Supporting Information

Phoban-Containing Ru-Complexes: Efficient Pre-Catalysts for Olefin Metathesis Reactions (Phoban = Phosphabicyclononane)

Fabien Boeda,§ Hervé Clavier,§ Margaritha Jordaan, † Wolfgang H. Meyer, † and Steven P. Nolan*,§

§Institute of Chemical Research of Catalonia (ICIQ), Av. Països Catalans, 16, 43007 Tarragona (Spain)

†Sasol Technology (Pty), Ltd., R&D Division, 1 Klasie Havenga Road, Sasolburg, 1947 (South Africa)

snolan@iciq.es

Table of Contents

General considerations........................................................................................................ S2
NMR spectras..................................................................................................................S3-S80
General considerations: All reagents were used as purchased. Dichloromethane (DCM) was obtained from an Innovative Technology solvent purification system. Other used solvents as well as 1-octene and nonane were dried and deoxygenated using common laboratory practices. Flash column chromatography were performed on silica gel 60 (230-400 mesh, Silicycle). $^1$H, $^{31}$P and $^{13}$C Nuclear Magnetic Resonance (NMR) spectra were recorded on a Bruker Avance 400 Ultrashield NMR spectrometer or on a Varian 400 MHz or 600 MHz spectrometers. Analysis of the self-metathesis reaction mixtures were performed on an Agilent Technologies 6890N Network GC system using a Pona column. Neolyst™ M3 (3-phenyl-1H-inden-1-ylidenedichloro[bis(i-butylphoban)]ruthenium) 6 was used without further purification. The synthesis and characterization of 4 (benzylidenedichlorobis(9-cyclohexyl-9-phosphabicyclo-[3.3.1]-nonane)ruthenium) has been previously described.1,2 3-phenyl-1H-inden-1-ylidenedichlorobis[triphenylphosphine]ruthenium complex has been previously described in the literature3 as well as complex 5.4 Compounds 7 to 40 have previously been described.5

SpinWorks 2.4: 13C with proton decoupling
SpinWorks 2.4: 13C with proton decoupling
SpinWorks 2.4: 13C with proton decoupling

freq. of 0 ppm: 75.487751 MHz
processed size: 68535 complex points
LB: 1.0000  GB: 0.0000
Helm: 718.424  ppm/cm: 9.53192