

Accepted Manuscript

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L.A. Rodríguez Palomino, J. Dawidowski, J.I. Márquez Damián,
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PII: S0168-9002(17)30769-6
DOI: <http://dx.doi.org/10.1016/j.nima.2017.07.027>
Reference: NIMA 59976

To appear in: *Nuclear Inst. and Methods in Physics Research, A*

Received date: 9 May 2017
Revised date: 14 July 2017
Accepted date: 14 July 2017

Please cite this article as: L.A. Rodríguez Palomino, J. Dawidowski, J.I. Márquez Damián, G.J. Cuello, G. Romanelli, M. Krzystyniak, Neutron total cross-section of hydrogenous and deuterated 1- and 2-propanol and n-butanol measured using the VESUVIO spectrometer, *Nuclear Inst. and Methods in Physics Research, A* (2017), <http://dx.doi.org/10.1016/j.nima.2017.07.027>

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Neutron total cross-section of hydrogenous and deuterated 1- and 2-propanol and n-butanol measured using the VESUVIO spectrometer

L. A. Rodríguez Palomino, J. Dawidowski*, J. I. Márquez Damián

Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Comisión Nacional de Energía Atómica-Universidad Nacional de Cuyo, Argentina

G. J. Cuello

Institut Laue Langevin, 71, Av. des Martyrs, 38042 Grenoble, France

G. Romanelli, M. Krzystyniak

ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire OX11 0QX, United Kingdom

Abstract

This work presents the total cross sections of a set of normal and deuterated alcohols (hydrogenous 1- and 2-propanol and n-butanol, 1-propanol(OD) and fully deuterated 2-propanol and n-butanol), measured at spectrometer VESUVIO (ISIS spallation neutron source, United Kingdom). Granada's Synthetic Model was applied to describe those systems and a satisfactory agreement with the measured total cross section was achieved in the range of energies from 10^{-3} to 100 eV. The input parameters of the model were determined from the essential features of the vibrational spectra of the atoms that compose the systems, which were studied using Molecular Dynamics.

Keywords: Neutron transmission, Total cross section, 1-propanol, 2-propanol, n-butanol

*Corresponding author

Email address: javier@cab.cnea.gov.ar (J. Dawidowski)

1. Introduction

The study of the structural properties of alcohols by neutron scattering, has been the recent subject of a renewed interest [1]. Although already extensively studied, the availability of varied experimental resources allow new degrees of refinement in the existing knowledge. Thus, to the customary use of deuteration to enhance the coherent signal, the possibility to perform polarized neutron experiments up to fairly large values of momentum transfer, opened the possibility to assess the total spin-incoherent contribution to the diffractograms in a direct way [2]. This also helps to overcome the drawbacks of isotopic substitution in the analysis of correlation functions, where one can never be sure whether a given observed feature comes from an isotopic effect or whether it is indeed a real feature. The task undertaken following this idea involved a set of experiments at the Spin Polarized Hot Neutron Beam Facility (D3) of the ILL (Institut Laue Langevin, Grenoble, France) [3].

The search for accurate results from neutron diffraction experiments, leads to the creation of precise analysis tools that contain the most updated information on the neutron-system interaction. The reason for such requirement is that the Monte Carlo techniques employed in the corrections for multiple scattering and sample attenuation, involve tracking the neutron histories along a series of interactions, where the neutron exchanges energy and momentum [4, 5], what makes it to change its mean free path. This fact is overlooked by common processing correction procedures employed for neutron diffraction, that were originally developed for X-rays techniques in times when computer resources were limited. Thus, the knowledge of the total cross section as a function of the energy is essential, since it has a direct influence on the intensity of the multiple scattering components. For that reason, a suitable neutron-molecule interaction model is a requirement of such simulation programs. Granada's Synthetic Model [6] has been favorably employed for that end due to its simple formulation and its fast performance in calculation. The model, based on a basic knowledge of the vibrational frequency spectra, can be benchmarked by comparison of the

predicted and measured total cross sections.

