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THE SOLVATION STRUCTURE OF LITHIUM ION IN WATER-AMMONIA MIXTURE  
BY MONTE CARLO METHOD

MISS SUCHADA KHEAWSRIKUL

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พิมพ์ต้นฉบับบทความวิจัยวิทยานิพนธ์ภายในกรอบสี่เหลี่ยมนี้เพียงแผ่นเดียว



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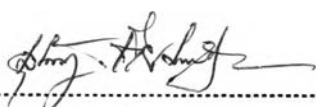
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0.9307 กรัมต่อลูกบาศก์เซนติเมตร ความยาวของลูกบาศก์ซึ่งมีคุณสมบัติปริมาตรมีค่าเท่ากับ  
18.56 อังสตรอม ได้นำสมการศักย์ฟังก์ชันทั้งหมด 5 สมการที่ได้จากการคำนวณโดยวิธีแอบ อินนิช-  
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ประกอบด้วยน้ำ 4 โมเลกุล และ แอมโมเนีย 2 โมเลกุล ส่วนในชั้นที่สองประกอบด้วยน้ำและ  
แอมโมเนีย 8 และ 4 โมเลกุล ตามลำดับ ซึ่งสามารถเขียนแทนได้ด้วย  $\text{Li}[(\text{H}_2\text{O})_4(\text{NH}_3)_2]^{\text{I}}$   
 $[(\text{H}_2\text{O})_8(\text{NH}_3)_4]^{\text{II}}$  นอกจากนี้ยังได้วิจารณ์ผลจากการกระจายของเลขโคออร์ดิเนชัน และการ  
กระจายพลังงานในลักษณะของกลไกการแลกเปลี่ยน

ภาควิชา .....เคมี.....

สาขาวิชา .....เคมีอนินทรีย์.....

ปีการศึกษา .....2531.....

ลายมือชื่อนิสิต 

ลายมือชื่ออาจารย์ที่ปรึกษา 

พิมพ์ต้นฉบับบทคัดย่อวิทยานิพนธ์ภายในกรอบสี่เหลี่ยมนี้เพียงแผ่นเดียว



SUCHADA KHEAWSRIKUL : THE SOLVATION STRUCTURE OF LITHIUM ION IN WATER-AMMONIA MIXTURE BY MONTE CARLO METHOD. THESIS ADVISOR : SUPOT HANNONGBUA, Ph.D. 153 PP.

The solvation structure of lithium ion in 18.45 mole % aqueous ammonia at 20 °C is investigated, using the Metropolis Monte Carlo method. The system consists of 202 particles, one lithium ion, 37 ammonia and 164 water molecules. The experimental density of 18.45 mole % aqueous ammonia ( $0.9307 \text{ g.cm}^{-3}$ ) was used, leading to a periodic sidelength of 18.56 Å and half of this length was chosen as spherical cut-off. Five pair potential functions, based on ab initio calculations, are used in order to represent all pairs of interactions, four of them were taken from the literatures while the lithium ion/ammonia pair potential was newly constructed in this work. The results show that lithium ion is preferentially solvated by water molecule. There are 4 water and 2 ammonia molecules in the first shell of lithium ion, the second one 8 water and 4 ammonia molecules. The fully solvated lithium ion in 18.45 mole % aqueous ammonia can be characterized by  $\text{Li}[(\text{H}_2\text{O})_4(\text{NH}_3)_2]^{\text{I}}[(\text{H}_2\text{O})_8(\text{NH}_3)_4]^{\text{II}}$ . Distribution of coordination numbers and binding energies have been discussed with respect to exchange mechanisms.

ภาควิชา .....เคมี.....  
สาขาวิชา .....เคมีอนินทรีย์.....  
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