be sufficient to test the theory, as indicated in Fig. 6. The temperature range over which the experiment may be carried out is unfortunately relatively narrow, since below liquid nitrogen temperatures only small changes in binding energy are expected from from the nature of the exponent in the expression for $N(T, p)$, while above liquid nitrogen temperature, it becomes increasingly difficult to locate the position of peak A_2.

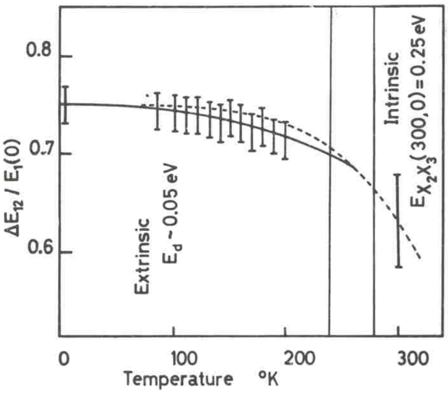

Fig. 7. The variation in the separation of the A_1 and A_2 exciton peaks with temperature. The transition from extrinsic to intrinsic behaviour occurs at about 250°K.

Figure 7 shows the separation of exciton peaks A_1 and A_2 at temperatures between 4° and 200°K. The separation at 300°K was that deduced from the pressure measurements. As expected, the separation is reduced as the temperature is increased, but by using (1) and (2), a more quantitative analysis is possible. We can write

$$\delta(T, 0) = \delta(T_s, 0)\left(\frac{T}{T_s}\right)^{1/4} \times \exp\left[\frac{E(T_s, 0)}{2k}\left\{\frac{1}{T_s} - \frac{1}{T}\frac{E(T, 0)}{E(T_s, 0)}\right\}\right] \quad (6)$$

in which T_s is a specified, fixed temperature in either the extrinsic or intrinsic region and $E(T_s, 0)$ is the activation energy, defined in Section 4, in the conduction region containing T_s. If the temperature variation of $E_{x_2x_3}$ and E_d are neglected, then (6) may be expressed as

$$\delta(T, 0) = \delta(T_s, 0)\left(\frac{T}{T_s}\right)^{1/4} \times \exp\left[\frac{E(T_s, 0)}{2k}\left\{\frac{1}{T_s} - \frac{1}{T}\right\}\right] \quad (7)$$

to a good degree of accuracy.

The variation $\delta(T, 0)$, and, accordingly in the separation of peaks A_1 and A_2, owing to changes in the intrinsic carrier concentration, is shown as the dotted line in Fig. 7. In this calculation, the value of $\delta(300, 0)$ is taken from the pressure measurements. We see that at low temperatures, the reduction in separation is underestimated, owing to the dominance of extrinsic effects. The electrical measurements available suggest that E_d is $(0{\cdot}05 \pm 0{\cdot}03)$ eV, so that, with the value of $\delta(250, 0)$ taken from the intrinsic curve, the change in binding energy, owing to an extrinsic carrier concentration, can be calculated. The calculation, however, is relatively insensitive at low temperatures to the exact value of E_d within this range, and therefore the result for E_d equal to 0·05 eV, shown as the solid curve, brings the theoretical calculations in line with the experimental observations.

6. CONCLUSION

The excitonic doublet below the fundamental absorption edge of MoS_2 has been explained in terms of transitions from a spin-orbit split valence band X_1 to a doubly degenerate conduction band X_3, lying on each side of a full narrow *d*-band X_2, (Fig. 3). The effect of pressure on the intensity and width of each absorption peak is well described by an increase in electron-hole screening, caused by a reduction of $E_{x_2x_3}$ with pressure, and it is evident that $E_{x_2x_3}$ is always greater than the exciton binding energy. However, at liquid helium temperatures, the free carrier density is sufficiently reduced for the binding energy of the B_1 exciton to be equal to $E_{x_2x_3}$ at about

60 kbars. Under these conditions, the original ground state is expected to become unstable against exciton formation, and a new ground state is formed[26–29]. This might be observed as a crystallographic phase change.

The pressure coefficients of the excitonic doublets in the related family of materials have also been measured, but these will be published later, together with the pressure coefficients of the absorption peaks at higher energies.

Acknowledgements—The authors are grateful to Professor F. P. Bowden and Professor Sir Nevil Mott for helpful discussions, and to the Science Research Council for a grant to the laboratory.

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