

**ASPECTS OF ADSOLUBILIZATION OF NEUTRAL ORGANIC SOLUTES  
INTO CATIONIC ADMICELLES**



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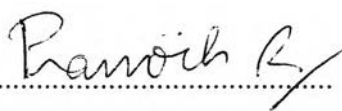
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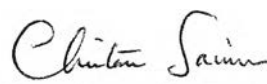
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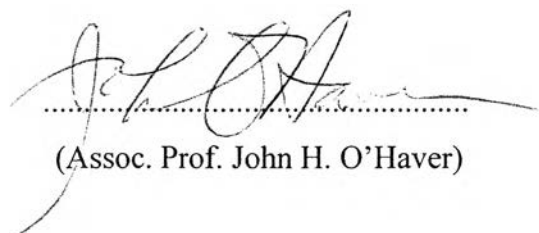
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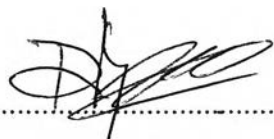
  
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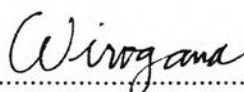
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## ABSTRACT

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Solubilization in adsorbed surfactant aggregates (admicelle) at solid/liquid interfaces has been well studied for decades, launching many related fundamental and applied studies. A related phenomenon, when admicelles solubilize solutes, is called adsolubilization. This work aims to study temperature effects on adsolubilization and elucidate the nature of molecular interactions or microenvironment in the admicelle. The preferential loci of adsolubilization for hydrophobic and hydrophilic solutes are the admicellar core and palisade/headgroup regions, respectively. The partition coefficient is affected by temperature change in three primary ways, (1) changing aqueous solubility of solute (2) changing surfactant packing density in the admicelle and (3) changing the strength of attractive interactions between solute and surfactant molecules. The third factor appears to have a strong impact on the 2-D structure of admicelles. Highly hydrophobic solutes show a higher partition coefficient in high region II of surfactant adsorption than that in region III. A preference of surfactant adsorption region (high region II or region III) for adsolubilization of hydrophilic p-tolunitrile would be governed by cation- $\pi$  and dipole-dipole attractive forces and surfactant packing density in admicelle. Differential scanning calorimetry shows 3 loci of micellar solubilization, whereas, it cannot distinguish the sharp difference between each loci in admicelle possibly due to uniform packing density in admicelle although the composition and hydrophobicity of microenvironment in admicelle are different. Based on this knowledge, a simple thermodynamic model of adsolubilization is developed.

## บทคัดย่อ

วสันต์ สภานุชาติ : ลักษณะการละลายของสารอินทรีย์ที่เป็นกลางเข้าไปในแอดไมเซลล์แคทไอออนิก (Aspects of Adsolubilization of Neutral Organic Solutes into Cationic Admicelles) อ. ที่ปรึกษา : รศ.ดร. จินตนา สายวรรณ และ รศ.ดร. จอห์น เอช โอเฮเวอร์ 127 หน้า

หลายสิบปีที่ผ่านมาได้มีการศึกษาการละลายโซลูบิลไลเซชันในกลุ่มสารลดแรงตึงผิวที่ถูกดูดซับบนพื้นผิวของแข็ง (แอดไมเซลล์) อย่างแพร่หลาย ทำให้มีการตีพิมพ์ผลงานที่เกี่ยวข้องกับองค์ความรู้และการวิจัยประยุกต์อย่างต่อเนื่อง ปรากฏการณ์ที่แอดไมเซลล์ละลายสารได้เรียกว่า “แอดโซลูบิลไลเซชัน” งานวิจัยนี้มุ่งศึกษาผลของอุณหภูมิต่อแอดโซลูบิลไลเซชันและศึกษาสภาพแวดล้อมระดับไมครอนในแอดไมเซลล์ที่อาจมีผลต่อแอดโซลูบิลไลเซชัน การทดลองพบว่สารอินทรีย์ที่มีความเป็นไฮโดรโฟบิกชอบที่จะละลายเข้าไปในบริเวณใจกลางของแอดไมเซลล์ ขณะที่สารอินทรีย์ที่มีความเป็นไฮโดรฟิลิกชอบที่จะละลายเข้าไปในบริเวณพาลีเสด การเพิ่มอุณหภูมิมีผลต่อค่าสัมประสิทธิ์ของการกระจายตัวของสารแบบแอดโซลูบิลไลเซชัน 3 ทางได้แก่ 1) เพิ่มการละลายของสารในน้ำ 2) เปลี่ยนแปลงการจับตัวของสารลดแรงตึงผิวในแอดไมเซลล์ให้เป็นไปอย่างหลวมๆ และ 3) แรงดึงดูดระหว่างโมเลกุลของสารลดแรงตึงผิวและสารอินทรีย์แรงดึงดูดดังกล่าวเป็นปัจจัยหลักที่ควบคุมการเปลี่ยนโครงสร้างสองมิติของแอดไมเซลล์ สารอินทรีย์ที่มีความเป็นไฮโดรโฟบิกสูงชอบที่จะละลายเข้าไปแอดไมเซลล์ในโซนที่ 2 มากกว่าในโซนที่ 3 ของการดูดซับสารลดแรงตึงผิว สารพาราโทลูไนไตรซึ่งมีความเป็นไฮโดรฟิลิกสูงชอบละลายเข้าไปในแอดไมเซลล์ในโซนใด ขึ้นอยู่กับแรงดึงดูดระหว่างโมเลกุลชนิดแคทไอออน-ไพและแรงดึงดูดระหว่างขั้วโมเลกุลระหว่างสารลดแรงตึงผิวและสารอินทรีย์ และความหนาแน่นของกลุ่มโมเลกุลในแอดไมเซลล์นั้น ผลการวิเคราะห์จากดีฟเฟอเรนเชียลสแกนนิ่งแคลอริมิเตอร์ แสดง ตำแหน่งของการละลายโซลูบิลไลเซชันในไมเซลล์ 3 ตำแหน่ง ขณะที่ตำแหน่งดังกล่าวในแอดไมเซลล์ไม่สามารถแยกความแตกต่างได้อย่างชัดเจน ทั้งนี้อาจเป็นเพราะความหนาแน่นของกลุ่มโมเลกุลในแอดไมเซลล์น่าจะมีค่าสม่ำเสมอตลอดทั้งแอดไมเซลล์แม้ว่าองค์ประกอบและความเป็นไฮโดรโฟบิกของสภาพแวดล้อมในส่วนต่างๆของแอดไมเซลล์จะต่างกัน จากองค์ความรู้ที่ได้ก็นำมาพัฒนาแบบจำลองเชิงอุณหพลศาสตร์ของแอดโซลูบิลไลเซชันอย่างง่าย

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