Hydrogen Bonding and Dynamics of Methanol by High-pressure Diamond Anvil Cell NMR

<u>Takuo Okuchi</u>, George D. Cody, Ho-kwang Mao, Russell J. Hemley, Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015, USA. E-mail: t.okuchi@gl.ciw.edu

Liquid methanol at densities up to $\tilde{n}/\tilde{n}_0 = 1.7$ was studied by NMR with a specially designed diamond anvil cell and radio frequency probe [1-2]. Methyl and hydroxyl resonances have been separately observed at pressures to 43 kbar which exceeds equilibrium freezing pressure of methanol. The chemical shift difference between methyl and hydroxyl protons increases nonlinearly with increasing density, indicating an accelerative decrease in hydrogen bond length (Figure). Analysis of spin-lattice relaxation rates of hydroxyl and methyl protons indicates that compression enhances intermolecular proton exchange and selectively reduces motion of the hydroxyl protons. Collectively these observations reveal that hydrogen bonding interaction in liquid methanol increases significantly with

compression, inhibiting the liquid-solid transition even above the freezing pressure.

 Okuchi T., *Phys. Earth Planet. Inter.* 2004, **143-144**, 611.
Okuchi T., Hemley R.J., Mao H.K., *Rev. Sci. Instum.* 2005, **76**, 026111.
Keywords: methanol,

NMR, high pressure

