Stereoselective Olefin Metathesis Processes Using Cyclometalated Ruthenium Alkylidene Complexes

Thesis by

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In Partial Fulfillment of the Requirements for
the Degree of
Doctor of Philosophy

CALIFORNIA INSTITUTE OF TECHNOLOGY
Pasadena, CA

2017
(Defended December 7, 2016)

For Padre

(March 10, 1961 – October 23, 2014)

ACKNOWLEDGEMENTS

I'd like to start by thanking Bob for accepting me into his group and offering me his unconditional support and guidance over the last five years. Grad school has comprised some of the more challenging years of my life, and I've been incredibly fortunate to have such a caring and generous advisor during this time. I am similarly grateful for my committee, composed of Profs. Dave Tirrell, Harry Gray, and Doug Rees. Their kindness, enthusiasm, and knowledge have been invaluable during my time at Caltech and will undoubtedly continue to be as I navigate the world beyond.

The Grubbs group is a special place at Caltech and in the world of chemistry. I'd like to extend special thanks to both Myles Herbert and B. Keith Keitz. Myles was the first face I saw when I sat down for lunch at my visiting weekend, and his welcoming enthusiasm and advice greatly eased my transition into the group. Keith was both an excellent desk-mate and mentor, and I am grateful for his help and patience during my first year in the group. I would also like to thank Dr. Vanessa Marx, who was not only instrumental in my development as an independent researcher and thinker but also an important friend. Crystal Chu, Brendon McNicholas, Zainab Al-Saihati, Dr. T. Patrick Montgomery, Dr. Karthish Manthiram, Dr. Chris Marotta, and Raymond Weitekamp in particular have been both good friends and good labmates and made Church 211 an excellent home for five years. Thank you also to Linda Syme for keeping our group running smoothly despite our best efforts. Finally, I'd like to thank all of the members of the group I've overlapped with over the years for their (countless) helpful conversations, words of encouragement, and time and energy, always freely given. Simply put, the Grubbs group is great because of the people in it.

The work in this thesis was made possible only through the support of so many others. Our group's ongoing collaboration with the Houk group at UCLA proved vital for the latter half of my thesis, and I would like to specifically recognize Peng Liu for his hard work and invaluable contributions. I am also grateful to everyone involved in keeping the Caltech chemistry department running on a day-to-day basis. Dr. Dave VanderVelde is especially appreciated for making the NMR facility such a fantastic resource in the department and for always willingly answering my many NMR questions. In addition, I would like to thank Dr. Mona Shahgholi and Naseem Torian for their help with mass spectrometry, Dr. Mike Takase and Larry Henling for their assistance with X-ray crystallography, and Dr. Scott Virgil for his general wisdom and helpfulness.

Finally, I would like to thank the friends and family who have provided me with continuous love and support over the years, including my dad Chris Rosebrugh (to whom this thesis is dedicated); my mom; my sister; and my aunts, uncles, and grandparents. A special thank you to the Janzen clan for always welcoming me with open arms. I am also incredibly grateful for the warmth, caring, and friendship I've found in the Pasadena community of ultimate frisbee players these past two years. Last but not least, I want to thank the members of my immediate family, Noby, Buster, and Jacob Janzen, the latter of whom is someone I am thankful for everyday to call my best friend and partner. I look forward to the many adventures to come.

ABSTRACT

The recent development of a class of *Z*-selective ruthenium metathesis catalysts containing a crucial cyclometalated *N*-heterocyclic carbene (NHC) ligand has extended the applicability of ruthenium-mediated olefin metathesis to the production of a variety of useful *Z*-olefin-containing small molecules, polymers, and natural products. This thesis explores the synthesis and application of a number of novel *Z*-selective cyclometalated ruthenium alkylidene complexes displaying enhanced activity and selectivity across a range of metathesis transformations. Mechanistic investigations aimed at understanding and controlling stereoselectivity specifically in ring-opening metathesis polymerization (ROMP) are also detailed.

Chapter 2 describes the preparation of new *Z*-selective cyclometalated ruthenium metathesis catalysts via an improved method employing sodium carboxylates. Effects of the cyclometalated NHC ligand on catalyst activity and selectivity in several cross metathesis assays, as well as macrocyclic ring-closing metathesis and other industrially relevant transformations, are investigated.

Chapter 3 relates a story in two parts: the first details the synthesis and activity of a series of novel cyclometalated ruthenium alkylidenes displaying unprecedented *cis,syndio*-selectivity in the ROMP of norbornene- and norbornadiene-derived monomers. The second comprises an extensive study into the origins of stereoselectivity in ROMP in these and related cyclometalated ruthenium initiators. Experimental results are used in conjunction with a computational analysis of propagation transition states to develop a complete stereochemical model for *cis,syndio*-selctivity in these systems.

PUBLISHED CONTENT AND CONTRIBUTIONS

Rosebrugh, L. E.; Herbert, M. B.; Marx, V. M.; Keitz, B. K.; Grubbs, R. H. *J. Am. Chem. Soc.* **2013**, *134*, 1276–1279. DOI: 10.1021/ja311916m.
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L.E.R. participated in the conception of the project, synthesized and characterized the catalysts as well as evaluated them in homodimerization reactions, prepared and analyzed the data, and participated in the writing of the manuscript.

Rosebrugh, L. E.; Marx, V. M.; Keitz, B. K.; Grubbs, R. H. *J. Am. Chem. Soc.* **2013**, *135*, 10032–10035. DOI: 10.1021/ja405559y.
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L.E.R. participated in the conception of the project, synthesized and characterized the cyclometalated *N*-^{t}Bu-*N*-mesityl catalyst, synthesized the chiral norbornene, evaluated the catalysts in ring-opening metathesis polymerization (ROMP) reactions, prepared and analyzed the data, and participated in the writing of the manuscript.

Marx, V. M.; Rosebrugh, L. E.; Herbert, M. B.; Grubbs, R. H. *Top. Organomet. Chem.* **2014**, *48*, 1–17. DOI: 10.1007/3418_2014_76.
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L.E.R. participated in the writing of the manuscript.

Rosebrugh, L. E.; Ahmed, T. S.; Marx, V. M.; Hartung, J.; Liu, P.; López, J. G.; Houk, K. N.; Grubbs, R. H. *J. Am. Chem. Soc.* **2016**, *138*, 1394–1405.
DOI: 10.1021/jacs.5b12277.
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L.E.R. participated in the conception of the project, evaluated the catalysts in ROMP reactions, prepared and analyzed the data, and participated in the writing of the manuscript.

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Chapter 1

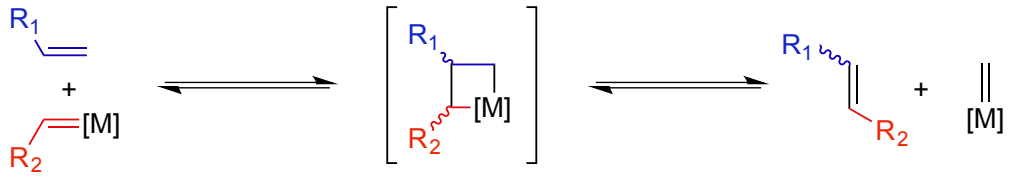
Introduction to *Z*-Selective Cyclometalated Ruthenium Metathesis Catalysts

Adapted in part from:
Marx, V. M.; Rosebrugh, L. E.; Herbert, M. B.; Grubbs, R. H. *Top. Organomet. Chem.* **2014**, *48*, 1–17.

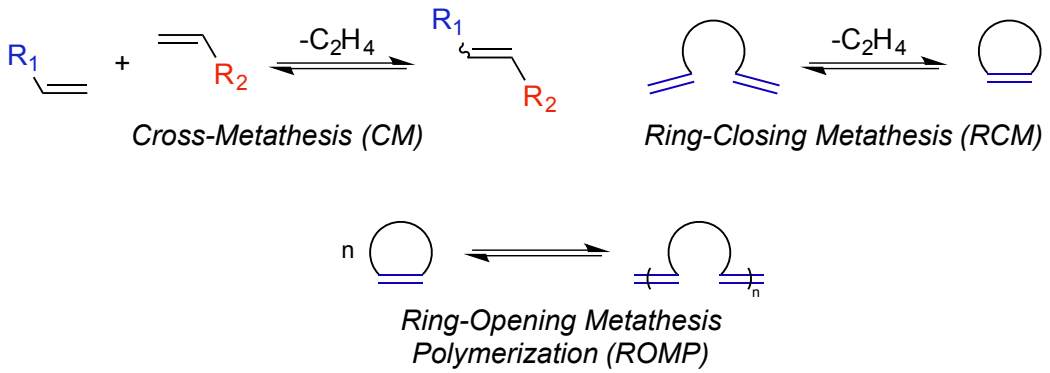
Link to article: 10.1007/3418_2014_76

Introduction

Over the past half-century, olefin metathesis has emerged as an indispensable methodology for the construction of new carbon–carbon bonds.[1] The olefin metathesis reaction proceeds via the [2 + 2] addition of an alkene substrate to a metal alkylidene, forming a metallacyclobutane intermediate that can collapse in a productive fashion to afford a new olefinic product (Scheme 1.1). This reaction is incredibly versatile due to the wide variety of olefins that can be employed in or generated via metathesis; for example, two terminal olefins can undergo an intermolecular reaction to form a new internal alkene product in a process known as cross-metathesis (CM), while α,ω-dienes can react in an intramolecular fashion to yield cyclic olefins via ring-closing metathesis (RCM) (Scheme 1.2). Furthermore, polymeric olefins can be produced by the ring-opening metathesis polymerization (ROMP) of strained, mono- or polycyclic olefins. CM, RCM, and ROMP represent the three main classes of olefin metathesis reactions.



Scheme 1.1. Mechanism of olefin metathesis.



Scheme 1.2. General schemes for common metathesis reactions.

Seminal work in the 1970s identified early transition metal carbene complexes as proficient olefin metathesis catalysts.[2] This initial discovery led to the development of a number of well-defined systems that allowed for thorough mechanistic investigations, including elucidation of the factors affecting catalyst activity and selectivity. Capitalizing on these results, present-day olefin metathesis catalysts are straightforward to employ, air- and moisture-tolerant, and highly active across a broad range of olefin substrates. Furthermore, through judicious choice of metal and ligands, these catalysts can be readily tailored to specific applications or classes of substrates, and many of these systems are now either readily accessible or commercially available. As a result, olefin metathesis has been employed with great success in a number of fields, including biochemistry,[3] polymer and materials science,[4] and natural product synthesis.[5]

Due to the reversible nature of the olefin metathesis reaction, however, an ongoing challenge in the field has been the control of stereoselectivity.[6] At high

conversions, the product distribution generally reflects the thermodynamic energy differences between olefin isomers, resulting in the predominant formation of *E*-olefins (ca. 80-90% *E*-selectivity). Many relevant natural products and pharmaceutical targets, on the other hand, contain functionality derived from *Z*-olefins. Moreover, the activity and properties of such molecules often depend heavily on the alkene geometry and can be adversely affected by even minute amounts of stereoisomeric impurities. While mixtures of *E*- and *Z*-isomers may be separated by chromatography or crystallizations, this often requires extensive optimization for each substrate and is not economical; additionally, purification is not possible in polymeric olefins containing both *E* and *Z* double bonds. Thus, it is highly desirable to develop catalyst systems that are not only kinetically selective for the formation of *Z*-olefins, but that are also capable of producing *stereopure* *Z*- or *E*-olefins. While indirect methods have been developed, including alkyne metathesis followed by highly *Z*-selective semireduction[7] and substrate-controlled macrocyclic-RCM of vinylsiloxanes followed by desilylation, the scope of these transformations is limited.[8]

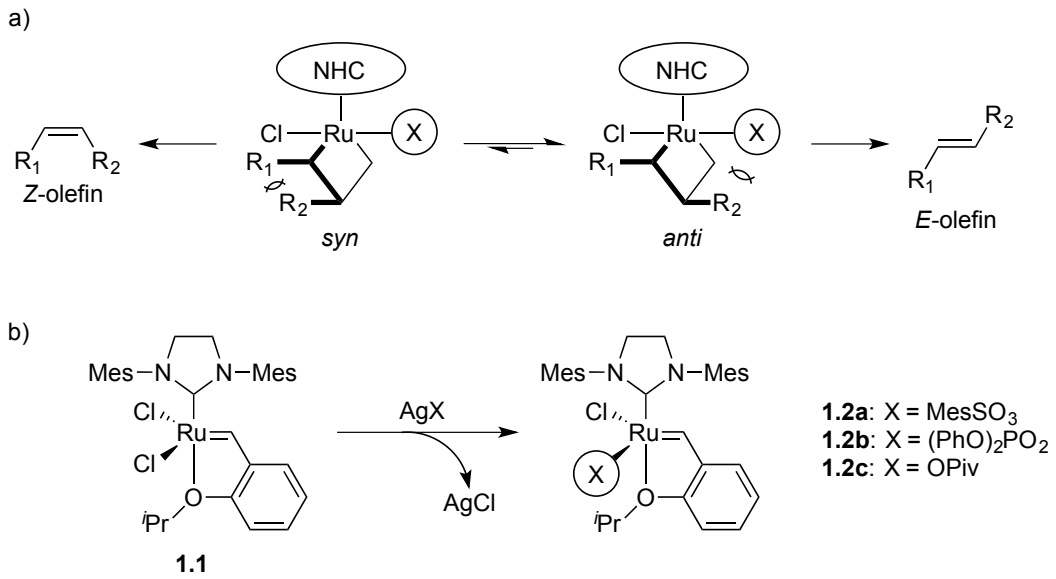
Considerable effort has therefore been dedicated to the search for metathesis catalysts exhibiting kinetic selectivity for the formation of *Z*-olefins. Consequently, the Schrock and Hoveyda groups recently developed the first *Z*-selective metathesis catalysts using molybdenum and tungsten,[9] a groundbreaking development allowing for the effective synthesis essentially pure *Z*-olefins via metathesis for the first time. Efforts to develop comparable ruthenium-based systems have resulted in the discovery of a number of highly *Z*-selective catalysts,[10,11] including the class of cyclometalated ruthenium metathesis catalysts described in detail below. Many of these systems exhibit consistently

high levels of activity and selectivity across a broad range of substrates and transformations, thus providing synthetic chemists with the ability to tackle a wide range of challenging and high-value targets derived from *Z*-olefins.

Development of *Z*-Selective Ruthenium Metathesis Catalysts

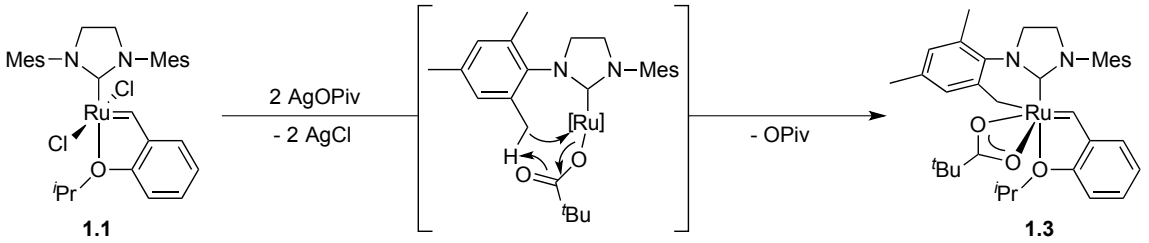
Original Strategy for the Design of Z-Selective Ruthenium Alkylidenes

Kinetic selectivity for *Z*-olefins results from the preferential formation of *syn*-metallacyclobutanes, in which the olefin substituents are on the same side of the metallacycle, following olefin binding (*anti*-metallacycles are those in which the substituents are positioned on *opposite* sides of the metallacycle). Cycloreversion of a *syn*-metallacycle produces *Z*-olefins; *anti*-metallacycles generate *E*-olefins. Importantly, for many ruthenacyclobutanes, such as those formed by prior generation *N*-heterocyclic carbene (NHC)-substituted metathesis catalyst **1.1** (Scheme 1.3b), the metallacycle is "bottom-bound," meaning that it is positioned opposite the NHC ligand in the equatorial plane, while the chloride ligands are located in apical positions (Scheme 1.3a).[12] As a result, initial attempts at synthesizing a *Z*-selective Ru-based catalyst focused on replacing one chloride ligand of **1.1** with a bulkier sulfonate (**1.2a**), phosphonate (**1.2b**), or carboxylate ligand (**1.2c**), anionic ligands which could be expected to experience significant steric interactions with *anti*-metallacycles (Scheme 1.3b).[13] This could, in turn, potentially increase preference for the formation of *syn*-metallacycles and thus *Z*-olefins (Scheme 1.3a).



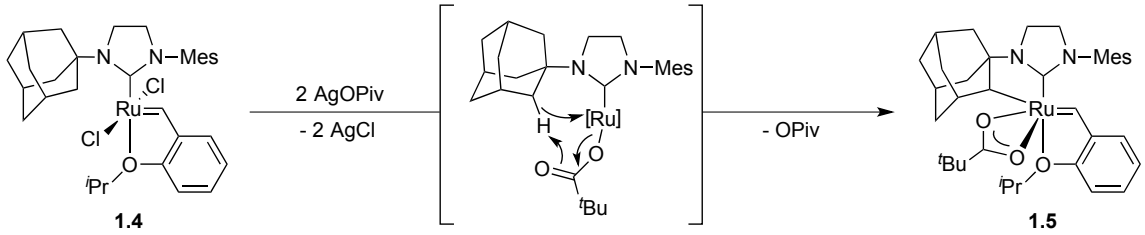
Scheme 1.3. (a) Proposed steric interactions for bottom-bound ruthenacycles. (b) Preparation of *Z*-selective ruthenium metathesis catalysts **1.2a–1.2c** with large X-type ligands. Mes = 2,4,6-trimethylphenyl.

Complexes **1.2a** and **1.2b** did exhibit slightly increased *Z*-selectivity relative to **1.1** but were still overall selective for the formation of *E*-olefins. (It was eventually discovered, however, that employing a sterically hindered 2,4,6-triphenyl-thiophenol ligand in place of one chloride ligand yielded a moderately *Z*-selective catalyst).[11a] Computational models predicted that the use of an anionic pivalate ligand, such as in **1.2c**, might dramatically increase *Z*-selectivity. Attempts to synthesize catalyst **1.2c** from **1.1** using silver pivalate (AgOPiv), however, did not lead to the formation of the desired mono-substituted product; instead, di-substitution of the chlorides by pivalate ligands followed by a carboxylate-assisted C–H bond insertion generated cyclometalated complex **1.3** (Scheme 1.4).[14] Notably, this marked the first time a cyclometalated ruthenium-based complex was isolated in which the ruthenium alkylidene remained intact (previously reported examples of cyclometalated complexes were the result of decomposition processes and were found to be metathesis inactive).[15]



Scheme 1.4. Mechanism of carboxylate-driven C–H bond insertion to form catalyst **1.3**. Mes = 2,4,6-trimethylphenyl.

Initial studies with catalyst **1.3** revealed unprecedented *Z*-selectivity (41% *Z*) in the standard CM reaction of allylbenzene and *cis*-1,4-diacetoxybutene.[14] It was proposed that increasing the steric bulk of the non-cyclometalated substituent on the NHC might result in a more *Z*-selective catalyst; accordingly, activation of **1.4** containing a bulky *N*-adamantyl group was attempted using AgOPiv (Scheme 1.5). In the resulting cyclometalated catalyst **1.5**, however, the C–H activated substituent was not the *N*-mesityl group as anticipated but rather the *N*-adamantyl group. While this result was initially unexpected, it could be explained by the relatively short distance (2.80 Å) between the C12 carbon of the adamantyl group and Ru, which resulted in rapid C–H activation to form the adamantyl chelate. Unlike the air- and moisture-stable, dark green complex **1.1**, catalyst **1.5** was isolated as an air-sensitive, bright purple solid. Remarkably, the new cyclometalated catalyst **1.5** was found to be highly *Z*-selective (91% *Z*) in the CM of allylbenzene and *cis*-1,4-diacetoxybutene. Despite its promising selectivity, however, catalyst **1.5** exhibited a maximum of only 50 turnovers.



Scheme 1.5. Preparation of cyclometalated ruthenium catalyst **1.5**. Mes = 2,4,6-trimethylphenyl.

Model for Z-Selectivity in Cyclometalated Ruthenium Complexes

To better understand the mechanism and origins of *Z*-selectivity in cyclometalated ruthenium systems, catalysts **1.3** and **1.5** were studied using computational methods.[16] In contrast to the bottom-bound metallacycles (**1.6**) observed with catalyst **1.1** and prior generations of ruthenium metathesis catalysts, computational studies suggest that **1.3** and **1.5** adopt "side-bound" ruthenacycles (**1.7**) (Figure 1.1). This is thought to be the result of two factors: (1) a side-bound conformation avoids significant steric interactions that are present between the *N*-adamantyl group and a bottom-bound metallacycle, and (2) the side-bound conformation is electronically stabilized relative to the bottom-bound conformation. Namely, while the bottom-bound conformation requires back-donation from the same ruthenium d-orbital that back-donates into the NHC, a separate metal d-orbital is available for back-donation into the side-bound metallacycle.[16a]

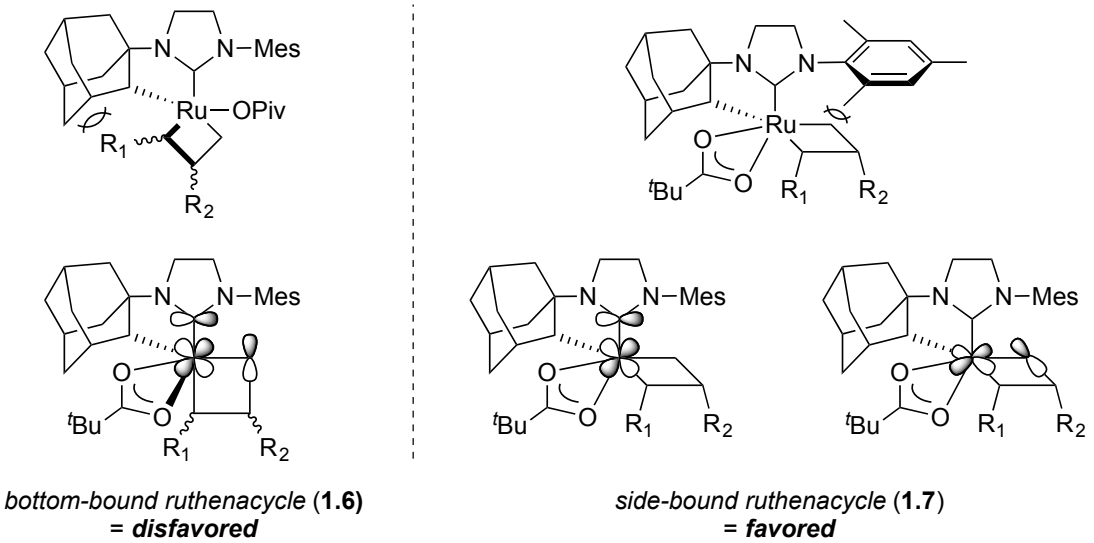
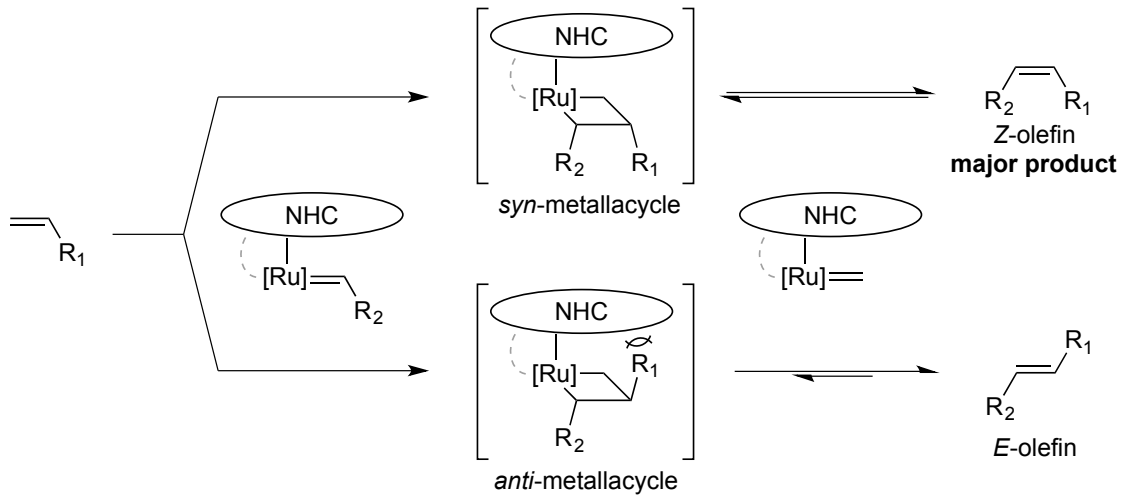


Figure 1.1. Comparison of the proposed steric and electronic interactions for side- and bottom-bound ruthenacycles. Mes = 2,4,6-trimethylphenyl.

Significantly, the adoption of the side-bound conformation **1.7** in catalysts **1.3** and **1.5** places the metallacycle directly below the *N*-aryl substituent of the NHC. As a result, it is proposed that *syn*-metallacycles (leading to the formation of *Z*-olefins) would form in preference to *anti*-metallacycles (leading to the formation of *E*-olefins), as the latter would presumably experience substantial steric interactions with the *N*-aryl substituent (Scheme 1.6). Indeed, *anti*-metallacycles derived from catalyst **1.5** have been computed to be much higher in energy than their *syn* counterparts.[16,17] Moreover, the congested steric environment about the alkylidene further discourages the formation of trisubstituted metallacycles, which in turn is hypothesized to slow the rate of *Z*-degradation caused by secondary metathesis events in cyclometalated systems. This property, combined with the inherent kinetic selectivity for *Z*-olefins in catalysts **1.3** and **1.5**, ensures that *Z*-selectivity remains high even at high conversions.[17]

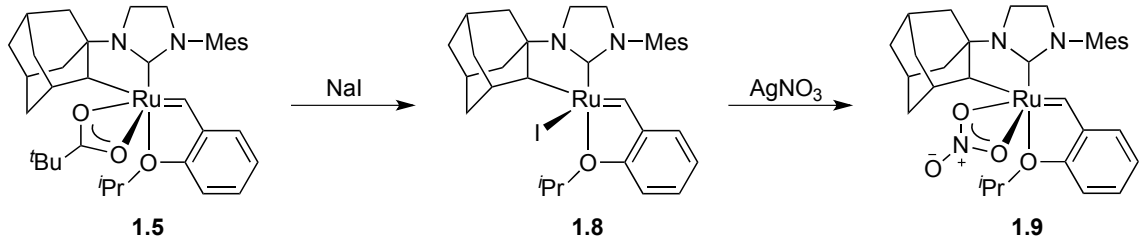


Scheme 1.6. Origins of *Z*-selectivity in cyclometalated ruthenium metathesis catalysts.

Evolution of Cyclometalated Ruthenium Complexes

Encouraged by the promising *Z*-selectivity observed with catalyst **1.5** in preliminary metathesis assays,[14,18] the syntheses of a variety of new cyclometalated complexes were attempted. Efforts focused specifically on the design of more active and *Z*-selective catalysts through the variation of three key structural elements of the catalyst: the X-type ligand, the chelate, and the *N*-aryl group.

It was determined that the most straightforward way to synthesize and assay a large number of new cyclometalated catalysts would be through variation of the X-type ligand.[19] Unfortunately, only carboxylate-type ligands were shown to be capable of inducing C–H activation. As a workaround, catalysts with monodentate (κ^1) ligands such as iodo-complex **1.8** were prepared by the treatment of catalyst **1.5** with sodium or potassium salts (Scheme 1.7). Catalyst **1.8** could in turn undergo transmetallation with a variety of silver (I) salts to give stable chelated species with new anionic, bidentate (κ^2) ligands, such as nitrato-complex **1.9**. Other new cyclometalated systems containing mono- or bidentate ligands (catalysts **1.10–1.12**) are shown in Figure 1.2.



