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ENERGY DEPENDENCE OF THE TOTAL NEUTRON CROSS SECTION
OF HYDROGEN BOUND IN SEVERAL ORGANIC MOLECULES

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1. In the past few years considerable effort has been spent on measuring the influence of chemical binding on the scattering of slow neutrons in several hydrogenous liquids. This is important from practical point of view since the spectrum shape of neutrons in hydrogenous reactors depends on the binding effect. The quantitative understanding of neutron thermalization requires a fairly good knowledge of scattering law for slow neutrons in hydrogenous liquids. At the same time these measurements are important for the study of the dynamics of hydrogen atoms in molecules.

It is well known that the use of Fermi approximation separates the scattering cross section into a factor depending on the initial and final neutron energy, and a "scattering law" $S(\kappa, \omega)$ which depends only on the dynamics of scattering system. Unfortunately the determination of the scattering law is accompanied by rather large experimental difficulties. The measurement of integral scattering cross section is more simple but it is not so sensitive to the details of the scattering system.

2. In our experiments the energy dependence of the total neutron cross section is measured in several hydrogenous liquids in the energy interval of 0,1-0,001 eV. It is expected that understanding of neutron scattering by these liquids will provide a reasonable basis for the quantitative estimates of some integral parameters /as transport mean free path, diffusion length/.

The energy dependence of the total neutron cross section was measured by time of flight technique. The collimated beam of neutrons coming out from the reactor was interrupted by a mechanical selector. The target /1-3 mm thick/ was placed behind a second collimator. The neutrons not scattered or absorbed in the target material were detected by a set of BF_3 counters the pulses of which were analysed by a 128 channel time-analyser. The distance between the selector and detector was 4,7 m; the duration of the neutron pulse produced by the selector was 126 μsec , the whole time-resolution of the

apparatus was 190 μ sec.

3. As a check of the apparatus the energy dependence of the total cross section in water was measured and the results were compared with the measurements of Melkonian /1949/, Hughes /1958/, and Heinloth et al. /1961/. In Fig.1. the very good agreement of our results can be seen with those obtained by other authors.

The energy dependence of the total cross section per hydrogen atom in benzene can be seen in Fig.2. Kovner et al. /1961/ and Boffi et al. /1963/ calculated the scattering cross section for benzene, their results are in good agreement with our experimental results.

The energy dependence of the cross-section in toluene is nearly the same as that in benzene but there is a significant difference between the cross sections in benzene and cyclohexane. In Figs.3. and 4. our experimental results are presented. For the sake of comparison in Fig.5. each of the curves is plotted showing the energy dependence of the neutron scattering cross section per hydrogen atom in different molecules.

4. A knowledge of the neutron transport cross section in hydrogenous moderators is needed to calculate the nuclear characteristics of experimental critical assemblies in which hydrogenous moderators are used. The temperature dependent transport cross section can be obtained from the total scattering cross section using the Radkowsky /1950/ prescription. This is useful, but not theoretically rigorous. In the prescription an energy-dependent transport cross section is calculated from the energy-dependent reduced mass of the scattering center obtained from the measured variation of the total cross section with energy. A Maxwellian average of the transport cross section obtained from the total cross section measurements was taken for comparison with the results of direct measurements.

5. Direct measurements were performed with the pulsed source method /Ádám et al. 1961/ the principle of which is very simple: the asymptotic decay constant α of a neutron pulse is measured in moderator blocks with different bucklings B^2 ; the resulting α vs. B^2 curve is plotted and using a least squares method, fitted by

$$\alpha = \langle v \Sigma_a \rangle + \frac{1}{3} \langle \frac{v}{\Sigma_{tr}} \rangle B^2 - CB^4$$

In this way, the average absorption cross section $\langle \Sigma_a \rangle$, the average transport cross section $\langle \Sigma_{tr} \rangle$, and the diffusion cooling coefficient C are determined.

6. From the diffusion approximation of transport theory one obtains for the transport cross section

$$\sum_{tr}(E) = \sum_t(E) - \langle \cos \theta \rangle \sum_s(E) \quad /1/$$

where $\sum_t(E)$ is the macroscopic total cross section at energy E , $\sum_s(E) = \sum_t(E) - \sum_a(E)$ is the macroscopic scattering cross section at energy E , and $\langle \cos \theta \rangle$ is the average cosine of scattering angle at energy E .