From that point of view, the interest in determining the total cross sections is twofold, not to mention that it is a normal requirement of calculations employed in Nuclear Engineering [7, 8, 9]. The transmission technique to determine the total cross sections, although simple, is not available in many facilities around the world. The spectrometer VESUVIO at ISIS facility [10] (Rutherford Appleton Laboratory, UK) has this capability and cross sections over five decades in energy can be determined by time of flight. It is worth to comment that the development plans for its proposed next-generation upgrade called ETNA (after Epithermal and Thermal Neutron Analysis), contemplates the use of the transmission technique concurrently with mass-resolved neutron spectroscopy, and diffraction [11, 12], as well as the implementation of techniques unique to pulsed neutrons such as γ -ray dopplerimetry and energy-resolved prompt- γ activation analysis, to explore the properties of complex functional materials.

In this work we present experimental total cross sections of hydrogenous 1-propanol, 2-propanol and n-butanol, as well as deuterated species of them. We show a procedure to elaborate the corresponding input parameters for the Synthetic Model based on frequency spectra generated by the code GROMACS [13]. Finally we calculate the total cross sections, which were benchmarked with the experimental data.

2. Experimental

The samples studied in this work were liquid high-purity 1-propanol ($\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$), 2-propanol ($\text{CH}_3\text{CHOHCH}_3$), n-butanol ($\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{OH}$), 1-propanol-OD ($\text{CH}_3\text{CH}_2\text{CH}_2\text{OD}$), 2-propanol-D8 ($\text{CD}_3\text{CDODCD}_3$) and n-butanol-D10 ($\text{CD}_3\text{CD}_2\text{CD}_2\text{CD}_2\text{OD}$) (Table 1), bought from Sigma Aldrich company, with 99% deuteration in the case of the last three. The experiments were carried out in two batches, the first with hydrogenated samples and the second with the deuterated ones. The great similarity in the results of hydrogenous 1- and 2- propanol, (that led us to conclude that they can be modeled by the same parameters) in the first batch,

led us not to choose both deuterated 1- and 2- propanol for the second batch, and to study 1-propanol (OD) and 2-propanol-D8 instead.

All the measurements were carried out at room temperature. The samples were poured into aluminum flat cells of square sections 65 mm inner side and 90 mm outer side, arranged to cover the penumbra of the neutron beam. The thicknesses were 1.5 mm in the case of normal and 2 mm in the case of the deuterated samples.

The experiment was carried out at VESUVIO spectrometer, placed at target station 1 (TS1) of the ISIS spallation neutron source at Rutherford Appleton Laboratory (United Kingdom). The general setup of VESUVIO is shown in Fig. 1, where the transmission facility employed in this work is highlighted. The transmission monitor S2 is a ^6Li -doped glass scintillator placed at 13.43 m from the neutron moderator. The beam monitor S1 (also a ^6Li scintillator) is placed at 8.60 m from the moderator, and its count rate is employed to normalize the spectra registered by the transmission monitor. The sample, placed into an evacuated bell jar, is at 11 m from the moderator.

Sample	Formula	Molecular mass (amu)	Density (g/cm ³)	Number density (Å ⁻³)	σ_{free} (barn)
1-propanol	CH ₃ CH ₂ CH ₂ OH	60.095	0.804	0.00806	183.28
2-propanol	CH ₃ CHOHCH ₃	60.095	0.785	0.00787	183.28
n-butanol	CH ₃ CH ₂ CH ₂ CH ₂ OH	74.12	0.81	0.00658	229.35
1-propanol (OD)	CH ₃ CH ₂ CH ₂ OD	61.096	0.817	0.00805	166.02
2-propanol (D8)	CD ₃ CDODCD ₃	68.14	0.89	0.00787	45.23
n-butanol (D10)	CD ₃ CD ₂ CD ₂ CD ₂ OD	84.12	0.92	0.00659	56.79

Table 1: Samples studied in this work, with their basic parameters of interest: molecular mass, density, number density per molecule, and free-atom scattering cross section per molecule.

