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THE $B(^3\Sigma_u^-)$–$X(^3\Sigma_g^-)$ BAND SYSTEM OF THE Se_2 MOLECULE

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[Plates 61 to 64]

CONTENTS

A detailed rotational analysis has been carried out of a large number of bands of the *B*–*X* system of the Se_2 molecule. Isotopically pure samples of ^{78}Se and of ^{80}Se were used, and observations were made both in absorption and in emission. The analysis shows that the bands arise from a transition which, in Hund's case *b*, may be represented as $B^3\Sigma_u^-$–$X^3\Sigma_g^-$. However, in Se_2, the states approach case *c*, and the splitting constants λ'' and λ' are so large that the system divides into two subsystems: (i) $B\,0_u^+$–$X\,0_g^+$ and (ii) $B\,1_u$–$X\,1_g$, of which the former is stronger and more developed than the latter. The transitions 1_u–0_g^+ and 0_u^+–1_g have not been observed.

The correct vibrational analysis of the Se_2 bands is given for the first time, and is amply confirmed, both by the vibrational isotope effect and by the rotation analysis. The structure of all the vibrational levels in $B\,0_u^+$ possessing discrete rotational levels, from $v = 0$ to $v = 21$, has been examined. Two kinds of perturbation are recognized, one sharp and one diffuse, and two distinct sets of predissociation are observed. From the limiting curves of predissociation, the dissociation energy, D_0^0 is found to be $72{\cdot}94 \pm 0{\cdot}03$ kcal/mole. The upper state, $B\,0_u^+$, possesses a potential maximum.

Values of some of the constants derived for $^{80}Se_2$ are given below. Although a good estimate of the difference $2\lambda''$–$2\lambda' = 434{\cdot}51$ cm^{-1}, has been obtained, the absolute values of λ'' and of λ' have not been determined.

Constants for $^{80}Se_2$ (cm^{-1})

(i) $B\,0_u^+$–$X\,0_g^+$

$\nu_e = 25980{\cdot}36$
$\omega_e' = 246{\cdot}291$ $\omega_e'' = 385{\cdot}3028$
$x_e'\omega_e' = 1{\cdot}016$ $x_e''\omega_e'' = 0{\cdot}96363$
$y_e'\omega_e' = -5{\cdot}49 \times 10^{-3}$ $y_e''\omega_e'' = -8{\cdot}184 \times 10^{-4}$
$B_e' = 0{\cdot}07048$ $B_e'' = 0{\cdot}08992$
$\alpha_e' = 0{\cdot}000345$ $\alpha_e'' = 0{\cdot}000288$
$\gamma_e'' = -6{\cdot}10 \times 10^{-7}$
$D' = 4 \times 10^{-8}$ $D_v'' = 10^{-8}\,[2{\cdot}4 - 0{\cdot}023\,(v+\tfrac{1}{2})]$
$r_e' = 2{\cdot}4464$ Å $r_e'' = 2{\cdot}1661$ Å.

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(ii) $B1_u$–$X1_g$

$$\begin{array}{rlrl}
\nu_e &= 25545{\cdot}85 & & \\
\omega_e' &= 246{\cdot}42 & \omega_e'' &= 386{\cdot}43 \\
x_e'\omega_e' &= 1{\cdot}225 & x_e''\omega_e'' &= 0{\cdot}9058 \\
 & & y_e''\omega_e'' &= -13{\cdot}13\times10^{-4} \\
B_e'(F_2) &= 0{\cdot}07067 & B_e''(F_2) &= B_e''(F_3) \\
B_e'(F_3) &= 0{\cdot}07105 & &= 0{\cdot}09012 \\
\alpha'(F_2) &= \alpha'(F_3) & \alpha''(F_2) &= \alpha''(F_3) \\
 &= 0{\cdot}000553 & &= 0{\cdot}000297 \\
r_e'(F_2, F_3) &= 2{\cdot}4400\ \text{Å} & r_e''(F_2, F_3) &= 2{\cdot}1631\ \text{Å}.
\end{array}$$

INTRODUCTION

A strong system of red-degraded bands of the Se_2 molecule, which lies in the region 3250 to about 6700 Å, has been known for very many years, and has been observed in absorption, emission and in fluorescence. However, the complexity of the spectrum of the natural mixture of selenium isotopes is such that no satisfactory analysis of the system has yet been advanced and even the number of systems was in doubt at the beginning of the present work.

Olsson (1934) studied isotopic shifts, and his work was essentially confirmed by Nevin (1935). Later, Olsson (1938) gave the following equation for the origins of a few emission bands (assigned incorrectly, as 10–6, 10–5, 10–4, 9–7, 8–6) of $^{80}Se_2$ from high resolution measurements in the ultraviolet region near 3900 Å:

$$\nu = 26083 + 271{\cdot}1(v'+\tfrac{1}{2}) - 2{\cdot}19(v'+\tfrac{1}{2})^2 - 391{\cdot}9(v''+\tfrac{1}{2}) + 1{\cdot}04(v''+\tfrac{1}{2})^2.$$

The agreement between calculated and observed isotopic shifts between $^{80}Se_2$ and $^{80}Se^{78}Se$ was not satisfactory, but no better vibrational numbering was found. The rotational analysis of bands of $^{80}Se_2$ showed that they possessed single R and P branches, and that lines of odd J'' were absent. Olsson therefore concluded that the transition is $^1\Sigma_u^+$–$^1\Sigma_g^+$. Rosen (1939) summarized his extensive work on the absorption, emission and fluorescence spectra of Se_2 and found that the bands between 2800 and 5200 Å constituted a single system, in agreement with the conclusions of Asundi & Parti (1937), who gave the following equation for the band-heads:

$$\nu = 26035 + 281{\cdot}11(v'+\tfrac{1}{2}) - 2{\cdot}65(v'+\tfrac{1}{2})^2 - 391{\cdot}77(v''+\tfrac{1}{2}) + 1{\cdot}06(v''+\tfrac{1}{2})^2 - 0{\cdot}002(v''+\tfrac{1}{2})^3.$$

It was not easy to accept the conclusion from the rotational analysis that the ground state is $^1\Sigma_g^+$. Some observations (Bhatnagar, Lessheim & Khanna 1937) suggested that the vapour of selenium was paramagnetic, although the partial pressure of Se_2 was unknown. Massen, Weigts & Poulis (1964) studied the temperature dependence of the magnetic susceptibility of saturated selenium vapour and concluded that the Se_2 component is paramagnetic. This indicates that the ground state is $^3\Sigma_g^-$. Rosen (1939), Asundi & Parti (1937) and others also suggested that the main system of Se_2 must be $^3\Sigma_u^-$–$^3\Sigma_g^-$ by analogy with O_2 and S_2. Davis & Jenkins (1951) were the first to use separated isotopes of selenium in a high resolution study of the rotational structure of some of the emission bands in the ultraviolet region. Davis (1954) concluded that the transition is $^1\Sigma_u^+$–$^1\Sigma_g^+$, and found that perturbations in the upper state affected the isotopic shifts.

The possibility of reconciling the simple singlet structure of the ultraviolet emission bands of selenium with the paramagnetic susceptibility expected for a $^3\Sigma$ state was provided by studies of the structures of the $^3\Sigma^-$ ground states of the related molecules S_2 (Barrow & Ketteringham 1963) and SeO (Barrow & Deutsch 1963), and, more recently, TeO (Chandler, Hurst & Barrow 1965). The rotational energy levels of a $^3\Sigma$ state in

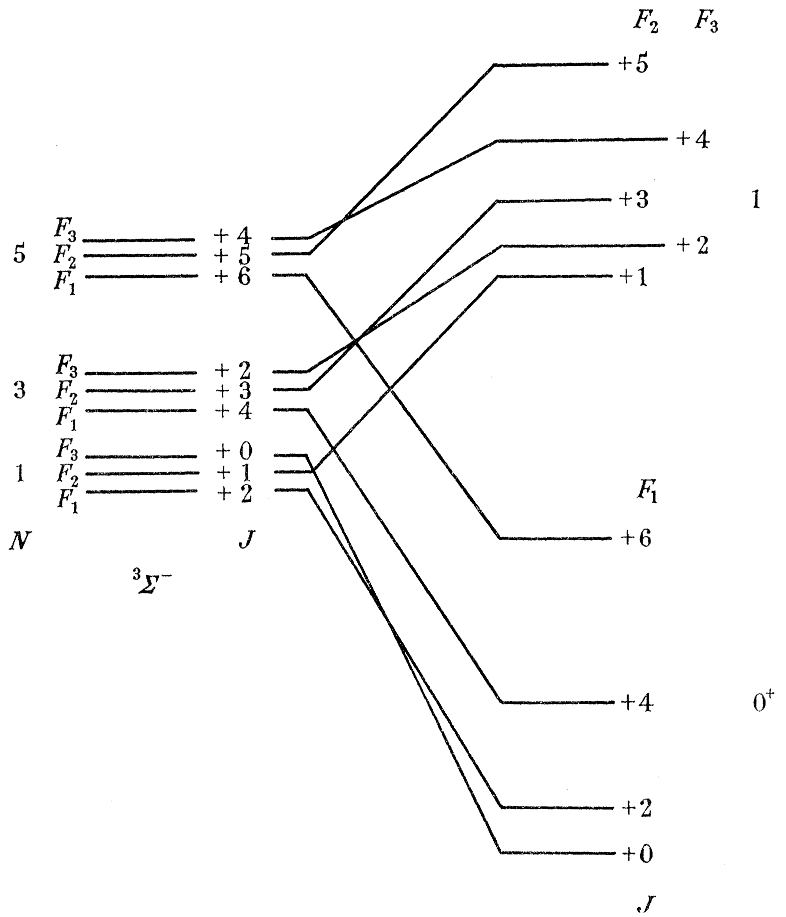


Figure 1. The correlation between the rotational levels of a $^3\Sigma_g^-$ state and the case $c\,0_g^+$ and $1g$ states for a homonuclear molecule with zero nuclear spin.

Hund's case *b* are given to sufficient approximation (Herzberg 1950; additional small terms, irrelevant here, are given by Townes & Schawlow 1955) as follows:

$$\begin{aligned} F_1(N) &= BN(N+1)+(2N+3)\,B-\lambda-[(2N+3)^2\,B^2+\lambda^2-2\lambda B]^{\frac{1}{2}}+\gamma(N+1), \\ F_2(N) &= BN(N+1), \\ F_3(N) &= BN(N+1)-(2N-1)B-\lambda+[(2N-1)^2B^2+\lambda^2-2\lambda B]^{\frac{1}{2}}-\gamma N, \end{aligned}$$

where, for F_1, $J = N+1$, for F_2, $J = N$, and for F_3, $J = N-1$. Of the two magnetic splitting constants it is commonly observed that $\lambda \gg \gamma$: for example, in the level $v = 6$ of the ground state $X^3\Sigma_g^-$ of S_2, $\lambda = 12{\cdot}23$, $\gamma = -0{\cdot}0067\ \mathrm{cm}^{-1}$. In what follows, we will assume γ to be negligibly small. The values of λ for the ground states of O_2 (Townes & Schawlow 1955), SO (Powell & Lide 1964), S_2 and SeO are, respectively, 1·985, 5·276, 11·65 and 86·4 cm^{-1}. λ therefore increases dramatically with atomic number for the ground states of these related molecules, and, for the heavier members, assumes values of the order expected for spin-orbit coupling constants. We can expect that the value of λ for $X^3\Sigma_g^-$ in Se_2 will be of the order of 100 cm^{-1} or more.

As λ^2 becomes large compared with $4N^2B^2-2B\lambda$, the F_1 levels of a $^3\Sigma^-$ state form a state with $\Omega = 0^+$, and the F_2, F_3 levels converge to form the doublets of a state with $\Omega = 1$. To a first approximation, and neglecting higher terms,

$$F_1(^3\Sigma^-) \rightarrow F(0^+) = BJ(J+1)-2\lambda,$$
$$F_2, F_3(^3\Sigma^-) \rightarrow F(1) = BJ(J+1).$$

The correlation between case *b* (λ small) and case *c* (λ large) is illustrated in figure 1 for the case of a $^3\Sigma_g^-$ state of a homonuclear molecule with zero nuclear spin. Here, as in the case of $^{78}Se_2$ or $^{80}Se_2$, only the levels with odd values of N will exist in a $^3\Sigma_g^-$ state. We will then expect to find, in a $^3\Sigma_u^-$–$^3\Sigma_g^-$ transition of such a molecule where λ' and λ'' are both large, two sub-systems, (i) 0_u^+–0_g^+, with single R and P branches, and even values of J'', and (ii) 1_u–1_g, containing single staggered R and P branches with both even and odd values of J''. This proves to be the pattern of the B–X systems of $^{78}Se_2$ and of $^{80}Se_2$.

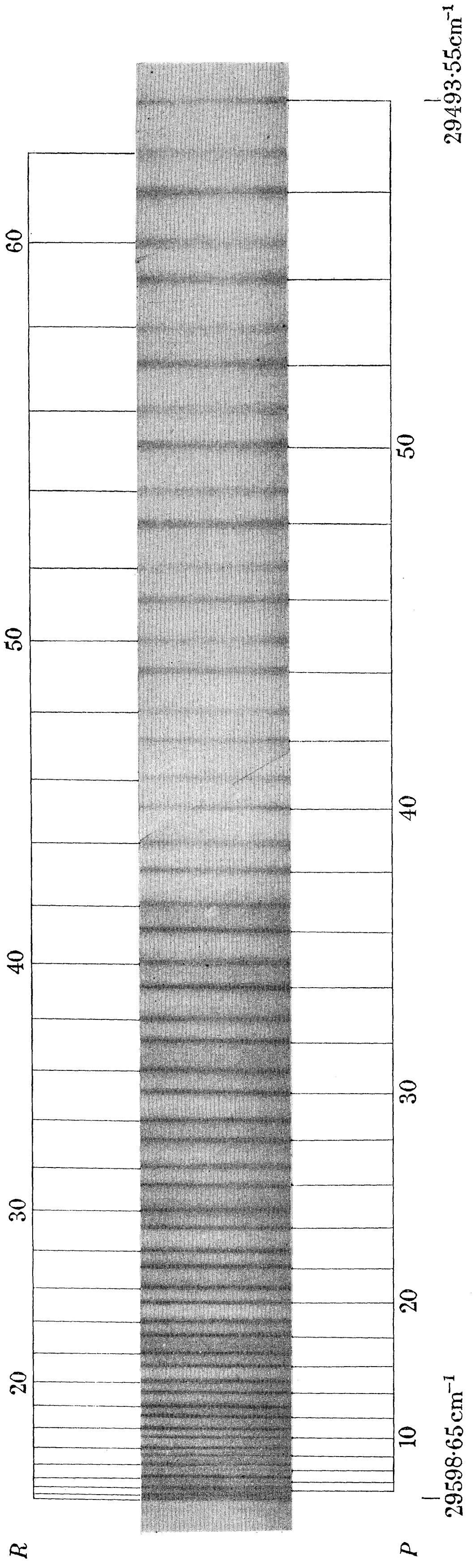
EXPERIMENTAL

Electromagnetically separated samples of ^{78}Se and of ^{80}Se (of isotopic purity $\geqslant 96\,\%$) were used for the work both in emission and in absorption. For the emission experiments, which were carried out at the University of California, Berkeley, a few milligrams of selenium were heated to about 650 °C in an evacuated quartz tube, and the spectrum was excited by a microwave generator. High resolution plates were taken on a 20 ft. plane grating spectrograph giving reciprocal plate dispersions of about 0·4 Å/mm in 9th order in a region around 6100 Å and 0·2 Å/mm in 15th order in a region around 3800 Å. Some lower dispersion plates were taken on a 21 ft. concave grating spectrograph giving 1·3 Å/mm in 1st order in the range 3600 to 5100 Å and 0·7 Å/mm in 2nd order between 4500 and 6200 Å. Kodak 103 aO and 103 aF plates were used.

For the absorption experiments, about $2{\cdot}5\times10^{-4}$g of selenium was placed in a sealed quartz tube 22 cm long and diameter 1 cm, provided with a side arm about 12 cm long. The main tube and the end windows were heated as evenly as possible. The minimum temperature required for observation of absorption bands from low vibrational levels in the ground state proved to be 400 °C. For the observation of bands at higher values of v'', temperatures up to 800 °C were used, with side-arm temperatures up to 500 °C. Photographs were taken in the region 3200 to 4550 Å in a third order of a 6·65 m concave grating spectrograph at Oxford University. The reciprocal plate dispersion was about 0·3 Å/mm. A 900 W xenon lamp was used as source of continuum, and satisfactory exposures were obtained in 2 to 6 min on Ilford N 50 plates. Thorium or iron arc standards were used, and the measurements were converted to wavenumbers in the usual way.

ANALYSIS OF BANDS OF THE SUBSYSTEM $B\,0_u^+$–$X\,0_g^+$

Bands of this system are strong, both in emission and in absorption. The ground state levels were found to be regular, but the upper state is extensively perturbed and also predissociated in several levels. All vibrational levels in $B\,0_u^+$ possessing discrete rotational



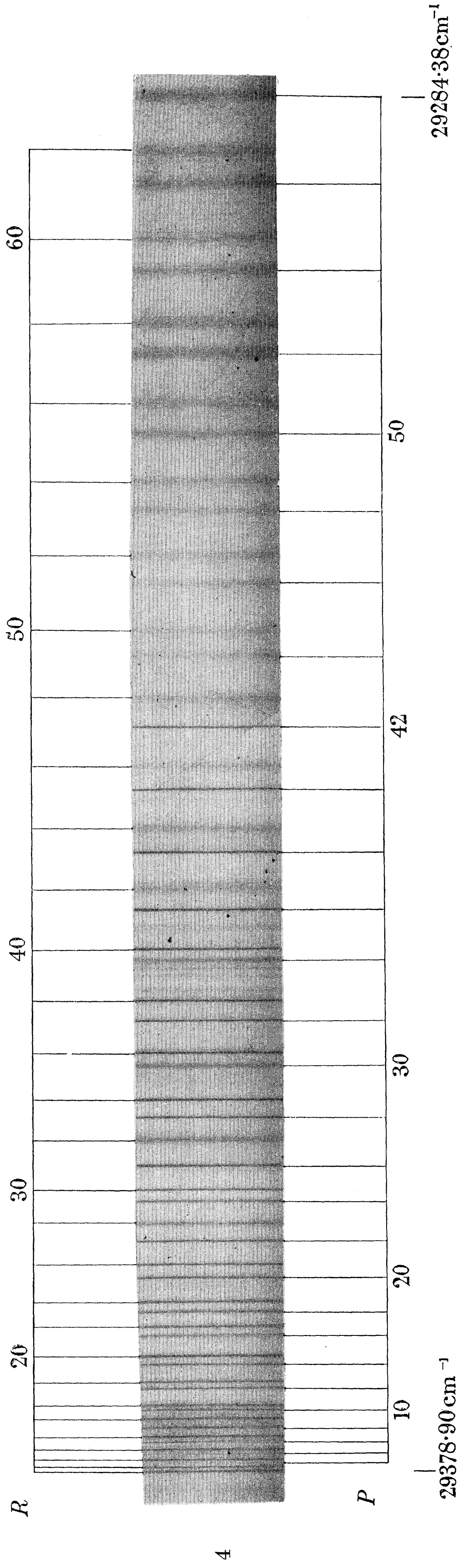


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FIGURE 2. The 16–0 band of the system $B0_u^+–X0_g^+$ of $^{78}\mathrm{Se}_2$ observed in absorption.

FIGURE 4. The 15–0 band of the system $B0_u^+–X0_g^+$ of $^{78}\mathrm{Se}_2$ observed in absorption.

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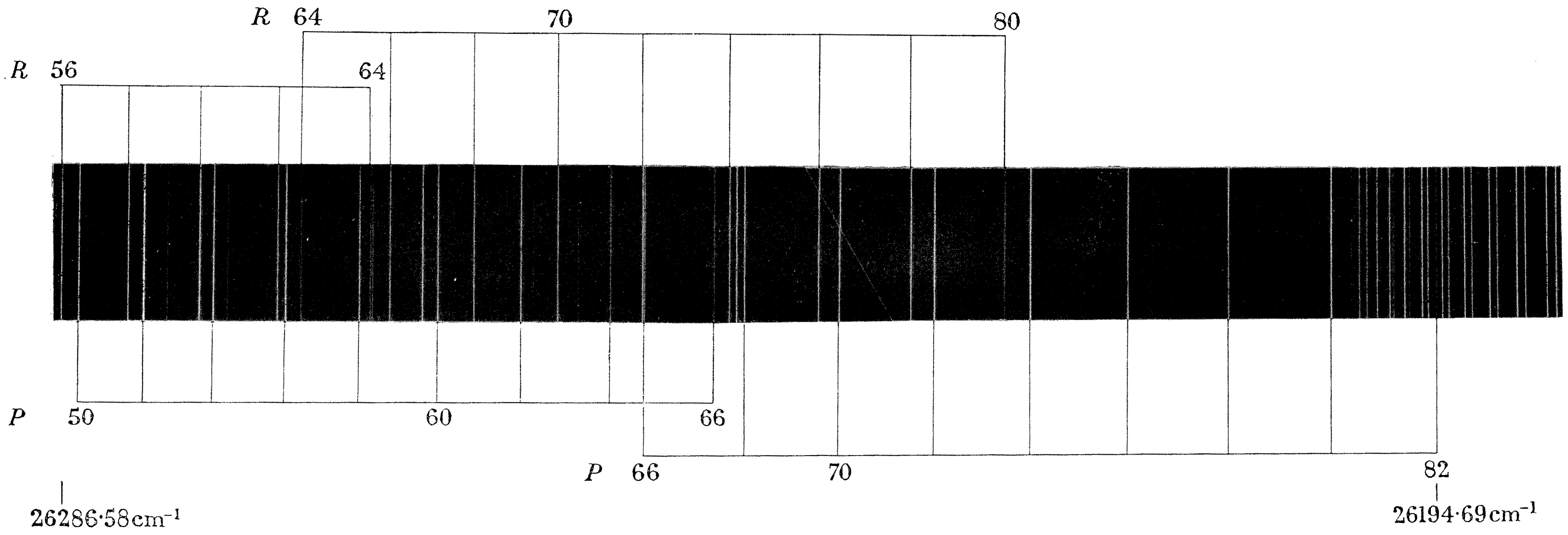

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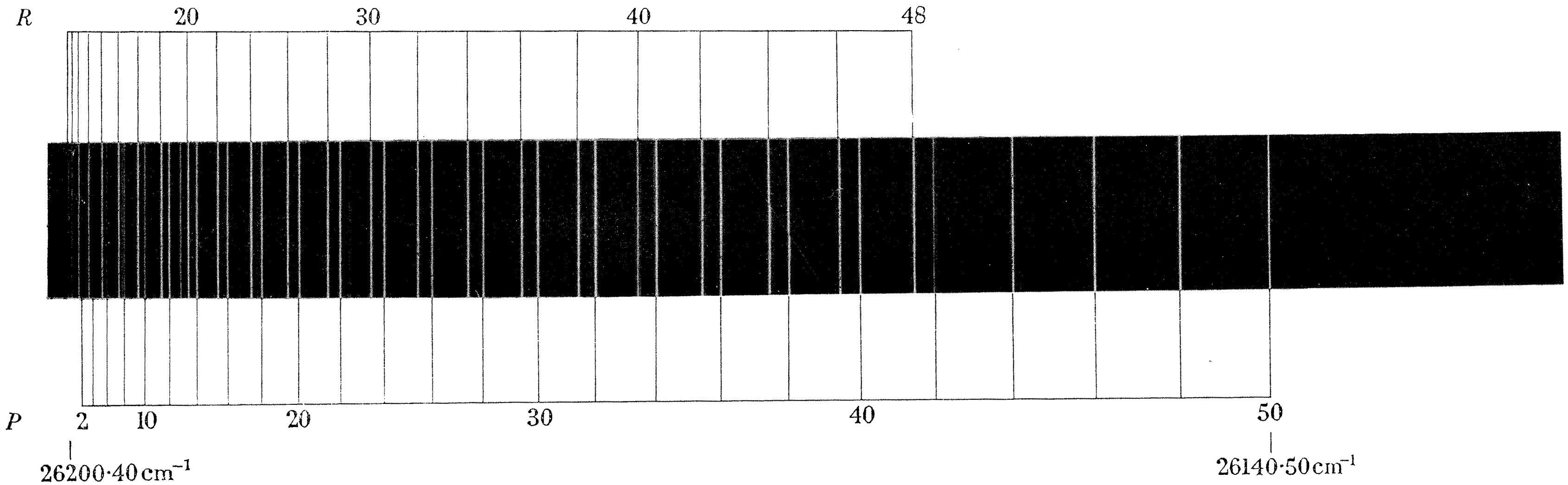

FIGURE 5. The 5–2 band of the system $B\,0_u^+–X\,0_g^+$ of $^{80}Se_2$ observed in emission.

FIGURE 6. The 6–3 band of the system $B\,0_u^+–X\,0_g^+$ of $^{80}Se_2$ observed in emission.