The calculation can be extended easily to cover the case in which more than one element is present. The expression for the transport cross section in hydrocarbon is then:

$$\sum_{tr}(E) = \left[\sum_{tC}(E) + \sum_{tH}(E) \right] \left[1 - \langle \cos \theta \rangle_H \frac{\sum_{sH}(H)}{\sum_{tC}(E) + \sum_{tH}(H)} - \langle \cos \theta \rangle_C \frac{\sum_{sC}(E)}{\sum_{tC}(E) + \sum_{tH}(E)} \right] \quad /2/$$

For carbon $A = 12$ the average cosine of the scattering angle is given by

$$\langle \cos \theta \rangle_C = \frac{2}{3A} = \frac{1}{18},$$

and the scattering cross section can be taken as constant in the 0,1-0,001 eV energy interval.

It remains necessary to evaluate the average cosine of the scattering angle from hydrogen. We are concerned here only with S-wave scattering, therefore,

$$\langle \cos \theta \rangle_H = \frac{2}{3 M_{eff}(E)} \quad /3/$$

in the laboratory system. The reduced mass M_{eff} depends on the chemical binding of the hydrogen in the molecule. From the asymptotic properties of the cross section for large and small energies it follows that the effective reduced mass can be given as

$$M_{eff}(E) = \frac{\sqrt{\sigma_{sH}(E)}}{\sqrt{80} - \sqrt{\sigma_{sH}(E)}} \quad /4/$$

Using the formulae (2), (3), and (4) we computed the transport cross section $\sum_{tr}(E)$ from the scattering cross section $\sigma_{sH}(E)$ measured in benzene, toluene and cyclohexane.

To calculate the value of the transport mean free path that can be compared with a direct experimental determination of this quantity, one must take into account that the measured transport mean free path is an average over thermal energies. Therefore, we have to take:

$$\langle \lambda_{tr} \rangle = \left\langle \frac{1}{\Sigma_{tr}} \right\rangle = \frac{\int_0^{\infty} \Phi_M(E) / \Sigma_{tr}(E) dE}{\int_0^{\infty} \Phi_M(E) dE} \quad /5/$$

where $\Phi_M(E)$ is the Maxwellian energy density function.

7. The results of our calculations for room temperature ($kT = 0,0253$ eV) are summarized in Tables I. and II. It is seen that the calculated values of the transport mean free path are in fairly good agreement with those of the direct measurements but there is a relatively large error /about 8 percent/ in the calculated value for cyclohexane.

For the sake of comparison the values of $\langle \lambda_{tr} \rangle$ are calculated from the data of $\sigma_{SH}(E)$ for 1,3-butadiene since Petrie et al./1957/ proposed the use of these data for the calculation of the diffusion length in various organic materials until more extensive cross section data are available. It is seen that in our case the use of the 1,3-butadiene data results a relatively large error in the calculated values, therefore, the employment of the 1,3-butadiene data is strongly limited.

8. As a conclusion it should be emphasized that the Radkowsky prescription is to be considered as useful device, not as theoretically rigorous treatment of the scattering of neutrons in moderators. In a comparison between prescription and experimental values of the transport mean free path, however, more confidence must be placed on the experimental values than on the prescription values.

Table I.

Calculated and measured values of $\langle \lambda_{tr} \rangle$ in several hydrogenous liquids

Material	$\langle \lambda_{tr} \rangle$ cm calculated from the proper σ_{SH}	$\langle \lambda_{tr} \rangle$ cm calculated using σ_{SH} from 1,3-butadiene	$\langle \lambda_{tr} \rangle$ cm measured using the pulsed neutron source technique
Benzene	0,587	0,651	0,584 \pm 0,017
Toluene	0,557	0,596	0,531 \pm 0,010
Cyclohexane	0,330	0,419	0,359 \pm 0,017

