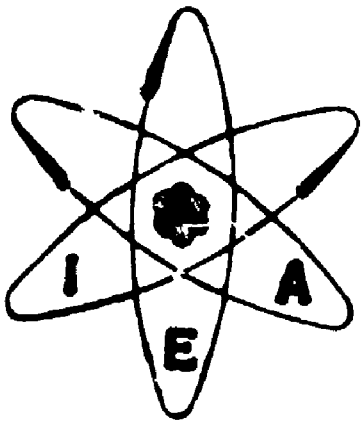

SLOW NEUTRON SCATTERING CROSS SECTION OF DEOXYRIBONUCLEIC ACID, EX-THYMUS

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ABSTRACT

In order to study the dynamics of water present in biological molecules and the freedom of motion of the hydrogen atoms, the neutron transmission through a DNA sample was measured in the neutron wavelength interval 4.0 to 6.5 Å using a crystal spectrometer.

The knowledgement of the bounding state of the water present in DNA is very useful to study the structures and the functions of biological macromolecules. NMR studies suggest some form of ice-like coordination for H_2O in biological molecules, where as results obtained from neutron inelastic scattering in polyglutamic acid suggest a behaviour similar to liquid water. In the present work, measurements were performed at room temperature for a dry sample and for a wet sample with 7.8% moisture. The total cross sections, σ_T, and the scattering cross sections per hydrogen atom, $\sigma_{S/H}$, were determined in each case, thus obtaining the cross section of H_2O present in DNA. This ross section shows that the water in DNA presents a behaviour similar to that of liquid water. By analysing the $\sigma_{S/H}$ curve for dry DNA it is observed that the hydrogen atoms have not much freedom of motion in this biological molecule.

I. Introduction

Information about rotational motions in molecules and crystals can be obtained from total cross section measurements with sufficiently slow neutrons (energy $<<$ 0.025 eV or neutron wavelength longer than 4Å).

The neutron scattering in hydrogenous compounds is essentially incoherent and due to the hydrogen atoms. From the total cross section, measured by neutron transmission, it is possible to obtain the incoherent scattering cross section per proton $\sigma_{S/H}$, that varies linearly with the neutron wavelength λ[1,8]. The slope of this cross section line depends on the incoherent inelastic scattering that comes from processes in which the neutron gains energy from molecules in populated excited states. At room temperature the main contribution to the inelastic scattering is due to de-excitation of energy levels corresponding to torsional or free rotational motion of the molecule or molecular groups containing hydrogen atoms. The slope $\sigma_{S/H} \times \lambda$ increases with the freedom of motion of the H atoms. This slope has been empirically correlated with the barrier hindering the internal rotation of defined molecular groups (NH_4 and CH_3) and calibration curves were obtained[9,18]. However, for the complicated DNA molecule, well characterized hydrogenous groups do not exist; therefore it is not possible to associate any barrier with the slope, and only the freedom of motion of the H atoms in a DNA tetranucleotide unit can be estimated.

It is well known the interest in the state and role of water in structures and functions of biological macromolecules[4]; since neutrons are very sensitive to the water presence in a sample, it is possible to obtain an indication of the dynamical behaviour of water in DNA samples from neutron transmission measurements through dry and wet samples.

II. General

II.1. The DNA Structure

The general term macromolecule characterizes large size molecules with molecular weight larger than 5000. If a macromolecule is of biological interest it is named biopolymer. The term includes the polymer concept, i.e, a large size molecule whose origin can be described by means of covalent unions between relatively small molecules called structural units.

One class of biopolymers are the nucleic acids, which, as their name indicates, are found as the major chemical constituents of the cell nucleus. Two classes of nucleic acids are present in the nucleus: deoxyribonucleic acid (DNA) and ribonucleic acid (RNA), but they are found elsewhere in the cell as well.

The nucleic acids are polynucleotides, i.e, linear polymers formed by a combination of structural units called nucleotides. Each nucleotide consists of three parts: a nitrogenous base (purine or pyrimidine side group), a five carbon sugar, and a phosphate group (fig. 1).

The backbone of the polynucleotide chain is formed by alternating phosphate and sugar groups - ribose in RNA and deoxyribose in DNA - bound by ester linkages between phosphoric acid and the 3' and 5' - hydroxyl groups of successive furanose rings. A purine or pyrimidine base is attached to the cyclic sugar through the 1' carbon atom to complete the nucleotide.

The purine bases adenine and guanine occur in both RNA and DNA, but the two nucleic acids differ somewhat in their pyrimidine composition: thymine occurs only in DNA and uracil only in RNA, while cytosine is a constituent of both nucleic acids.

In figure 2 the four bases constituents of DNA are shown.

The primary structure of nucleic acids, referent to the problem of establishing the sequence of nucleotides within the polynucleotide chain, still persists at the present time as the object of incessant studies. Since DNA is the bearer of genetic information, the specific biological role of a given macromolecule of DNA must be in the sequence of its structural units.

At the beginning it was thought that DNA contained the four bases, adenine and guanine (purines) and cytosine and thymine (pyrimidines) in equal proportions, and the suggestion was made that the fundamental unit was a tetranucleotide. However, careful analysis by Chargaff[3] has shown this not to be true.

Using the technique of paper chromatography, the base composition of DNA of several species was determined (Table I)[17].

From the data in Table I, the following conclusions might be drawn: 1) the base composition of DNA is a characteristic of the species, differing in composition for different species, but not for the different tissues of anyone specie; 2) for all DNA samples the amount of adenine equals thymine (A = T) and cytosine equals guanine (C = G). It follows then that A + G (purines) = T + C (pyrimidines). These regularities are well-known as Chargaff's base pairing rules.

In contrast with the primary structure, the macro molecular structure of DNA is at the

Table I

The base composition of DNA of several species*

Source of DNA	Adenine A	Guanine G	Cytosine C	Thymine T
Salmon sperm	29.7	20.8	20.4	29.1
E. coli (bacteria)	25.2	25.0	25.5	24.3
Yeast	31.7	18.1	17.6	32.6
Micrococus (bacteria)	14.5	36.1	35.9	13.5
Calf thymus	29.8	20.4	20.7	29.1
Calf thyroid	29.6	20.8	20.7	29.1
Calf spleen	29.6	20.4	20.8	29.2
	PURINES		PYRIMIDINES	

*The above results are expressed as mole percent, which is equal to the number of molecule of one base divided by the total number of molecules of all four bases, times 100

present time very well established. Using X-Ray diffraction technique, the following fine details of the DNA macromolecules were revealed[23]: 1) DNA from different species give identical X-Ray patterns, despite the fact that their base composition varies; 2) the actual length of the DNA molecule is greater than 30μ, whereas it is only about 20 Å thick; 3) DNA has a repetitive structure every 34 Å; that is, proceeding along the lengthwise axis of the molecule at regular intervals of 34 Å, there is a repetition of the basic structure.

