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QUANTUM-MECHANICAL CALCULATIONS FOR THE ELECTRON - IMPACT BROADENING AND SHIFT OF SOME LINES OF NEUTRAL HELIUM IN A HOT PLASMA

by

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ABSTRACT

In this paper we apply the quantum-mechanical formalism developed by Bassalo and Cattani to calculate the broadening and shift produced by electronic collisions of some lines (5876, 5048, 5015, 4713, 3964 and 3889 Å) of neutral Helium in a plasma. The effect of the ions are also taken into account. Our theoretical predictions are compared with the experimental results of Bötticher, Roder and Wobig and with the semi-classical estimates of Griem, Baranger, Kolb and Oertel.

(1) Introduction

In a preceding paper (Bassalo, Yamamoto and Cattani 1975) we have applied the quantum-mechanical formalism developed by Bassalo and Cattani (1972, 1974) to calculate the broadening and shift of the neutral Helium line $4^3s \rightarrow 2^3p$ (4713 Å). This formalism has been carried out to determine the broadening and shift of isolated atomic lines produced by electronic collisions. To take into account the contribution of the ions we have used the approach developed by GBKO (Griem, Baranger, Kolb and Oertel 1962) and Griem (1962).

In the present paper, following the procedure used in the preceding paper, we calculate the half-width $\Delta\nu$ and shift S of the lines $4^1s \rightarrow 2^1p$ (5048 Å), $4^3s \rightarrow 2^3p$ (4713 Å), $4^1p \rightarrow 2^1s$ (3964 Å), $3^3d \rightarrow 2^3p$ (5876 Å), $3^3p \rightarrow 2^3s$ (3889 Å) and $3^1p \rightarrow 2^1s$ (5015 Å). The half-width and the shift of the 4713 Å line will be recalculated because Bassalo, Yamamoto and Cattani (1975) have made a mistake in the estimation of the ions effect.

These transitions of neutral Helium were chosen because their shifts and widths have been extensively studied by Bötticher, Roder and Wobig (1963) in the temperature range from $T = 13000$ K to 19000 K, and in the electron density range from $N = 5.10^{15}/cm^3$ to $35.10^{15}/cm^3$.

The experimental results of Bötticher et al. (1963) are compared with our theoretical estimates and with the predictions obtained with the semi-classical approach of GBKO (1962) and Griem (1962).

(2) Calculation of $\Delta\nu$ and S

Let us indicate by $|n^{\sigma}\ell)$ and $|n'^{\sigma}\ell')$, where $\sigma = 1$ for the para-Helium and $\sigma = 3$ for the orto-Helium, the initial and final states, respectively, of the analyzed transition. The final state $|n'^{\sigma}\ell')$ will be chosen as the lowest energy level; and as it is much less polarizable than the initial state, its contribution to the broadening and shift will be negligible compared with that of the initial state.

According to Bassalo and Cattani (1972, 1974) and Bassalo, Yamamoto and Cattani (1975) the half-width $\Delta\nu_e$ and the shift S_e , produced by electronic collisions, of the line $|n^{\sigma}\ell) \to$ $\to |n'^{\sigma}\ell')$ are given by:

$$\Delta\nu_e = 16\, N\, e^4 \left(\frac{\beta m}{2\pi}\right)^{1/2} \left(\frac{a_o}{\hbar}\right)^2 \int_0^{\infty} \frac{y\, dy}{(y^2+\delta^2)^2} \sum_{\ell'} F_{n^{\sigma}\ell,\, n^{\sigma}\ell'}(y) \cdot \exp\left[-\left(\frac{\xi\Delta_{n^{\sigma}\ell,\, n^{\sigma}\ell'}}{y} - \eta y\right)^2\right] \qquad (1)$$

and

$$S_e = \frac{32}{\sqrt{\pi}}\, N\, e^4 \left(\frac{\beta m}{2\pi}\right)^{1/2} \left(\frac{a_o}{\hbar}\right)^2 \int_0^{\infty} \frac{y\, dy}{(y^2+\delta^2)^2} \sum_{\ell'} F_{n^{\sigma}\ell,\, n^{\sigma}\ell'}(y) \cdot D\left(\frac{\xi\Delta_{n^{\sigma}\ell,\, n^{\sigma}\ell'}}{y} - \eta y\right) \qquad (2)$$

where N is the electronic density, $\beta = 1/k_B T$, k_B the Boltzmann constant, T the absolute temperature of the plasma, m the reduced mass of the electron and Helium atom, a_o the Bohr radius, $\delta = 2a_o/\ell_D$, ℓ_D the Debye radius, $\xi = (2\beta m)^{1/2}\, a_o/\hbar$ and $\eta = (\beta/2m)^{1/2}\, \hbar / 4a_o$.

