

# 以核磁共振光譜法鑑別鎔氧六甲基丙烯胺肟非鏡像立體異構物之研究

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## 摘要

由  $^1\text{H-NMR}$  及  $^{13}\text{C-NMR}$  光譜圖知，僅有  $^{13}\text{C-NMR}$  可以分辨 d,l-型和 meso-型 CB-PAO 配位子，因為就環丁烯基上的三個甲烯基而言，由於 meso-型分子的對稱結果，形成三個  $^{13}\text{C-NMR}$  訊號分別為  $\delta 15.18(\text{CrH}_2)$ ， $\delta 28.18(\text{C}\alpha, \text{H}_2)$  以及  $\delta 28.28(\text{C}\beta\text{H}_2)$ ，而 d,l-型卻只產生兩個訊號分別為  $\delta 15.18(\text{CrH}_2)$ ， $\delta 28.11(\text{C}\alpha, \beta\text{H}_2)$ 。此外，d,l-CBPAO 有 8 組碳種類，而 meso-CB-PAO 則有 9 組，亦可明顯鑑別不同種類立體異構物。就  $^{99}\text{TcO-d,l-CBPAO}$  之  $^1\text{H-NMR}$  光譜圖而言，在不對稱碳上的兩個氫原子(bH; jH) 其與鎔氧核上的氧以及另一個不對稱碳上的甲基(iCH<sub>3</sub>, CCH<sub>3</sub>)所形成之立體化學環境不相同，彼此屬於非化學不等價，故受甲基上三個氫原子影響而分裂為兩個四重峰。就  $^{99}\text{TcO-meso-CB-PAO}$  而言，bH 與 jH，對鎔氧核上的氧及相關之 iCH<sub>3</sub> 及 CCH<sub>3</sub> 甲基所形成之立體化學環境相同，彼此屬於化學等價，因此受甲基上三個氫原子分裂為一個四重峰。此外，就  $^{99}\text{TcO-d,l-CBPAO}$  之 CH<sub>2</sub>N 上的四個氫原子(2dH, 2hH)而言，其所處鎔氧核上的氧及不對稱碳上的甲基之立體化學環境皆不相同，屬於化學不等價，故受同一碳上的另一氫原子影響，分裂為四個二重峰，然而，對於  $^{99}\text{TcO-meso-CB-PAO}$  而言，接在同一碳上的兩個氫原子，屬於非化學不等價，但其各別卻又和另一碳上的兩個氫原子分別屬於化學不等價，因而受到同一碳上另一氫原子影響，只分裂為兩個二重峰。就  $^{13}\text{C-NMR}$  光譜顯示  $^{99}\text{Tc-d,l-CB-PAO}$  有 12 組不同環境之碳種類，而  $^{99}\text{Tc-meso-CB-PAO}$  只有 9 組，根據上述實驗結果，以核磁共振光譜法可有效鑑別及確認 d,l-CB-PAO 與 meso-CB-PAO 非鏡像立體異構之鎔錯合物。

關鍵字：核磁共振，非鏡像立體異構物，鎔錯合物，非化學等價

# Identification and Characterization of CB-PAO Diastereoisomers of Technetium (v) Complexes by Using NMR

## Spectroscopy Method

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### Abstract

$^{13}\text{C}$ -NMR spectroscopy is only suitable to identify the stereochemical isomers of CB-PAO due to the different NMR signals of  $-\text{CH}_2-$  on the same cyclobutyl group. Because of the symmetry of meso-form molecular structure, it appears three  $^{13}\text{C}$ -NMR signal on  $\delta$  15.18 (CrH<sub>2</sub>) ,  $\delta$  28.18(C  $\alpha$  , H<sub>2</sub>) and  $\delta$  28.28(C  $\beta$  H<sub>2</sub>) for meso-CB-PAO. However, it appears just only two  $^{13}\text{C}$ -NMR signal on  $\delta$  15.18(CrH<sub>2</sub>) ,  $\delta$  28.11(C  $\alpha$  ,  $\beta$  H<sub>2</sub>) for d,l-CB-PAO. In addition,  $^{13}\text{C}$ -NMR spectroscopy of meso-CB-PAO displays nine kinds of carbon type, but that of d,l-CB-PAO displays only eight kinds of C type. For  $^{99}\text{TcO}$ -d,l-CB-PAO complex, the stereochemical environments on the unsymmetrical carbon are different between two H(bH,jH);O (Tc=O) and methyl group (iCH<sub>3</sub>; cCH<sub>3</sub>). They are belong to chemical non-equivalence and splitted into two quartet on the influence of three hydrogen atoms. For  $^{99}\text{Tc}$ -meso-CB-PAO complex, they are belong to chemical equivalence and splitted into one quartet. For  $^{99}\text{TcO}$ -d,l-CB-PAO complex, the stereochemical environment of the four hydrogen (2dH, 2hH) on  $-\text{CH}_2\text{N}-$  group is different between oxygen (Tc=O) and methyl (unsymmetrical carbon). They are belong to chemical non-equivalence and splitted into four doublet. For  $^{99}\text{TcO}$ -meso-CB-PAO complex, the two hydrogen on the same carbon are belong to chemical non-equivalence and splitted into two doublet.  $^{13}\text{C}$ -NMR measurements on  $^{99}\text{TcO}$ -d,l-CB-PAO complex displays 12 kinds of different environment of carbon types. However, it provides only 9 kinds of carbon types for  $^{99}\text{TcO}$ -meso-CB-PAO complex. According to the results of NMR spectroscopy, it is qualitatively feasible for the identification and characterization of CB-PAO diastereoisomers of technetium complexes.

KeyWords : nuclear magnetic resonance (NMR) , diastereoisomer , technetium complex , chemical non-equivalence

