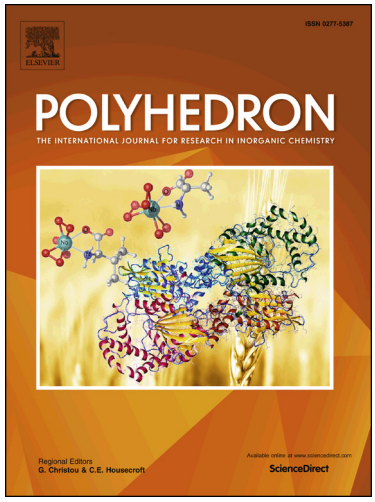

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A VARIABLE TEMPERATURE NMR ANALYSIS AND RESONANCE ASSIGNMENT OF THE GRUBBS SECOND GENERATION CATALYST

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Abstract

The Grubbs second generation catalyst [$RuCl_2(PCy_3)(H_2IMes)CHPh$] was analysed in solution in order to identify and assign all of the ^{1}H and ^{13}C NMR resonances. This was achieved through utilizing various 2D NMR techniques and by acquiring spectra at a range of different temperatures (-40 to 60 °C). These assignments will aid researchers in future NMR studies of catalytic systems that employ the Grubbs catalyst by eliminating the resonances belonging to the catalyst and thus enabling the identification of any intermediates and/or new catalytic species. Restricted conformations and π-stacking arrangement within the catalyst was also confirmed during this study.

Keywords: Grubbs second generation catalyst; NMR; ^{1}H; ^{13}C; 2D techniques

Introduction

With metathesis reactions being an indispensable tool in synthetic chemistry for carbon-carbon double bond formation,[1-3] various catalyst variations of Grubbs'[4-13] (and Schrock')[14,15] catalysts have been and are being studied in order to improve these catalysts' lifetime, activity, reactivity and stability.