The regularities observed by Chargaff added to the exhaustive construction of theoretical models, led Watson and Crick to propose a coherent description for the organization of the DNA three-dimensional structure[14,20,21].

Figure 3 shows the Watson-Crick model for DNA. The most significant features of the model are DNA is a double helix composed by two helicoidal polynucleotide chains with the maximum possible number of hydrogen bonds joining the purine and pyrimidine side chains which are packed into the space between the two helical strands (Fig. 2 and 3). The steric relationships specially the similar overall dimensions of the side groups, require that a pyrimidine on one chain be opposite a purine on the other chain. Combining this with the maximization of hydrogen bonding, one concludes that these conditions are satisfied only by the pairs adenine: thymine (two H–bonds) and guanine: cytosine (three H–bonds) as illustrated in fig. 2. An interesting consequence of this is that the nucleotide sequences of the two helices are not independent of each other in the double stranded model. Specification of a nucleotide

base in one chain defines the one opposite to it in the second chain: adenine must lie opposite thymine, and guanine opposite cytosine Both A:T and G:C base pairs have exactly the same dimension perpendicular to the axis, a necessary condition for regularity of the double helix Moreover, the two molecular strands are antiparallel with respect to one another, defining the sense of the chain according to the orientation of the deoxyribose along the polynucleotide backbone

The celebrated Watson-Click model of DNA structure was confirmed time after time in many different ways until it became a fundamental principle of molecular biology.

When accurate measurements were made on scale models of the double helix, the diameter turned out to be 20 Å and the length for a complete turn was 34 Å There were ten bases on each chain for every complete turn of the helix The distance between bases on the same chain was thus 3 4 Å

II.2. Water in DNA

A kind of "bound water" is found, to a large extent, in biological matter, like living cells or muscles; by bound water is meant[4] the water which does not freeze out on cooling and does not melt on subsequent heating of a solution, although it can be removed by conventional technics of dehydration Nuclear magnetic resonance and others evidences have demonstrated that the mobility of these H_2O molecules, or a certain fraction of them, is smaller than the mobility in the liquid; this suggests some form of ice-like coordination for H_2O close to the surface of biological molecules[19] The degree of crystallinity of DNA fibres has been found to be highly sensitive to the humidity of the surrounding atmosphere[6]; the ionic phosphate groups are considered as the primary hydration sites[5,6] Jacobson[12] pointed out the excellent fit of the Watson-Crick model for DNA to the ice-I lattice and suggested that the water hydrated to DNA have an "ice-like" structure This fact was partially corraborated by the neutron scattering measurements for NaDNA performed by Dahlborg and Rupprecht[4]. However, Whittemore[22] also using neutron inelastic scattering, investigated the motion of water molecules in samples of polyglutamic acid, and his results have provided evidence that the water molecule is tightly bound to the polypeptide with a behaviour similar to that of liquid water. Also Falk et al[5] concluded from infrared study that the water molecules hydranting DNA samples have the same behaviour The state and role of water in the structure and functions of biological macromolecules is a subject of great interest and controversy Since slow neutron are very sensitive to the presence of water in any sample, the neutron transmission technique was used on DNA sample in order to obtain additional informations on the behaviour of H_2O molecules present in the deoxyribonucleic acid in powder form

III Experimental

III.1. Crystal spectrometer

The neutron source for this work was the Instituto de Energia Atômica swimming pool research reactor operated at 2 MW Neutron transmissions through DNA samples were measured using the IEA crystal spectrometer[17].

The spectrometer operation is based on the seletive diffraction from a single crystal, governed by the Bragg equation for coherent elastic scattering

$$\lambda = (2\,d\,\sin\theta)/n \quad \text{with} \quad n = 1,2,3, \ldots \qquad (1)$$

where: n is the order of reflection, λ is the neutron wavelength, d is the spacing of the appropriate crystal planes and θ is the glancing angle of the neutron beam with respect to these planes The several neutron wavelengths are selected changing the Bragg angle θ. Figure 4 shows the schematic diagram of the IEA neutron crystal spectrometer; the polyenergetic neutron beam from the reactor passes through the first collimator, is diffracted by the crystal in a reflection geometry, passes through the second collimator and reaches a boron trifluoride detector placed at the end of the spectrometer arm.

Since any neutron satisfying equation (1) can be diffracted, higher order contamination are always present in the reflected beam, that has neutrons with the desired wavelength λ and also wavelengths $\lambda/2$, $\lambda/3$, etc

Polycrystalline filters, that transmit only neutrons with wavelength greater than the cut-off given by twice the larger interplanar spacing, are commonly used to eliminate or attenuate higher order contamination.

In our case a beryllium polycrystalline filter, with cut-off 3.96 Å, is placed inside the beam hole, after the first collimator.

A magnetite crystal monochromator was used because the magnetic scattering amplitude falls rapidly with $\sin\theta/\lambda$ and the relative amount of higher order contamination is smaller.

Through the combination of this monochromator and the Be filter (10 cm thick) it is possible to perform transmission measurements for neutrons in the wavelength range 4.0 – 6.5 Å, without contamination; this was checked measuring the total neutron cross section of H_2O, chosen as standard.

III.2. Transmission Measurements

The total neutron cross section at each wavelength is obtained measuring the transmission of the specimen with monochromatic neutrons When a collimated neutron beam is perpendicularly incident to the plane surface of a sample, the measured transmission, or the ratio between the transmited and the incident intensities is given by:

$$T = \exp(-N \times \sigma_T)$$

where N is the number of atoms (or molecules) per cm^3 of the sample, x is the sample thickness and σ_T is the microscopic total cross section of the atom (or molecule), composed by the absorption cross section σ_a and by the scattering cross section σ_s: $\sigma_T = \sigma_a + \sigma_s$ N is given by

$$N = \frac{\rho\, N_0}{A}$$

where N_0 is the Avogadro's number, A is the atomic (or molecule) weigth and ρ is the density of the sample.

For samples in powder form, which is the case for DNA, the density to be used in the calculation depends on the powder compactation, and is computed from mass and volume

measurements.

The product $Nx = m\,N_0/SA = n$ is the number of atoms (or molecules) per barn*, where m is the mass of the sample and S is the surface area of the sample container.

In the case of hygroscopic samples like DNA, equation (2) must be rewritten for the wet sample

$$\ln T_{wet}^{-1} = n_{DNA}\,\sigma_{DNA} + n_{H_2O}\,\sigma_{H_2O} = \ln T_{DNA}^{-1} + \ln T_{H_2O}^{-1} \qquad (4)$$

We can assume that the water presence does not influence in a sensible way the interaction of DNA with the neutrons, since the water molecules are primary bound to phosphate groups[5,6]. Therefore we can use $n_{DNA}\,\sigma_{DNA} = n_{dry}\,\sigma_{dry}$.