The ISIS spallation neutron source produces pulses at a repetition rate of 50 Hz in such a way to provide both target stations 1 (TS1) and 2 (TS2). In every set of five pulses, the first four (with a period of 20 msec per pulse) go

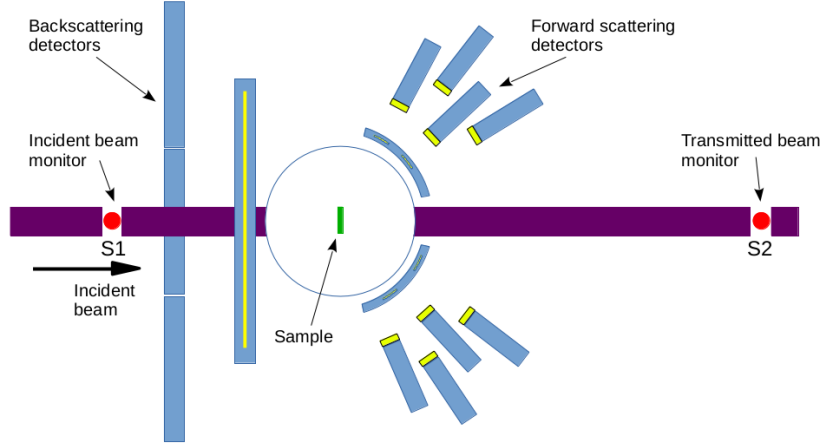


Figure 1: VESUVIO general setup, showing the forward scattering and backscattering detectors. The transmission line with monitors S1 and S2 employed in this work is highlighted.

to TS1 and the fifth to TS2. For the measurement of the deuterated samples, the acquisition software was setup to record the slow neutrons produced after the fourth pulse, taking advantage of the 40 msec time lapse available, which allowed to extend the energy range down to about 1 meV.

The spectra were recorded as a function of the time of flight, and converted to energy employing programs based on the Open Genie display and data analysis suite, developed for the neutron scattering instruments at the ISIS facility [14]. The sample transmissions $T(E)$ were determined by measuring the transmitted beam $S(E)$, and the empty cell $C(E)$. The background, checked by measuring the transmitted beam of a 1 mm thick cadmium sheet, was considered negligible. The transmission, determined from

$$T(E) = \frac{S(E)}{C(E)}, \quad (1)$$

is related to the total cross section $\sigma_{\text{tot}}(E)$ via

$$T(E) = \exp(-n d \sigma_{\text{tot}}(E)), \quad (2)$$

where n is the number density and d the sample thickness. Both n (shown in Table 1) and σ_{tot} are determined per molecule. Thus, the cross sections are determined from

$$\sigma_{\text{tot}}(E) = -\frac{1}{nd} \ln \left(\frac{S(E)}{C(E)} \right). \quad (3)$$

3. Model

Granada's Synthetic Model was extensively discussed elsewhere [6] and successfully applied in a variety of cases [8, 15]. The Synthetic Model is based on a set of parameters that define a synthetic vibrational spectrum represented by a set of Einstein oscillators. Such parameters are discrete frequencies and widths and their corresponding weights, that describe the essential features of the vibrational spectrum.

The procedure followed to formulate the model for each system was to determine the vibrational spectra of each atomic species obtained through molecular dynamics (MD) using the GROMACS code [16]. The spectra thus obtained was represented by Einstein oscillators at frequencies located approximately at the barycenters of their main sections, and with weights proportional to their areas. This served to formulate an input dataset for the Synthetic Model which was benchmarked with the measured total cross sections. Small corrections were applied to the input data until a satisfactory comparison was reached.