Scheme 1.7. Preparation of mono- and bidentate cyclometalated catalysts. Mes = 2,4,6-trimethylphenyl.

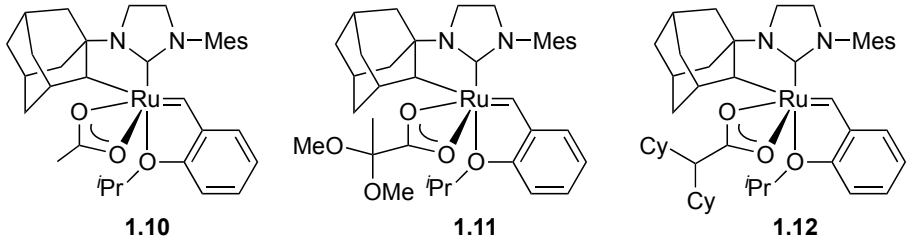


Figure 1.2. Cyclometalated ruthenium metathesis catalysts **1.10–1.12**. Mes = 2,4,6-trimethylphenyl.

Of the newly synthesized derivatives, nitrate-substituted catalyst **1.9** was found to be the highest performing, catalyzing a variety of CM reactions with near 1000 turnovers and ca. 90% *Z*-selectivity across the board.[19] Additionally, **1.9** produced highly *cis* polynorbornenes and norbornadienes (up to >95% *cis*);[20] however, the polymers were not highly tactic, a result in line with prior generation Ru-based metathesis catalysts. In contrast to pivalate-substituted catalyst **1.5** that decomposed in solution within 2 h upon exposure to air, complex **1.9** exhibited significantly improved stability, remaining active in solution for up to 12 h. Furthermore, **1.9** was found to be air- and moisture-stable in the solid-state for a minimum of 10 days.[19]

Following the discovery of the superior stability and activity afforded by the nitrate ligand, a number of derivatives of **1.9** containing different *N*-aryl groups were targeted.[19] Alterations to the *para*-substituent of the *N*-aryl group were found to have a limited effect on activity and selectivity: catalysts **1.13** and **1.14**, containing a *p*-chloro

and *p*-methoxy group, respectively, displayed similar metathesis activity to catalyst **1.9** (Figure 1.3). Similarly, installation of an *N*-2,6-diethylphenyl group (**1.15**) resulted in minimal change in reactivity relative to catalyst **1.9**.

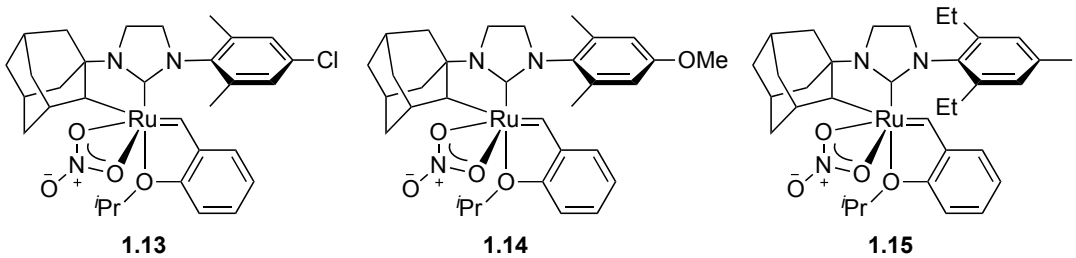


Figure 1.3. Cyclometalated ruthenium metathesis catalysts **1.13–1.15**.

Computational data suggested that further increasing the bulk of the *ortho*-substituents on the *N*-aryl group might result in enhanced *Z*-selectivity. Unfortunately, however, it appeared that only subtle steric and electronic modifications of the *N*-aryl group were possible when using AgOPiv, as attempts to C–H activate a precursor complex bearing an *N*-2,6-diisopropylphenyl (DIPP) group resulted in the formation and eventual decomposition of a metastable complex.[21] Similar results were observed when significant modifications to the cyclometalated group were attempted. As such, an alternative method to access new cyclometalated *Z*-selective catalysts was highly desired.

In this dissertation, a milder method to effect the salt metathesis and C–H activation of cyclometalated ruthenium metathesis catalysts using sodium carboxylates in place of silver (I) carboxylates is presented. As a result of this advance, a variety of new catalyst architectures were synthesized and studied. *Chapter 2* describes the development of this new approach and its application to the synthesis of the most active, *Z*-selective cyclometalated ruthenium complexes to date, including the previously inaccessible *N*-DIPP-*N*-adamantyl complex described above. *Chapter 3* is composed of two sections: the

first details the synthesis of a series of cyclometalated initiators displaying unprecedented activity and selectivity in ROMP, and the second comprises a detailed mechanistic study of these new complexes and prior cyclometalated systems in stereoselective ROMP. Work in this chapter was performed in conjunction with the Houk group at UCLA, who performed computational studies that were essential to the development of a complete mechanistic picture.

References

1. (a) Fürstner, A. *Angew. Chem., Int. Ed.* **2000**, *39*, 3013. (b) Trnka, T. M., Grubbs, R. H. *Acc. Chem. Res.* **2001**, *34*, 18. (c) Schrock, R. R. *Chem. Rev.* **2002**, *102*, 145. (d) Schrock, R. R.; Hoveyda, A. H. *Angew. Chem., Int. Ed.* **2003**, *42*, 4592. (e) Grubbs, R. H., Ed. *Handbook of Metathesis*; Wiley-VCH: Weinheim, Germany, 2003. (f) Nicolaou, K. C.; Bulger, P. G.; Sarlah, D. *Angew. Chem., Int. Ed.* **2005**, *44*, 4490. (g) Samojlowicz, C.; Bieniek, M.; Grela, K. *Chem. Rev.* **2009**, *109*, 3708. (h) Vougioukalakis, G.; Grubbs, R. H. *Chem. Rev.* **2010**, *110*, 1746. (i) Lozano-Vila, A. M.; Monsaert, S.; Bajek, A.; Verpoort, F. *Chem. Rev.* **2010**, *110*, 4865. (j) Cossy, J.; Arseniyadia, S.; Meyer, C., Eds. *Metathesis in Natural Product Synthesis: Strategies, Substrates, and Catalysts*; Wiley-VCH: Weinheim, Germany, 2010.

2. (a) Hérisson, J.-L.; Chauvin, Y. *Makromol. Chem.* **1970**, *141*, 161. (b) Casey, C. P.; Burkhardt, T. J. *J. Am. Chem. Soc.* **1974**, *96*, 7808. (c) Katz, T. J.; McGinnis, J. *J. Am. Chem. Soc.* **1975**, *97*, 1592. (d) Grubbs, R. H.; Burk, P. L.; Carr, D. D. *J. Am. Chem. Soc.* **1975**, *97*, 3265.

3. Binder, J. B.; Raines, R. T. *Curr. Opin. Chem. Biol.* **2008**, *12*, 767.

4. (a) Leitgeb, A.; Wappel, J.; Slugovc, C. *Polymer* **2010**, *51*, 2927. (b) Sutthasupa, S.; Shiotsuki, M.; Sanda, F. *Polym. J.* **2010**, *42*, 905.

5. Cossy, J.; Arseniyadis, S.; Meyer, C., Eds. *Metathesis in Natural Product Synthesis: Strategies, Substrates, and Catalysts*, 1st ed.; Wiley-VCH: Weinhein, Germany, 2010.

6. (a) Gottumukkala, A. L.; Madduri, A. V. R.; Minnaard, A. J. *ChemCatChem.* **2012**, *4*, 462. (b) Fürstner, A. *Science* **2013**, *341*, 1357. (c) Shahane, S.; Bruneau, C.; Fischmeister, C. *ChemCatChem.* **2013**, *5*, 3436.

7. (a) Fürstner, A.; Davies, P. W. *Chem. Commun.* **2005**, 2307. (b) Zhang, W.; Moore, J. S. *Adv. Synth. Catal.* **2007**, *349*, 93.

8. (a) Wang, Y.; Jimenez, M.; Hansen, A. S.; Raiber, E.-A.; Schreiber, S. L.; Young, D. W. *J. Am. Chem. Soc.* **2011**, *133*, 9196. (b) Fürstner, A.; Gallenkamp, D. *J. Am. Chem. Soc.* **2011**, *133*, 9232.

9. (a) Flook, M. M.; Jiang, A. J.; Schrock, R. R.; Müller, P.; Hoveyda, A. H. *J. Am. Chem. Soc.* **2009**, *131*, 7962. (b) Ibrahem, I.; Yu, M.; Schrock, R. R.; Hoveyda, A. H. *J. Am. Chem. Soc.* **2009**, *131*, 3844. (c) Jiang, A. J.; Zhao, Y.; Schrock, R. R.; Hoveyda, A. H. *J. Am. Chem. Soc.* **2009**, *131*, 16630. (d) Meek, S. J.; O'Brien, R. V.; Llaveria, J.; Schrock, R. R.; Hoveyda, A. H. *J. Am. Chem. Soc.* **2011**, *133*, 11512. (e) Marinescu, S. C.; Levine, D. S.; Zhao, Y.; Schrock, R. R.; Hoveyda, A. H. *J. Am. Chem. Soc.* **2011**, *133*, 11512. (f) Peryshkov, D. V.; Schrock, R. R.; Takase, M. K.; Müller, P.; Hoveyda, A. H. *J. Am. Chem. Soc.* **2011**, *133*, 20754. (g) Marinescu, S. C.; Schrock, R. R.; Müller, P.; Takase, M. K.; Hoveyda, A. H. *Organometallics*, **2011**, *30*, 1780. (h) Flook, M. M.; Ng, V. W. L.; Schrock, R. R. *J. Am. Chem. Soc.* **2011**, *133*, 1784. (i) Yu, M.; Wang, C.; Kyle, A. F.; Jakubec, P.; Dixon, D. J.; Schrock, R. R.; Hoveyda, A. H. *Nature* **2011**, *479*, 88. (j) Yu, M.; Ibrahem, I.; Hasegawa, M.; Schrock, R. R.; Hoveyda, A. H. *J. Am. Chem. Soc.* **2012**, *134*, 2788. (k) Townsend, E. M.; Schrock, R. R.; Hoveyda, A. H. *J. Am. Chem. Soc.* **2012**, *134*, 11334. (l) Wang, C.; Yu, M.; Kyle, A. F.; Jakubec, P.; Dixon, D. J.; Schrock, R. R.; Hoveyda, A. H. *Chem. Eur. J.* **2013**, *19*, 2726. (m) Keisewetter, E. T.; O'Brien, R. V.; Yu, E. C.; Meek, S. J.; Schrock, R. R.; Hoveyda, A. H. *J. Am. Chem. Soc.* **2013**, *135*, 6026. (n) Wang, C.; Haeffner, R. R.; Schrock, R. R.; Hoveyda, A. H. *Angew. Chem., Int. Ed.* **2013**, *52*, 1939. (o) Yuan, J.; Schrock, R. R.; Gerber, L. C. H.; Müller, P.; Smith, S. *Organometallics* **2013**, *32*, 2983. (p) Mann, T. J.; Speed, A. W. H.; Schrock, R. R.; Hoveyda, A. H. *Angew. Chem., Int. Ed.* **2013**, *32*, 2983.

10. (a) Khan, R. K. M.; O'Brien, R. V.; Torker, S.; Li, B.; Hoveyda, A. H. *J. Am. Chem. Soc.* **2012**, *134*, 12774. (b) Khan, R. K. M.; Zhugralin, A. R.; Torker, S.; O'Brien, R. V.; Lombardi, P. J.; Hoveyda, A. H. *J. Am. Chem. Soc.* **2012**, *134*, 12438. (c) Khan, R. K. M.; Torker, S.; Hoveyda, A. H. *J. Am. Chem. Soc.* **2013**, *135*, 10258. (d) Koh, M. J.; Khan, R. K. M.; Torker, S.; Hoveyda, A. H. *Angew. Chem., Int. Ed.* **2014**, *53*, 1968. (e) Torker, S.; Khan, R. K. M.; Hoveyda, A. H. *J. Am. Chem. Soc.* **2014**, *136*, 3439. (f) Khan, R. K. M.; Torker, S.; Hoveyda, A. H. *J. Am. Chem. Soc.* **2014**, *136*, 14337. (g) Koh, M. J.; Khan, R. K. M.; Torker, S.; Yu, M.; Mikus, M. S.; Hoveyda, A. H. *Nature* **2015**, *517*, 181. (h) Mikus, M. S.; Torker, S.; Hoveyda, A. H. *Angew. Chem., Int. Ed.* **2016**, *55*, 4997.

11. (a) Occhipinti, G.; Hansen, F. R.; Törnroos, K. W.; Jensen, V. R. *J. Am. Chem. Soc.* **2013**, *135*, 3331. (b) Nelson, J. W.; Grundy, L. M.; Dang, Y.; Wang, Z.-X.; Wang, X. *Organometallics* **2014**, *33*, 4290. (c) Smit, W.; Koudriavtsev, V.; Occhipinti, G.; Törnroos, K. W.; Jensen, V. R. *Organometallics* **2016**, *35*, 1825.

12. (a) Romero, P. E.; Piers, W. E.; McDonald, R. *Angew. Chem., Int. Ed.* **2004**, *43*, 6161. (b) Wenzel, A. G.; Grubbs, R. H. *J. Am. Chem. Soc.* **2006**, *128*, 16048. (c) Romero, P. E.; Piers, W. E. *J. Am. Chem. Soc.* **2007**, *129*, 1698. (d) Rowley, C. N.; van der Eide, E. F.; Piers, W. E.; Woo, T. K. *Organometallics* **2008**, *27*, 6043. (e) van der Eide, E. F.; Romero, P. E.; Piers, W. E. *J. Am. Chem. Soc.* **2008**, *130*, 4485. (f) Leitao, E. M.; van der Eide, E. F.; Romero, P. E.; Piers, W. E.; McDonald, R. *J. Am. Chem. Soc.* **2010**, *132*, 2784. (g) van der Eide, E. F.; Piers, W. E. *Nat. Chem.* **2010**, *2*, 571. (h) Wenzel, A. G.; Blake, G.; VanderVelde, D. G.; Grubbs, R. H. *J. Am. Chem. Soc.* **2011**, *133*, 6429. (i) Keitz, B. K.; Grubbs, R. H. *J. Am. Chem. Soc.* **2011**, *133*, 16277.

13. Teo, P.; Grubbs, R. H. *Organometallics* **2010**, *29*, 6045.

14. Endo, K.; Grubbs, R. H. *J. Am. Chem. Soc.* **2011**, *133*, 8525.

15. (a) Trnka, T. M.; Morgan, J. P.; Sanford, M. S.; Wilhelm, T. E.; Scholl, M.; Choi, T.-L.; Ding, S.; Day, M. W.; Grubbs, R. H. *J. Am. Chem. Soc.* **2003**, *125*, 2546. (b) Leitao, E. M.; Dubberley, S. R.; Piers, W. E.; Wu, Q.; McDonald, R. *Chem. Eur. J.* **2008**, *14*, 11565.

16. (a) Liu, P.; Xu, X.; Dong, X.; Keitz, B. K.; Herbert, M. B.; Grubbs, R. H.; Houk, K. N. *J. Am. Chem. Soc.* **2012**, *134*, 1464. (b) Dang, Y.; Wang, Z-.X.; Wang, X. *Organometallics* **2012**, *31*, 7222.

17. Miyazaki, H.; Herbert, M. B.; Liu, P.; Dong, X.; Xu, X.; Keitz, B. K.; Ung, T.; Mkrtumyan, G.; Houk, K. N.; Grubbs, R. H. *J. Am. Chem. Soc.* **2013**, *135*, 5848.

18. Keitz, B. K.; Endo, K.; Herbert, M. B.; Grubbs, R. H. *J. Am. Chem. Soc.* **2011**, *133*, 9686.

19. Keitz, B. K.; Endo, K.; Patel, P. R.; Herbert, M. B.; Grubbs, R. H. *J. Am. Chem. Soc.* **2012**, *134*, 693.

20. Keitz, B. K.; Federov, A.; Grubbs, R. H. *J. Am. Chem. Soc.* **2012**, *134*, 2040.

21. Herbert, M. B.; Lan, Y.; Keitz, B. K.; Liu, P.; Endo, K.; Day, M. W.; Houk, K. N.; Grubbs, R. H. *J. Am. Chem. Soc.* **2012**, *134*, 7861.

Chapter 2

Synthesis and Activity of New *Z*-Selective Cyclometalated Ruthenium Metathesis Catalysts

Adapted from:
Rosebrugh, L. E.; Herbert, M. B.; Marx, V. M.; Keitz, B. K.; Grubbs, R. H. *J. Am. Chem. Soc.* **2013**, *134*, 1276–1279.

Link to article: 10.1021/ja311916m

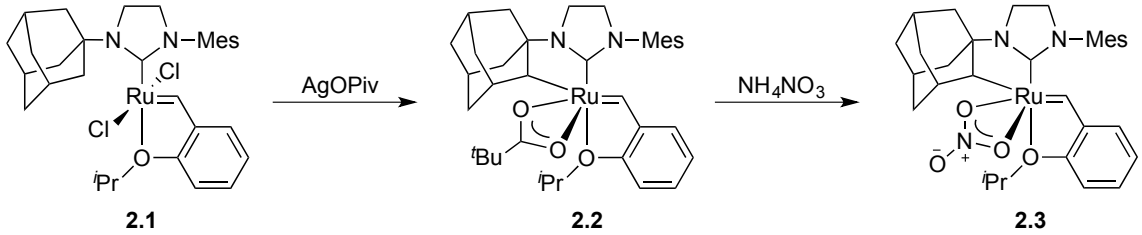
Abstract

A novel cyclometalated ruthenium-based metathesis catalyst bearing an *N*-2,6-diisopropylphenyl group was synthesized and subsequently shown to give near-perfect selectivity for the *Z*-olefin (>95% in most cases), as well as unparalleled TONs of up to 7400, in a variety of homodimerization and industrially relevant metathesis reactions. This derivative and other new catalytically active species were synthesized using an improved method employing sodium carboxylates to induce the salt metathesis and C–H activation of these cyclometalated complexes. All of these new ruthenium-based catalysts were highly *Z*-selective in the homodimerization of terminal olefins.

Introduction

As described in *Chapter 1*, a persistent challenge in olefin metathesis reactions is the control of stereoselectivity, as metathesis catalysts generally favor formation of the thermodynamically preferred *E*-olefin.[1] Recently, the synthesis and activity of the first examples of ruthenium-based *Z*-selective metathesis catalysts (**2.2**, **2.3**) containing a

cyclometalated *N*-heterocyclic carbene (NHC) ligand were reported.[2] The Ru-adamantyl bond is formed via an intramolecular C–H activation induced by the addition of silver pivalate (AgOPiv) (Scheme 2.1). Prior to the work outlined in this chapter, nitrato-catalyst **2.3** was the best *Z*-selective ruthenium-based metathesis catalyst, with turnover number (TONs) approaching 1000 and *Z*-selectivity on average around 90%. This catalyst has been shown to be effective for the synthesis of homo- and hetero-cross-products, highly *cis* polymers, and a variety of insect pheromones and macrocyclic musks.[2c,3]



Scheme 2.1. Synthetic route to previously reported C–H activated metathesis catalysts **2.2** and **2.3**. Mes = 2,4,6-trimethylphenyl.

Inspired by computational data, we hypothesized that increasing the steric bulk of the *N*-aryl group of **2.3** would further destabilize the *E*-selective transition state, thereby enhancing *Z*-selectivity.[4] However, as mentioned in *Chapter 1*, previous attempts to make significant alterations to the NHC substituents, both to the cyclometalated group and to the *N*-aryl group, generally resulted in decomposition upon exposure to AgOPiv.[5] In order to access stable cyclometalated species with various modifications to the NHC substituents, we sought to develop a milder approach to form this ruthenium–carbon bond. In this chapter, an improved method to induce the salt metathesis and C–H activation of ruthenium alkylidene complexes employing mild and economically viable sodium carboxylates is described, and the superior activity and selectivity of several new

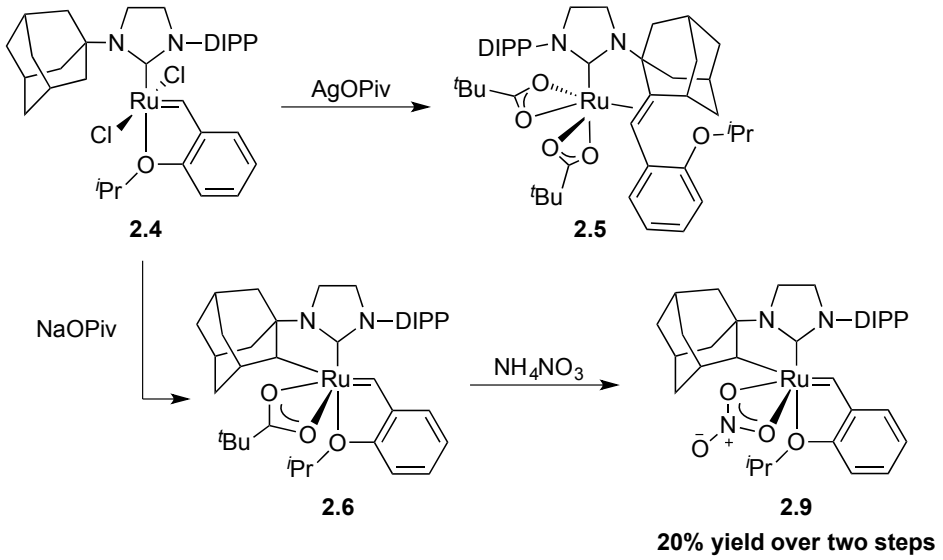
cyclometalated metathesis-active catalysts are explored. Through the use of this improved approach, we have uncovered the highly active catalyst **2.9**, which gives on average >95% *Z*-selectivity and TONs up to 7400 in the homodimerization of terminal olefin substrates. Significantly, this represents a near tenfold increase in activity relative to nitrato-catalyst **2.3**. Moreover, **2.9** meets or exceeds TONs reported for the most active *Z*-selective molybdenum- and tungsten-based systems in similar metathesis reactions.[6]

Results and Discussion

We initiated our studies by first employing sodium pivalate (NaOPiv) in place of AgOPiv during the C–H activation step. It was discovered that exposing the unactivated dichloride catalyst **2.1** to excess NaOPiv in a 1:1 mixture of THF and MeOH resulted in the clean formation of the desired cyclometalated catalyst **2.2** after heating at 40 °C for 6 h; this complex could then be converted to the nitrato-form (**2.3**) in 60% overall yield through the addition of excess ammonium nitrate. In comparison, the two-step synthesis of **2.3** using AgOPiv proceeds in 48% yield. It was additionally found that other sodium carboxylates could be used to effect the salt metathesis and C–H activation steps: Reaction of **2.1** with excess sodium acetate also resulted in complete conversion to **2.2**, although the C–H activation failed to reach full conversion with some of the catalysts described later in this chapter. Reducing the steric bulk of the carboxylate even further by employing sodium formate or sodium bicarbonate in the C–H activation of **2.1** resulted in no discernable conversion to the desired cyclometalated product.

In order to explore the utility and mildness of this new approach, we revisited a number of ruthenium complexes containing a variety of *N*-aryl and *N*-carbocyclic groups

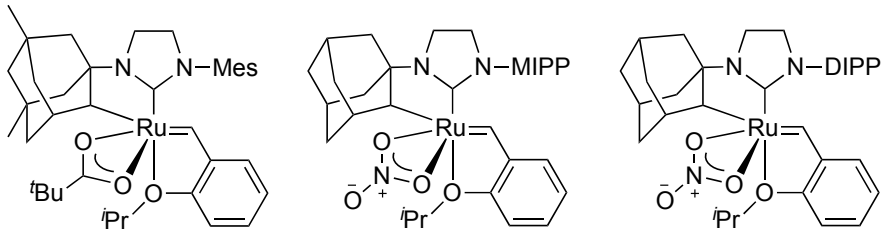
that had decomposed when exposed to AgOPiv. As described in *Chapter 1*, attempts to replace the *N*-mesityl group of **2.3** with a bulkier *N*-2,6-diisopropylphenyl (DIPP) group, as in **2.4**, had resulted in substantial decomposition to **2.5** during the C–H activation step. Using NaOPiv, however, we were able to cleanly form the stable *N*-adamantyl-*N*-DIPP pivalate precursor (**2.6**) of catalyst **2.9** (Scheme 2.2).



Scheme 2.2. Decomposition and C–H activation pathways of precatalyst **2.4**. DIPP = 2,6-diisopropylphenyl.

We were also able to generate C–H activated *N*-3,5-dimethyladamantyl-*N*-mesityl (**2.7**) and *N*-adamantyl-*N*-2,6-methylisopropylphenyl (MIPP) (**2.8**) derivatives via this improved method. More extreme alterations to the chelating group, however, including exchanging the *N*-adamantane for an *N*-cyclohexyl or *N*-1-methylcyclohexyl group, resulted in the formation of cyclometalated catalysts that were inherently unstable. When these reactions were monitored by ^{1}H NMR spectroscopy, these complexes were seen to either decompose immediately to a ruthenium hydride species upon introduction of NaOPiv or form a metastable activated complex that was unisolable without noticeable decomposition.

Complexes observed to form a stable cyclometalated architecture were subsequently converted to the nitrato-form via ligand exchange with the pivalate group (Scheme 2.2), as past experience with catalyst **2.3** suggested that the nitrato-complexes would likely be more stable and show increased activity.[2c] However, while this was the case for complexes possessing a cyclometalated *N*-adamantyl group (complex **2.6** and the pivalate analogue of catalyst **2.8** were isolated and assayed to confirm this), catalyst **2.7** was more stable and easier to isolate in the pivalate-substituted form. Catalysts successfully synthesized using the NaOPiv method are depicted in Figure 2.1.



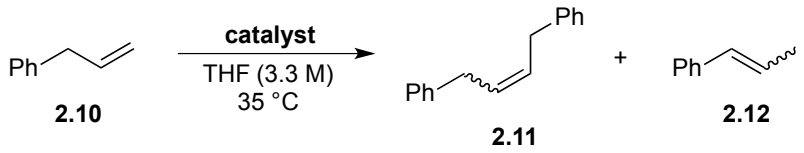
2.7 **2.8** **2.9**

Figure 2.1. Catalysts **2.7–2.9**: Mes = 2,4,6-trimethylphenyl (**2.7**); MIPP = 2,6-methylisopropylphenyl (**2.8**); DIPP = 2,6-diisopropylphenyl (**2.9**).

In order to analyze the efficacy of these new complexes for metathesis, we first evaluated their performance in the homodimerization of allylbenzene (**2.10**, see Table 2.1). While a relatively facile substrate for homodimerization, allylbenzene is also prone to olefin isomerization to form **2.12**. Importantly, the extent of this side reaction depends heavily on the identity and stability of the catalyst, making **2.10** a good benchmark substrate.[7] Homodimerization reactions were generally run in THF at 35 °C with a high substrate concentration (3.3 M in **2.10**) and a catalyst loading varying between 0.1 and 2 mol %. Catalyst **2.8** was not soluble in THF, however; thus, all reactions using **2.8** were run in 1,2-dichloroethane (DCE). Experimentation with catalyst **2.9** demonstrated that using DCE in place of THF provided analogous results (see Table 2.2). For the

homocoupling of **2.10**, excellent conversions and near-perfect *Z*-selectivities (96-98%) were seen by ^{1}H NMR spectroscopy when using catalysts **2.7–2.9**, with **2.8** and **2.9** being the most selective for the homodimer **2.11** over the olefin isomerization product **2.12**.

