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ACCEPTED MANUSCRIPT

Water, the special liquid

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ABSTRACT:

Some prominent special properties of liquid water are summarized and related to the characteristics of the water molecule. It is shown that the substance appears to be anomalous only when compared to hard-sphere models with molecular interactions restricted to excluded-volume effects. Besides the electric charge distribution and the balanced number of hydrogen bond donating and accepting sites, the strength of the hydrogen bonds and also of the covalent bonds are identified significant factors in making water so special. As another major feature the small size of the water molecule is emphasized. It is often neglected but is relevant in every respect. It contributes, for example, to the large permittivity of water which plays an important role in the solvent behavior of water. The paper also demonstrates that the smallness of the water molecule is a key property in the molecular mobility of the liquid. The single-dipole (molecular) reorientation time is deduced from the experimentally available relaxation time of the macroscopic dielectric polarization and is discussed in terms of the socalled wait-and-switch model of dielectric relaxation. By comparison of the waiting periods of the model with structure relaxation times from ultraviolet and X-ray Brillouin spectra, close coupling between the reorientational motions and translational motions, i.e. the hydrogen network fluctuations in water, is disclosed. This finding confirms the idea of the wait-andswitch model. In addition, the waiting period is seen to nicely follow Eyring behavior, indicating an activated switch (or jump) mechanism.

Keywords:

Water, hydrogen bond, dipole moment, molecular reorientation, wait-and-switch model, translation – orientation coupling

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