IV. Results and Discussion

IV.1. Hydration

The sample used in the transmission measurements was a Deoxiribonucleic acid ex thymus in powder form (from Koch. Light Laboratories Ltd.) whose approximate moisture is 6%

Using conventional technique of dehydration one can remove the water present in DNA, including the bounded[4] water. A DNA quantity of 8.0399 g was placed in a dissecator in vacuum with calcium chloride for two months, and 0.4755 g of water was eliminated (5.9%); therefore the remaining mass of dry DNA was $m_{dry} = 7.5644$ g.

This dry DNA was placed in a sealed container (with $S = 15.9\ cm^2$) and the neutron transmission in the 4.0 – 6.5 Å wavelength-range was measured.

Figure 5 shows the experimental points of $\ln T_{dry}^{-1}$ vs λ. The straight line equation adjusted by a least-square fit is given by

$$\ln T_{dry} = (0.82 \pm 0.02) + (0.076 \pm 0.003)\lambda \qquad (5)$$

After these transmission measurements, the same sample of powdered DNA was treated to become hydrated. The DNA was exposed for fifteen days to a surrounding atmosphere whose relative humidity was approximately 85%. Through successive weighting a gradual increase of mass due to the water presence, was observed until the saturation with a final total mass of 8.1783 g, that corresponds to 0.6139 g of water (7.5%) or $n_{H_2O} = 1.292 \times 10^{-3}$ molecules/barn This is equivalent to 5.6 water molecules per tetra nucleotide.

The transmission through this hydrated sample was measured for the same neutron wavelength range. In figure 5 the experimental points of $\ln T_{wet}^{-1}$ vs λ are shown and the straight line adjusted by least-square fit is

$$\ln T_{wet} = (0.96 \pm 0.02) + (0.092 \pm 0.004)\lambda \qquad (6)$$

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* 1 barn = $10^{-24}\ cm^2$ is the unit used for cross sections.

From equations (4), (5) and (6) results

$$\ln T^{-1}_{H_2O} = (0.14 \pm 0.03) + (0.016 \pm 0.005)\lambda$$

Thus the contribution of water to $\ln T^{-1}_{wet}$ is about 15%. The total cross section for H_2O molecules in Deoxyribonucleic acid ex thymus calculated using the above value of n_{H_2O} is given by equation (7):

$$\sigma_{H_2O}(\text{in DNA}) = (108 \pm 23) + (12 \pm 4)\lambda \quad \text{barns} \tag{7}$$

The neutron scattering cross section per proton for H_2O molecules in DNA, $\sigma_{S/H}$, is obtained from the total cross section, eq. (7), by subtracting the absorption cross sections of oxygen and hydrogen, proportional to the neutron wavelength, known from tabulated values at thermal energy (0.025 eV)[10] and dividing the remaining cross section value by the number of hydrogen atoms in the molecule. The $\sigma_{S/H}$ equation for H_2O in wet DNA is given by

$$\sigma_{S/H} = (54 \pm 12) + (6 \pm 2)\lambda \quad \text{barns} \tag{8}$$

The slope of $\sigma_{S/H}$ is determined by the dynamics of the H atoms. For the water the obtained slopes varie between 6.1 and 6.8[10,15] and is considerably larger than the slope of 2.9 b/Å obtained for ice[15].

Therefore the slope here obtained for water in wet DNA agrees with the slope for liquid water This suggests that the water molecules in DNA execute approximately the same kind of hindered rotation or torsional motions as in liquid water, what would confirm the results obtained by Whittemore[22].

IV.2. Cross Section of DNA

The empirical formula for a tetranucleotide monomeric unit estimated from the base composition of Deoxyribonucleic acid ex thymus (Table 1) and from the number of atoms of each element that constitute the bases (fig. 2) is $C_{39}\,H_{49}\,O_{24}\,N_{15}\,P_4$, with an average molecular weight 1235.8 amu.

The number of tetranucleotide monomeric units per barn of the DNA sample according to eq. (3) is $n = 2.3187 \times 10^{-4}$ units/barn.

In figure 6 the experimental points, σ_T for dry DNA are plotted in the 4.0 – 6.5 Å neutron wavelength range; the straight line is just eq. (5) divided by the number of monomeric units

The total cross section curve represents the interaction probability between DNA ex thymus and neutrons, by scattering and absorption, in that wavelength range.

From σ_T for the tetranucleotide unit, the scattering cross section per hydrogen atom, $\sigma_{S/H}$, can be obtained by a procedure similar to that used for water: subtracting the absorption cross sections of the atoms in the tetranucleotide unit dividing by number of hydrogen atoms.

Experimental points of $\sigma_{S/H}$ vs. λ are shown in figure 7 and the straight line, adjusted by

least square-fit, is given by

$$\sigma_{S/H} = (72.5 \pm 1.4) + (6.1 \pm 0.3)\lambda \quad \text{barns}$$

The slope obtained for $\sigma_{S/H}$ in dry DNA is very similar to the slope obtained for water in DNA. Therefore, the slope for $\sigma_{S/H}$ in wet DNA should be also the same, what has been actually found following the same procedure, but considering the 5.6 water molecules per DNA tetranucleotide unit.

The slope 6.1 b/Å indicates that the freedom of motion for H atoms is not large, since free motion of protons would correspond to slopes larger than 11 b/Å[9,18].

The relatively small value for the slope, 6.1 b/Å, and its similarity to the slope of liquid water, can be attributed partially to the existence of hydrogen bonding in DNA, although only 10% of the protons in this compound are located in these bounds. As it is well known the presence of hydrogen bonding in hydrogenous compounds restricts the freedom of motions of H atoms[16].

However, the small hydrogen motion in DNA is mainly due to torsional motions with origin in molecular nonplanarity[8], stretching of C = O and N – H bondings[2] and other motions that can be identified through the peaks occurring in a range of 30 - 600 cm^{-1} of frequency distribution measured by optical techniques[13] or neutron inelastic scattering[8].

The similarity of the slopes of $\sigma_{S/H}$ for DNA and water shows that in the average, the torsional motions of H in DNA are similar to those in liquid water.

V. Conclusion

Measurements of neutron transmission through dry and wet samples of DNA allowed the determination of neutron scattering cross section of the water bound to the biopolymer. This cross section shows that the water in DNA presents a behaviour more similar to that of liquid water.