Table 2.1. Homodimerization of Allylbenzene (2.10)



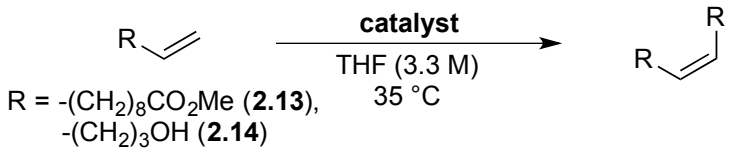
catalyst	loading, mol %	time, h	conv, %[a]	*Z*-**2.11**, %[a]	**2.11/2.12**[a]
2.7	2	1.5	94	96	16.6
2.8[b]	0.1	2	78	98	50
2.9	0.1	2	96	98	50

[a]Determined by ^{1}H NMR spectroscopy. [b]DCE was used in place of THF.

In order to differentiate between these very active catalysts, we turned to two more challenging homodimerization substrates, methyl 10-undecenoate (**2.13**) and the primary alcohol 4-pentenol (**2.14**), the latter of which has been indirectly implicated in the decomposition of previous generations of ruthenium metathesis catalysts.[8] Reactions were run utilizing the standard conditions described previously. Of the three catalysts, **2.9** gave the best results (see Table 2.2), providing the homodimerization products in high conversions (97% and 77% for **2.13** and **2.14**, respectively) with 98% *Z*-selectivity for both substrates. Catalyst **2.8** also demonstrated excellent selectivity (97% and 99% *Z* for **2.13** and **2.14**, respectively) but low conversions, particularly in the homodimerization of **2.14** (7%). The almost exclusive selectivity for the *Z*-olefin observed with **2.8** and **2.9** is likely a result of the steric bulk of the *N*-MIPP or *N*-DIPP group positioned over the alkylidene, which ensures that any approach of the terminal olefin in a manner that would produce an *E*-olefin is extremely disfavored.[4] Previously, the homodimer of **2.14** was

isolated in 67% yield with only 81% selectivity for the *Z*-olefin using catalyst **2.3**; thus, the development of **2.9** represents a significant improvement in the field of ruthenium-mediated *Z*-selective metathesis.

Table 2.2. Homodimerization of 10-Methyl Undecenoate (2.13) and 4-Pentenol (2.14)

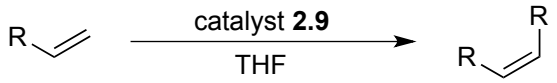


substrate	catalyst	loading, mol %	time, h	conv, %[a]	*Z*, %[a]
2.13	**2.7**	2	3	77	91
	2.8[b]	0.1	6	65	97
	2.9	0.1	6	97	98
2.14	**2.7**	2	1.5	83	80
	2.8[b]	0.1	2	7	99
	2.9	0.1	2	77	98
	2.9[b]	0.1	2	79	92

[a]Determined by ^{1}H NMR spectroscopy. [b]DCE was used in place of THF.

In order to further quantify the activity of the highly *Z*-selective catalyst **2.9**, we assayed its performance at room temperature (r.t.) and lower concentration (1 M in substrate). Under these conditions, similar conversions and *Z*-selectivities were observed compared to those recorded under standard conditions, although significantly longer reaction times were necessary. We additionally tested **2.9** at 0.01 mol % and were pleased to discover that it performed exceptionally well, reaching turnover numbers as high as 5800 and 7400 in the homodimerizations of **2.13** and **2.10**, respectively, while maintaining between 96 and >99% *Z*-selectivity in all cases. This is in comparison to previously reported TONs of up to 1000 for catalyst **2.3** in conjunction with ca. 90% *Z*-selectivity.[2c] Finally, isolated yields were obtained for all reactions employing catalyst **2.9**, including those run using the standard conditions, and are reported in Table 2.3.

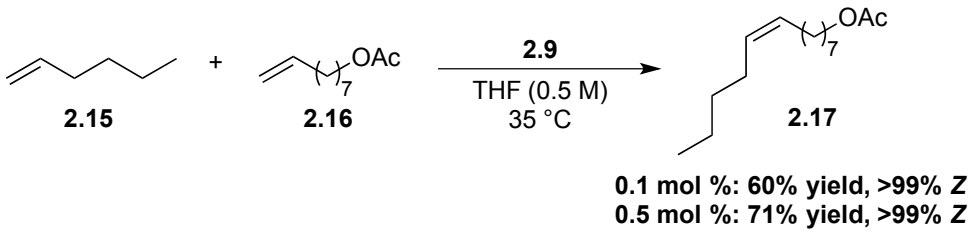
Table 2.3. Homodimerization of Terminal Olefin Substrates Using Catalyst 2.9



substrate	loading, mol %	conc., M	temp, °C	time, h	isolated yield, %	*Z*, %[a]	TON
2.10	0.1	3.3	35	2	84	96	840
	0.1	1	23	6.5	91	96	910
	0.01	7	35	2.5	74	98	7400
2.13	0.1	3.3	35	6.5	87	>99	870
	0.1	1	23	12	85	>99	850
	0.01	3.3	35	12	58	98	5800
2.14	0.1	3.3	35	2.5	81	98	810
	0.1	1	23	12	80	99	800
	0.01	3.3	35	4.5	15	98	1500

[a]Determined by ^{1}H NMR spectroscopy.

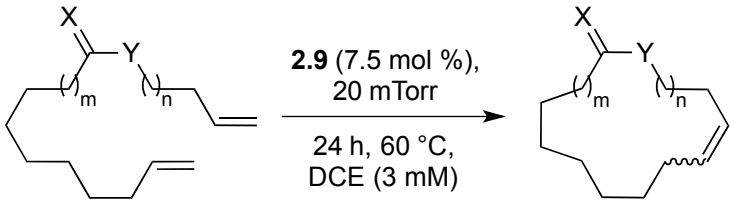
Having established the effectiveness of **2.9** in homodimerization reactions, we set about to further evaluate its activity and *Z*-selectivity by exploring more complex transformations. The reaction of 1-hexene (**2.15**) and 8-nonenyl acetate (**2.16**) to form the pheromone derivative **2.17** was previously described using catalyst **2.3**, proceeding in good yield (67%) with high *Z*-selectivity (91%) at a low catalyst loading (0.5 mol %).[2c] Catalyst **2.9** was able to catalyze this transformation with no observable formation of the *E*-isomer and in slightly higher yield (71%) at the same catalyst loading. Additionally, the catalyst loading could be lowered to 0.1 mol % and still provide a good yield of **2.17** (60%) while maintaining >99% *Z*-selectivity (Scheme 2.3). The expansion of this methodology to produce more complicated cross products with presumably total *Z*-selectivity should further enable its widespread use in the synthesis of *Z*-olefin-containing pheromones and other natural products.



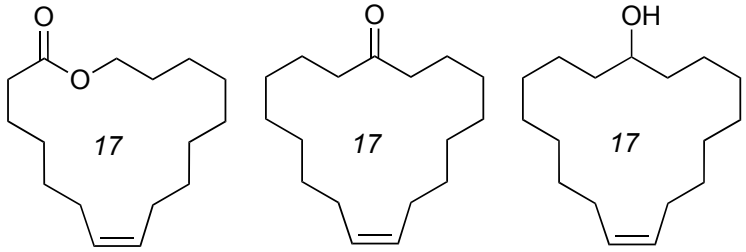
Scheme 2.3. Synthesis of pheromone **2.17** using catalyst **2.9**.

We next evaluated catalyst **2.9** in macrocyclic ring-closing metathesis (mRCM).[9] Although *Z*-selective W- and Mo-based systems exhibit *Z*-selectivities as high as 97% for mRCM reactions,[10,11] catalyst **2.3** yields only ca. 85% *Z*-selectivity.[3c] Particularly problematic for **2.3** are substrates containing ketone or alcohol functionality, in which it is observed that the *Z*-isomer is readily degraded at high conversions. Thus, we were delighted to find that when dienes **2.18a–2.20a** were exposed to catalyst **2.9**, macrocycles **2.18–2.20** were all obtained in modest yields and with only trace amounts of the *E*-isomer evident by ^{1}H and ^{13}C NMR spectroscopy (Table 2.4). It is expected that this methodology will be applicable to the synthesis of a variety of natural products and pharmaceuticals, including a unique class of olfactory compounds known as macrocyclic musks. Many of these compounds contain a macrocyclic backbone either featuring a *Z*-olefin or bearing functionality stereospecifically installed using a *Z*-olefin.[9,12] In fact, **2.18** and **2.19** are both currently in demand by the perfume industry (marketed as ambrettolide and civetone, respectively).[12]

Table 2.4. *Z*-Selective Macrocyclizations Employing Catalyst 2.9[a]



2.18a-2.20a **2.18-2.20**



2.18	**2.19**	**2.20**
64% yield	36% yield	45% yield
(98% *Z*)	(99% *Z*)	(97% *Z*)

[a]Isolated yields (*E*/*Z* ratios determined by ^{1}H- or ^{13}C-NMR spectroscopy).

Conclusions and Future Outlook

In summary, we have developed a new method to effect the salt metathesis and C–H activation of *Z*-selective ruthenium-based metathesis catalysts using sodium carboxylates. This approach has been used to synthesize several new stable cyclometalated species, all of which were found to be highly *Z*-selective in the homodimerizations of terminal olefin substrates. Notably, installation of an *N*-2,6-diisopropylphenyl group on the NHC led to significant improvements in activity and selectivity in the homocouplings of terminal olefins as well as industrially relevant metathesis reactions. Near-perfect selectivity for the *Z*-olefin (>95% in almost all cases) and unmatched TONs of up to 7400 were observed with catalyst **2.9**, all while retaining the ease of use associated with the ruthenium family of metathesis catalysts.

Since this paper was published in the *Journal of the American Chemical Society* in 2013, catalyst **2.9** has been studied extensively in a variety of transformations. Notably, this catalyst has been shown to effectively facilitate chemoselective cross-metathesis, reacting preferentially with terminal and internal *Z*-olefins in the presence of internal *E*-olefins.[13] Complex **2.9** is also effective for the cross-metathesis of allylic-substituted olefins, a challenging class of substrates for *Z*-selective metathesis due to their inherent bulk.[14] Finally, catalyst **2.9** exhibits high *cis,syndio*-selectivity in the ring-opening metathesis polymerization of norbornenes and norbornadienes, particularly when compared to previous cyclometalated systems such as **2.3** (see *Chapter 3*).[15] Additionally, in recent years, the NaOPiv method has been successfully extended to complexes containing cyclometalated *N*-2-adamantane and *N*-bornyl group.[16] Despite these achievements, however, there is still room for the continued development of *Z*-selective ruthenium metathesis catalysts. For example, the cyclometalated systems presented in this chapter are ineffective for the *Z*-selective cross-metathesis of two internal olefins or the formation of trisubstituted *Z*-olefins, transformations that have been reported for both *Z*-selective Mo- and W-based catalysts.[11,17] Overall, it is hoped that the insights gained in this study will contribute to new developments and discoveries in the ever-expanding field of ruthenium-mediated *Z*-selective olefin metathesis.

References

1. (a) Gottumukkala, A. L.; Madduri, A. V. R.; Minnaard, A. J. *ChemCatChem* **2012**, *4*, 462. (b) Fürstner, A. *Science* **2013**, *341*, 1357. (c) Shahane, S.; Bruneau, C.; Fischmeister, C. *ChemCatChem* **2013**, *5*, 3436.

2. (a) Endo, K.; Grubbs, R. H. *J. Am. Chem. Soc.* **2011**, *133*, 8525. (b) Keitz, B. K.; Endo, K.; Herbert, M. B.; Grubbs, R. H. *J. Am. Chem. Soc.* **2011**, *133*, 9686. (c)

Keitz, B. K.; Endo, K.; Patel, P. R.; Herbert, M. H.; Grubbs, R. H. *J. Am. Chem. Soc.* **2011**, *134*, 693.

3. (a) Keitz, B. K.; Fedorov, A.; Grubbs, R. H. *J. Am. Chem. Soc.* **2012**, *134*, 2040. (b) Herbert, M. B.; Marx, V. M.; Pederson, R. L.; Grubbs, R. H. *Angew. Chem., Int. Ed.* **2012**, *52*, 310. (c) Marx, V. M.; Herbert, M. B.; Keitz, B. K.; Grubbs, R. H. *J. Am. Chem. Soc.* **2013**, *135*, 94.

4. Liu, P.; Xu, X.; Dong, X.; Keitz, B. K.; Herbert, M. B.; Grubbs, R. H.; Houk, K. N. *J. Am. Chem. Soc.* **2012**, *134*, 1464.

5. Herbert, M. B.; Lan, Y.; Keitz, B. K.; Liu, P.; Endo, K.; Day, M. W.; Houk, K. N.; Grubbs, R. H. *J. Am. Chem. Soc.* **2012**, *134*, 7861.

6. (a) Peryshkov, D. V.; Schrock, R. R.; Takase, M. K.; Müller, P.; Hoveyda, A. H. *J. Am. Chem. Soc.* **2011**, *133*, 20754. (b) Mougel, V.; Pucino, M.; Copéret, C. *Organometallics* **2015**, *34*, 551. (c) Schowner, R.; Wolfgang, F.; Buchmeiser, M. R. *J. Am. Chem. Soc.* **2015**, *137*, 6188.

7. Ritter, T.; Hejl, A.; Wenzel, A. G.; Funk, T. W.; Grubbs, R. H. *Organometallics* **2006**, *25*, 5740.

8. (a) Trnka, T. M.; Morgan, J. P.; Sanford, M. S.; Wilhelm, T. E.; Scholl, M.; Choi, T. L.; Ding, S.; Day, M. W.; Grubbs, R. H. *J. Am. Chem. Soc.* **2003**, *125*, 2546. (b) Beach, N. J.; Lummiss, J. A. M.; Bates, J. M.; Fogg, D. E. *Organometallics* **2012**, *31*, 2349.

9. (a) Gradillas, A.; Pérez-Castells, J. *Angew. Chem., Int. Ed.* **2006**, *45*, 8086. (b) Majumdar, K. C.; Rahaman, H.; Roy, B. *Curr. Org. Chem.* **2007**, *11*, 1339. (c) Diederich, F.; Stang, P. J.; Tykwinshi, R. R. *Modern Supramolecular Chemistry: Strategies for Macrocycle Synthesis*; Wiley-VCH: Weinheim, Germany, 2008. (d) Cossy, J.; Arseniyadis, S.; Meyer, C. *Metathesis in Natural Product Synthesis: Strategies, Substrates, and Catalysts*, 1st ed.; Wiley-VCH: Weinheim, Germany, 2010.

10. (a) Yu, M.; Wang, C.; Kyle, A. F.; Jakubec, P.; Dixon, D. J.; Schrock, R. R.; Hoveyda, A. H. *Nature* **2011**, *479*, 88.

11. For more recent examples of W- and Mo-catalyzed *Z*-selective macrocyclic ring-closing metathesis and its application to natural product synthesis, see: (a) Wang, C.; Yu, M.; Kyle, A. F.; Jakubec, P.; Dixon, D. J.; Schrock, R. R.; Hoveyda, A. H. *Chem.—Eur. J.* **2013**, *19*, 2726. (b) Wang, C.; Haeffner, F.; Schrock, R. R.; Hoveyda, A. H. *Angew. Chem., Int. Ed.* **2013**, *52*, 1939. (c) Yu, M.; Schrock, R. R.; Hoveyda, A. H. *Angew. Chem., Int. Ed.* **2014**, *54*, 215. (d) Zhang, H.; Yu, E. C.; Torker, S.; Schrock, R. R.; Hoveyda, A. H. *J. Am. Chem. Soc.* **2014**, *136*, 16493.

12. (a) Rowe, D. J. *Chemistry and Technology of Flavors and Fragrances*; Blackwell: Oxford, 2005. (b) Ohloff, G.; Pickenhagen, W.; Kraft, P. *Scent and Chemistry—The Molecular World of Odors*; Verlag Helvectica Acta: Zurich, 2011.

13. Cannon, J. S.; Grubbs, R. H. *Angew. Chem., Int. Ed.* **2013**, *52*, 9001.

14. Quigley, B. L.; Grubbs, R. H. *Chem. Sci.* **2014**, *5*, 501.

15. Rosebrugh, L. E.; Ahmed, T. S.; Marx, V. M.; Hartung, J.; Liu, P.; López, J. G.; Houk, K. N.; Grubbs, R. H. *J. Am. Chem. Soc.* **2016**, *138*, 1394.

16. Herbert, M. B.; Suslick, B. A.; Liu, P.; Zou, L,; Dornan, P. K.; Houk, K. N.; Grubbs, R. H. *Organometallics* **2015**, *34*, 2858.

17. Flook, M. M.; Jiang, A. J.; Schrock, R. R.; Müller, P.; Hoveyda, A. H. *J. Am. Chem. Soc.* **2009**, *131*, 7962.

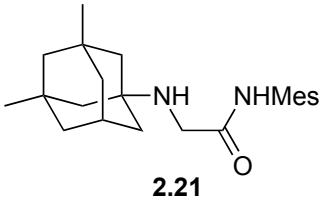
18. Breitmaier, E.; Voelter, W. *Carbon-13 NMR Spectroscopy: High-Resolution Methods and Applications in Organic Chemistry and Biochemistry*, 3rd Ed.; Wiley-VCH: Weinheim, Germany, 1987.

Supporting Information

General Information: All reactions were carried out in dry glassware under an argon atmosphere using standard Schlenk techniques or in a Vacuum Atmospheres Glovebox under a nitrogen atmosphere, unless otherwise specified. All solvents were purified by passage through solvent purification columns and further degassed by bubbling argon. C_6D_6 was purified by passage through a solvent purification column. $CDCl_3$ and CD_2Cl_2 were used as received. All substrates for olefin cross-metathesis (**2.10**, **2.13**, and **2.14**) were degassed with argon and filtered through a plug of neutral alumina prior to use. Dienes **2.18a–2.20a** were synthesized as disclosed previously.[3c] $RuCl_2(PCy_3)$(=CH-*o*-$O^iPrC_6H_4$) (**2.24**) was obtained from Materia, Inc. Precatalyst **2.4** was synthesized according to the literature procedure.[5] Other commercially available reagents and silica gel were used as received.

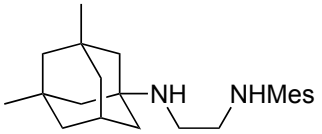
^{1}H NMR spectra were acquired at 400 or 500 MHz and ^{13}C NMR spectra at 101 or 126 MHz as $CDCl_3$ or C_6D_6 solutions unless otherwise noted. Chemical shifts are reported in ppm downfield from Me_4Si by using the residual solvent peak as an internal standard. Spectra were analyzed and processed using MestReNova Ver. 7.1.

High-resolution mass spectra (HRMS) were provided by the California Institute of Technology Mass Spectrometry Facility using a JEOL JMS-600H High Resolution Mass Spectrometer. All HRMS were by positive-ion EI or FAB.



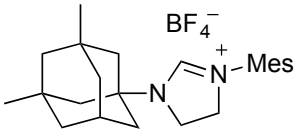
2.21

Preparation of 2.21: A three-neck 250 mL round-bottom flask equipped with a condenser was flame dried and charged with 2-chloro-*N*-mesitylacetamide (3.5 g, 17 mmol), memantine hydrochloride (3.0 g, 14 mmol, OChem Incorp.), and K_2CO_3 (4.8 g, 35 mmol). MeCN (110 mL) was added and the suspension was heated to 100 °C under an argon atmosphere for 24 h. After cooling to r.t., the mixture was filtered through celite, washing with CH_2Cl_2, and the filtrate was concentrated to a white powder. The crude mixture was dry loaded onto a silica gel column and purified via flash chromatography (SiO_2, eluent Et_2O) to give **2.21** (3.0 g, 60%) as a white powder. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.97 (br s, 1H), 6.88 (s, 2H), 3.38 (s, 2H), 2.26 (s, 3H), 2.18 (s, 6H), 2.17 (m, 1H), 1.53 (br s, 1H), 1.49 (br d, J = 3.2 Hz, 2H), 1.31–1.27 (m, 8H), 1.14 (br q, J = 11.6 Hz, 2H), 0.86 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.5, 136.4, 134.7, 131.4, 128.8, 52.8, 50.7, 49.0, 44.3, 42.8, 41.3, 32.4, 30.2, 30.1, 20.9, 18.5. HRMS (FAB+, (M+H)): Calculated—355.2749, Found—355.2766.



2.22

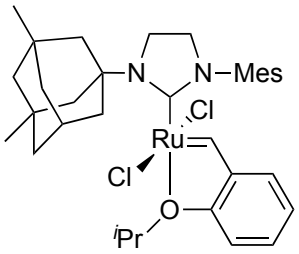
Preparation of 2.22: A two-neck 100 mL RB flask equipped with a condenser was dried and charged with $LiAlH_4$ (1.3 g, 34 mmol) and THF (50 mL). A separate 25 mL RB flask was dried and charged with **2.21** (3.0 g, 8.4 mmol) and THF (20 mL). The solution of **2.21** was then added dropwise to the $LiAlH_4$ suspension. After the addition was complete, the suspension was heated to 80 °C for 24 h, after which it was cooled to r.t. and carefully quenched via the sequential, dropwise addition of H_2O (1.3 mL), 15% NaOH solution (1.3 mL), and H_2O (4.0 mL). The quenched reaction was stirred for 5 h under air and then filtered through celite, washing with Et_2O. The filtrate was concentrated to give **2.22** (2.8 g, 98%), which was used without further purification. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.86 (s, 2H), 3.04 (t, *J* = 4.4 Hz, 2H), 2.85 (t, *J* = 4.8 Hz, 2H), 2.34 (s, 6H), 2.28 (s, 3H), 2.20 (br s, 1H), 1.55 (s, 2H), 1.38–1.32 (m, 8H), 1.19–1.17 (m, 2H), 0.92 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.0, 130.6, 129.4, 129.2, 52.1, 51.0, 49.5, 49.2, 43.1, 41.4, 40.9, 32.4, 30.4, 30.3, 20.6, 18.6. HRMS (FAB+, (M+H)): Calculated—341.2957, Found—341.2964.



2.23

Preparation of 2.23: A 100 mL round-bottom flask was dried and charged with **2.22** (1.0 g, 2.9 mmol), NH_4BF_4 (0.34 g, 3.2 mmol), and $CH(OMe)_3$ (6.0 mL, 28 mmol). The solution was heated to 100 °C for 4 h, cooled to r.t., and concentrated. The resulting

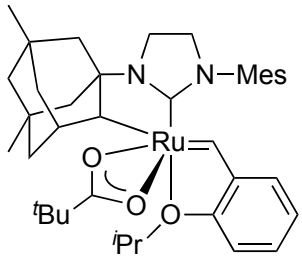
orange-red residue was washed with cold ^{n}BuOH:toluene (1:1) to give a white precipitate that was collected by filtration. Drying the precipitate under vacuum gave **2.23** (0.49 g, 44%) as an off-white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (s, 1H), 6.89 (s, 2H), 4.31–4.13 (m, 4H), 2.27 (m, 1H), 2.26 (s, 3H), 2.22 (s, 6H), 1.65 (br s, 2H), 1.61 (br q, *J* = 11.6 Hz, 4H), 1.36 (br q, *J* = 14.4 Hz, 4H), 1.21 (br s, 2H), 0.91 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.7, 139.9, 135.2, 130.7, 129.6, 59.3, 50.4, 49.6, 46.3, 44.9, 41.6, 39.0, 32.6, 29.7, 29.4, 20.8, 17.4. HRMS (FAB+, (M-BF_4)): Calculated—351.2800, Found—351.2755.



2.25

Preparation of 2.25: In a glovebox, a solution of **2.23** (0.49 g, 1.1 mmol) in hexanes (30 mL) was treated with $KCOMe_2Et$ (0.14 g, 0.91 mmol), and the mixture was allowed to stir at 35 °C for 1.5 h. To the reaction mixture was then added **2.24** (0.64 g, 1.1 mmol), upon which the mixture was removed from the glovebox and allowed to stir at 65 °C for 3.5 h. The precipitated solids were filtered and washed well with warm hexanes and pentane to give **2.25** (0.54 g, 89%) as a green powder. ^{1}H NMR (500 MHz, $CDCl_3$) δ 16.90 (s, 1H), 7.55 (ddd, *J* = 8.8, 7.3, 1.9 Hz, 1H), 7.06 (s, 2H), 6.95–6.88 (m, 2H), 6.86 (dd, *J* = 7.5, 1.8 Hz, 1H), 5.09 (hept, *J* = 6.3 Hz, 1H), 4.12 (s, 2H), 4.06–3.98 (m, 2H), 3.90–3.82 (m, 2H), 2.70 (p, *J* = 3.1 Hz, 1H), 2.46 (s, 3H), 2.25 (s, 6H), 2.04 (dd, *J* = 11.9, 1.8 Hz, 2H), 1.81 (d, *J* = 12.2 Hz, 2H), 1.74 (dt, *J* = 12.6, 2.8 Hz, 2H), 1.63 (d, *J* = 6.1 Hz, 6H), 1.47 (dt, *J* = 12.6, 2.4 Hz, 2H), 1.31–1.17 (m, 2H), 0.97 (s, 6H). ^{13}C NMR (126

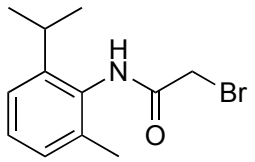
MHz, $CDCl_3$) δ 312.4, 207.8, 152.4, 145.9, 139.6, 138.5, 138.1, 130.8, 129.8, 123.9, 122.8, 113.5, 74.4, 58.9, 51.2, 50.7, 47.3, 44.7, 42.4, 42.2, 33.0, 31.3, 30.4, 22.6, 21.3, 18.5. HRMS (FAB+, (M)): Calculated—670.2031, Found—670.2028.



2.7

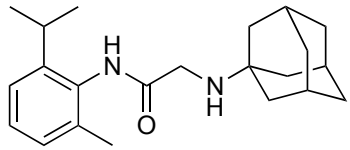
Preparation of 2.7: In a glovebox, a 20 mL scintillation vial was charged with **2.25** (0.10 g, 0.16 mmol), NaOPiv (0.19 g, 1.5 mmol), THF (2.0 mL), and MeOH (2.0 mL). The vial was capped, removed from the glovebox, and heated to 40 °C for 4.5 h, during which a color change from green to brown to dark purple was observed. The vial was then returned to the box, where the solvent was removed under high vacuum and the residue dissolved in CH_2Cl_2 (15 mL), filtered through celite, and concentrated to a deep purple residue. The residue was recrystallized from Et_2O at -35 °C. The resulting crystals were washed with cold Et_2O (3 x 5 mL) to give **2.7** (20 mg, 18%) as a bright purple solid. ^{1}H NMR (400 MHz, C_6D_6) δ 14.83 (s, 1H), 7.46 (dd, *J* = 7.2, 1.6 Hz, 1H), 7.26 (t, *J* = 7.6 Hz, 1H), 6.92 (t, *J* = 7.6 Hz, 1H), 6.83 (br s, 1H), 6.76 (br s, 1H), 6.70 (d, *J* = 8.4 Hz, 1H), 4.79 (sept, *J* = 6.8 Hz, 1H), 3.91 (s, 1H), 3.47–3.40 (m, 2H), 3.27–3.14 (m, 2H), 2.57 (br s, 1H), 2.43 (s, 3H), 2.29 (s, 3H), 2.21 (s, 3H), 1.73 (br d, *J* = 11.2 Hz, 1H), 1.60 (br d, *J* = 10.8 Hz, 1H), 1.53–1.51 (m, 4H), 1.43–1.39 (m, 2H), 1.26 (s, 9H), 1.18 (q, *J* = 6.4 Hz, 4H), 1.03 (d, *J* = 9.6 Hz, 1H), 0.89 (br s, 4H), 0.77 (br d, *J* = 12.8 Hz, 1H), 0.67 (br d, *J* = 10.4 Hz, 1H), 0.62 (s, 3H), 0.31 (br d, *J* = 9.6 Hz, 1H). ^{13}C NMR (101 MHz, C_6D_6) δ 259.0, 214.9, 154.2, 143.8, 138.0, 137.0, 136.8, 136.5, 129.9, 129.7, 125.6,

123.1, 122.8, 113.9, 74.5, 66.5, 64.1, 52.1, 51.7, 48.8, 46.6, 42.6, 41.3, 39.8, 39.1, 38.6, 33.4, 32.1, 30.8, 30.7, 28.9, 27.8, 21.6, 21.2, 21.0, 19.1, 19.0. HRMS (FAB+, [(M+H)-H_2]): Calculated—700.3178, Found—700.3181.