These vibrational spectra were obtained employing a box of 216 molecules modeled using the OPLSAA (optimized potential for liquid simulations all-atom) force field [17]. The system was equilibrated using a Nose-Hoover thermostat at 300 K and a Parrinello-Rahman barostat at 1 bar for 300 ps with a 0.2 fs time-step, and then a production run was computed in the NVE microcanonical ensemble with a 0.1 fs time-step for 10 ps. Velocity values were captured every 0.2 fs and used to compute the velocity auto-correlation function, which

was then used to compute the generalized frequency spectra by cosine Fourier transform.

Figures 2 and 3 show the vibrational spectra of the different atomic species for the hydrogenous and deuterated alcohols respectively. Hydrogenous 1- and 2-propanol were modeled with the same parameters since both molecules have the same elementary molecular units (CH_3 , CH_2 , OH), being different only the location of OH unit. Due to this characteristic, its vibrational modes are very similar, which is corroborated by the similar cross sections found (as described in Sect. 4). In both Figures the energies representing the main features of the spectra, employed to build the inputs for the Synthetic Model are indicated. In the case of hydrogenous samples, the same discrete energy set applies for H, C and O. This is not the case for the deuterated samples. Especially, in 1-propanol (OD) some frequencies corresponding to H modes do not correspond with D modes.

The effective masses employed in the Synthetic Model for each mode are inversely proportional to the areas of the portion of the frequency spectrum that they represent. To determine them, after normalizing the frequency spectra, as shown in Figs. 2 and 3, we apply the relation that links the different masses [6]

$$\frac{1}{M_j} = \frac{1}{M_{\text{mol}}} + \sum_{\lambda} \frac{1}{M_{\lambda}^j}, \quad (4)$$

where M_j is the mass of the j th atom, M_{mol} is the molecular mass, and M_{λ}^j is the mass associated with the vibrational mode λ of the j th atom.

Tables 2, 3, 4, 5 and 6 show the input parameters of hydrogenous 1- and 2-propanol, n-butanol, 1-propanol (OD), and deuterated 2-propanol and n-butanol, respectively.

4. Results

Figures 4 and 5 show the experimental neutron total cross-sections for the hydrogenous and the deuterated samples respectively, compared with the Synthetic

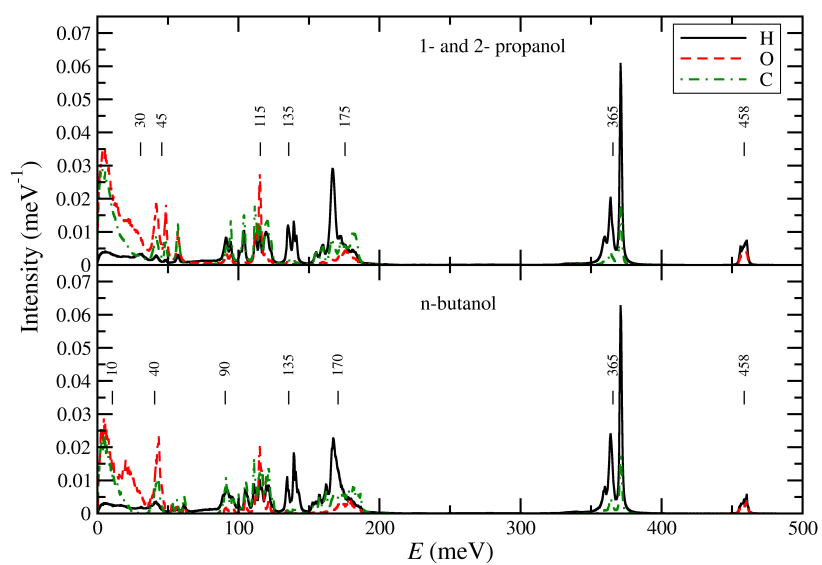


Figure 2: Frequency spectra for the atoms that compose the hydrogenous alcohols studied in this work determined by molecular dynamics (GROMACS). Upper frame: hydrogenous 1- and 2- propanol; lower frame: n-butanol. Also indicated are the frequencies employed in the formulation of the Synthetic Model.

