Supporting Information

for

Synthesis of Ru alkylidene complexes

Renat Kadyrov*¹ and Anna Rosiak¹,²

Address: ¹Evonik Degussa GmbH, Rodenbacher Chaussee 4, 63457 Hanau-Wolfgang, Germany and ²present address: ASM Research Chemicals, Feodor-Lynen-Str. 31, 30625 Hannover, Germany.

Email: renat.kadyrov@evonik.com

*Corresponding author

Detailed experimental data
Variable-temperature spectra of the solution of 1e in CD₂Cl₂.
Experimental (top) and calculated (bottom) spectrum parts (7.4-9.0 ppm) for exchanging signals H3', H5, H5' and H3 of the thienyl fragment in 1e.

- T = 193 K
- k = 0 (w = 10 Hz)
- T = 213 K
- k = 0.25
- T = 233 K
- k = 4.7
- T = 253 K
- k = 59 (∆G ≠ = 12.7 kcal/mol)
- T = 303 K
- k = 5400 (∆G ≠ = 12.6 kcal/mol)
\[ \ln K = -669.92 \left( \frac{1}{T} \right) + 1.9303 \]

Arrhenius plot for 1e interconversion based on line-shape analysis.

\[ \Delta H = 1.3 \text{ kcal/mol} \]

\[ \ln \left( \frac{k}{T} \right) = -6910.6 \left( \frac{1}{T} \right) + 25.75 \]

Eyring plot of the rate constants obtained from line shape analysis for 1e interconversion.

\[ \Delta H^\# = 13.7 \text{ kcal/mol} \]
Variable-temperature spectra of the solution of 1g in CD₂Cl₂.

Dichlorobis(tricyclohexylphosphine)(ethylidene)ruthenium(II) (1a):
Dichlorobis(tricyclohexylphosphine)(cyclopenten-1-ylmethylidene)ruthenium(II) (1b):
Dichlorobis(tricyclohexylphosphine)(cyclohexen-1-ylmethylidene)ruthenium(II)-toluene adduct (1c-toluene):
Dichlorobis(tricyclohexylphosphine)(thien-2-ylmethylidene)ruthenium(II) (1e): 1H in CD$_2$Cl$_2$

13C in CDCl$_3$
Dichlorobis(tricyclohexylphosphine)(fur-2-ylmethylidene)ruthenium(II) (1f):
Dichlorobis(tricyclohexylphosphine)(naphth-2-ylmethylidene)ruthenium(II) (1g):
1H in CD₂Cl₂

13C in CDCl₃
Dichlorobis(tricyclohexylphosphine)(inden-2-ylmethylidene)ruthenium(II) (1h):
Dichlorobis(tricyclohexylphosphine)(norpinanylmethylidene)ruthenium(II) (1i)
1H in CD$_2$Cl$_2$

13C in CDCl$_3$
Dichlorobis(tricyclohexylphosphine)(2-phenylvinylidene)ruthenium(II) (2):

Dichlorobis(tricyclohexylphosphine)(2-butylvinylidene)ruthenium(II) (3):