2.26

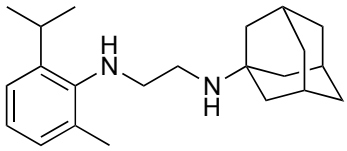
Preparation of 2.26: Bromoacetyl chloride (2.8 mL, 34 mmol) was added dropwise to a 0 °C solution of 2-isopropyl-6-methylaniline (5.0 g, 34 mmol) and K_2CO_3 (9.4 g, 68 mmol) in MeCN (70 mL). The solution was warmed to r.t., stirred overnight, filtered over celite, and concentrated. Recrystallization from CH_2Cl_2/hexanes provided **2.26** (5.5 g, 60%) as a colorless solid. ^{1}H NMR δ 7.77 (br s, 1H), 7.24 (m, 1H), 7.18 (m, 1H), 7.11 (m, 1H), 4.08 (s, 2H), 3.06 (m, 1H), 2.24 (s, 3H), 1.21 (d, J = 6.9 Hz, 6H). ^{13}C NMR δ 164.3, 145.7, 135.9, 131.6, 128.4, 128.3, 123.7, 29.2, 28.7, 23.5, 18.5. HRMS (FAB+, (M+H)): Calculated—270.0493, Found—270.0480.



2.27

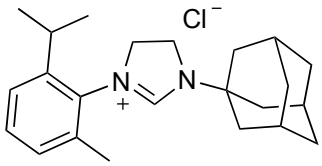
Preparation of 2.27: Compound **2.26** (2.4 g, 8.9 mmol) and 1-adamantylamine (92.0 g, 13 mmol) were dissolved in MeCN (30 mL), K_2CO_3 (1.9 g, 14 mmol) was added, and the solution was refluxed for 24 h. After cooling to r.t., the mixture was filtered over celite and concentrated. The residue was then dissolved in CH_2Cl_2 and filtered over a pad of silica gel (eluent 10% MeOH in CH_2Cl_2). Removal of the solvent *in vacuo* provided **2.27** (3.0 g, 94%) as a peach solid. ^{1}H NMR δ 9.15 (br s, 1H), 7.18 (m, 1H), 7.16 (m, 1H),

7.09 (m, 1H), 3.44 (s, 2H), 3.04 (m, 1H), 2.23 (s, 3H), 2.11 (m, 3H), 1.58–1.72 (m, 14H), 1.20 (d, J = 6.9 Hz, 6H). ^{13}C NMR δ 171.9, 145.2, 135.6, 132.8, 128.1, 127.5, 123.3, 51.1, 44.0, 42.9, 36.5, 29.5, 28.7, 23.4, 18.8. HRMS (FAB+, (M+H)): Calculated—341.2593, Found—341.2603.



2.28

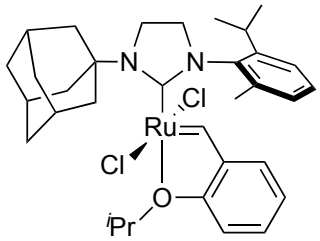
Preparation of 2.28: $LiAlH_4$ (1.0 g, 26 mmol) was added portion-wise to a 0 °C solution of compound **2.27** (3.0 g, 8.8 mmol) in THF (45 mL), and the resulting solution was brought to r.t. and refluxed for 72 h. The mixture was then cooled to 0 °C and carefully quenched via the sequential, dropwise addition of H_2O (1.0 mL), 10% *aq*. NaOH (1.0 mL), and H_2O (1.0 mL). The solution was then dried with $MgSO_4$, filtered, and concentrated. Flash chromatography of the residue (SiO_2, eluent 66% Et_2O in pentanes) provided **2.28** (1.8 g, 62%) as a yellow oil. ^{1}H NMR δ 7.08 (m, 1H), 6.98 (m, 1H), 6.91 (m, 1H), 3.30 (m, 1H), 3.06 (m, 2H), 2.86 (m, 2H), 2.32 (s, 3H), 2.08 (m, 3H), 1.59–1.73 (m, 15H), 1.23 (d, J = 6.9 Hz, 6H). ^{13}C NMR δ 145.1, 140.8, 130.6, 128.4, 123.6, 122.4, 51.1, 50.1, 42.9, 42.5, 40.7, 36.6, 29.5, 27.5, 24.0, 19.1. HRMS (FAB+, (M+H)): Calculated—327.2800, Found—327.2800.



2.29

Preparation of 2.29: A solution of compound **2.28** (1.3 g, 4.0 mmol) in Et_2O (7.0 mL) was treated with HCl (4.0 mL, 2.0 M in Et_2O) and stirred for 15 min at r.t. The resulting

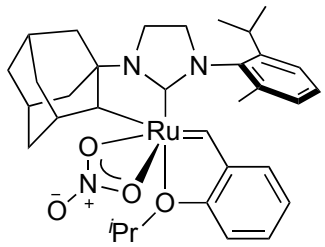
solid was filtered, washed with Et_2O, and dried, then suspended in $CH(OEt)_3$ and refluxed for 2 h. After cooling to r.t. and concentrating, the solid residue was washed rigorously with Et_2O to provide **2.29** (0.75 g, 50%) as a tan powder. ^{1}H NMR δ 8.79 (br s, 1H), 7.32 (m, 1H), 7.22 (m, 1H), 7.13 (m, 1H), 4.55 (m, 1H), 4.43 (m, 2H), 4.25 (m, 1H), 2.93 (m, 1H), 2.41 (s, 3H), 2.27 (m, 3H), 2.18–2.08 (m, 6H), 1.74 (m, 6H), 1.28 (d, J = 6.8 Hz, 6H). ^{13}C NMR δ 156.0, 146.5, 135.9, 132.0, 130.6, 129.2, 124.8, 58.2, 52.1, 45.5, 41.1, 35.4, 29.2, 28.7, 24.8, 24.2, 18.7. HRMS (FAB+, (M-Cl)): Calculated—337.2644, Found—337.2652.



2.30

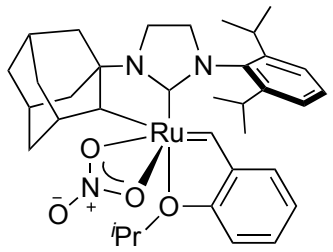
Preparation of 2.30: In a glovebox, $KCOMe_2Et$ (75 mg, 0.57 mmol) was added to a suspension of compound **2.29** (0.19 g, 0.52 mmol) in hexanes (6.0 mL). The solution was stirred at 35 °C for 30 minutes before adding **2.24** (0.31 g, 0.52 mmol), at which point the solution was removed from the glovebox. The solution was stirred for 2 h at 65 °C and then cooled to r.t. The resulting precipitate was filtered and washed thoroughly with warm hexanes to provide **2.30** (0.22 g, 65%) as a green solid. ^{1}H NMR δ 16.9 (s, 1H), 7.54 (m, 1H), 7.49 (m, 1H), 7.22 (m, 1H), 6.92 (m, 1H), 6.87 (m, 1H), 6.85 (m, 1H), 5.07 (m, 1H), 3.98–4.11 (m, 2H), 3.84–3.92 (m, 2H), 3.15 (m, 1H), 2.96 (m, 5H), 2.42 (m, 2H), 2.32 (s, 3H), 1.94 (m, 3H), 1.83 (m, 3H), 1.69 (d, J = 6.2 Hz, 3H), 1.60 (d, J = 6.2 Hz, 3H), 1.18 (d, J = 6.8 Hz, 3H), 0.89 (d, J = 6.8 Hz, 3H). ^{13}C NMR δ 310.5, 208.2, 152.5, 148.7, 145.2, 140.6, 137.9, 130.6, 129.1, 128.9, 124.8, 123.8, 122.5, 113.2, 74.2,

57.2, 52.7, 44.5, 42.2, 36.1, 30.0, 27.6, 25.5, 23.8, 22.7, 22.3, 18.9. HRMS (FAB+, (M)): Calculated—656.1875, Found—656.1894.



2.8

Preparation of 2.8: In a glovebox, a solution of NaOPiv (0.30 g, 1.5 mmol) in MeOH (2.0 mL) was added to a solution of **2.30** (0.15 g, 0.15 mmol) in THF (2.0 mL). The mixture was removed from the glovebox, heated at 50 °C for 21 h, and then brought back into the glovebox and concentrated. The resulting residue was taken up in CH_2Cl_2, filtered over a pad of celite, and concentrated. The solid was then dissolved in THF (8.0 mL), and NH_4NO_3 (0.12 g, 1.5 mmol) was added. After stirring for 3 h, the mixture was concentrated, taken up in CH_2Cl_2, filtered over a pad of celite, and concentrated again. Rigorous washing of the resulting solid with Et_2O provided **2.8** (0.70 g, 72%) as a purple solid. ^{1}H NMR δ 15.0 (s, 1H), 7.48 (m, 1H), 7.42 (m, 1H), 7.13 (m, 1H), 7.08 (m, 1H), 6.99 (m, 1H), 6.97 (m, 1H), 5.10 (m, 1H), 3.95 (m, 1H), 3.78–3.99 (m, 4H), 3.72 (m, 1H), 3.15 (m, 1H), 2.23 (m, 1H), 2.18 (s, 3H), 2.18 (*overlapped*, 1H), 2.06 (m, 1H), 1.99 (m, 1H), 1.92 (m, 1H), 1.72 (m, 1H), 1.65 (m, 1H), 1.59 (m, 1H), 1.55 (m, 2H), 1.48 (d, J = 6.2 Hz, 3H), 1.23 (d, J = 6.8 Hz, 3H), 1.17 (d, J = 6.2 Hz, 3H), 1.12 (d, J = 6.8 Hz, 3H), 0.98 (m, 2H), 0.24 (m, 1H). ^{13}C NMR δ 266.4, 213.1, 154.7, 147.6, 143.1, 138.0, 137.3, 128.7, 128.3, 127.1, 124.0, 123.4, 123.4, 112.9, 74.4, 67.6, 52.6, 43.2, 42.3, 40.3, 37.9, 37.7, 37.6, 33.3, 31.0, 29.8, 28.3, 26.3, 23.6, 21.4, 20.6, 17.5. HRMS (FAB+, [(M+H)-H_2]): Calculated—646.2219, Found—646.2239.



2.9

Preparation of 2.9: In a glovebox, a 250 mL Schlenk flask was charged with **2.4** (0.50 g, 0.73 mmol), NaOPiv (0.92 g, 7.4 mmol), THF (32 mL), and MeOH (16 mL). The flask was sealed, removed from the glovebox, and heated to 40 °C for 4 d, during which the solution was observed to change color from green to brown to dark purple. The solvent was removed under high vacuum and the Schlenk flask transferred back into the glovebox. The residue was then dissolved in CH_2Cl_2 (80 mL), filtered through celite, and concentrated to a deep purple residue consisting of a mixture of the C–H activated product and pivalic acid. To this mixture was added NH_4NO_3 (0.72 g, 9.0 mmol) and THF (35 mL). The reaction was allowed to stir for 3 h and then concentrated. The resulting residue was dissolved in C_6H_6 (70 mL), filtered through celite, and concentrated. Trituration with Et_2O (3 x 15 mL) provided **2.9** (100 mg, 20%) as a bright purple powder. ^{1}H NMR (500 MHz, C_6D_6) δ 15.21 (s, 1H), 7.45 (dd, *J* = 7.4, 1.7 Hz, 1H), 7.19 (qd, *J* = 5.8, 5.2, 2.5 Hz, 3H), 7.00 (dd, *J* = 6.8, 2.5 Hz, 1H), 6.85 (t, *J* = 7.4 Hz, 1H), 6.47 (d, *J* = 8.4 Hz, 1H), 4.54 (hept, *J* = 6.3 Hz, 1H), 4.10 (s, 1H), 3.83–3.71 (m, 2H), 3.59 (ddd, *J* = 11.7, 10.1, 8.1 Hz, 1H), 3.36 (ddd, *J* = 11.0, 9.7, 8.1 Hz, 1H), 3.26–3.15 (m, 2H), 2.25 (t, *J* = 3.0 Hz, 1H), 2.06 (p, *J* = 3.3 Hz, 1H), 1.94 (tt, *J* = 11.9, 2.4 Hz, 2H), 1.77 (*overlapped*, 2H), 1.75 (d, *J* = 6.7 Hz, 3H), 1.63 (p, *J* = 3.4 Hz, 1H), 1.55–1.44 (m, 2H), 1.43 (*overlapped*, 1H), 1.42 (d, *J* = 6.4 Hz, 3H), 1.20 (d, *J* = 6.9 Hz, 3H), 1.16 (d, *J* = 6.8 Hz, 3H), 1.14 (*overlapped*, 1H), 1.13 (d, *J* = 6.8 Hz, 3H), 1.10 (*overlapped*, 1H),

0.97 (d, J = 6.1 Hz, 3H), 0.58 (dt, J = 12.2, 2.6 Hz, 1H). ^{13}C NMR (126 MHz, C_6D_6) δ 267.5, 211.9, 154.8, 147.5, 147.4, 143.4, 135.6, 129.2, 126.9, 124.8, 124.2, 123.4, 123.4, 113.2, 74.4, 66.4, 63.2, 54.1, 43.0, 41.6, 40.3, 38.0, 37.8, 37.7, 33.3, 30.9, 29.8, 29.0, 28.7, 27.9, 26.8, 23.6, 23.1, 21.1, 20.3. HRMS (FAB+, [(M+H)-H_2]): Calculated—674.2566, Found—674.2532.

General Procedure for Homodimerization Reactions: In a glovebox, a 4 mL vial was charged with catalyst (0.014 mmol) and THF (1.0 mL) to make a stock solution (0.014 M). A portion of the catalyst stock solution (70 µL, ca. 1.0 µmol, 0.1 mol %) was then added to a 4 mL vial containing substrate (1.0 mmol) and THF (100 µL, *ca.* 3.3 M). The reaction was placed into an aluminum block on an IKA temperature-controlled hotplate preheated to 35 °C and stirred while open to the glovebox atmosphere. After the completion of the reaction (as determined by ^{1}H NMR spectroscopy), the vial was removed from the glovebox and quenched with oxygen. The product was then isolated either via flash chromatography on silica gel or by removal of the starting material *in vacuo* according to literature procedures. The percentage of *Z*-olefin product was determined by ^{1}H NMR spectroscopy. All spectra were consistent with previous literature reports.[2b]

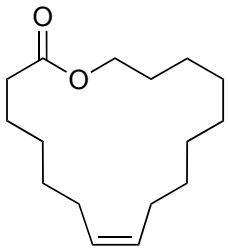
General Procedure for the Synthesis of 2.17 Using Catalyst 2.9: In a glovebox, a 20 mL vial was charged with **2.15** (3.1 mL, 25 mmol), **2.16** (520 µL, 2.5 mmol), and THF (1.4 mL). **2.9** (8.5 mg, 0.013 mmol, 0.5 mol %) was added, and the reaction was stirred at 35 °C in an open vial. After 2 h, the vial was removed from the glovebox, quenched with

excess ethyl vinyl ether (1.5 mL) and stirred for 1 h. The solvent was then removed *in vacuo*. The crude mixture was purified by flash chromatography (SiO_2, eluent hexanes to 4% ethyl acetate in hexanes) two times to provide the pure *Z*-isomer of **2.17** (430 mg, 71%) as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.34 (m, 2H), 4.05 (t, J = 6.8 Hz, 2H), 2.00–2.04 (m, 7H), 1.60–1.63 (m, 2H), 1.29–1.36 (m, 12H), 0.88–0.91 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.4, 130.1, 129.9, 64.8, 32.1, 29.8, 29.3, 28.7, 27.3, 27.1, 26.0, 22.5, 21.2, 14.1. HRMS (EI+, (M+H)): Calculated—241.2168, Found—241.2174.

Synthesis of 2.17 at 1 mol % Catalyst Loading: Following the general procedure, **2.9** (1.7 mg, 2.5 μmol, 0.1 mol %) was added to a solution of **2.15** (3.1 mL, 25 mmol) and **2.16** (520 μL, 2.5 mmol) in THF (1.4 mL) to produce the pure *Z*-isomer of **2.17** (360 mg, 60%) as a colorless oil.

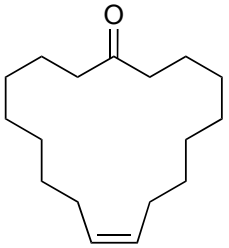
General Procedure for Macrocyclizations Using Catalyst 2.9: In a glovebox, a 500 mL Strauss flask was charged with a solution of diene (0.45 mmol) in DCE (90 mL), and a solution of **2.9** (0.034 mmol, 7.5 mol %) dissolved in DCE (1.0 mL) was added. The flask was sealed, brought out of the glovebox, and subjected to a single freeze-pump-thaw cycle. Keeping the flask under a static vacuum of *ca.* 20 mTorr, the reaction was heated at 60 °C. After 24 h, the mixture was cooled, quenched with excess ethyl vinyl ether, and concentrated. Flash chromatography of the residue (SiO_2, eluent 2% Et_2O in pentanes for compounds **2.18** and **2.19** and 10% Et_2O in pentanes for compound **2.20**) provided the product. The percentage of *Z*-olefin product was determined by ^{1}H or

quantitative ^{13}C NMR spectroscopy.[18] Quantitative ^{13}C measurements were acquired at 126 MHz (decoupled, without NOE, 13 second delay time).



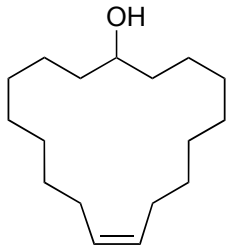
2.18

Preparation of 2.18: According to the general procedure for macrocyclizations, diene **2.18a** (62 mg, 0.22 mmol) was reacted with **2.9** (12 mg, 0.018 mmol) to provide **2.18** (35 mg, 64% yield, 98% *Z*) as a colorless oil. ^{1}H NMR δ 5.32 (m, 2H), 4.13 (t, *J* = 5.4 Hz, 2H), 2.33 (t, *J* = 6.5 Hz, 2H), 2.04 (m, 4H), 1.63 (m, 4H), 1.21–1.43 (m, 14H). ^{13}C NMR δ 174.0, 130.2, 130.0, 63.7, 34.6, 29.4, 28.8, 28.7, 28.5 (2C), 28.4, 27.7, 27.0, 26.8, 25.3 (2C). HRMS (EI+, (M)): Calculated—252.2089, Found—252.2084.



2.19

Preparation of 2.19: According to the general procedure for macrocyclizations, diene **2.19a** (60 mg, 0.22 mmol) was reacted with **2.9** (12 mg, 0.018 mmol) to provide **2.19** (20 mg, 36% yield, 99% *Z*) as a colorless solid. ^{1}H NMR δ 5.34 (m, 2H), 2.40 (t, *J* = 6.7 Hz, 4H), 2.01 (m, 4H), 1.62 (m, 4H), 1.21–1.39 (m, 16H). ^{13}C NMR δ 212.6, 130.2 (2C), 42.5 (2C), 29.0 (2C), 28.6 (2C), 28.2 (2C), 28.1 (2C), 26.7 (2C), 23.9 (2C). HRMS (EI+, (M)): Calculated—250.2297, Found—250.2289.



2.20

Preparation of 2.20: According to the general procedure for macrocyclizations, diene **2.20a** (62 mg, 0.22 mmol) was reacted with **2.9** (12 mg, 0.018 mmol) to provide **2.20** (23 mg, 42% yield, 97% *Z*) as a colorless solid. ^{1}H NMR δ 5.34 (m, 2H), 3.72 (m, 1H), 2.04 (m, 4H), 1.50 (m, 4H), 1.22–1.40 (m, 21H). ^{13}C NMR δ 130.2 (2C), 70.4, 35.7 (2C), 29.0 (2C), 28.2 (2C), 28.0 (2C), 27.9 (2C), 26.8 (2C), 23.5 (2C). HRMS (EI+, (M)): Calculated—252.2453, Found—252.2463.

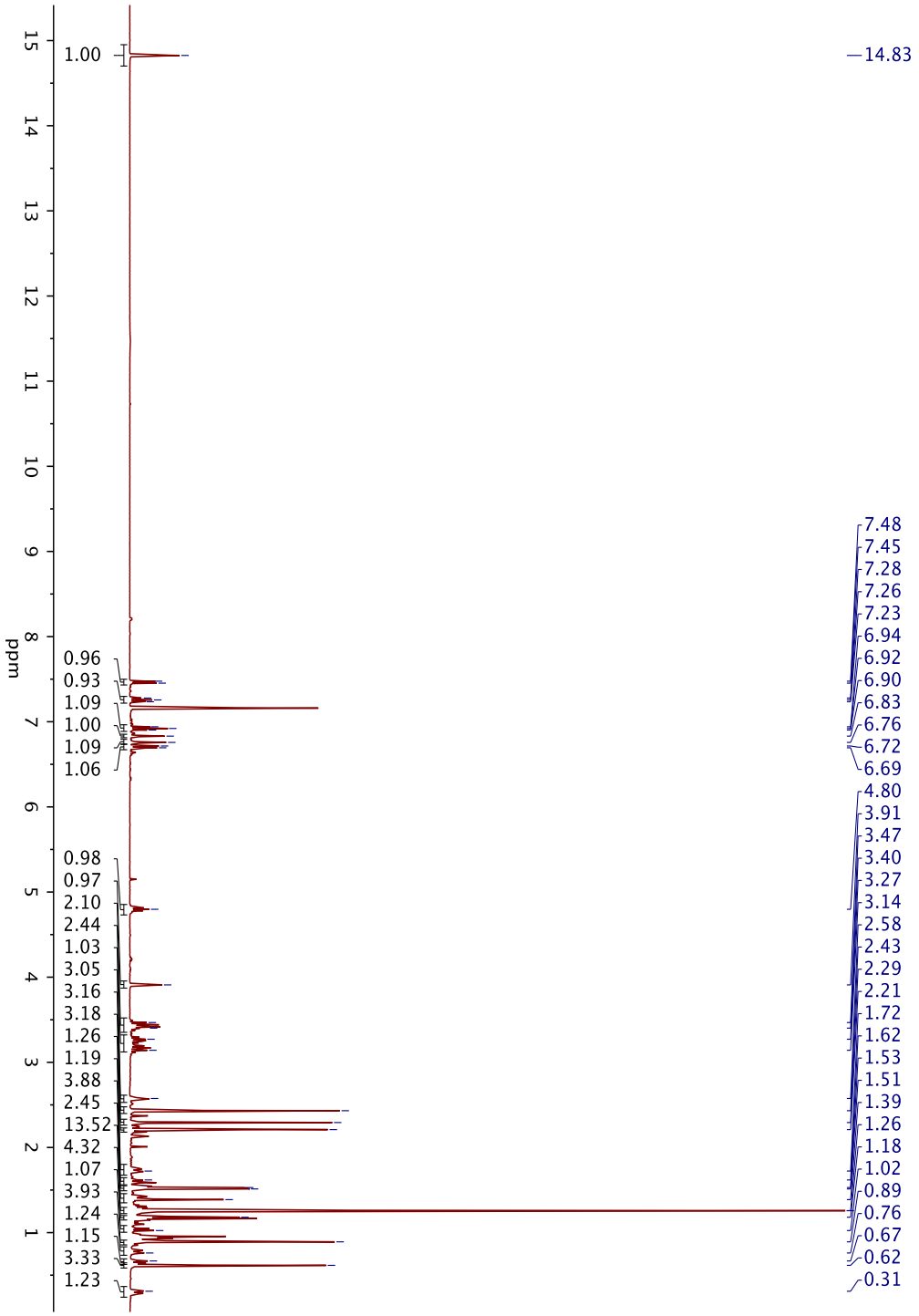


Figure 2.2. ^{1}H NMR (400 MHz, C_6D_6) spectrum of **2.7**.

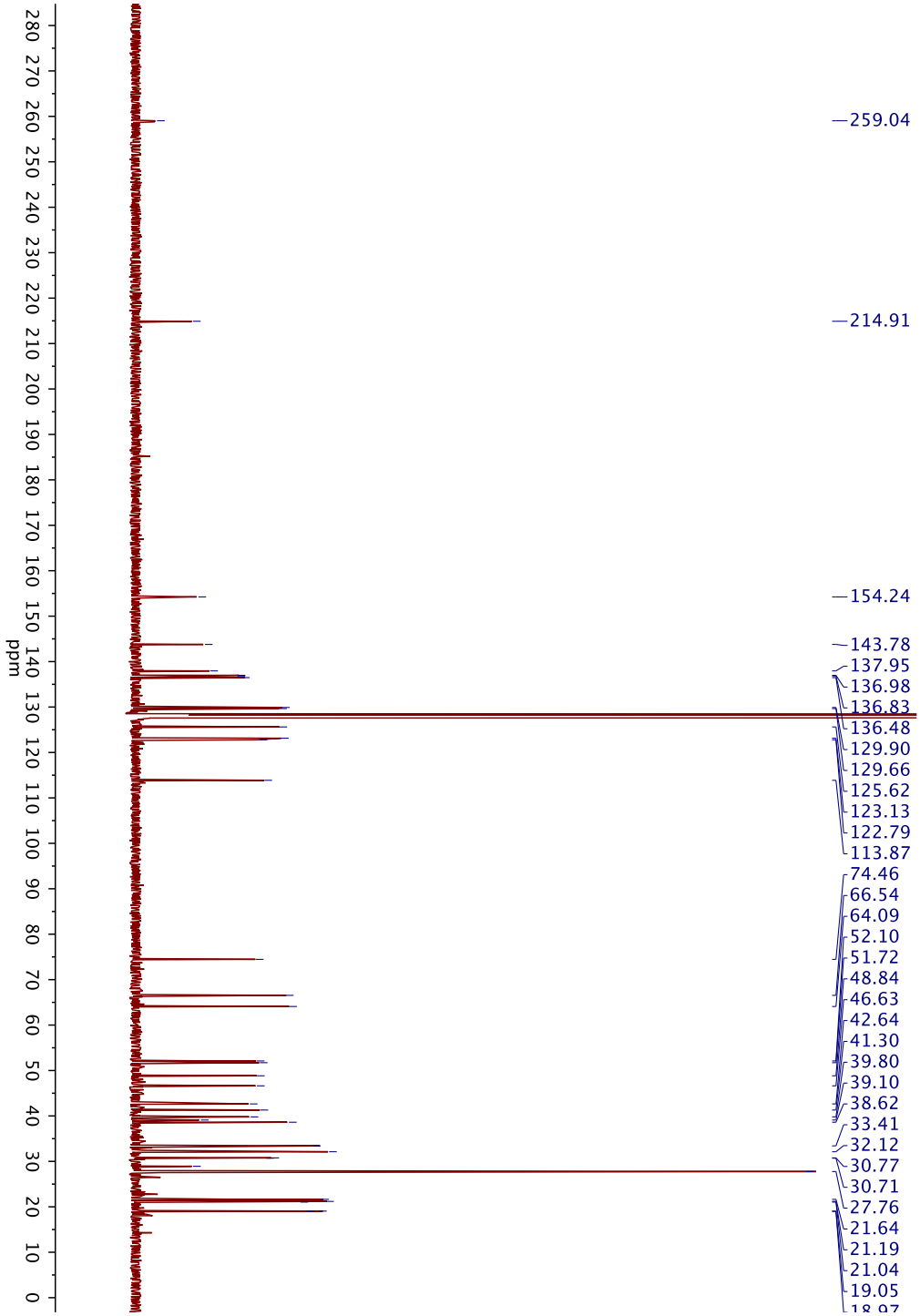


Figure 2.3. ^{13}C NMR (101 MHz, C_6D_6) spectrum of **2.7**.