The form-factors $F_{n^{\sigma}\ell, n^{\sigma}\ell'}(y)$, that are given in the Appendix, have been calculated assuming that the more excited electron is bound to a nucleus with effective charge $Z_{eff} = 1$ and with a hydrogen-like wave function. So, the form-factors have the same form for orto and para-Helium. The energy differences $\Delta_{n^{\sigma}\ell, n^{\sigma}\ell'}$ between the states $|n^{\sigma}\ell)$ and $|n^{\sigma}\ell')$ are given, for instance, by Bethe and Salpeter (1957) and the Dawson's integral $D(x)$ is defined and tabulated by Abramowitz and Segun (1969).

We verified that, if the screening parameter $\delta = 2a_o/\ell_D$ is put equal to zero, which means that ℓ_D is infinite, our theoretical predictions for $\Delta\nu_e$ and S_e are modified only by a few percent.

With equations (1) and (2) we can calculate the half-width and the shift produced by electronic collisions. To calculate the effect of the ions we use the approach developed by GBKO (1962) and Griem (1962). Following these authors, the total half-width and total shift S are given by:

$$\Delta\nu \cong \Delta\nu_e \left[1 + 1.75\, \alpha\, (1 - 0.75\, R) \right] \tag{3}$$

and

$$S \cong S_e \pm 2.0\, \alpha\, (1 - 0.75\, R)\, \Delta\nu_e \tag{4}$$

where the parameters α and R are defined in those papers. The signal in equation (4) is equal to that of the low-velocity limit for S_e (Griem 1974).

Our quantum-mechanical estimates do not coincide with the semi-classical predictions of GBKO (1962) and Griem (1962) only for the widths of the 3889 Å and 5876 Å lines and for the shift of the 5048 Å line. This is shown in Figures 1, 2 and 3, respectively, where the experimental results of Bötticher et al. (1963) are compared with our theoretical predictions and with the semi-classical estimates.

The figures of the remaining cases (where quantum - mechanical and semi - classical predictions coincide) can be seen in the paper of Bötticher et al. (1963).

(Insert figures 1, 2 and 3)

We see from figures 1, 2 and 3 that the quantum - mechanical estimates are in better agreement with the experimental results than the semi-classical predictions. Indicating by $\Delta\nu_i$ and S_i the contributions of the ions to the half-width and to the shift, respectively, we verify that $\Delta\nu_e \sim 15\ \Delta\nu_i$ and $S_e \sim -2.5\ S_i$.

From figures 1, 2 and 3 and from those given by Bötticher et al. we observe that only for $\Delta\nu$ is there a reasonable agreement between theory and experiment. For the shifts, in practically all cases, no good agreement is found.

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APPENDIX

We present here the form-factors $F_{n^{\sigma}\ell, n^{\sigma}\ell'}(y)$ that have been calculated assuming that the more excited electron is bound to a nucleus with effective charge Z_{eff} and with a hydrogen-like function. In this approximation, the form-factors have the same form for orto and para-Helium. We remember that the form-factor is defined by:

$$F_{n\ell,n\ell'}(y) = |Z_{eff}\ \delta_{\ell,\ell'} - < n\ell 0 \,|\, \exp(i\Delta q\ z/\hbar) \,|\, n\ell' 0 > |^2$$

So, we have:

$$F_{4s,4s} = \left[Z_{eff} - (4y^{12} - 46y^{10} + 166y^8 - 215y^6 + 109y^4 - 19y^2 + 1)/(y^2+1)^8\right]^2$$

$$F_{4s,4p} = 45\ (2y^{10} - 18y^8 + 43y^6 - 37y^4 + 11y^2 - 1)^2\ y^2/(y^2+1)^{16}$$

$$F_{4s,4d} = \frac{1}{16}\ (-\ 64y^8 + 568y^6 - 992y^4 + 536y^2 - 80)^2\ y^4/(y^2+1)^{16}$$

$$F_{4s,4f} = \frac{1}{320}\ (-\ 160y^6 + 1470y^4 - 2240y^2 + 560)^2\ y^6/(y^2+1)^{16}$$

$$F_{4p,4p} = \left[Z_{eff} + (50y^{10} - 272y^8 + 425y^6 - 223y^4 + 37y^2 - 1)/(y^2+1)^8\right]^2$$

