Supplementary material

The Study of Correlations between Hydrogen Bonding Characteristics in Liquid, Sub- and Supercritical Methanol. Molecular Dynamics Simulations and Raman Spectroscopy Analysis

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Table S1. H1 united-atom potential models for methanol. CH_3, CH_2, O and H denote the methyl group, methylene group, hydroxyl oxygen and hydrogen, respectively. $R_{min}/2$ (in Å) and ε (in kcal/mol) are parameters of Lennard-Jones potential ($R_{min}/2$ equal to the position of the minimum on Lennard-Jons potential divided by 2), q (in e) are partial charges.

	H1
q_O	-0.728
q_{CH2}	-
q_{CH3}	0.297
q_H	0.431
ε_O	0.174
ε_{CH2}	-
ε_{CH3}	0.181
$(R_{min}/2)_O$	1.73
$(R_{min}/2)_{CH2}$	-
$(R_{min}/2)_{CH3}$	2.17

Table S2. Charmm22 potential model and polarizable model of Anisimov et al. for alcohols. C(O), H(CO), Calc(CH2), Halc(CH2), Calc(CH3) and Halc(CH3) denote carbon connected to hydroxyl oxygen, hydrogen connected to C(O), carbon in methylene group, hydrogen in methylene group, carbon in methyl group, and hydrogen in methyl group, respectively. Other designations and the units are the same as in table S1.

	Methanol Charmm22	Methanol Anisimov et al.	Ethanol Charmm22	Ethanol Anisimol et al.	1-Propanol Charmm22	1-Propanol Anisimol et al.
q_O	0.0	-0.66	0.0	-0.66	0.0	-0.66
$q_{lone\text{-}pair}$	-0.23	-	-0.23	-	-0.23	-
$q_{H(O)}$	0.36	0.43	0.36	0.43	0.36	0.43
$q_{C(O)}$	-0.14	-0.04	-0.06	0.05	-0.06	0.05
$q_{H(CO)}$	0.08	-	0.08	0.09	0.08	0.09
$q_{Calc(CH2)}$	-	-	-	-	-0.12	-0.18

$q_{Halc(CH2)}$	-	-	-	-	0.06	0.09
$q_{Calc(CH3)}$	-	-	-0.18	-0.27	-0.18	-0.27
$q_{Halc(CH3)}$	-	0.09	0.06	0.09	0.06	0.09
ε_{O}	0.150	0.152	0.150	0.152	0.150	0.152
$\varepsilon_{H(O)}$	0.035	0.046	0.035	0.046	0.035	0.046
$\varepsilon_{C(O)}$	0.110	0.080	0.032	0.080	0.032	0.055
$\varepsilon_{H(CO)}$	0.035	0.022	0.045	0.022	0.045	0.022
$\varepsilon_{Calc(CH2)}$	-	-	0.056	-	0.056	0.055
$\varepsilon_{Halc(CH2)}$	-	-	0.035	-	0.035	0.022
$\varepsilon_{Calc(CH3)}$	-	-	0.078	0.022	0.078	0.08
$\varepsilon_{Halc(CH3)}$	-	-	0.024	0.022	0.024	0.022
$(R_{min}/2)_{O}$	1.77	1.77	1.77	1.77	1.77	1.77
$(R_{min}/2)_{H(O)}$	1.34	0.22	1.34	0.22	1.34	0.22
$(R_{min}/2)_{C(O)}$	2.0	2.06	2.0	2.06	2.0	2.18
$(R_{min}/2)_{H(CO)}$	1.34	0.22	1.34	0.22	1.34	1.32
$(R_{min}/2)_{Calc(CH2)}$	2.01	-	2.01	1.32	2.01	2.18
$(R_{min}/2)_{Halc(CH2)}$	1.34	-	1.34	1.32	1.34	1.32
$(R_{min}/2)_{Calc(CH3)}$	2.04	-	2.04	1.32	2.04	2.06
$(R_{min}/2)_{Halc(CH3)}$	1.34	-	1.34	1.32	1.34	1.32

Figure S1. Typical deconvolution of experimental Raman spectrum on constituent profiles (CH3 band, free and 1-, 2-, 3-bonded molecules) on the example of methanol spectrum for 83 bar isobar and T=393K