The measurements allowed also the determination of the average scattering cross section per proton $\sigma_{S/H}$ for DNA, which slope 6.1 b/Å, very similar to the liquid water, shows that the hydrogen atoms don't have much freedom of motion in this macromolecule. This can be attributed to the existence of hydrogen bonding in DNA, where 10% of protons are located, and to torsional motions of the remaining protons, giving as a net result an average freedom of motion for protons in DNA very similar to that in liquid water.

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RESUMO

Com a finalidade de estudar a dinâmica da água absorvida em moléculas biológicas e a liberdade de movimento dos átomos de hidrogênio, foi medida a transmissão para neutrons de uma amostra de DNA, utilizando um espectrômetro de cristal no intervalo de comprimento de onda entre 4,0 e 6,5 Å.

O conhecimento do estado em que se encontra a água presente no DNA é de grande interesse para o estudo de estruturas e funções de macromoléculas biológicas. Estudos de NMR sugerem que a coordenação da água no DNA é do tipo gelo, enquanto que resultados obtidos através do espalhamento inelástico de neutrons pelo ácido poliglutâmico sugerem um comportamento do tipo água líquida. No presente trabalho, foram realizadas medidas, à temperatura ambiente, para uma mostra seca de DNA e para uma amostra com 7,8% de umidade. As seções de choque totais, σ_T, e as de espalhamento por átomo de hidrogênio, $\sigma_{S/H}$, foram determinadas em cada caso, obtendo-se a seção de choque da água no DNA. Esta seção de choque mostra que a água no DNA apresenta um comportamento do tipo da água líquida. Analisando-se a curva $\sigma_{S/H}$ para o DNA seco observa-se que os átomos de hidrogênio nesta molécula biológica não têm muita liberdade de movimento.

RÉSUMÉ

Ayant pour but l'étude de la dynamique de l'eau present dans les molécules biologiques et la liberté de mouvement des atomes d'hydrogène, la transmission neutronique à travers une echantillon de DNA a été mesurée, employant un spectromètre à cristal dans l'intervalle de longueuer d'onde de 4,0 à 6,5 Å.

La connaissance de l'état de l'eau présent dans le DNA est très utile pour l'étude de structures et fonctions des macromolécules biologiques. Études de NMR ont suggéré que la coordination de l'eau dans le DNA est du type glace, tandis que résultats obtenus pour la dispersion inelastique de neutrons ont suggéré un comportement type eau liquide. Dans le présent travail sont presentées mesures a la temperature ambiante pour un enchantillon sec et pour un enchatillon avec 7,8% d'humidité. La section efficace totale, σ_T, et de dispersion per atome d'hidrogène, $\sigma_{S/H}$, ont été determinées dans chaque cas. La section efficace obtenuée pour l'eau dans le DNA présente un comportement type eau liquide. L'analyse de la courbe de $\sigma_{S/H}$ pour le DNA sec montre que les atomes d'hydrogène dans la molécule biologique n'ont pas beaucoup de liberté de mouvement.