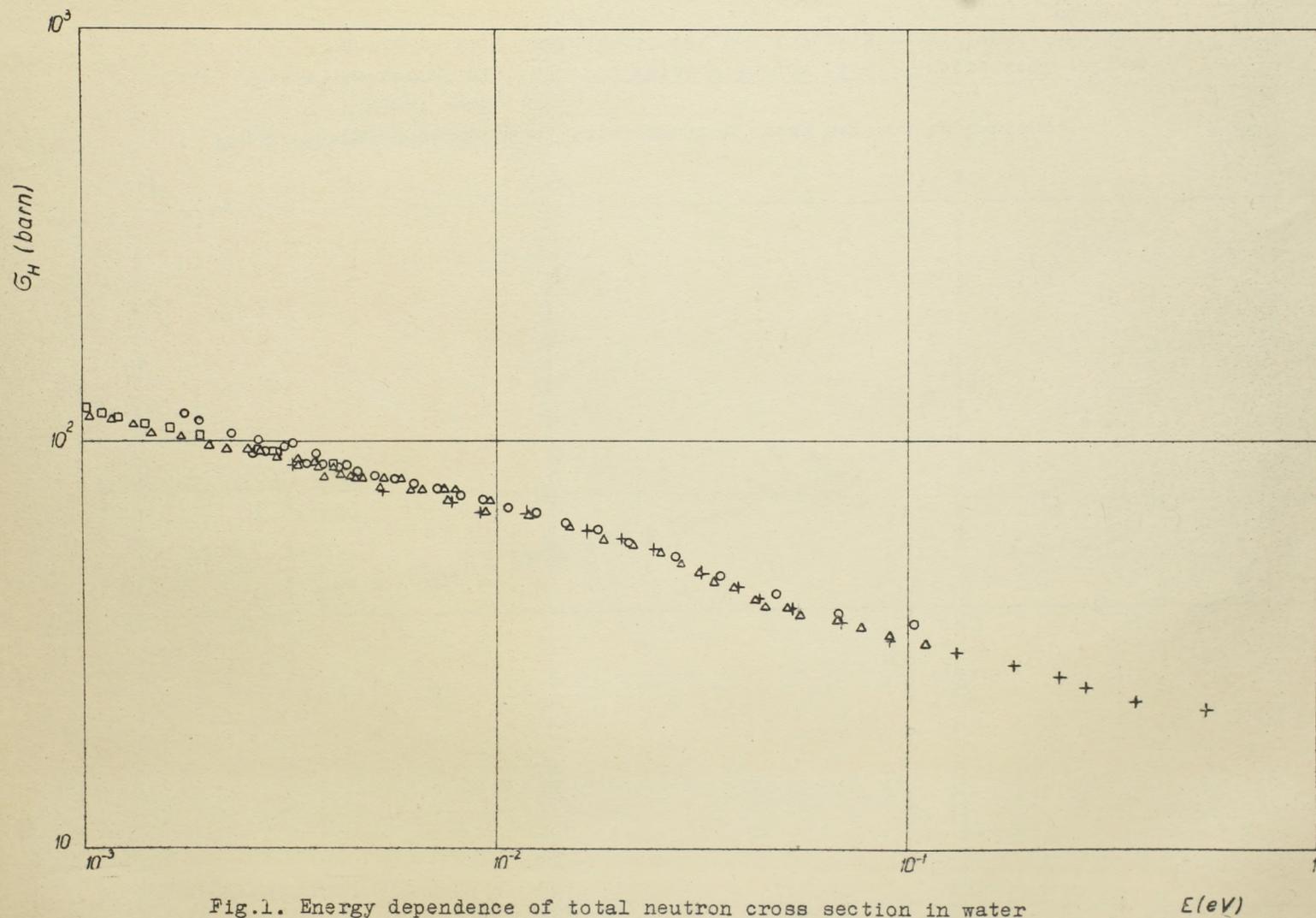
Table II.

