Supporting Information for
“On the relationship between structure and reaction rate in olefin ring-closing metathesis”

Ashworth, Carboni, Hillier, Nelson, Percy, Rinaudo and Vincent

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### T₁ Values for Dienes and Cycloalkenes

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Octadiene is representative of all diene substrates; olefinic protons exhibited the highest T₁ values in each molecule. D₁ = 35 s was selected, being the longest T₁ x 5.
Procedure for Kinetic Experiments

Grubbs’ second generation pre-catalyst 9 and 1,3,5-trimethoxybenzene were purchased from Sigma Aldrich and used as supplied. The pre-catalyst was handled under a flow of dry oxygen-free nitrogen at all times. Deuterated chloroform and dichloromethane were purchased from Sigma Aldrich and Goss Scientific respectively; solvents were dried over activated 4 Å molecular sieves for at least 12 h before use. Karl-Fischer analysis confirmed that water content in both solvents was < 10 ppm.

The use of disposable plastic syringes was avoided to prevent contamination of the chlorinated solvents with plasticisers that might interfere with the metathesis catalyst.

A clean and dry volumetric flask was flushed with nitrogen and charged with an appropriate mass of 1,3,5-trimethoxybenzene and an appropriate mass of diene. The flask was made up to volume with dry solvent under a gentle nitrogen flow. This concentrated stock solution(s) (typically approx. 100 mM total diene concentration) was then diluted to an appropriate concentration in a second volumetric flask, using a clean and dry gastight syringe. The flask was made up to volume using dry solvent. This solution (typically 10 mM total diene concentration) was used as a stock solution.

A clean, oven-dried NMR tube was flushed with nitrogen using a balloon. The 10 mM stock solution (600 µL) was added and the tube capped. The tube was inserted into the magnet and the instrument internal temperature was set to 298K and allowed to equilibrate. NMR analysis was carried out before pre-catalyst addition to confirm that the solution did not contain acetone (δ_H = 2.2 ppm) or water (broad peak at δ_H = 1.5 ppm) and that it contained the correct concentration of diene with respect to the internal standard.
A dry volumetric flask was flushed with nitrogen and charged with an appropriate mass of Grubbs’ second generation pre-catalyst 9 and stored in a bag filled with nitrogen. The flask was made up to volume using dry solvent approximately 5 minutes before charging the solution to the NMR tube.

This catalyst solution was charged to the NMR tube via a dry glass syringe and the time noted. The tube was shaken vigorously for approx. 15 seconds before the cap was exchanged for a pierced cap.

The sample was then analysed at appropriate intervals using a Bruker Topspin automated script, multi_zgvd2b. Samples were automatically shimmed using topshim 1dFast between acquisitions.

NMR spectra were acquired on a Bruker AV400 instrument fitted with BBFO-z-ATMA probe or a Bruker AV600 instrument fitted with a TBI-z or BBO-z-ATMA probe; both instruments are fitted with temperature control units. Settings for spectra acquisition were as follows: NS = 4 scans; D1 = 35 s; SW = 24 ppm and O1P = 10 ppm. The sample was held at 298 K for the duration of the experiment.
Kinetic Data

*Ternary Competition RCM in Chloroform*

3.3 mM heptadiene 7b, 3.4 mM octadiene 7c, 3.5 mM nonadiene 7d, 0.1 mM pre-catalyst 9

*Analysis was by $^1$H NMR at 600 MHz using a Bruker AV600 equipped with TBI-z probe; the temperature was maintained at 298 K throughout.*

Sample spectra:

(1) Before pre-catalyst addition.

(2) Approx. 2 h after addition.
(3) After approx. 2h: signals used for quantification
Concentration/time data for the RCM of heptadiene 7b, octadiene 7c, nonadiene 7d with pre-catalyst 9 in CDCl$_3$ at 298 K (AV600, TBI-z probe); 4 scans with $D_1 = 35$ s; $TE = 298$ K; concentrations obtained by integration of the appropriate signal and the internal standard (see above).
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**Ternary Competition RCM in Dichloromethane**

3.4 mM heptadiene 7b, 3.4 mM octadiene 7c, 3.5 mM nonadiene 7d, 0.1 mM pre-catalyst 9

Analysis was by $^1$H NMR at 600 MHz using a Bruker AV600 equipped with BBO-z-ATMA probe; the temperature was maintained at 298 K throughout.

