# Measurements of the Down-Scattering of Neutrons from Molecules with a Methyl Group

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**Abstract**

The down-scattering of thermal neutrons into the cold energy region was measured in an attempt to investigate the usefulness of methyl molecules as cold moderators. Neutron spectroscopy of a Be-detector coupled with the TOF method was used. Typical molecules $CH_3CCl_3$, $CH_3OH$ and $CH_3NO_2$ were selected with differently barriered internal rotations.

## 1. Introduction

Cold neutrons, which have energies lower than approximately 5 meV, are widely used for the investigation of a condensed system by the inelastic neutron scattering, as well as in neutron physics. They are more effectively produced in a cold moderator by the further slowing-down of thermal neutrons. The cold moderator, slightly different from a thermal moderator, consists of materials taking away a small quantity of energy from neutrons through downscattering at very low temperatures. There are some reports on the usage of solid methane and hydrogen[1].

However some molecules with methyl groups such as methanol might be useful for a cold moderator because of simpler handling. For these molecules, the internal rotation of methyl group plays an important role in the slowing-down of neutrons. To date total cross section of neutrons heve been investigated for the internal rotation of the methyl group[2].

The down-scattering of thermal neutrons is, in the present paper, described depending on the internal rotation of the differently barriered methyl groups. Neutron spectroscopy, consisting of a Be-detector using the time of flight (TOF) method, has been used directly to measure the down-scattering of thermal neutrons into the cold energy range.

## 2. Samples

The potential is written for the internal rotation of the methyl group with threehold rotational symmetry[3].

$$V(\alpha)=\frac{V_3}{3}(1-\cos 3\alpha)+\frac{V_6}{6}(1-\cos 6\alpha)+\cdots\cdots, \qquad (1)$$

where $\alpha$ is the angle around the axis of rotation and where in usual molecules,

$V_3 \gg V_6$. We have selected the following typical molecules with different heights of rotational barrier.

**$CH_3CCl_3$**

Methylchloroform has a very high barrier. Hence the torsional motion of the methyl group can well be approximated by the Mathieu equation. The energy transfer of neutrons caused by the transition of the tortional state $V=0\rightarrow 1$ will be so large that this molecule may be less preferable as a cold moderator. Rush reports $V_3=5.8$ kcal/mol by the up-scattering experiment of cold neutrons[4)], but there are large differences from the optical data[5)].

**$CH_3NO_2$**

Regarding nitromethane in a gas state, $V_3$ is always zero due to the plane symmetry of the $NO_2$- group. The next term, $V_6$ is extremely small so that the motion of the $CH_3$- group can well be considered to be a free rotation. A small energy transfer will possibly take place through the scattering of neutrons with the nearly free $CH_3$- group. However the circumstances will be different in the condensed state where intermolecular coupling might affect the rotation. We have no information on intermolecular coupling of the molecule in the condensed state.

**$CH_3OH$**

Methanol has an intermediate barrier height between the two preceding molecules, and in fact are used as a cold moderator. Although the up-scattering of cold neutrons was measured for this molecule at room temperature[6)], we are interested in the low temperature solid phase from a standpoint of a cold moderator.

**$TiH_2$**

This sample was measured in order to examine the characteristics of the neutron spectroscopy, because of the simple frequency distribution.

## 3. Experimental Arrangement

The down-scattering of thermal neutrons into a cold energy range was measured by the neutron spectroscopy using the Be-detector coupled with the TOF method. This spectroscopy, in spite of the lower energy resolution, is preferred in this case because of the direct detection of cold neutrons through the Be-filter.

The arrangement of the spectroscopy is shown in Fig. 1. A linear accelerator* is used for the production of the pulsed fast neutrons via $e^- \rightarrow \gamma \rightarrow n$ process. Thermal neutrons are produced in the boron poisoned moderator of light water ($\sim$0.0035 B/H), whose effective size is $50\times 200\times 200$ mm$^3$. The flight path of thermal neutrons is about 5 m. Only cold neutrons through the Be-filter were measured. Two systems of the Be-detector were used, and those outputs were added each other. The Be-filter consists of sandwich layers of Be blocks ($50\times$

* These measurements were made by using the linear accelerator at Kyôto University Reactor Institute.