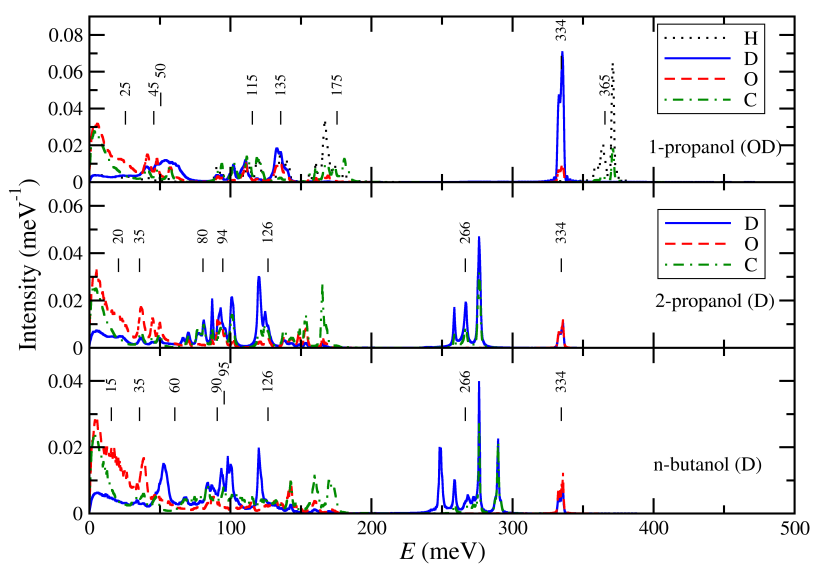


Figure 3: Frequency spectra for the atoms that compose the deuterated alcohols studied in this work determined by molecular dynamics (GROMACS). Upper frame: 1-propanol (OD); middle frame: 2-propanol (D); lower frame: n-butanol (D). Also indicated are the frequencies employed in the formulation of the Synthetic Model.

$\hbar\omega_\lambda$ (meV)	$\hbar\sigma_\lambda$ (meV)	M_H (amu)	M_O (amu)	M_C (amu)
30	15	10.17	218.18	150.0
45	10	25.42	545.45	375.0
115	35	4.75	101.95	70.1
135	5	12.71	272.73	187.5
175	25	4.00	85.90	59.1
365	35	3.77	80.81	55.6
458	35	24.21	519.48	357.1

Table 2: Input parameters for the Synthetic Model for hydrogenated 1- and 2-propanol. Columns list the vibrational frequency ($\hbar\omega_\lambda$), their associated widths ($\hbar\sigma_\lambda$), and the H, O and C effective masses, respectively.

$\hbar\omega_\lambda$ (meV)	$\hbar\sigma_\lambda$ (meV)	M_H (amu)	M_O (amu)	M_C (amu)
10	7	20.68	416.61	292.3
40	15	18.43	371.16	260.4
90	30	4.43	89.14	62.5
135	10	10.45	210.45	147.7
170	30	3.96	79.74	56.0
365	20	3.54	71.38	50.1
458	10	36.20	729.06	511.52

Table 3: Input parameters for the Synthetic Model for hydrogenated n-butanol. Columns list the vibrational frequency ($\hbar\omega_\lambda$), their associated widths ($\hbar\sigma_\lambda$), and the H, O and C effective masses, respectively.

$\hbar\omega_\lambda$ (meV)	$\hbar\sigma_\lambda$ (meV)	M_H (amu)	M_D (amu)	M_O (amu)	M_C (amu)
25	10	9.87	18.14	38.73	38.70
45	10	29.05	-	111.22	137.05
50	10	-	7.15	-	-
115	35	5.21	14.36	258.20	63.57
135	5	9.68	12.76	249.30	574.57
175	25	3.90	-	637.91	84.88
334	5	-	7.11	542.22	219.69
365	35	3.38	-	-	-

Table 4: Input parameters for the Synthetic Model for 1-propanol (OD). Columns list the vibrational frequency ($\hbar\omega_\lambda$), their associated widths ($\hbar\sigma_\lambda$), and the H, D, O and C effective masses, respectively.