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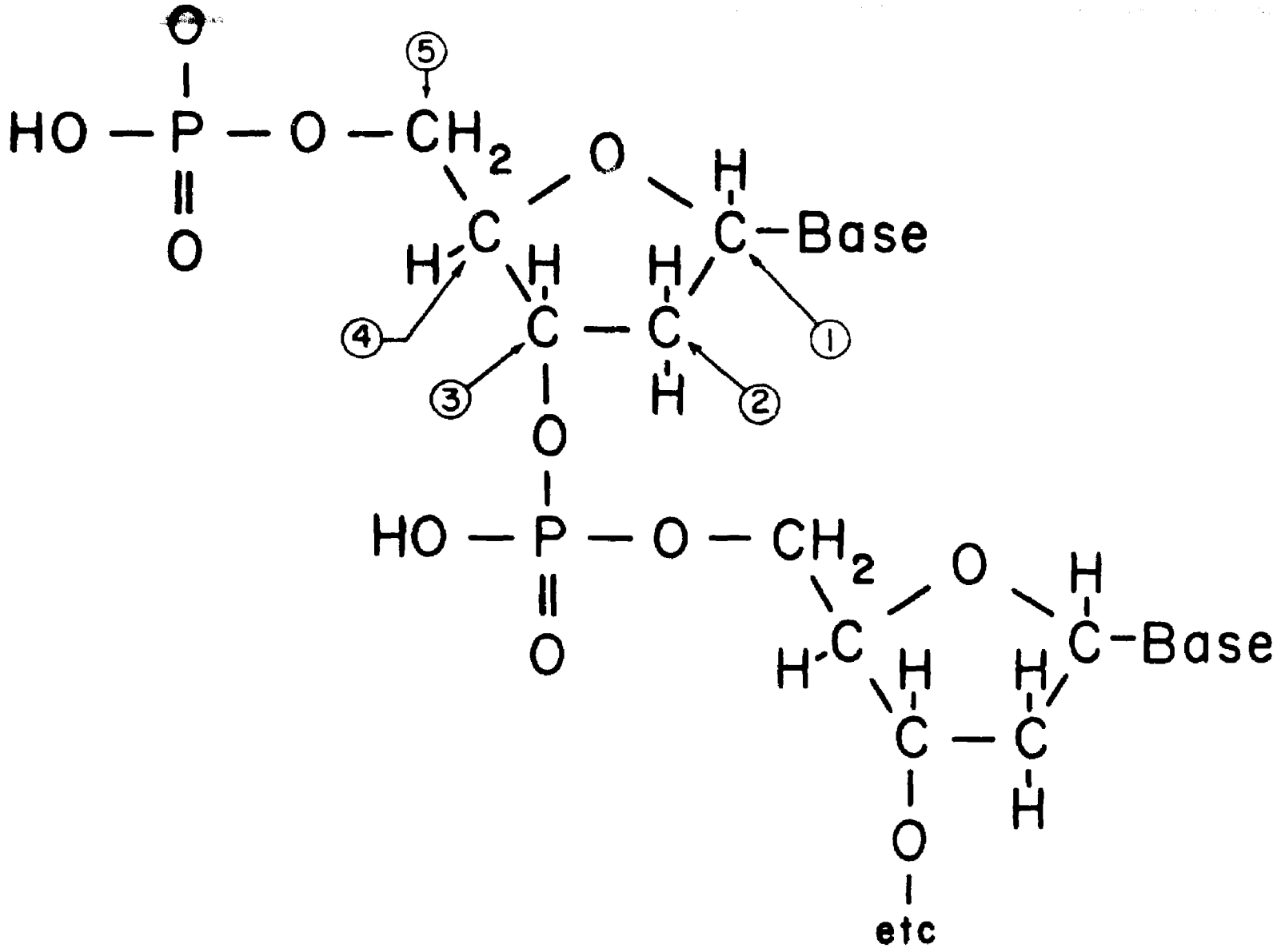
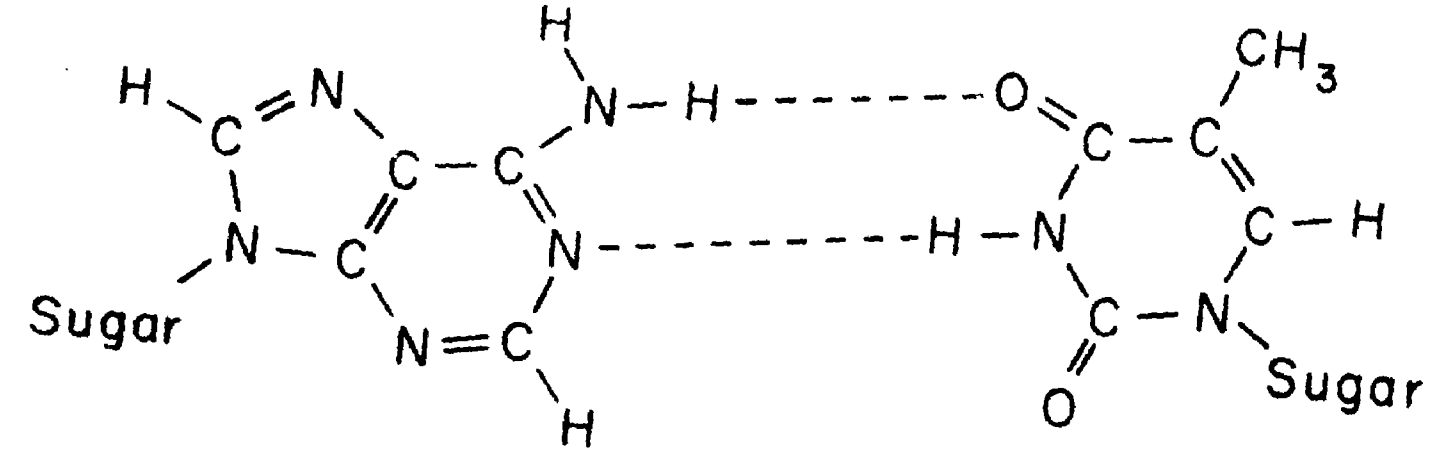
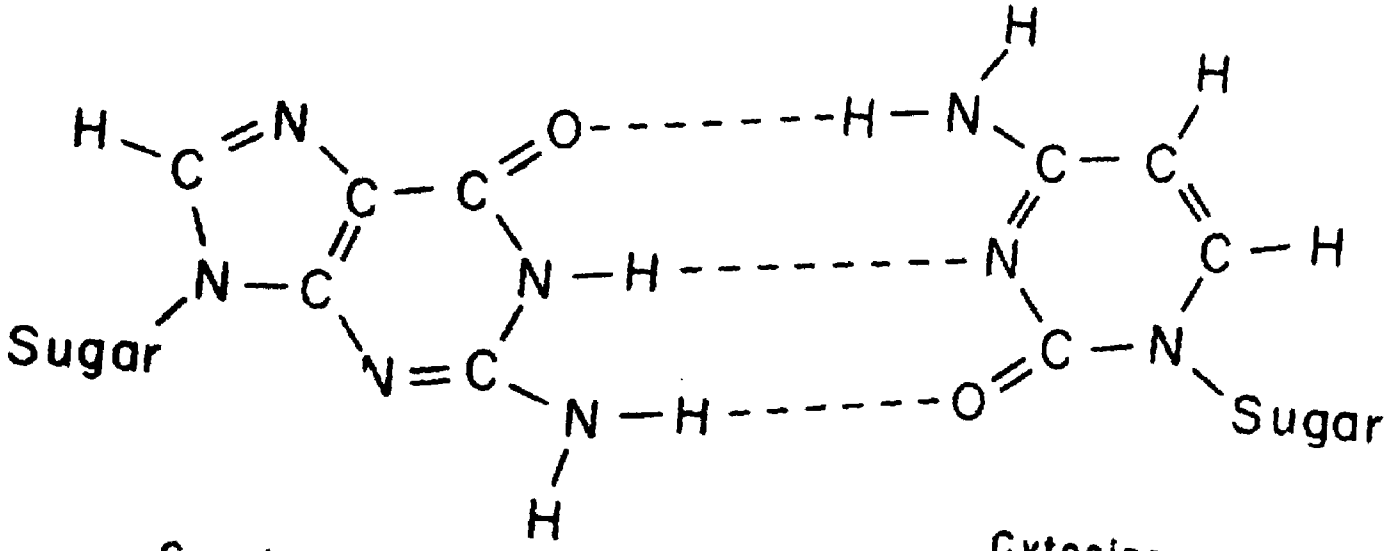


Figure - 1 Structure of Nucleotides; the sugar stretch is for Deoxyribose in DNA; Deoxyribose is distinguished from ribose by the absence of a hydroxy' group on 2' - carbon atom of the sugar.



Adenine Thymine



Guanine Cytosine

Figure - 2 The component bases of DNA. Adenine and Thymine are held together by two hydrogen bonds, while Cytosine and Guanine are held together by three hydrogen bonds; Uracil in RNA has a hydrogen atom substituting CH_3 of Thymine.