Sample spectra:

(1) Before pre-catalyst addition.

![Sample spectrum 1](image1)

(2) Approx 2 h after addition.

![Sample spectrum 2](image2)
(3) After approx. 2h: signals used for quantification

Pre-catalyst 9 cannot be detected due to the lower sensitivity of the BBO-z-ATMA probe.
Concentration/time data for the RCM of heptadiene 7b, octadiene 7c, nonadiene 7d with pre-catalyst 9 in CD2Cl2 at 298 K (AV600, BBO-z-ATMA probe); 4 scans with D1 = 35 s; TE = 298 K; concentrations obtained by integration of the appropriate signal and the internal standard (see above).
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Heptadiene RCM in Chloroform

9.1 mM heptadiene 7b (dataset 1) or 9.2 mM heptadiene 7b (dataset 2); both with 0.1 mM pre-catalyst 9. Analysis was by $^1$H NMR at 400 MHz using a Bruker AV400 equipped with BBFO-z-ATMA probe; the temperature was maintained at 298 K throughout.

Sample Spectra

(1) Before pre-catalyst addition

(2) Approx. 1 h after addition
(3) Signals used for quantification

- Ethene
- Diene
- Internal Standard
- Cyclopentene

(Not quantified)
Concentration/time data for the RCM of heptadiene 7b with pre-catalyst 9 in CDCl₃ at 298 K (AV400, BBFO-z-ATMA probe); 4 scans with D₁ = 35 s; TE = 298 K; concentrations obtained by integration of the appropriate signal and the internal standard (see above).

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Concentration/time data for the RCM of heptadiene \textit{7b} with pre-catalyst \textit{9} in CDCl\textsubscript{3} at 298 K (AV400, BBFO-z-ATMA probe); 4 scans with \(D_1 = 35\) s; TE = 298 K; concentrations obtained by integration of the appropriate signal and the internal standard (see above).

\textbf{Dataset 2}

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Heptadiene RCM in Dichloromethane

9.6 mM heptadiene 7b (dataset 1) or 9.2 mM heptadiene 7b (dataset 2); both with 0.1 mM pre-catalyst 9. Analysis was by \(^1\)H NMR at 600 MHz using a Bruker AV600 equipped with BBO-z-ATMA probe; the temperature was maintained at 298 K throughout.

Sample Spectra

(1) Before pre-catalyst addition

(2) Approx. 1 h after addition
(3) Signals used for quantification

- Ethene
- Diene
- Internal Standard
- Cyclopentene
Concentration/time data for the RCM of heptadiene \(7b\) with pre-catalyst \(9\) in CD_{2}Cl_{2} at 298 K (AV600, BBO-z-ATMA probe); 4 scans with \(D_{1} = 35\) s; \(TE = 298\) K; concentrations obtained by integration of the appropriate signal and the internal standard (see above).

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Concentration/time data for the RCM of heptadiene 7b with pre-catalyst 9 in CD$_2$Cl$_3$ at 298 K (AV600, BBO-z-ATMA probe); 4 scans with $D_1 = 35$ s; $TE = 298$ K; concentrations obtained by integration of the appropriate signal and the internal standard (see above).

