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Simulations of vapor water clusters at vapor-liquid equilibrium[1]
KIM BOLTON, School of Engineering, University College of Boras, SE-501 90, Boras, Sweden; Physics Department, Goteborg University, SE-412 96, Goteborg, Sweden, PETER AHLSTROM, ERIK JOHANSSON, School of Engineering, University College of Boras, SE-501 90, Boras, Sweden, ARNE ROSEN, Physics Department, Goteborg University, SE-412 96, Goteborg, Sweden — Clustering of water molecules is important, for example, in the nucleation of water drops and in the penetration of water into hydrophobic polymers where water trees can be formed. Monte Carlo methods have been used to study the clustering of water under vapour-liquid equilibrium conditions between 300 and 600 K. The number of clusters, as well as the cluster size, increases with increasing temperature. In addition, due to entropic effects, the percentage of clusters that have linear (or open) topologies increases with temperature and dominate over the minimum-energy cyclic topologies at the temperatures studied here.

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Arne Rosen
Physics Department, Goteborg University, SE-412 96, Goteborg, Sweden

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