Calculated and measured values of D and L

Material	D cm ² sec ⁻¹		L cm	
	calculated	measured	calculated	measured
Benzene	48917	48649 \pm 1373	4,12	4,11 \pm 0,14
Toluene	46417	44229 \pm 847	3,74	3,63 \pm 0,06
Cyclohexane	27500	29944 \pm 1382	2,36	2,47 \pm 0,06

R e f e r e n c e s

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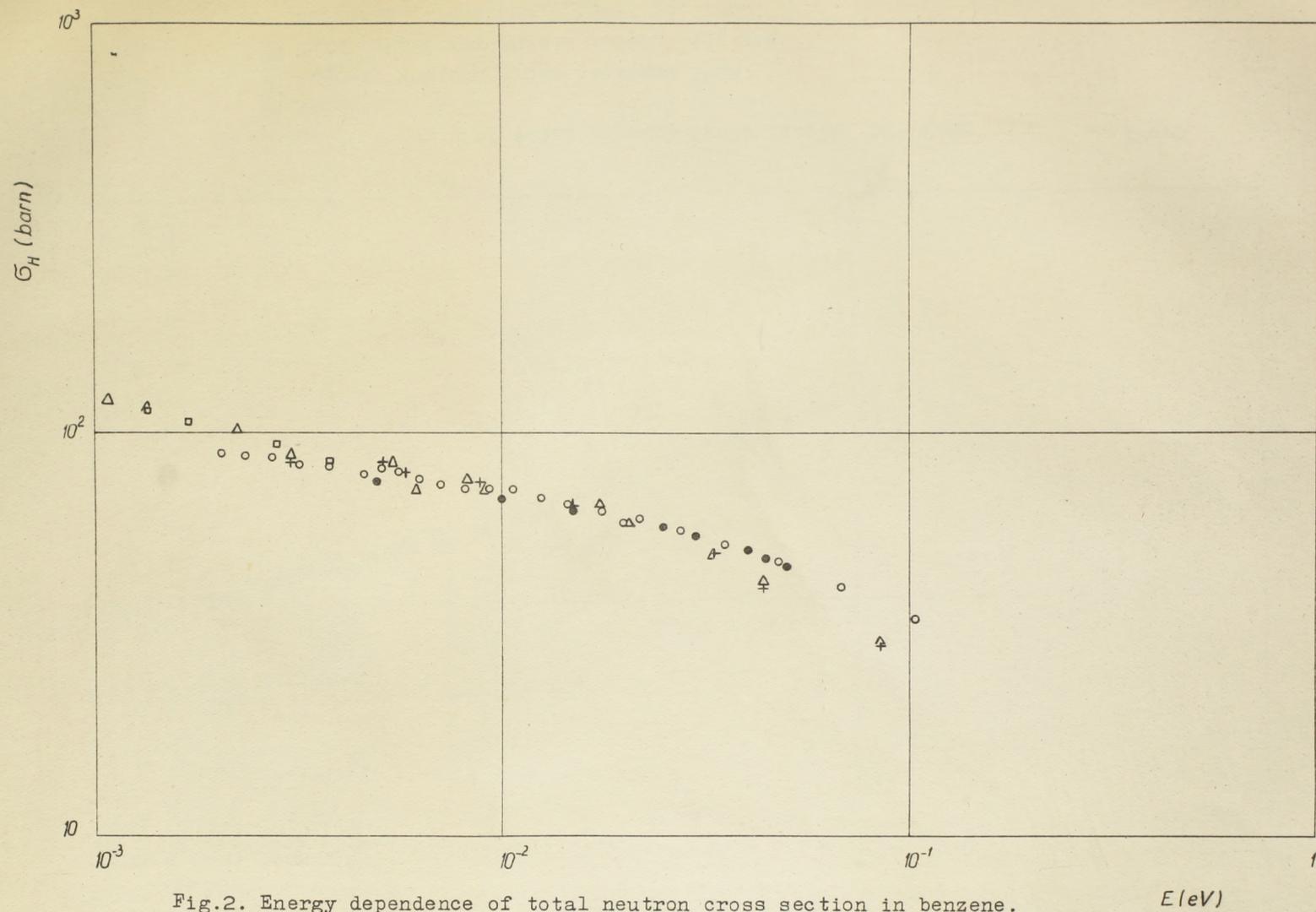


Fig.2. Energy dependence of total neutron cross section in benzene.

