

It is well known fact, that kind of intermolecular interaction govern molecular dynamics of the material and their properties. Consequently, features of van der Waals liquids are different than associated ones. Classification of materials according to recently developed the isomorph theory distinguish group of materials, called Roskilde simple liquids for whom there are curves in the phase diagram along which structure and dynamics are invariant in reduced units. This is consequence of genre of intermolecular bounds in the material and to this group of simple materials belongs van der Waals liquids, polymers and some ionic liquids. On the other hands, hydrogen bonded materials, due to characteristic behavior of hydrogen bonds at various thermodynamic conditions, cannot be classified as simple.

Experimentally, in the materials that are classified as simple are observed e.g. density scaling of the relaxation dynamics and isochronal superposition of the loss spectra of the structural relaxation. These features are violated e.g. in H-bonded materials, but also some exceptions are observed for van der Waals liquids. Because in associated materials exist hydrogen bonded supramolecular structures, therefore molecular dynamics of these materials changes when the architecture and size of the structures is modified. It happens during variation of thermodynamic conditions. But, because temperature and pressure changes these structures in different manner, then even for the same structural relaxation time their architecture can be different and principles of simple liquids are not fulfilled. Moreover, in some H-bonded materials, like primary alcohols, these changes becomes visible, e.g. in dielectric spectroscopy results, only at some thermodynamic conditions, e.g. at high enough pressures. Consequently, it can be possible, that for low pressure limit these materials can be classified as simple.

Unfortunately, up to now some properties of materials are specified only in limited range of temperature or pressure. Especially, density data from PVT experiments, necessary for test of so called thermodynamic scaling are limited to pressure range up to ca. 200MPa and only for temperatures from ambient to high. Consequently, large extrapolation of the density data in high pressure/low temperature range is necessary to test scaling principles in some materials. It is definitely much below pressure limit, at which changes of H-bonded structures are observed e.g. in monoalcohols. Then conclusions about some properties of associated liquids and other materials, based on presently accessible data can be misleading. Unfortunately, until now there is lack of high pressure and low temperature results from the PVT experiments. Moreover, commercially accessible PVT equipment is difficult to use due to application of the mercury as medium.

The main goals of the project will be: 1) preparation of new kind of the PVT equipment, that will work in the pressure and temperature range inaccessible for commercial apparatus and enable investigations of density at thermodynamic conditions for whom changes of the supramolecular structures becomes important; the apparatus will not use the mercury so will be user friendly; 2) test of some principles of the isomorph theory in various H-bonded materials by combination of results from PVT and dielectric spectroscopy measurements, also performed in our laboratory at various p-T conditions; moreover, PVT data collected at thermodynamic conditions at which changes in molecular dynamics of the supramolecular structures was detected by other experimental methods, enable us to check if also density reflect these changes, and 3) check of properties of non-associated liquids in which some exception to the rules of the isomorph theory were observed.

It has to be emphasized, that the PVT equipment developed during realization of the project will be useful not only for investigations of associated and van der Waals materials. It will be excellent experimental tool to study properties of e.g. liquid crystals, ionic liquids, polymers, critical mixtures, biomaterials and high pressure chemical reactions.