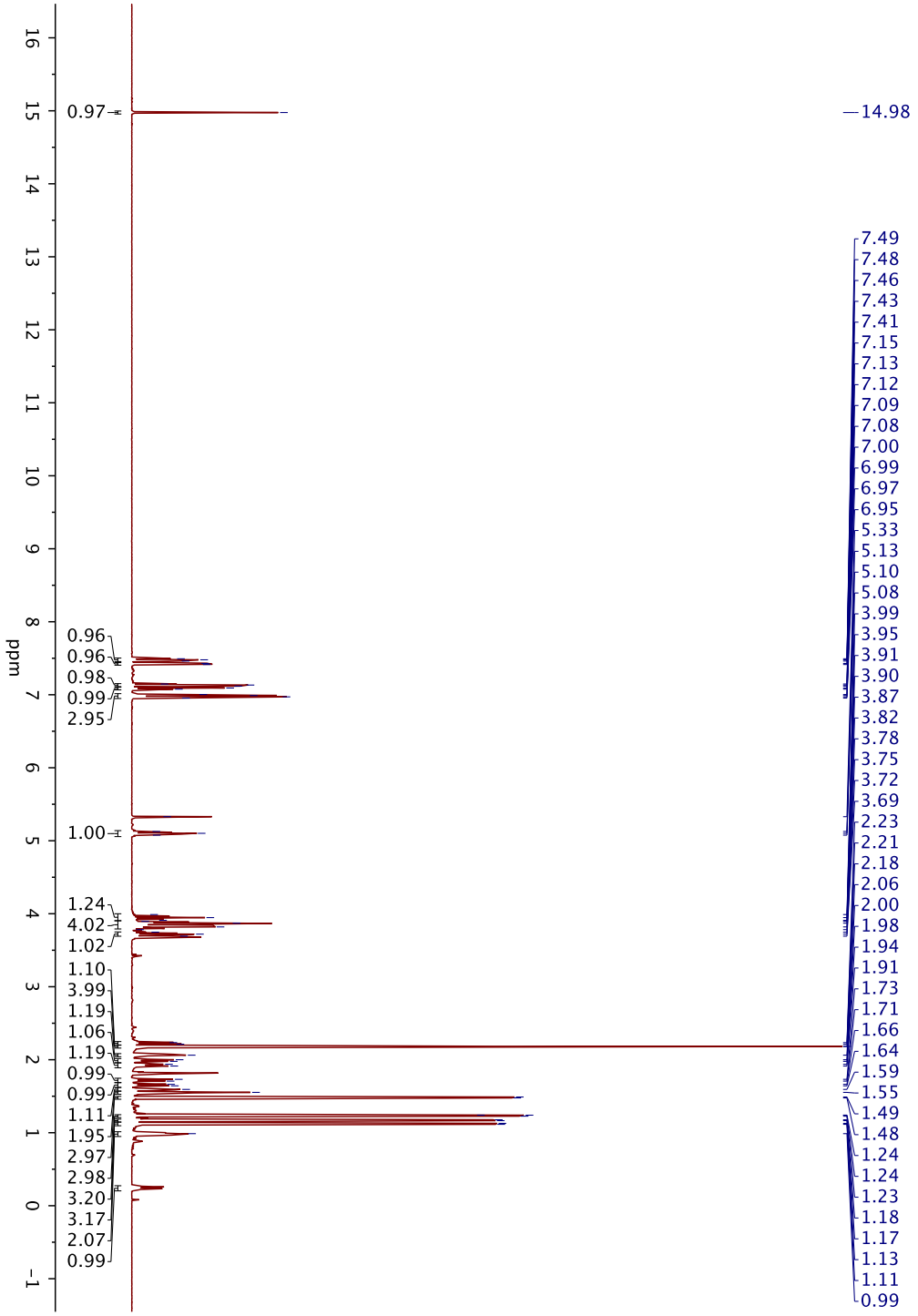


Figure 2.4. ^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of **2.8**.

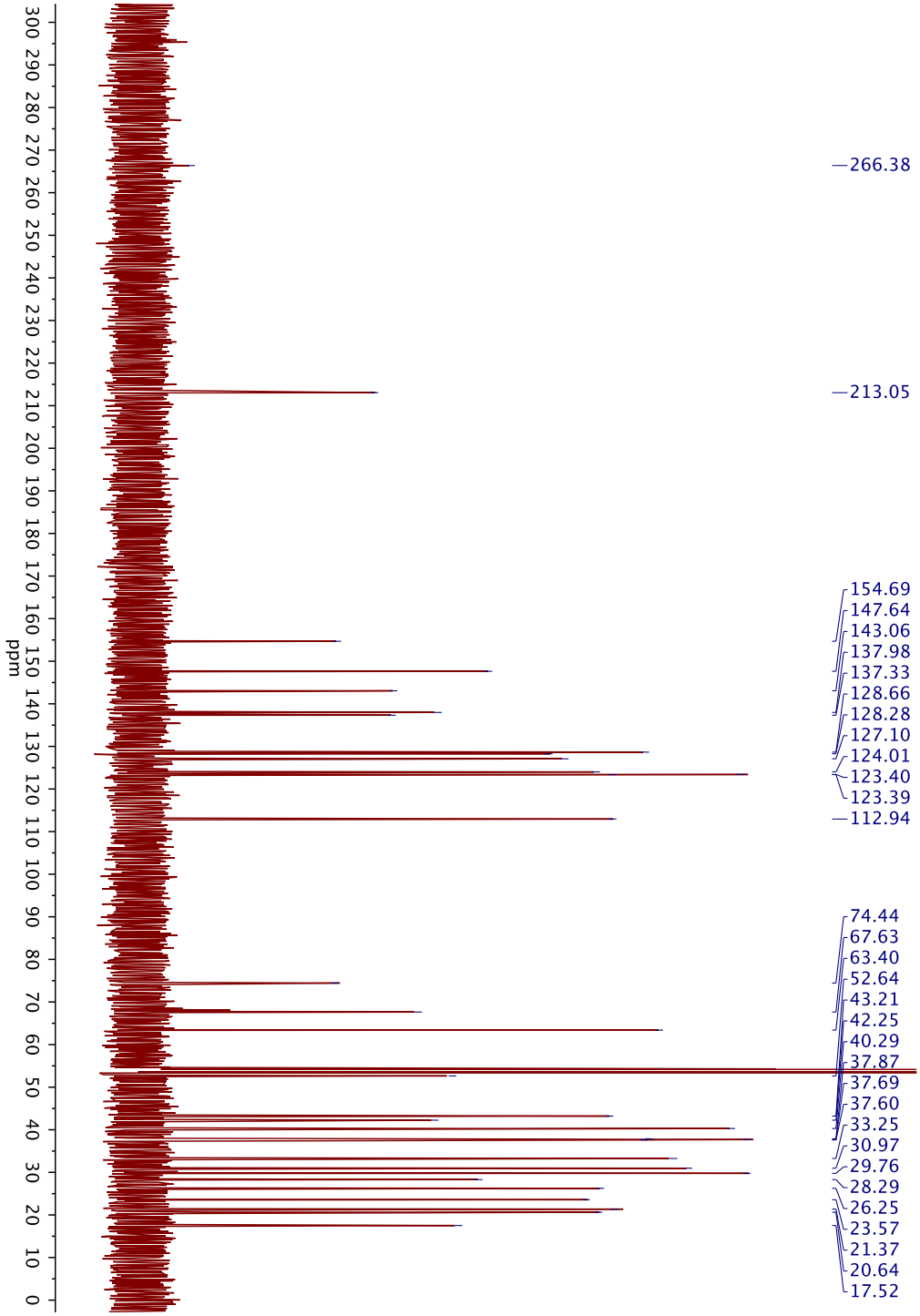


Figure 2.5. ^{13}C NMR (126 MHz, CD_2Cl_2) spectrum of **2.8**.

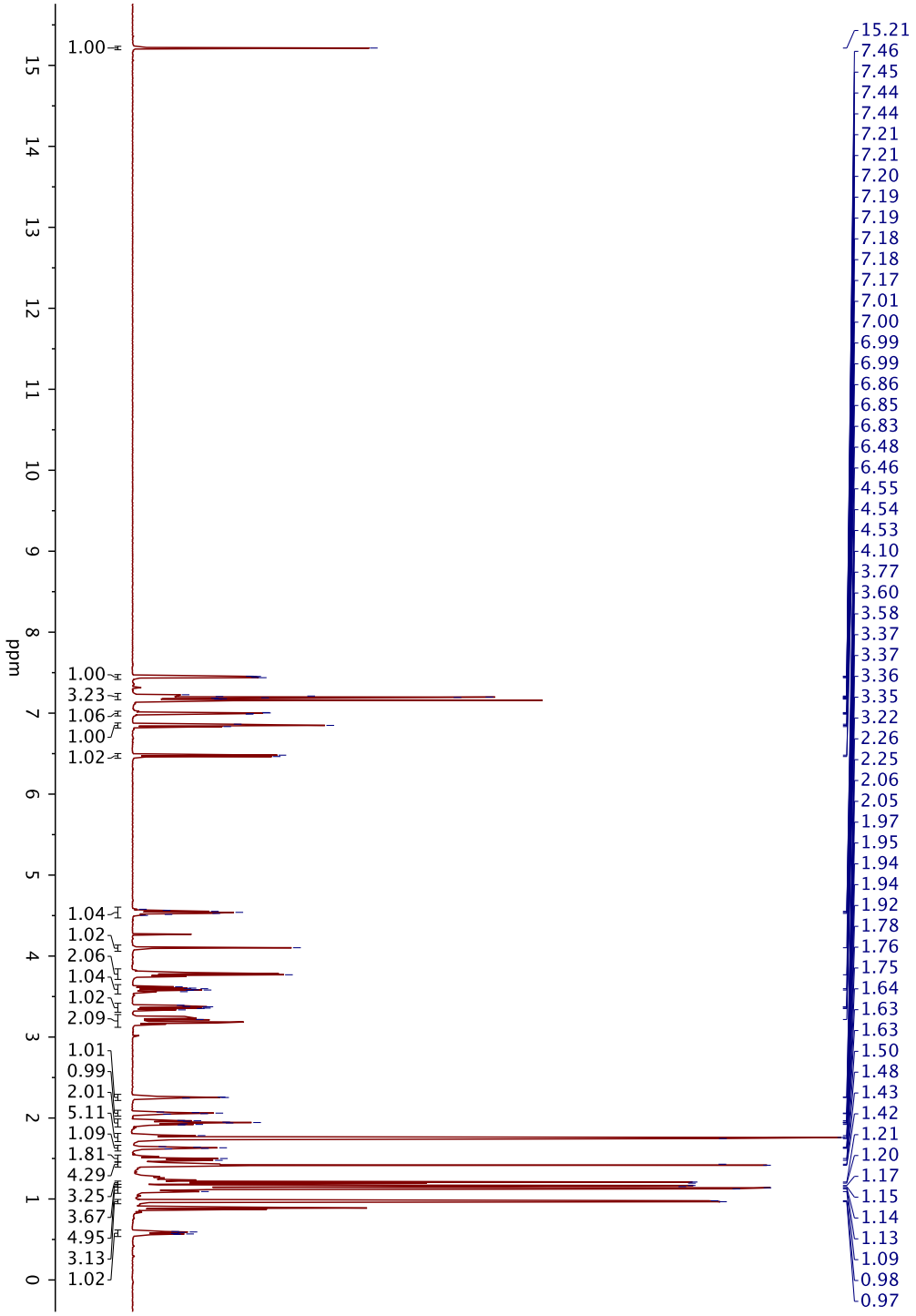


Figure 2.6. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **2.9**.

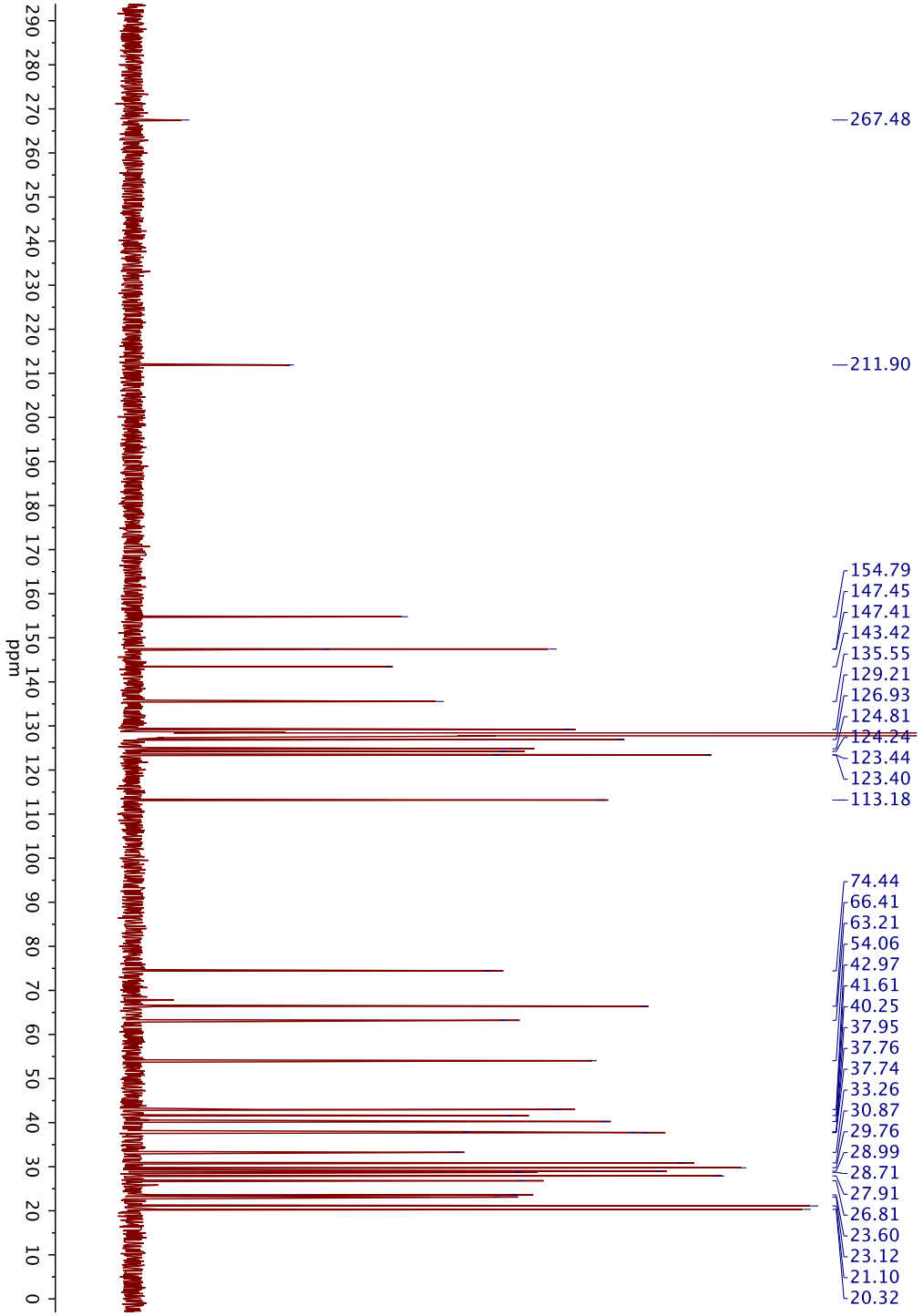


Figure 2.7. ^{13}C (126 MHz, C_6D_6) spectrum of **2.9**.

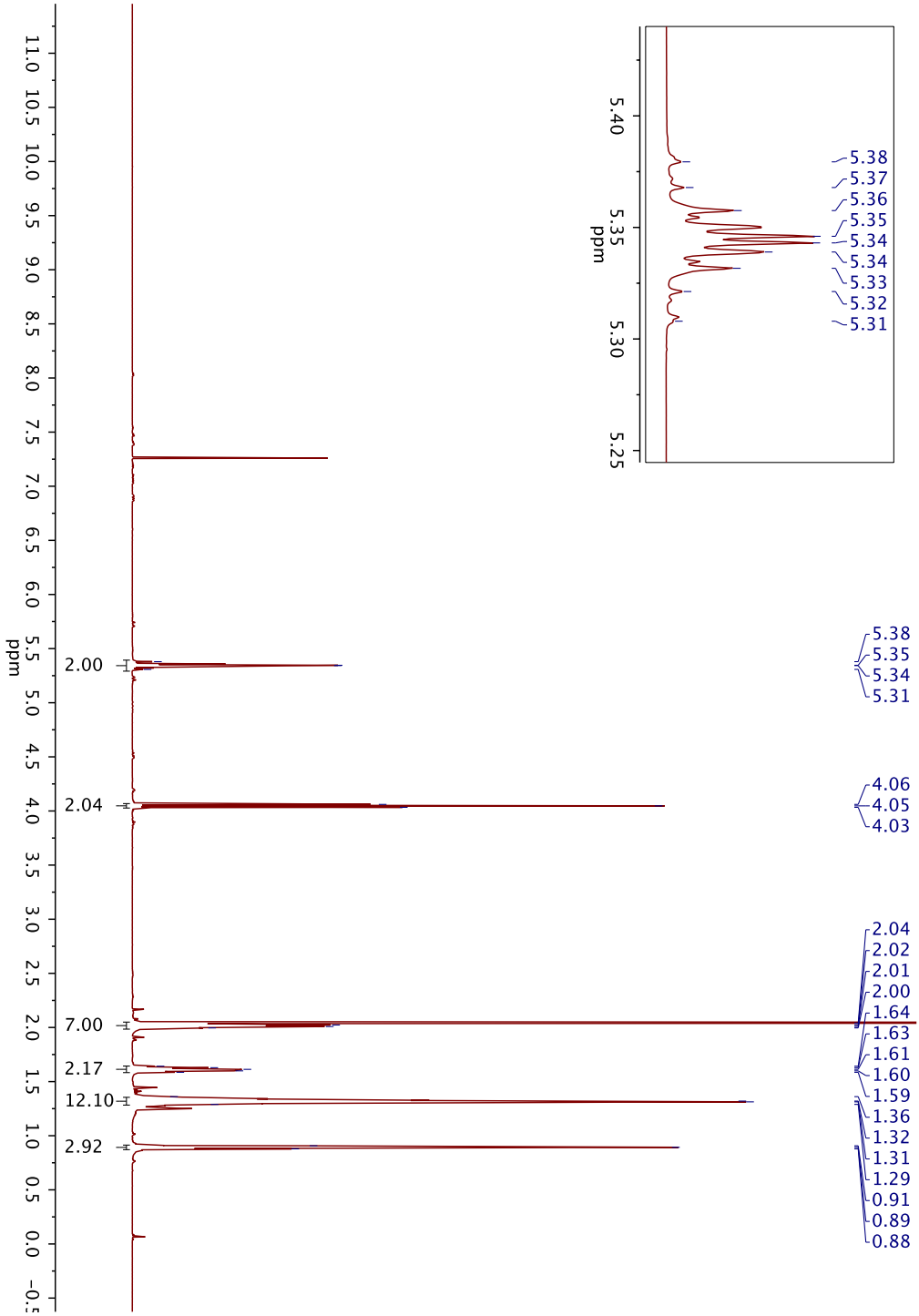


Figure 2.8. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **2.17**.

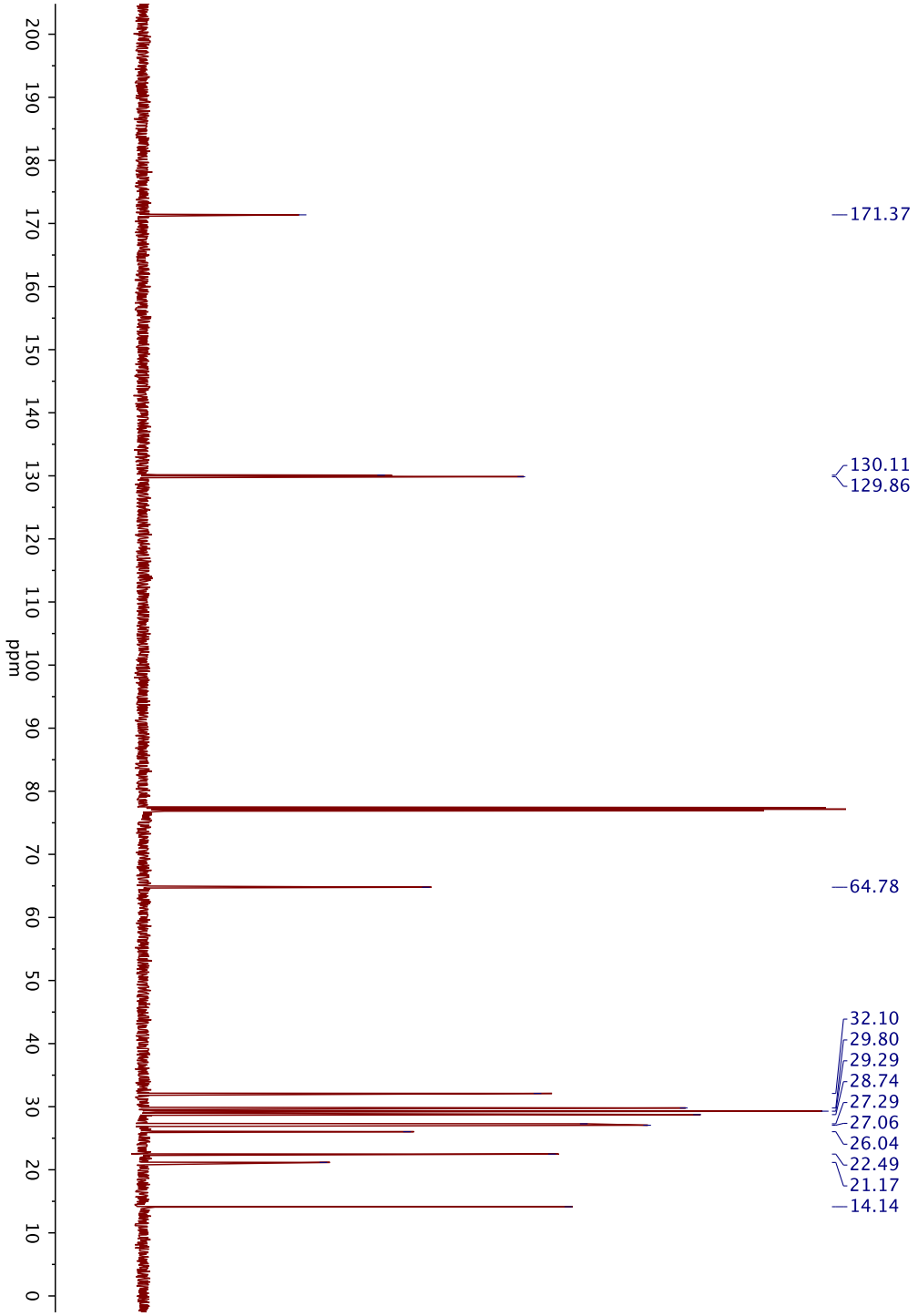


Figure 2.9. ^{13}C (126 MHz, $CDCl_3$) spectrum of **2.17**.

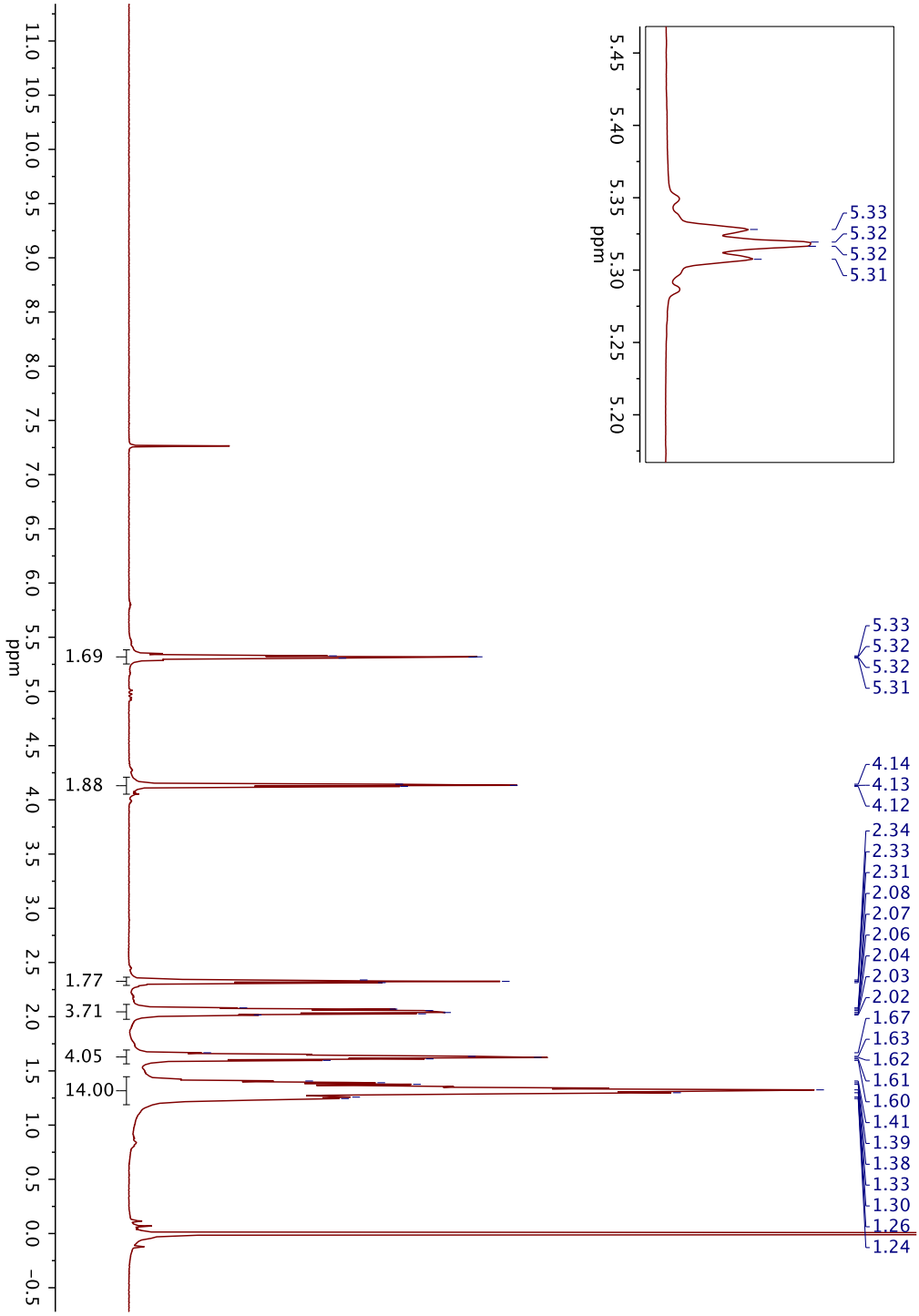


Figure 2.10. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **2.18**.

