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CHARGE TRANSFER BETWEEN A PROTON AND A HEAVY METAL ATOM

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Recently there has been heavy demand for cross section data for charge transfer between a proton and a heavy metal element. This is because the heavy metal atom originating from plasma-wall interaction plays an important role in plasma cooling. Unfortunately at present experimental data on charge transfer involving these elements are sparse because of experimental difficulty. Therefore theoretical estimation of these cross sections may be useful even though these are rather crude.

In this report, we present some approximate theoretical data on cross section for the title process in the graphical form, ie,

$$H^+ + M \rightarrow H + M^+ \tag{1}$$

$$(M = Cr, Mo, W, Fe, Ni, Au)$$

using the formula given by Rapp and Francis[1]. The main features of the approximations adopted by these authors are summarized as follows;

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i) Approximate solution of coupled equations

ii) Single electron approximation and adoption of the Slater 1s type wave function

iii) Classical straight-line trajectory for relative motion.

The final expression obtained can be computed as a function of an incident energy if difference ΔE and some suitable mean I of the ionization potentials I_H, I_M of the atoms involved are given. There is some ambiguity to choice of I. Here we have adopted $I = (I_H+I_M)/2$ and tested this ambiguity by computing the cross section for M=Mo with different choice of I, ie, $I=I_H, I_M \ (I_H+I_M)/2$. The computations indicate that deviation from the case for $I=(I_H+I_M)/2$ is at most 40%. In the present calculation, we have corrected an error of the original expression pointed out by Dewangan[2]. The values of I_M, ie, the first ionization potentials was adopted from Moore's Table[3].

Numerical results are shown in Fig.1-6 together with the results for incident deuteron or triton, which can be easily computed from the relation between the cross sections $\sigma_p(v)=\sigma_d(v)=\sigma_t(v)$. Here v is the velocity of an incident ion.

Finally we wish to make some comments on accuracy of the present results. Rapp and Francis[1] compared their results with experimental data for H^+ + rare gas systems. They argued that qualitative agreement is good, but did not claim quantitative agreement between theory and experiment, which also applies to the present results. For example, for the case of $H^+ + X_e$, there exists a factor of 4-9 discrepancy for the cross section between theory and experiment. (See fig.8, ref.1) This might be used as a very rough estimate of the error to the present results. Further the results are most reliable near the peak. At lower energy region, the results become less reliable because of assumption of the straight-line trajectory.

