The *T, p*-Dependence of the Chemical Shift of the Hydroxyl Protons in Deeply Supercooled Methanol and Water

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The hydroxyl proton chemical shifts δ (H – O) of supercooled methanol (T_{min} = 149 K) and water have been determined (T_{min} = 183 K), and the pressure dependence of these shifts was measured up to 200 MPa. In both compounds the downfield shift of δ (H – O) continues down to the lowest temperatures reached. This result disagrees with the two state models for the hydrogen bond formation in both liquids. The isotherms δ (H_2O) show for $T \leq 273$ K an upfield shift that becomes more pronounced with decreasing temperature. For δ (H – O – CH_3), increasing p causes at all temperatures a downshift.

Key words: NMR; Supercooling; Pressure; Methanol; Water.