp\ ^1P_1^0$
		8		$-4dnp\ ^3P_1^0$
			8	$-4dnp\ ^3D_1^0$
			5	$-4d(^2D_{5/2})nf\ \left[\frac{3}{2}\right]_1^0$
			5	$-4d(^2D_{5/2})nf\ \left[\frac{1}{2}\right]_1^0$
	6			$-4d(^2D_{3/2})nf\ \left[\frac{3}{2}\right]_1^0$

EMISSION SPECTRUM
OF ZINC VAPOUR

Analysis of Autoionization Resonance Structure
in the $5s^2 \ ^1S_0 - 4dnp, nf$ Spectrum of Sr I

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Abstract

The absorption spectrum of strontium vapor in the quartz ultraviolet and Schumann region has been obtained at good dispersion, leading to extension of the singlet principal series to $n = 33$, and discovery of ninety-four lines due to double-electron transitions, most of which are classifiable within six series converging on the Sr II 4^2D metastable term. Pronounced autoionization resonance effects occur in the Schumann region. We re-classify as $4d6p^3D^o$ a triplet term previously listed as $4d6p^3F^o$.

1. Introduction

For reasons explained in the preceding paper, viz., that the full description of a spectrum containing strongly autoionized lines and/or perturbed series necessarily includes simultaneous specification of the detail of the relative photoionization cross section, we have obtained photometric scans of the main portion of the Sr I absorption spectrum in the Schumann region, and have used a computer program to unfold the absorption cross section into individual "resonance" profiles according to the prescription given by Fano (1961) and Fano and Cooper (1965).

2. Experimental

A McPherson one-meter, normal incidence vacuum spectrometer, provided with a 1200 line/mm grating was employed for the photometry. The instrument, used with slit width of 20 microns, resolved to about 0.16\AA . The light source employed was a positive-column hydrogen discharge, run at a few hundred milli-amps from a 3 kV source. For detector, at the exit slit, we used an ASCOP "end-window" photomultiplier, type 541 F, sensitive to 1200\AA .

A stainless steel tube, 2 inches in diameter and 48 inches long, was held along the core of a horizontal wire-wound commercial "tube-furnace", with an effective hot zone of 22 inches. The metal tube carried end fittings in which fused quartz lenses of high ultraviolet transmission were mounted to focus the light source at the center of the vapour column, and again on the entrance slit. The end fittings also carried side tubes for evacuation and gas inlet. Helium, scavenged over hot CuO and charcoal, and passed into the stainless steel tube at a pressure of about 50 mm, served to prevent almost entirely diffusion of the strontium vapour towards the end fittings and

lenses. The strontium metal was introduced into the furnace tube in small boats, and temperatures between 650° and 950° were employed in the photometric scans.

The scans were made from the series limit at 2177Å and extended to embrace the line 4d9p $^1P_1^o$ at 1722Å; below the latter wavelength the spectrum became too crowded for reliable data to be obtained at the dispersion available. The output of the photomultiplier, after amplification, was transmitted to a chart recorder, from which the intensities were reduced manually to relative absorption cross sections on an arbitrary scale. Values of relative absorption cross section at intervals 0.25Å in the case of the dominant 4d6p $^1P_1^o$ feature at about 1970Å, and 0.12Å elsewhere, were fed to a computer programmed to unfold the observed cross sections into an assigned number of Fano resonance profiles as explained below.

3. Reduction of Relative Absorption Cross Section to Fano Resonance Profiles

Inspection of the spectrum of the preceding paper indicated how many resonances were to be included between the long wavelength end of the two-electron spectrum, i.e., the line 4d6p $^3D_1^o$ at 2024Å, and the line 4d9p $^1P_1^o$ at 1722Å.

Fano's (1961) formula for an autoionized line shape, written in arbitrary units in our case, is

$$\sigma = \sigma_b + \sigma_a \frac{(q+\epsilon)^2}{1+\epsilon^2}$$

where q = "line profile index",

$$\epsilon = 2 \frac{(\nu_r - \nu)}{\Gamma},$$

with Γ = half-width of the resonance at frequency ν_r , wavelength λ_r .