References

1. D. Rapp and W.E. Francis, J. Chem. Phys. 37 2631 (1962).

2. D.P. Dewangan, J. Phys. B. Atom. Molec. Phys. 6 L20 (1973).

3. C.E. Moore, Atomic Energy Levels NBS Circular No. 467.

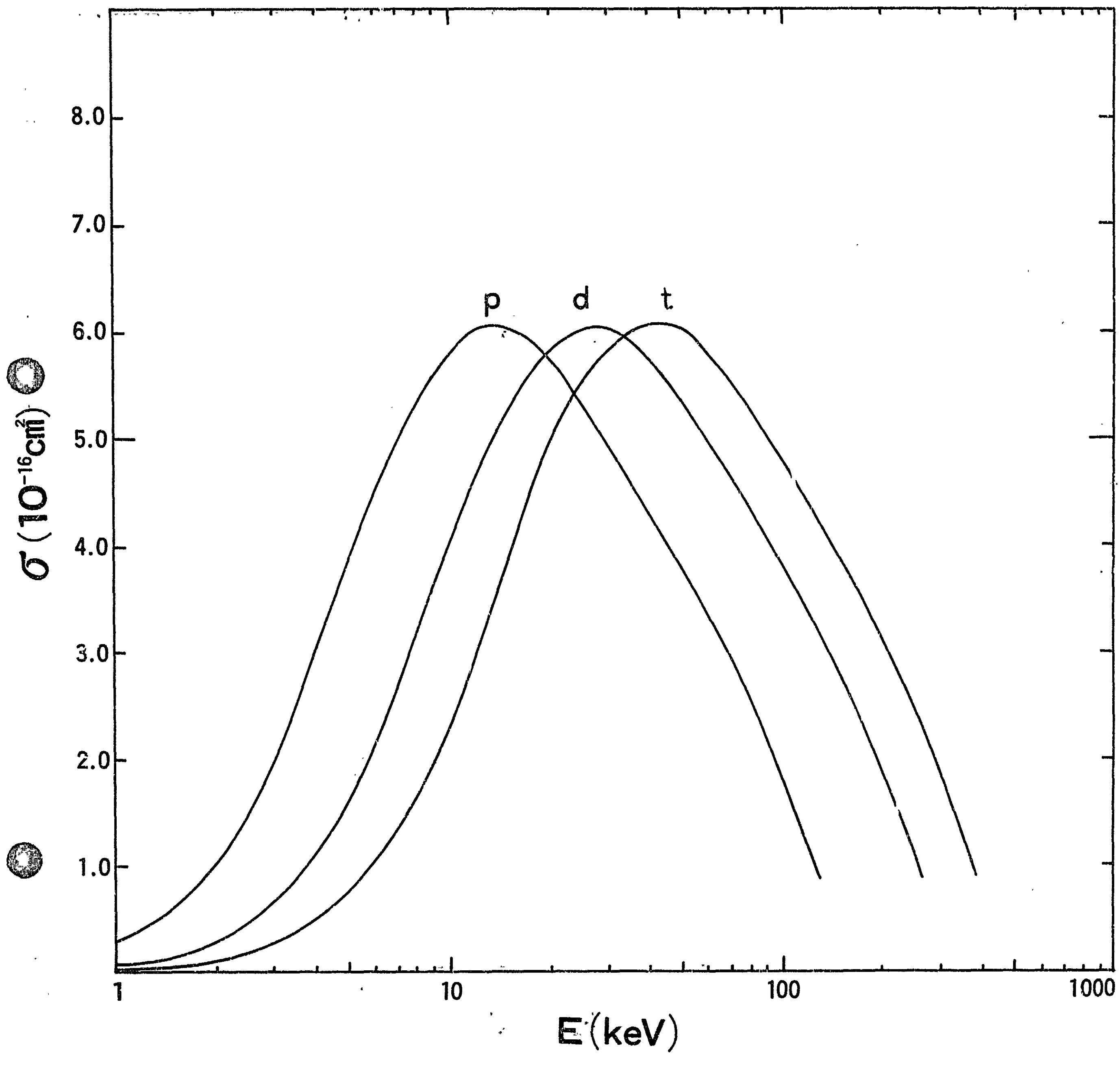

Fig. I Cross section for charge transfer

$$\begin{matrix} p \\ d \\ t \end{matrix} + Cr \longrightarrow \begin{matrix} H \\ D \\ T \end{matrix} + Cr^{+}$$

energy defect of the process $\Delta E = 6.8$eV
average ionization potential $I = 10.2$eV

