Restricted Rotational Motion of Interlayer Water Molecules in Vanadium Pentoxide Hydrate, $V_2O_5 \cdot nD_2O$, as Studied by Deuterium NMR

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The rotational behavior of the interlayer water molecules of deuterated vanadium pentoxide hydrate, $V_2O_5 \cdot nD_2O$, was studied by solid-state deuterium NMR for the mono- and double-layer structures of the adsorbed water molecules. The rotational motion was anisotropic even at 355 K for both the mono- and double-layer structures. The 180° flipping motion about the C_2-symmetry axis of the water molecule and the rotation around the figure axis, which makes an angle θ with the C_2-axis, occurred with the activation energy of (34 ± 4) and (49 ± 6) kJmol^{-1}, respectively. The activation energies were almost independent of the mono- and double-layer structures of the water molecules, but the angle θ made by the two axes varied from 33° for the monolayer to 25° for the double-layer at 230 K. The angle started to decrease above 250 K (e. g. the angle was 17° at 355 K for the double-layer structure). The results indicate that the average orientation of the water molecules in the two dimensional interlayer space depends on the layer structure and on the temperature. From the deuterium NMR spectrum at 130 K, the quadrupole coupling constant e^2Qq/h = 240 kHz and the asymmetry parameter η = 0.12 were deduced. These values indicate the average hydrogen bond distance R(O···H) = 2.0 Å for the D_2O molecules in the 2D-interlayer space.

Key words: Rotational Motion; Interlayer Water; $V_2O_5 \cdot nD_2O$; Solid-State Deuterium NMR.