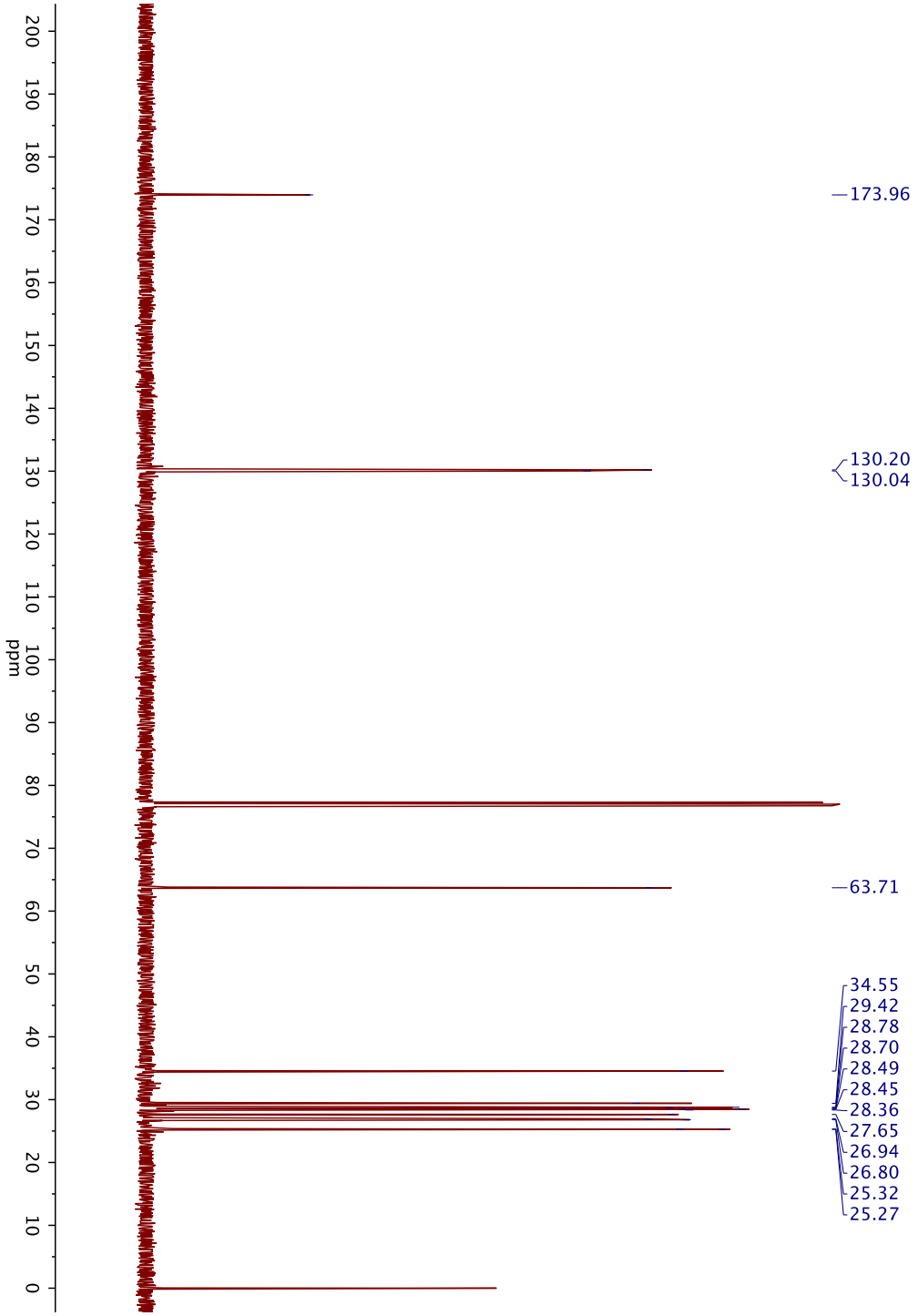


Figure 2.11. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **2.18**.

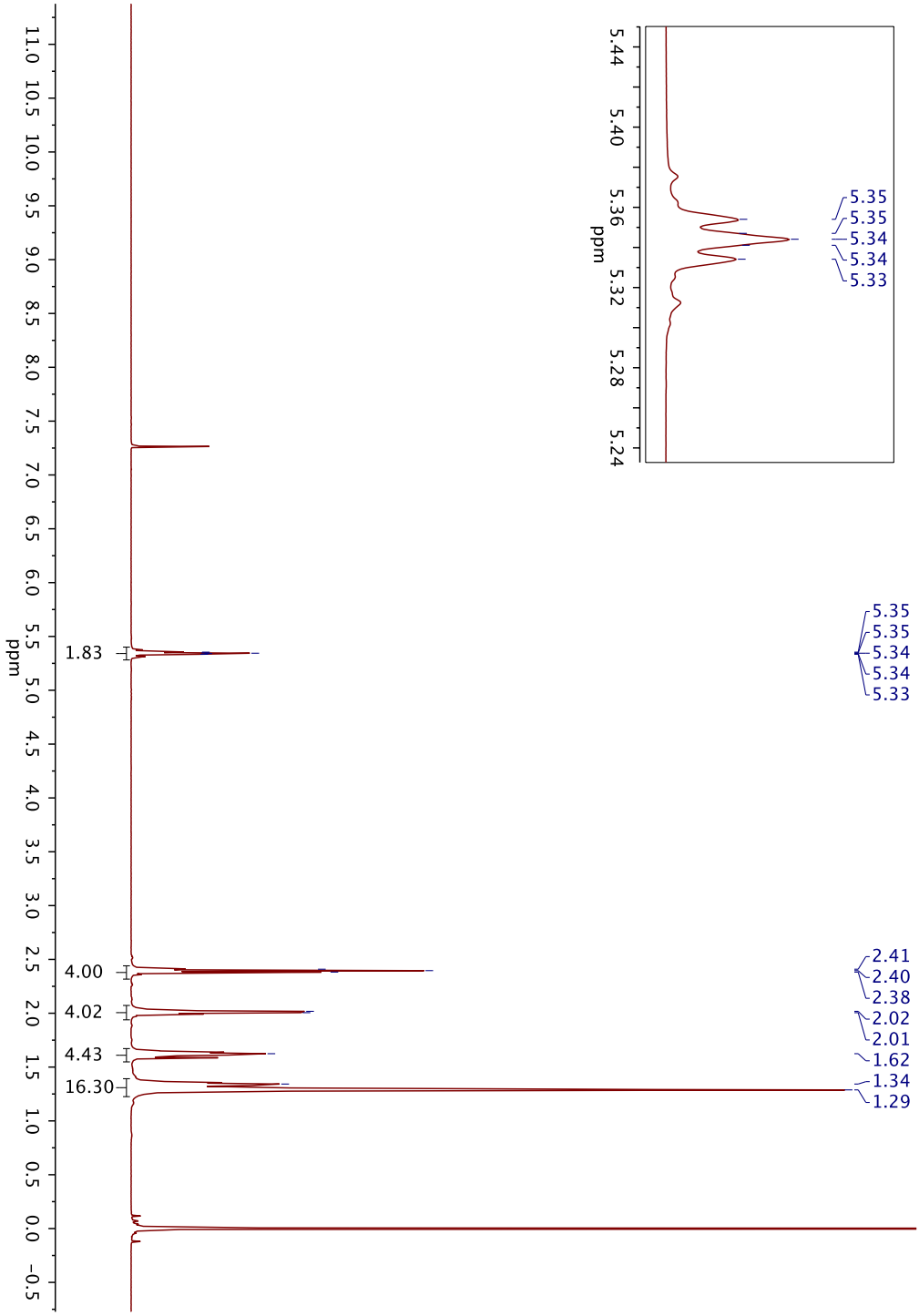


Figure 2.12. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **2.19**.

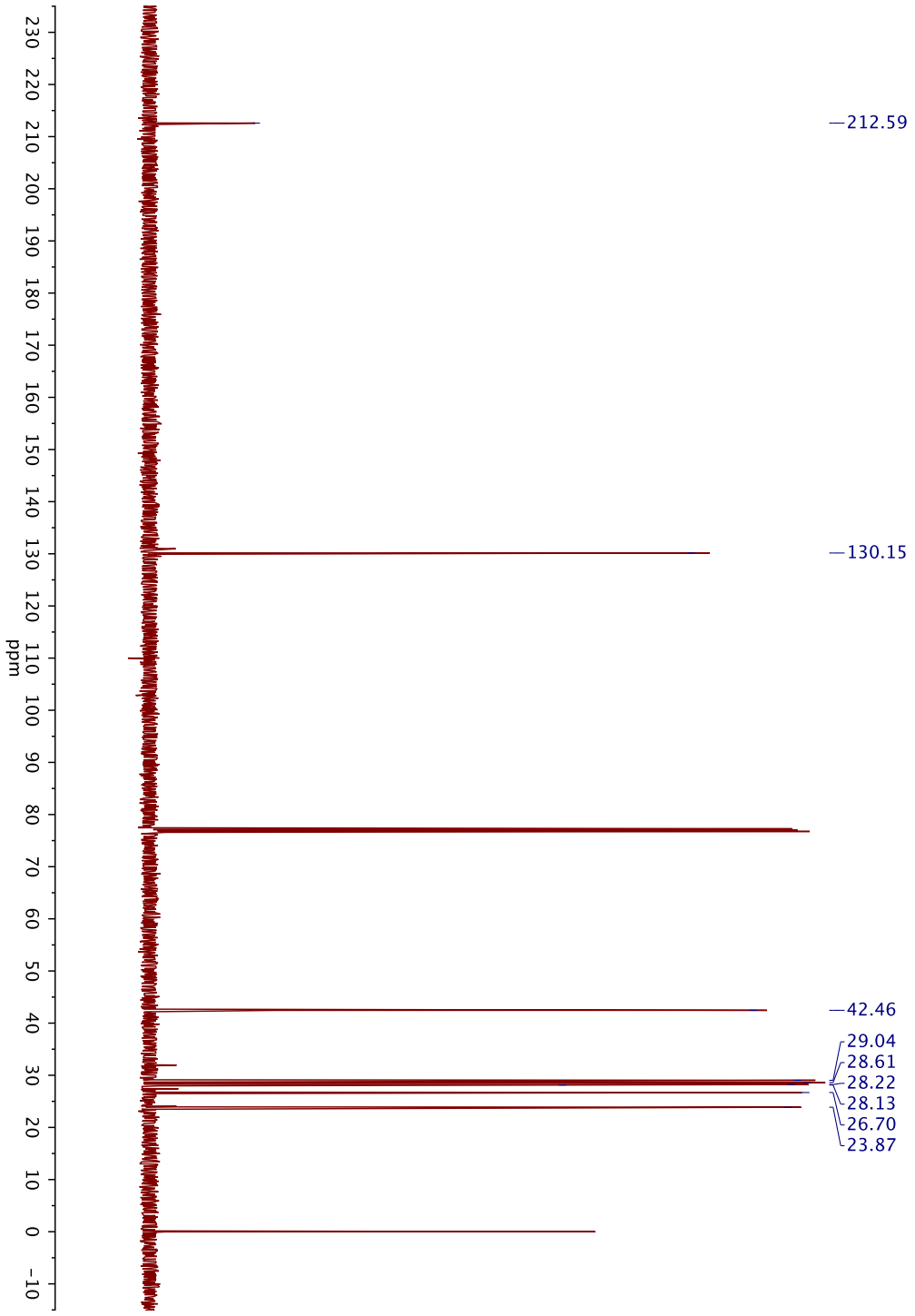


Figure 2.13. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **2.19**.

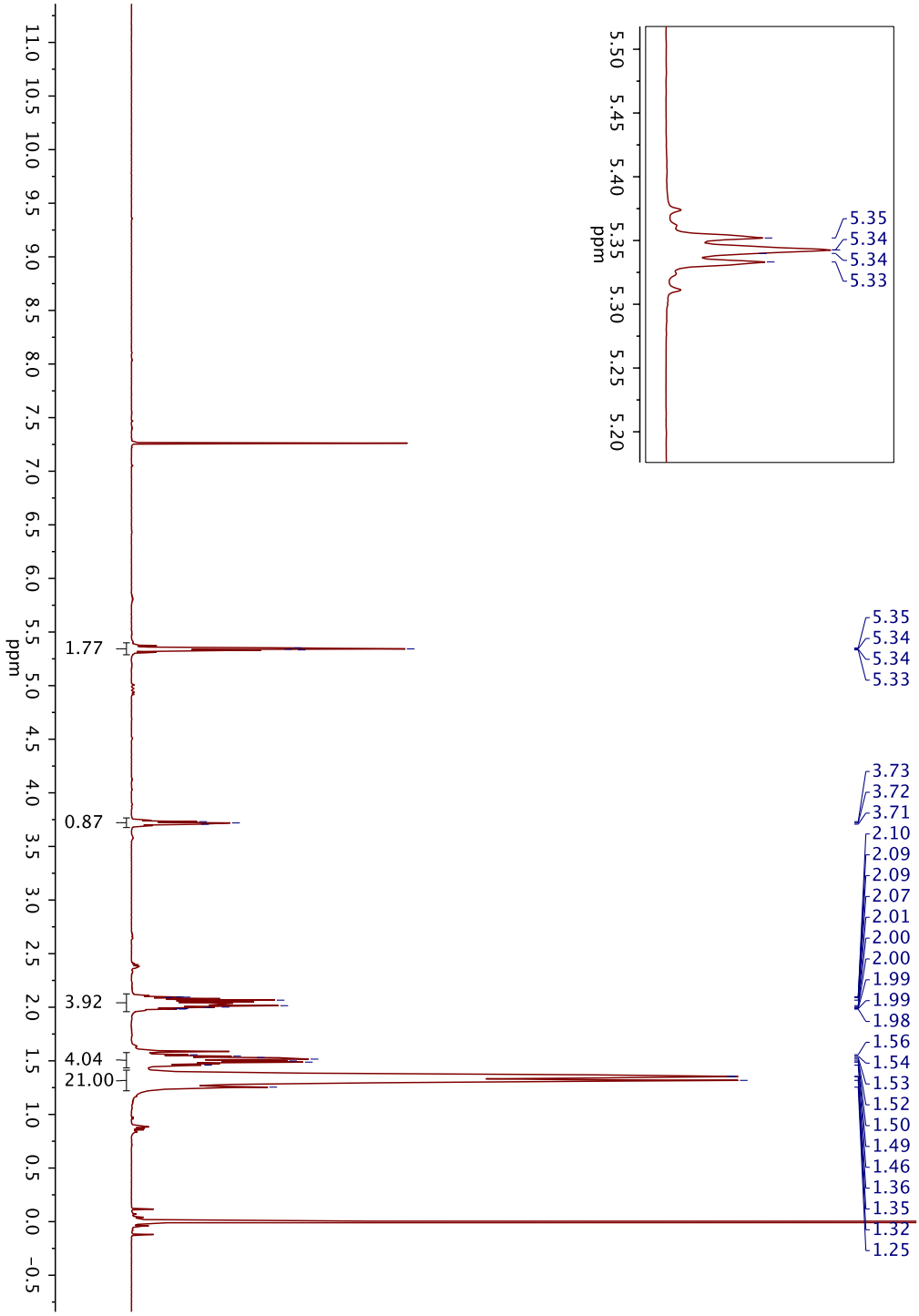


Figure 2.14. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **2.20**.

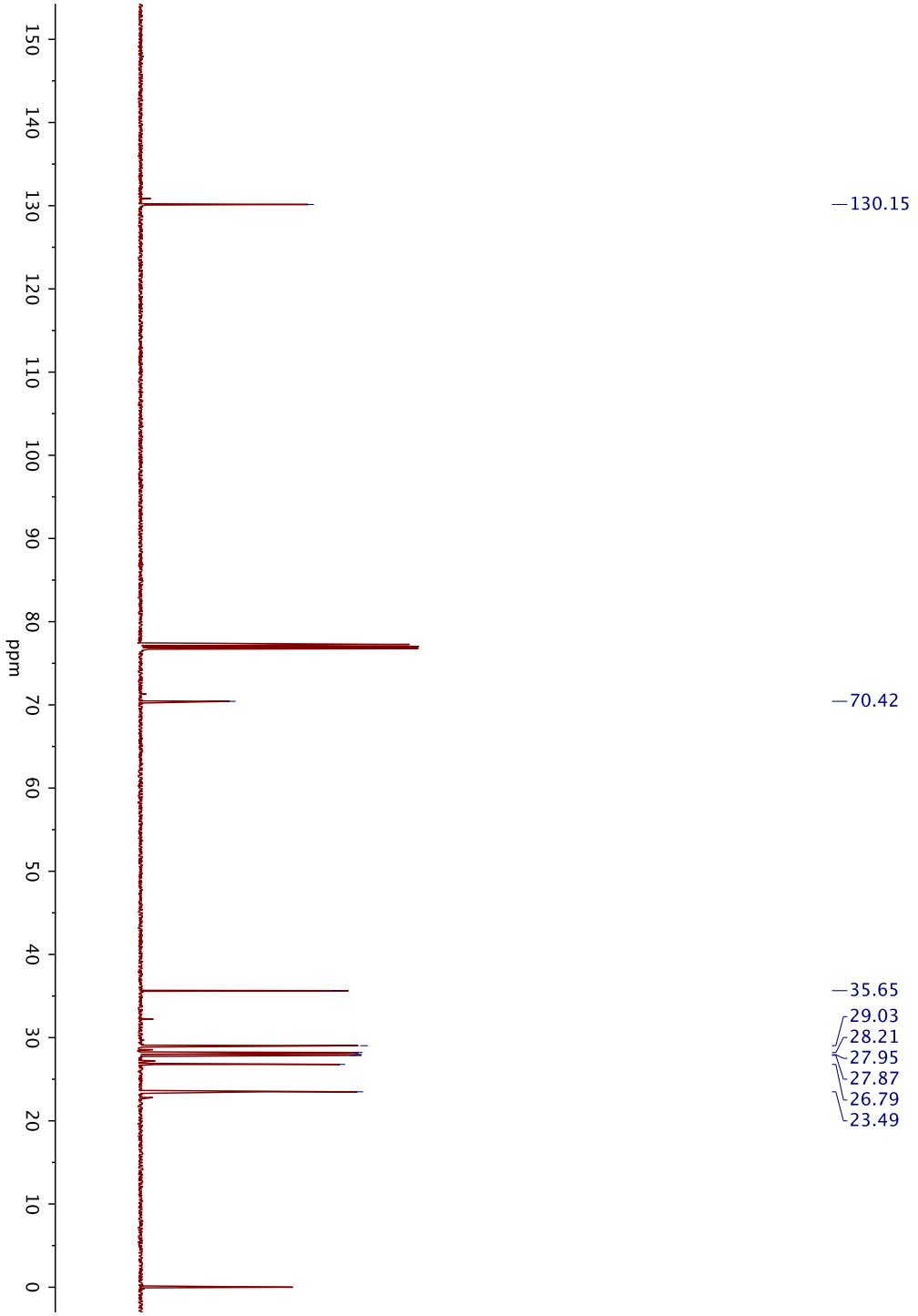


Figure 2.15. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **2.20**.

Chapter 3

Stereoselective Ring-Opening Metathesis Polymerization Using Cyclometalated Ruthenium Metathesis Catalysts

Adapted from:
Rosebrugh, L. E.; Marx, V. M.; Keitz, B. K.; Grubbs, R. H. *J. Am. Chem. Soc.* **2013**, *135*, 10032–10035.

Link to article: 10.1021/ja405559y

Rosebrugh, L. E.; Ahmed, T. S.; Marx, V. M.; Hartung, J.; Liu, P.; López, J. G.; Houk, K. N.; Grubbs, R. H. *J. Am. Chem. Soc.* **2016**, *138*, 1394–1405.

Link to article: 10.1021/jacs.5b12277

Abstract

Using the sodium pivalate method outlined in *Chapter 2*, a series of previously inaccessible ruthenium alkylidene complexes containing a cyclometalated *N*-^{t}Bu group was synthesized. These systems were shown to produce highly *cis*, highly tactic polymers (>95% *cis,syndiotactic* in some cases) via ring-opening metathesis polymerization (ROMP), marking the first time any norbornene- or norbornadiene-based polymer with >95% a single structure had been synthesized using a Ru-based olefin metathesis catalyst. Polymerization of an enantiomerically pure 2,3-dicarboalkoxynorbornadiene confirmed a syndiotactic microstructure. In order to elucidate the exact origin of tacticity in these and related cyclometalated ruthenium alkylidene initiators, experimental and computational methods were employed to develop a complete model of stereoselectivity in ROMP. Of the cyclometalated systems surveyed, most produced highly *cis,syndiotactic* polymers (>95% in many cases). Microstructural errors, when present, were generally in the form

of *trans,syndiotactic* or *cis,isotactic* dyads. These experimental data, in conjunction with computational analyses of the propagation transition states, strongly suggest that polymer stereoselectivity in these systems is a consequence of stereogenic metal control, while errors in the polymer structure primarily result from rotation about the ruthenium alkylidene bond.

Introduction

The precise control of polymer microstructures resulting from the ring-opening metathesis polymerization (ROMP) reactions of mono- and polycyclic olefins is critical for the development of polymers with well-defined characteristics.[1] With respect to norbornene- and norbornadiene-derived ROMP polymers in particular, these microstructures include *cis* or *trans* double bonds; isotactic (*m*) or syndiotactic (*r*) dyads; and, in the case of polymers derived from unsymmetrically substituted monomers, head–tail (HT) dyads or head–head (HH) and tail–tail (TT) dyads (Figure 3.1). These primary structural elements have a significant impact on the physical and mechanical properties of ROMP polymers.[2] For example, *cis,syndiotactic* poly(norbornene) is a crystalline polymer with a high melting point, while atactic *trans*-poly(norbornene) is amorphous and low-melting in comparison.[3] Accordingly, the development of olefin metathesis catalysts capable of producing highly stereoregular polymers (comprised of >95% a single structure) via ROMP is of great interest.

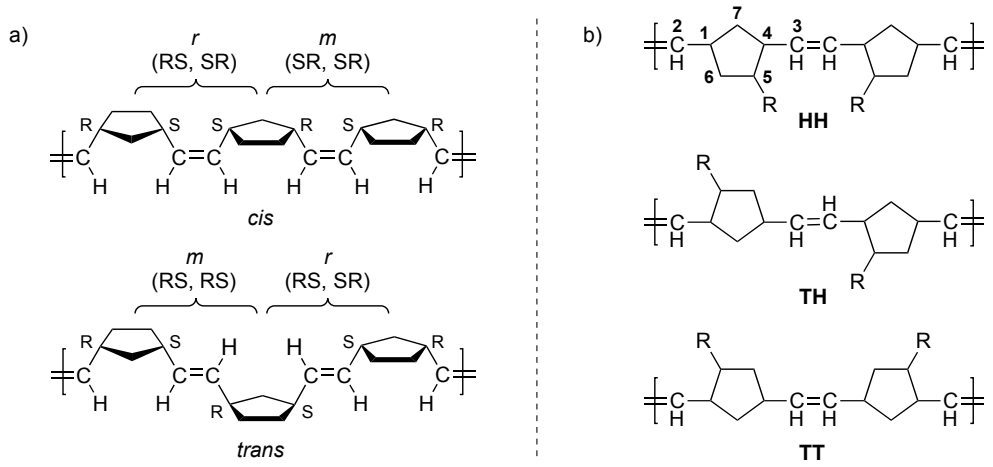


Figure 3.1. (a) Structural possibilities of norbornene-derived ROMP polymers. (b) Head–head (HH), head–tail (HT), and tail–tail (TT) dyads resulting from polymerization of unsymmetrically substituted norbornenes.

Significant microstructural control of norbornene- and norbornadiene-based polymers was first achieved using classical, metal-salt type initiators (e.g., $RuCl_3$, $ReCl_5$, and $OsCl_3$), in which selectivity is usually a result of chain-end control.[1] However, because this type of control results from an influence of the polymer chain on the propagation step, whether through steric crowding or the coordination of recently formed double bonds to the metal center, the stereoselectivity of these systems can vary dramatically depending on the type of monomer and/or reaction conditions employed. As a result, examples of ROMP polymers composed predominately of a single structure produced by these systems are rare.

More recently, the development of molybdenum- and tungsten-based initiators with discrete ligand environments and mechanisms of action has led to the preparation of an increasing number of ROMP polymers with singular microstructures.[4–7] Fully *cis,isotactic* polymers can be produced from a range of norbornene- and norbornadiene-based monomers using W and Mo biphenolate and binaphtholate initiators, which operate

through enantiomorphic site control, a primarily steric directing effect derived from the chirality of the biphenolate or binaphtholate ligand.[5] Additionally, pure *cis,syndiotactic* microstructures are accessible through the use of monoaryloxide pyrrolide (MAP) alkylidene complexes as a result of stereogenic metal control, arising from the inversion of the absolute configuration of the metal center that occurs with each forward metathesis step.[6] Finally, a few examples of predominantly *trans,syndiotactic* and *trans,isotactic* polymers have been prepared with certain Mo initiators as a consequence of chain-end control and a "turnstile-like" nonmetathesis-based polytopal rearrangement, respectivity.[5b,6c,7]

In contrast, only limited control of *cis*/*trans* content and tacticity has been realized with discrete ruthenium alkylidenes, and, much like the classical initiators, this stereochemical control is generally dependent on the use of specialized monomers or reactions conditions.[8] A prevailing theory for the overall lack of stereoselectivity in these systems is that the low calculated barriers of rotation for Ru alkylidenes result in the inability of the Ru=C bond to enforce the steric pressures necessary for the formation of tactic ROMP polymers.[4a,6b,9] Recently, we reported the *Z*-selective ruthenium metathesis catalyst **3.4** (highlighted in *Chapter 1* of this thesis) containing a crucial cyclometalated *N*-heterocyclic carbene (NHC) ligand (Figure 3.2) in which the Ru–C bond is formed via C–H activation induced by the addition of silver pivalate (AgOPiv).[10] This catalyst was shown to give on average 80-95% *cis* content in the ROMP of norbornene and norbornadiene derivatives, thus demonstrating for the first time the *cis*-selective ROMP of a wide range of monomers with a single Ru-based metathesis catalysts.[11] However, these polymers were originally thought to be atactic.

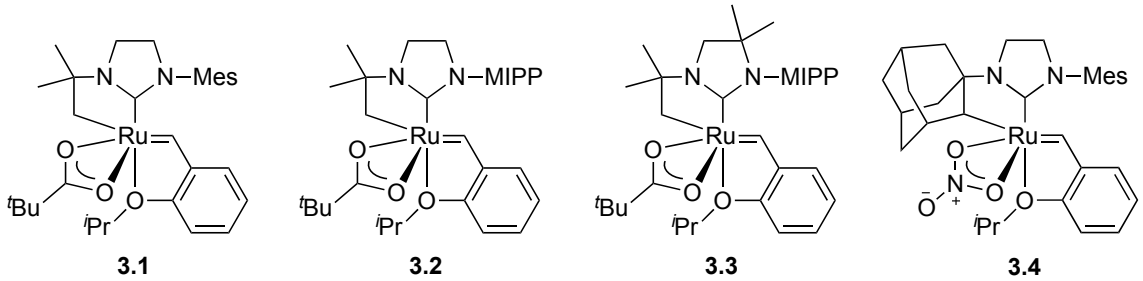


Figure 3.2. Catalysts **3.1–3.4**: Mes = 2,4,6-trimethylphenyl (**3.1**, **3.4**); MIPP = 2-methyl-6-isopropylphenyl (**3.2**, **3.3**).