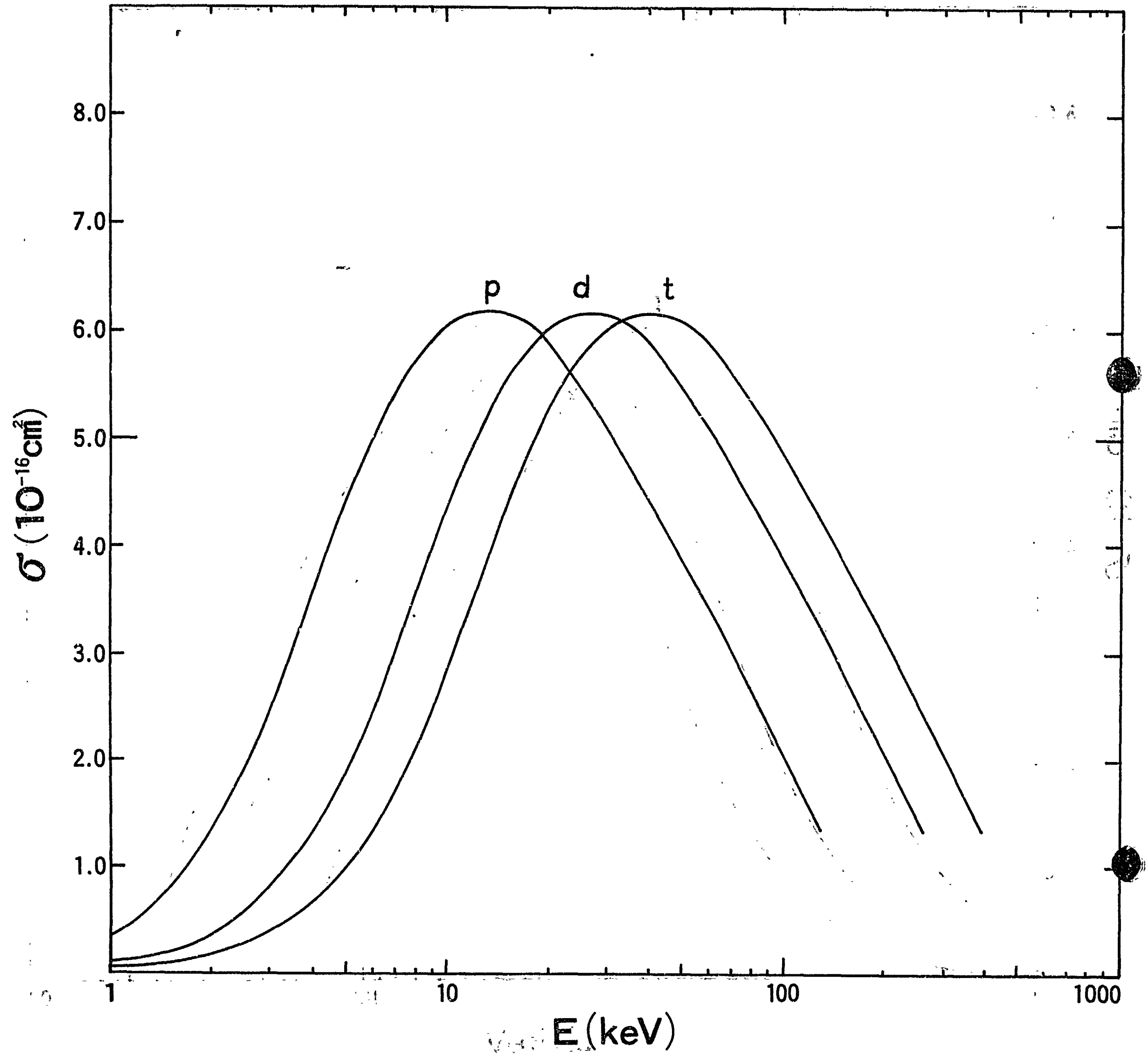

Fig. 2 Cross section for charge transfer

$$\begin{matrix} p \\ d \\ t \end{matrix} + Mo \longrightarrow \begin{matrix} H \\ D \\ T \end{matrix} + Mo^{+}$$

