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STRUCTURAL DETERMINATION OF COBALT TUNGSTATE

BY X-RAY DIFFRACTION METHOD



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หัวข้อวิทยานิพนธ์    การหาโครงสร้างของโคบอลต์ทังสเตนโดยวิธีดิฟแฟรกชันของรังสีเอกซ์  
 ชื่อ                      นางสาวอัญชรี มีทอง    แผนกวิชาเคมี  
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บทคัดย่อ



โคบอลต์ทังสเตน ( $\text{CoWO}_6$ ) ภายสภาวะแม่เหล็กเดี่ยว โดยมีค่ามิติของเซลล์  $a = 4.678 \pm 0.001$ ,  $b = 5.684 \pm 0.001$ ,  $c = 4.949 \pm 0.001$  อังสตรอม  $\beta = 90.04 \pm 0.03$  องศา, ปริมาตรของเซลล์ = 131.61 ลูกบาศก์อังสตรอม ค่าความหนาแน่น  $D_m = 7.75 \pm 0.02$  กรัมต่อลูกบาศก์เซนติเมตรที่อุณหภูมิ 28 องศาเซลเซียส  $D_x = 7.744$  กรัมต่อลูกบาศก์เซนติเมตร หมู่สมมาตรสามมิติ  $P2/c$  และ  $Z = 2$  การหาโครงสร้างโดยดิฟแฟรกชันของรังสีเอกซ์ใช้วิธีฟูเรียร์และอะตอมหนัก (Fourier and heavy atom methods) ตำแหน่งอะตอมของออกซิเจนได้จากการสังเคราะห์  $\Delta F$  การปรับค่าอย่างละเอียดของตำแหน่งและพารามิเตอร์เนื่องจากความร้อนแบบไอโซโทรปิกของอะตอมต่าง ๆ ใช้วิธีสี่สแควร์เมทริกครบถ้วน (full matrix least squares method) ซึ่งให้ค่า  $R = 0.09$  สำหรับจุดสะท้อนที่  $2\theta$  จาก 10 ถึง 25 องศาจากการทดลอง

ผลการทดลองพบว่า อะตอมของออกซิเจนจะจัดตัวซ้อนกันแบบเฮกซะโกนอลที่บิดไป (distorted hexagonal close packing) โดยมีอะตอมของโคบอลต์และทังสเตนบรรจุอยู่ในช่องว่างของออกตะฮีดรอน ออกตะฮีดรอนของ  $\text{CoO}_6$  หรือ  $\text{WO}_6$  อย่างเดียวกันจะ เชื่อมกันด้วยขอบ แต่ถ้าต่างชนิดกันจะ เชื่อมกันด้วยมุม

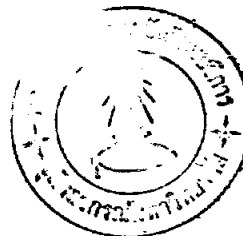
Thesis Title      Structural Determination of Cobalt Tungstate by  
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## ABSTRACT

Cobalt tungstate,  $\text{CoWO}_4$ , crystallizes in the monoclinic system with cell dimensions  $a = 4.678 \pm 0.001$ ,  $b = 5.684 \pm 0.001$ ,  $c = 4.949 \pm 0.001 \text{ \AA}$ ,  $\beta = 90.04 \pm 0.03^\circ$ ,  $V = 131.61 \text{ \AA}^3$ ,  $D_m = 7.75 \pm 0.02 \text{ g.cm}^{-3}$  at  $28^\circ\text{C}$ ,  $D_x = 7.744 \text{ g.cm}^{-3}$ , space group  $P2/c$  and  $Z = 2$ . The structure has been determined by X-ray diffraction using Fourier and heavy atom methods. The difference synthesis was used to locate the oxygen atoms. Positional and isotropic thermal parameters were refined by the full matrix least squares method to a final R index of 0.09 for 225 independent observed reflections.

The structure of  $\text{CoWO}_4$  is based on a distorted hexagonal close packing of oxygen atoms with cobalt and tungsten atoms each occupying one-fourth of the octahedral interstices. The similar octahedra of  $\text{CoO}_6$  or  $\text{WO}_6$  are joined by edges and the different octahedra by corners.

## Acknowledgements



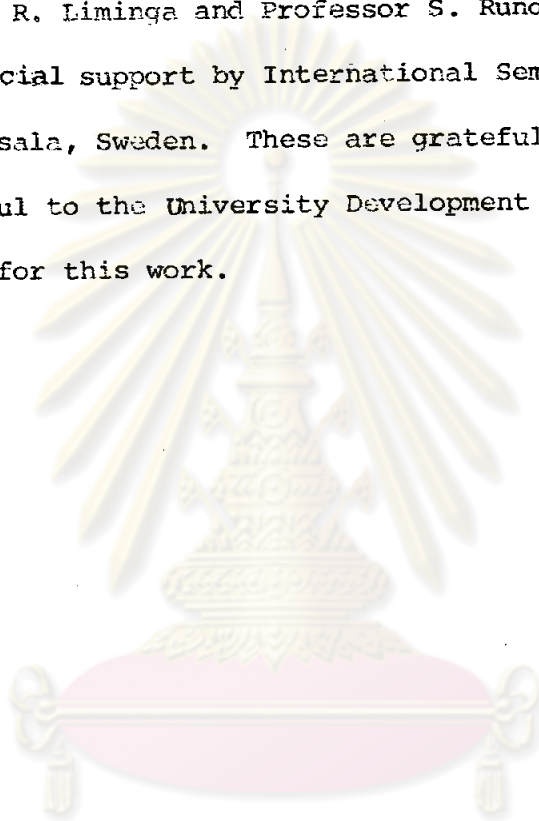
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