Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

The microwave heating mechanism of N-(4-methoxybenzyliden)-4-butylaniline in liquid crystalline and isotropic phases as determined by *in situ* microwave irradiation NMR spectroscopy

Yugo Tasei[1], Fumikazu Tanigawa[1], Izuru Kawamura[1], Teruaki Fujito[2], Motoyasu Sato[3], Akira Naito[1,*]

[1]Graduate School of Engineering, Yokohama National University, 79-5 Tokiwadai, Hodogaya-ku, Yokohama 240-8501, Japan. [2]Probe Laboratory Inc., 1-7-17, Kawasaki, Haruma, Tokyo, 205-0021, Japan. [3]Faculty of Engineering, Chubu University, 200 Matsumoto-cho, Kasugai 457-8501, Japan.

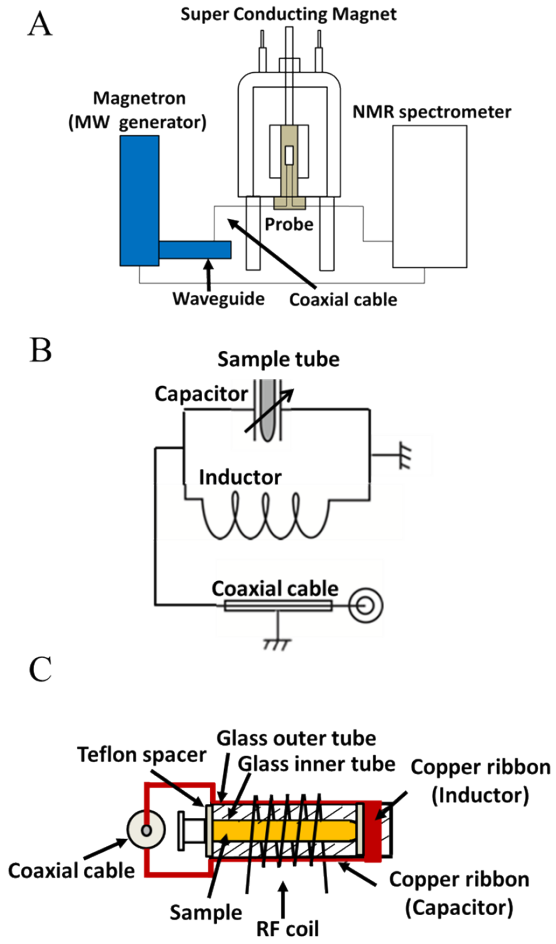

Figure S1. (A) Schematic diagram of the *in situ* microwave irradiation solid state NMR spectrometer (CMX Infinity 400, Chemagnetics) equipped with a microwave transmitter (IDX, 1.3 kW, Tokyo Electronic Co). Continuous wave (CW) and pulsed microwaves were gated by pulses from the spectrometer's pulse programmer. Microwaves were transferred from the microwave transmitter via the wave-guide and coaxial cable and introduced to the microwave resonance circuit in the probe. (B) The equivalent microwave resonance circuit consisting of inductor and capacitor. The sample was inserted in the capacitor in the microwave resonance circuit. (C) A schematic diagram of the sample tube, microwave capacitor and inductor, and radio wave coil. An inner sample tube was inserted into a glass outer tube to insulate the sample from the temperature regulated air. The microwave resonance circuit was attached on the surface of the glass outer tube.