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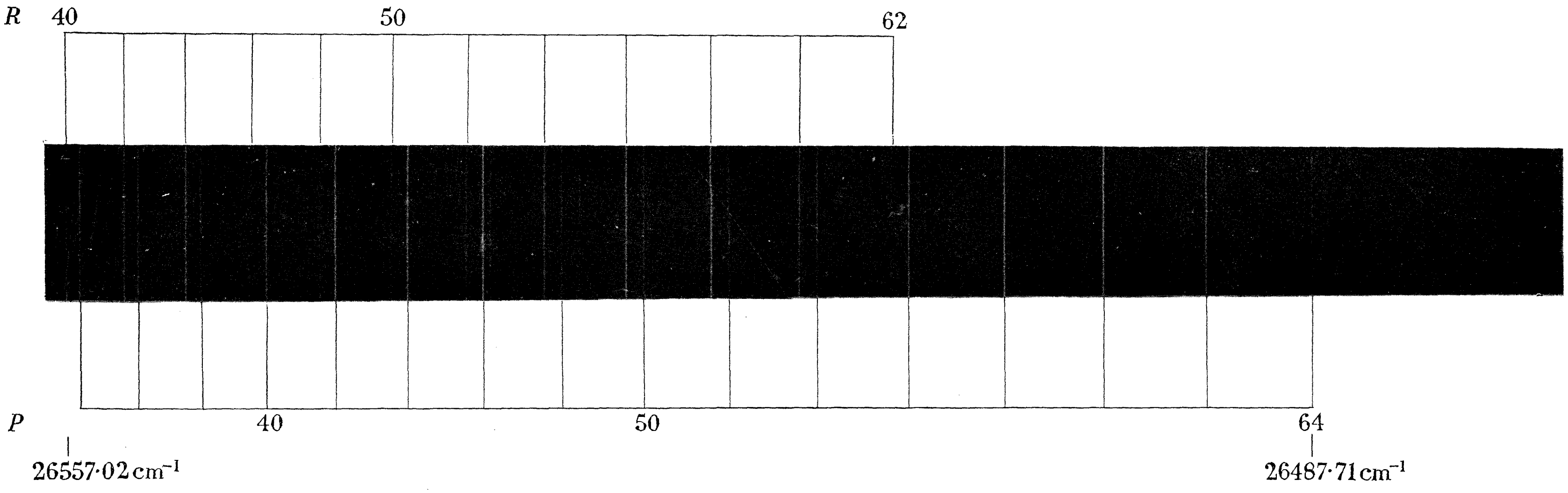

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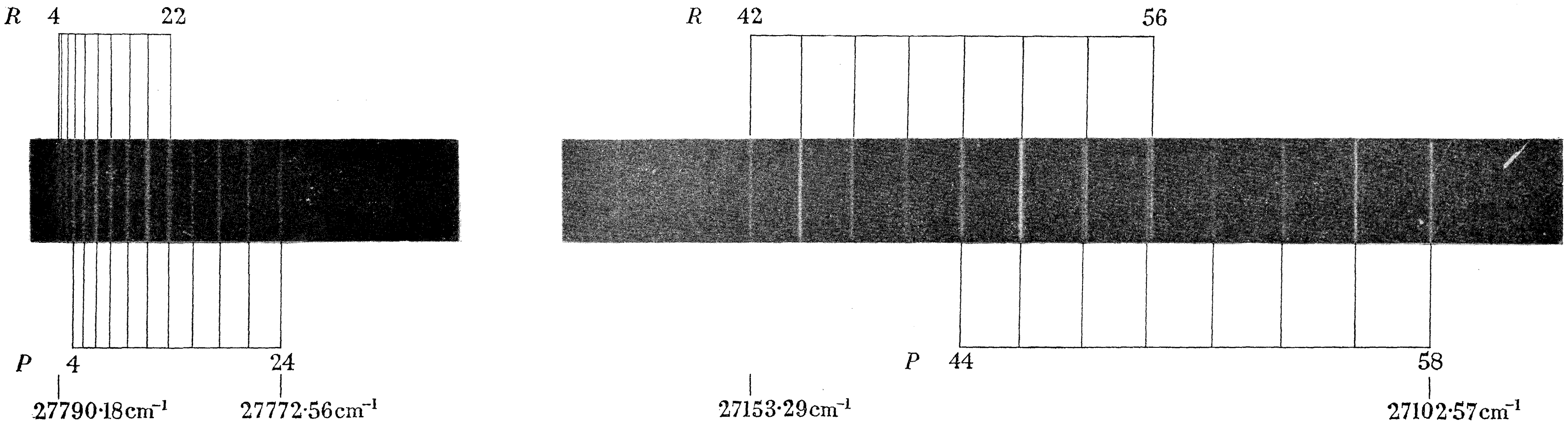

(*a*) (*b*)

FIGURE 7. The 6–2 band of the system $B0_u^+$–$X0_g^+$ of $^{78}Se_2$ observed in emission.

FIGURE 8. (*a*) The 13–3, (*b*) the 12–4 bands of the system $B0_u^+$–$X0_g^+$ of $^{78}Se_2$ observed in emission.

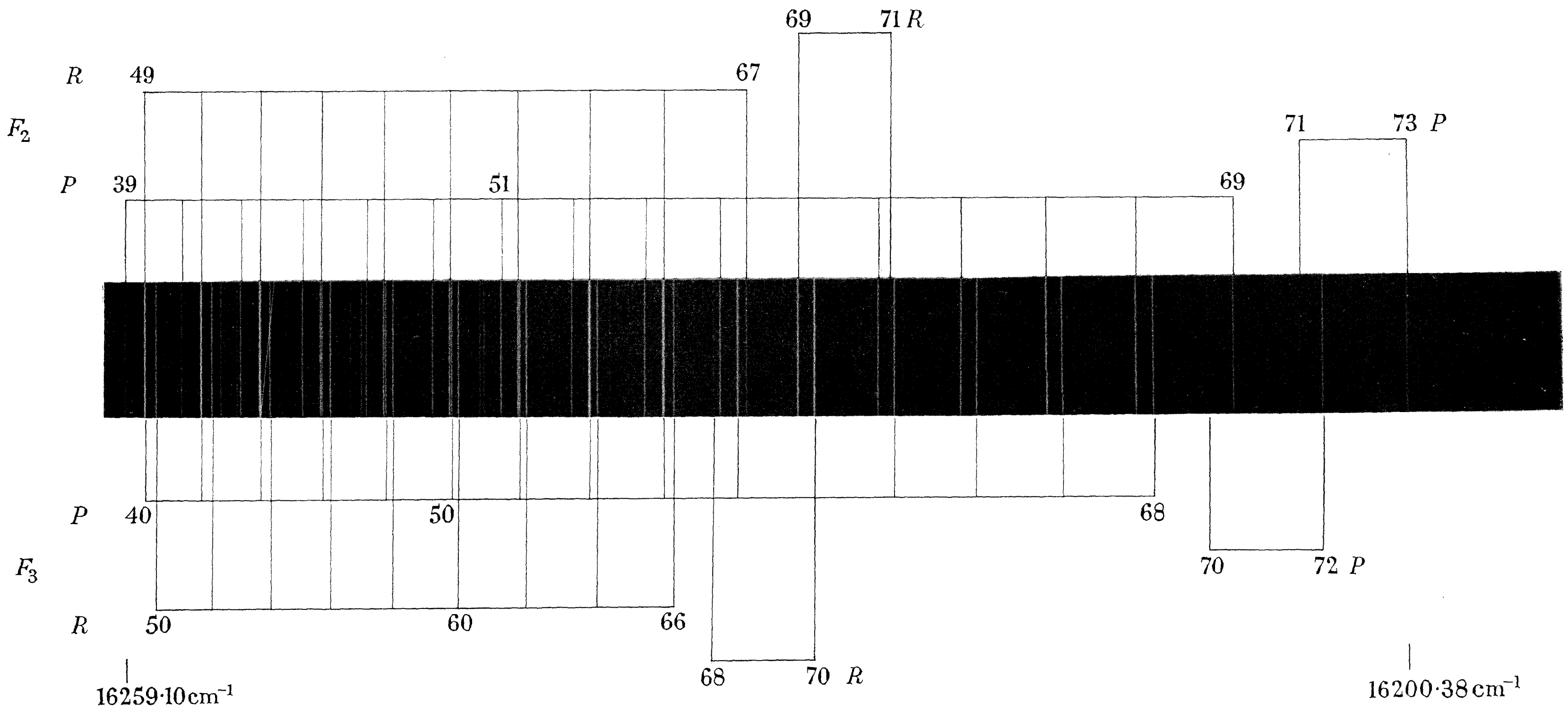

FIGURE 12. The 5–29 band of the system $B1_u$–$X1_g$ of $^{80}Se_2$ observed in emission.

levels have been analysed, both in $^{78}Se_2$ and in $^{80}Se_2$ and individual features are summarized in table 1. Values of $\Delta_2F''(J)$ for $v = 0$ in $X\,0_g^+$, $^{78}Se_2$, are given in the appendix, table A1 and wavenumbers of lines of $^{78}Se_2$ and of $^{80}Se_2$ in tables A3 and A4. Some comments on the levels in $B\,0_u^+$ follow.

Table 1. A summary of features observed in the state $B\,0_u^+$

			values of J at		
v	observed in absorption (A) emission (E)	range of J analysed	(i) diffuse perturbation	(ii) perturbation	(iii) predissociation
		$^{78}Se_2$			
15	A	1–67	16, 24, 30, 34	—	42
14	A	3–71	24, 36, 40, 46, 56, 64	—	72
13	A	3–87	36, 54, 66, 88	—	24
	E	3–23	—	—	—
12	A	3–79	34, 64	80	—
	E	43–55	—	—	—
11	A	3–79	58, 80	—	—
	E	5–27	—	—	—
10	A	11–107	70, *ca.* 114	—	—
9	A	5–37		diffuse throughout	
8	A	7–67	68	—	—
7	A	7–67	64	—	—
6	E	5–63	—	—	46
5	A	7–93	—	70	78
	E	7–77	—	—	—
4	A	9–87	—	60, 74	—
3	A	11–89	—	34	—
2	A	11–89	—	—	—
1	A	13–73	—	*ca.* 74	—
0	A	29–95	—	28, 68	—
		$^{80}Se_2$			
15	A	7–49	8, 22, 34, 46	—	50
14	A	3–77	20, 34, 48, 54, 58, 66	—	78
13	A	3–95	42, 58	72	34, 96
12	A	45–79	44, 68, 80	—	—
11	A	5–77	54, 78	—	—
10	A	37–99	38, *ca.* 74	—	—
9	A	7–49	diffuse throughout		
8	A	7–55	diffuseness increases at $J' > 38$		
7	A	7–71	72 diffuseness initially decreases at $J' > 6$		
6	E	1–49	—	—	50
5	E	1–81	—	66	82
4	E	3–105	—	40, 54	106
3	A	19–91	—	18	—
2	A	11–97	—	—	—
1	A	15–93	—	68	—
0	A	25–89	—	24, 66, *ca.* 90	—

(*a*) $v = 22$ *to* $v = 16$

These levels are observed only in absorption, and appear, for each isotope, by transitions from $v'' = 0$ at the ultraviolet end of the system. There are no rotational perturbations in the range $0 \leqslant J \lesssim 60$, but in each level the line width increases with J to such an extent that accurate measurement of lines with $J > 60$ becomes impossible (see figure 2, plate 61). The diffuseness also increases with v, so that the level $v = 21$ is the last to show rotational structure, and the 22–0 band appears only as an absorption continuum with a short wavelength head at low dispersion.

(*b*) $v = 15$ *to* $v = 0$: *perturbations*

Perturbations are found throughout these levels, but few extra lines are observed so that little information can be derived about the perturbing states. One exception is the perturbation at $J \sim 66$ in $v = 5$ of $B\,0_u^+$, illustrated in figure 3. From the crossing-point in the plot of $\Delta_2F/(J+\frac{1}{2})$ against J, the B value of the perturbing state is estimated to be about 0·055 cm^{-1}. It is indeed characteristic of the perturbations that in all cases B (perturbing state) $< B_v$ of $B\,0_u^+$. The distribution of the perturbations is significant. This shows that the potential energy curve of the perturbing state extends at least as low as $v = 0$ in $B\,0_u^+$. Secondly, the number of perturbations observed in each vibrational level increases with v until $v = 15$; no perturbations are observed at $v > 15$. This indicates that the vibrational levels of the perturbing state converge to a dissociation limit close to the level $v = 15$ or 16 in $B\,0_u^+$.

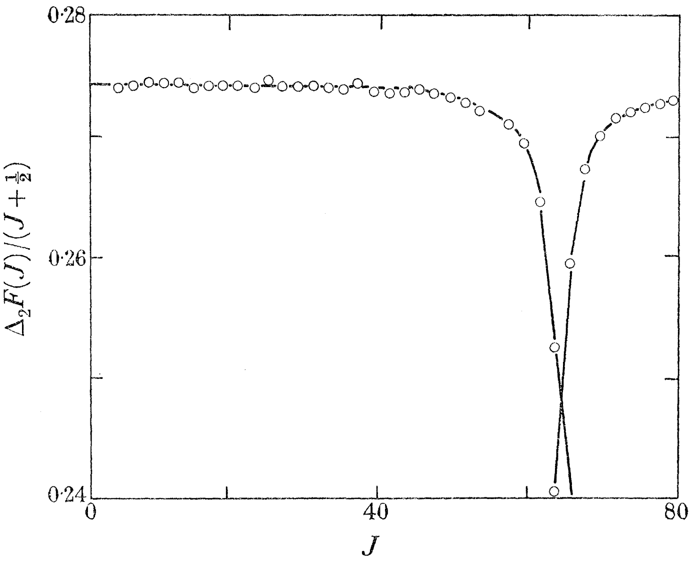

FIGURE 3. $\Delta_2F(J)/(J+\frac{1}{2})$ is plotted against J for $v = 5$ in $B\,0_u^+$ of $^{80}Se_2$, illustrating the perturbation at $J \sim 66$.

(*c*) $v = 15$ *to* $v = 7$: *diffuse perturbations*

These levels are distinguished by the presence of groups of diffuse lines in absorption. The diffuseness often, but not invariably, accompanies the line displacement characteristic of a perturbation. Diffuse perturbations which appear in $v = 15$ before a predissociation are illustrated in figure 4, plate 61. It is suggested that these are accidental predissociations in which the perturbing state is predissociated by a third unstable state to which direct radiationless transfer from $B\,0_u^+$ is forbidden. The effect in emission is that some lines have reduced or zero intensity and in absorption these transitions give diffuse lines: the energy shifts of the levels may be negligibly small. In some cases, for example in $v = 10$ and 12 of $B\,0_u^+$ for $^{80}Se_2$, the lines are so diffuse that no analyses were found at J values below that of the perturbation.

(*d*) *Predissociations*

(i) $v = 15$, 14 *and* 13

In absorption, these levels show sharp increases in diffuseness at certain J values for each isotope, above which all the lines are diffuse and become broader with increasing J. No perturbations have been observed after the onset of diffuseness. These effects arise from predissociation, and occur at decreasing values of J for increasing values of v. A limiting curve of predissociation may be drawn which indicates that the levels $v \geqslant 16$ should be completely predissociated. The effect in $v = 15$ of $B0_u^+$ in $^{78}Se_2$ is illustrated in figure 4, plate 61. The lines at low J in $v = 15$ are indeed much sharper than those in $v = 16$ (see figure 2). In table 1, the predissociations are indicated at even values of J, intermediate between the last sharp (odd J) level and the first diffuse level.

(ii) $v = 6$, 5 *and* 4

Observations of $^{80}Se_2$ show that these levels are sharply predissociated in emission. The predissociations have been carefully differentiated from perturbations by (*a*) the regularity of the rotational term values to the point of cut-off, (*b*) the absence of lines at higher values of J in different bands with common values of v'. The predissociation at $J = 50$ in $v = 6$ was earlier recognized by Olsson (1938) and by Davis (1954), but their assignment of this level as $v = 10$ is shown below to be incorrect. In absorption the first level to appear diffuse is $J = 55$, and the line width reaches a maximum, with no perturbation, at $J = 65$.

The predissociations in $v = 5$ and 4 were not previously identified because the rotational structure at lower J values in these levels is confused by perturbations. The analysis of the perturbation, and the predissociation, in $v = 5$ is illustrated in figure 5, plate 62. In $v = 4$, perturbations are observed at $J \sim 40$ and 54; regular structure then extends to a sharp predissociation at $J \sim 106$.

For $^{78}Se_2$, the predissociations are less pronounced. In $v = 6$ there is a sharp drop in the emission intensity at $J = 46$, but the branches continue and their intensity rises to a normal value at about $J = 59$. There follows a slow decrease of intensity, and lines with $J > 62$ are absent. No perturbations are observed throughout this range of J. In absorption the lines $R(48)$ and $P(50)$ are somewhat stronger than normal, and this may reflect a slight broadening.

In $v = 5$ the observation of predissociation is complicated by a perturbation at $J \sim 70$. However, in absorption the branches continue strongly after the perturbation, and unequivocal assignments of emission lines may be made. The last R line in emission is $R(74)$, but P lines are found up to $P(78)$. The emission bands are here very free from overlapping, and later lines would surely have been observed if present. It is concluded that this level is predissociated at $J \sim 78$.

In addition to these predissociations Davis (1954) reported the weakening in emission of single R and P lines in $v = 6$ for the three species $^{77}Se_2$, $^{78}Se_2$ and $^{80}Se_2$ and suggested that these might be caused by accidental predissociations. For $^{80}Se_2$ the weak lines are $R(40)$ and $P(42)$. The new spectrograms show that these lines are in fact split into two components, perhaps by a perturbation. For $^{78}Se_2$ the weak lines are $R(36)$ and $P(38)$ and our observations confirm this. For neither isotope is any effect noticed in absorption in this region, perhaps because of the overlapping of branches. The weakening of these single lines and the predissociations in $v = 6$ for $^{80}Se_2$ and $^{78}Se_2$ may be compared in figure 6, plate 62 and figure 7, plate 63 respectively.

(iii) $v = 13, 12, 11$ *and* 7

From the predissociations in $v = 6$, 5 and 4 a limiting curve may be drawn which indicates that $v > 6$ should not appear in emission. Such bands have, however, been reported. Rosen (1939) found that $v = 7$ was present but weak, $v = 8$ appeared strongly in emission and resonance spectra; $v = 9$ was very weak; $v \geqslant 10$ did not appear. Olsson (1938) found no trace of $v \geqslant 7$. To check these observations Davis (1954) searched for $v = 7$ and 8 on heavily exposed plates using separated isotopes and high dispersion. He found and analysed very weak 7–2 and 7–3 bands but only for one species, $^{77}Se_2$; he found no bands from $v = 8$. The evidence of this high dispersion work must be accepted in preference to Rosen's low dispersion studies on natural selenium; he gave no rotational analysis so that his identifications cannot be checked.

On the present emission plates no bands for $7 \leqslant v \leqslant 10$ appear. But several bands arising from $v = 11$, 12 and 13 occur weakly on the low dispersion plates in emission. Analysis was only possible for $^{78}Se_2$ because the similar region for $^{80}Se_2$ was overlapped by impurity bands.

(*a*) $v = 13$. The bands are very short and show sharp cutoffs assigned as a predissociation at $J' = 24$. In absorption the $R(26)$ and $P(28)$ are the first diffuse lines—revealed by a marked increase in intensity—in agreement with the usual observation that diffuseness in absorption is a less sensitive test for predissociation than cutoff in emission. The diffuseness increases thereafter and reaches a maximum at $J = 36$ where there is a perturbation. It is concluded that there is a predissociation at $J \sim 24$ and a diffuse perturbation at $J = 36$.

(*b*) $v = 12$. The emission bands are headless since only lines for $43 \leqslant J \leqslant 57$ occur. The absence of lines in emission is here ascribed to accidental predissociations—in absorption there are diffuse perturbations at $J = 34$ and 64 so that the emission cutoffs occur about eight rotational levels from the centres of perturbation.

(*c*) $v = 11$. The emission bands are short but no common cutoff point is observed so the absence of further lines is ascribed to accidental predissociations. Emission bands for $v = 12$ and 13 of $^{78}Se_2$ are illustrated in figure 8, plate 63.

Determination of rotational constants

Values of the ground state constants were determined, over the whole range of observed values of J, by a least squares method on the Oxford KDF 9 computer. The results are given in table 2 with derived rotational constants; the error estimates, here and elsewhere in this paper, are one standard error. Parentheses denote values where the value of D is clearly incorrect: this occurs when both branches are blended throughout the band, giving a systematic rather than a random error.

Since the upper state is perturbed, the constants for this state have been found where possible from values of ΔB and ΔD in what appear to be unperturbed regions by multiple linear regression on the line given by

$$R(J)+P(J) = 2\nu_0+2B'+2(B'-B'')J(J+1)-2(D'-D'')J^2(J+1)^2.$$

A plot of B_v against v for $B\,0_u^+$ revealed that, for each isotope there is a marked change of slope for $v > 15$: values above this could not be fitted to the expression

$$B_v = B_e - \alpha_e(v+\tfrac{1}{2}) + \gamma_e(v+\tfrac{1}{2})^2.$$

Table 2. Rotational constants for $X\,0_g^+$ (cm^{-1})

	^{80}Se$_2$		^{78}Se$_2$	
v	$10^2\,B$	$10^8\,D$	$10^2\,B$	$10^8\,D$
0	8·976 ± 0·006	2·0 ± 1·3	9·206 ± 0·004	2·0 ± 0·6
1	8·950 ± 0·004	2·7 ± 1·0	9·170 ± 0·004	1·8 ± 0·6
2	8·920 ± 0·007	2·8 ± 1·2	9·145 ± 0·007	2·4 ± 1·9
3	8·890 ± 0·004	2·2 ± 0·5	9·115 ± 0·009	2·0 ± 1·5
4	8·859 ± 0·005	2·3 ± 0·8	(9·008 ± 0·013	− 8·1 ± 2·1)
5	8·825 ± 0·007	1·9 ± 1·0	9·054 ± 0·009	2·4 ± 1·5
6	—	—	(9·034 ± 0·049	20·3 ± 88·7)
7	(8·731 ± 0·010	−0·5 ± 1·2)	8·979 ± 0·009	1·2 ± 1·1
8	8·744 ± 0·010	2·4 ± 1·5	8·959 ± 0·010	0·6 ± 1·9
29	8·089 ± 0·005	1·7 ± 0·6	—	—
30	8·059 ± 0·005	1·6 ± 0·5	—	—
31	8·026 ± 0·004	1·7 ± 0·6	—	—

		calculated from ^{80}Se$_2$
$B_e = 0{\cdot}08992 \pm 0{\cdot}00001$	$B_e = 0{\cdot}09219 \pm 0{\cdot}00002$	0·09223
$\alpha_e = 0{\cdot}000288$	$\alpha_e = 0{\cdot}000299$	0·000299
$\gamma_e = -6{\cdot}1 \times 10^{-7}$	$\gamma_e = -6 \times 10^{-7}$	—
$D_v = 2{\cdot}4 \times 10^{-8} - 0{\cdot}023 \times 10^{-8}\,(v+\frac{1}{2})$	$D = 1{\cdot}8 \times 10^{-8}$	—
$r_e = 2{\cdot}1659 \pm 0{\cdot}0001$ Å	$r_e = 2{\cdot}1663 \pm 0{\cdot}0002$ Å	—

Table 3. Rotational constants for $B\,0_u^+$ (cm^{-1})

	^{80}Se$_2$	^{78}Se$_2$
v	$10^2\,B$	$10^2\,B$
0	7·032 ± 0·005	7·241 ± 0·028
1	7·000 ± 0·010	7·167 ± 0·010
2	6·962 ± 0·007	7·138 ± 0·009
3	6·925 ± 0·005	7·120 ± 0·009
4	6·887 ± 0·005	7·075 ± 0·009
5	6·857 ± 0·005	7·026 ± 0·005
6	6·826 ± 0·005	6·993 ± 0·005
7	6·794 ± 0·004	6·945 ± 0·007
8	6·752 ± 0·004	6·920 ± 0·004
9	6·719 ± 0·004	6·862 ± 0·004
10	6·774 ± 0·006	6·930 ± 0·004
11	6·678 ± 0·005	6·837 ± 0·004
12	6·583 ± 0·019	6·834 ± 0·004
13	6·615 ± 0·005	6·776 ± 0·004
14	6·536 ± 0·007	6·686 ± 0·004
15	6·460 ± 0·011	6·636 ± 0·007
16	6·471 ± 0·006	6·629 ± 0·004
17	6·424 ± 0·006	6·583 ± 0·004
18	6·376 ± 0·006	6·533 ± 0·004
19	6·325 ± 0·006	6·473 ± 0·004
20	6·265 ± 0·006	6·397 ± 0·004
21	6·178 ± 0·006	6·297 ± 0·009

		calculated from ^{80}Se$_2$
$B_e = 0{\cdot}07048 \pm 0{\cdot}00002$	$B_e = 0{\cdot}07228$	0·07229
$\alpha_e = 0{\cdot}000345$	$\alpha_e = 0{\cdot}000363$	0·000358
$D = 4 \times 10^{-8}$	$D = 5 \times 10^{-8}$	—
$r_e = 2{\cdot}4464 \pm 0{\cdot}0003$ Å	$r_e = 2{\cdot}4465$ Å	—

In addition the values of B in the region $9 < v < 16$ show so much scatter, because of the perturbations at low J values, that little regularity is apparent. The constants B_e and α_e for each isotope were therefore evaluated for the region $0 \leqslant v \leqslant 8$, over which the term in γ_e is found to be negligibly small. The values are given in table 3. Using the derived constants, we have drawn in figure 9 a plot of $10^5(B_{v,\,\mathrm{obs.}} - B_{v,\,\mathrm{calc.}})$ against v for each isotope. The deviations of B_v from the expected values for $v > 15$ are clear.