$\Delta E = 6.5 eV$, $I = 10.4 eV$

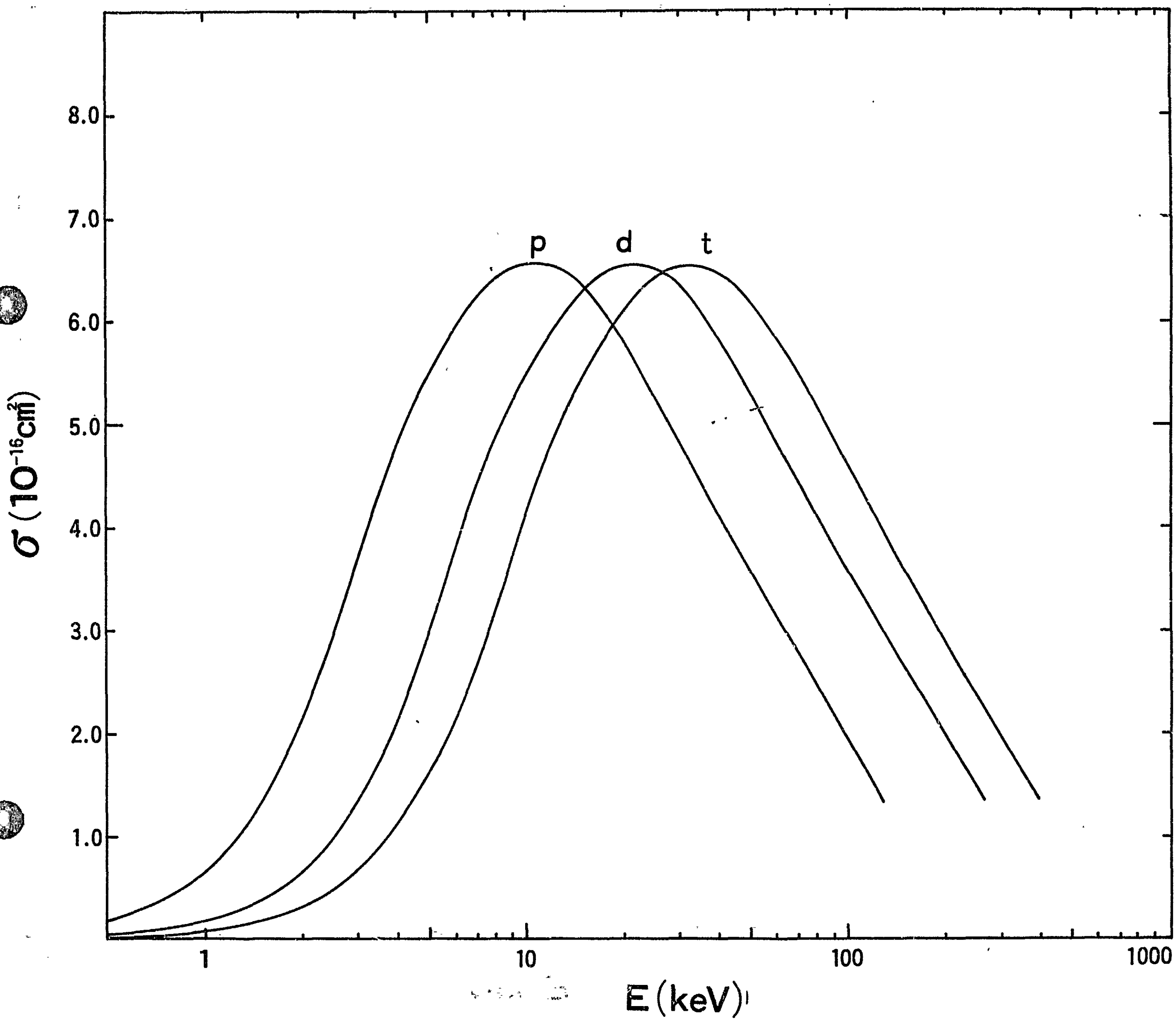

Fig. 3 Cross section for charge transfer

$$\begin{matrix} p \\ d \\ t \end{matrix} + W \longrightarrow \begin{matrix} H \\ D \\ T \end{matrix} + W^{+}$$