$$F_{4p,4d} = \frac{1}{5}\ (150y^8 - 648y^6 + 666y^4 - 204y^2 + 12)^2\ y^2/(y^2+1)^{16}$$

$$F_{4p,4f} = (42y^6 - 168y^4 + 114y^2 - 12)^2\ y^4/(y^2+1)^{16}$$

$$F_{4d,4d} = \left[Z_{eff} - (102y^8 - 263y^6 + 169y^4 - 25y^2 + 1)/(y^2+1)^8\right]^2$$

$$F_{4d,4f} = \frac{1}{5}\ (161y^6 - 287y^4 + 103y^2 - 9)^2\ y^2/(y^2+1)^{16}$$

$$F_{3p,3p} = \left[Z_{eff} + (14580y^6 - 53136y^4 + 41472y^2 - 4096)/(9y^2/4 + 4)^6\right]^2$$

$$F_{3p,3s} = \frac{128}{3}(615.09y^6 - 4374y^4 + 6264y^2 - 2304)^2\, y^2/(9y^2/4 + 4)^{12}$$

$$F_{3p,3d} = \frac{256}{3}(1822.5y^4 - 4752y^2 + 1152)^2\, y^2/(9y^2/4 + 4)^{12}$$

$$F_{3d,3d} = \left[Z_{eff} - (22032y^4 - 19968y^2 + 4096)/(9y^2/4 + 4)^6\right]^2$$

$$F_{3d,3s} = 32768\,(22.78y^4 - 162y^2 + 120)^2\, y^4/(9y^2/4 + 4)^{12}$$

The parameter y, seen above, is defined by $y = \frac{2\Delta q}{\hbar}\left(\frac{a_o}{Z_{eff}}\right)$, where Δq is the momentum transfer between electron and atom in a collision (Bassalo and Cattani 1972).

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FIGURE CAPTIONS

Figures 1 and 2 - Experimental results of Bötticher et al. (× × ×) for the half-width compared with the semi-classical estimates of Griem et al. (———) , with the quantum-mechanical predictions $\Delta\nu$ (—— ● ——) given by equation (3) and with $\Delta\nu_e$ (— — — —) given by equation (1).

Figure 3 - Experimental results of Bötticher et al. (× × ×) for the shift compared with the semi-classical estimates of Griem et al. (———) , with the quantum-mechanical predictions S (—— ○ ——) given by equation (4) and with S_e (— — — —) given by equation (2).