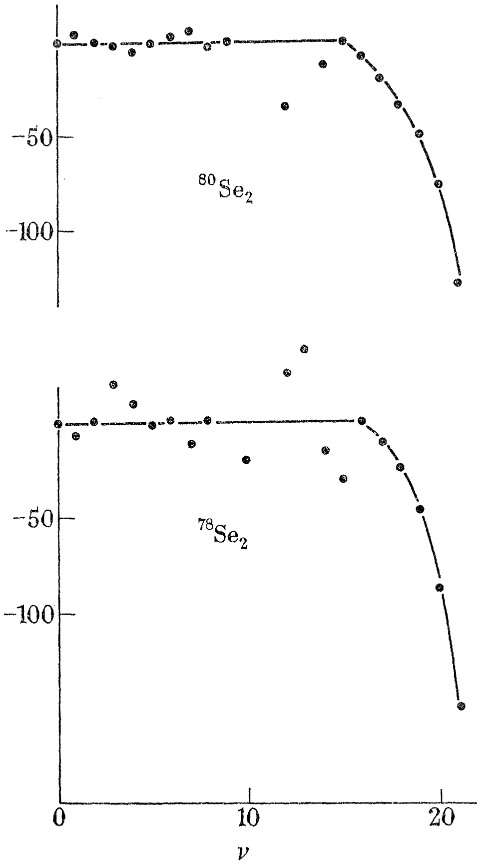

FIGURE 9. Values of 10^5 B_v (observed–calculated) plotted against v for the state $B\,0_u^+$ of $^{78}Se_2$ and $^{80}Se_2$.

Vibrational analysis

The complexity arising from the use of natural selenium was not recognized by all the previous workers on this molecule: furthermore, the present work shows that the B–X system consists of two overlapping subsystems with very similar vibrational constants. It is not fruitful, therefore, to give detailed comparisons with the early analyses, since there is agreement in some regions and disagreement in others. As an example may be taken the vibrational analysis of Rosen (1939) which is the most comprehensive of the early work and which in fact refers to the 0_u^+–0_g^+ subsystem. As a result of the present study it has been shown that for the $v' = 0$ and 1 progressions, Rosen's analysis is correct, for the $v'' = 0$ and 1 progressions, the v' numbering is too low by 1, while for intermediate bands, v'' should be reduced by 3 and v' by 4.

Three points may be made before the correct vibrational analysis is given:

(1) The region 5450 to 5950 Å has been described by Rosen & Montford (1936) as consisting of 'fluctuation bands'. We have observed this region in emission and there are no fluctuations of intensity when separated isotopes are used. However, both subsystems occur strongly, and medium dispersion plates appear extremely complex, with observed isotopic shifts between the band-heads of $^{78}Se_2$ and $^{80}Se_2$ of about 100 cm^{-1}. With natural selenium, the complexity of this region would of course be very much greater.

(2) A study of the medium dispersion emission plates in the region 4000 to 6040 Å, in which no bands have been analysed rotationally, reveals many bands of which most are assigned to the 0^+–0^+ and some to the 1–1 subsystem. The features distinguishing the 0^+–0^+ and 1–1 bands are only apparent at high dispersion. However, so many bands are present that some of the unassigned bands must be assigned to the 1–1 system, at least at wavelengths above 4000 Å. At $\lambda < 4000$ Å, all the bands have been analysed rotationally, and are found to be 0^+–0^+ bands. It therefore appears that the 1–1 subsystem is predissociated below about 4000 Å.

(3) In the region around 6000 Å where 1–1 emission bands have been analysed rotationally, the overlapping of bands is less, and it is suggested that earlier workers, using low dispersion, assigned the 1–1 bands to a new system, for example the system at 5900 to 6800 Å reported by Leelavathi & Rao (1955). Using separated isotopes, this region is found to contain only B–X bands when the spectrum is excited in a microwave discharge: this method usually produces spectra rather similar to those excited in a high frequency discharge such as was used by Leelavathi & Rao.

To determine the correct vibrational analysis, it was first assumed that the long progression of 0^+–0^+ bands at the short wavelength end of the absorption spectrum is a $v'' = 0$ progression. The rotational analysis of these bands, together with those of $v'' = 1$ which occur at somewhat longer wavelengths provided reliable values of B''_0 and of B''_1. Comparison with the values of B'' obtained by Olsson (1938) and by Davis (1954) showed that the v'' numbering used by them was three units too high. The position of the system origin previously obtained was assumed to be roughly correct, and to maintain this value and reduce v'' by 3 requires a reduction of 4 in v'. Test calculation of the isotope shifts of the emission bands, extending to $v'' = 30$, gave excellent agreement with observation, implying that at least the new v'' numbering was correct.

However, numerous vibrational perturbations were reported by almost all the previous workers and the values for the upper state vibrational constants were considered unreliable until it had been shown that the vibrational levels used to derive them were unperturbed. We proceeded as follows. First, band origins of the bands with $v = 5$ in $^{80}Se_2$, i.e. the 5–1, 5–2, 5–3, 5–4, 5–30 and 5–31 bands, were used to determine accurate ground state constants by fitting to the polynomial

$$T_{5,e} = (\nu_0)_{5,v} + \omega''_e(v+\tfrac{1}{2}) - x''_e\omega''_e(v+\tfrac{1}{2})^2 + y''_e\omega''_e(v+\tfrac{1}{2})^3.$$

Using these values, the upper state term values for $^{80}Se_2$ were derived from

$$T' = \nu_0 + G''_v.$$

For $^{78}Se_2$, no information was available at high values of v'', and the ground state constants were therefore calculated from those of $^{80}Se_2$ by the isotope relationships using

$\mu(^{78}Se_2) = 38{\cdot}97116$ and $\mu(^{80}Se_2) = 39{\cdot}97103$ (Townes & Schawlow 1955). The calculated values of $\Delta G''$ were checked by comparison with those observed at low values of v''. Upper state term values for $^{78}Se_2$ were then calculated from the band origins. A test plot of the upper state term values against v showed a marked change of slope for $v > 15$, for both isotopes. In the determination of upper state vibrational constants, term values for $v > 15$ were therefore omitted from the calculation: in addition, the values for $v = 10$ and 12 for $^{80}Se_2$ were also omitted because no analysis was available at low values of J for these levels.

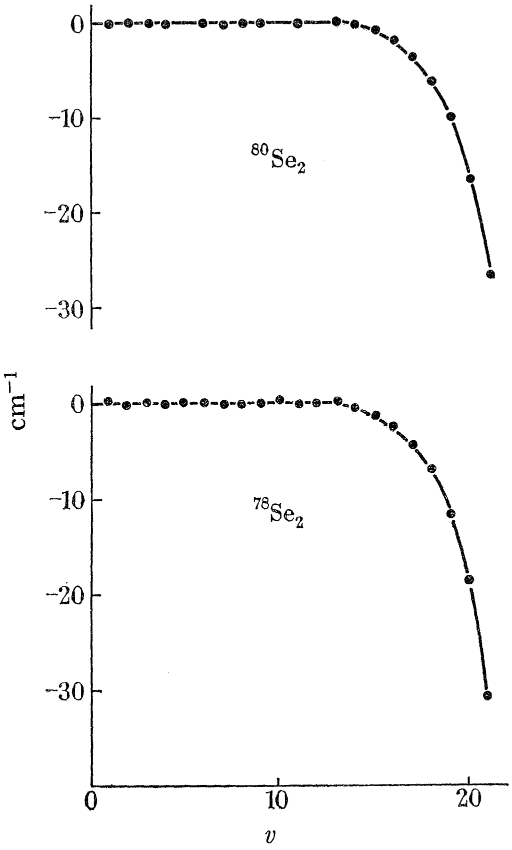

Figure 10. Term values (observed–calculated) plotted against v for the state $B\,0_u^+$ of $^{78}Se_2$ and $^{80}Se_2$.

Constants were then derived by a least squares method, the term values being fitted to the equation

$$T' = T_e + \omega_e'(v+\tfrac{1}{2}) - x_e'\omega_e'(v+\tfrac{1}{2})^2 + y_e'\omega_e'(v+\tfrac{1}{2})^3.$$

Term values were then back calculated from the vibrational constants, and a plot of T' (observed–calculated) against v' for each isotope is given in figure 10. The excellent agreement shows that there are no appreciable perturbations of the origins for $v < 15$. Values of the band origins are given in table 4 and the derived vibrational constants are given in table 5. The agreement between the constants derived for $^{78}Se_2$ with those calculated from $^{80}Se_2$ is seen to be excellent.

Observed and calculated isotope shifts are also given in table 4. The bands of the two isotopes have usually been measured from different photographic plates. This procedure gives rise to larger errors than are obtained by direct comparison on the same plate. None

Table 4. Band origins, band heads and vibrational isotope effect, $B0_u^+ - X0_g^+$, $^{78}Se_2$, $^{80}Se_2$

band	$^{80}Se_2$	$^{78}Se_2$	$\Delta\nu_{\text{obs.}}$	$\Delta\nu_{\text{calc.}}$	$\Delta\nu_{\text{obs.}-\text{calc.}}$
21–0	30 532·27	30 579·08	−46·81	−50·89	4·08
20–0	30 346·08	30 392·95	−46·87	−49·13	2·26
19–0	30 153·28	30 199·13	−45·85	−47·28	1·43
18–0	29 955·52	30 000·03	−44·51	−45·36	0·85
17–0	29 753·69	29 796·40	−42·71	−43·37	0·66
16–0	29 548·24	29 589·20	−40·96	−41·29	0·33
15–0	29 339·93	29 378·63	−38·70	−39·16	0·46
14–0	29 128·30	29 165·21	−36·91	−36·94	0·03
13–0	28 914·21	28 948·67	−34·46	−34·66	0·20
13–1	28 530·79	28 560·38	−29·59	−29·80	0·21
13–3	—	27 789·91	—	—	—
13–4	—	27 407·63	—	—	—
13–5	—	27 027·45	—	—	—
13–6	—	26 649·15	—	—	—
12–0	(28 699·54)	28 729·41	−29·87	−32·30	—
12–1	(28 315·71)	28 341·11	−25·40	−27·44	—
11–0	28 477·65	28 507·57	−29·92	−29·88	−0·04
11–1	28 094·26	28 119·26	−25·00	−25·02	0·02
11–2	—	27 733·08	—	—	—
11–3	—	27 348·85	—	—	—
11–4	—	26 966·67	—	—	—
10–0	(28 256·21)	28 283·33	−27·12	−27·39	—
10–1	(27 872·91)	27 895·09	−22·18	−22·53	—
9–1	27 647·98	27 667·93	−19·95	−19·98	0·03
9–2	27 266·49	27 281·72	−15·23	−15·17	−0·06
8–0	27 804·70	27 826·97	−22·27	−22·23	−0·04
8–1	27 421·27	27 438·65	−17·38	−17·37	−0·01
7–1	27 192·26	27 206·99	−14·76	−14·68	−0·08
6–1	26 960·99	26 973·00	−12·01	−11·94	−0·07
6–2	26 579·54	26 586·58	−7·04	−7·13	0·09
6–3	26 200·12	26 202·46	−2·34	−2·37	0·03
6–27	—	17 591·09 H	—	—	—
6–28	17 358·26 H	17 257·90 H	100·36	99·92	0·44
6–29	17 031·05 H	—	—	—	—
6–31	16 381·47	—	—	—	—
5–1	26 727·45	26 736·67	−9·22	−9·13	−0·09
5–2	26 346·12	26 350·38	−4·26	−4·32	0·06
5–3	25 966·64	—	—	—	—
5–4	25 588·94	25 584·35 H	4·6	5·16	−0·6
5–25	—	18 025·64 H	—	—	—
5–26	17 785·86 H	17 689·50 H	96·36	95·76	0·60
5–27	17 454·43 H	17 354·80 H	99·63	99·27	0·36
5–28	17 125·08 H	17 021·64 H	103·44	102·73	0·71
5–30	16 471·19	—	—	—	—
5–31	16 147·99	—	—	—	—
4–3	25 730·80	25 727·57	3·23	3·30	−0·07
4–4	25 353·30 H	25 345·65 H	7·65	8·02	−0·37
4–5	24 978·27 H	24 963·87 H	14·40	12·67	1·73
4–24	18 218·69 H	18 127·37 H	91·32	91·44	−0·12
4–25	17 883·59 H	17 787·86 H	95·73	95·05	0·68
4–26	17 549·82 H	17 451·42 H	98·40	98·62	−0·22
4–27	17 218·30 H	17 117·32 H	100·98	102·13	−1·15
4–29	16 560·73	—	—	—	—
4–30	16 235·48	—	—	—	—
3–4	25 115·53	25 104·47	11·06	10·94	0·12
3–22	—	18 570·03 H	—	—	—
3–23	18 319·19 H	18 227·99 H	91·20	90·70	0·50
3–24	17 981·13 H	17 886·35 H	94·78	94·36	0·42
2–5	24 499·78	24 481·23	18·55	18·56	−0·01
2–19	19 449·90 H	—	—	—	—
2–20	19 103·35 H	19 021·31 H	82·04	82·34	−0·30
2–21	18 760·87 H	18 673·87 H	87·00	86·15	0·85
2–22	—	18 328·37 H	—	—	—
1–8	23 142·59	23 107·40	35·19	35·29	−0·10
1–17	19 904·31 H	19 830·48 H	73·83	73·56	0·27
1–18	19 555·96 H	19 476·82 H	79·14	77·55	1·59
1–19	19 206·59 H	19 124·92 H	81·67	81·49	0·18
0–7	23 267·98	23 233·85	34·13	33·88	0·25

H indicates band head: other measurements are of band origins.
Values in parentheses are uncertain because of perturbations.

the less, there is good agreement for upper state levels $0 \leqslant v' \leqslant 15$ and over a wide range of ground state levels: this confirms the vibrational analysis.

It is interesting to consider why the upper state levels with $v > 15$ show, for both isotopes, such marked deviations both in vibrational term values and also in B_v. It is suggested that the effect is caused by the avoidance of crossing of two potential curves of the same symmetry, equivalent to a homogeneous perturbation by an unstable state. The magnitude of the perturbation evidently increases with v, and the overall effect is the formation of a potential energy maximum in $B\,0_u^+$. The dissociation limit of the unstable state must lie at a lower energy than that of $v = 15$ in $B\,0_u^+$, where its effect is already noticeable and it may be assumed that this limit must lie considerably below for there to be significant interaction between the two states.

TABLE 5. VIBRATIONAL CONSTANTS FOR $B\,0_u^+–X\,0_g^+$ (cm^{-1})

		$^{80}Se_2$	$^{78}Se_2$ (obs.)	$^{78}Se_2$ (calc.)
$B\,0_u^+$	ν_e	25 980·36	25 980·25	—
	ω_e	246·291	249·436	249·430
	$x_e\omega_e$	1·016	1·035	1·042
	$y_e\omega_e$	$-5{\cdot}49\times10^{-3}$	$-6{\cdot}27\times10^{-3}$	$-5{\cdot}7\times10^{-3}$
$X\,0_g^+$	ω_e	385·3028		390·2143
	$x_e\omega_e$	0·96363		0·98835
	$y_e\omega_e$	$-8{\cdot}184\times10^{-4}$		$-8{\cdot}501\times10^{-4}$

ANALYSIS OF BANDS OF THE SUBSYSTEM $B\,1_u–X\,1_g$

Emission bands of the 1–1 system at around 6000 Å have been analysed for the $^{80}Se_2$ molecule: these include bands with $v' = 3$, 4 and 5. Absorption bands in the region of the 0–8, 0–9 and 0–10 bands of the $0_u^+–0_g^+$ subsystem have been analysed for both isotopes. Wave numbers of the lines are given in tables A5 and A6.

TABLE 6. ROTATIONAL CONSTANTS (cm^{-1}), for $B\,1_u–X\,1_g$

		$^{80}Se_2$		$^{78}Se_2$	
	v	$10^2B(F_2)$	$10^2B(F_3)$	$10^2B(F_2)$	$10^2B(F_3)$
$B\,1_u$	0	$7{\cdot}041\pm0{\cdot}006$	$7{\cdot}085\pm0{\cdot}007$	$7{\cdot}219\pm0{\cdot}006$	$7{\cdot}260\pm0{\cdot}007$
	1	$6{\cdot}980\pm0{\cdot}007$	$7{\cdot}019\pm0{\cdot}007$	$7{\cdot}153\pm0{\cdot}006$	$7{\cdot}193\pm0{\cdot}008$
	3	$6{\cdot}887\pm0{\cdot}009$	$6{\cdot}918\pm0{\cdot}011$	—	—
	4	$6{\cdot}809\pm0{\cdot}010$	$6{\cdot}846\pm0{\cdot}010$	—	—
		$B_e(F_2) = 0{\cdot}07067$	$B_e(F_3) = 0{\cdot}07105$	$B_e(F_2) = 0{\cdot}07244$	$B_e(F_3) = 0{\cdot}07284$
		$\alpha(F_2) = \alpha(F_3) = 0{\cdot}000553$		[$\alpha(F_2) = \alpha(F_3) = 0{\cdot}000574$: calc. from $^{80}Se_2$]	
		B_e(m.v.) = 0·07086 r_e(m.v.) = 2·4398 Å		B_e(m.v.) = 0·07264 r_e(m.v.) = 2·4405 Å	
$X\,1_g$	8	$8{\cdot}758\pm0{\cdot}008$	$8{\cdot}762\pm0{\cdot}007$	$8{\cdot}993\pm0{\cdot}006$	$8{\cdot}996\pm0{\cdot}010$
	9	$8{\cdot}736\pm0{\cdot}006$	$8{\cdot}737\pm0{\cdot}007$	$8{\cdot}943\pm0{\cdot}007$	$8{\cdot}954\pm0{\cdot}007$
	27	$8{\cdot}193\pm0{\cdot}009$	$8{\cdot}193\pm0{\cdot}012$	—	—
	28	$8{\cdot}167\pm0{\cdot}010$	$8{\cdot}158\pm0{\cdot}004$	—	—
	29	$8{\cdot}141\pm0{\cdot}007$	$8{\cdot}140\pm0{\cdot}011$	—	—
		$B_e(F_2) = B_e(F_3) = 0{\cdot}9012$ $\alpha(F_2) = \alpha(F_3) = 0{\cdot}000297$		$B_e(F_2) = B_e(F_3) = 0{\cdot}09250$ [$\alpha(F_2) = \alpha(F_3) = 0{\cdot}000309$: calc. from $^{80}Se_2$]	
		$r_e = 2{\cdot}1635$ Å		$r_e = 2{\cdot}1626$ Å	

$D = 2\times10^{-8}$ for both states of each isotope.

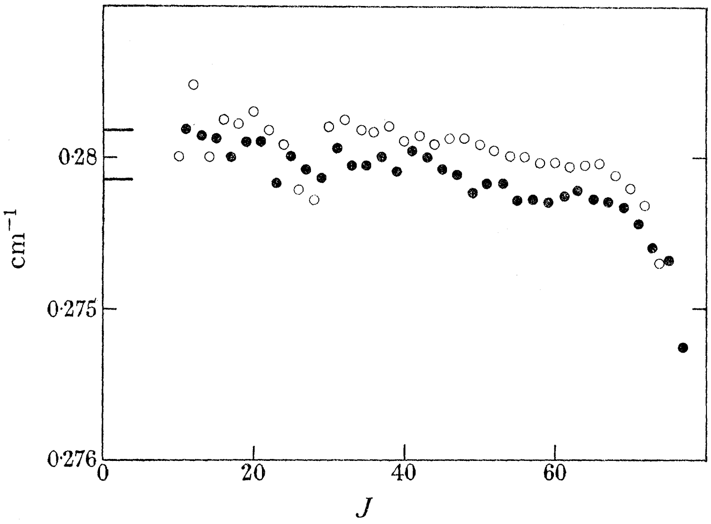

FIGURE 11. $\Delta_2F(J)/(J+\frac{1}{2})$ is plotted against J for the F_2 component ●, and the F_3 component ○, of $v = 1$ in $B\,1_u$ of $^{80}Se_2$. The computed values of $4B$ are 0·2792 and 0·2808 cm^{-1} for F_2 and F_3 respectively.

TABLE 7. A SUMMARY OF FEATURES OBSERVED IN THE STATE $B\,1_u$

				J values at	
v		observed in absorption (A) emission (E)	range of J analysed	(i) perturbations	(ii) predissociations
			$^{78}Se_2$		
1	F_2	A	14–78	79	—
	F_3	A	19–75	76	—
0	F_2	A	14–82	83	—
	F_3	A	11–79	80	—
			$^{80}Se_2$		
5	F_2	E	10–72	9, 69	73
	F_3	E	1–71	8, 68	72
4	F_2	E	2–86	71, 87	—
	F_3	E	7–83	68, 84	—
3	F_2	E	14–74	73	—
	F_3	E	11–71	72	—
2	F_2	—	—	—	—
	F_3	—	—	—	—
1	F_2	A	10–78	79	—
	F_3	A	9–75	76	—
0	F_2	A	14–72	73	—
	F_3	A	13–73	74	—

Rotational analysis

The analysis was straightforward: the F_2 branches are numbered by odd values of J'' and the F_3 branches by even values of J''. The relative numbering in each band is fixed by observation of a perturbation which occurs at about the same J value for each component. B'_v is again found to be greater than B_p. Values of $\Delta_2F(J)$ for $v'' = 28$, $X\,1_g$ of $^{80}Se_2$ are given in table A2. The absolute numbering was determined by assigning trial values of J until $\Delta_2F''(J)/(J+\frac{1}{2})$ was linear in $(J+\frac{1}{2})^2$, and likewise for $\Delta_2F'(J)/(J+\frac{1}{2})$ in unperturbed regions. An example is illustrated in figure 11. The rotational constants were evaluated for each component separately and values are given in table 6.

Features observed in the analysed levels of $B1_u$ are summarized in table 7. The absence of 1–1 bands in the region near 4000 Å analysed in emission may be explained by predissociation. The level $v = 5$ in $B1_u$, the highest level of this state to be observed, is sharply predissociated at two rotational levels after a perturbation (see figure 12, plate 64). A search was made for bands with $v' = 6$. The Franck–Condon parabola is such that the 6–29 and 6–30 bands at 16518 and 16190 cm^{-1} respectively, and the 6–1 and 6–2 bands near 4000 Å, should be strong. However, none of these bands are observed on the emission plates. The analysis of $v' = 4$ could not be extended far enough to observe the predissociation expected at high J values.

Vibrational analysis

The band origins of the F_2 and F_3 components are found to be identical so that both follow the same vibrational scheme. The most probable *relative* vibrational numbering of the bands followed from the values of B'' and of B', and a first approximation to the *absolute* numbering was provided by comparison of the isotope shifts of the bands at low v'' with those determined from the 0^+–0^+ bands. The correct absolute numbering was finally obtained by comparing trial values of G''_v $(X1_g)$ with those of G''_v $(X0^+_g)$. There are strong indications that the latter should be slightly smaller than the former. Thus in S_2, the splitting constant λ'' increases somewhat with v in the ground state $X^3\Sigma^-_g$ (Barrow & Ketteringham 1963), and the same effect is observed in SeO (Barrow & Deutsch 1963). Likewise in TeO, ω_e for the $\Omega = 1$ component of the ground state is a little larger than ω_e for the 0^+ component. With this assumption, values of v'' could be assigned unambiguously, and the assignment of values of v' followed from the isotope separations. Band origins and derived rotational constants are given in table 8.

TABLE 8. BAND ORIGINS AND VIBRATIONAL CONSTANTS (cm^{-1}), FOR $B1_u$–$X1_g$

	$^{80}Se_2$		$^{78}Se_2$	
band	F_2	F_3	F_2	F_3
0–9	22 080·59	22 080·59	22 037·61	22 037·61
1–9	22 324·57	22 324·56	22 284·98	22 284·94
1–8	22 694·38	22 694·37	22 659·39	22 659·33
3–27	16 478·72	16 478·74	—	—
3–28	—	16 146·12	—	—
4–28	16 382·86	16 382·74	—	—

Derived constants for $^{80}Se_2$

$\nu_e = 25545{\cdot}85$

$\omega'_e = 246{\cdot}42$

$x'_e\omega'_e = 1{\cdot}225$

$\omega''_e = 386{\cdot}43$

$x''_e\omega''_e = 0{\cdot}9058$

$y''_e\omega''_e = -13{\cdot}13 \times 10^{-4}$

Upper state term values, relative to the minimum of the potential curve for $X1_g$ have been calculated from the derived constants and are compared with values of $(\nu_{0,\,\mathrm{obs.}} + G''_v)$ in table 9. The observed value for $v' = 1$ of $^{78}Se_2$ is anomalous and it seems likely that there is a perturbation at low J which makes the extrapolation for ν_0 of $v' = 1$ uncertain. This is supported by the failure to analyse this level of $^{78}Se_2$ to the low J values found elsewhere. The isotope shifts are also shown in table 9: there is good agreement for $v' = 0$, but not for $v' = 1$ as expected. The derived value of $\nu_e(1\text{–}1)$ is smaller than $\nu_e(0^+\text{–}0^+)$ by 434·5 cm: this is formally equal to $2\lambda''$–$2\lambda'$.