$\Delta E = 5.6\,\mathrm{eV}$, $I = 10.8\,\mathrm{eV}$

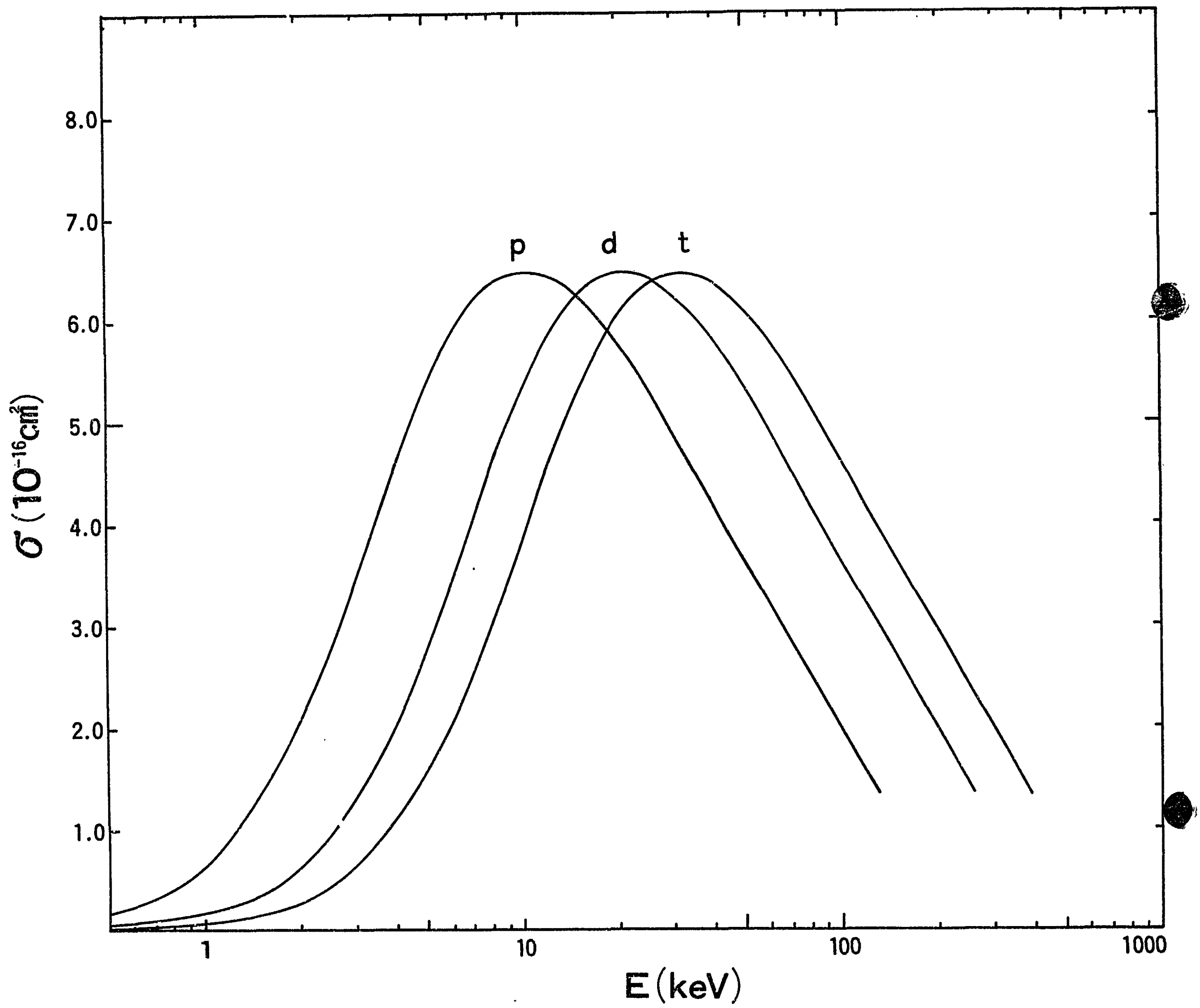

Fig. 4 Cross section for charge transfer

$\begin{matrix} p \\ d \\ t \end{matrix} + Fe \longrightarrow \begin{matrix} H \\ D \\ T \end{matrix} + Fe^+$