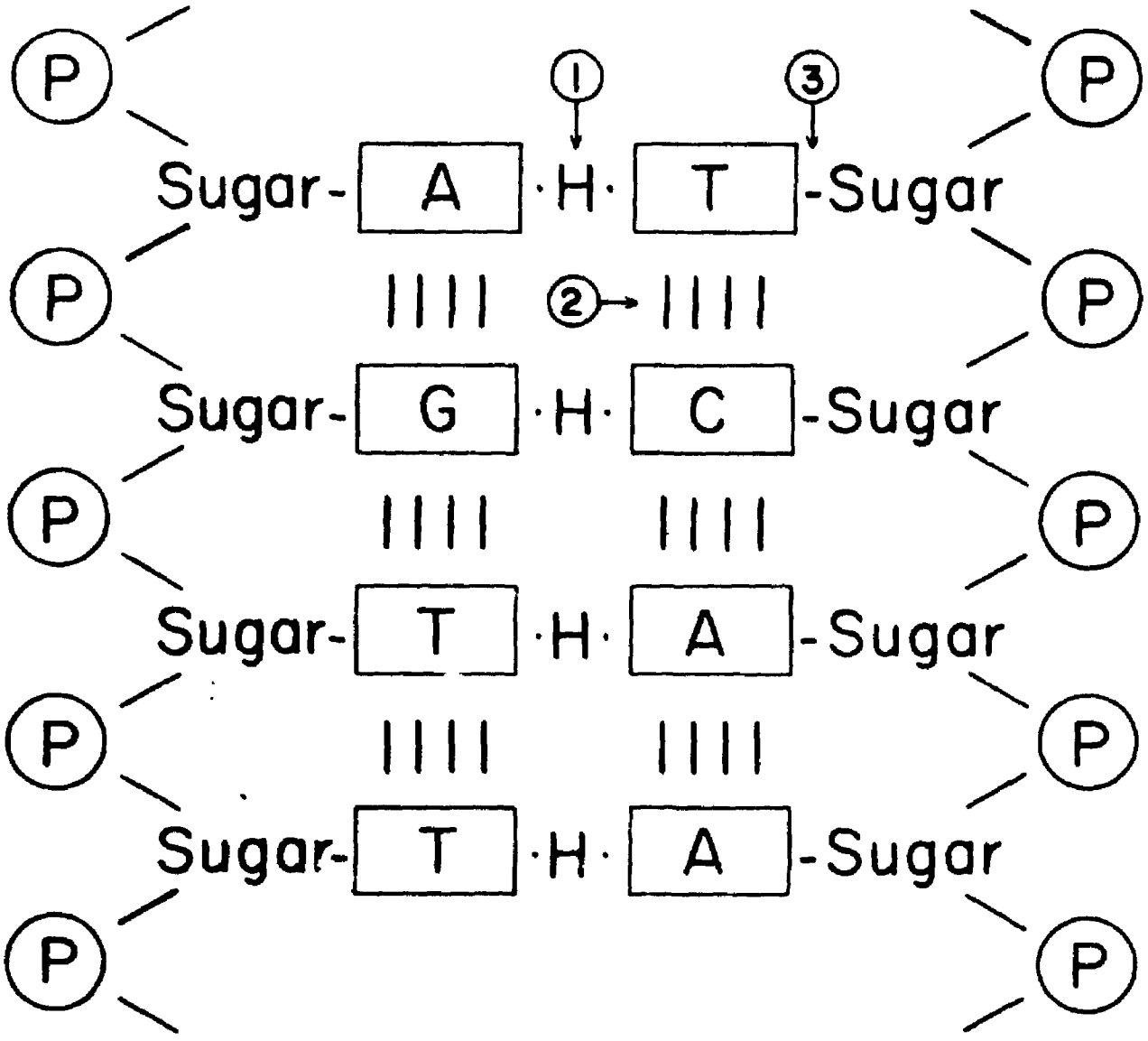


Figure - 3(a) The Watson Crick model for DNA. A two-dimensional representation of a segment of double stranded DNA(1) hydrogen bonds between the complementary bases, adenine (A) and thymine (T), or guanine (G) and cytosine (C); (2) stocking interaction between the bases, moderated by the supporting water envelope; (3) N-glycosidic bonds;

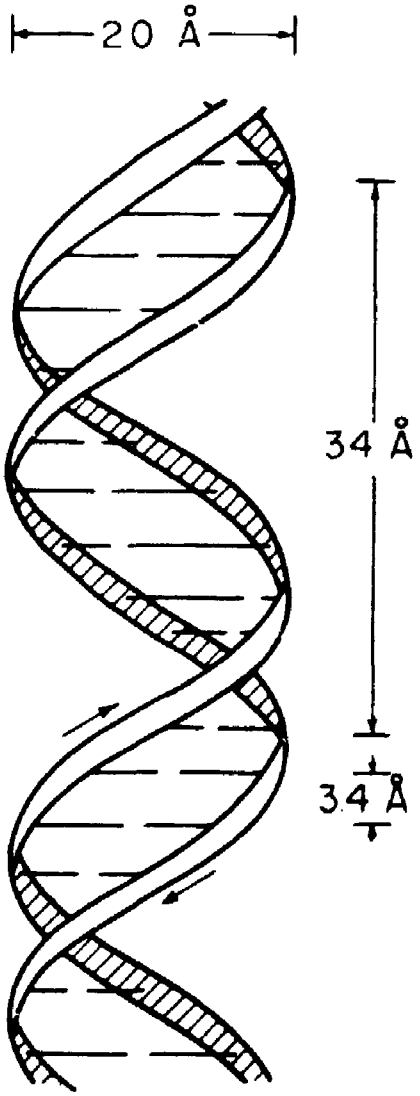


Figure - 3(b) The Watson Crick model for DNA: the three-dimensional structure of double stranded DNA, the horizontal bars being the pairs of bases holding the chain together.

