

ERASMUS MUNDUS MASTER OF SCIENCES

“ADVANCED SPECTROSCOPY IN CHEMISTRY”

Master Thesis 2010-2011

University : Lille1	
Title: Hydrogen bond in supercritical fluids	
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Subject

In the proposed project we will concentrate on discovering the general relationships between H-bond characteristics in supercritical fluids using both Raman spectroscopy and molecular dynamics simulations. Particularly, we will focus on the correlations between various topological characteristics of H-bonded clusters and the mole fraction of H-bonded molecules (XHB).

We will start by analysing the structure in neat aliphatic alcohols. There are several intermolecular potential models of these molecules that predict more or less thermodynamic and structural properties. Some of them were developed to predict structural properties of liquid state and are good for describing of the radial distribution functions, structure factors, etc. At the same time they fail to predict the thermodynamic parameters closely to the critical point and along the liquid-gas coexistence curve.

The first objective of the investigations is to obtain the liquid-gas coexistence curves for all the intermolecular potential models by the use of the Grand Canonical Monte-Carlo simulations using Towhee program package in order to choose the adequate model which describes the thermodynamic behavior near the critical point.

The second step is to carry out a detailed structural analysis along the liquid-gas coexistence curve and along the critical isochore in order to provide insights of the relative importance of hydrogen bonding versus non-hydrogen bonded interactions that govern the structure of aliphatic alcohols. To this end, we will use approaches such as ranked radial distribution function, orientation, interaction energy distributions, structure factors, Voronoi polyhedra analysis.

Keywords:

Molecular dynamics simulation, quantum calculations, Raman spectroscopy