$\Delta E = 5.7 eV, \; I = 10.8 eV$

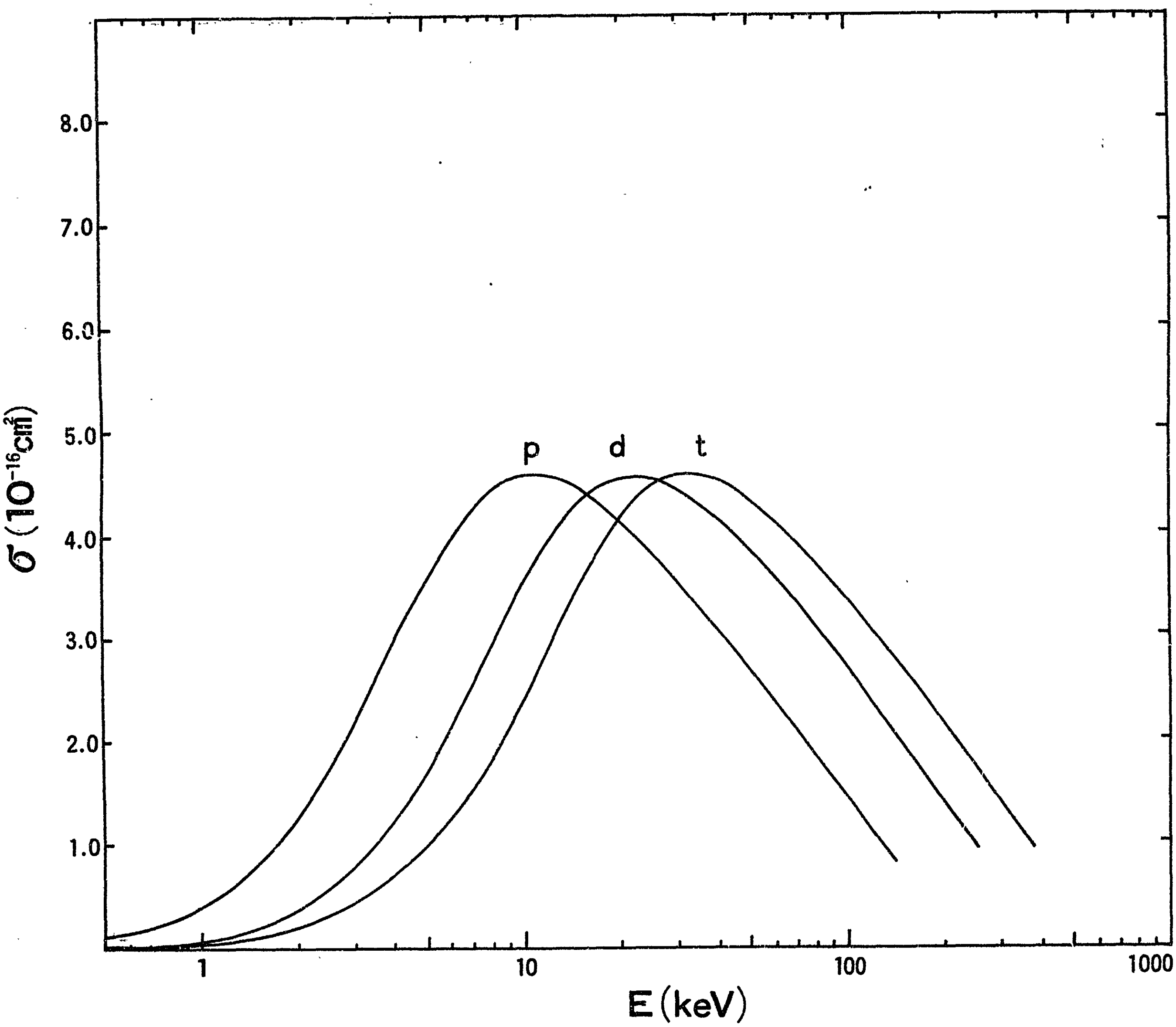

Fig. 5 Cross section for charge transfer

$$\begin{matrix} p \\ d \\ t \end{matrix} + Ni \longrightarrow \begin{matrix} H \\ D \\ T \end{matrix} + Ni^{+}$$