σ_a represents the cross section of the unperturbed continuum which interacts with the doubly-excited state, and σ_b is the residue of continuum which does not so interact.

Equation 1 is written more conveniently for our purpose as

$$\begin{aligned}\sigma &= \sigma_b + \sigma_a + \sigma_a \left[\frac{(q+\epsilon)^2}{1+\epsilon^2} - 1 \right] \\ &= \sigma_b + \sigma_a + \sigma_\ell\end{aligned}$$

where $\sigma_\ell = \sigma_a \left[\frac{(q+\epsilon)^2}{1+\epsilon^2} - 1 \right]$ 2

represents the absorption cross section contribution by the resonance divorced from the continuum.

If σ_a becomes small in the neighbourhood of a particular resonance, the profile tends to dispersion shape, the Fano parameter q becoming indeterminate. In this case, it is more convenient to employ the parameters a and b suggested by Shore (1967), the profile being then represented by

$$\sigma = \sigma_a + \sigma_b + \sigma_\ell = (\sigma_b + \sigma_a) + \frac{a\epsilon + b}{1+\epsilon^2} \quad 3$$

the relations between a , b , q , and σ_a being generally

$$a = 2 \sigma_a q; \quad b = \sigma_a (q^2 - 1) \quad 4$$

Reference to equations (15) and (16) of Shore's (1967) paper shows that a vanishes with σ_a , but b can remain non-zero, and the σ_ℓ in (3) reduces to $b/1+\epsilon^2$, b being positive for an absorption resonance and negative for a "window".

The computer program, to be described elsewhere, has been devised by one of us (G.L.G.) and L. Toy, to perform a least-squares iteration, providing values for λ_r , Γ , σ_a and q or b , when supplied with approximate values, obtained by rough manual calculation, for the number of resonances assigned after inspection of the spectrum. Moreover, the program permits insertion of a

linear course of $(\sigma_a + \sigma_b)$ versus λ , and computes the slope. The non-interacting background continuum σ_b is thereafter obtained from the computed results by subtraction from the measured absorption cross section. In all cases, σ_a has been assumed uniform over each individual resonance; this is only seriously questionable for the strong wide absorption $5^1S_0 - 4d6p^1P_1^0$ around 1970\AA .

4. Results

The results of the photometric work and its unfolding are given in the curves of Fig. 1 and in Table 1. The points marked along the profiles are taken from the actual measured values of relative absorption coefficient, and the curve drawn in is constructed from summation of the computed profiles, for which the parameters are given in the table. Obviously, the overall agreement is excellent.

In the spectral range examined only two resonances of plate 1 in the preceding paper have been omitted. The first of these is the longest wavelength member of the 2-electron transitions, viz., $5^1S_0 - 4d6p^3D_1^0$ at 2024\AA . This line was rather too narrow for reliable measurement at the dispersion available, and additionally suffered from the proximity of an impurity line (Mg I). The other omitted feature is the very weak resonance $5^1S_0 - 4d(2^2D_{5/2})5f[\frac{1}{2}]_1^0$ at 1782\AA .

An interesting detail which has emerged from the photometric work, but was not recognizable from the photographic spectrum, occurs in the region 1860\AA , i.e., in the neighbourhood of the $5^1S_0 - 5p6s^1P_1^0$ resonance. In the spectra and tables of the paper preceding, one of the three resonances ascribed to $4dnf$ is missing from the identifications, at $n = 4$. The photometric trace of Fig. 1 of the present paper shows an undoubted secondary

peak on the long wavelength side of the $5p6s \ ^1P_1^o$ resonance, which can thus be reasonably accommodated as $4d \ (^2D_{\frac{5}{2}}) \ 4f \ [\frac{1}{2}]_1^o$. The structure of the spectrum in this region is obviously especially complicated.

The "resonance" wavelengths λ_r in table 1 conform very well with the measurements listed from the photographic work in tables 3 - 8 in the preceding paper, with the exception of the resonance $5 \ ^1S_0 - 4d6p \ ^1P_1^o$, for which the photometry gives 1970Å in place of the 1957Å estimate from the plates. The asymmetry of this very wide strong absorption feature, of course, accounts for the difference, and 1970Å (50760 cm^{-1}) is a more realistic placing for the "line center".

