

**THE ORIGIN OF HOST-GUEST INTERACTION  
IN METAL/BENZOXAZINE SYSTEMS**



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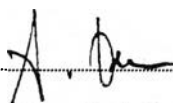
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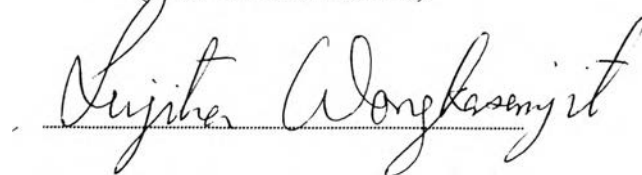
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## บทคัดย่อ

นายพิทยา ถกถักถัก: การศึกษาปฏิกิริยาที่มีต่อกันของสารหลัก-รองในระบบโลหะและเบนซอกซาซีน (The Origin of Host-Guest Interaction in Metal/Benzoxazine Systems) อาจารย์ที่ปรึกษา: ผศ. ดร. สุวบุญ จิรชาณูชัย ศ. ดร. ฮัทสึโอะ อิชิดะ (Prof. Hatsuo Ishida), 69 หน้า ISBN 974-334-188-9

อนุพันธ์เบนซอกซาซีนมอนอเมอร์ประเภท (3,4-dihydro-2H-1,3-benzoxazines) และอนุพันธ์ของการเปิดวงของเบนซอกซาซีนมอนอเมอร์ (ไดเมอร์) ประเภท (N,N-Bis (2-hydroxybenzyl) amine) โดยมีหมู่ที่ตำแหน่ง ortho หรือ para ของวงฟีนอลและหมู่เอมีนที่แตกต่างกัน สมบัติของการตอบรับไอออนโลหะหมู่ 1 ของเบนซอกซาซีนมอนอเมอร์ถูกศึกษาโดยใช้วิธีเพ็ดersen (Pedersen's Technique) และวิเคราะห์ข้อมูลโดยใช้เครื่อง UV/Vis. การจับโลหะขึ้นอยู่กับปัจจัยคือ ความเข้มข้นของเบนซอกซาซีน ชนิดของเอมีน และชนิดของฟีนอล สารประกอบ 3,4-dihydro-3,6,8-trimethyl-2H-1,3-benzoxazine (1) และ 3,4-dihydro-6-*t*-butyl-3-methyl-2H-1,3-benzoxazine (4) ให้ผลในการจับโลหะสูงสุดเมื่อเทียบกับอนุพันธ์ประเภทอื่น อนุพันธ์เบนซอกซาซีนไดเมอร์เกิดสารประกอบเกิดสารประกอบเชิงซ้อนกับคิวปริกคลอไรด์ (CuCl<sub>2</sub>) แคลเซียมคลอไรด์ (CaCl<sub>2</sub>) และ แบเรียมคลอไรด์ (BaCl<sub>2</sub>) ซึ่งสามารถยืนยันผลโดยใช้ ESIMS, FTIR และ XRD ESIMS ได้พิสูจน์ให้เห็นว่าอนุพันธ์เบนซอกซาซีนมอนอเมอร์ที่เปิดวงนี้เกิดการรวมตัวเป็นคลัสเตอร์ (cluster) กันตั้งแต่ 2 ถึง 7 โมเลกุล ผลการวิเคราะห์ด้วย FTIR แสดงว่าไดเมอร์มีการรวมตัวเป็นกลุ่มโมเลกุลได้โดยการสร้างพันธะไฮโดรเจนทั้งภายในและระหว่างภายนอกโมเลกุล ผลการวิเคราะห์ด้วย XRD แสดงถึงการเปลี่ยนแปลงทางโครงสร้างอย่างเด่นชัดหลังการเป็นสารประกอบเชิงซ้อน

**ABSTRACT**

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**KEYWORDS** : Benzoxazine Monomers/ Benzoxazine Dimer/ Molecular Assembly/ Metal Picrates/ Ion Interaction.

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A series of benzoxazine monomer derivatives, 3,4-dihydro-2H-1,3-benzoxazines, and ring opening of benzoxazine monomer derivatives (dimer derivatives), N,N-Bis (2-hydroxybenzyl) amine, with different functional groups at ortho and/or para positions on the phenol ring and amine groups were prepared. Ion interaction properties of the monomer derivatives for alkali metal were studied by using Pedersen's technique and characterized by UV/Vis. Ion extraction percentage depend on main factors; benzoxazine concentration and structure of benzoxazine. 3,4-dihydro-3,6,8-trimethyl-2H-1,3-benzoxazine, **1**, and 3,4-dihydro-6-*t*-butyl-3-methyl-2H-1,3-benzoxazine, **4**, gave the highest extraction comparing to the other monomers. Benzoxazine dimers formed the complex with CuCl<sub>2</sub>, CaCl<sub>2</sub>, and BaCl<sub>2</sub> as confirmed by the ESIMS, FTIR and XRD. ESIMS clarified that benzoxazine dimers assembly as a series of clusters of 2-7 molecules. The peak shifting of OH group in FTIR implied that the molecular assembly of benzoxazine dimer was presented by inter and intramolecular hydrogen bonding. The XRD patterns implied after the change in the packing structure of benzoxazine complexation with metal guests.

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