FOREWORD

Water - the essential molecule

Water is the subject of basic studies in physics, chemistry and biology. Such a very simple molecule, H_2O, presents an enormous complexity in its properties. It is normally said that water is an anomalous liquid because of the variety of distinctions with other regular liquid systems.

One of the most intriguing properties is its density maximum around 4 ^{o}C. Underwater life depends on this anomaly. But there are many others. It has a large heat capacity that contributes to thermal regulations, a large dielectric constant dissolving ionic compounds and making an excellent solvent. The behavior with temperature and pressure also presents several curious properties: pressure reduces the melting point; the already large viscosity increases as the temperature decreases; the variation of the heat capacity with temperature presents a minimum, etc. In addition, water freezes in many different crystal structures. Whereas most small molecules (N_2, O_2, HCN, NH_3, CH_4 etc.) are found as a gas in normal conditions, water is a clear liquid. In fact, it is a liquid in a very broad range of temperature. This is one of the consequences of the intermolecular forces between the water molecules. One of these, of particular importance, is the hydrogen bond. Again, water shows how it is unique. Having only three atoms it is able to form around 4 hydrogen bonds. The nature of the hydrogen bonds are closely related to some of the anomalous behavior of water. To mention one, of great interest in biology, it is the hydrophobic (and the complementary hydrophilic) effect. This is at the heart of the formation of micelles and biological membranes and to a large extent, in the folding of proteins. Proton exchange regulates the *pH* of water which regulates the structure of aminoacids. Water is, indeed, essential to all molecular processes related to life.

One may wonder that for no other reason Nature selected water, such a simple, yet so beautifully complex molecule, as the biological solvent.

The central question that intrigues every one that has ever studied the water molecule is how such a simple three-atom system can present such a diversity of unique properties. In recent years there has been a considerable increase in the number of studies dedicated to water. This is an outcome of the advances in experimental techniques and the progress in hardware/software technology that has made computer simulation a very important theoretical tool. As a consequence some progress is being achieved. The idea of this special issue is to collect in a single volume different aspects such as thermodynamic and dynamic properties, physico-chemical properties, hydrogen bond, solvent effects, biomolecular implications, micelles, colloids, hydration problems, protein-folding, etc. The contributing authors are experts in their fields and promptly reacted to the idea of this special issue. It is expected that this collection will give some of the scope of present research work.

We thank all the authors and the Brazilian Journal of Physics for the success of this endeavor.

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Guest editors