Table 9. Vibrational term values and isotope effect (cm^{-1}) for $B1_u$–$X1_g$

values of $T'_{v,e}$

v	$^{80}Se_2$ obs.	$^{80}Se_2$ calc.	$^{78}Se_2$ obs.	$^{78}Se_2$ calc.
0	25 668·80	25 668·75	25 670·48	25 670·31
1	25 912·78	25 912·72	25 917·88	25 917·36
3	26 393·25	26 393·31	—	—
4	26 629·86	26 629·93	—	—

values of $\Delta\nu(^{80}Se_2$–$^{78}Se_2)$ (cm^{-1})

band	obs.	calc.
0–9	42·98	43·10
1–9	39·61	40·02
1–8	35·02	35·52

Discussion

Predissociations in $B\,0_u^+$

The predissociations in levels $v = 13$, 14 and 15 have been described: they occur at decreasing values of J for increasing v. Mulliken (1960) has discussed the possible types of predissociation in diatomic spectra, and of these, only two, namely c^+ and b^+, have the observed J dependence. Both types involve intersection of a second state A with the right hand limb of the potential energy curve of $B\,0_u^+$. In c^+, the intersection would occur above the asymptote of A, while in b^+ the intersection would occur below that asymptote. For a heavy molecule like Se_2, where the rotational constant B is very small, the differences in J dependence between these two types of predissociation are quite small, but they may be described as follows.

The effective potential energy $U_J(r)$, including rotation, is given by

$$U_J(r) = U_0(r) + \frac{h}{8\pi^2 c\mu r^2} J(J+1).$$

In c^+ predissociations, these J dependent potential curves for each state intersect at the same critical value, r_c, independent of J. Predissociation of $B\,0_u^+$ by A occurs for all rotational levels above the critical one, J_c, for which the intersection coincides with an actual level of $B\,0_u^+$. Thus if predissociations are observed in different vibrational levels the difference in their term values depends only on the rotational energy $B_c J(J+1)$, where $B_c = h/8\pi^2 c\mu r_c^2$. A plot of term value of predissociation against $J(J+1)$ therefore gives a straight line of slope B_c. This slope can be calculated since r_c is about equal to $r_{\max.}$ of $B\,0_u^+$ for the particular vibrational levels. The term value obtained by extrapolation of the plot to $J = 0$ is that for the intersection of the two rotationless potential energy curves. Since this represents a potential maximum, it only sets a maximum value on the energy of the asymptote of A.

In b^+, critical J values occur in the same way, but the energy for some values of v lie below the asymptote of A: no predissociation can occur and these intersections therefore give rise, by the same selection rules, to perturbations. With rotation, the potential curves of A and $B\,0_u^+$ possess potential maxima of increasing height at large internuclear distances. These maxima occur at smaller values of r, r^*, for increasing J. Predissociation of $B\,0_u^+$

occurs sharply when the energy is equal to that of the potential maximum of A (assuming that no tunnelling occurs for a molecule as heavy as Se_2). A plot of term values of predissociation against $J(J+1)$ therefore gives a curve whose slope is smaller than for c^+, since $r^* > r_c$, and the slope tends to zero with increasing J as r^* tends to infinity. Extrapolation of this limiting curve of predissociation to $J = 0$ therefore gives an accurate estimate of the limit of the predissociating state A.

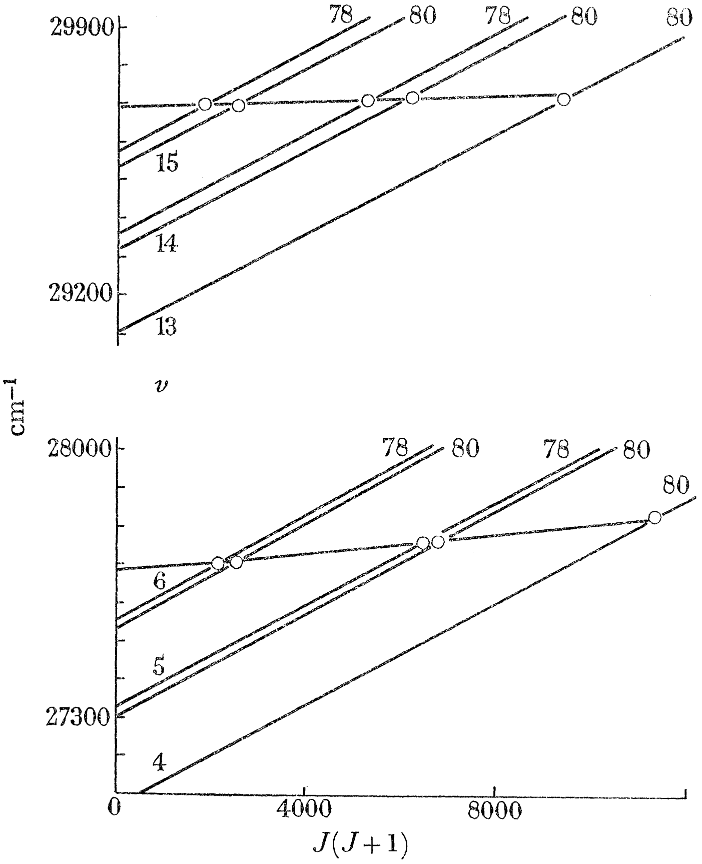

FIGURE 13. Limiting curves of predissociation in the states $B\,0_u^+$ of $^{78}Se_2$ and $^{80}Se_2$. Term values with respect to the minima of $X\,0_g^+$ are plotted against $J(J+1)$.

The different variations of the slope with J are commonly used to distinguish cases c^+ and b^+. However, in a molecule as heavy as Se_2 differentiation between c^+ and b^+ is best made by consideration of the slopes of the limiting curves of predissociation, and, perhaps, by the observation of perturbations before the predissociation together with the absence of perturbations in the predissociated levels.

The two limiting curves of predissociation, for $v = 13$, 14 and 15 and 4, 5 and 6 are drawn in figure 13, where the straight lines represent the calculated term values for $B\,0_u^+$. The observation that the predissociations for both isotopes fall on the same curve supports the assumption that tunnelling is quite unimportant. For $v = 13$, 14 and 15, the slope at $J \sim 70$ is about $0{\cdot}006\ \text{cm}^{-1}$, which may be compared with $B' = 0{\cdot}07\ \text{cm}^{-1}$ and B_c (calculated for c^+ from $r_c = r_{\text{max.}} = 2{\cdot}85$ Å, from figure 13) $= 0{\cdot}05\ \text{cm}^{-1}$. The observed slope is thus much smaller than for c^+, and is equivalent to a value of r^* of about 8 Å. It is therefore established that the predissociations in $v = 13$, 14, and 15 are of type b^+, and this is confirmed by the distribution of perturbations previously mentioned which indicated that the perturbing state is also the predissociating state. Extrapolation of the limiting curve of predissociation gives a dissociation limit at 29690 cm^{-1}, with an estimated error, partly caused by the absence of alternate levels, of $\pm$ 20 cm^{-1}.

For the predissociations in $v = 4$, 5 and 6, the observed slope at $J \sim 70$ is about 0·009 cm^{-1}, compared with $B' = 0{\cdot}07$ and $B_c = 0{\cdot}06\ \mathrm{cm}^{-1}$ ($r_{\mathrm{max.}} \sim 2{\cdot}7$ Å). Thus the value of r^* is about 7 Å, indicating that these predissociations are also of type b^+. Extrapolation to $J = 0$ gives a value for the limit of $27700 \pm 20\ \mathrm{cm}^{-1}$.

The difference between the two limits, $29690 - 27700 = 1990\ \mathrm{cm}^{-1}$ should agree with the difference between two low lying terms of Se I. Values of these, taken from Moore (1952), are as follows: $^3P_2$, 0 cm^{-1}; $^3P_1$, 1989·5 cm^{-1}; $^3P_0$, 2534·3 cm^{-1}; $^1D_2$, 9576·1 cm^{-1}. The interval $^3P_1$–$^3P_2$ in Se I is seen to correspond exactly to the difference between the two predissociation limits in Se_2. This agreement confirms the identification of the predissociations as being of type b^+, caused by two different, stable, electronic states.

The higher of these two predissociating states is, very probably, responsible for some of the observed perturbations. The lower predissociating state does not, however, appear to be otherwise observed, and it is interesting to consider the reasons for this. The presence of emission lines *after* the predissociation has been observed in $v = 6$ for $^{78}\mathrm{Se}_2$, but not for $^{80}\mathrm{Se}_2$. These lines are still sharp, and the bands showing predissociation are no weaker than others, so that the behaviour does not arise from a disturbance of thermal equilibrium (Farkas 1931) nor from the effect of deactivating collisions (Olsson 1938). That the predissociation at $v = 6$ is weak is supported by the relative sharpness of absorption lines of bands with $v > 6$ and by the observation in emission of weak bands with $v = 7$ of $^{77}\mathrm{Se}_2$ (Davies 1954), and with $v = 11$, 12 and 13 in $^{78}\mathrm{Se}_2$. Although pressure effects may be important in weakly allowed predissociations (Herzberg & Mundie 1940), it is difficult to see how they can be responsible for the effects observed here. It seems more likely that the differences between the different isotopic species are to be explained by the assumption that the predissociation is weak, heterogeneous and, therefore, J-dependent. In this case, the strength of the predissociation is expected to increase in the order of the critical J values, that is, in the order $^{77}\mathrm{Se}_2 < {}^{78}\mathrm{Se}_2 < {}^{80}\mathrm{Se}_2$, as is observed. Since the interaction of the predissociating state with $B\,0_u^+$ is evidently very weak, it is not surprising that no strong perturbations have been recognized before this predissociation.

An unrelated predissociation is observed at low J in $v = 13$, corresponding to an energy of about 29180 cm^{-1}. Numerous diffuse perturbations in levels $v = 12$ and 11 prevented further study of these predissociations.

Predissociation in $B\,1_u$

The predissociation at $J' \sim 72$ in $v = 5$ occurs at a term value, relative to the minimum of $X\,0_g^+$, of $(27201 + 2\lambda'')\ \mathrm{cm}^{-1}$. The term value of $v = 6$, $J = 0$ is estimated to lie at $(27096 + 2\lambda'')\ \mathrm{cm}^{-1}$: bands with $v = 6$ have not been observed, either in emission or in absorption. The difference between these term values, 105 cm^{-1}, divided by $J(J+1) \sim 5000$ gives a *lower* limit for the limiting slope of predissociation of 0·02 cm^{-1}, far larger than that of the predissociation in $B\,0_u^+$ at 27700 cm^{-1}. The two predissociations, in $B\,0_u^+$ and in $B\,1_u$, are not therefore caused by the same state: most probably that in $B\,1_u$ arises from an interaction of type c^+ with an unstable state.

Diffuse perturbations in $B\,0_u^+$

Diffuse perturbations are observed for the absorption bands in the region $7 \leqslant v \leqslant 15$. They are assigned as accidental predissociations involving a third unstable state as well as the perturbing state. Kovács & Budó (1947) have given a discussion of this type of interaction from which it is clear that if the interaction between the perturbing state and $B\,0_u^+$ is strong then the lines at an accidental predissociation can be perturbed and broadened. Similarly, the weakness of emission lines from a single rotational level in $v = 6$ can be correlated with the observed splitting of this level in $^{80}Se_2$, in a similar manner to the accidental predissociation observed in one of the excited $^1\Pi$ states of HBr (Barrow & Stamper 1961). The asymptote of the unstable state may be 27 700 cm^{-1}, but if the weak lines in $v = 6$ arise by interaction with the same state, it lies below 27 700 cm^{-1}.

Triplet splitting

The relation
$$\begin{aligned} B_v(F_3) - B_v(F_2) &= B_v(F_2) - B_v(F_1) \\ &= 2B^2/(\lambda^2 - 2\lambda B)^{\frac{1}{2}} \end{aligned}$$
for case b (large λ) was found to hold, at least approximately for the ground state of SeO (Barrow & Deutsch 1963). Inspection of tables 2 and 6 reveals that this approximation does not apply to the ground state of Se$_2$, where
$$B_v(F_3) \simeq B_v(F_2) > B_v(F_1).$$
It seems then that the ground state of Se$_2$ is better described by Hund's case c than by case b (large λ). The Ω doubling in the 1_g state is presumably caused mainly by interaction with the lower 0_g^+ state, so that the order of the levels is expected to be $F_3(J) > F_2(J)$ or $1_g^+ > 1_g^-$. The very small difference in the values of B suggests that this Ω doubling is very small. Recently, Åslund (1965) has developed a method for the direct determination of term values by a least squares method which makes a more complete use of experimental measurements than is done in calculations based upon combination differences. This method has been used to derive very precise values of B for $v = 9$ of $X\,1_g$ for $^{80}Se_2$. For this level, a least squares treatment of combination differences gave
$$B(F_2) = 0{\cdot}08736 \pm 0{\cdot}00006 \text{ cm}^{-1},$$
$$B(F_3) = 0{\cdot}08737 \pm 0{\cdot}00007 \text{ cm}^{-1},$$
values which may be compared with the results of the term value calculation:
$$B(F_2) = 0{\cdot}087385 \pm 0{\cdot}000009 \text{ cm}^{-1},$$
$$B(F_3) = 0{\cdot}087401 \pm 0{\cdot}000008 \text{ cm}^{-1}.$$
Direct determination of the slope of $F_3(J)$–$F_2(J)$ plotted against $J(J+1)$ gives $0{\cdot}000021 \pm 0{\cdot}000002$ cm^{-1}, which is the Ω doubling constant, q, for $X\,1_g$.

In case c, if the Ω doubling is due only to the 0_g^+ state, the case of pure precession discussed by van Vleck (1929) may apply: q is then given by $q = 2B^2 l(l+1)/\nu(\Pi\Sigma)$. Here

$\nu(\Pi\Sigma)$ is the separation $(1_g$–$0_g^+) = 2\lambda''$. If $l = 1$, $q = 2B^2/\lambda''$. Few examples of $^3\Sigma^-$ states in case c are available to test this result. However, the ground state of BiH is one such state, and for this Heimer (1935) derives $q = 0{\cdot}020\ \mathrm{cm^{-1}}$ and $B = 5{\cdot}141\ \mathrm{cm^{-1}}$. The calculated separation $X1$–$X0^+$ is then 5290 cm^{-1}, in satisfactory agreement with the observed separation of 4917 cm^{-1}. For Se_2, a similar calculation gives $\lambda'' = 727\ \mathrm{cm^{-1}}$, corresponding to a separation $X1_g$–$X0_g^+$ of 1454 cm^{-1}. For obvious reasons (Mulliken & Christy 1931), the error in this estimate may be large. However, it seems safe to conclude that λ'' is of the order of several hundred wavenumbers.

In the upper state, comparison of the B values (tables 3 and 6) shows that $B_v(F_3)$–$B_v(F_2)$ is about twice as large as $B_v(F_2)$–$B_v(F_1)$. This may indicate that $B\,^3\Sigma_u^-$ is nearer to case b than is $X\,^3\Sigma_g^-$, but has limited significance in the determination of the sign or magnitude of λ'.

Electronic states of Se_2

The selection rules permit interactions with $B\,0_u^+$ of 1_u and 0_u^+ states only. The vibrational perturbations in $B\,0_u^+$ for $v > 15$ have been assigned as homogeneous perturbations so that the unstable state causing the potential maximum in $B\,0_u^+$ is a second 0_u^+ state. The perturbing state, with a limit at 29 690 cm^{-1} causes no marked change in the potential curve of $B\,0_u^+$, but the perturbations are strong so that it is assigned as a 1_u state. This assignment is supported by the increasing diffuseness of the lines with increasing J in bands above 29 690 cm^{-1}: both predissociations and perturbations are therefore heterogeneous. The accidental predissociations in $B\,0_u^+$ could thus arise by interactions with a third unstable state 2_u. No direct inference from the perturbations and predissociations in $B\,1_u$ has been made.

The equivalent case b states may be derived from the low lying m.o. configurations

$$\ldots(\pi_u\,4p)^4(\pi_g^*\,4p)^2, \quad {}^3\Sigma_g^-,\ {}^1\Delta_g,\ {}^1\Sigma_g^+,$$
$$\ldots(\pi_u\,4p)^3(\pi_g^*\,4p)^3, \quad {}^1\Sigma_u^+,\ {}^1\Sigma_u^-,\ {}^3\Sigma_u^+,\ {}^3\Sigma_u^-,\ {}^1\Delta_u,\ {}^3\Delta_u.$$

The $^3\Delta_u$ state is expected to lie below $^3\Sigma_u^-$. In S_2, the state perturbing $B\,^3\Sigma_u^-$ has been assigned by Barrow & du Parcq (1965) as $^3\Pi_u$, with the possible configuration $\ldots(\sigma_g 3p)^2 (\pi_u 3p)^4(\pi_g 3p)\ (\sigma_u 3p)$. If the analogy with S_2 is close, then the state perturbing $B\,0_u^+$ in Se_2 is also $^3\Pi_u$ which gives, among others, the required 1_u state in case c.

The dissociation energy

Two methods have been previously used to study the dissociation energy of Se_2: (1) equilibrium studies; (2) ultraviolet spectroscopy by (*a*) band convergence studies, and (*b*) predissociation studies.

(1) Early equilibrium studies were used by Goldfinger, Jeunehomme & Rosen (1936) to obtain an approximate value for the dissociation energy of either 60 or 70 kcal. The value depended on the statistical weight of the ground state and since this is now known to be 3, at least at high temperatures, the derived value is 60 kcal.

(2) Band convergence and predissociation studies require accurate assessment of dissociation limits and correct assignment of atomic and molecular states. Previous analyses have been shown to be wrong on both counts so that their conclusions are unreliable: however, some points are relevant.

(*a*) Linear (Birge–Sponer) extrapolation of the ground state vibrational levels of Rosen (1939) gives the value $D'' = 104$ kcal. In the other group VI molecules, O_2 and S_2, this method gives values which are about 25% too high; application of this rough correction gives $D'' = 83$ kcal. Vibrational levels in the upper state are now known to converge to a potential maximum so that this limit cannot be used to derive a dissociation limit.

(*b*) Rosen (1939) reported predissociations in $v' = 6$ to 10 at decreasing values of J and deduced a limit at 29500 cm^{-1}. Our failure to observe these predissociations in the recent high dispersion emission work has already been discussed. Rosen also studied the intense absorption predissociations for $v' \geqslant 22$ and deduced a limit at 30865 cm^{-1}. The absorption maximum was studied by Asundi & Parti (1937) who gave a limit at 31557 cm^{-1}. Nevin (1935) suggested that there was an induced predissociation with a limit at 30535 cm^{-1}. In 1963 Herman & Herman restudied the last few absorption bands with high dispersion but using natural selenium; their conclusions about the crossing of the potential curves were indefinite.

Olsson (1938) and Davis & Jenkins (1951) correctly assigned the cutoff in the emission bands with $v' = 6$ as a predissociation, and this was used to give an upper limit to D''_e of 28670 cm^{-1} but the vibrational numbering of the $v' = 6$ bands was incorrect—being assigned, for example, as 10–6 instead of 6–3. The incorrect assignment of v' does not affect the dissociation limit but that for v'' does; correction lowers the value given by about 1100 cm^{-1}. However, the observation of only one predissociation cannot provide information about the stability of the state causing it.

Using the results from these methods, Gaydon (1953) concluded that a value of 65 kcal was probably correct. Using the same information, Détry (1963–64) recently deduced a value of 74 ± 3 kcal. Both these conclusions must be rejected because the upper state converges to a potential maximum and the increase in diffuseness arises from a quite different interaction with a perturbing state. Also there is the failure to differentiate between the various isotopic species, and the non-recognition of the triplet nature of the transition.

The dissociation energy may be derived, however, by using the results of the present analysis of the $^3\Sigma_u^-$–$^3\Sigma_g^-$ transition. It has been shown that λ'' is large and positive. The F_1 component therefore lies below the F_2, F_3 components of $^3\Sigma_g^-$ so that in the case *c* limit the 0_g^+ component lies below the 1_g component. The potential curves for these components are then independent but they may be quite similar.

The dissociation limits of the two states which predissociate $B\,0_u^+$ lie at 27700 and 29690 cm^{-1}, with a separation equal to the interval $^3P_1$–$^3P_2$ in the Se atom. There are then three possibilities, according to the state of excitation of the second selenium atom, for the configurations of the atoms at these limits:

I	II	III
$^3P_1 + {}^3P_2$	$^3P_1 + {}^3P_1$	$^3P_1 + {}^3P_0$
$^3P_2 + {}^3P_2$	$^3P_2 + {}^3P_1$	$^3P_2 + {}^3P_0$
$D_e = 27700$	25710	25166 cm^{-1}
or 79·18	73·49	71·94 kcal/mole

Recent mass-spectroscopic studies of the dissociation equilibrium have been used by Jeunehomme (1962) and by Détry (1963–64) to derive the values 77·2 ± 5 and 74 ± 3 kcal respectively. J. Drowart, in a personal communication (1965), considers that the best value at present available is $D_0''(Se_2) = 75 \pm 2$ kcal, equivalent to $D_e(Se_2) = 26430 \pm 700$ cm^{-1}. This supports assignment II above, but the value is hardly precise enough to serve to eliminate I and III which would require errors of no more than ±4 kcal in the mass-spectroscopic value. To proceed we must consider more detailed spectroscopic arguments.

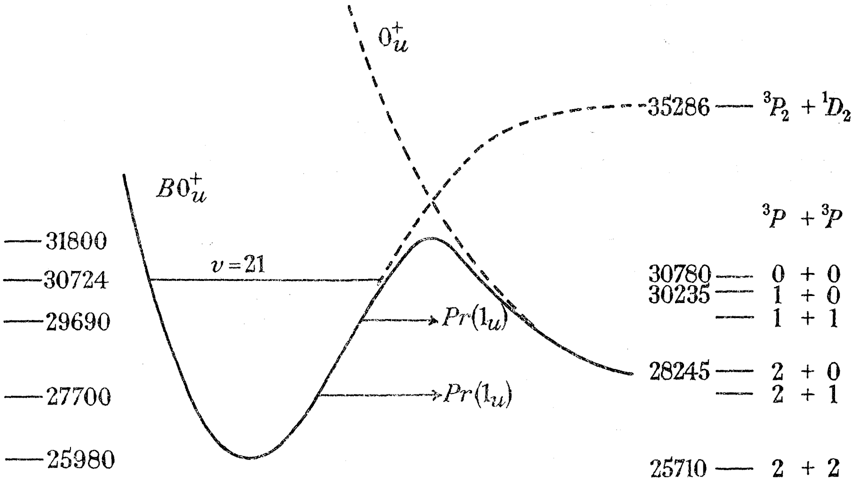

FIGURE 14. Correlations of molecular states with the states of the separated atoms.

Gaydon (1953) lists the correlation of molecular Ω values with atomic J. Now assignment *I* may be eliminated as follows. The displacement of the levels $v > 15$ of $B0_u^+$ from their expected positions is most readily interpreted as a homogeneous perturbation with an unstable 0_u^+ state whose asymptote must lie *lower* than the first level in $B0_u^+$ which is clearly perturbed: i.e. below $v = 14$ at $T' > 29320$ cm^{-1}. According to assignment I, the only atom pair below this limit is $^3P_2 + {}^3P_2$: this pair does not combine to give a 0_u^+ state. Even if it were, improbably, supposed that there were appreciable interaction at $v = 14$ in $B0_u^+$ with the 0_u^+ state arising from $^3P_2 + {}^3P_1$ at 29690 cm^{-1}, the evidence from the spectrum of S_2 would suggest that this 0_u^+ state is a component of the $^3\Pi_u$ state which perturbs and predissociates $B^3\Sigma_u^-$ in S_2. This is not then the repulsive state which is required to explain the strong homogeneous perturbation of the upper levels of $B0_u^+$ in Se_2. Assignment I may then be rejected, and we consider now assignments II and III. The energy relations according to II are illustrated in figure 14.

Both II and III provide molecular states of the correct symmetry in the right relative positions. For example, considering II, the combination $^3P_1 + {}^3P_1$ gives rise to only one state 1_u, which can interact with $B0_u^+$. This may be identified with the stable state which perturbs and predissociates $B0_u^+$ with a limit at 29690 cm^{-1}. The combination $^3P_2 + {}^3P_0$ gives rise to single 1_u and 0_u^+ states, amongst others, of which the 0_u^+ state is considered to be responsible for the homogeneous perturbation of $B0_u^+$ at $v > 15$. $^3P_2 + {}^3P_1$ atoms give a single 0_u^+ and three 1_u states. The former is expected to be a component of a shallow $^3\Pi_u$ state: one of the latter may be assigned as the stable state with a predissociation limit at 27700 cm^{-1}. The 2_u state responsible for the accidental predissociations may be correlated either with $^3P_2 + {}^3P_2$ or $^3P_2 + {}^3P_1$. Similar statements may be made about assignment III:

however, we favour II on the ground that the natural correlation between molecular and atomic states is that which relates the lowest molecular terms to the lowest atomic states of the correct symmetry.

The derived value for $D''_e(\mathrm{Se_2})$ is thus $25710 \pm 20\ \mathrm{cm^{-1}}$, so that $D^0_0(\mathrm{Se_2}) = 25518 \pm 20\ \mathrm{cm^{-1}}$, equivalent to $72{\cdot}94 \pm 0{\cdot}03$ kcal/mole.

Potential energy curves for $B\,0_u^+$ and $X\,0_g^+$

A potential energy curve for $B\,0_u^+$ was required for consideration of the predissociations in this state. The Rydberg–Klein method, as described by Richards & Barrow (1964), was used. The data for $B\,0_u^+$ were taken from observed values where known and from interlated values for others, e.g. for $v = 10$ and 12 of $^{80}\mathrm{Se_2}$. The method becomes unreliable at low values of v, and values of $r_{\mathrm{min.}}$ and $r_{\mathrm{max.}}$ were computed for $v \geqslant 8$. The resulting curve is given in figure 15 together with the Morse curve, which may be used at lower values of v. The value of D'_0 used for the Morse curve was calculated from the limit at $\mathrm{Se}(^3P_2) + \mathrm{Se}(^1D_2)$ and the derived value of D''_0. The agreement between the two curves is not good, but the difference is about the same as for $X\,0_g^+$ (see figure 16).