- present work
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- + Boffi et al., Inelastic Scatt.Vol.I.IAEA Vienna /1963/ /theoretical values/
- Heinloth,Z.für Physik /1961/ 163, 218.
- △ Pauli et al., Inelastic Scatt.Vol.I.IAEA Vienna /1963/

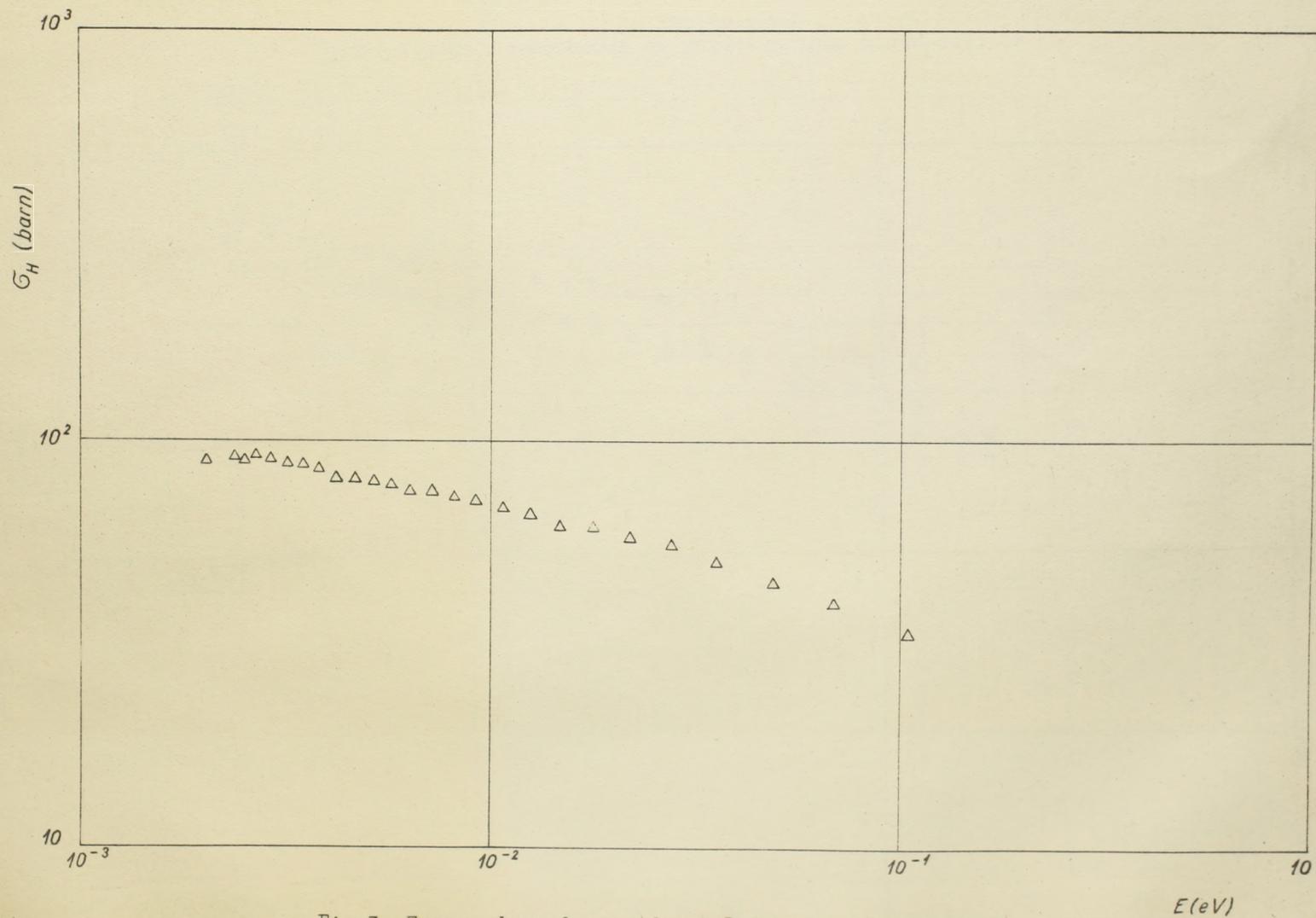


Fig.3. Energy dependence of total neutron cross-section in toluene

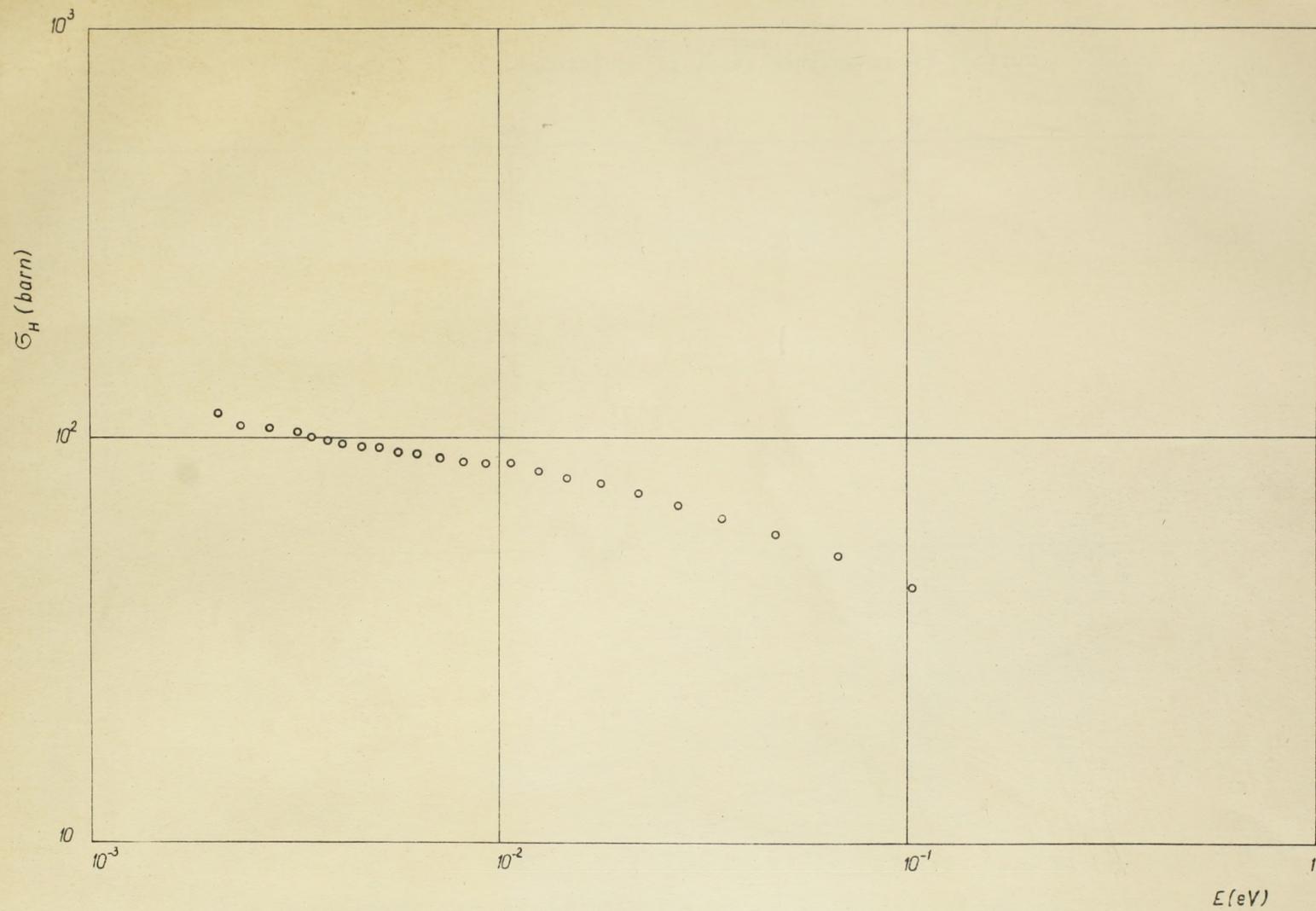


Fig.4. Energy dependence of total neutron cross-section in cyclohexane