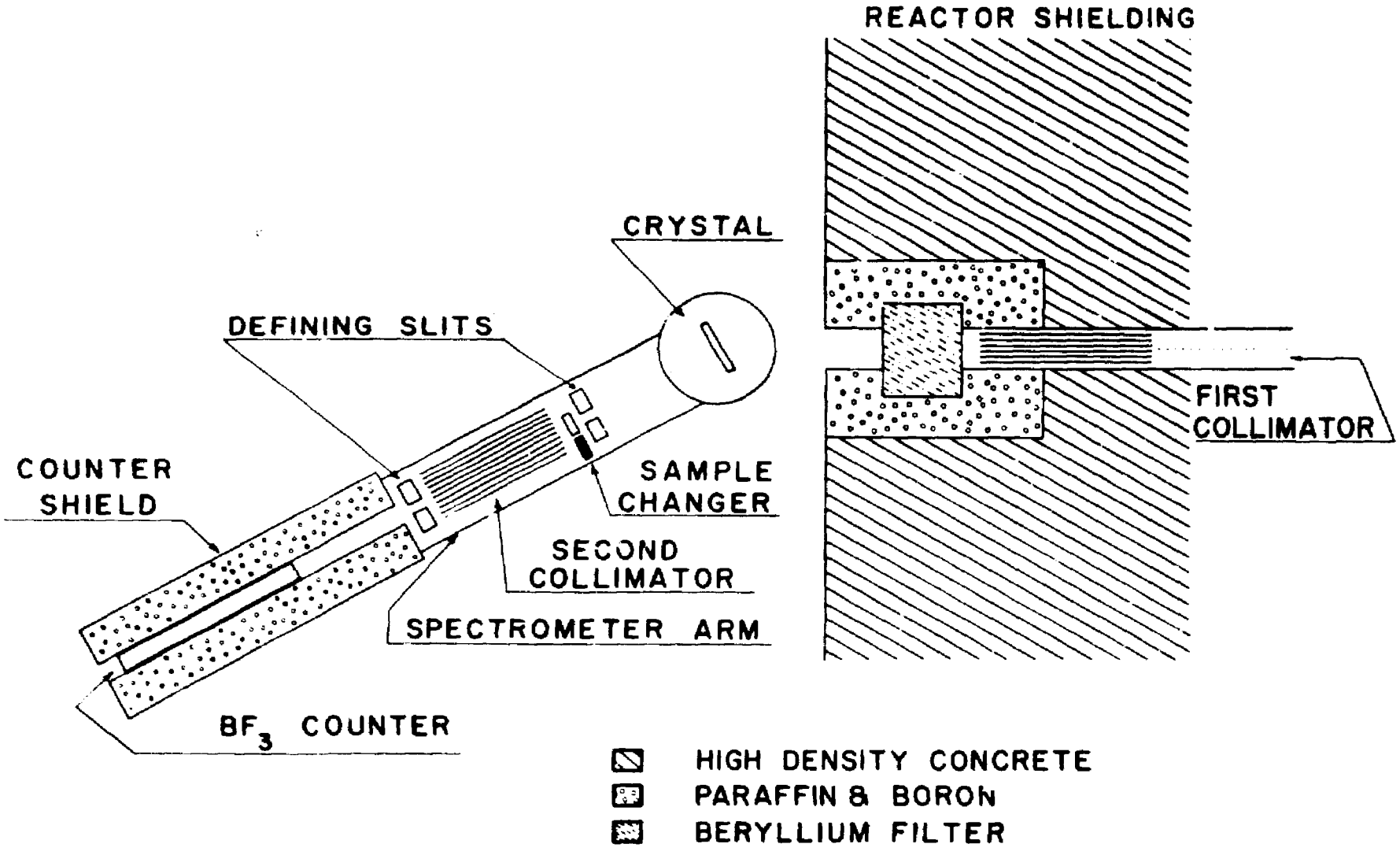


Figure - 4 Schematic diagram of the IEA neutron crystal spectrometer.

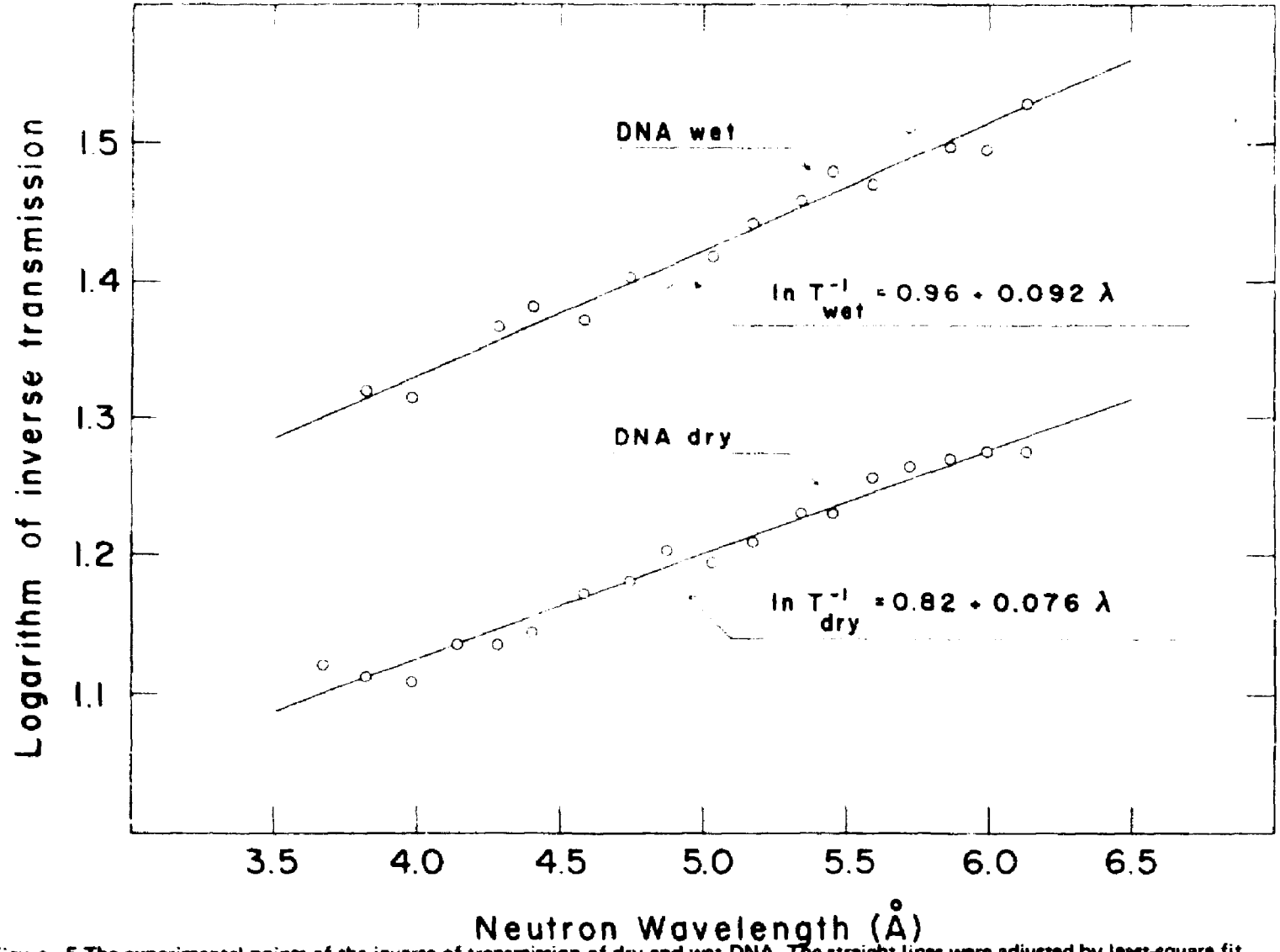


Figure - 5 The experimental points of the inverse of transmission of dry and wet DNA. The straight lines were adjusted by least-square fit.