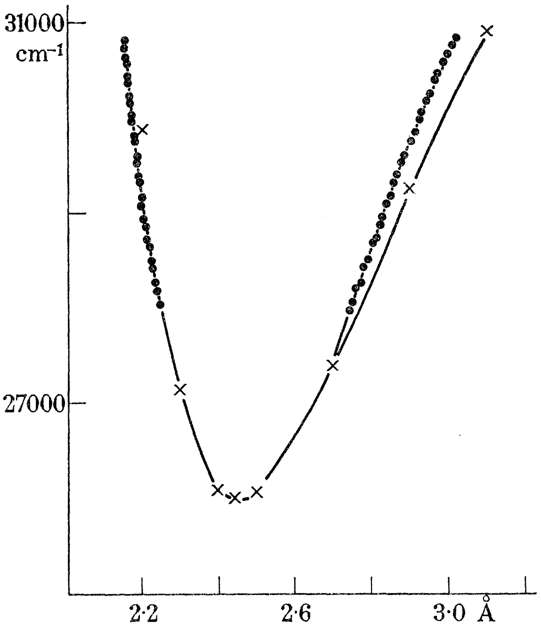

FIGURE 15. Potential energy curve for the state $B\,0_u^+$. ×, Morse curve; ●●●, calculated by the Rydberg–Klein method.

The Rydberg–Klein calculations for $B\,0_u^+$ of $^{78}\mathrm{Se_2}$ and $^{80}\mathrm{Se_2}$ were done separately, and the agreement is seen to be excellent. This shows that the method may be used satisfactorily in a region of homogeneous perturbation: for $v > 15$ in $B\,0_u^+$ the right hand limb shows increasing curvature with increasing v, while the left hand limb remains regular. Indeed the vibrational intervals in $B\,0_u^+$ converge quite rapidly to a limit at about $31800\ \mathrm{cm^{-1}}$ above the minimum of $X\,0_g^+$. However, the separations between the limits, for example, $31800 - 27700 = 4100\ \mathrm{cm^{-1}}$ do not correspond to any intervals in the term scheme of the low lying states of Se I. It is clear, then, that, as has been remarked above, the limit at 31 800 cm^{-1} represents a potential maximum, formed by the avoided crossing of an unstable 0_u^+ state arising from $^3P_2+{}^3P_0$ with a stable 0_u^+ state from $^3P_2+{}^1D$. Indeed the *low* vibrational levels of $B\,0_u^+$ may be extrapolated very naturally to a limit corresponding to Se $^3P_2$+Se $^1D_2$. This behaviour is in sharp contrast to that of the case b $^3\Sigma_u^-$ state of O_2. The atom pair $^3P+{}^3P$ does not yield a case b $^3\Sigma_u^-$ state, and B $^3\Sigma_u^-$ in O_2 dissociates to O ^3P+O ^1D and no potential maximum is formed (Brix & Herzberg 1954).

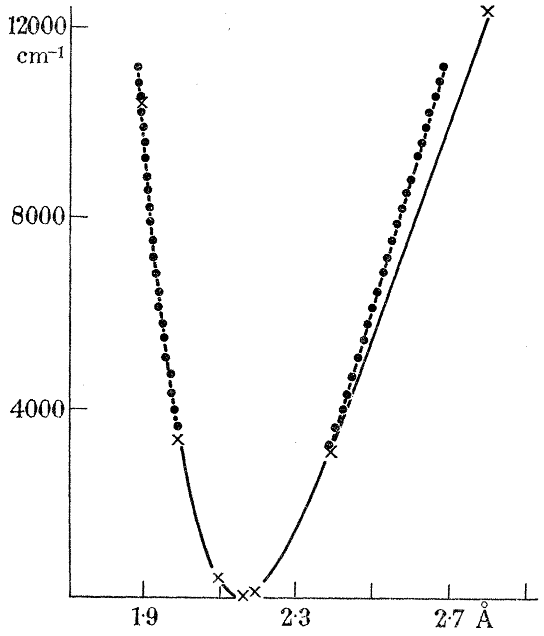

FIGURE 16. Potential energy curve for the ground state $X\,0_g^+$. ×, Morse curve; ●●●, calculated by the Rydberg–Klein method.

CONCLUSIONS

The main system, $B-X$, of the Se_2 molecule is found to arise from transitions 0_u^+–0_g^+, 1_u–1_g, the case c analogues of a $^3\Sigma_u^-$–$^3\Sigma_g^-$ transition. Related predissociations in $B\,0_u^+$ enable a precise value for the dissociation energy in the ground state, $X\,0_g^+$, to be determined. These predissociations also enable it to be shown that the state $B\,0_u^+$ dissociates to a potential maximum formed by the avoided crossing of a stable and an unstable 0_u^+ state. $B\,1_u$ is still more strongly predissociated than $B\,0_u^+$, and only one predissociation has been observed. The indications are that $X\,1_g$ lies above $X\,0_g^+$ by some hundreds of wavenumbers, but a precise value for this separation has not yet been determined. Thus at low temperatures the Se_2 molecule will behave thermodynamically as if the ground state were a singlet state and at high temperatures as if the ground state were a triplet. Observation of the 1_u–1_g bands in absorption with short paths at $t < 800$ °C shows that this temperature is not too high.

The case c character of the states of Se_2 leads to qualitative differences between the spectra of O_2 and S_2 on the one hand and of Se_2 on the other. Present indications are that the spectrum of Te_2 is, as expected, similar to that of Se_2, but that the separation $X\,1_g$–$X\,0_g^+$ is still larger in Te_2: however, further work on this molecule is in progress.

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APPENDIX

TABLE A1. VALUES OF Δ_2F FOR $v = 0$, $X0_g^+$ OF $^{78}Se_2$

J	$v' = 21$	20	19	18	17	16	15	14	13	12	11	10	8	m.v.
7	2·73	2·76	2·77	2·75	2·80	2·76	2·75	2·76	2·75	2·78		2·73		2·755
9	3·24	3·56	3·56	3·52	3·51	3·48	3·51	3·51	3·48	3·49	3·49		3·46	3·49
11	4·03	4·36	4·19	4·28	4·21	4·23	4·25	4·24	4·24	4·24	4·26	4·26	4·21	4·24
13	4·73	5·02	5·05	5·94	4·93	4·93	4·96	4·98	4·96	4·98	4·97	4·97	4·90	4·96
15	5·32	5·69	5·75	5·78	5·71	5·72	5·71	5·73	5·74	5·70	5·70	5·71	5·67	5·71
17	6·24	6·34	6·52	6·49	6·43	6·44	6·43	6·45	6·45	6·43	6·45	6·44	6·40	6·44
19	7·06	7·16	7·18	7·21	7·22	7·23	7·18	7·16	7·18	7·17	7·18	7·24	7·16	7·18
21	7·89	7·91	7·94	7·91	7·90	7·92	7·91	7·91	7·94	7·91	7·90	7·92	7·92	7·92
23	8·70	8·70	8·71	8·55	8·67	8·65	8·64	8·61	8·64	8·64	8·65	8·62	8·63	8·63
25	9·34	9·36	9·39	9·41	9·37	9·44	9·38		9·38	9·38	9·38	9·33	9·37	9·37
27	10·17	10·16	10·14	10·11	10·07	10·15	10·13	10·12	10·13	10·21	10·10	10·09	10·09	10·12
29	10·84	10·83	10·88	10·82	10·82	10·80	10·85	10·84	10·88	10·86	10·86	10·81	10·85	10·85
31	11·51	11·57	11·66	11·57	11·60	11·66	11·61	11·57	11·62	11·62	11·60	11·55	11·59	11·59
33	12·39	12·33	12·35	12·32	12·38	12·28	12·34	12·31	12·35	12·32	12·33	12·26	12·35	12·32
35	13·04	13·08	13·12	13·04	13·10	13·07	13·03	13·00	13·07	13·08	13·07	13·01	13·10	13·06
37	13·74	13·89	13·72	13·76	13·75	13·81	13·82		13·79	13·82	13·83	13·78	13·80	13·81
39	14·63	14·61	14·53	14·51	14·58	14·62	14·53		14·55	14·54	14·55	14·53	14·54	14·54
41	15·12	15·31	15·29	15·22	15·23	15·34	15·26	15·21	15·28	15·27	15·27	15·27	15·29	15·27
43	16·13	16·12	16·10	15·99	15·91	16·04	16·01	16·02	16·01	15·99	16·01	16·03	16·03	16·01
45	16·67	16·77	16·68	16·72	16·71	16·68				16·73	16·74	16·76	16·77	16·75
47	17·46	17·49	17·48	17·50	17·40	17·43	17·49	17·47	17·47	17·46	17·46	17·47	17·49	17·47
49	18·20	18·18	18·30	18·23		18·24	18·20	18·21	18·20	18·22	18·20	18·26	18·22	18·22
51		18·97	18·88	18·96		18·94		18·94	18·95	18·95	18·93	18·97	18·95	18·95
53		19·62	19·73	19·87		19·69		19·67	19·70	19·68		19·66	19·69	19·68
55		20·49	20·46	20·44		20·50		20·41		20·41		20·43	20·42	20·42
57		21·17	21·11	21·10		21·07		21·14		21·15		21·13	21·15	21·14
59		21·83	21·91	21·97		21·96		21·81		21·88		21·83	21·91	21·86
61								22·62		22·61		22·62	22·61	22·615
63								23·36		23·31	23·35	23·33		23·34
65								24·11			24·07	24·07	24·13	24·09
67								24·84		24·85	24·79	24·85	24·79	24·82
69								25·54		25·54	25·50	25·50		25·52
71								26·28		26·28	26·23			26·26
73										26·98	26·99			26·985
75									27·73	27·75	27·73	27·76		27·74
77									28·47	28·47	28·47	28·49		28·475
79									29·19	29·18	29·23	29·22		29·205
81									29·95			29·94		29·945
83									30·66			30·65		30·655
85									31·39			31·38		31·385
87									32·09			32·08		32·085

Values only for $8 \leqslant v' \leqslant 15$ were used in determining the means.

TABLE A2. VALUES OF Δ_2F FOR $v = 28$, $X1_g$ OF $^{80}\mathrm{Se}_2$

J	F_2			J	F_3		
	$v' = 3$	4	5		3	4	5
10				11			3·75
12		4·20		13			4·42
14		4·84		15			5·04
16		5·48		17	5·74		5·68
18		6·12	6·03	19	6·35	6·40	6·36
20		6·74	6·70	21	7·04	6·98	7·02
22		7·35	7·36	23	7·69	7·63	7·68
24		8·00	7·99	25	8·34	8·30	8·31
26		8·63	8·64	27	8·99	8·96	8·97
28	9·32	9·29	9·30	29	9·65	9·63	9·63
30	9·95	9·92	9·95	31	10·31	10·25	10·29
32	10·60	10·59	10·62	33	10·93	10·91	10·93
34	11·25	11·24	11·26	35	11·59	11·56	11·60
36	11·90	11·88	11·92	37	12·25	12·22	12·24
38	12·55	12·52	12·57	39	12·88	12·87	12·88
40	13·17	13·16	13·19	41	13·56	13·53	13·52
42	13·85	13·83	13·84	43	14·17	14·18	14·19
44	14·50	14·49	14·48	45	14·82	14·83	14·83
46	15·15	15·12	15·15	47	15·47	15·49	15·49
48	15·81	15·75	15·80	49	16·13	16·15	16·14
50	16·47	16·44	16·47	51	16·80	16·80	16·80
52	17·12	17·08	17·08	53	17·44	17·47	17·45
54	17·77	17·78	17·75	55	18·09	18·12	18·10
56	18·40	18·43	18·41	57	18·74	18·80	18·73
58	19·05	19·07	19·05	59	19·40	19·42	19·39
60	19·70	19·77	19·71	61	20·05	20·10	20·04
62	20·34	20·41	20·35	63	20·72	20·75	20·68
64	21·01	21·05	20·99	65	21·33	21·36	21·32
66	21·63	21·69	21·63	67	22·00	22·02	21·97
68	22·29	22·33	22·30	69	22·65	22·67	
70	22·94	22·95		71	23·29	23·29	
72		23·57		73		23·91	
74		24·19		75		24·53	
76		24·80		77		25·14	
78		25·46		79		25·78	
80		26·11		81		26·42	
82		26·75					
84		27·46					
86		28·02					

TABLE A3. WAVENUMBERS OF LINES OF $B\,0_u^+$–$X\,0_g^+$, ^{78}Se$_2$

	21–0 band		20–0 band	
J	R_{11}	P_{11}	R_{11}	P_{11}
2			30 393·45	
4			93·32	30 392·15
6			92·91	91·32
8			92·35	90·18
10			91·52	88·79
12			90·48	87·16
14			89·22	85·46
16	30 573·42	30 569·76	87·68	83·53
18	71·68	67·18	85·98	81·34
20	69·76	64·62	84·06	78·82
22	67·50	61·87	81·93	76·15
24	64·96	58·80	79·52	73·23
26	62·29	55·62	77·00	70·16
28	59·27	52·12	74·09	66·84
30	56·08	48·43	71·03	63·26
32	52·67	44·57	67·73	59·46
34	49·04	40·28	64·24	55·40
36	45·09	36·00	60·57	51·16
38	40·91	31·35	56·54	46·68
40	36·50	26·28	52·36	41·93
42	32·06	21·38	47·96	37·05
44	29·96	15·93	43·27	31·84
46	21·91	10·29	38·34	26·50
48	16·64	04·45	33·13	20·85
50	10·96	498·44	27·85	14·94
52	05·00		22·23	08·88
54	499·03		16·55	02·61
56			10·62	296·06
58			04·26	89·45
60			297·75	82·43
62			91·08	75·06
64			84·19	67·90
66				60·08

	19–0 band		18–0 band	
J	R_{11}	P_{11}	R_{11}	P_{11}
4	30 199·53		30 000·44	
6	99·12	30 197·43	00·08	29 998·39
8	98·63	96·36	29 999·55	97·31
10	97·78	95·07	98·85	96·03
12	96·86	93·59	97·81	94·57
14	95·61	91·81	96·70	92·87
16	94·21	89·86	95·26	90·91
18	92·48	87·69	93·59	88·77
20	90·63	85·30	91·84	86·38
22	88·58	82·69	89·71	83·93
24	86·22	79·87	87·54	81·16
26	83·69	76·83	85·04	79·13
28	80·95	73·55	82·36	74·93
30	77·98	70·07	79·46	71·54
32	74·76	66·32	76·34	67·89
34	71·39	62·41	73·06	64·02
36	67·63	58·27	69·44	60·02
38	63·88	53·91	65·70	55·68
40	59·77	49·35	61·77	51·19
42	55·57	44·48	57·59	46·55
44	50·96	39·47	53·17	41·60
46	46·31	34·28	48·57	36·45
48	41·39	28·83	43·75	31·07
50	36·16	23·09	38·66	25·52
52	30·74	17·28	33·44	19·70
54	25·11	11·01	27·84	13·57
56	19·27	04·65	22·14	07·40
58	13·26	098·16	16·29	01·04
60	06·90	91·35		
62	00·52	84·23		

TABLE A 3 (*cont.*)

	17–0 band		16–0 band	
J	R_{11}	P_{11}	R_{11}	P_{11}
2		29 796·25		29 589·04
4	29 796·82	95·59	29 589·65	88·35
6	96·49	94·74	89·31	87·58
8	95·94	93·74	88·78	86·51
10	95·21	92·43	88·07	85·30
12	94·37	91·00	87·13	83·84
14	93·12	89·34	86·04	82·20
16	91·76	87·41	84·69	80·32
18	90·20	85·33	83·17	78·25
20	88·42	82·98	81·42	75·94
22	86·43	80·52	79·45	73·50
24	84·22	77·76	77·34	70·80
26	81·77	74·85	74·95	67·90
28	79·14	71·70	72·35	64·80
30	76·38	68·32	69·68	61·55
32	73·34	64·78	66·62	58·02
34	70·02	60·96	63·44	54·34
36	66·56	56·92	60·06	50·37
38	62·94	52·81	56·53	46·25
40	59·02	48·36	52·66	41·91
42	54·90	43·79	48·62	37·32
44	50·59	38·99	44·37	32·58
46	46·14	33·88	39·93	27·69
48		28·74	35·37	22·50
50			30·47	17·13
52			25·44	11·53
54			20·28	05·75
56			14·62	499·78
58			09·07	93·55
60			03·46	87·11
62			497·31	80·57

	15–0 band				14–0 band			
J	R_{11}		P_{11}		R_{11}		P_{11}	
2	29 379·01		29 378·32					
4	78·90		77·70		29 165·47		29 164·28	
6	78·61		76·89		65·20		63·48	
8	78·11		75·85		64·73		62·45	
10	77·40		74·60		64·03		61·22	
12	76·46		73·15		63·15		59·79	
14	75·23		71·50		62·07		58·17	
16		74·30	69·52		60·76		56·34	
18		72·68		67·87	59·25		54·31	
20		70·90		65·50	57·51		52·09	
22		68·89		62·99	55·48		49·60	
24	67·17			60·25			46·87	
26	64·60		57·79			52·23		
28	61·78		54·47			49·19		42·11
30		59·44	50·93			46·17		38·35
32		56·03		47·83		43·14		34·60
34	53·23			43·69		39·78		30·83
36	50·04		40·20					26·78
38	46·45		36·22					
40	*42·89*		31·92		31·00			
42	38·77		*27·63*		25·86		15·79	
44	34·63		22·76				09·84	
46	30·34		17·81			17·97		
48	25·72		12·85			13·86		00·50
50	20·97		07·52			09·03		095·65
52	15·85		01·94			04·02		90·09
54	10·73		296·42			098·45		84·35
56	05·45		90·54		93·66			78·04
58	299·90		84·38		87·73		72·52	
60	94·16		78·09		82·31		65·92	
62	88·09		71·44		76·75		59·69	
64	81·96		65·01			69·86	53·39	
66	76·00		57·95			63·57		45·75
68						57·24		38·73
70						*51·54*		31·70
72								*25·26*

Lines printed in italics are the last lines observed in emission before predissociation. Perturbations are indicated by discontinuities in the columns.

TABLE A 3 (*cont.*)

	13–0 band				13–1 band			
J	R_{11}		P_{11}		R_{11}		P_{11}	
4			28 947·79		28 560·60		28 559·40	
6	28 948·76		46·99		60·34		58·59	
8	48·27		46·00		59·90		57·59	
10	47·63		44·79		59·20		56·40	
12	46·78		43·39		58·40		55·03	
14	45·71		41·82		57·38		53·46	
16	44·49		40·01		56·17		51·68	
18	43·05		38·04		54·73		49·73	
20	41·43		35·87		53·11		47·59	
22	39·58		33·49		51·32		45·24	
24	37·54		30·94		49·32		42·70	
26	35·30		28·16		47·09		39·96	
28	32·92		25·17		44·78		37·01	
30	30·31		22·04		42·17		33·93	
32	27·47		18·69		39·37		30·63	
34	24·41		15·12		36·35		27·10	
36		21·33	11·34			33·35	23·33	
38		17·85		07·54		29·92		19·54
40		14·22		03·30		26·33		15·38
42		10·37		898·94		22·52		11·07
44		06·34		94·36		18·54		06·55
46		02·08		89·61		14·31		01·84
48		897·62		84·61		09·93		496·93
50		92·90		79·42		05·27		91·76
52		88·01		73·97		00·40		86·39
54				68·31				80·81
56	78·30							
58	72·64		57·18					
60	66·81		50·75					
62	60·63		44·17					
64	54·30		37·23					
66			30·20					
68								
70								
72						445·11		
74						37·92		418·23
76		17·06				30·46		10·29
78		09·41		788·59		22·90		02·10
80		01·58		80·22		15·97		393·82
82		793·53		71·63		07·23		85·36
84		85·28		62·87		399·08		76·69
86		76·96		53·89		90·81		67·85
88				44·87				58·70

TABLE A3 (*cont.*)

	13–3 band		13–4 band	
J	R_{11}	P_{11}	R_{11}	P_{11}
4	27 790·18	27 788·87		
6	89·93	88·05		
8	89·47	87·09		
10	88·87	85·92	27 406·71	
12	88·05	84·62	05·87	27 402·38
14	87·09	83·05	04·92	00·87
16	85·92	81·34	03·73	399·19
18	84·62	79·46	02·38	97·30
20	82·98	77·36	00·87	95·30
22	*81·21*	75·06	*399·19*	93·02
24		*72·56*		*90*·56

	13–5 band		13–6 band	
J	R_{11}	P_{11}	R_{11}	P_{11}
4	27 027·73	27 026·46	26 649·38	26 648·14
6	27·45	25·67	49·14	47·39
8	27·03	24·75	48·74	46·44
10	26·46	23·56	48·14	45·34
12	25·67	22·24	47·39	44·00
14	24·75	20·78	46·44	42·51
16	23·56	19·07	45·34	40·83
18	22·24	17·19	44·00	38·99
20	20·78	15·26	42·51	36·97
22	19·07		*40·83*	34·76
24				*32·37*

	12–0 band		12–1 band	
J	R_{11}	P_{11}	R_{11}	P_{11}
4	28 729·63		28 341·33	
6	29·37	28 727·60	41·10	28 339·27
8	28·94	26·62	40·65	38·32
10	28·32	25·45	40·07	37·16
12	27·50	24·08	39·27	35·82
14	26·47	22·52	38·26	34·25
16	25·27	20·77	37·08	32·56
18	23·86	18·84	35·71	30·65
20	22·28	16·69	34·12	28·53
22	20·49	14·37	32·32	26·22
24	18·49	11·85	30·38	23·72
26	16·43	09·11	28·35	21·03
28	14·11	06·22	26·07	18·17
30	11·54	03·25	23·54	15·24
32	08·79	699·92	20·85	11·96
34	05·85	96·47	17·93	08·56
36	02·71	92·77	14·82	04·91
38	699·35	88·89	11·49	01·07
40	95·81	84·81	08·02	297·03
42	92·06	80·54	04·34	92·80
44	88·13	76·07	00·45	88·38
46	84·01	71·40	296·38	83·78
48	79·69	66·55	92·11	78·97
50	75·16	61·47	87·66	73·97
52	70·44	56·21	82·98	68·77
54	65·50	50·76	78·14	63·40
56	60·35	45·09	73·03	57·79
58	55·06	39·20	67·84	51·98
60	49·44	33·18	62·29	46·03
62	43·67	26·83		39·77
64		20·36		
66	32·04			
68	25·64	07·19	38·82	20·37
70	19·05	00·01	32·33	13·38
72	12·22	592·77	25·59	06·16
74	05·28	85·24	13·73	198·70
76	597·98	77·53	11·51	91·09
78	90·24	69·51	03·90	83·17
80		61·06		74·80

TABLE A 3 (*cont.*)

	12–6 band	
J	R_{11}	P_{11}
42	26 396·01	
44	92·37	26 380·36
46	88·58	76·01
48	84·62	71·52
50	80·36	66·79
52	76·01	61·87
54		56·80

	12–4 band	
J	R_{11}	P_{11}
42	27 153·39	
44	49·61	27 137·57
46	45·74	33·12
48	41·68	28·47
50	37·57	23·67
52	33·12	18·74
54	28·22	13·55
56	23·35	08·17
58		02·57

	11–0 band		11–1 band	
J	R_{11}	P_{11}	R_{11}	P_{11}
4	28 507·83	28 506·55		
6	07·57	05·78	28 119·37	28 117·48
8	07·10	04·79	18·82	16·50
10	06·49	03·61	18·19	15·34
12	05·65	02·23	17·39	14·01
14	04·64	00·68	16·40	12·45
16	03·43	498·94	15·21	10·72
18	02·05	96·98	13·87	08·81
20	00·46	94·87	12·31	06·70
22	498·71	92·56	10·59	04·43
24	96·75	90·06	08·65	01·97
26	94·59	87·37	06·55	099·32
28	92·27	84·49	04·23	96·45
30	89·75	81·41	01·76	93·44
32	87·02	78·15	099·08	90·21
34	84·11	74·69	96·21	86·79
36	81·02	71·04	93·16	83·19
38	77·72	67·19	89·88	79·40
40	74·23	63·17	86·47	75·44
42	70·54	58·96	82·84	71·27
44	66·66	54·53	79·01	66·90
46	62·57	49·92	75·00	62·32
48	58·32	45·11	70·79	57·59
50	53·84	40·12	66·39	52·65
52		34·91		47·55
54				
56				
58				
60				
62	23·58		36·55	
64	17·66	00·23	30·71	13·30
66	11·61	393·59	24·73	06·72
68	05·36	86·82	18·58	00·02
70	398·91	79·86	12·21	27 993·13
72	92·26	72·68	05·63	86·03
74	85·36	65·27	27 998·83	78·72
76	78·22	52·63	91·77	71·18
78	70·81	49·75	84·50	63·44
80		41·58		55·43

TABLE A 3 (*cont.*)

J	11–2 band R_{11}	11–2 band P_{11}	11–3 band R_{11}	11–3 band P_{11}	11–4 band R_{11}	11–4 band P_{11}
6	27 733·17	27 731·26			26 966·56	
8	32·64	30·30			66·26	26 963·96
10	32·02	29·10	27 347·80	27 344·99	65·69	62·83
12	31·26	27·82	47·10	43·63	64·91	61·55
14	30·30	26·27	46·17	42·16	63·96	60·05
16	29·10	24·55	44·99	40·48	62·83	58·37
18	27·82	22·71	43·63	38·61	61·55	56·55
20	26·27	20·65	42·16	36·55	60·05	54·56
22		18·36	40·48		58·37	52·27
24					56·55	49·87
26					54·56	47·35
28						44·69