**Dataset 2**

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**Octadiene RCM in Chloroform**

9.3 mM octadiene 7c (dataset 1) or 8.8 mM octadiene 7c (dataset 2); both using 0.1 mM pre-catalyst 9. *Analysis was by* $^1$H NMR *at 400 MHz using a Bruker AV400 equipped with BBFO-z-ATMA probe; the temperature was maintained at 298 K throughout.*

Sample Spectra

(1) Before pre-catalyst addition

![Sample Spectrum Before Pre-catalyst Addition](image1)

(2) Approx. 1 h after addition

![Sample Spectrum After Pre-catalyst Addition](image2)
(3) Signals used for quantification

- Ethene
- Diene
- Internal Standard
- Cyclohexene

Mes~N\(\text{Cl}\)\(\text{PCy}_3\)Ph

(Not quantified)
Concentration/time data for the RCM of octadiene 7c with pre-catalyst 9 in CDCl₃ at 298 K (AV400, BBFO-z-ATMA probe); 4 scans with $D_1 = 35$ s; TE = 298 K; concentrations obtained by integration of the appropriate signal and the internal standard (see above).

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Concentration/time data for the RCM of octadiene 7c with pre-catalyst 9 in CDCl3 at 298 K (AV400, BBFO-z-ATMA probe); 4 scans with $D_1 = 35$ s; $TE = 298$ K; concentrations obtained by integration of the appropriate signal and the internal standard (see above).

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Octadiene RCM in Dichloromethane

10.1 mM octadiene 7c (dataset 1) or 10.3 mM octadiene 7c (dataset 2); both using 0.1 mM pre-catalyst 9. Analysis was by $^1$H NMR at 600 MHz using a Bruker AV600 equipped with BBO-z-ATMA probe; the temperature was maintained at 298 K throughout.

Sample Spectra

(1) Before pre-catalyst addition

(2) Approx. 1 h after addition
(3) Signals used for quantification

- Ethene
- Diene
- Internal Standard
- Cyclohexene
Concentration/time data for the RCM of octadiene 7c with pre-catalyst 9 in CD₂Cl₂ at 298 K (AV600, BBO-z-ATMA probe); 4 scans with D₁ = 35 s; TE = 298 K; concentrations obtained by integration of the appropriate signal and the internal standard (see above).

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Concentration/time data for the RCM of octadiene 7c with pre-catalyst 9 in CD$_2$Cl$_2$ at 298 K (AV600, BBO-z-ATMA probe); 4 scans with $D_1 = 35$ s; $TE = 298$ K; concentrations obtained by integration of the appropriate signal and the internal standard (see above).

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**Nonadiene RCM in Chloroform**

10.2 mM nonadiene 7d (dataset 1) or 9.7 mM nonadiene 7d (dataset 2); both using 0.1 mM pre-catalyst 9. Analysis was by $^1$H NMR at 600 MHz using a Bruker AV600 equipped with BBO-z-ATMA probe or 400 MHz using a Bruker AV400 equipped with BBFO-z-ATMA probe; the temperature was maintained at 298 K throughout.

Sample Spectra

(1) Before pre-catalyst addition

(2) Approx. 1 h after addition
(3) Signals used for quantification
Concentration/time data for the RCM of nonadiene 7d with pre-catalyst 9 in CDCl₃ at 298 K (AV600, BBO-z-ATMA probe); 4 scans with \( D_1 = 35 \text{ s} \); \( TE = 298 \text{ K} \); concentrations obtained by integration of the appropriate signal and the internal standard (see above).

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Concentration/time data for the RCM of nonadiene 7d with pre-catalyst 9 in CDCl3 at 298 K (AV400, BBFO-z-ATMA probe); 4 scans with D1 = 35 s; TE = 298 K; concentrations obtained by integration of the appropriate signal and the internal standard (see above).

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Nonadiene RCM in Dichloromethane

9.8 mM nonadiene 7d (dataset 1) or 9.9 mM nonadiene 7d (dataset 2); both using 0.1 mM pre-catalyst 9. Analysis was by $^1$H NMR at 600 MHz using a Bruker AV600 equipped with BBO-z-ATMA probe; the temperature was maintained at 298 K throughout.

Sample Spectra (600 MHz)

(1) Before pre-catalyst addition

(2) Approx. 1 h after addition
(3) Signals used for quantification

- Ethene
- Diene
- Internal Standard
- Cyclohexene
Concentration/time data for the RCM of nonadiene 7d with pre-catalyst 9 in CD$_2$Cl$_2$ at 298 K (AV600, BBO-z-ATMA probe); 4 scans with $D_1 = 35$ s; $TE = 298$ K; concentrations obtained by integration of the appropriate signal and the internal standard (see above).