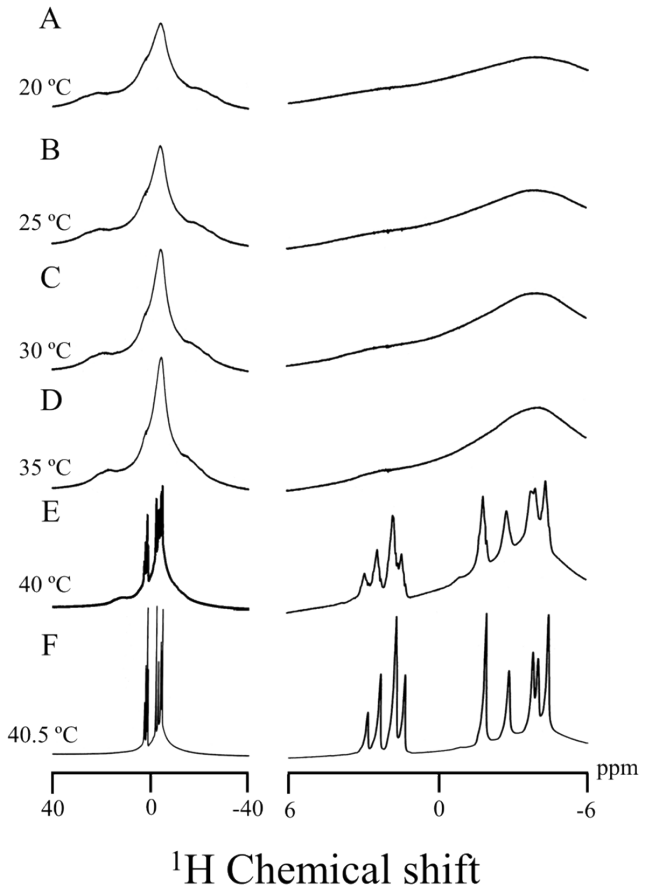

Figure S2. Temperature variation of ^{1}H NMR spectra (left) and expanded spectra (right) of liquid crystalline MBBA varying (A) 20, (B) 25, (C) 30, (D) 35, (E) 40 and (F) 40.5 °C using temperature control unit of the spectrometer. Isotropic phase was coexisted at 40 °C and the phase transition was completed at 40.5 °C, and hence the phase transition temperature, Tc, was determined to 40.5 °C.

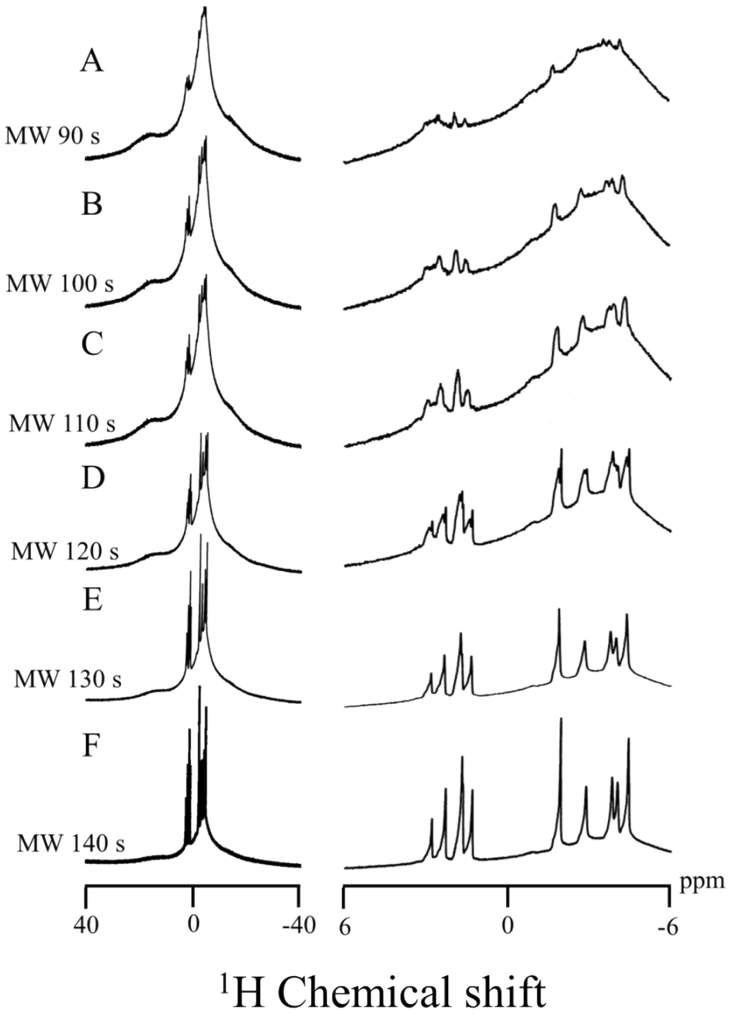

Figure S3. ^{1}H NMR spectra (left) and expanded spectra (right) of liquid crystalline MBBA under CW microwave irradiation of 130 W for (A) 90, (B) 100, (C) 110, (D) 120, (E) 130 and (F) 140 sec. A small amount of isotropic phase appeared in (A) and the phase transition was completed at (F). The temperature of the liquid crystalline phase was determined to 35 °C, which is 5.5 °C below the Tc of 40.5 °C.