In the first part of this chapter, a new series of cyclometalated catalysts (**3.1–3.3**) derived from the sodium pivalate (NaOPiv)-mediated C–H activation of an *N*-^{t}Bu group is reported. These complexes display stereoselectivity in ROMP that is unprecedented for Ru-based metathesis catalysts, as they yield polymers that not only have generally higher *cis* contents that those obtained using **3.4** (>95% in many cases) but also are highly syndiotactic. This provides a further demonstration that like their W- and Mo-based counterparts, Ru-based metathesis catalysts are capable of producing polymers with singular microstructures *without* the use of specialized monomers or reaction conditions.

Because the stereochemical information contained in any given ROMP polymer represents a chronological "road map" of every catalytic cycle that took place over the course of the polymerization, careful microstructural analysis of the dyads and triads in a ROMP polymer can shed light on the exact nature of the propagation transitions state(s). ROMP, therefore, presents a powerful tool in which to gain additional insight into the mode-of-action of cyclometalated ruthenium catalysts in *cis*-selective metathesis transformations. To this end, we additionally conducted an experimental and computational study focused on elucidating the precise mechanisms responsible for *cis*-selectivity and tacticity in Ru-based catalysts such as **3.1–3.3** and **3.4** by determining how

variation of the cyclometalated group, *N*-aryl substituent, and X-type ligand affects the resulting polymer microstructure. The results of these mechanistic studies, along with a proposed general model for *cis*-selectivity and tacticity in cyclometalated Ru-based initiators, are detailed in the second part of this chapter. Overall, the results contained in both sections of this chapter provide a fundamental understanding of the mode-of-action of these catalysts and, as such, are generally applicable to other transformations mediated by cyclometalated Ru-based catalysts.

Results and Discussion

Initial Discovery of cis,syndio-Selective Cyclometalated Ruthenium Complexes

As described in *Chapter 2*, the recent development of a milder method of effecting the salt metathesis and C–H activation of cyclometalated ruthenium metathesis catalysts using NaOPiv has enabled the synthesis of previously inaccessible complexes with significant alterations to the cyclometalated *N*-alkyl group of the NHC.[12] Using this new approach, we were able to prepare the less sterically encumbered *N*-^{t}Bu catalysts **3.1–3.3** (Figure 3.2). While a nitrato ligand afforded increased activity, stability, and selectivity to **3.4** compared with other X-type ligands, catalysts **3.1–3.3** were significantly more stable in the pivalate form compared to the analogous nitrato species. It is also important to note that complexes **3.1–3.3** quickly decomposed upon exposure to terminal olefins and were therefore ineffective at mediating cross metathesis. As such, the focus of this investigation is on the effectiveness and stereoselectivity of **3.1–3.3** in ROMP. Single crystal X-ray diffraction of **3.2** confirmed the cyclometallation of the *N*-^{t}Bu substituent as well as the bidentate coordination of the pivalate ligand and also revealed that the *N*-aryl

ring is positioned in such a way that the isopropyl substituent resides on the same face at the benzylidene (Figure 3.3). The structural parameters, including bond lengths and angles, were consistent with those for **3.4** and its pivalate derivative.[10]

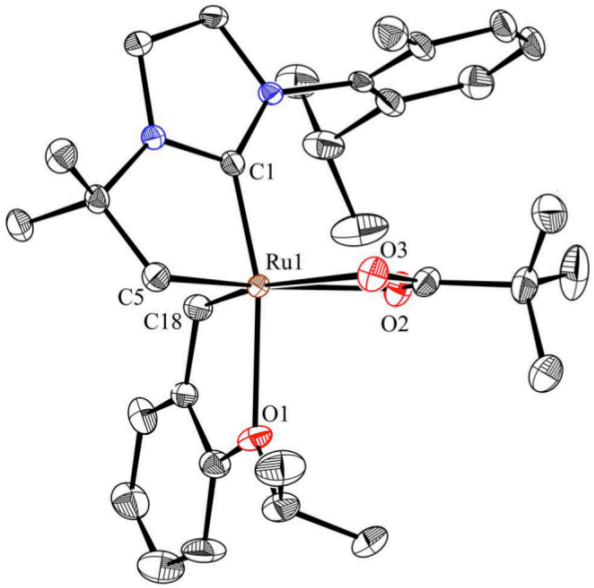
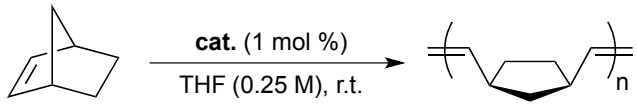


Figure 3.3. Solid-state structure of **3.2** with thermal ellipsoids drawn at 50% probability. For clarity, H atoms have been omitted. Selected bond lengths (Å) for **3.2**: C1–Ru, 1.932; C5–Ru, 2.071; C18–Ru, 1.798; O1–Ru, 2.334; O2–Ru, 2.202; O3–Ru, 2.398.

We initiated our ROMP studies by adding **3.1** (1 mol %) to a solution of norbornene (NBE, **3.5**) in tetrahydrofuran (THF) (0.25 M) at room temperature (r.t.), upon which the resulting solution rapidly became viscous. Importantly, while catalyst solutions were prepared in the glovebox for convenience, **3.1** was determined to be relatively air-stable in the solid state, exhibiting minimal decomposition after exposure to air for 3 h. ^{1}H NMR spectroscopy revealed that the isolated **poly(3.5)** produced by **3.1** was almost exclusively *cis* (σ_c = 0.97; Table 3.1).[13] While resolution of the *m*/*r* peaks is not observed in the NMR spectra of poly(NBE), a qualitative distinction between syndiotactic and atactic microstructures can be made in the case of highly *cis* poly(NBE)

(>90%) by looking at the relative peak heights of the signals corresponding to the $C_{1,4}$ and $C_{5,6}$ carbons: approximately equal heights and widths correspond to a highly syndiotactic polymer, while differing heights/widths suggest the presence of *m* dyads in the sample.[14] A sample in which the $C_{1,4}$ line is half the height and twice the width of the $C_{5,6}$ peak is completely atactic. Examination of the $C_{1,4}$ and $C_{5,6}$ peaks in the ^{13}C NMR spectrum of **poly(3.5)** prepared with **3.1** showed nearly equal heights and widths consistent with highly syndiotactic poly(NBE) (see Figure 3.14 in the Supporting Information [SI] section).

Table 3.1. Polymerization of Norbornene (3.5) with Catalysts 3.1–3.3



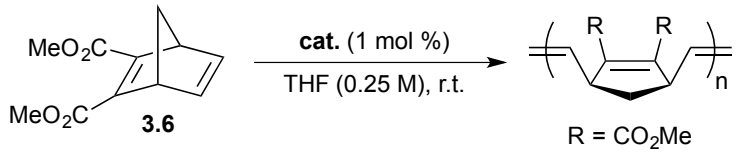
3.5

catalyst	σ_c[a]	M_n (kDa)[b]	PDI[b]
3.1	0.97	605[c]	1.41
3.2	0.99	521[c]	1.49
3.3	0.99	424[c]	1.45

[a]Fraction of double bonds having *cis* configuration; average of four values derived from $C_{2,3}$, $C_{1,4}$, C_7, and $C_{5,6}$ resonances, with agreement generally within ±0.02. [b]Determined by gel-permeation chromatography (GPC) with a multiangle light scattering detector. [c]The specific refractive index increment (d*n*/d*c*) was determined to be 0.139 ± 0.005 mL/g.

In order to quantify the extent of tacticity in polymers produced by these initiators, we turned to the more complex monomer 2,3-dicarbomethoxynorbornadiene (DCMNBD, **3.6**). DCMNBD has been used extensively for this purpose, as the *cis* $C_{1,4}$ peak displays *m*/*r* splitting that is sufficiently resolved for quantitative analysis.[15] **Poly(3.6)** produced by catalyst **3.1** was found to be highly *cis* (σ_c = 0.99) and highly syndiotactic (the *cis* regions were comprised of 99% *r* dyads) (see Figure 3.7a in the second portion of this chapter) (Table 3.2).

Table 3.2. Polymerization of Monomer 3.6 with Catalysts 3.1–3.3



catalyst	σ_c[a]	% *r* (*cis*)[b]
3.1	0.99	99
3.2	>0.99	97
3.3	>0.99	98

[a]Fraction of double bonds having *cis* configuration; average of two values derived from $C_{2,3}$ and $C_{1,4}$ resonances, with agreement generally within ±0.02. [b]Derived from *cis* $C_{1,4}$ peaks.

To probe the effect of the symmetry of the *N*-aryl group on *cis* content and tacticity, we next evaluated catalysts **3.2** and **3.3** containing a cyclometalated *N*-^{t}Bu group as in **3.1** but also an asymmetric *N*-aryl group (Figure 3.1). The geminal dimethyl backbone of **3.3** was installed to prevent any rotation of the *N*-aryl group that might occur in **3.2**. Similar results to **3.1** were observed in the polymerization of **3.5** with catalysts **3.2** and **3.3**; both produced poly(NBE) that was highly *cis* (σ_c = 0.99) and consistent with highly syndiotactic poly(NBE) by NMR (Table 3.1). Polymerization of **3.6** with catalysts **3.2** and **3.3** also yielded samples of **poly(3.6)** that were composed of almost exclusively *cis, r* dyads (97% and 98%, respectively) (Table 3.2).

As had previously been observed with **3.4**, the experimental number-average molecular weights (M_n) for **poly(3.5)** prepared using catalysts **3.1–3.3** were significantly higher than the theoretical values (Table 3.1). This indicates that the propagation rate constant (k_p) of **3.5** exceeds the initiation rate constants (k_i) of **3.1–3.3**, which would lead to the broad polydispersity indexes (PDIs) observed; this is likely a result of incomplete catalyst initiation. This might be expected on the basis of the relatively low k_i values of **3.1–3.3**: The initiation rate constants of catalysts **3.1–3.3** at 25 °C were calculated to be

2.8 x 10^{-3}, 4.1 x 10^{-4}, and 1.1 x 10^{-4} s^{-1}, respectively. For comparison, k_i = 8.4 x 10^{-4} s^{-1} for catalyst **3.4** and k_i > 0.2 s^{-1} for $RuCl_2(C_5H_5N)_2(IMesH_2)(CHPh)$, the latter of which is the preferred catalyst for ROMP.[16]

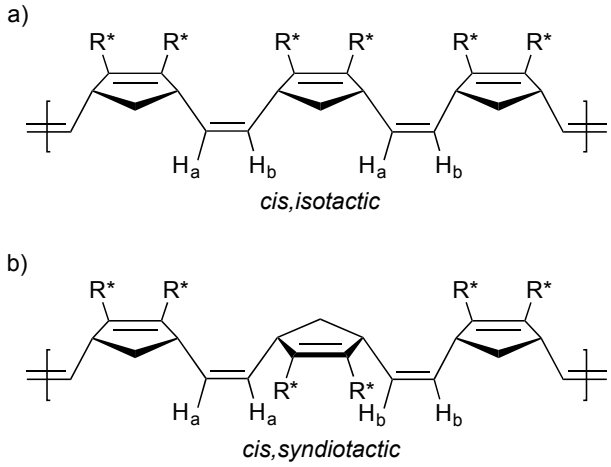
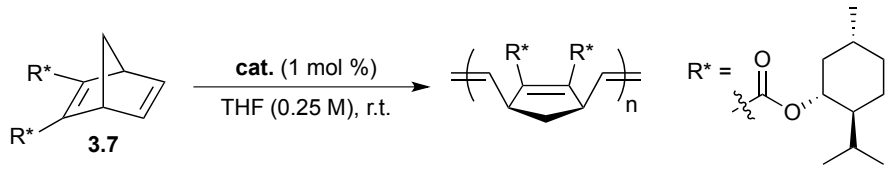


Figure 3.4. Olefinic protons in (a) *cis,isotactic* and (b) *cis,syndiotactic* polymers made from an enantiomerically pure 2,3-disubstituted norbornadiene.

To further verify the syndiotactic nature of the norbornene- and norbornadiene-based polymers produced by catalysts **3.1–3.3**, we turned to chiral monomer **3.7**. Due to the lack of mirror planes relating the monomeric unit in polymers derived from monomer **3.7**, it is expected that if samples of **poly(3.7)** produced by **3.1–3.3** were *cis,isotactic*, then the olefinic protons would be inequivalent (Figure 3.4a), and a coupling characteristic of olefinic protons would be observed in a COSY NMR spectrum.[5b] Conversely, in *cis,syndiotactic* **poly(3.7)**, the *cis* olefinic protons are related by a C_2 axis passing through the midpoint of the double bond, meaning the protons would be equivalent and therefore uncoupled (Figure 3.4b). Samples of **poly(3.7)** produced by catalysts **3.1–3.3** were only moderately *cis* (σ_c = 0.76–0.83) (Table 3.3); however, no coupling was observed by COSY NMR between the *cis* olefinic protons (clearly resolved from the *trans* resonances in the COSY spectrum) confirming that the *cis* regions of

poly(3.7) were syndiotactic in all cases (Figure 3.5). Furthermore, the *trans* olefinic protons were also uncoupled, similarly consistent with a syndiotactic microstructure.

Table 3.3. Polymerization of Monomer 3.7 with Catalysts 3.1–3.3



catalyst	σ_c^a
3.1	0.76
3.2	0.78
3.3	0.83

[a]Fraction of double bonds having *cis* configuration; derived from olefinic proton resonances in ^{1}H NMR spectrum.

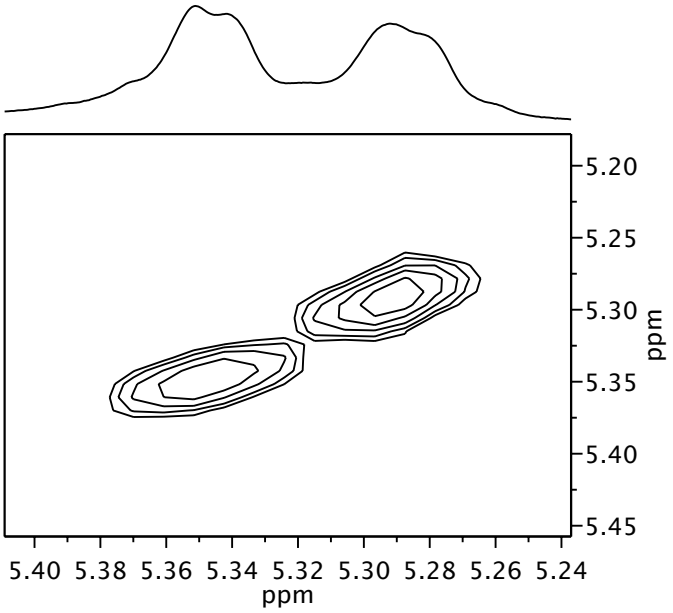


Figure 3.5. *Cis* olefinic proton region of the COSY spectrum of **poly(3.7)** prepared with catalyst **3.1**. The absence of olefinic coupling suggests that the *cis* regions of the polymer are predominantly syndiotactic.

Finally, we briefly explored the physical properties of the tactic ROMP polymers in comparison with their atactic counterparts using differential scanning calorimetry

(DSC) and thermogravimetric analysis (TGA). The glass-transition temperature (T_g) of atactic *trans*-poly(NBE) is 37 °C.[3a] As expected, the T_g of *cis,syndiotactic* **poly(3.5)** produced by catalyst **3.1** was significantly higher at ca. 70 °C, consistent with a higher packing order due to the increased stereoregularity of the polymer. Both the *trans,atactic* and *cis,syndiotactic* polymers decomposed at ca. 430 °C (see the SI).

Mechanistic Studies into cis,syndio-Selective ROMP Mediated by Cyclometalated Ruthenium Complexes

In order to elucidate the origin of tacticity in catalysts **3.1–3.3** and understand the enhanced stereoselectivity in these initiators relative to **3.4**, we undertook a combined experimental and computational study in collaboration with the Houk group at the University of California, Los Angeles (UCLA). Initial work focused on examining the microstructures of polymers produced by a selection of cyclometalated catalysts with varying NHC architectures and X-type ligands in order to gain a comprehensive view of activity and selectivity in this class of complexes. The information gained from this investigation then informed the computational work, which examined the propagation transition states of a select few cyclometalated complexes to better understand the role of alkylidene isomerization in ROMP stereoselectivity. Combined, these results have allowed us to develop a complete model for *cis*-selectivity and tacticity in cyclometalated Ru-based initiators such as **3.1–3.3** and **3.4**.

General Reactivity, *cis*-Selectivity, and Blockiness of ROMP Polymers Produced by Cyclometalated Ruthenium Metathesis Catalysts: Reactions of a variety of cyclometalated catalysts (**3.1**, **3.4**, **3.8–3.13**, Figure 3.6) with norbornene (**3.5**) were

screened to study general reactivity and *cis*-selectivity.[13] Consistent with previous ROMP reactions, all polymerizations were performed at r.t. in THF (0.25 M) at a ratio of [monomer]/[initiator] = 100 (1 mol %). In general, quantitative conversion of monomer to polymer was observed when using catalysts **3.1**, **3.4**, and **3.8–3.11**, whereas monodentate catalysts **3.12** and **3.13** were less active that their bidentate counterparts, giving only 20-50% yield. All of the catalysts were found to yield polymers with moderate to high *cis* contents (σ_c > 0.95 in many cases) (Table 3.4).

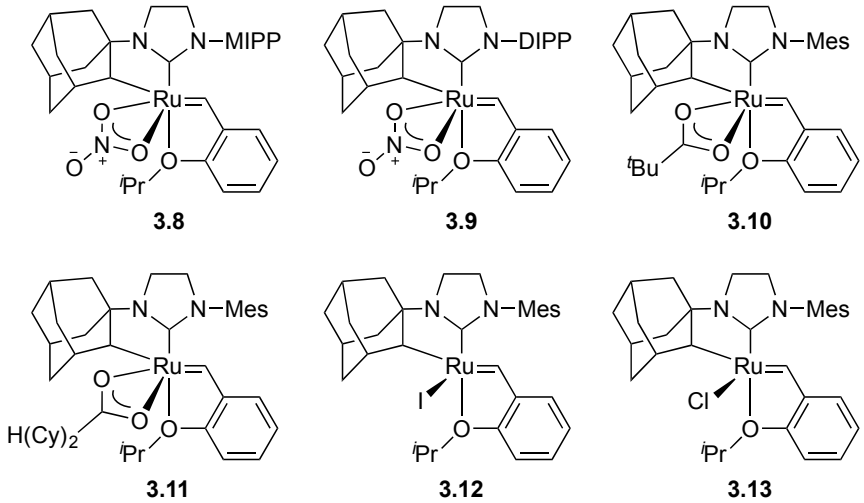
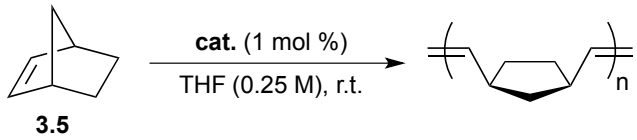


Figure 3.6. Catalysts **3.8–3.13**: MIPP = 2,6-methylisopropylphenyl (**3.8**); DIPP = 2,6-diisopropylphenyl (**3.9**); Mes = 2,4,6-trimethylphenyl (**3.10–3.13**).

Table 3.4. Polymerization of Norbornene (3.5) with Catalysts 3.1, 3.4, and 3.8–3.13



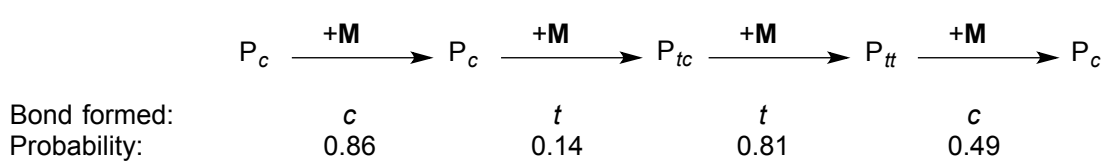
catalyst	σ_c[a]	r_t[b]	r_c[b]	$r_t r_c$
3.1	0.97	--	--	--
3.4	0.92	0.27	6.5	1.7
3.8	0.97	--	--	--
3.9	0.99	--	--	--
3.10	0.74	0.52	2.4	1.2
3.11	0.74	0.94	3.9	3.7
3.12	0.88	0.45	6.5	2.9
3.13	0.82	0.53	4.8	2.5

[a]Fraction of double bonds having *cis* configuration; average of four values derived from $C_{2,3}$, $C_{1,4}$, C_7, and $C_{5,6}$ resonances, with agreement generally within ±0.02. [b]Average of two values derived from $C_{1,4}$ and $C_{5,6}$ peaks.

In the case of poly(NBE) and related polymers, the distribution of *cis* and *trans* double bonds in a given chain can be readily determined from ^{13}C NMR, which provides information on the proportions of double-bond dyads in the polymer.[13b,17] This distribution, known as blockiness, is represented by the relationship $r_t r_c$, where r_t = (*tt*)/(*tc*) and r_c = (*cc*)/(*ct*). Understanding the nature of the double bond distribution in any ROMP polymer affords significant mechanistic insight: a random distribution, characterized by $r_t r_c = 1$, suggests that the formation of a *cis* double bond is independent of any previously formed double bonds, whereas a blocky distribution ($r_t r_c > 1$) may indicate some influence of the polymer chain in the propagation step (i.e., chain-end control).

In general, predominantly *cis* ($\sigma_c > 0.50$) polymers of norbornene and related monomers formed by early generation ROMP catalysts are somewhat-to-highly blocky, with values of $r_t r_c$ ranging from 5 to 8 or more.[17a] Significantly, r_t is almost always

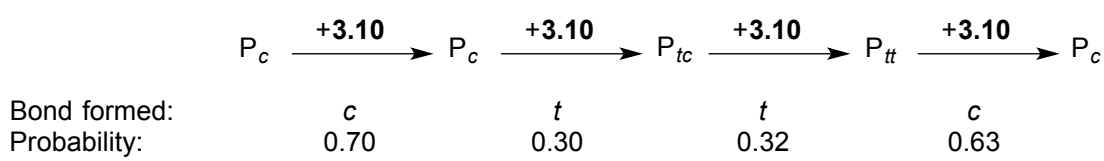
greater that 1 (i.e., *tt* > *tc*), indicating a preference for *trans* double bonds to occur in pairs. One postulate for this observed behavior is the existence of multiple kinetically distinct propagating species each having a different selectivity for the formation of *cis* or *trans* double bonds. This is supported by careful examination of the proportions of double bond triads in the polymers (readily derived from the known proportions of dyads), from which it can be shown that in the classical systems, the probability of *cis* or *trans* double bond formation at any given propagation step varies greatly depending on the identity of the last- and/or second-to-last formed double bond; this is presumably due to some interaction of these recently formed double bonds with the metal center or alkylidene.[18] Propagating species in which the most recently formed double bond is *cis* (P_c) are highly *cis*-directing, whereas the selectivity of species in which the last-formed double bond is *trans* depends on whether the configuration of the penultimate double bond is *cis* (P_{tc}, highly *trans*-directing) or *trans* (P_{tt}, essentially nonselective) (Scheme 3.1).[1b] These relative selectivities are ultimately responsible for the high incidence of *trans–trans* double bond pairs observed in poly(NBE) samples produced by many classical metathesis catalysts.



Scheme 3.1. Probabilities of forming *cis* or *trans* double bonds in the $W(CO)_6/h\nu$-catalyzed ROMP of norbornene (**3.5**). P_c refers to a propagating species that has just formed a *cis* double bond, while P_{tc} and P_{tt} describe species that have just formed a *trans* double bond but have different penultimate double bonds (*cis* and *trans*, respectively). Adapted with permission from ref. 1b. Copyright 1997 Academic Press.

Values of $r_t r_c$ calculated for the poly(NBE)s produced by catalysts **3.1**, **3.4**, and **3.8–3.13** ranged from 1.2 to 3.7 (Table 3.4), indicating only modest deviations from

randomness in the *cis*/*trans* double bond distributions of the polymers. Moreover, all of the highly *cis* polymers produced by catalysts **3.1**, **3.4**, and **3.8–3.13** had r_t values that were less than unity; in conjunction with the overall low values of $r_t r_c$, these low r_t values suggest that *trans* double bonds occur as single, random errors throughout the polymers rather than in pairs as observed with the classical systems. Furthermore, calculation of the probabilities of forming a *cis* or *trans* double bond according to the identity of the last- or last-but-one double bond revealed no significant dependence of *cis*-selectivity on the configurations of these previously formed double bonds in the polymerization of norbornene (Scheme 3.2). This suggests that chain-end control is most likely *not* the driving force behind the stereoselectivity in ROMP observed with initiators **3.1**, **3.4**, and **3.8–3.13**.

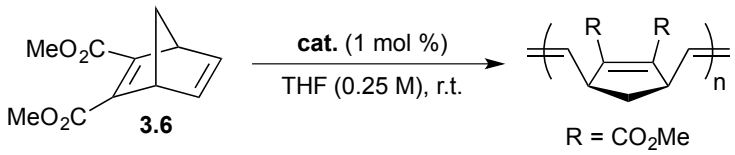


Scheme 3.2. Probabilities of forming *cis* or *trans* double bonds in the ROMP of norbornene (**3.5**) by catalyst **3.10** (σ_c = 0.74).

Tacticity and Head–Tail Bias of ROMP Polymers Produced by Catalysts 3.1, 3.4, and 3.8–3.13: To fully understand the origins of selectivity in cyclometalated catalysts **3.1**, **3.4**, and **3.8–3.13**, a complete microstructural picture, taking into account not only *cis*/*trans* content but also tacticity and, in some cases, head–tail selectivity across dyads and triads, is essential. As such, we once again turned to DCMNBD (**3.6**) in order to quantify tacticity in the polymers produced by these systems. For polymerizations of **3.6** with catalysts **3.1**, **3.4**, and **3.8–3.13**, the fraction of *cis, r* dyads in each highly *cis* polymer was easily determined using the *m*/*r* splitting displayed by the *cis* $C_{1,4}$ peak

(Table 3.5; Figure 3.7). Surprisingly, the *cis* portions of the polymers produced by catalysts **3.4** and **3.8–3.13** were found to be highly syndiotactic and not atactic as previously thought. In fact, monodentate catalysts **3.12** and **3.13** yielded polymers that were almost exclusively *cis,syndiotactic*.

Table 3.5. Polymerization of Monomer 3.6 with Catalysts 3.1, 3.4, and 3.8–3.13



catalyst	σ_c^a	% *r* (*cis*)[b]
3.1	0.99	99
3.4	0.87	85
3.8	0.84	84
3.9	0.91	85
3.10	0.72	68
3.11	0.65	68
3.12	0.98	96
3.13	0.94	96

[a]Fraction of double bonds having *cis* configuration; average of two values derived from $C_{2,3}$ and $C_{1,4}$ resonances, with agreement generally within ±0.02. [b]Derived from *cis* $C_{1,4}$ peaks.