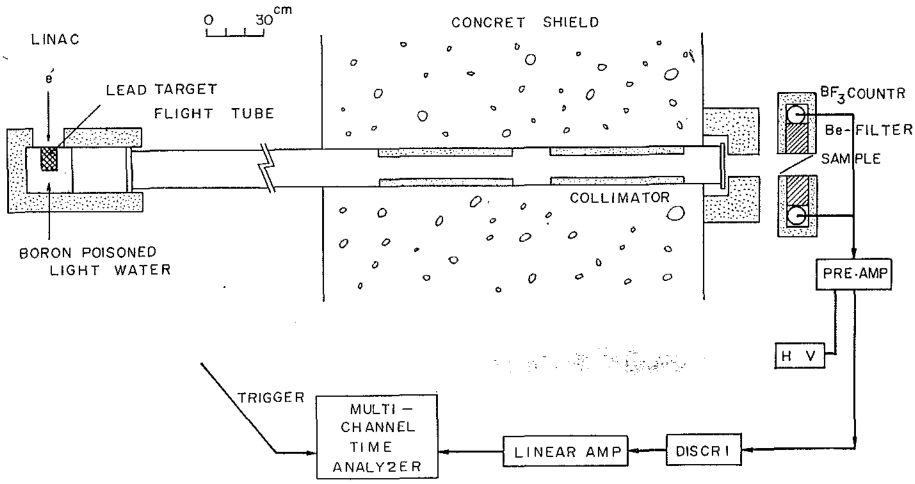


**Fig. 1.** Arrangement of neutron spectroscopy.

$20 \times 150\,mm^3$) and Cd sheets (0.5 mm thick), whose overall size is about $100 \times 100 \times 150\,mm^3$. The filters are used at room temperature. The samples of the methyl molecules are cooled in a can of Al (0.5 mm thick) by liquid nitrogen and the temperature was controled within $\pm 1°C$. The other sample $TiH_2$ coated on a thin Al plate was measured at room temperature.

## 4. Results and Discussions

### $TiH_2$

Figure 2 shows a result for $TiH_2$. Two peaks at the 300 th and 330 th channels are due to the elastic scattering of cold neutrons. A peak observed at the 79 th channel is due to the down-scattering from the corresponding energy

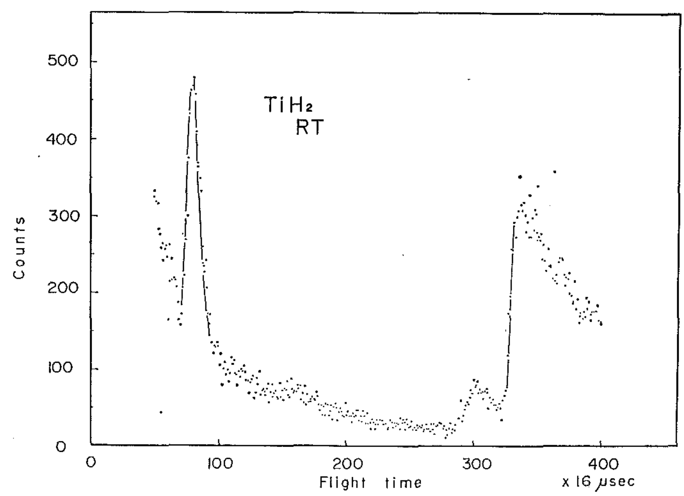


**Fig. 2.** TOF spectrum of down-scattered neutron for $TiH_2$.

into the cold energy region by the optical vibration. The optical energy is 143 meV, and the width is 50 meV. Although the resolution of this spectroscopy is somewhat inferior, it should be sufficient for the investigation of cold moderator.

**$CH_3CCl_3$**

Figure 3 shows a measurement of $CH_3CCl_3$ at 148°K. A peak at the 136 th channel corresponds to the transition of the torsional state $V=0\rightarrow1$, the transfer energy of which is 36.4 meV (294 $cm^{-1}$). This value is in good agreement with the

