Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information for

Hydrogen bond network topology in liquid water and methanol: a graph theory approach

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Structure of liquid methanol

The molecules with 3 HB neighbors and the bonds to these molecules are omitted. These are referenced as “without branch points”.

Table S1. The fraction of bonds between molecules with different number of hydrogen bonds.

$n_{HB,1}$	$n_{HB,2}$	$P(n_{HB,all})$[a]	$P(n_{HB,wobp})$[b]
1	1	0.016	0.066
1	2	0.200	0.384
1	3	0.044	---
2	2	0.546	0.548
2	3	0.181	---

[a]All molecules were considered
[b] Wobp stands for without branch points. Methanol molecules with three hydrogen bonds (branch points) were converted to monomers in the statistical analysis. Hydrogen bonds to these molecules were omitted.

Cyclic and non-cyclic entities: ratio of non-cyclic entities 0.977; ratio of isolated cyclic entities 0.022; and ratio of cyclic entities with shared atom: negligible (1.26E-4)

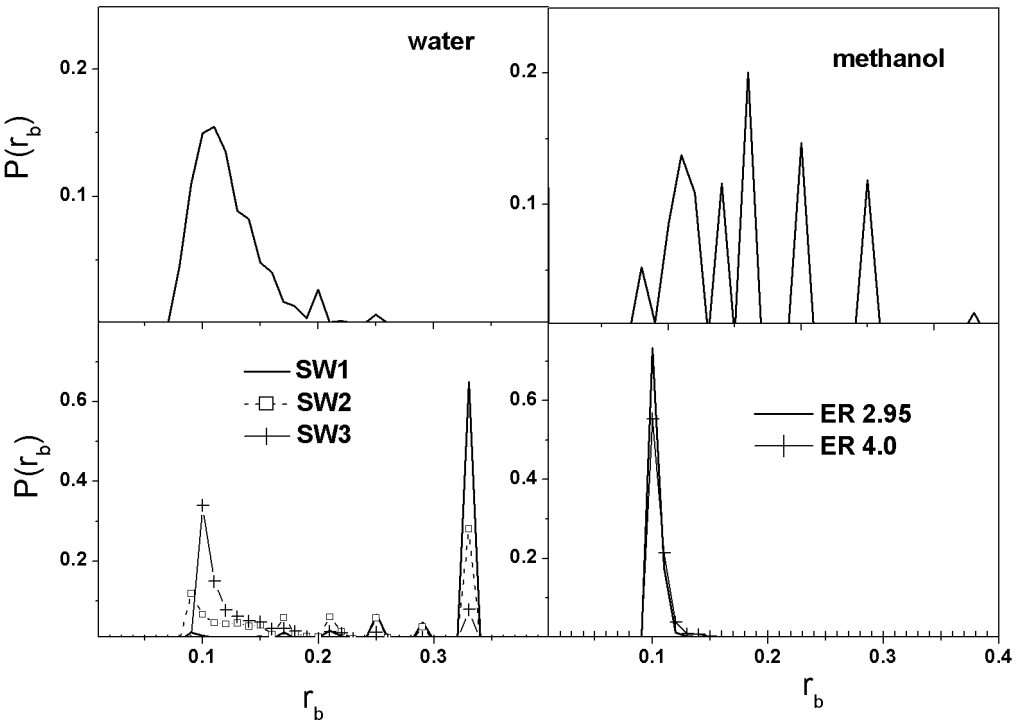

Fig. S1. The histogram of the local bonding coefficient (r_b) for the investigated systems.

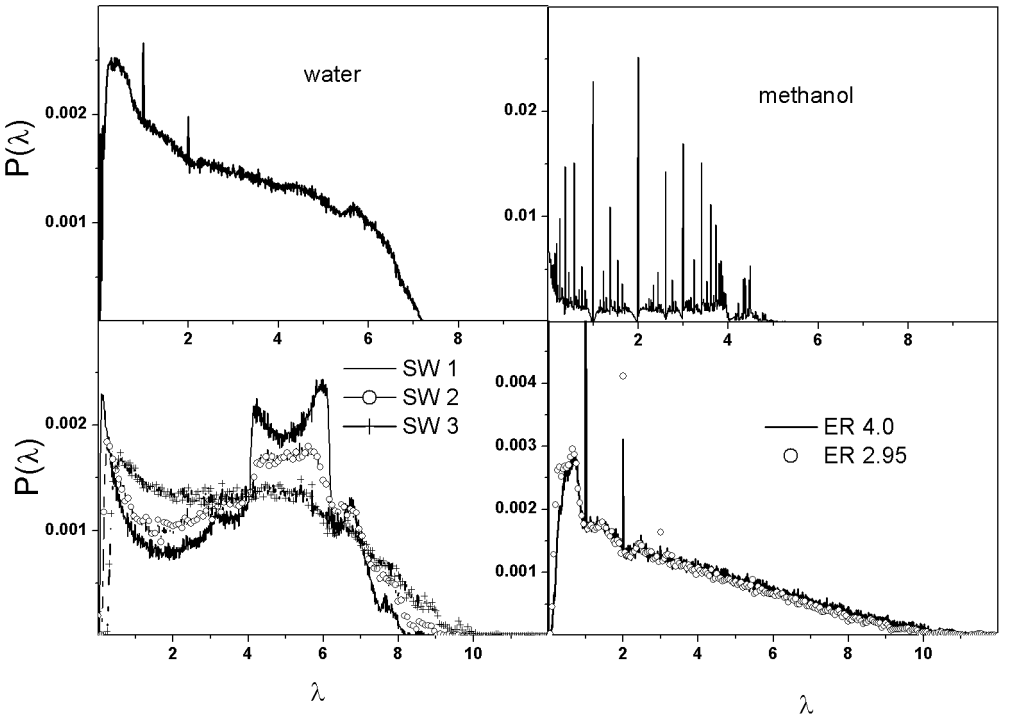

Fig. S2. Spectral density of the Laplace matrix for the investigated systems. .

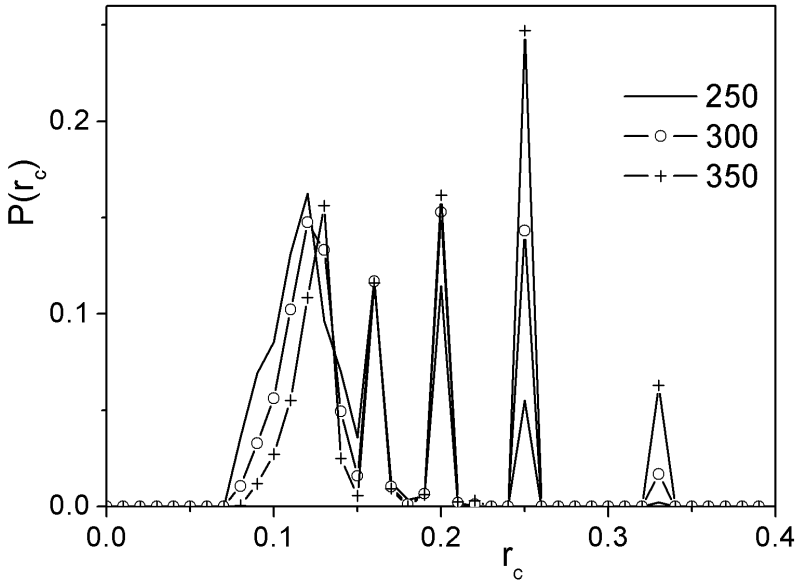

Fig. S3. The histogram of local cyclic coefficients (r_c) for the low-density patch of water at various temperatures (in K).