



**University  
of Victoria**

Graduate Studies

Notice of the Final Oral Examination  
for the Degree of Doctor of Philosophy

of

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**“Exploring the Binding of Small Guest Molecules in Sodium  
Deoxycholate Hydrogels”**

Department of Chemistry

Thursday, October 20, 2016

12:00 P.M.

David Turpin Building

Room A136

Supervisory Committee:

Dr. Cornelia Bohne, Department of Chemistry, University of Victoria (Supervisor)

Dr. Irina Paci, Department of Chemistry, UVic (Member)

Dr. Matthew Moffitt, Department of Chemistry, UVic (Member)

Dr. Richard Keeler, Department of Physics and Astronomy, UVic (Outside Member)

External Examiner:

Dr. Alex Adronov, Department of Chemistry and Chemical Biology, McMaster University

Chair of Oral Examination:

Dr. Julie Zhou, Department of Mathematics and Statistics, UVic

Dr. David Capson, Dean, Faculty of Graduate Studies

## **Abstract**

Bile salts are supramolecules with amphiphilic properties. Bile salts form aggregates in aqueous solutions. The primary aggregates of bile salts are hydrophobic and the secondary aggregates which form at higher concentrations are relatively hydrophilic. Among bile salts, sodium deoxycholate (NaDC) has been known to form hydrogels at pHs close to the neutral pH and within a certain concentration range.

The aim of this work was to provide insight into the properties of a NaDC hydrogel as a supramolecular gel system through three different projects. Pyrene is a hydrophobic polycyclic aromatic compound which was used as a fluorescent probe and the guest for these projects. 1,1'-dioctadecyl-3,3,3',3'-tetramethylindodicarbocyanine perchlorate (DiD) is another fluorescent compound which was used as another guest.

The objective of the first project was to understand the mobility of a small guest molecule in NaDC gel in the presence of curcubit[6]uril (CB[6]) compound as an additive for the gel. Curcubit[n]urils are macrocyclic compounds with a hydrophobic cavity and two hydrophilic portals. The presence of CB[6] provides another binding site for pyrene in addition to the primary aggregates of the bile salts. The results showed that the mobility of the guest from water and CB[6] to the bile salts network happens when the temperature is raised. The release of the guest back into the water happens when the gel is cooled.

The objective of the second project was to investigate the effect of surfaces with different hydrophilicity on the NaDC gel properties. The results of fluorescence correlation spectroscopy (FCS) experiments revealed that either the hydrophilicity of the surface does not affect the NaDC gel network or the FCS is insensitive to the structural changes induced by the hydrophilicity of the surface. These experiments depicted that the aggregates involved in the gel's network are the same as those formed in the aqueous solutions. Moreover, results of the steady-state and time-resolved fluorescence experiments showed that the bulk gel properties are not affected by the hydrophilicity of the surface.

The objective of the last project was to determine the effect of ions on NaDC gel properties. The results showed that cations with different charge density have different effects on the gel formation and properties. The presence of inorganic salts with a monovalent cation leads to the formation of a kinetically favored gel sample within a few hours after sample preparation. The extension of the network occurs overtime and a thermodynamically stable gel forms a couple of days after sample preparation.