J	10–0 band R_{11}	10–0 band P_{11}	10–1 band R_{11}	10–1 band P_{11}
12	28 281·54	28 278·14	27 893·36	27 889·85
14	80·60	76·57	92·44	88·43
16	79·47	74·89	91·33	86·73
18	78·23	73·03	90·06	84·89
20	76·69	70·99	88·58	82·91
22	74·99	68·77	86·92	80·70
24	73·12	66·37	85·09	78·31
26	71·08	63·79	83·06	75·74
28	68·83	60·99	80·86	72·98
30	66·40	58·02	78·48	70·05
32	63·79	54·85	75·91	66·95
34	60·99	51·53	73·14	63·61
36	58·02	47·98	70·19	60·14
38	54·85	44·24	67·07	56·47
40	51·53	40·32	63·86	52·59
42	47·98	36·26	60·31	48·63
44	44·24	31·95	56·62	44·40
46	40·32	27·48	52·74	40·00
48	36·26	22·85	48·70	35·40
50	31·95	18·00	44·40	30·60
52	27·43	12·98	40·00	25·62
54	22·78	07·77	35·40	20·46
56	17·89	02·35	30·60	15·09
58	12·82	196·76	25·62	09·55
60	07·60	90·98	20·46	03·79
62	02·13	84·98	15·09	797·91
64	196·49	78·80	09·55	91·81
66	90·70	72·42	03·79	85·53
68	84·59	65·85	797·82	79·05
70		59·09		72·35
72				
74	65·75		79·18	
76	58·87	37·99	72·41	51·54
78	51·85	30·38	65·51	44·04
80	44·68	22·63	58·43	36·37
82	37·28	14·74	51·15	28·59
84	29·73	06·63	43·69	20·56
86	21·96	098·35	36·03	12·38
88	14·01	89·88	28·19	04·00
90	05·90	81·20	20·13	695·42
92	097·55	72·33	11·92	86·66
94	89·03	63·27	03·48	77·71
96	80·30	54·02	694·87	68·56
98	71·35	44·56	86·04	59·23
100	62·32	34·91	77·06	49·68
102	52·97	25·09	67·88	40·02
104	43·44	15·06	58·49	30·13
106	33·71	04·80	48·90	20·03

TABLE A3 (*cont.*)

	9–1 band		9–2 band	
J	R_{11}	P_{11}	R_{11}	P_{11}
6	27 668·05	27 666·11		27 279·96
8	67·50	65·18	27 281·33	79·02
10	66·90	63·99	80·73	77·86
12	66·11	62·65	79·96	76·53
14	65·18	61·12	79·09	75·05
16	63·99	59·44	77·86	73·37
18	62·65	57·54	76·53	71·51
20	61·12	55·46	75·05	69·45
22	59·44	53·20	73·37	67·20
24	57·54	50·72	71·51	64·70
26	55·46	48·02	69·45	62·10
28	53·20	45·22		59·35
30	50·72	42·28		
32	48·02	39·10		
34	45·22	35·68		
36	42·28	32·05		
38		28·30		

	8–0 band		8–1 band	
J	R_{11}	P_{11}	R_{11}	P_{11}
6	27 826·96			
8	26·55	27 824·23	27 438·30	27 435·98
10	25·98	23·09	37·69	34·79
12	25·19	21·77	36·91	33·47
14	24·23	20·29	35·98	31·99
16	23·09	18·56	34·86	30·32
18	21·77	16·69	33·57	28·46
20	20·29	14·61	32·09	26·41
22	18·56	12·37	30·42	24·20
24	16·69	09·93	28·56	21·80
26	14·61	07·32	26·53	19·22
28	12·37	04·52	24·32	16·45
30	09·93	01·52	21·92	13·51
32	07·32	798·34	19·33	10·37
34	04·52	94·97	16·58	07·07
36	01·52	91·42	13·61	03·56
38	798·34	87·72	10·47	399·87
40	94·97	83·80	07·15	96·00
42	91·42	79·68	03·64	91·94
44	87·66	75·39	399·93	87·69
46	83·70	70·89	96·04	83·27
48	79·58	66·21	91·98	78·63
50	75·25	61·36	87·72	73·83
52	70·72	56·30	83·27	68·85
54	66·00	51·04	78·63	63·67
56	61·09	45·58	73·79	58·30
58	55·99	39·94	68·75	52·72
60	50·67	34·08	63·50	46·95
62	45·13	28·06	58·06	40·98
64	39·40	21·73	52·40	34·81
66	33·38	15·27	46·51	28·40
68		08·59		21·79

TABLE A3 (*cont.*)

	7–1 band		4–3 band			
J	R_{11}	P_{11}	R_{11}		P_{11}	
6	27 207·03					
8	06·66	27 204·27				
10	06·07	03·17	25 726·91		25 723·84	
12	05·35	01·86	26·22		22·71	
14	04·41	00·36	25·41		21·32	
16	03·32	198·72	24·41		19·77	
18	02·05	96·89	23·24		18·05	
20	00·59	94·89	21·95		16·18	
22	198·96	92·70	20·50		14·14	
24	97·15	90·34	18·82		11·89	
26	95·16	87·79	17·03		09·55	
28	92·99	85·07	15·06		07·01	
30	90·64	82·17	12·91		04·31	
32	88·11	79·09	10·60		01·45	
34	85·41	75·84	08·14		698·39	
36	82·52	72·38	05·51		95·22	
38	79·45	68·77	02·70		91·87	
40	76·21	64·98	699·74		88·33	
42	72·78	61·01	96·62		84·61	
44	69·17	56·84	93·30		80·77	
46	65·38	52·50	89·83		76·71	
48	61·42	47·98	86·21		72·52	
50	57·27	43·28	82·35		68·15	
52	52·93	38·38	78·34		63·59	
54	48·41	33·31	74·14		58·86	
56	43·71	28·08	69·62		53·90	
58	38·81	22·62	64·72		48·70	
60	33·73	17·01		62·89	43·06	
62	28·42	11·24		57·33		40·49
64		05·21		52·07		34·20
66		099·00		46·81		28·25
68		92·60		41·48		22·29
70				35·99		16·17
72				30·34		09·97
74			24·87			03·61
76			18·65		597·44	
78			12·51		90·45	
80			06·24		83·61	
82			599·79			
84			93·19			
86			86·40			

TABLE A3 (*cont.*)

	6–1 band		6–2 band		6–3 band	
J	R_{11}	P_{11}	R_{11}	P_{11}	R_{11}	P_{11}
4	26 973·39		26 586·85	26 585·63	26 202·73	
6	73·18		86·70	84·84	02·59	26 200·69
8	72·74	26 970·47	86·29	83·90	02·17	199·83
10	72·26	69·31	85·77	82·82	01·64	98·73
12	71·45	67·95	85·01	81·56	00·98	97·47
14	70·61	66·56	84·17	80·12	00·10	96·07
16	69·53	64·91	83·13	78·51	199·07	94·46
18	68·28	63·13	81·93	76·72	97·87	92·69
20	66·90	61·12	80·51	74·79	96·49	90·77
22	65·23	58·96	78·94	72·64	94·95	88·68
24	63·49	56·55	77·20	70·32	93·25	86·39
26	61·55	54·11	75·26	67·86	91·35	83·94
28	59·44	51·44	73·20	65·21	89·31	81·34
30	57·11	48·59	70·90	62·42	87·10	78·56
32	54·56	45·54	68·46	59·44	84·68	75·58
34	51·99	42·34	65·84	56·25	82·13	72·48
36	49·11	38·94	63·07	52·90	79·33	69·16
38	46·14	35·39	60·18	49·37	76·44	65·67
40	42·96	31·70	57·02	45·70	73·37	62·03
42	39·59	27·73	53·70	41·85	70·10	58·22
44	*36·07*	23·67	*50·22*	37·82	*66·68*	54·26
46		*19·38*	46·57	*33·60*	63·11	*50·09*
48			42·74	29·20	59·28	(45·77)
50			38·73	24·64	(55·35)	41·25
52			34·55	19·92	51·19	(36·59)
54			30·18	15·00	46·99	31·84
56	11·15	895·31	25·63	09·90	42·43	26·76
58	06·32	89·98	20·90	04·63	37·80	(21·55)
60			15·99	499·18	33·03	
62			10·88	93·55		
64				87·71		

	5–2 band			5–2 band (*cont.*)	
J	R_{11}	P_{11}	J	R_{11}	P_{11}
8	26 350·12	26 347·75	52	26 299·36	26 284·66
10	49·60	46·65	54	95·05	79·83
12	48·90	45·40	56	90·59	74·80
14	48·03	43·96	58	85·92	69·59
16	47·01	42·37	60	81·09	64·21
18	45·80	40·60	62	75·97	58·62
20	44·42	38·67	64	70·53	52·80
22	42·87	36·54	66	64·39	46·64
24	41·19	34·30	68	56·63	39·73
26	39·29	31·86	70		31·27
28	37·25	29·24	72	(50·72)	
30	35·04	26·46	74	44·21	24·03
32	32·65	23·51	76	(37·79)	16·66
34	30·07	20·37	78	(31·36)	09·54
36	27·36	17·11	80	(24·86)	(02·38)
38	24·46	13·65	82	(18·08)	(195·13)
40	21·40	10·03	84	(11·24)	(87·66)
42	18·16	06·24	86	(04·21)	(80·06)
44	14·75	02·27	88	(197·02)	(72·36)
46	11·15	298·13	90	(89·67)	(64·40)
48	07·40	93·80	92	(82·30)	(56·27)
50	03·47	89·32	94		(48·01)

Wavenumbers of lines observed only in absorption are given in parentheses.

Table A3 (*cont.*)

	3–4 band		2–5 band	
J	R_{11}	P_{11}	R_{11}	P_{11}
10	25 103·89		24 480·66	
12	03·24	25 099·70	80·09	24 476·52
14	02·45	98·36	79·34	75·20
16	01·51	96·85	78·43	73·74
18	00·41	95·18	77·37	72·08
20	099·14	93·36	76·18	70·32
22	97·72	91·37	74·81	68·39
24	96·13	89·23	73·29	66·31
26	94·38	86·91	71·62	64·08
28	92·45	84·44	69·81	61·68
30	90·35	81·79	67·83	59·13
32	88·03	78·96	65·70	56·42
34		75·91	63·42	53·58
36			60·99	50·56
38	81·23		58·38	47·41
40	78·24	66·95	55·64	44·09
42	75·17	63·24	52·75	40·62
44	71·98	59·45	49·69	37·01
46	68·63	55·53	46·50	33·21
48	65·14	51·45	43·13	29·29
50	61·49	47·24	39·61	25·21
52	57·69	42·85	35·93	20·98
54	53·73	38·33	32·11	16·59
56	49·62	33·64	28·12	12·04
58	45·34	28·79	24·00	07·35
60	40·89	23·77	19·72	02·51
62	36·29	18·59	15·28	397·49
64	31·54	13·26	10·69	92·34
66	26·61	07·75	05·94	87·04
68	21·52	02·09	01·04	81·58
70	16·26	24 996·26	396·00	75·95
72	10·84	90·26	90·78	70·18
74	05·26	84·10	85·41	64·24
76	24 999·52	77·78	79·90	58·15
78	93·60	71·26	74·21	51·91
80	87·52	64·61	68·40	45·48
82	81·24		62·40	
84	74·88		56·24	
86	68·30		49·94	
88	61·54		43·45	

Table A3 (*cont.*)

	1–8 band		0–7 band			
J	R_{11}	P_{11}	R_{11}		P_{11}	
14	23 105·77	23 101·62				
16	04·96	00·23				
18	03·99	098·70				
20	02·89	97·01				
22	01·62	95·18				
24	00·23	93·21	perturbed			
26	098·70	91·10				
28	97·01	88·84	23 223·84			
30	95·18	86·44	22·04		23 213·18	
32	93·21	83·88	20·04		10·73	
34	91·10	81·21	17·90		08·04	
36	88·84	78·36	15·67		05·21	
38	86·44	75·39	13·27		02·25	
40	83·88	72·26	10·80		199·13	
42	81·21	69·01	08·11		95·87	
44	78·36	65·59	05·29		92·48	
46	75·39	62·05	02·30		88·90	
48	72·26	58·36	199·20		85·25	
50	69·01	54·53	95·96		81·43	
52	65·59	50·55	92·56		77·45	
54	62·05	46·44	89·01		73·34	
56	58·36	42·20	85·31		69·11	
58	54·53	37·80	81·50		64·67	
60	50·55	33·24	77·52		60·14	
62	46·40	28·55	73·40		55·44	
64	42·14	23·70	69·11		50·61	
66	37·74	18·69	64·67		45·60	
68	33·14	13·55		60·41	40·45	
70	28·42	08·22		55·59		35·47
72	23·50	02·79		50·74		29·94
74		22 997·17		45·75		24·39
76				40·65		18·69
78				35·34		12·85
80				29·94		06·86
82				24·39		00·76
84				18·69		094·47
86				12·85		88·06
88				06·86		81·50
90				00·76		74·78
92				094·47		67·94
94				88·06		60·96

TABLE A4. WAVENUMBERS OF LINES OF $B\,0_u^+–X\,0_g^+$, $^{80}\mathrm{Se}_2$

J	21–0 band R_{11}	21–0 band P_{11}	20–0 band R_{11}	20–0 band P_{11}
6			30 346·04	
8			45·42	30 343·47
10			44·75	42·06
12	30 529·75	30 526·73	43·75	40·63
14	28·44	24·98	42·53	38·86
16	26·97	23·00	41·10	36·92
18	25·26	20·76	39·47	34·84
20	23·37	18·29	37·58	32·46
22	21·14	15·62	35·48	29·84
24	18·80	12·74	33·22	27·02
26	16·13	09·67	30·64	24·00
28	13·39	06·31	27·90	20·79
30	10·28	02·74	24·92	17·31
32	06·98	498·94	21·80	13·67
34	03·42	94·89	18·37	09·75
36	499·71	90·67	14·70	05·66
38	95·68	86·22	10·86	01·31
40	91·47	81·50	06·84	
42	87·01	76·58	02·58	
44	82·33	71·38		
46	77·46	66·05		
48	72·28	60·38		
50	66·91	54·62		
52	61·53	48·53		
54	55·50	42·22		
56	49·48			

J	19–0 band R_{11}	19–0 band P_{11}	18–0 band R_{11}	18–0 band P_{11}
4	30 153·68	30 152·55	29 955·91	29 954·79
6	53·32	51·60	55·55	53·95
8	52·77	50·59	55·02	52·86
10	51·98	49·32	54·33	51·63
12	51·06	47·92	53·38	50·19
14	49·84	46·20	52·27	48·55
16	48·47	44·30	50·90	46·68
18	46·93	42·20	49·31	44·58
20	45·05	39·86	47·54	42·32
22	43·00	37·29	45·52	39·81
24	40·77	34·59	43·35	37·12
26	38·34	31·68	40·99	34·22
28	35·64	28·46	38·39	31·09
30	32·80	25·10	35·54	27·78
32	29·69	21·53	32·53	24·25
34	26·38	17·70	29·30	20·48
36	22·91	13·65	25·85	16·55
38	19·14	09·42	22·20	12·37
40	15·17	05·00	18·38	08·05
42	11·05	00·32	14·31	03·49
44	06·66	095·44	10·02	898·68
46	02·02	90·35	05·56	93·68
48	097·29	85·04	00·89	88·47
50	92·31	79·54	895·97	83·11
52	87·08	73·75	90·83	77·51
54	81·61	67·95	85·53	71·67
56	76·00	61·68	79·96	
58	70·03		74·22	
60	63·98			

TABLE A4 (*cont*)

J	17–0 band		16–0 band	
	R_{11}	P_{11}	R_{11}	P_{11}
4	29 754·13	29 752·90	29 548·69	29 547·55
6	53·77	52·11	48·35	46·67
8	53·27	51·08	47·82	45·65
10	52·55	49·87	47·14	44·41
12	51·62	48·42	46·28	43·03
14	50·48	46·79	45·18	41·43
16	49·19	44·96	43·87	39·65
18	47·68	42·89	42·41	37·59
20	45·90	40·65	40·70	35·37
22	44·02	38·21	38·79	32·93
24	41·86	35·54	36·68	30·37
26	39·52	32·72	34·40	27·56
28	36·95	29·63	31·90	24·55
30	34·21	26·35	29·21	21·31
32	31·26	22·91	26·31	17·93
34	28·06	19·23	23·27	14·33
36	24·70	15·34	19·94	10·50
38	21·15	11·27	16·44	06·48
40	17·38	06·94	12·79	02·30
42	13·41	02·49	08·84	497·88
44	09·19	697·80	04·72	93·26
46	04·86	92·94	00·43	88·45
48	00·27	87·78	495·96	83·47
50	695·49	82·54	91·24	78·19
52	90·41	76·99	86·39	
54		71·26		

J	15–0 band				14–0 band			
	R_{11}		P_{11}		R_{11}		P_{11}	
4					29 128·49		29 127·26	
6					28·18		26·51	
8	29 339·35				27·70		25·46	
10	38·59		29 335·91		27·08		24·30	
12	37·67		34·44		26·21		22·94	
14	36·57		32·81		25·11		21·36	
16	35·28		31·03		23·86		19·58	
18	33·80		29·00		22·26	23·43	17·60	
20	32·07		26·79			21·01	15·29	16·48
22			24·36			19·12	12·78	13·31
24		28·16				17·10		10·70
26		26·11		18·99		14·84		07·93
28		23·55		16·25		12·43		05·00
30		20·74		12·97		09·76		01·85
32		17·62		09·40		06·85		098·46
34	15·24			05·63				94·83
36	11·77		02·39		00·80			
38	08·53		298·31		097·54		87·31	
40	04·76		94·36		93·87		83·33	
42	00·90	00·76	89·89		89·94		78·96	
44	297·47	296·96	85·30	85·16	85·88		74·32	
46		93·64	81·12	80·62	81·21		69·50	
48		*87·97*		75·56			64·16	
50				*70·22*				
52								
54						64·80		
56								44·90
58					54·44			
60					48·32		33·08	
62					42·52		26·29	
64					36·69		19·78	
66						30·21	13·26	
68						23·65		06·09
70						17·13		28 998·78
72						10·40		91·54
74						03·31		84·13
76						*28 996·83*		76·30
78								*69·09*

TABLE A4 (*cont.*)

	13–0 band				13–1 band			
J	R_{11}		P_{11}		R_{11}		P_{11}	
4	28 914·44		29 813·31					
6	14·16		12·45		28 530·74		28 529·07	
8	13·71		11·47		30·31		28·07	
10	13·04		10·25		29·68		26·92	
12	12·23		08·93		28·85		25·55	
14	11·23		07·38		27·87		24·03	
16	10·01		05·65		26·69		22·33	
18	08·62		03·73		25·30		20·41	
20	07·04		01·62		23·76		18·34	
22	05·27		899·31		21·99		16·05	
24	03·30		96·80		20·08		13·60	
26	01·09		94·13		17·92		10·94	
28	898·78		91·25		15·61		08·08	
30	96·44		88·15		13·11		05·05	
32	93·46		84·91		10·40		01·81	
34	90·55		81·43		07·51		498·41	
36	87·45		77·82		04·42		94·79	
38	84·11		73·95		01·14		91·00	
40	80·54		69·92		497·64		87·00	
42		77·25	65·66			94·38	82·80	
44		73·01		61·61		90·21		78·82
46		68·90		56·69		86·15		73·93
48		64·59		51·86		81·89		69·17
50		60·11		46·84		77·46		64·20
52		55·38		41·63		72·82		59·04
54		50·45		36·21		67·95		53·69
56		45·27		30·59		62·83		48·11
58				24·68				
60		34·93						
62		29·14		12·88				
64		23·28		06·44				
66		17·11		799·81				
68		10·73		92·93				
70		03·72		85·80				
72				78·09				
·								
·								
84	757·32							
86	48·64		26·72					
88	40·01		17·34					
90	31·42		07·96					
92	22·49		698·62					
94	*13·56*		89·00					
96			*79·37*					

	12–0 band				12–1 band	
J	R_{11}		P_{11}		R_{11}	P_{11}
		perturbation			perturbation	
44	28 657·91				28 275·04	
46	53·72		28 641·59		70·91	28 258·79
48	49·41		36·66		66·66	53·94
50	44·94		31·64		62·27	48·97
52	40·32		26·47		57·71	43·87
54	35·51		21·14		52·96	38·60
56	30·50		15·61		48·03	33·14
58	25·33		09·90		42·92	27·51
60	19·85		03·99		37·53	21·67
62	14·42		597·79		32·18	15·57
64	08·64		91·65		26·46	09·50
66	02·65		85·15			03·09
68			78·44			
70		590·29				
72		83·76		64·69		
74		77·01		57·44		
76		69·90		49·96		
78		62·86		42·15		
80				34·40		

Table A4 (*cont.*)

	11–0 band		11–1 band	
J	R_{11}	P_{11}	R_{11}	P_{11}
6	28 477·64	28 475·93	28 094·26	
8	77·21	74·94	93·84	28 091·57
10	76·60	73·80	93·23	90·44
12	75·80	72·47	92·46	89·12
14	74·83	70·96	91·48	87·62
16	73·67	69·27	90·35	85·95
18	72·32	67·39	89·03	84·09
20	70·79	65·31	87·52	82·06
22	69·08	63·07	85·83	79·82
24	67·18	60·65	83·98	77·42
26	65·11	58·03	81·92	74·85
28	62·83	55·23	79·68	72·07
30	60·39	52·25	77·26	69·13
32	57·75	49·08	74·66	66·00
34	54·93	45·73	71·88	62·68
36	51·91	42·19	68·92	59·18
38	48·72	38·47	65·77	55·51
40	45·35	34·55	62·45	51·65
42	41·78	30·45	58·90	47·60
44	38·03	26·18	55·21	43·37
46	34·08	21·70	51·33	38·97
48	29·94	17·04	47·25	34·35
50	25·61	12·20	42·97	29·55
52	21·07	07·16	38·49	24·59
54				
56			perturbation	
58				
60	01·53	385·68		
62	396·01	79·51		
64	90·39	73·24		
66	84·54	66·89		
68	75·52	60·34		
70	72·25	53·58		
72	65·85	46·64		
74	59·23	39·50		
76	52·32	32·16		
78		24·62		
	perturbation			

Table A4 (*cont.*)

J	10–0 band R_{11}	10–0 band P_{11}	10–1 band R_{11}	10–1 band P_{11}
	perturbation		perturbation	
36			27 848·81	
38	28 228·63		45·74	27 835·46
40	25·39	28 214·53	42·47	31·59
42	21·95	10·52	39·08	27·62
44	18·37	06·34	35·46	23·52
46	14·53	01·96	31·74	19·27
48	10·52	197·44	27·79	14·78
50	06·34	92·75	23·65	10·12
52	01·96	87·88	19·32	05·23
54	197·44	82·83	14·85	00·20
56	92·65	77·52	10·18	794·99
58	87·73	72·05	05·29	89·62
60	82·58	66·40	00·24	84·04
62	77·25	60·56	794·99	78·27
64	71·70	54·49	89·49	72·29
66	65·88	48·22	83·75	66·10
68		41·67		59·64
70				
72	perturbation			
74				
76				
78				
80			40·12	18·64
82			33·03	11·08
84			25·77	03·28
86			18·34	695·34
88			10·72	87·16
90			02·92	78·82
92			694·94	70·31
94			86·74	61·58
96			78·38	52·70
98			69·80	43·62

J	9–1 band R_{11}	9–1 band P_{11}	9–2 band R_{11}	9–2 band P_{11}
6	27 647·98			
8	47·56	27 645·30	27 266·14	
10	47·02	44·19	65·52	27 262·75
12	46·25	42·87	64·76	61·45
14	45·30	41·41	63·85	60·00
16	44·19	39·73	62·75	58·35
18	42·87	37·92	61·45	56·52
20	41·41	35·85	60·00	54·54
22	39·73	33·71	58·35	52·35
24	37·92	31·30	56·52	50·01
26	35·85	28·75	54·54	47·42
28	33·61	25·99		44·69
30	31·19	23·04		
32	28·63	19·90		
34	25·81	16·58		
36	22·86	13·11		
38	19·65	09·43		
40	16·31	05·56		
42	12·72	01·46		
44	08·97	597·20		
46	05·07	92·72		
48	00·96	88·10		

Table A4 (*cont.*)

	8–0 band		8–1 band	
J	R_{11}	P_{11}	R_{11}	P_{11}
6	27 804·69		27 421·27	27 419·51
8	04·31	27 802·02	20·90	18·59
10	03·71	00·90	20·36	17·49
12	02·95	799·62	19·60	16·22
14	02·02	98·14	18·70	14·78
16	00·90	96·49	17·60	13·14
18	799·62	94·66	16·32	11·33
20	98·14	92·64	14·87	09·36
22	96·49	90·47	13·25	07·18
24	94·66	88·08	11·45	04·85
26	92·64	85·50	09·47	02·32
28	90·47	82·80	07·31	399·62
30	88·08	79·89	04·97	96·75
32	85·50	76·80	02·45	93·69
34	82·80	73·53	399·75	90·47
36	79·89	70·06	96·86	87·04
38	76·80	66·41	93·83	83·48
40	73·53	62·61	90·61	79·70
42			87·17	75·75
44			83·58	71·64
46			79·81	67·33
48			75·85	62·84
50			71·68	58·15
52			67·38	53·28
54			62·84	48·22
56				42·99

perturbation

	7–1 band	
J	R_{11}	P_{11}
6	27 192·28	
8	91·94	27 189·63
10	91·38	88·51
12	90·66	87·27
14	89·76	85·82
16	88·69	84·23
18	87·45	82·45
20	86·05	80·48
22	84·46	78·35
24	82·69	76·05
26	80·76	73·58
28	78·64	70·92
30	76·36	68·10
32	73·91	65·11
34	71·29	61·94
36	68·47	58·59