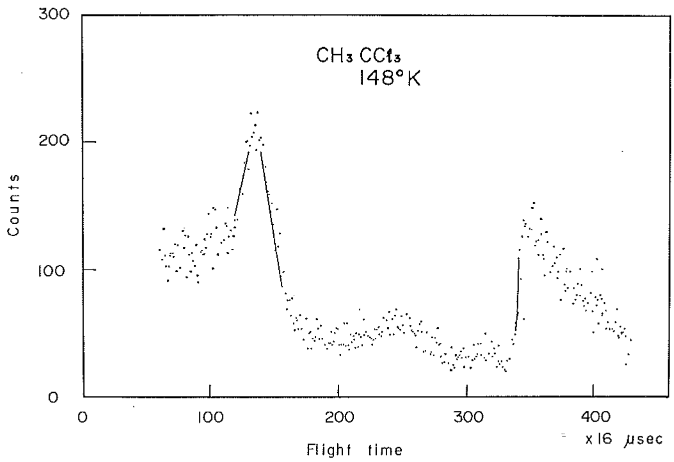


**Fig. 3.** TOF spectrum of down-scattered neutron for $CH_3CCl_3$.

up-scattering value 297 $cm^{-1}$ at 194°K obtained by Rush. Further there are little contribution of the acoustic mode, say between the 160 th and 300 th channels, to the production of cold neutrons. The molecule $CH_3CCl_3$ is not suitable for the cold moderator.

**$CH_3OH$**

Figure 4 shows a result for $CH_3OH$ at 153°K. The TOF spectrum of the down-scattered neutrons are very different between $CH_3OH$ and $CH_3CCl_3$. In case of $CH_3OH$, the contribution is large from the fairly lower energy i. e., near the 100 th channel. Further, the peak due to the elastic scattering of cold neutrons becomes comparatively smaller. This fact indicates that the scattering with the small energy transfer takes place frequently in $CH_3OH$, and supports the usefulness of $CH_3OH$ for a cold moderator.

**$CH_3NO_2$**

Figure 5 shows the result for $CH_3NO_2$ at 171°K. The TOF spectrum is similar to that of $CH_3OH$. In case of $CH_3NO_2$, a broad inelastic peak and a weaker elastic peak appear. This fact indicates that $CH_3NO_2$ is more suitable as a cold moderator than $CH_3OH$, from a view of down-scattering.

From the foregoing measurements, the usefulness of $CH_3OH$ and $CH_3NO_2$ is justified for a cold moderator. A neutron spectroscopy with higher resolution

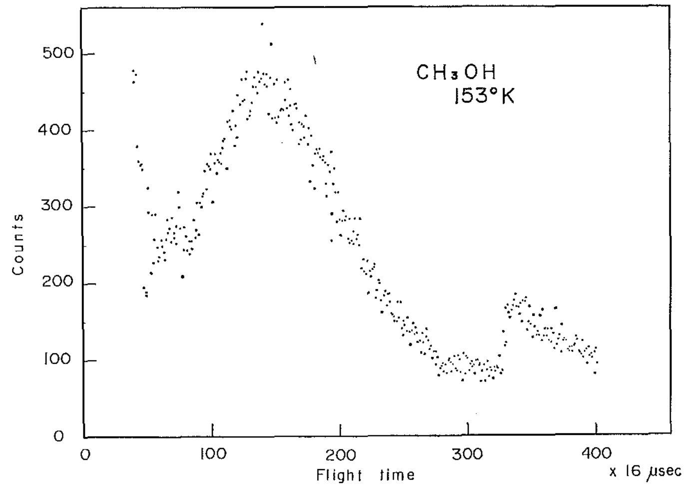


**Fig. 4.** TOF spectrum of down-scattered neutron for $CH_3OH$.

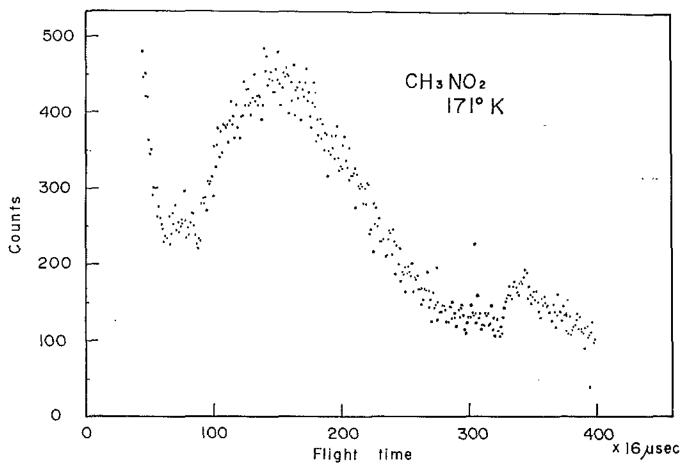


**Fig. 5.** TOF spectrum of down-scattered neutron for $CH_3NO_2$.

is required for a detailed investigation of the internal rotation with a low barrier height sucn as $CH_3OH$ and $CH_3NO_2$.

## References

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