

Supplementary Material for Network topology of deeply supercooled water

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To investigate the origin of the small peak associated with large 18-membered rings, we ran EPSR simulations identical in every respect but varied the box size. The associated -O-H-O- ring distributions for five models containing 500, 1000, 1800, 2500 and 3000 molecules are shown in figure S3. Anomalous large peaks are observed for ring sizes of 13 for a box size of 500 molecules and 16 for a box containing 1000 molecules. The anomalous peak shifts to a ring size of 18 for a box of 1800 molecules, the same as observed by Soper⁹, but of higher intensity. For boxes of 2500 and 3000 molecules the anomalous peak disappeared. As a consequence the EPSR models reported in this paper were run using boxes containing 2500 molecules.

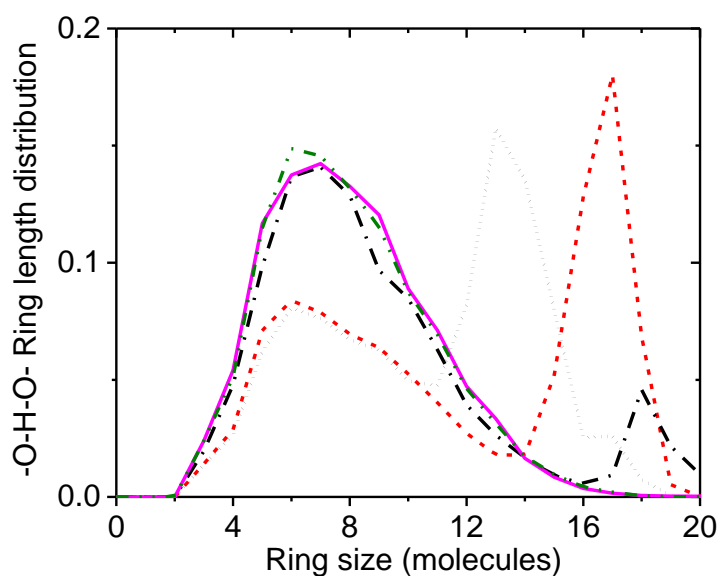


Figure S1. The box size dependence of ring distributions for -O-H-O- rings from the EPSR models at 293 K, using the cutoff $r_{\text{O-H}} = 2.4 \text{ \AA}$. The number of molecules in each box were 500 (black dotted line), 1000 (red dashed line), 1800 (black dash-dot line), 2500 (magenta solid line) and 3000 (green dash-dot-dot line).

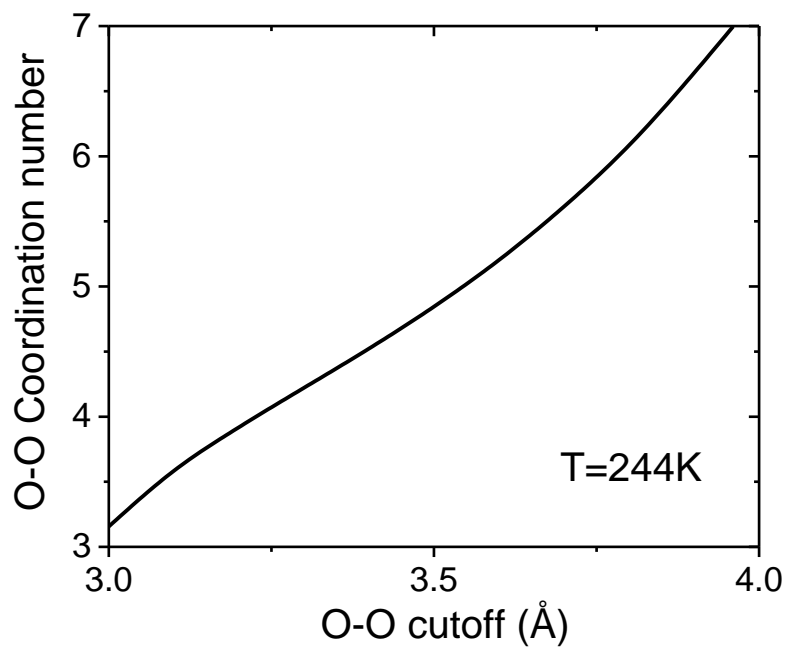
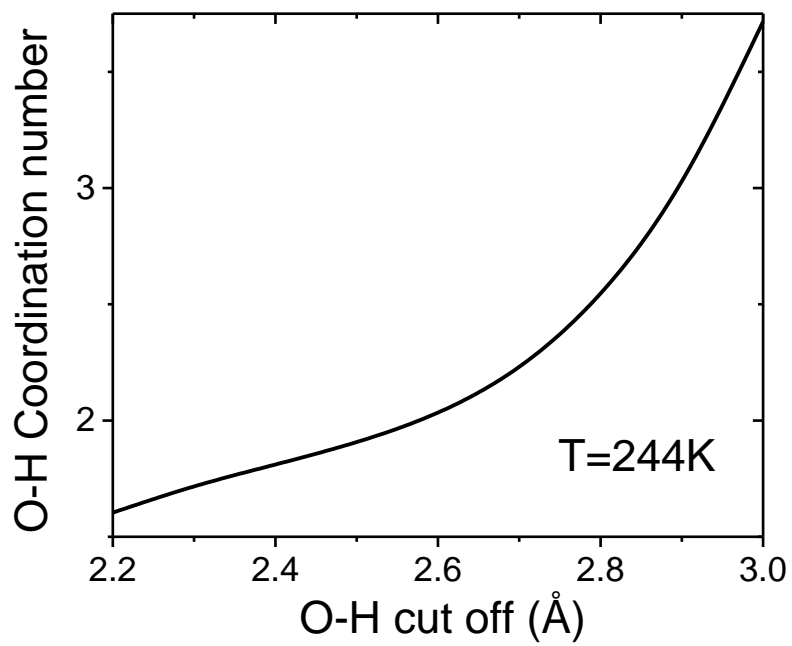