$\hbar\omega_\lambda$ (meV)	$\hbar\sigma_\lambda$ (meV)	M_D (amu)	M_O (amu)	M_C (amu)
20	10	14.31	40.55	45.54
35	10	42.05	107.85	196.91
80	10	17.61	475.52	182.14
94	10	10.30	246.15	127.82
126	10	9.91	175.82	52.60
266	20	8.41	-	107.94
334	5	55.69	498.17	-

Table 5: Input parameters for the Synthetic Model for 2-propanol (D). Columns list the vibrational frequency ($\hbar\omega_\lambda$), their associated widths ($\hbar\sigma_\lambda$), and the D, O and C effective masses, respectively.

$\hbar\omega_\lambda$ (meV)	$\hbar\sigma_\lambda$ (meV)	M_D (amu)	M_O (amu)	M_C (amu)
15	10	16.26	39.21	46.20
35	10	51.22	140.17	164.70
60	10	11.71	208.05	-
90	10	-	-	61.95
95	10	8.43	244.01	-
126	10	14.95	140.17	51.85
266	20	8.13	-	120.69
334	5	75.88	520.12	-

Table 6: Input parameters for the Synthetic Model for n-butanol (D). Columns list the vibrational frequency ($\hbar\omega_\lambda$), their associated widths ($\hbar\sigma_\lambda$), and the D, O and C effective masses, respectively.

Model calculations for the total scattering cross sections plus an “ $1/v$ ” absorption component [19]. The cross sections were calculated at $k_B T = 0.00253$ eV, with the scattering cross sections $\sigma_b^H = 82.020$ barn, $\sigma_b^O = 4.232$ barn, $\sigma_b^C = 5.551$ barn, $\sigma_b^D = 7.64$ barn; and the absorption cross sections $\sigma_{abs}^H = 0.3326$ barn, $\sigma_{abs}^O = 0.0002$ barn, $\sigma_{abs}^C = 0.0035$ barn, $\sigma_{abs}^D = 0.000519$ barn (Reference [19]).

As commented above (Section 2) we observe that in the measurements of the deuterated samples, the experimental data reach lower energies. As seen in Fig. 4 there are no significant differences between the cross sections of hydrogenous 1- and 2-propanol, nor are there any differences in their calculated vibrational frequency spectra, which corroborates the modeling of both systems with the same parameters of the Synthetic Model. Fig. 6 allows a better inspection of the results. To highlight the differences between the cross sections, in the upper frame we display them normalized by their respective value of σ_{free} (taken from Table 1). A comparison of the different calculations can be seen in the lower frame, where the ratio of the different cross sections with respect to the one of 1-propanol (H) is shown. 2-propanol (H) is not included in this last graph since the model for it is the same as that of 1-propanol (H).

The general good agreement observed between experimental and calculated total cross sections serves as benchmarks of the proposed models. It is worth noting that an oscillatory behavior of the cross sections apparent in the fully deuterated samples 2-propanol (D) and n-butanol (D) (Fig. 5) is typically due to the coherence effects that are not described by the Synthetic Model. A similar effect was observed on ethanol in Ref. [8].

