

Supporting information

Harnessing Nuclear Magnetic Resonance Spectroscopy to Decipher Structure and Dynamics of Clathrate Hydrates in Confinement: A Perspective

Maarten Houilleberghs^{1,§}, Sambhu Radhakrishnan^{1,2,§}, C. Vinod Chandran^{1,2}, Alysson F. Morais^{1,2}, Johan A. Martens¹, and Eric Breynaert^{1,2,*}

¹ Centre for Surface Chemistry and Catalysis—Characterization and Application Team (COK-KAT),

KU Leuven, Celestijnenlaan 200F - box 2461, 3001 Leuven, Belgium.

² NMR/X-ray Platform for Convergence Research (NMRCORE), KU Leuven, Celestijnenlaan 200F - box 2461, 3001 Leuven, Belgium

* Correspondence: eric.breynaert@kuleuven.be; Tel.: +32 16 321598

Experimental details

Figure 6: The experiments were done in Bruker 800 Neo NMR spectrometer using 5mm BBO probe. The operating Larmor frequencies of ¹H and ¹³C were 801.25 MHz and 201.47 MHz, respectively. The sample in sapphire tube was pressurized up to 80 bar of methane. The RF strength used for ¹H was 18 kHz and for ¹³C was 25 kHz. Power gated decoupling was used. ¹H experiments used recycle delay of 10 s and 8 scans. The ¹³C experiments used recycle delay of 30 s and 8 scans. The resonances were referenced against those of TMS.

Figure 7: The experiments were performed using a Bruker 400 Neo NMR spectrometer in combination with a Phoenix NMR high-pressure NMR probe in combination with 5mm WHiMS high pressure MAS rotors (Phoenix NMR). The operating Larmor frequencies of ¹H and ¹³C were 400.30 MHz and 100.66 MHz, respectively. The 5mm Phoenix rotor with sample under 60 bar of methane pressure was spun up to 4 kHz. The RF strength used for ¹H was 80 kHz and for ¹³C was 50 kHz. ¹H decoupling was achieved with SPINAL-64 sequence. ¹H experiments used recycle delay of 6.2 s and 8 scans. The ¹³C experiments used recycle delay of 26.3 s and 20 scans. The resonances were referenced against those of adamantane.