Little significance can be attached to the course of σ_b as represented by the lower curve traced in Fig. 1. The analysis presented is obviously of the nature of first approximation, because it assumes each resonance may be treated as interacting with one continuum which remains flat over the width of the feature concerned. A more sophisticated and much more difficult treatment of the measured values would take into account that the shape of one resonance would affect directly the background continuum presented to those adjacent. However, the results presented illustrate the successful performance of a Fano-type analysis on a fairly complex autoionized structure. It is plainly not possible to give all the detail of measured relative cross sections in this paper, but the material remains on file at Harvard College Observatory for future examination by others if required.

5. Acknowledgements

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6. References

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Fano, U. and Cooper, J.W., 1965, Phys. Rev., 137, A1364.

Shore, B.W., 1967, Rev. Mod. Phys., 39, 439.

Table 1

Resonance No.	Transition	λ Å	$\Gamma \times 10^{12}$ sec ⁻¹	σ_a arbit. units	q	b arbit. units
	5 ¹ S ₀ -					
1	4d6p ³ D ₁ ^o	2024	too narrow for analysis			
2	³ P ₁ ^o	2018	10.0			1.1
3	¹ P ₁ ^o	1970	78. ₂	0.18	-5.2	
X	6s5p ³ P ₁ ^o	1891	15. ₈	0.29	0.10	
5	4d(² D _{3/2}) 4f [^{3/2}] ₁ ^o	1878.0	3.28	0.11	4.6 ₀	
6	4d(² D _{5/2}) 4f [^{3/2}] ₁ ^o	1867.9	3.82	0.15	3.5 ₆	
Y ₁ } Y ₂ }	6s5p ¹ P ₁ ^o +	1865.5	9.3 ₃	0.07	-1.9 ₆	
	4d(² D _{3/2}) 4f [^{1/2}] ₁ ^o ?	1859.6	54. ₈	0.003	-13. ₇	
8	4d7p ³ P ₁ ^o	1827.2	9.6 ₃	0.12	2.5 ₆	
9	¹ P ₁ ^o	1810.1	132			0.84
10	4d(² D _{3/2}) 5f [^{3/2}] ₁ ^o	1791.4	12.9	0.09	-2.6 ₄	
11	4d(² D _{5/2}) 5f [^{3/2}] ₁ ^o	1780.1	14.2	0.02	4.8 ₈	
12	4d8p ³ D ₁ ^o	1772.8	3.5 ₂	0.01	7.1 ₄	
13	³ P ₁ ^o	1766.7	6.9 ₁	0.002	27. ₅	
14	¹ P ₁ ^o	1756.8	24.9	0.04	-6.2 ₇	
15	4d(² D _{3/2}) 6f [^{3/2}] ₁ ^o	1747.7	8.9 ₈	0.07	-3.1 ₉	
16	4d(² D _{5/2}) 6f [^{1/2}] ₁ ^o	1740.3	10. ₀			0.26
17	4d(² D _{5/2}) 6f [^{3/2}] ₁ ^o	1737.4	5.0			0.45
18	4d9p ³ D ₁ ^o	1735.1	2.7			0.84
19	³ P ₁ ^o	1732.2	4.6			1.4 ₇
20	4d(² D _{3/2}) 7f [^{3/2}] ₁ ^o	1723.5	5.8 ₅	0.13	3.7 ₆	
21	4d9p ¹ P ₁ ^o	1722.2	11.3	0.18	-2.5 ₄	