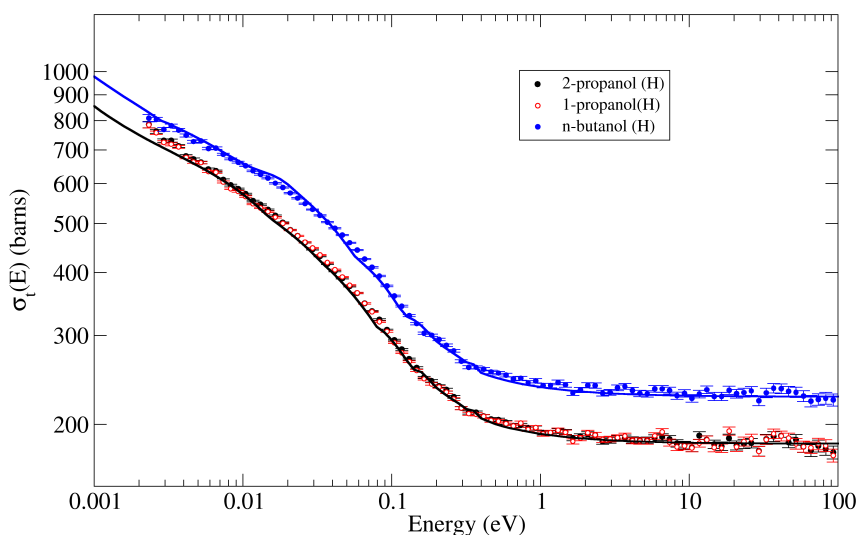


Figure 4: Experimental neutron total cross-sections for the hydrogenous 1- and 2-propanol and n-butanol (symbols), compared with their Synthetic Model calculations (lines).

5. Conclusions

In this work we presented experimental total cross sections of a set of alcohols and described them by Granada's Synthetic Model. In the process, the input data sets elaborated were extracted from vibrational spectra calculated with a MD model, and benchmarked through a comparison with experiment. This procedure is alternative to the ones presented in Refs. [3] and [8], where a constructive method was used for deuterated 1- and 2-propanol, based on pre-

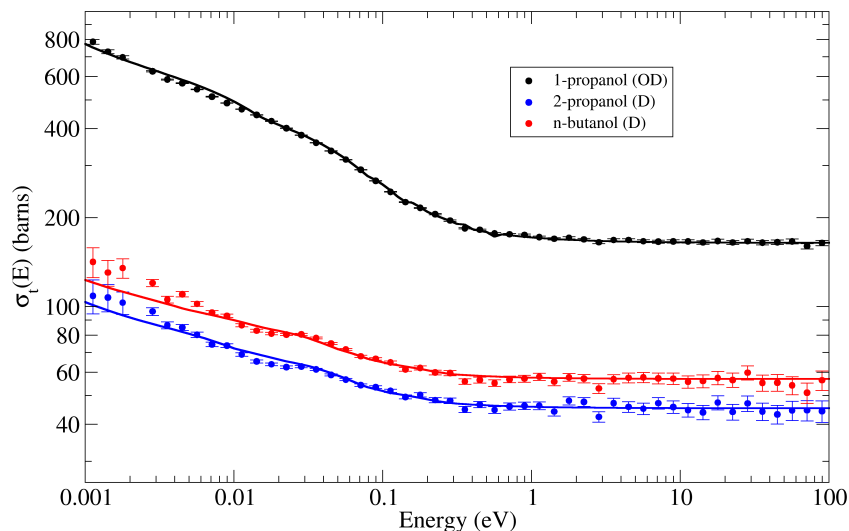


Figure 5: Experimental neutron total cross-sections for the hydrogenated 1-propanol (OD), 2-propanol (D) and n-butanol (D) (symbols), compared with their Synthetic Model calculations (lines).

vious knowledge of the vibrational spectra of molecular sub-units. While this method can provide a reasonable guess of the input parameters of the Synthetic Model when a more complete information is lacking, a method based either on MD results or experimental data is more accurate and should be preferred if possible.