Figure S2. The (a) O-H and (b) O-O intermolecular coordination numbers from the EPSR model at 244 K as a function of cut-off distance.

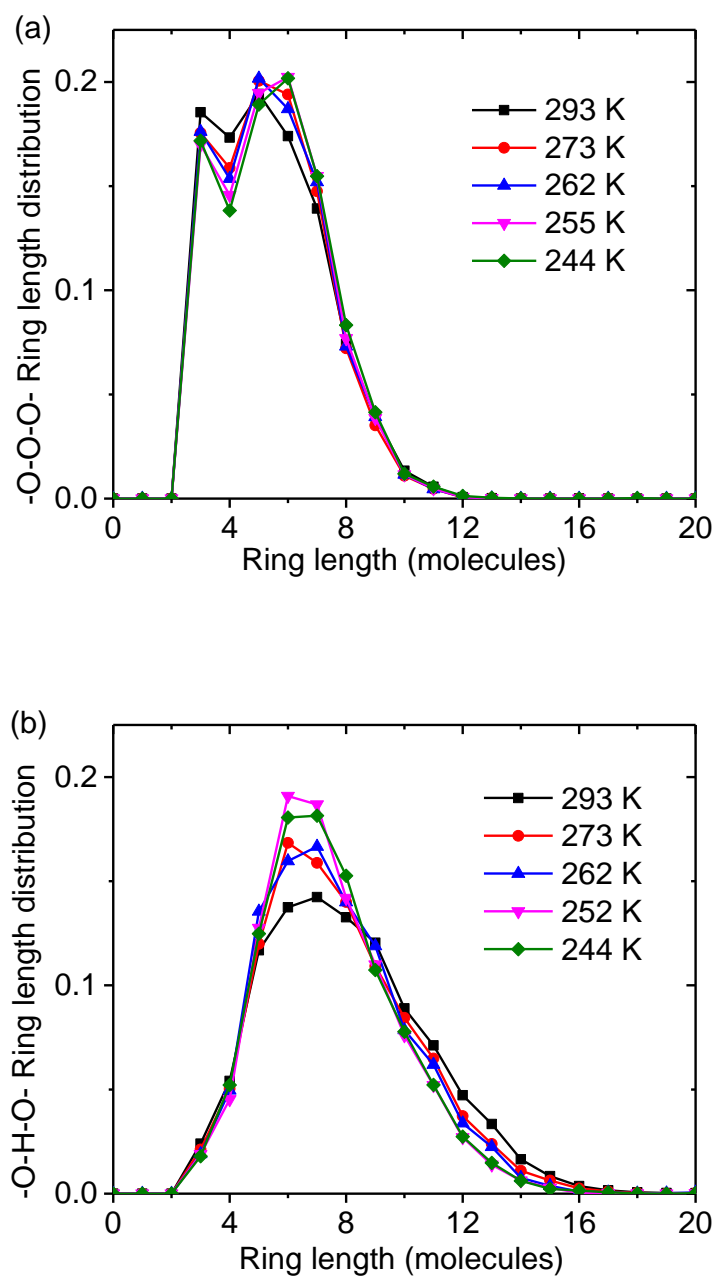


Figure S3. Temperature dependence of (a) the hydrogen bonded -O-O-O- distributions and (b) -O-H-O- ring distributions obtained from EPSR models. Shown here as continuous lines rather than a bar graph for clarity.