$\Delta E = 6.0 eV$, $I = 10.6 eV$

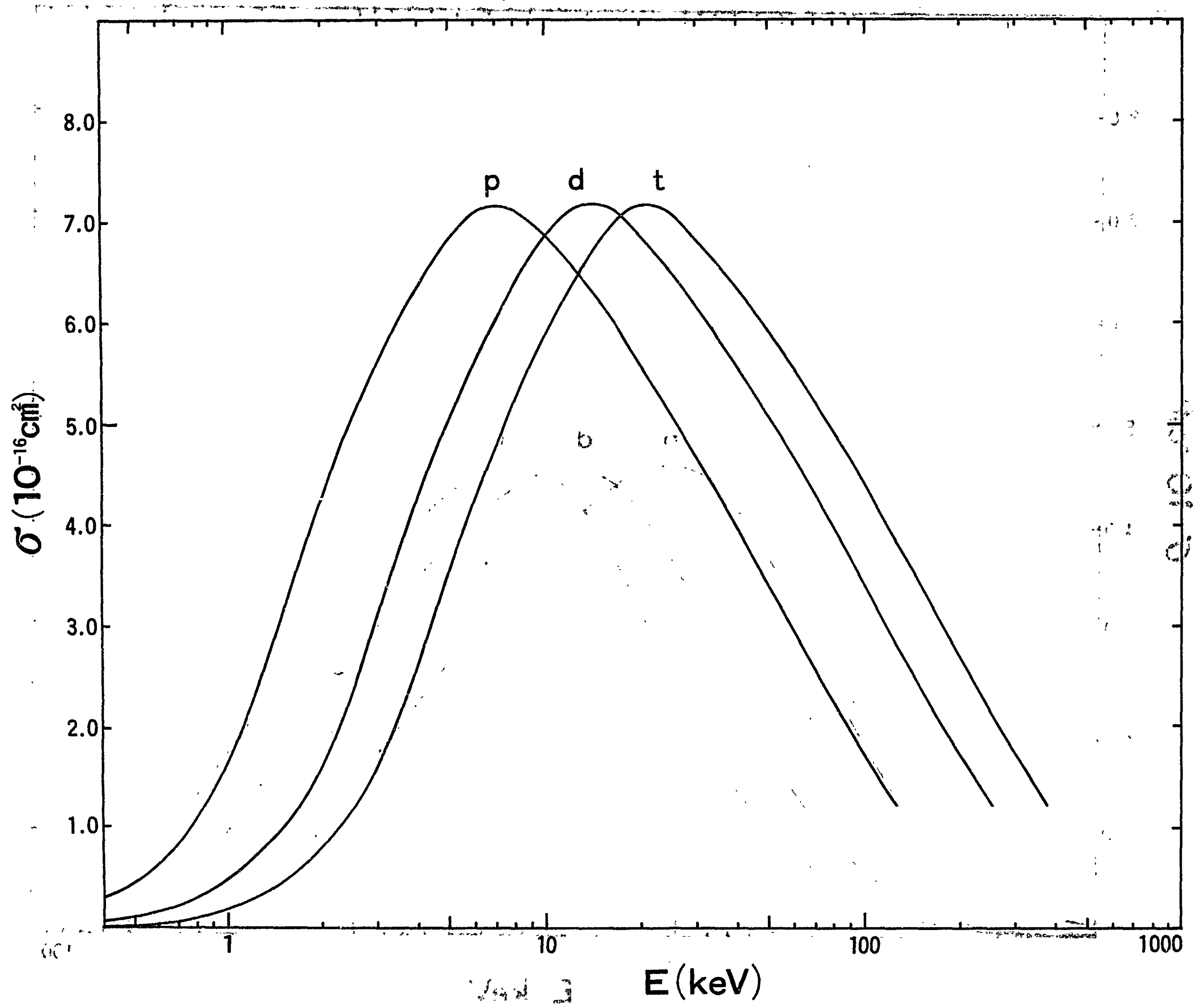

Fig. 6 Cross section for charge transfer

$$\begin{matrix}p\\d\\t\end{matrix} + Au \longrightarrow \begin{matrix}H\\D\\T\end{matrix} + Au^{+}$$

$\Delta E = 4.4eV$, $I = 11.4eV$