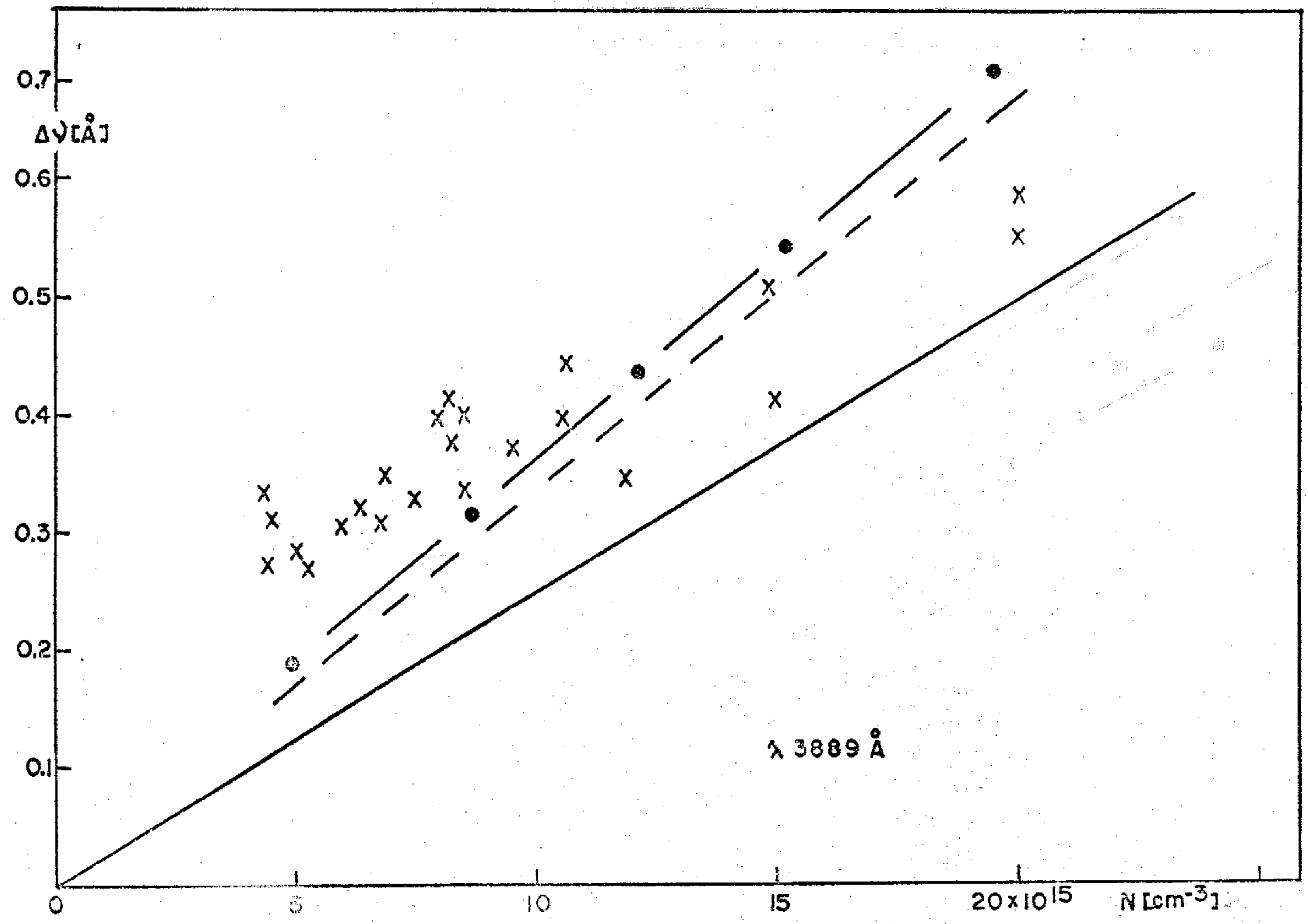

Fig. 1

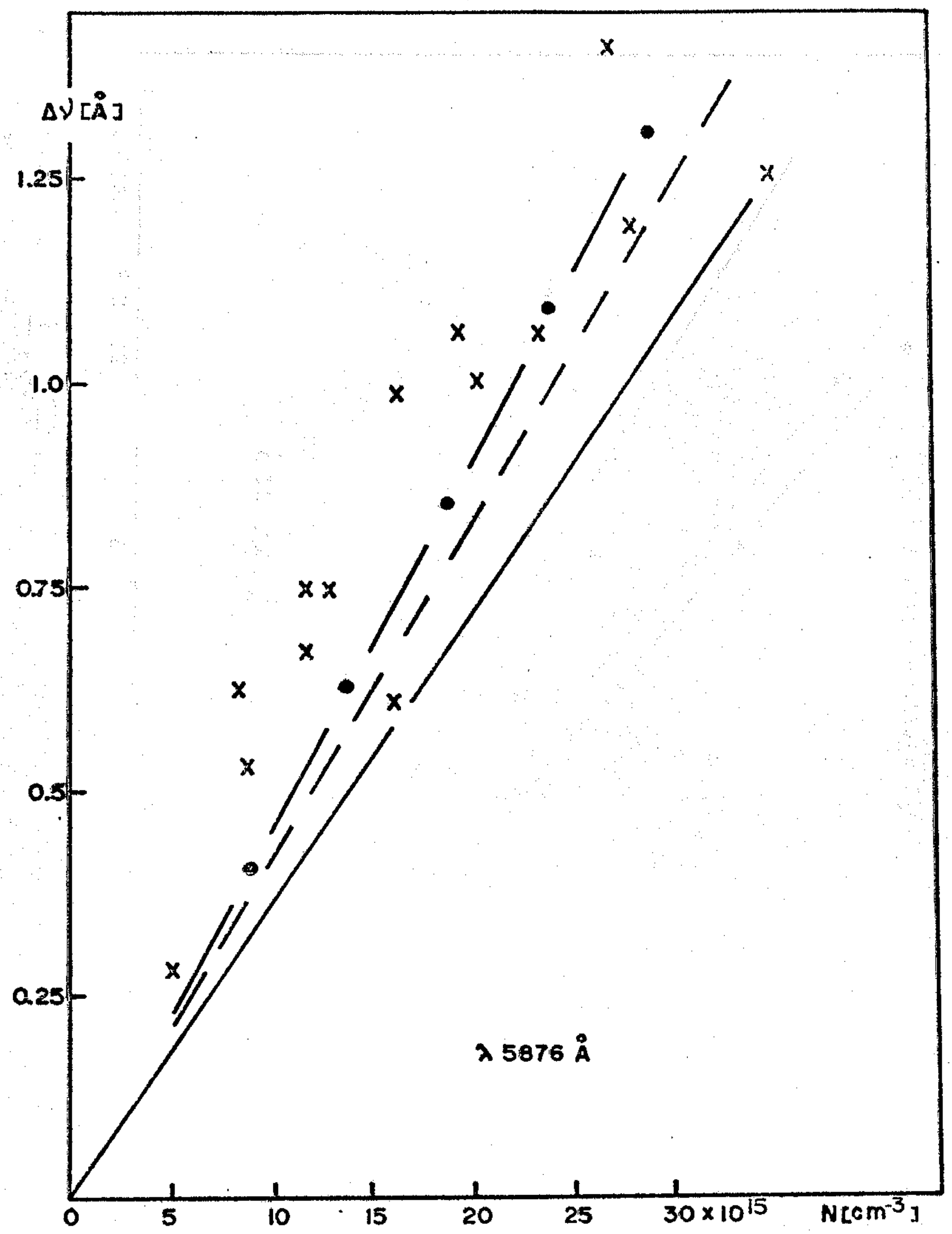