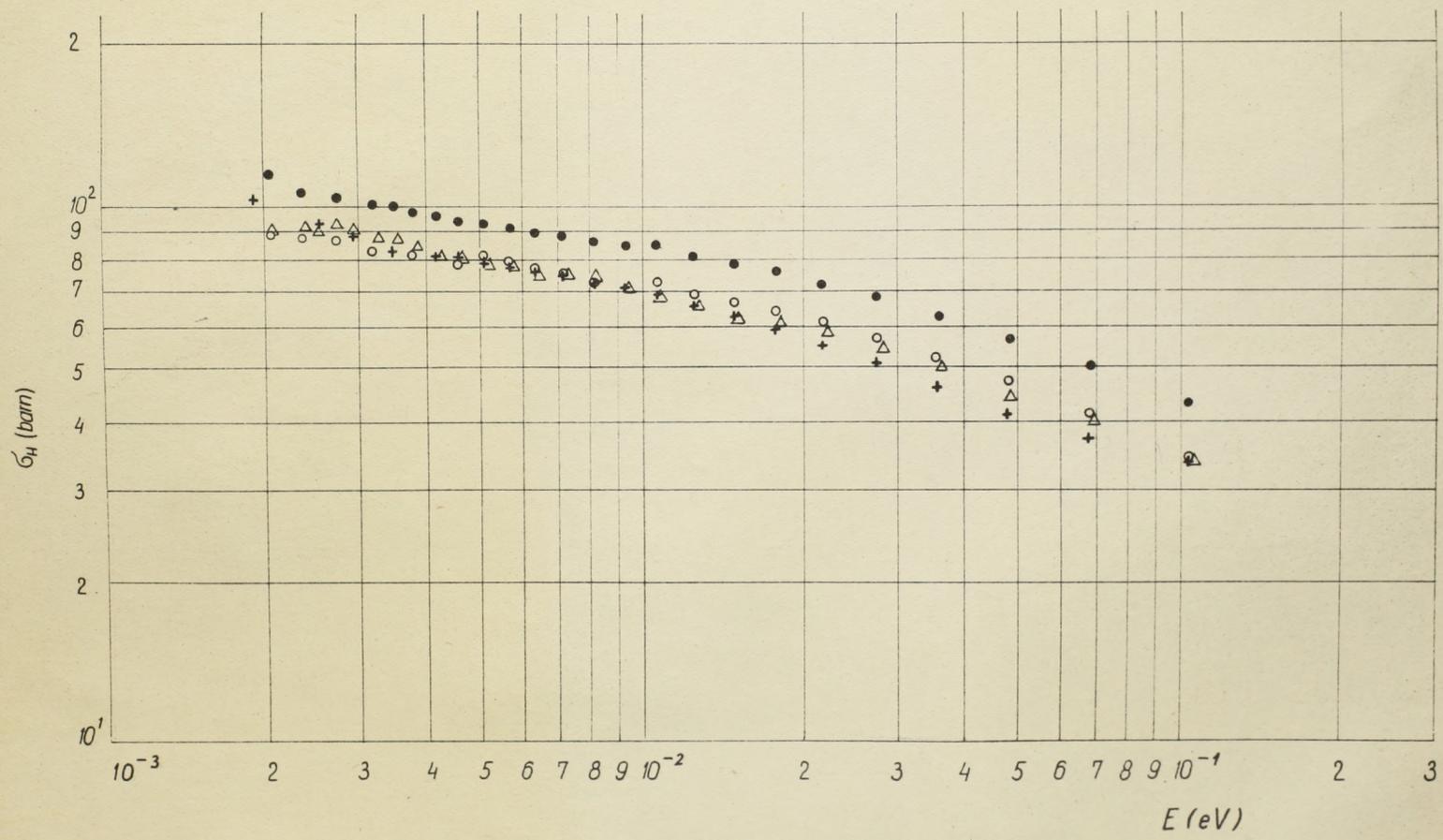


Fig.5. Comparison of the total neutron cross sections per one hydrogen atom bound in water (+) , benzene (o) , toluene (Δ) and cyclohexane (\bullet).

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