Figure 1 Autoionization Resonance Structure in Sr I

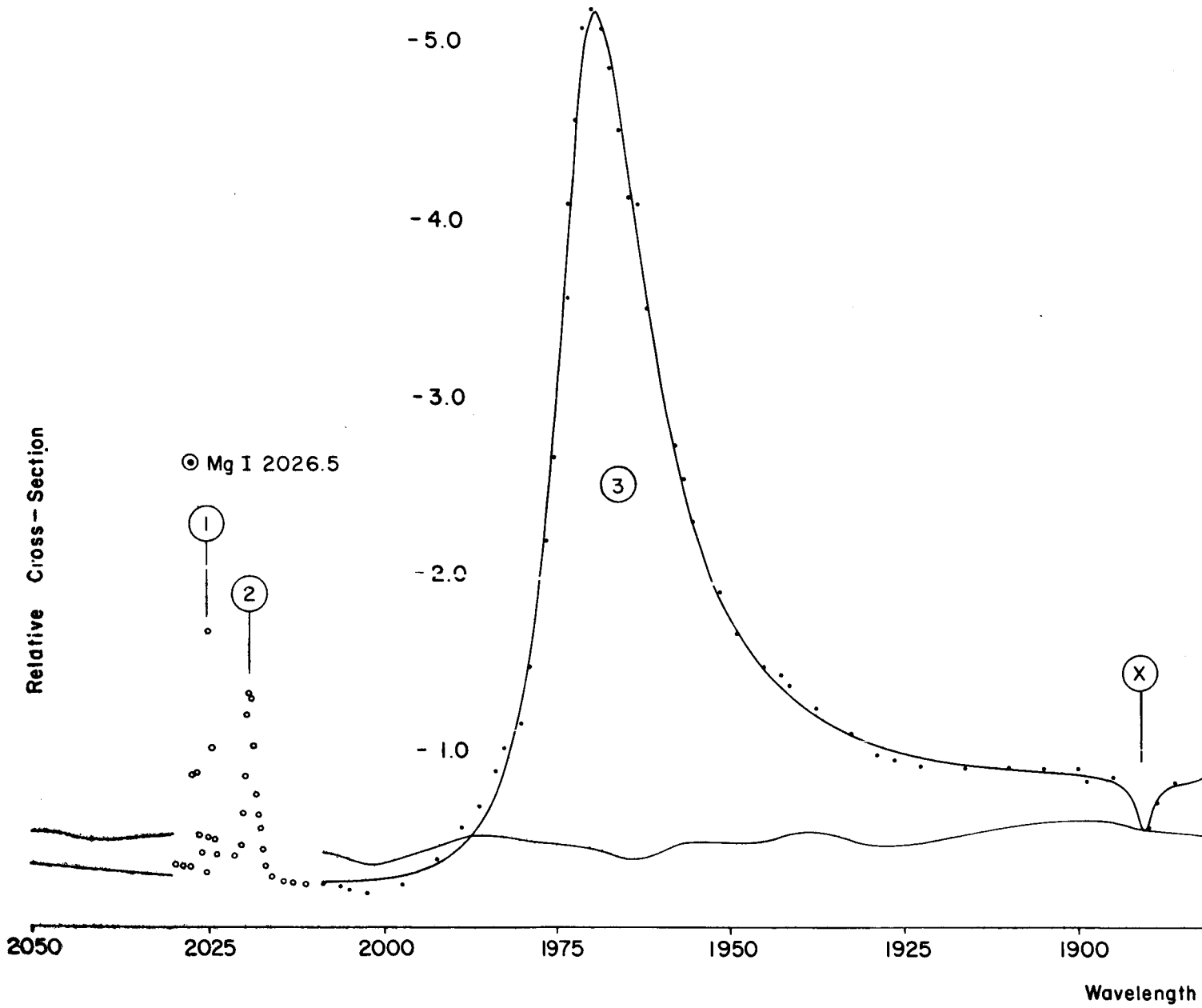


FIG. 1-1

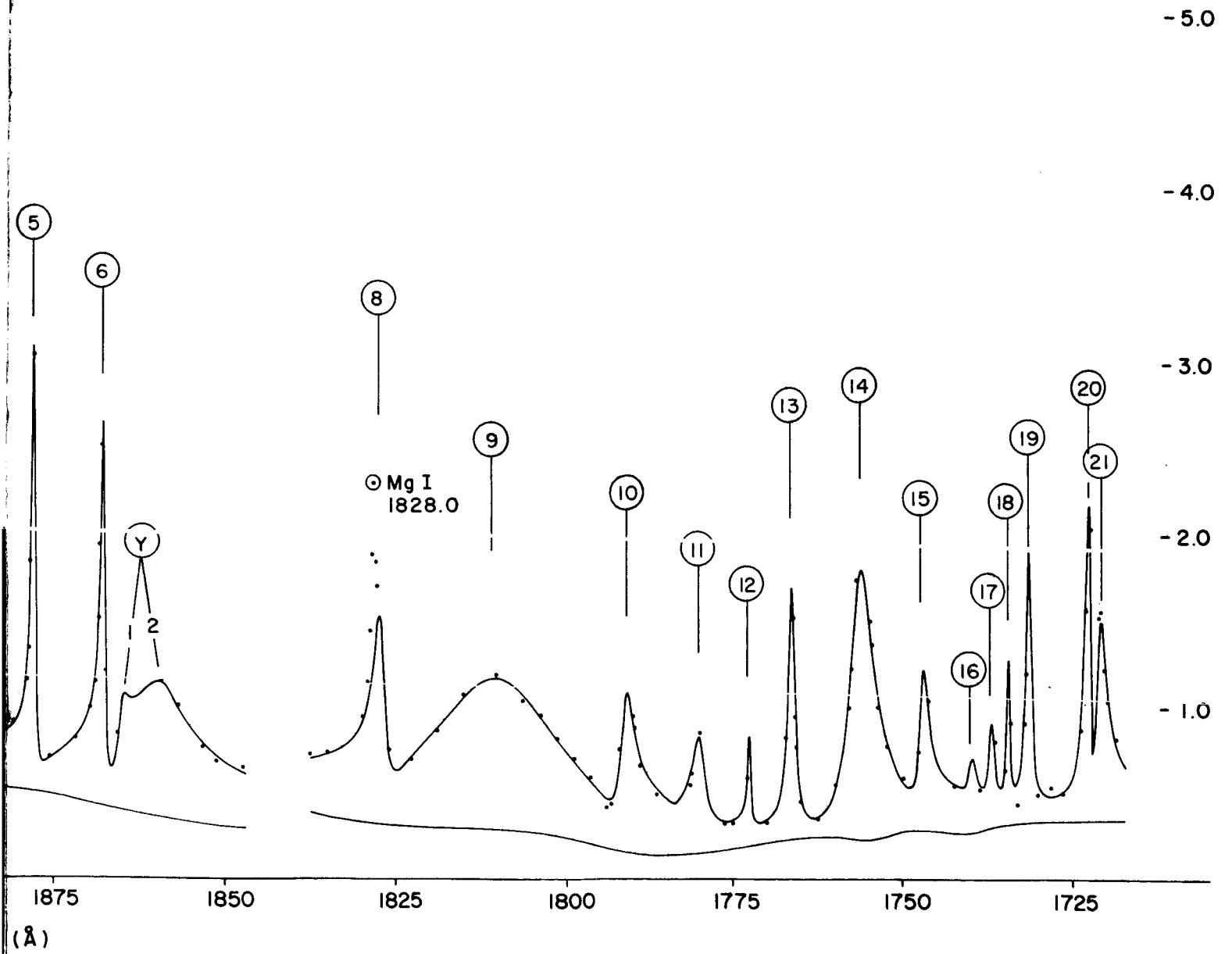


Fig. 1-2

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<p>The absorption spectrum of strontium vapor in the quartz ultraviolet and Schumann region has been obtained at good dispersion, leading to extension of the singlet principal series to $n=33$, and discovery of ninety-four lines due to double-electron transitions, most of which are classifiable within six series converging on the Sr II 2D metastable term. pronounced autoionization resonance effects occur in the Schumann region. We re-classify as $4d6p\ ^3D^o$ a triplet term previously listed as $4d6p\ ^3F^o$.</p> <p>A photoelectric spectrometer has been used to measure relative absorption cross-sections in the Sr I spectrum, over the region comprising about 22 of the autoionization resonances described in the preceding paper. The results are unfolded by a computer program into Fano-type or dispersion profiles, and values of "line-profile indices" and autoionization damping constants are derived. One additional resonance, not recognizable from the photographic spectrum, is reported.</p>			