	7–1 band (*cont.*)	
J	R_{11}	P_{11}
38	27 165·49	27 155·06
40	62·33	51·37
42	59·00	47·49
44	55·49	43·47
46	51·79	39·23
48	47·94	34·83
50	43·91	30·24
52	39·68	25·49
54	35·27	20·56
56	30·70	15·45
58	25·93	10·15
60	20·97	04·67
62	15·81	099·00
64	10·48	93·14
66	04·90	87·11
68	099·07	80·79
70	92·93	74·26
72		67·39

perturbation

Table A4 (*cont.*)

	6–3 band		6–31 band	
J	R_{11}	P_{11}	R_{11}	P_{11}
2		26 199·71		
4	26 200·40	99·19		
6	00·22	98·44		16 380·16
8	199·86	97·53	16 381·85	79·52
10	99·36	96·49	81·64	78·79
12	98·67	95·26	81·38	77·95
14	97·83	93·89	80·98	77·04
16	96·82	92·33	80·53	76·01
18	95·64	90·60	79·96	74·90
20	94·31	88·72	79·26	73·69
22	92·81	86·68	78·51	72·38
24	91·13	84·46	77·64	70·98
26	89·30	82·08	76·68	69·47
28	87·29	79·54	75·62	67·88
30	85·12	76·83	74·46	66·18
32	82·79	73·95	73·18	64·37
34	80·30	70·89	71·85	62·49
36	77·63	67·69	70·41	60·48
38	74·79	64·30	68·85	58·40
40	71·84	60·76	67·25	56·21
42	68·61	57·08	65·46	53·92
44	65·27	53·16	63·62	51·52
46	61·76	49·11	61·67	49·03
48	*58·06*	44·90	*59·60*	46·44
50		*40·50*		*43·73*

	5–2 band				5–4 band			
J	R_{11}		P_{11}		R_{11}		P_{11}	
2	26 346·40							
4	46·40		26 345·18		25 589·22		25 587·98	
6	46·23		44·44		89·06		87·28	
8	45·87		43·56		88·73		86·42	
10	45·36		42·49		88·25		85·37	
12	44·68		41·27		87·60		84·17	
14	43·84		39·87		86·79		82·81	
16	42·85		38·33		85·82		81·30	
18	41·69		36·62		84·70		79·63	
20	40·35		34·74		83·41		77·78	
22	38·85		32·69		81·96		75·79	
24	37·19		30·49		80·36		73·62	
26	35·36		28·09		78·57		71·29	
28	33·36		25·55		76·62		68·82	
30	31·20		22·85		74·54		66·18	
32	28·86		19·96		72·28		63·39	
34	26·38		16·94		69·87		60·43	
36	23·72		13·70		67·29		57·32	
38	20·88		10·34		64·56		54·03	
40	17·89		06·80		61·67		50·59	
42	14·72		03·09		58·60		46·98	
44	11·39		299·21		55·39		43·20	
46	07·89		95·17		51·97		39·28	
48	04·22		90·96		48·43		35·18	
50	00·36		86·58		44·70		30·93	
52	296·34		82·03		40·80		26·50	
54	92·10		77·30		36·69		21·90	
56	87·78		72·35		32·51		17·07	
58	83·16		67·32		28·04		12·17	
60	78·26		61·98		23·27		06·96	
62	72·91		56·38		18·07		01·53	
64	66·59	71·29	50·28		11·88	16·62	495·57	01·17
66		65·25	43·26	47·97		10·68		
68		59·55		41·21		05·15		
70		53·87		34·79		499·64		
72		48·10		28·41		94·04		
74		42·22		21·95				
76		36·19		15·38				
78		30·01		08·66				
80		*23·68*		01·74				
82				*194·67*				

TABLE A4 (*cont.*)

J	5–30 band				5–31 band			
	R_{11}		P_{11}		R_{11}		P_{11}	
6	16 471·65						16 146·72	
8	71·56		16 469·21		16 148·34		46·10	
10	71·36		68·49		48·21		45·34	
12	71·11		67·67		47·96		44·51	
14	70·71		66·76		47·60		43·60	
16	70·23		65·72		47·13		42·61	
18	69·65		64·61		46·58		41·51	
20	68·99		63·40		45·93		40·31	
22	68·23		62·08		45·19		39·04	
24	67·37		60·66		44·37		37·64	
26	66·42		59·15		43·43		36·17	
28	65·36		57·55		42·40		34·58	
30	64·21		55·85		41·30		32·92	
32	62·97		54·05		40·09		31·17	
34	61·61		52·16		38·77		29·32	
36	60·17		50·16		37·37		27·33	
38	58·62		48·07		35·89		25·33	
40	56·97		45·88		34·28		23·19	
42	55·23		43·60		32·58		20·96	
44	53·37		41·21		30·79		18·63	
46	51·43		38·71		28·92		16·20	
48	49·38		36·12		26·93		13·67	
50	47·25		33·45		24·84		11·05	
52	44·98		30·65		22·64		08·32	
54	42·63		27·74		20·30		05·49	
56	40·14		24·74		17·96		02·51	
58	37·48		21·63		15·37		099·52	
60	34·62		18·33		12·58		96·29	
62	31·35	36·84	14·81		09·39	14·95	92·86	
64	27·22	31·93	10·95	16·42	05·35	10·04	89·05	94·61
66		28·11	06·15	10·85		06·32	84·35	89·05
68		24·69		06·42		03·02		84·70
70		21·43		02·39		099·80		80·76
72		18·13		398·44		96·60		76·91
74		14·76		94·50		93·33		73·06
76		11·33		90·49		89·99		69·15
78		07·81		86·39		86·57		65·17
80		*04·19*		82·22		*82·92*		61·11
82				*77·98*				

J	4–3 band			
	R_{11}		P_{11}	
4			25 729·85	
6	25 730·95		29·13	
8	30·61		28·26	
10	30·11		27·20	
12	29·47		26·01	
14	28·65		24·65	
16	27·70		23·14	
18	26·56		21·49	
20	25·28		19·63	
22	23·84		17·63	
24	22·23		15·49	
26	20·48		13·17	
28	18·54		10·17	
30	16·46		08·05	
32	14·21		05·25	
34	11·79		02·29	
36	09·21		699·16	
38	06·44		95·88	
40	03·60		92·43	
42	00·50		88·88	
44	697·27		85·08	
46	93·86		81·11	
48	90·25		77·00	
50	86·40		72·69	
52	82·17	86·10	68·12	
54	77·15	80·58	63·19	67·12
56	25 675·71		25 657·44	60·87
58	71·09			55·28
60	66·47			49·96
62	61·75			44·63
64	56·88			39·20
66	51·88			33·63
68	46·71			27·92
70	41·40			22·05
72	35·94			16·05
74	30·31			09·87
76	24·51			03·53
78	18·59			597·06
80	12·46			90·39
82	06·21			83·58
84	599·77			76·61
86	93·18			69·45
88	86·42			62·16
90	79·49			54·71
92	72·40			47·10
94	65·14			39·28
96	57·74			31·37
98	50·15			23·27
100	42·40			14·95
102	34·45			06·49
104	*26·17*			497·83

Table A 4 (*cont.*)

	4–29 band				4–30 band			
J	R_{11}		P_{11}		R_{11}		P_{11}	
16	16 559·81		16 555·22					
18	59·24		54·12					
20	58·56		52·90					
22	57·79		51·58					
24	56·92		50·19					
26	55·96		48·68					
28	54·92		47·08					
30	53·78		45·38					
32	52·53		43·58					
34	51·18		41·70					
36	49·72		39·70					
38	48·16		37·60					
40	46·58		35·39					
42	44·81		33·19					
44	42·93		30·75		16 218·31		16 206·10	
46	40·97		28·23		16·39		03·65	
48	38·87		25·61		14·34		01·09	
50	36·58		22·87		12·10		198·39	
52	33·97		19·94					
54	30·67	34·09	16·70				92·36	96·31
56		30·98	12·74	16·19		06·70	88·45	91·91
58		28·18		12·41		04·00		88·21
60		25·46		08·99		01·34		84·83
62		22·69		05·62		198·66		81·55
64		19·86		02·20		95·89		78·20
66		16·94		498·71		93·06		74·81
68		13·94		95·14		90·13		71·33
70		10·83		91·48		87·12		67·79
72		07·64		87·73		84·00		64·14
74		04·36		83·89		80·80		60·40
76		00·96		79·96		77·50		56·54
78		497·48		75·93		74·12		52·62
80		93·88		71·79		70·66		48·58
82		90·20		67·57		67·09		44·46
84		86·43		63·27		63·43		40·23
86		82·54		58·85		59·67		35·93
88		78·57		54·33		55·81		31·53
90		74·50		49·71		51·84		27·02
92		70·31		44·98		47·78		22·42
94		66·04		40·18		43·60		17·75
96		61·70		35·29		39·34		12·95
98		57·20		30·27		34·98		08·04
100		52·60		25·16		30·52		03·02
102		47·89		19·92		25·93		097·97
104		*42·96*		14·59		*21·12*		92·75
106				*09·04*				*87·27*

Table A4 (*cont.*)

	3–4 band		2–5 band	
J	R_{11}	P_{11}	R_{11}	P_{11}
10			24 499·29	
12			98·67	24 495·20
14	perturbation		97·92	93·90
16			97·07	92·47
18	25 111·79		96·03	90·88
20	10·42	25 104·87	94·86	89·15
22	08·99	02·81	93·54	87·27
24	07·43	00·67	92·04	85·24
26	05·71	098·39	90·42	83·05
28	03·85	95·97	88·64	80·72
30	01·83	93·39	86·72	78·24
32	099·66	90·68	84·63	75·61
34	97·35	87·81	82·41	72·81
36	94·88	84·77	80·04	69·88
38	92·26	81·60	77·52	66·81
40	89·46	78·27	74·84	63·57
42	86·54	74·78	72·02	60·18
44	83·45	71·15	69·03	56·65
46	80·20	67·36	65·90	52·97
48	76·80	63·39	62·62	49·12
50	73·24	59·28	59·19	45·14
52	69·54	55·02	55·61	41·01
54	65·68	50·60	51·87	36·74
56	61·65	46·02	48·00	32·31
58	57·45	41·30	43·96	27·74
60	53·13	36·40	39·79	22·99
62	48·65	31·36	35·46	18·14
64	43·99	26·16	30·98	13·11
66	39·18	20·81	26·36	07·92
68	34·21	15·31	21·57	02·61
70	29·10	09·65	16·66	397·13
72	23·85	03·82	11·58	91·49
74	18·42	24 997·88	06·35	85·71
76	12·84	91·75	00·96	79·77
78	07·10	85·47	395·43	73·68
80	01·20	79·02	89·73	67·43
82	24 995·17	72·44	83·91	61·06
84	88·97		77·89	54·49
86	82·59		71·74	47·78
88	76·05		65·43	40·92
90	69·39		58·93	
92			52·24	
94			45·29	
96			38·39	

Table A4 (*cont.*)

	1–8 band				0–7 band			
J	R_{11}		P_{11}		R_{11}		P_{11}	
16	23 140·20		23 135·62					
18	39·29		34·11					
20	38·20		32·46		perturbation			
22	36·99		30·67					
24	35·62		28·77		23 261·05			
26	34·11		26·71		59·56		23 252·11	
28	32·46		24·50		57·88		49·93	
30	30·67		22·16		56·11		47·56	
32	28·77		19·69		54·17		45·10	
34	26·71		17·06		52·11		42·50	
36	24·50		14·30		49·93		39·73	
38	22·16		11·40		47·56		36·85	
40	19·69		08·35		45·10		33·80	
42	17·06		05·17		42·50		30·63	
44	14·30		01·86		39·73		27·30	
46	11·40		098·40		36·85		23·84	
48	08·35		94·79		33·80		20·25	
50	05·17		91·07		30·63		16·52	
52	01·86		87·18		27·30		12·65	
54	098·40		83·15		23·84		08·61	
56	94·77		78·99		20·25		04·45	
58	91·03		74·66		16·52		00·14	
60	87·09		70·23		12·65		195·71	
62	83·03		65·62		08·61		91·11	
64	78·81		60·87		04·45		86·44	
66	74·33		55·97				81·51	
68		71·01	50·82					
70		65·90		46·81				
72		61·08		40·99		186·52		
74		56·16		35·50		81·66		60·83
76		51·13		29·85		76·66		55·27
78		45·98		24·13		71·54		49·58
80		40·67		18·27		66·25		43·79
82		35·24		12·25		60·83		37·79
84		29·66		06·08		55·27		31·66
86		23·95				49·58		25·41
88		18·09				43·79		19·03
90		12·07						12·46
92		05·92						

TABLE A5. WAVENUMBERS OF LINES OF $B1_u$–$X1_g$, ^{78}Se$_2$

1–9 band

J	R_{22}	P_{22}	J	R_{33}	P_{33}
25			26	22 276·46	22 269·00
27	22 275·41	22 267·59	28	74·80	66·65
29	73·63	65·25	30	73·00	64·25
31	71·74	62·74	32	71·05	61·75
33	69·69	60·13	34	69·00	59·09
35	67·50	57·38	36	66·77	56·31
37	65·16	54·46	38	64·41	53·36
39	62·68	51·40	40	61·92	50·29
41	60·05	48·19	42	59·27	47·06
43	57·30	44·86	44	56·51	43·71
45	54·38	41·37	46	53·59	40·21
47	51·35	37·74	48	50·53	36·58
49	48·19	33·99	50	47·32	32·79
51	44·79	30·08	52	43·99	28·89
53	41·32	26·02	54	40·50	24·82
55	37·70	21·84	56	36·87	20·63
57	33·95	17·50	58	33·10	16·29
59	30·04	13·02	60	29·20	11·81
61	25·97	08·40	62	25·15	07·20
63	21·77	03·63	64	20·95	02·43
65	17·42	198·72	66	16·60	197·53
67	12·92	93·67	68	12·10	92·47
69	08·26	88·45	70	07·44	87·26
71	03·46	83·07	72	02·60	81·88
73	198·46	77·55	74	197·53	76·33
75	93·28	71·86	76		70·55
77	87·81	65·94			
79		59·78			

1–8 band

J	R_{22}	P_{22}	J	R_{33}	P_{33}
15	22 657·28	22 652·90	16		
17	56·39	51·39	18		
19	55·32	49·74	20	22 654·81	22 648·89
21	54·08	47·94	22	53·54	47·05
23	52·70	45·99	24	52·16	45·07
25	51·19	43·89	26	50·59	42·93
27	49·52	41·65	28	48·89	40·68
29	47·69	39·27	30	47·05	38·27
31	45·75	36·74	32	45·07	35·72
33	43·64	34·09	34	42·93	33·00
35	41·41	31·26	36	40·68	30·17
37	39·02	28·29	38	38·27	27·19
39	36·49	25·19	40	35·72	24·07
41	33·81	21·94	42	33·00	20·80
43	30·99	18·54	44	30·17	17·37
45	28·03	15·02	46	27·19	13·84
47	24·92	11·34	48	24·07	10·15
49	21·67	07·51	50	20·80	06·32
51	18·27	03·54	52	17·37	02·33
53	14·72	599·43	54	13·84	598·21
55	11·04	95·16	56	10·15	93·92
57	07·20	90·75	58	06·32	89·51
59	03·23	86·19	60	02·33	84·96
61	599·08	81·49	62	598·21	80·26
63	94·80	76·65	64	93·92	75·42
65	90·37	71·67	66	89·51	70·43
67	85·77	66·52	68	84·92	65·29
69	81·05	61·24	70	80·17	60·00
71	76·13	55·78	72	75·25	54·54
73	71·07	50·18	74	70·10	48·91
75	65·79	44·39	76		43·04
77	60·24	38·41			
79		32·13			

Table A5 (*cont.*)

0–9 band

J	R_{22}	P_{22}	J	R_{33}	P_{33}
9			10	22 037·34	
11			12	36·84	22 033·19
13	22 036·48		14	36·23	32·09
15	35·78	22 031·31	16	35·46	30·68
17	34·89	29·87	18	34·67	29·21
19	33·92	28·29	20	33·54	27·59
21	32·82	26·61	22	32·37	25·86
23	31·52	24·77	24	31·07	23·94
25	30·11	22·77	26	29·64	21·94
27	28·58	20·66	28	28·05	19·80
29	26·91	18·40	30	26·33	17·50
31	25·08	15·99	32	24·49	15·06
33	23·11	13·45	34	22·49	12·50
35	21·03	10·78	36	20·37	09·80
37	18·78	07·96	38	18·11	06·96
39	16·41	05·01	40	15·71	03·97
41	13·89	01·91	42	13·18	00·86
43	11·22	21 998·67	44	10·51	21 997·60
45	08·42	95·29	46	07·70	94·21
47	05·48	91·79	48	04·75	90·69
49	02·41	88·12	50	01·67	87·02
51	21 999·18	84·33	52	21 998·45	83·21
53	95·81	80·39	54	95·07	79·28
55	92·32	76·31	56	91·58	75·20
57	88·67	72·10	58	87·93	70·99
59	84·89	67·74	60	84·15	66·64
61	80·95	63·25	62	80·23	62·14
63	76·88	58·61	64	76·16	57·51
65	72·67	53·85	66	71·97	52·75
67	68·33	48·91	68	67·63	47·84
69	63·82	43·85	70	63·12	42·77
71	59·18	38·63	72	58·49	37·56
73	54·38	33·26	74	53·68	32·19
75	49·40	27·74	76	48·65	26·66
77	44·25	22·06	78	43·39	20·94
79	38·84	16·19	80		14·96
81	33·10				

TABLE A 6. WAVENUMBERS OF LINES OF $B\,1_u$–$X\,1_g$, $^{80}\mathrm{Se}_2$

5–28 band

J	R_{22}	P_{22}	J	R_{33}	P_{33}
1			2		16 619·04
3			4		18·46
5			6		17·74
7			8		17·03
9	16 619·04		10	16 618·82	16·12
11	18·57		12	18·31	15·07
13	17·95		14	17·65	13·89
15	17·26		16	16·86	12·61
17	16·45	16 611·85	18	16·01	11·18
19	15·44	10·36	20	15·00	09·65
21	14·37	08·74	22	13·89	07·98
23	13·15	07·01	24	12·66	06·21
25	11·85	05·16	26	11·31	04·35
27	10·44	03·21	28	09·87	02·34
29	08·90	01·14	30	08·33	00·24
31	07·28	598·95	32	06·67	598·04
33	05·53	96·66	34	04·94	95·74
35	03·70	94·27	36	03·09	93·34
37	01·76	91·78	38	01·14	90·85
39	599·71	89·19	40	599·09	88·26
41	97·57	86·52	42	96·97	85·57
43	95·31	83·73	44	94·72	82·78
45	92·98	80·83	46	92·39	79·89
47	90·53	77·83	48	89·95	76·90
49	87·99	74·73	50	87·42	73·81
51	85·30	71·52	52	84·79	70·62
53	82·56	68·22	54	82·04	67·34
55	79·69	64·81	56	79·19	63·94
57	76·71	61·28	58	76·24	60·46
59	73·62	57·66	60	73·16	56·85
61	70·40	53·91	62	69·97	53·12
63	67·06	50·05	64	66·63	49·29
65	63·55	46·07	66	63·05	45·31
67	59·70	41·92	68	61·14	41·08
69	57·25	37·40	70	*56·48*	38·52
71	*52·92*	34·31	72		*33·19*
73		*29·33*			

TABLE A6 (*cont.*)

5–29 band

J	R_{22}		P_{22}		J	R_{33}		P_{33}	
					6			16 287·46	
7					8	16 288·65		86·62	
9	16 288·49				10	88·29		85·67	
11	88·03		16 284·97		12	87·77		84·55	
13	87·46		83·94		14	87·15		83·39	
15	86·74		82·75		16	86·39		82·12	
17	85·91		81·39		18	85·54		80·71	
19	84·97		79·87		20	84·55		79·24	
21	83·94		78·32		22	83·47		77·58	
23	82·75		76·62		24	82·27		75·82	
25	81·48		74·79		26	80·97		73·99	
27	80·12		72·88		28	79·60		72·01	
29	78·62		70·84		30	78·06		69·98	
31	77·02		68·69		32	76·44		67·80	
33	75·32		66·43		34	74·74		65·53	
35	73·52		64·09		36	72·93		63·19	
37	71·63		61·64		38	71·04		60·72	
39	69·63		59·10		40	69·04		58·16	
41	67·52		56·47		42	66·96		55·56	
43	65·34		53·72		44	64·76		52·80	
45	63·05		50·87		46	62·48		49·97	
47	60·64		47·93		48	60·10		47·05	
49	58·16		44·87		50	57·63		42·99	
51	55·56		41·74		52	55·04		40·87	
53	52·85		38·49		54	52·37		37·66	
55	50·06		35·15		56	49·59		34·34	
57	47·15		31·70		58	46·71		30·90	
59	44·11		28·14		60	43·70		27·39	
61	40·96		24·47		62	40·57		23·72	
63	37·68		20·68		64	37·31		19·96	
65	32·47		16·76		66	33·82		16·05	
67	30·49		12·69		68		32·00	11·91	
69		28·14	08·27		70		*27·39*		09·44
71		*23·89*		05·26	72				*04·20*
73				*00·38*					

TABLE A6 (*cont.*)

4–28 band

J	R_{22}		P_{22}		J	R_{33}		P_{33}	
3			16 382·37						
5			81·85						
7			81·20		8			16 380·98	
9			80·46		10			80·16	
11	16 382·82		79·59		12			79·26	
13	82·37		78·62		14			78·27	
15	81·85		77·53		16			77·14	
17	81·20		76·37		18	16 380·98		75·91	
19	80·46		75·08		20	80·16		74·58	
21	79·59		73·72		22	79·26		73·18	
23	78·62		72·24		24	78·27		71·63	
25	77·53		70·62		26	77·18		69·97	
27	76·37		68·90		28	76·01		68·22	
29	75·08		67·08		30	74·69		66·38	
31	73·72		65·16		32	73·29		64·44	
33	72·24		63·13		34	71·78		62·38	
35	70·62		61·00		36	70·17		60·22	
37	68·90		58·74		38	68·46		57·95	
39	67·08		56·38		40	66·65		55·59	
41	65·16		53·92		42	64·73		53·12	
43	63·13		51·33		44	62·70		50·55	
45	61·00		48·64		46	60·58		47·87	
47	58·74		45·88		48	58·35		45·09	
49	56·38		42·99		50	56·00		42·20	
51	53·92		39·94		52	53·57		39·20	
53	51·38		36·84		54	51·00		36·10	
55	48·69		33·60		56	48·34		32·88	
57	45·88		30·26		58	45·54		29·54	
59	42·99		26·81		60	42·66		26·12	
61	39·94		23·22		62	39·63		22·56	
63	36·74		19·53		64	36·45		18·88	
65	33·37		15·69		66	33·10	33·37	15·09	
67	29·54		11·68		68		29·92	11·09	11·34
69	25·34	26·81	07·21		70		26·28		07·25
71		22·97	02·31	03·86	72		22·50		02·99
73		19·03		299·40	74		18·53		298·59
75		14·90		94·84	76		14·28		94·00
77		10·52		90·10	78		09·68		89·14
79		05·78		85·06	80		04·45		83·90
81		00·49		79·67	82		298·59		78·03
83		294·51		73·74	84				71·57
85		87·70		67·05					
87				59·68					

TABLE A6 (*cont.*)

3–27 band

J	R_{22}	P_{22}	J	R_{33}	P_{33}
9			10	16 478·95	
11			12	78·59	
13			14	78·14	16 474·12
15	16 477·80	16 473·52	16	77·62	73·05
17	77·21	72·37	18	77·01	71·89
19	76·49	71·11	20	76·26	70·60
21	75·71	69·77	22	75·43	69·21
23	74·82	68·33	24	74·52	67·74
25	73·81	66·76	26	73·52	66·18
27	72·69	65·12	28	72·37	64·48
29	71·46	63·36	30	71·11	62·68
31	70·13	61·48	32	69·77	60·81
33	68·70	59·50	34	68·33	58·85
35	67·16	57·42	36	66·76	56·70
37	65·52	55·23	38	65·11	54·48
39	63·72	52·93	40	63·40	52·16
41	61·96	50·45	42	61·53	49·83
43	59·97	48·07	44	59·54	47·25
45	57·86	45·38	46	57·44	44·64
47	55·66	42·63	48	55·23	41·91
49	53·37	39·81	50	52·93	39·06
51	50·92	36·84	52	50·51	36·12
53	48·36	33·74	54	47·96	33·03
55	45·69	30·54	56	45·25	29·81
57	42·88	27·22	58	42·48	26·46
59	39·94	23·75	60	39·51	23·01
61	36·84	20·16	62	36·39	19·39
63	33·58	16·42	64	33·03	15·62
65	30·13	12·51	66	29·50	11·65
67	26·46	08·41	68	25·69	07·47
69	22·49	04·09	70		02·98
71	18·13	399·48			
73		94·50			
75		88·87			

