



'n Elektrochemiese en berekeningschemiestudie van tenoïelbevattende Rh(I) β -diketonatokomplekse

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Note:

A selection of conference proceedings: Student Symposium in Science, 07 and 08 November 2013, University of Pretoria, South Africa. Organising committee: Mr Rudi W. Pretorius (Department of Geography, University of South Africa) and Ms Andrea Lombard (Department of Geography, University of South Africa), Dr Hertzog Bisset (South African Nuclear Energy Corporation [NECSA]) and Prof. Philip Crouse (Department of Chemical Engineering, University of Pretoria).

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An electrochemical and computational study of thenoyl-containing Rh(I) β -diketonat complexes. The electrochemical properties of $[\text{Rh}((\text{C}_4\text{H}_9\text{S})\text{COCHCO}(\text{R}))(\text{CO})(\text{PPh}_3)]$ (with $\text{R} = \text{C}_4\text{H}_9\text{S}, \text{C}_6\text{H}_5, \text{CF}_3$) were determined through cyclic voltammetry and the results were compared with Hammett constants and group electro-negativities. We obtained good correlations which enable the synthesis of rhodium complexes with specific characteristics through modelling with computational chemistry.

Sikliese voltammetrie (CV) is 'n populêre en eenvoudige elektro-analitiese metode wat gebruik word om inligting aangaande die fisiese en chemiese eienskappe van organiese, anorganiese en oorgangsmetaalkomplekse te bekom (Kissinger & Heineman 1983). Die oksidasie van Rh(I) na Rh(III) is belangrik in katalitiese siklusse (Cotton, Wilkinson & Gaus 1995:604).

In hierdie studie is die elektrochemiese eienskappe van $[\text{Rh}((\text{C}_4\text{H}_9\text{S})\text{COCHCO}(\text{R}))(\text{CO})(\text{PPh}_3)]$ (met $\text{R} = \text{C}_4\text{H}_9\text{S}, \text{C}_6\text{H}_5, \text{CF}_3$) bepaal en gekorreleer met die energie van die hoogs gevulde molekulêre orbitaal (HOMO) wat volgens die digtheidsfunksionaalteorie (DFT) bereken is. 'n Positiewe verskuiwing in die oksidasiepotensiale van die rodiumkomplekse is waargeneem namate die elektronegatiwiteit van die R-groep, wat aan die metaalsentrum gebind is, toeneem. Hierdie elektrochemiese resultate vergelyk goed met die DFT-berekende HOMO-energieë asook met Hammett-konstantes en groepelektronegatiwiteite. Die resultate wat verkry is, maak dit moontlik om rodiumkomplekse met spesifieke eienskappe te sintetiseer deur die komplekse eers met behulp van berekeningschemie te modelleer.

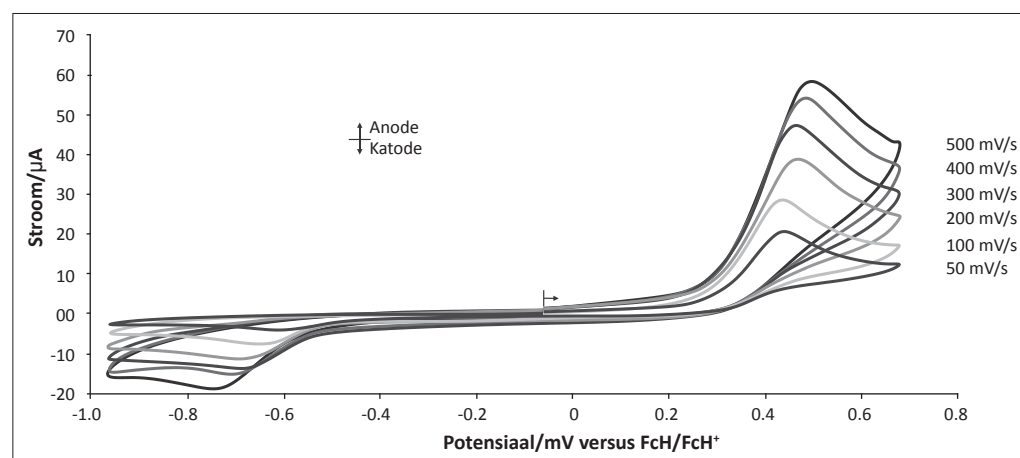
DFT-berekenings is met behulp van Gaussian se 2009-program deur middel van die PW91-funksionaal (Perdew & Wang 1992) en 'n TZP-basisstel uitgevoer.

Literatuurverwysings

Cotton, F.A., Wilkinson, G. & Gaus, P.A., 1995, *Basic Inorganic Chemistry*, 3rd edn., John Wiley, New York.

Kissinger, P.T. & Heineman, W.R., 1983, 'Cyclic voltammetry', *Journal of Chemical Education* 60, 702-706.

Perdew, J.P. & Wang, Y., 1992, 'Accurate and simple analytic representation of the electron-gas correlation energy', *Journal of American Chemical Society* 114(23), 244-249.



Nota: Daar is met skanderings teen verskillende tempo's in die positiewe rigting begin, soos met die pyltjie aangedui.

FIGUUR 1: Sikliese voltammogram van $[\text{Rh}((\text{C}_4\text{H}_9\text{S})\text{COCHCO}(\text{CF}_3))(\text{CO})(\text{PPh}_3)]$ met 'n konsentrasie van 1.0 mM in asetonitriël met 0.1 M-tetrabutielammonium-heksafluoorfosfaat as die steunelektroliet op 'n glasagtige koolstofwerkselektrode relatief tot die oksidasiepotensiaal van FcH/FcH^+ , $T = 25^\circ\text{C}$.

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