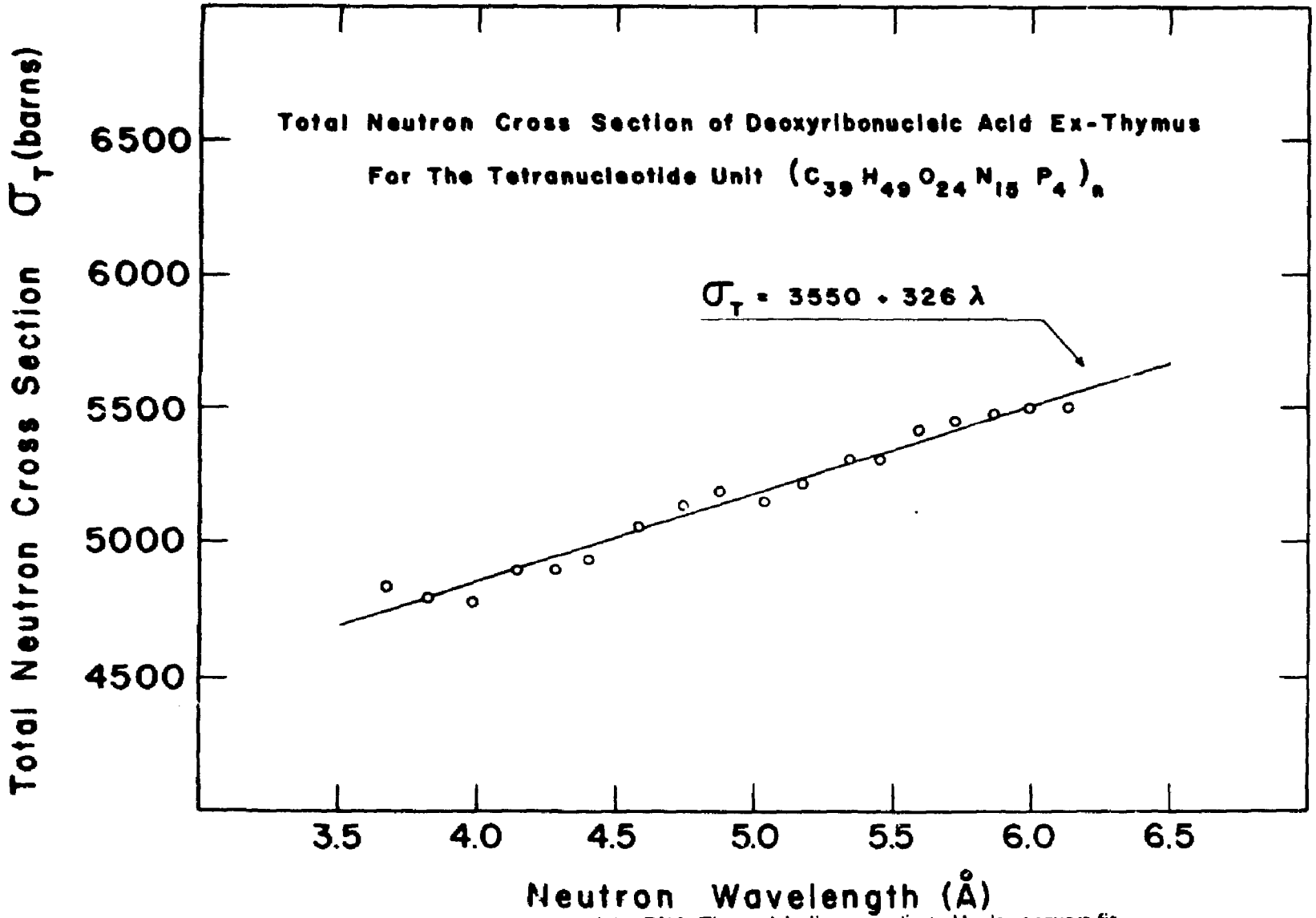


Figure - 6 Total neutron cross section of dry DNA. The straight line was adjusted by least-square fit.

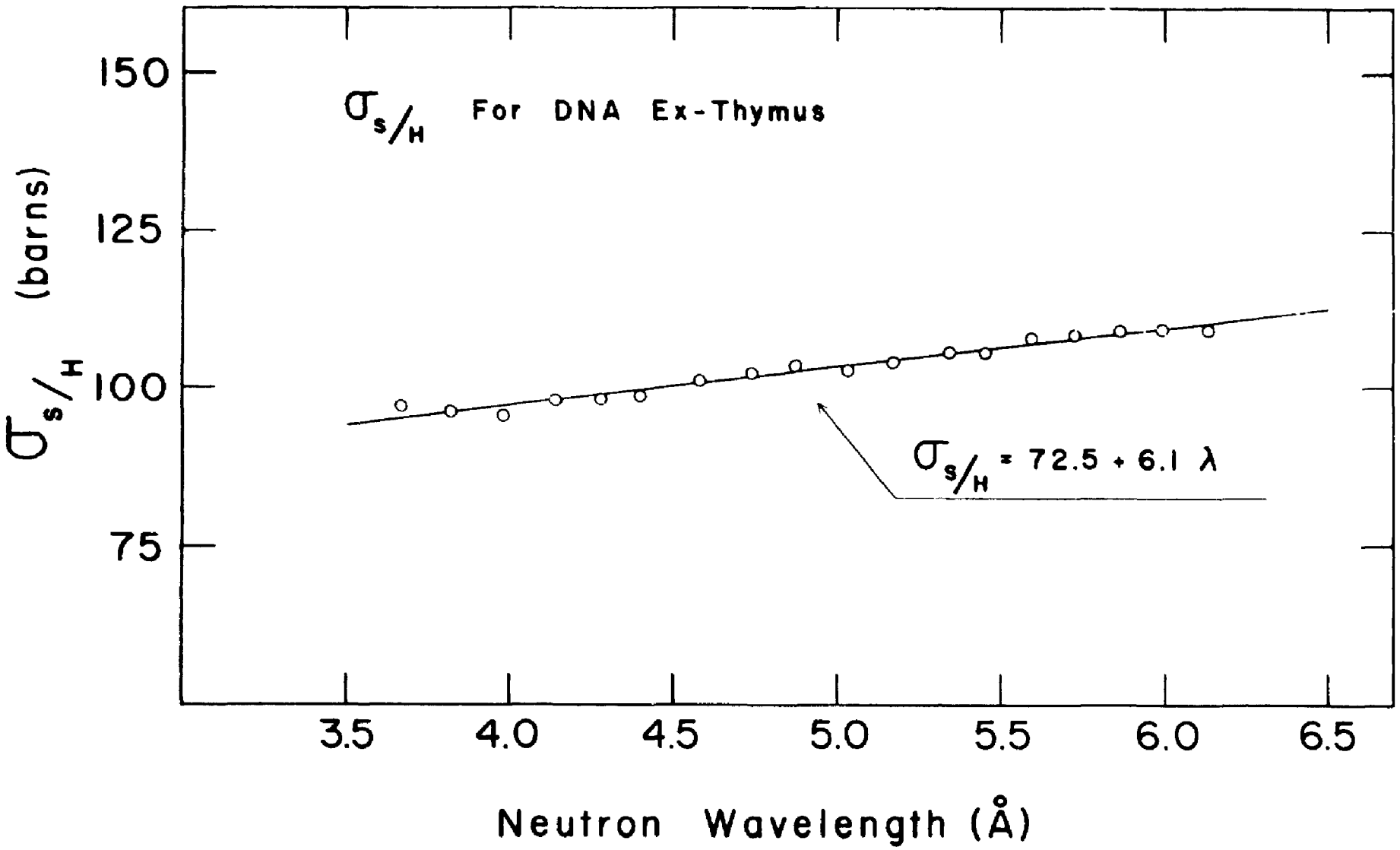


Figure - 7 Neutron scattering cross section per hydrogen atom of DNA. The straight line was adjusted by least-square fit.