3–28 band

J	R_{22}	P_{22}	J	R_{33}	P_{33}
9			10	16 146·29	
11			12	45·95	
13			14	45·56	
15			16	45·08	
17	16 144·68		18	44·46	16 139·34
19	44·04		20	43·78	38·11
21	43·27		22	43·01	36·74
23	42·42		24	42·09	35·32
25	41·38		26	41·09	33·75
27	40·31		28	39·99	32·10
29	39·12		30	38·77	30·32
31	37·82		32	37·47	28·46
33	36·42	16 127·22	34	36·07	26·54
35	34·92	25·17	36	34·58	24·48
37	33·31	23·02	38	32·92	22·33
39	31·53	20·76	40	31·31	20·04
41	29·84	18·36	42	29·46	17·75
43	27·90	16·00	44	27·53	15·29
45	25·87	13·40	46	25·51	12·71
47	23·74	10·72	48	23·35	10·04
49	21·48	07·93	50	21·12	07·22
51	19·11	05·01	52	18·76	04·32
53	16·63	01·99	54	16·27	01·32
55	14·02	098·86	56	13·67	098·18
57	11·28	95·62	58	10·93	94·93
59	08·42	92·23	60	08·04	91·53
61	05·39	88·72	62	04·97	87·99
63	02·21	85·05	64	01·73	84·29
65	098·81	81·20	66	098·27	80·40
67	95·23	77·18	68	94·53	76·27
69	91·36	72·94	70	90·44	71·88
71	87·07	68·42	72		67·15
73		63·56			

Table A 6 (*cont.*)

1–9 band

J	R_{22}	P_{22}	J	R_{33}	P_{33}
9			10	22 324·25	22 321·31
11	22 323·96	22 320·73	12	23·73	20·20
13	23·37	19·58	14	23·08	19·02
15	22·62	18·27	16	22·30	17·66
17	21·74	16·84	18	21·37	16·17
19	20·73	15·26	20	20·31	14·54
21	19·58	13·55	22	19·11	12·79
23	18·27	11·71	24	17·76	10·84
25	16·84	09·70	26	16·24	08·85
27	15·26	07·57	28	14·63	06·69
29	13·55	05·31	30	12·93	04·36
31	11·71	02·88	32	11·05	01·91
33	09·70	00·33	34	09·03	299·34
35	07·57	297·64	36	06·86	96·61
37	05·31	94·81	38	04·57	93·75
39	02·88	91·84	40	02·13	90·77
41	00·33	88·70	42	299·57	87·64
43	297·64	85·46	44	96·86	84·38
45	94·81	82·09	46	94·01	80·96
47	91·84	78·57	48	91·03	77·42
49	88·70	74·90	50	87·91	73·75
51	85·46	71·09	52	84·66	69·95
53	82·09	67·16	54	81·27	66·01
55	78·57	63·11	56	77·73	61·91
57	74·90	58·88	58	74·07	57·70
59	71·09	54·52	60	70·25	53·32
61	67·15	50·01	62	66·30	48·82
63	63·05	45·34	64	62·22	44·18
65	58·82	40·57	66	57·98	39·37
67	54·42	35·62	68	53·58	34·48
69	49·87	30·53	70	49·01	29·34
71	45·16	25·30	72	44·25	24·07
73	40·26	19·90	74	39·24	18·64
75	35·14	14·26	76		12·94
77	29·71	08·50			
79		02·36			

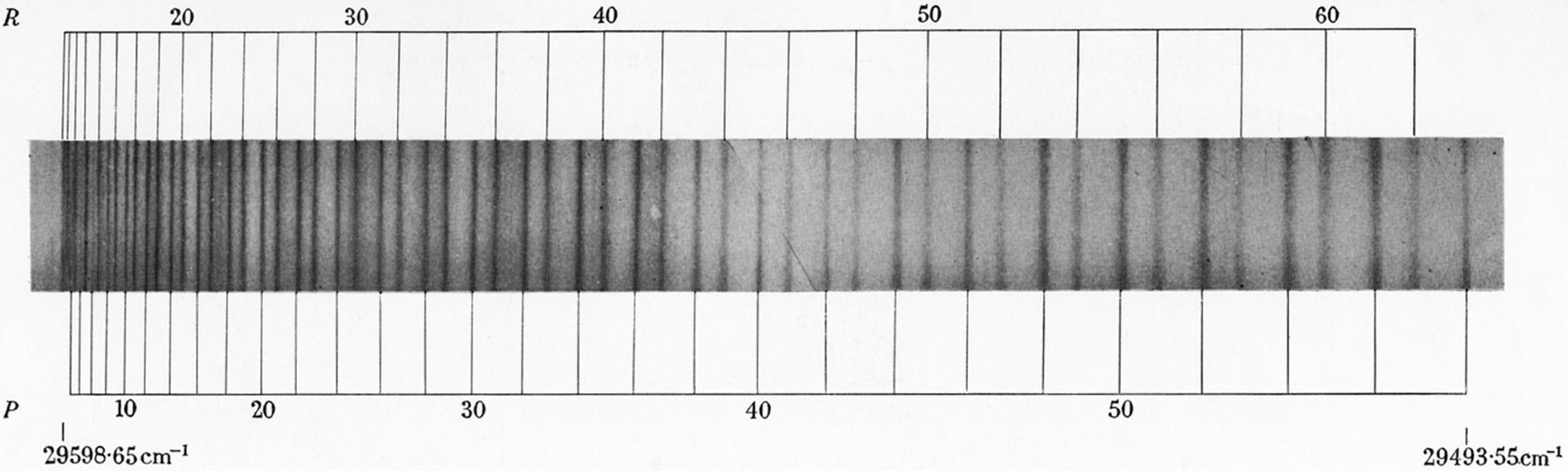
Table A6 (*cont.*)

1–8 band

J	R_{22}	P_{22}	J	R_{33}	P_{33}
13	22 693·13		14		
15	92·36	22 688·04	16	22 692·02	22 687·40
17	91·46	86·58	18	91·08	85·90
19	90·44	84·98	20	89·99	84·26
21	89·23	83·27	22	88·78	82·49
23	87·93	81·39	24	87·40	80·57
25	86·48	79·35	26	85·90	78·50
27	84·87	77·18	28	84·26	76·30
29	83·12	74·91	30	82·49	73·97
31	81·22	72·46	32	80·57	71·48
33	79·21	69·87	34	78·50	68·85
35	77·05	67·14	36	76·30	66·10
37	74·74	64·26	38	73·97	63·20
39	72·29	61·24	40	71·48	60·15
41	69·68	58·09	42	68·85	56·97
43	66·95	54·79	44	66·10	53·65
45	64·06	51·35	46	63·24	50·20
47	61·04	47·76	48	60·20	46·60
49	57·84	44·03	50	57·03	42·86
51	54·56	40·18	52	53·72	39·00
53	51·10	36·18	54	50·24	34·97
55	47·50	32·03	56	46·64	30·81
57	43·76	27·74	58	42·90	26·51
59	39·89	23·30	60	39·00	22·08
61	35·86	18·71	62	34·97	17·49
63	31·70	13·98	64	30·81	12·75
65	27·38	09·10	66	26·51	07·88
67	22·89	04·09	68	22·03	02·85
69	18·26	598·92	70	17·37	597·68
71	13·46	93·58	72	12·52	92·33
73	08·39	88·09	74	07·41	86·78
75	03·26	82·31	76		80·98
77	597·73	76·51			
79		70·31			

0–9 band

J	R_{22}	P_{22}	J	R_{33}	P_{33}
11			12	22 079·87	
13			14	79·26	22 075·14
15	22 078·79	22 074·45	16	78·51	73·86
17	77·99	73·06	18	77·63	72·40
19	77·02	71·52	20	76·63	70·82
21	75·91	69·85	22	75·48	69·10
23	74·67	68·06	24	74·20	67·26
25	73·29	66·15	26	72·80	65·30
27	71·77	64·04	28	71·23	63·18
29	70·12	61·83	30	69·57	60·95
31	68·35	59·48	32	67·76	58·56
33	66·42	57·01	34	65·80	56·05
35	64·37	54·39	36	63·73	53·41
37	62·19	51·65	38	61·51	50·62
39	59·86	48·75	40	59·17	47·73
41	57·38	45·71	42	56·69	44·67
43	54·78	42·56	44	54·07	41·48
45	52·04	39·25	46	51·31	38·17
47	49·16	35·81	48	48·43	34·72
49	46·14	32·24	50	45·40	31·13
51	43·00	28·53	52	42·25	27·41
53	39·70	24·67	54	38·94	23·56
55	36·28	20·68	56	35·51	19·58
57	32·70	16·57	58	31·93	15·43
59	28·97	12·30	60	28·22	11·18
61	25·12	07·90	62	24·34	06·77
63	21·11	03·34	64	20·33	02·20
65	16·96	21 998·63	66	16·13	21 997·50
67	12·63	93·78	68	11·76	92·60
69	08·10	88·75	70	07·06	87·51
71	03·30	83·53	72	01·84	82·11
73		78·02	74		76·21



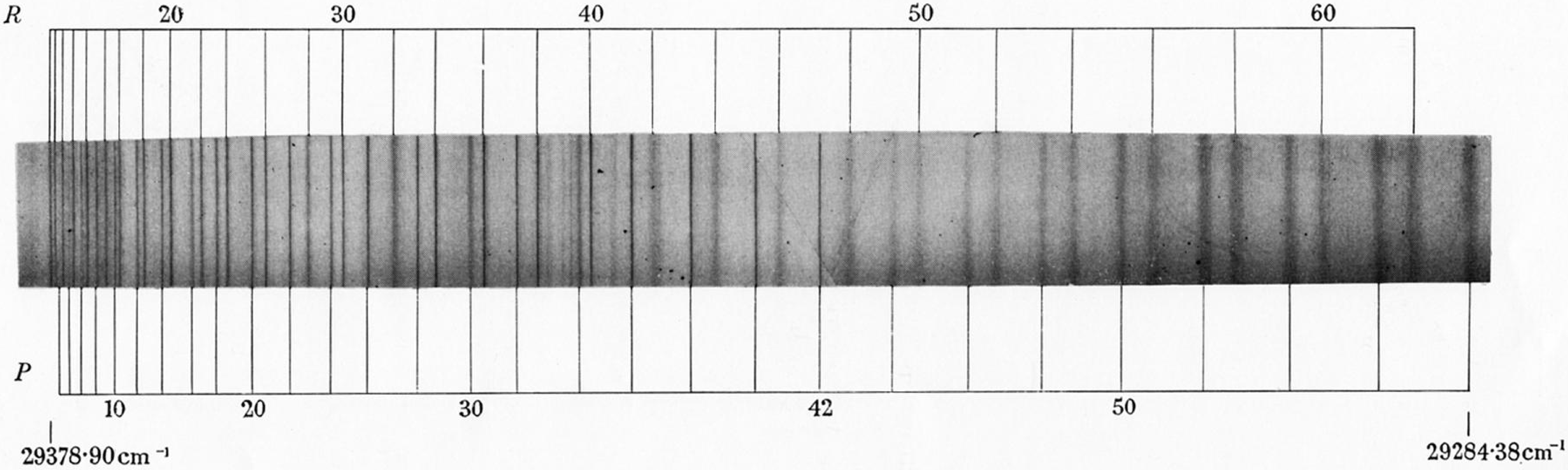
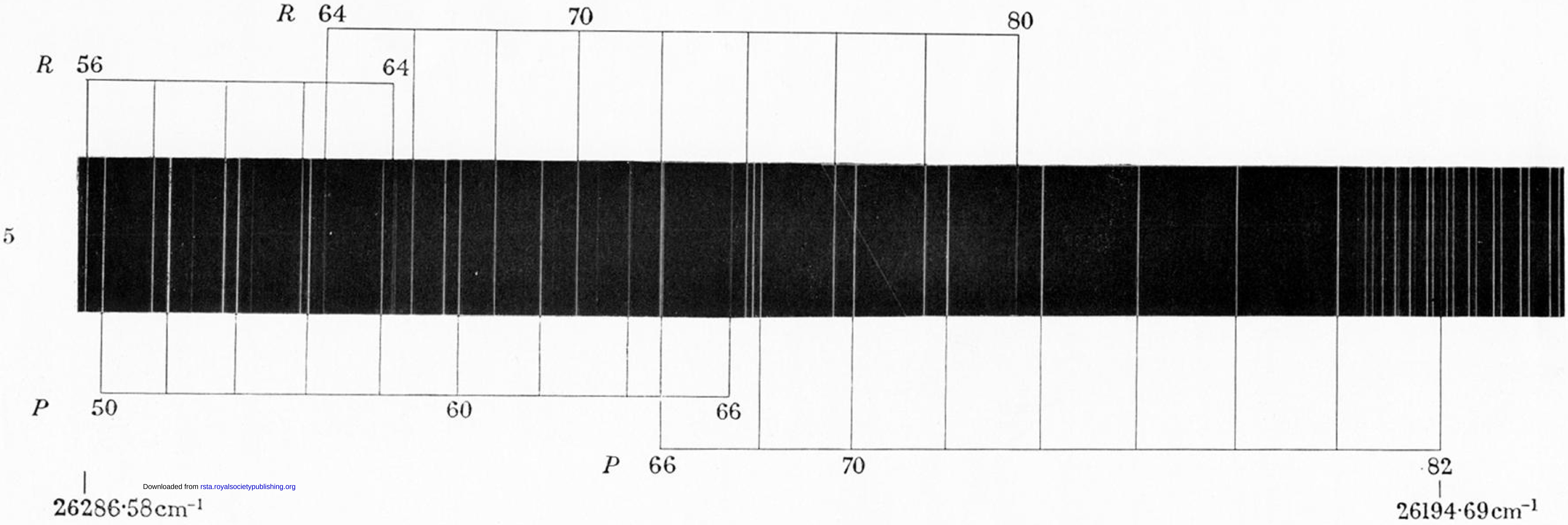


FIGURE 2. The 16–0 band of the system $B\,0_u^+ – X\,0_g^+$ of $^{78}Se_2$ observed in absorption.

FIGURE 4. The 15–0 band of the system $B\,0_u^+ – X\,0_g^+$ of $^{78}Se_2$ observed in absorption.



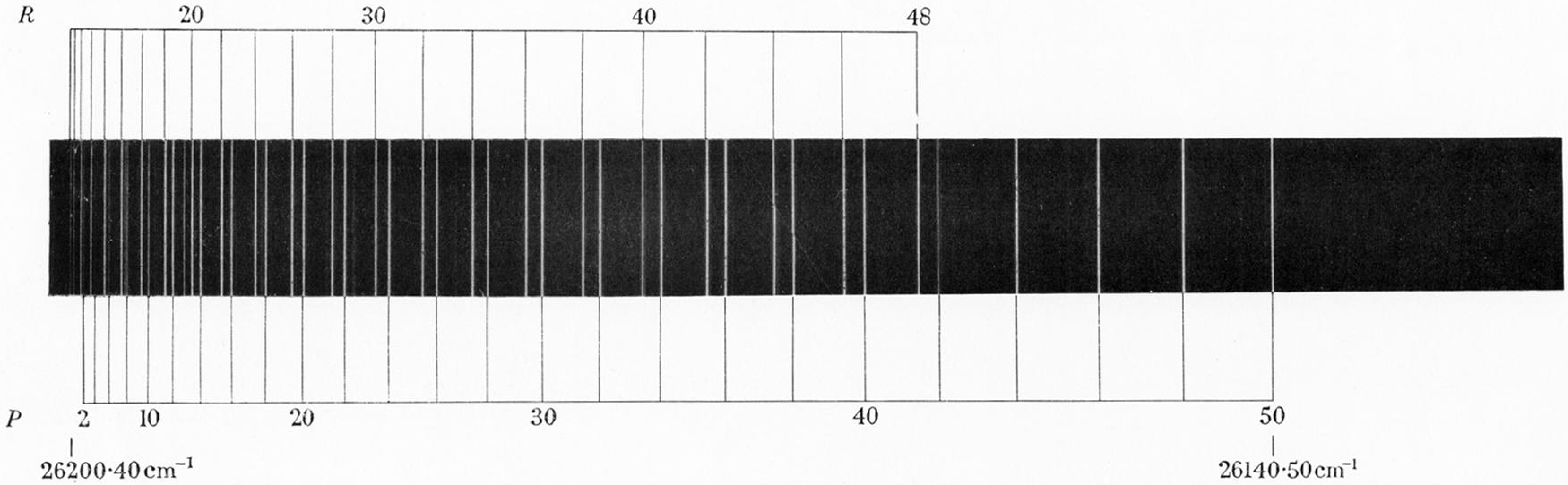


FIGURE 5. The 5–2 band of the system $B\,0_u^+–X\,0_g^+$ of $^{80}\mathrm{Se}_2$ observed in emission.

FIGURE 6. The 6–3 band of the system $B\,0_u^+–X\,0_g^+$ of $^{80}\mathrm{Se}_2$ observed in emission.

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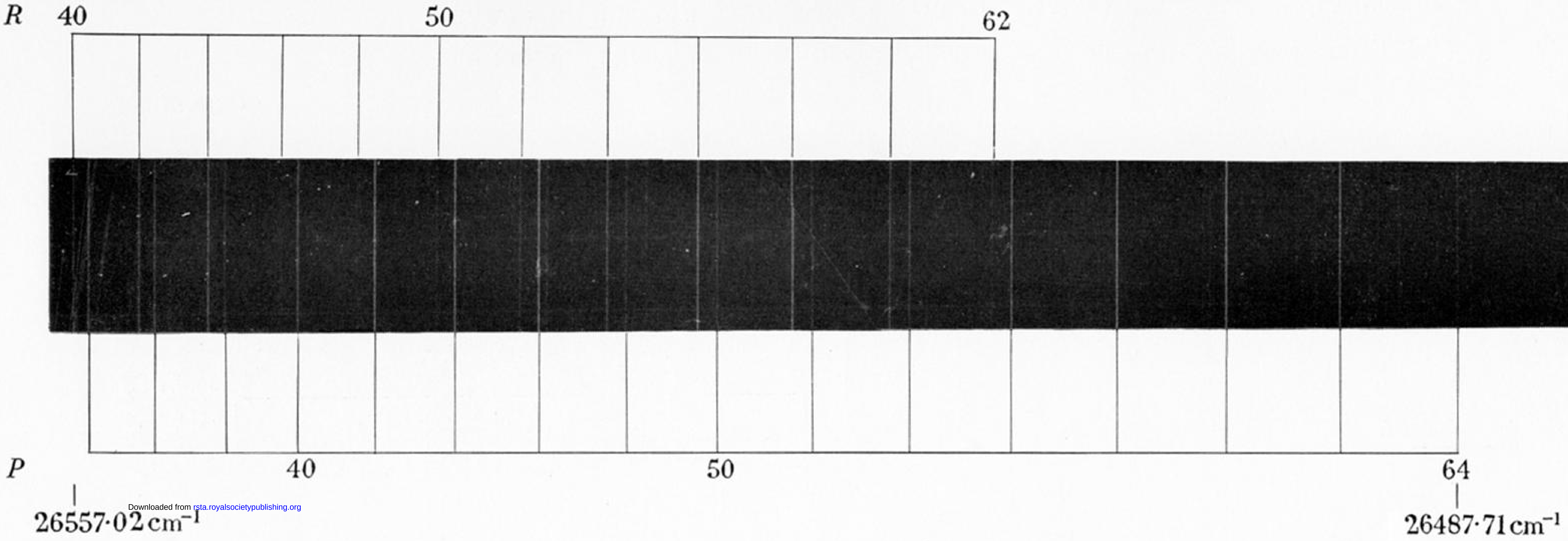

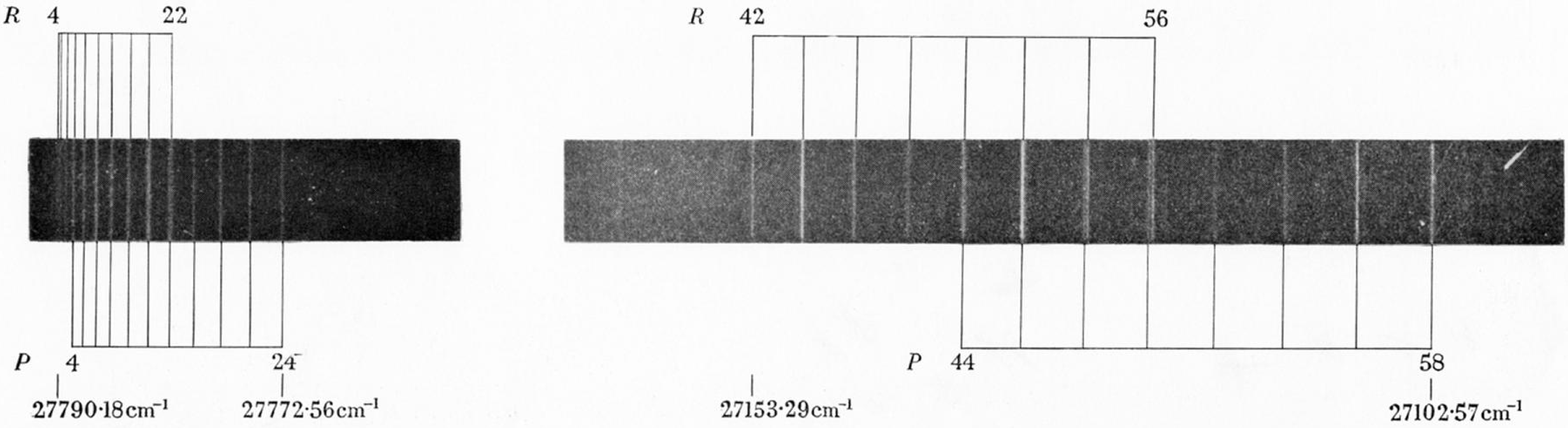

(a)

(b)

FIGURE 7. The 6–2 band of the system $B\,0_u^+–X\,0_g^+$ of $^{78}Se_2$ observed in emission.

FIGURE 8. (a) The 13–3, (b) the 12–4 bands of the system $B\,0_u^+–X\,0_g^+$ of $^{78}Se_2$ observed in emission.

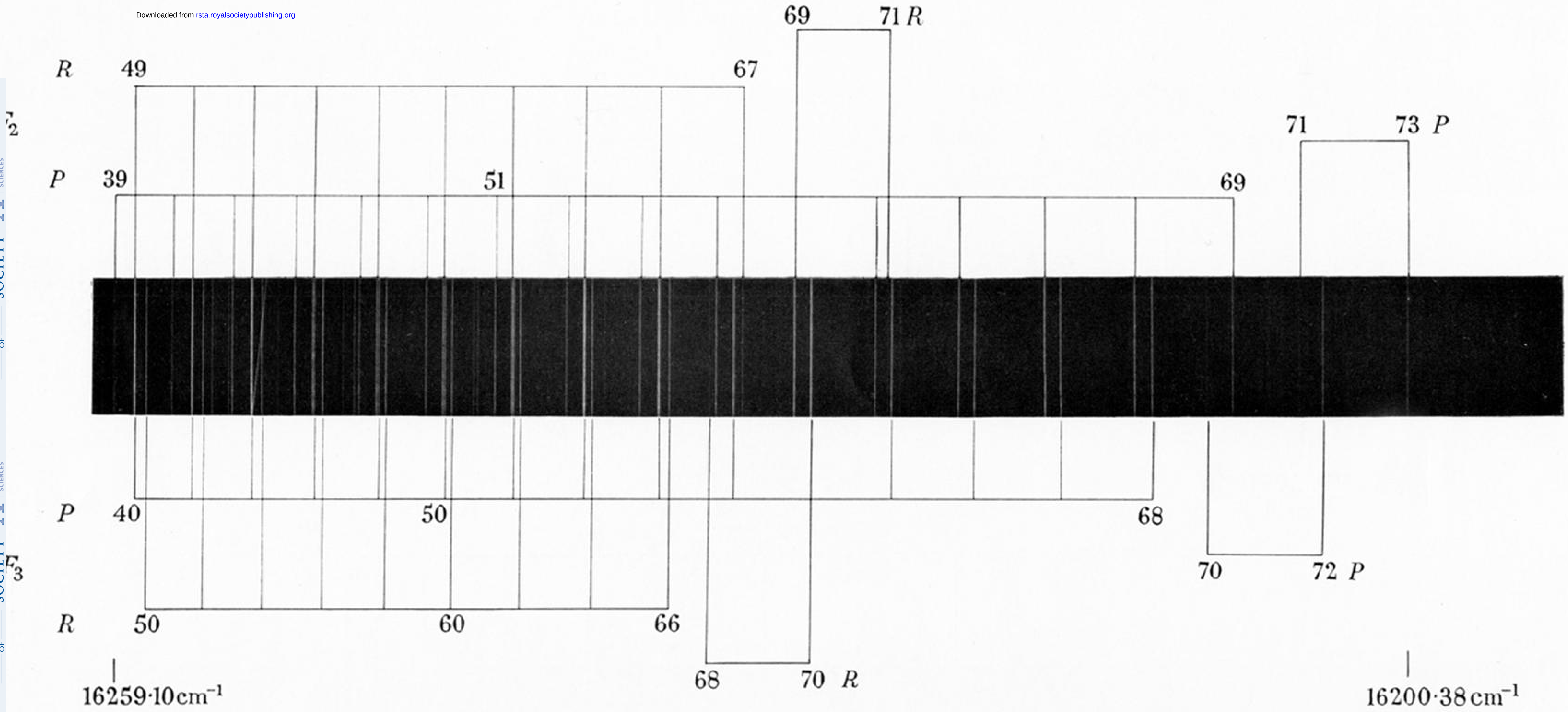

FIGURE 12. The 5–29 band of the system $B\,1_u$–$X\,1_g$ of $^{80}\mathrm{Se}_2$ observed in emission.