In this work we verified that from the point of view of the dynamics, (in order to built suitable synthetic vibrational spectra) there are no significant differences in the hydrogenous 1- and 2-propanol, what can be extrapolated to the deuterated species. For this reason the model elaborated here for the 2-propanol (D) is applicable to 1-propanol (D) also. A close exam of 1-propanol (OD) shows that the dynamics of the hydrogen is similar as in the fully hydrogenated system, and that the inclusion of deuterium affects in that the 458 meV O-H mode is replaced by a feature at 334 meV characteristic of the O-D vibration. Also the appearance of low-frequency features around 50 meV is a

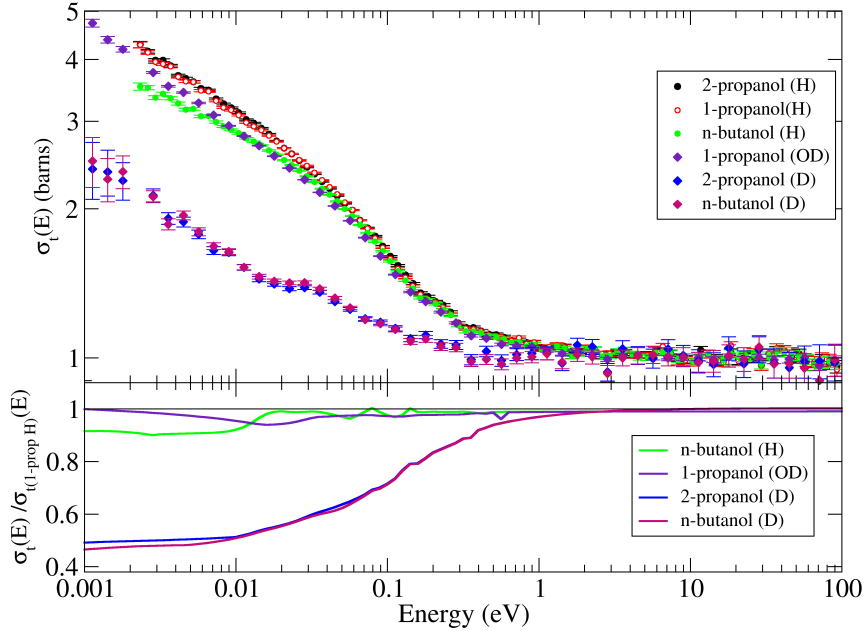


Figure 6: Upper frame: Experimental neutron total cross-sections for all the alcohols measured in this work, normalized by their respective σ_{free} (Table 1). Lower frame: Ratio of the calculated cross sections to 1-propanol (H).

distinctive footprint of the effect of deuterium not present in the hydrogenated case. These differences in the dynamics, lead to generate a synthetic spectrum (Table 4) that is somewhat different also in the lower frequencies from those of 1- and 2-propanol (Table 2).

We observe a correspondence between the high-frequency modes in case of n-butanol and 1- and 2-propanol in the hydrogenous as well as in the deuterated systems, with differences in the lower frequencies that are transferred to the synthetic spectra.

The benchmark of the synthetic vibrational spectrum through comparison with experimental total cross sections is a strong test of how the model works in different energy regimes, since the cross sections could be determined in five decades of energy in a single experiment, in the present case. This is an

outstanding feature of spectrometer VESUVIO, that originally was developed to work with epithermal neutrons, yet recently exploiting a good thermal and sub-thermal flux for neutron diffraction and transmission, which is the reason of new prospects of development in this spectrometer [20, 12]. Let us add that there is a lack of facilities to measure total cross sections around the world, and that accelerator-based pulsed neutron sources, have a distinctive advantage in this sense.

The results of this paper will be employed to develop further analysis of structural data of the alcohols, and also to trace a route on the steps needed to get the required information to perform a data analysis procedure in correspondence with high quality experimental diffraction data available nowadays.

Acknowledgments

The authors thank to Rutherford Appleton Laboratory for the beam time allowed (proposals 1520079 and 1620228). This work has been supported by CONICET (Project PIP 2011-0552), ANPCyT (Projects PICT 2011-0534 and PICT 2015-0937), and Universidad Nacional de Cuyo (Project 06C/420).

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