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Concentration/time data for the RCM of nonadiene 7d with pre-catalyst 9 in CD₂Cl₂ at 298 K (AV600, BBO-z-ATMA probe); 4 scans with D₁ = 35 s; TE = 298 K; concentrations obtained by integration of the appropriate signal and the internal standard (see above).

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**Attempted Hexadiene Metathesis in Chloroform**

8.7 mM hexadiene 7a, 0.1 mM pre-catalyst 9. Analysis was by $^1$H NMR at 400 MHz using a Brüker AV400 equipped with BBFO-z-ATMA probe; the temperature was maintained at 298 K throughout.

![Graph showing NMR spectra at different times](image_url)

- $t = 0$
- $t = 20$ min
- $t = 1$ h
- $t = 2.5$ h

Ethene
**Hexadiene Metathesis, Concentrated Solution in Chloroform**

252.6 mM hexadiene 7a, 4.7 mM pre-catalyst 9. *Analysis by $^1$H NMR at 400 MHz using a Brüker AV400 equipped with BBFO-z-ATMA probe; the sample was analysed periodically at 298K and stored on an auto-sampler carousel in a temperature controlled room 294 K when analysis was not being performed.*

(1) Before pre-catalyst addition

(2) Approx 8 h after addition

(Not quantified)
Approx. 8 h after addition (continued)
**Heptadiene/Octadiene Competition RCM in Chloroform**

4.4 mM heptadiene 7b and 4.5 mM octadiene 7c (dataset 1) and 4.5 mM heptadiene 7b and 4.6 mM octadiene 7c; both with 0.1 mM pre-catalyst 9. *Analysis by $^1$H NMR at 400 MHz using a Bruker AV400 equipped with BBFO-z-ATMA probe; the sample temperature was maintained at 298K throughout.*

(1) Before pre-catalyst addition

![NMR spectrum before pre-catalyst addition](image1)

(2) Approx. 1 h after addition

![NMR spectrum after pre-catalyst addition](image2)
(3) Signals used for quantification

- Ethene
- Diene
- Internal Standard
- Cyclopentene
- Cyclohexene
- Octadiene
- (Not quantified)
Concentration/time data for the RCM of heptadiene 7b and octadiene 7c with pre-catalyst 9 in CDCl₃ at 298 K (AV400, BBFO-z-ATMA probe); 4 scans with D₁ = 35 s; TE = 298 K; concentrations obtained by integration of the appropriate signal and the internal standard (see above), with the exception of heptadiene which was calculated from [diene]-[octadiene].

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Concentration/time data for the RCM of heptadiene 7b and octadiene 7c with pre-catalyst 9 in CDCl₃ at 298 K (AV400, BBFO-z-ATMA probe); 4 scans with D₁ = 35 s; TE = 298 K; concentrations obtained by integration of the appropriate signal and the internal standard (see above), with the exception of heptadiene which was calculated from [diene]-[octadiene].

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Inhibited Octadiene RCM in Chloroform

5.7 mM hexadiene 7a and 5.0 mM octadiene 7c with 0.1 mM pre-catalyst 9. Analysis by $^1H$ NMR at 400 MHz using a Brüker AV400 equipped with BBFO-z-ATMA probe; the sample temperature was maintained at 298K throughout.

(1) Before pre-catalyst addition

(2) Approx. 1 h after addition
(3) Signals used for quantification

- Ethene
- Internal Standard
- Hexadiene
- Cyclohexene
- Octadiene

(Not quantified)
Concentration/time data for the RCM of octadiene 7c with pre-catalyst 9 in the presence of hexadiene 7a, in CDCl₃ at 298 K (AV400, BBFO-z-ATMA probe); 4 scans with $D_1 = 35$ s; TE = 298 K; concentrations obtained by integration of the appropriate signal and the internal standard (see above).