Fig. 2

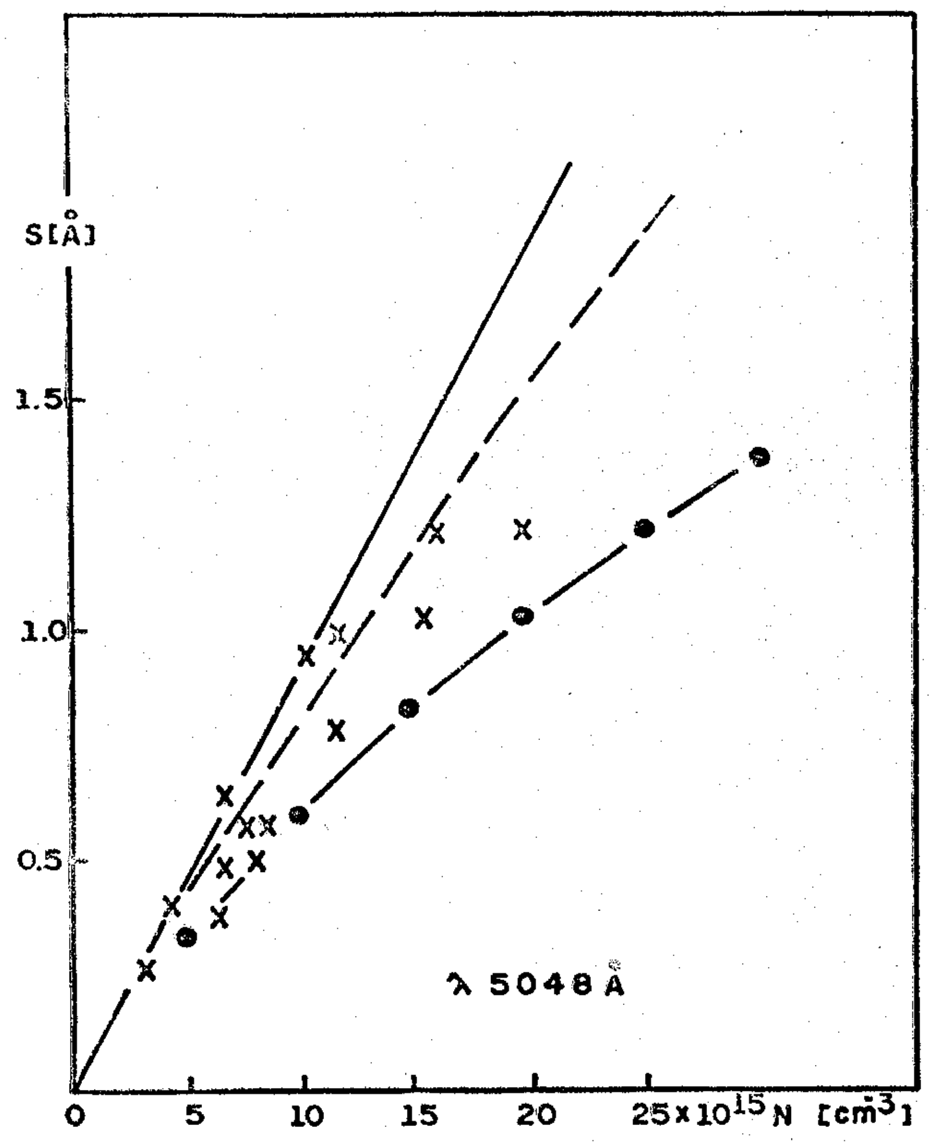

Fig. 3