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**Hexadiene-derived 14e Propagating Carbene 10a**

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Metallocyclobutane 12b from heptadiene

Energy: -2175.171237 au

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**Metallocyclobutane fragmentation transition structure 13b from heptadiene**
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4   6  0  -1.247738  1.887007  0.145282
5   1  0  -1.399093  2.498713  -0.754714
6   1  0  -1.987145  1.990610  0.950598
7   6  0   1.659144  2.091891  0.987264
8   1  0   1.994687  1.458359  1.808977
9   6  0   0.506551  2.893014  1.143923
10  1  0  -0.073124  2.853518  2.060503
11  6  0   2.641409  2.758600  0.056351
12  1  0   3.073348  2.074296  -0.679199
13  1  0   3.473055  3.139567  0.667312
14  6  0   0.666724  4.164962  0.347466
15  1  0  -0.236327  4.500437  -0.167748
16  1  0   0.907306  4.948942  1.079558
17  6  0   1.847741  3.900858  -0.594355
18  1  0   1.479138  3.571781  -1.566112
19  1  0   2.454725  4.795100  -0.754125
20  6  0  -0.321122  -1.184994  -0.277898
21  7  0  -1.501117  -1.816088  -0.386354
22  7  0   0.663970  -2.058945  -0.563463
23  6  0  -1.333960  -3.180356  -0.915756
24  1  0  -1.963066  -3.886982  -0.369456
25  1  0  -1.632240  -3.208811  -1.971858
26  6  0   0.159447  -3.425307  -0.727155
27  1  0   0.377213  -4.017905   0.172156
28  1  0   0.628415  -3.917408  -1.582817
29  6  0   2.037779  -1.690949  -0.408789
30  6  0   4.638124  -0.722144  -0.128038
31  6  0   2.797197  -1.427742  -1.561771
32  6  0   2.581403  -1.562615   0.879251
33  6  0   3.879219  -1.053121   0.988827
34  6  0   4.088933  -0.942912  -1.393554
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**Metallocyclobutane 12c from octadiene**

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5   1  0  1.929370  2.372360  -0.738749
6   1  0  1.321651  2.679006  0.979204
7   6  0  -1.420502  1.743474  -0.820207
8   1  0  -1.532570  1.574831  -1.897809
9   6  0  -0.250427  2.839794  -0.591279
10  1  0  -0.019589  3.135520  -1.620169
11  6  0  -2.719449  2.079573  -0.140028
12  1  0  -3.462666  1.324775  -0.415890
13  1  0  -2.619805  2.047650  0.946592
14  6  0  -0.818823  3.968250  0.268652
15  1  0  -0.979590  3.579841  1.280150
16  1  0  -0.064605  4.756219  0.357838
17  6  0  -3.171274  3.467374  -0.608093
18  1  0  -3.376752  3.427771  -1.684176
19  6  0  -2.108089  4.543170  -0.313112
20  1  0  -1.868494  5.093619  -1.230183
21  6  0  0.403582  -1.300527  0.152384
22  7  0  1.611404  -1.885456  0.150018
23  7  0  -0.545384  -2.249004  0.202240
24  6  0  1.506611  -3.340696  0.337740
25  1  0  2.175414  -3.866346  -0.347397
26  1  0  1.791817  -3.605564  1.365041
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Basis Set Details.
The calculations were carried out using a locally modified version of GAUSSIAN 03.\(^1\)

Ru has the SDD pseudopotential and SDD basis set. In addition it has an f-function with exponent 0.57800.

C, N, Cl and H have the 6-311G** basis set.

The functional is M06-L and the solvation model is COSMO (with the default Klamt radii and DCM as solvent).

The frequencies are with the B1 basis set.

Ru has the LANL2DZ pseudo potential and LANL2DZ basis set with an addition f-function of exponent 0.57800.

C, N, Cl and H have the 6-31G* basis set

(The frequencies were used to provide thermodynamic corrections to the solvation energies)

Reference