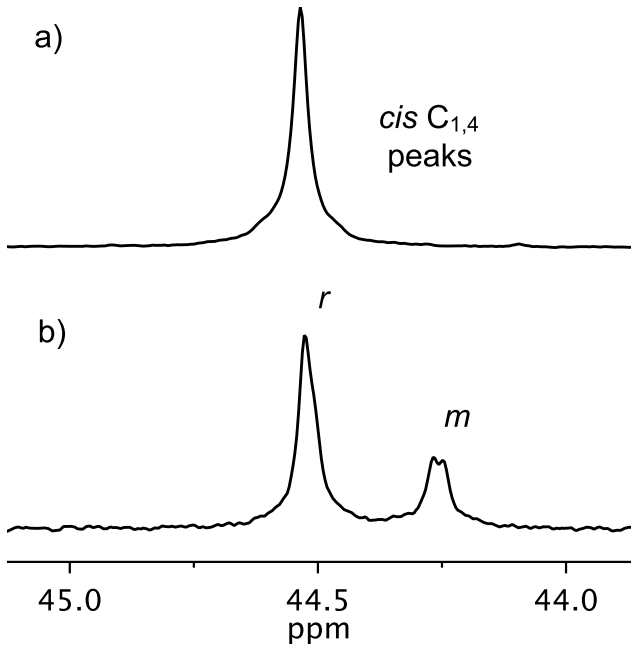


Figure 3.7. ^{13}C NMR spectra of (a) *cis,syndiotactic* **poly(3.6)** produced by catalyst **3.1** and (b) 72% *cis*, 68% syndiotactic (*cis* regions) **poly(3.6)** produced by catalyst **3.10**.

We next probed the effects of temperature and dilution on the polymerization of **3.6** by initiator **3.4**. If the propagation reaction is in competition with other processes occurring at the catalyst center, such as alkylidene isomerization, changes in *cis* content and/or tacticity can result from variations in temperature or monomer concentration.[1b] Decreasing monomer concentration in particular presents a simple method in which to slow propagation relative to these other processes. However, we found that the concentration of **3.6** had very little appreciable effect on the microstructures of the polymers produced by catalyst **3.4** (Table 3.6). Increasing the temperature from 25 to 40 °C, on the other hand, resulted in an approximately 5% decrease in both the *cis* content and the tacticity of **poly(3.6)/3.4**, while decreasing the temperature to 0 °C had the opposite effect. These results suggest that alkylidene isomerization might indeed be

occurring at a rate comparable to (or faster than) that of propagation and could therefore feasibly be a major contributor in the resulting stereoselectivity of the polymerization.

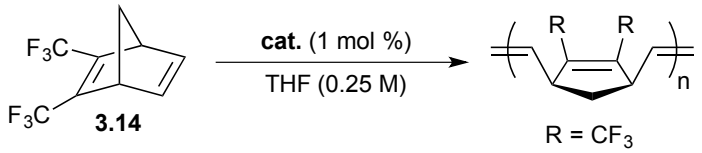
Table 3.6. Temperature and Concentration Effects on the Polymerization of Monomer 3.6 with Catalyst 3.4

temp (°C)	conc (M)	σ_c[a]	% *r* (*cis*)[b]
25	0.25	0.87	85
0	0.25	0.92	90
40	0.25	0.83	81
25	0.05	0.90	88
25	1.25	0.88	85

[a]Fraction of double bonds having *cis* configuration; average of two values derived from $C_{2,3}$ and $C_{1,4}$ resonances, with agreement generally within ±0.02. [b]Derived from *cis* $C_{1,4}$ peaks.

As catalysts **3.1**, **3.4**, and **3.9** were found to cover the general range of microstructures produced by **3.1**, **3.4**, and **3.8–3.13**, further polymerizations were performed using only these three systems. Results similar to monomer **3.6** were obtained when 2,3-bis(trifluoromethyl)-norbornadiene (**3.14**) was polymerized using catalysts **3.1**, **3.4**, and **3.9** (Table 3.7);[19] the resulting polymers were also *cis*-biased with highly syndiotactic *cis* regions.

Table 3.7. Polymerization of Monomer 3.14 with Catalysts 3.1, 3.4, and 3.9

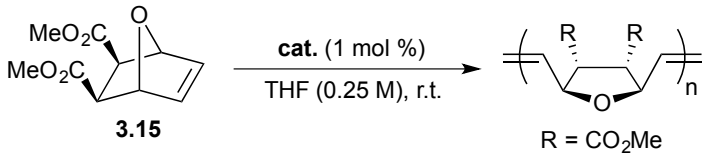


catalyst	σ_c[a]	% *r* (*cis*)[b]
3.1	0.79	99
3.4	0.63	99
3.9	0.55	>99

[a]Fraction of double bonds having *cis* configuration; average of three values derived from $C_{2,3}$, $C_{1,4}$, and C_7 resonances, with agreement generally within ±0.02. [b]Derived from *cis* C_7 peaks.

To obtain a comprehensive understanding of the origins of *cis*-selectivity and tacticity in cyclometalated catalysts **3.1**, **3.4**, and **3.8–3.13**, it is necessary to also determine the tacticity of the *trans* regions of polymers produced by these systems. However, the *trans* peaks in polymers derived from monomers **3.6** and **3.14** are too small and not sufficiently resolved for meaningful analysis. Thus, we next turned our attention toward polymers with more easily analyzable *trans* regions, specifically *exo,exo*-7-oxa-5-norbornene-2,3-dicarboxylic acid (**3.15**) and 7-methylnorbornene (7-MNBE, **3.16**).[15,20] Polymers produced from **3.15** had generally lower *cis* contents (σ_c = 0.73–0.94) (Table 3.8), allowing for facile qualitative analysis of the *trans* portions via the *trans* $C_{1,4}$ peak, which displays *m*/*r* tacticity splitting (the signals were still too small to allow for accurate integration, however). Although the *cis* peaks are not sensitive to tacticity splitting, a tacticity bias can be determined on the basis of comparison with data from catalyst **3.1**, shown to consistently produce predominantly syndiotactic polymers. All of the polymers produced by catalysts **3.1**, **3.4**, and **3.9** contained syndiotactic-biased *cis* regions. The tacticities of the *trans* regions, however, were found to differ somewhat depending on the specific catalyst/monomer combination being studied. Catalysts **3.1** and **3.9** produced polymers with *trans* regions that were largely syndiotactic, while **poly(3.15)** produced by catalyst **3.4** appeared to have negligible bias for either *m* or *r* dyads in the *trans* regions (Figure 3.8).

Table 3.8. Polymerization of Monomer 3.15 with Catalysts 3.1, 3.4, and 3.9



catalyst	σ_c [a]
3.1	0.94
3.4	0.73
3.9	0.93

[a]Fraction of double bonds having *cis* configuration; average of three values derived from CO_2Me, $C_{2,3}$, and $C_{1,4}$ resonances, with agreement generally within ±0.03.

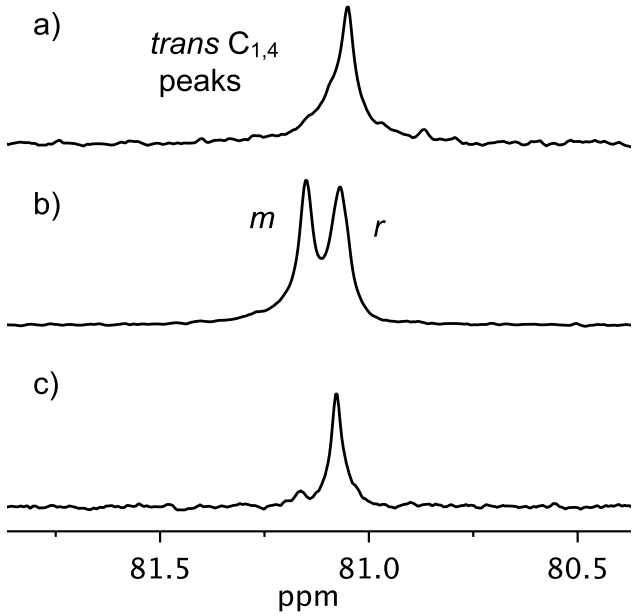
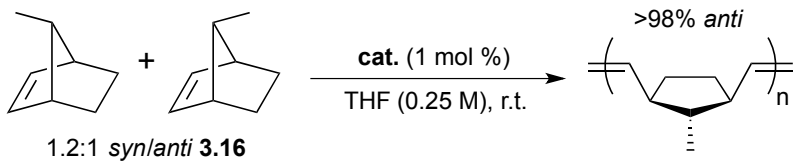


Figure 3.8. ^{13}C NMR spectra highlighting the *trans* $C_{1,4}$ regions of (a) 94% *cis* **poly(3.15)** produced by catalyst **3.1**, (b) 73% *cis* **poly(3.15)** produced by catalyst **3.4**, and (c) 93% *cis* **poly(3.15)** produced by catalyst **3.9**.

Next, we exposed catalysts **3.1**, **3.4**, and **3.9** to a 1.2:1 *syn*/*anti* mixture of **3.16**. It is generally accepted that norbornene and related compounds react at the less-hindered *exo* face in ROMP.[21] This was confirmed for catalysts **3.1** and **3.4** by the polymerization of **3.16**; both polymerized the *anti* monomer almost exclusively (<2% *syn*-derived

polymer was observed by ^{13}C NMR). This occurs because the 7-methyl group in the *syn* monomer is positioned directly over the *exo* face of the double bond; as a result, polymerization via *exo* attack is prohibitively high in energy, whereas this is avoided in the *anti* monomer. Gratifyingly, quantitative determination of tacticity was achieved for both the *cis* and the *trans* regions by analyzing polymers of *anti*-**3.16**, in which all of the carbons with the exception of C_7 are sensitive to tacticity. Samples of poly(*anti*-7-MNBE) produced by catalysts **3.1** and **3.4** were highly *cis* (σ_c = 0.97 and 0.87, respectively) with highly syndiotactic *cis* regions (90-95% *r*) and highly syndiotactic *trans* regions (>99% *r*) (Table 3.9). No appreciable amount of polymer was formed with initiator **3.9**; this is likely a result of the increased steric bulk associated with the *N*-2,6-diisopropylphenyl group of this catalyst.

Table 3.9. Polymerization of a 1.2:1 *syn*/*anti* Mixture of 7-Methylnorbornene (3.16) with Catalysts 3.1, 3.4, and 3.9



catalyst	σ_c[a]	tacticity[b]
3.1	0.97	*cis* regions, 95% *r*; *trans*, >99% *r*
3.4	0.87	*cis*, 90% *r*; *trans*, >99% *r*
3.9[c]	--	--

[a]Fraction of double bonds having *cis* configuration; derived from $C_{1,4}$ resonances. [b]Derived from *cis* and *trans* $C_{1,4}$ peaks. [c]No reaction.

Finally, we probed the extent of head-to-tail (HT) selectivity exhibited by catalysts **3.1**, **3.4**, and **3.9** in the polymerization of racemic unsymmetrically substituted norbornenes. HT bias is measured by determining the ratios of head–head/head–tail (HH/HT) and tail–tail/tail–head (TT/TH) dyads in both the *cis* and the *trans* regions of a

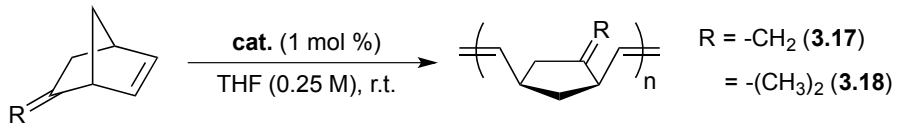
given polymer. The enantiomers are randomly distributed throughout the polymer (i.e., no bias is present) when these values are equal to unity.

The degree of HT bias in polymers derived from substituted norbornenes is delicately related to electronic and steric effects associated with both the monomer substituent(s) and the catalyst.[1b] Additionally, any catalyst relaxation or isomerization processes occurring on the same time scale as propagation may also contribute to HT bias, as different propagating species can exhibit different levels of HT discrimination. One way to probe the role of the catalyst in HT selectivity is via the polymerization of norbornene monomers substituted at the C_5 or C_6 position. These substituents are sufficiently remote from the double bond that they generally do not exert any intrinsic head-to-tail bias resulting from steric effects; thus, any observed bias with these monomers is likely catalyst-dependent. An HT bias in the polymerization of C_5- and C_6-substituted norbornene monomers with a given catalyst, then, particularly one that increases with decreasing rate of polymerization (or increasing dilution), may point toward the existence of two or more distinct propagating species with distinctive HT biases.

To test for HT-bias, catalysts **3.1**, **3.4**, and **3.9** were used to polymerize the unsymmetrically substituted racemic monomers 5-methylene-2-norbornene (**3.17**) and 5,5-dimethylnorbornene (DMNBE, **3.18**).[22,23] Although all of the catalysts were found to be essentially bias-free in the polymerization of monomer **3.17** (*cis* TT/TH ratios = 0.93–1.04), initiators **3.1** and **3.4** displayed more significant biases in the polymerization of **3.18** (*cis* TT/TH ratios = 1.11–1.51; *trans* TT/TH ratios = 0.20–1.00) (Table 3.10). Notably, the rate of polymerization of monomer **3.18** by initiators **3.1** and **3.4** was

significantly lower than that of **3.17** (1–4 h to full conversion vs minutes); additionally, as seen with monomer **3.16** no appreciable amount of **poly(3.18)** was formed using catalyst **3.9**. Both of these results are likely a consequence of the increased steric hindrance imparted by the *endo* substitution in monomer **3.18**. The increase in HT bias with decreasing rate suggests that there are multiple propagating species (perhaps resulting from alkylidene isomerization or a similar process), each with a different inherent HT bias.

Table 3.10. Polymerization of Monomers 3.17 and 3.18 with Catalysts 3.1, 3.4, and 3.9



catalyst	monomer	σ_c[a]	*cis* TT/TH[b]	*trans* TT/TH[c]
3.1	**3.17**	0.98	0.93	--[d]
3.4	**3.17**	0.87	0.95	--
3.9	**3.17**	0.94	1.0	--
3.1	**3.18**	0.78	1.1	0.20
3.4	**3.18**	0.77	1.5	0.50
3.9[e]	**3.18**	--	--	--

[a]Fraction of double bonds having *cis* configuration; derived from C_6 resonances (**3.17**) and C_2 resonances (**3.18**). [b]Derived from *cis* TT and TH $C_{2,3}$ peaks (**3.17**) and *cis* TT and TH C_2 peaks (**3.18**). [c]Derived from *trans* TT and TH C_2 peaks (**3.18**). [d]Here and below: overlap of *trans* TT and HH $C_{2,3}$ peaks in **poly(3.17)** precluded *trans* TT/TH or HH/HT analysis. [e]No reaction.

Computational Investigations of Reaction Pathways and Proposed Model for *cis*-Selectivity and Tacticity in Catalysts 3.1, 3.4, and 3.8–3.13: The selectivity for *cis,syndiotactic* polymers exhibited by catalysts **3.1**, **3.4**, and **3.8–3.13** is hypothesized to be due in large part to stereogenic metal control, as in the case of the Mo- and W-based MAP alkylidene complexes described earlier. Because initiators **3.1**, **3.4**, and **3.8–3.13** are stereogenic-at-Ru, the absolute configuration of the metal center is inverted with each

propagation step to generate enantiomeric (in the case of **3.1**) or diastereomeric (**3.4** and **3.8–3.13**) carbenes (Figure 3.9), resulting in the addition of incoming monomers to alternating sides of the Ru=C bond.

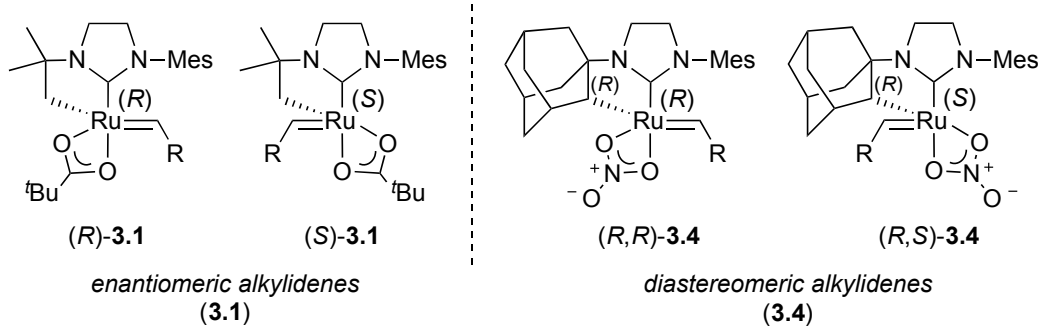
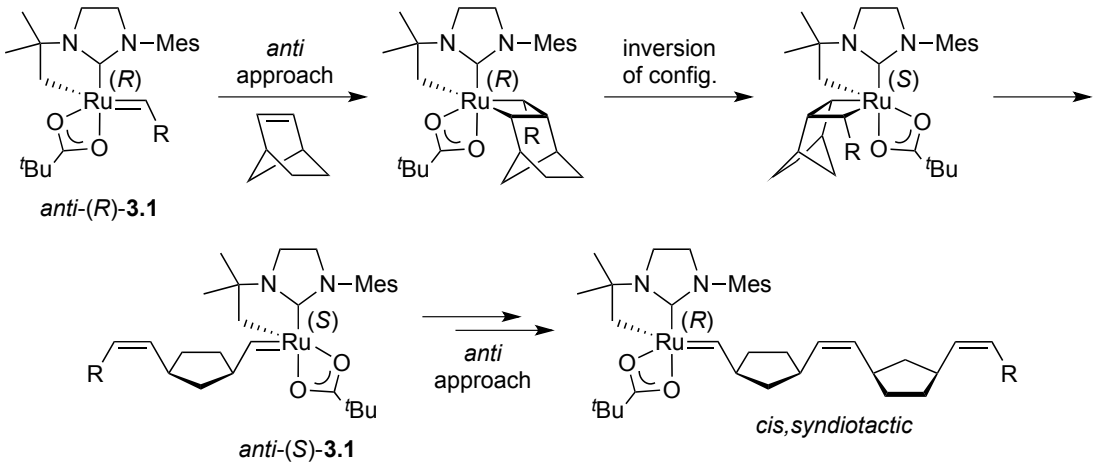


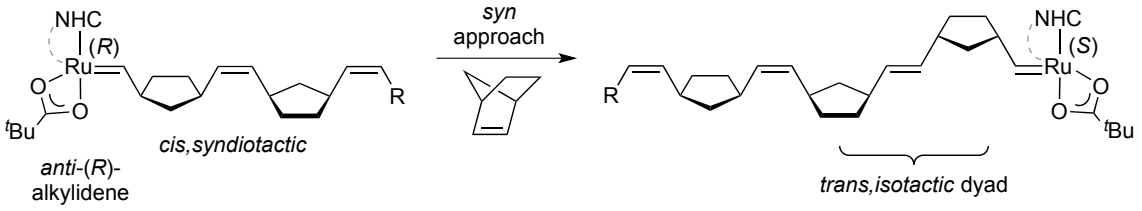
Figure 3.9. Enantiomeric (**3.1**) and diastereomeric (**3.4**) alkylidenes generated by the stereochemical inversion of the Ru metal center that occurs with each forward metathesis step.

Previous computational and experimental work has shown that *cis*-selectivity in cross metathesis reactions mediated by cyclometalated catalysts similar to **3.1** and **3.4** stems from the steric influence of the bulky *N*-aryl group positioned directly over the side-bound metallacycle, which results in the destabilization of the transition state leading to the formation of *trans* olefins (described in further detail in *Chapter 1* of this thesis).[24] It is likely that monomer approach in ROMP is similarly influenced by the presence of the *N*-aryl group, in that norbornene and related monomers would be expected to react at the less hindered *exo* face with the methylene bridge pointed away from the *N*-aryl "cap."[25] In the terminology employed by Schrock and co-workers in regards to well-defined Mo and W initiators, this approach is designated *anti*, in that the bulk of the monomer points away from the *N*-aryl group; the opposite approach is *syn*.[5c] Likewise, *syn* and *anti* Ru=CHR isomers are defined according to whether the R group of the alkylidene points towards or away from the *N*-aryl group, respectively. A consistently

anti monomer approach to alternate sides of an *anti* alkylidene as a result of stereogenic metal control leads to the formation of a *cis,syndiotactic* polymer (Scheme 3.3). However, if the incoming monomer were to occasionally adopt a *syn* approach to the *anti* alkylidene, a single *trans,isotactic* "error" would be produced (Scheme 3.4).



Scheme 3.3. Proposed mechanism for forming *cis,syndiotactic* polymers using cyclometalated catalyst **3.1**. Mes = 2,4,6-trimethylphenyl, R = *o*-isopropoxyphenyl.



Scheme 3.4. Formation of a *trans,isotactic* dyad in a predominantly *cis,syndiotactic* polymer following a *syn* approach of the monomer to an *anti* alkylidene. R = *o*-isopropoxyphenyl.

Mixed tacticities (i.e., *cis,isotactic* and *trans,syndiotactic* dyads) would result if isomerization of the *anti* alkylidene were to occur between propagation steps, either through rotation about the M=C double bond to adopt a *syn* configuration or via a nonmetathesis-based polytopal rearrangement[26] between the stereoisomeric metal alkylidenes (i.e., (*R*)-**3.1** and (*S*)-**3.1**). Moreover, the degree to which these "errors" occur would be related to the barrier to these processes, with an increase in regions of mixed

tacticity being observed when the rate of alkylidene isomerization occurs on a time scale that is comparable to the time scale for propagation. Competition between alkylidene isomerization and propagation would also provide a reasonable explanation for the HT bias detected in catalysts **3.1** and **3.4** as well as the temperature effect observed in the polymerization of **3.6** with catalyst **3.4**, as outlined previously.

To explore these possible alkylidene isomerization processes, as well as to better understand how they may lead to a loss in *cis*-selectivity and tacticity in some of these cyclometalated ruthenium-based systems, DFT calculations on polymerization reactions involving catalysts **3.1** and **3.4** were performed by the Houk group at UCLA.[27] All calculations were performed with Gaussian 09[28] at the M06/SDD-6-311+G(d,p)/SMD(THF)//B3LYP/SDD-6-31G(d) level of theory. See the SI for computational details.

We first investigated the likelihood of alkylidene isomerization through a nonmetathesis-based polytopal rearrangement pathway. The computed energy profile of the polytopal rearrangement of *N*-^{t}Bu-cyclometalated ruthenium alkylidene **3.19** to form its diastereomer **3.20** (using a 3-cyclopentenyl group as a model of the polymer chain) is shown in Figure 3.10. This multistep rearrangement process starts from alkylidene *anti* to *syn* isomerization via rotation (**3.21-TS**), which requires a relatively low barrier to form the *syn* alkylidene intermediate **3.22**. Isomerization of the alkylidene to the position *trans* to the NHC leads to highly unstable intermediate **3.24**. Complex **3.24** subsequently undergoes ring flip of the five-membered chelate (**3.25-TS**) and a very unfavorable rearrangement of the pivalate ligand (**3.27-TS**) to form complex **3.28**, which then

isomerizes to **3.20**. With the alkylidene *trans* to the NHC ligand, complexes **3.24**, **3.26**, and **3.28** are all highly unstable, and this process is overall highly disfavored.

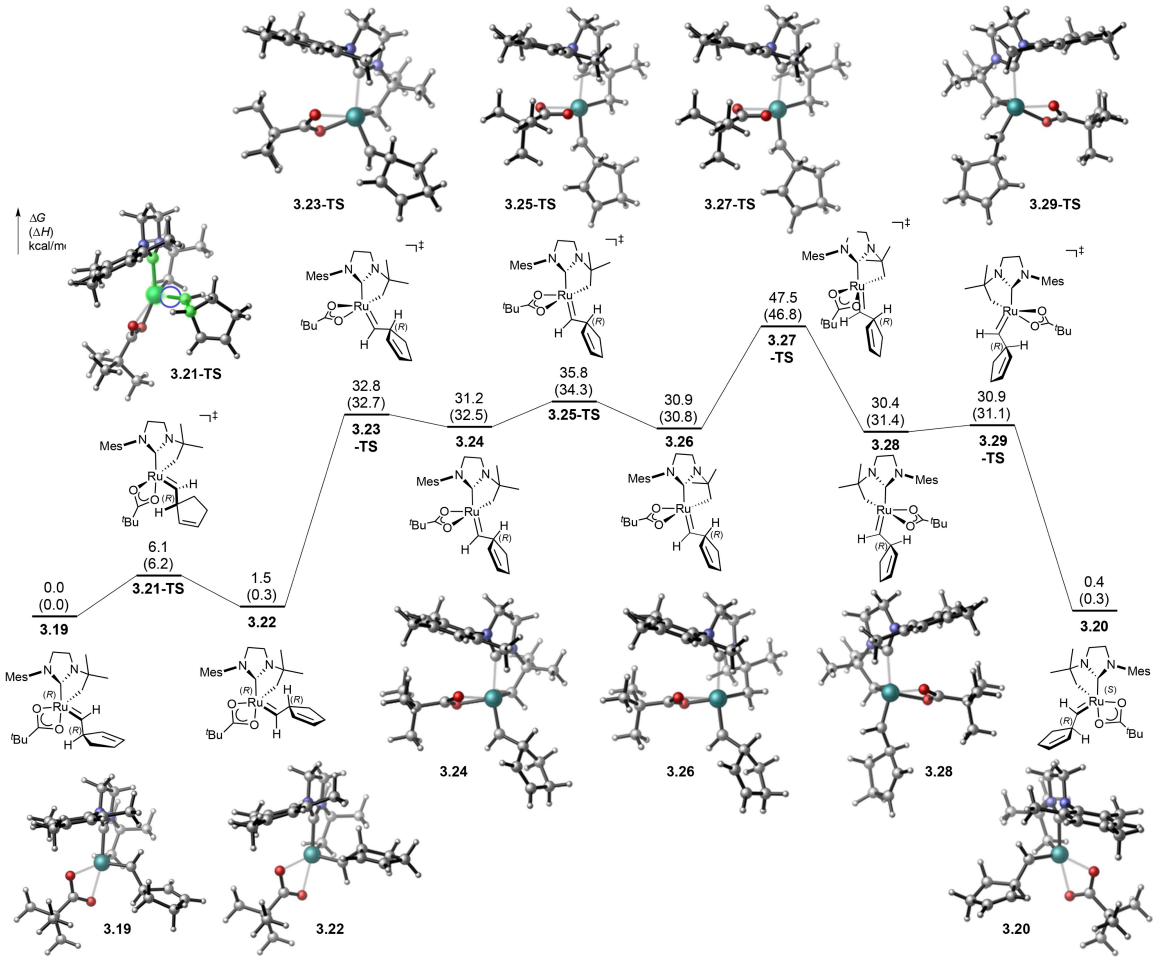
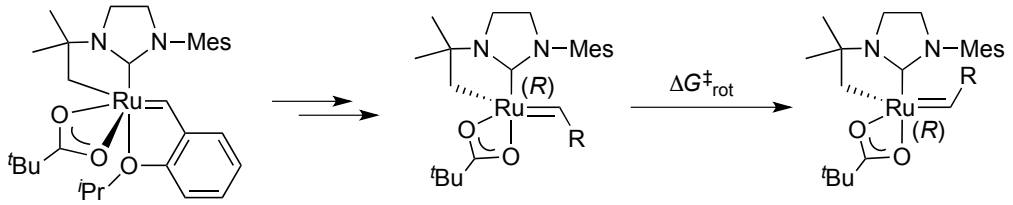
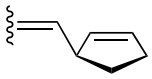
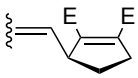
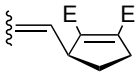
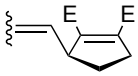


Figure 3.10. Nonmetathesis-based polytopal rearrangement of ruthenium alkylidene **3.19** to its diastereomer **3.20**.

We next explored the possibility of isomerization via rotation about the alkylidene Ru=C double bond. The computed rotational barriers for catalysts **3.1** and **3.4** are summarized in Table 3.11. Because of steric repulsions between the alkylidene R group and the *N*-aryl group, the *syn* alkylidene is less stable than the *anti* isomer. The alkylidene rotational barrier is only slightly affected by the steric bulk of the substituent on the alkylidene and the cyclometalated group on the catalyst. In general, the barrier to alkylidene rotation is comparable to the barrier for monomer addition (see below).

Table 3.11. Computed Alkylidene Rotational Barriers

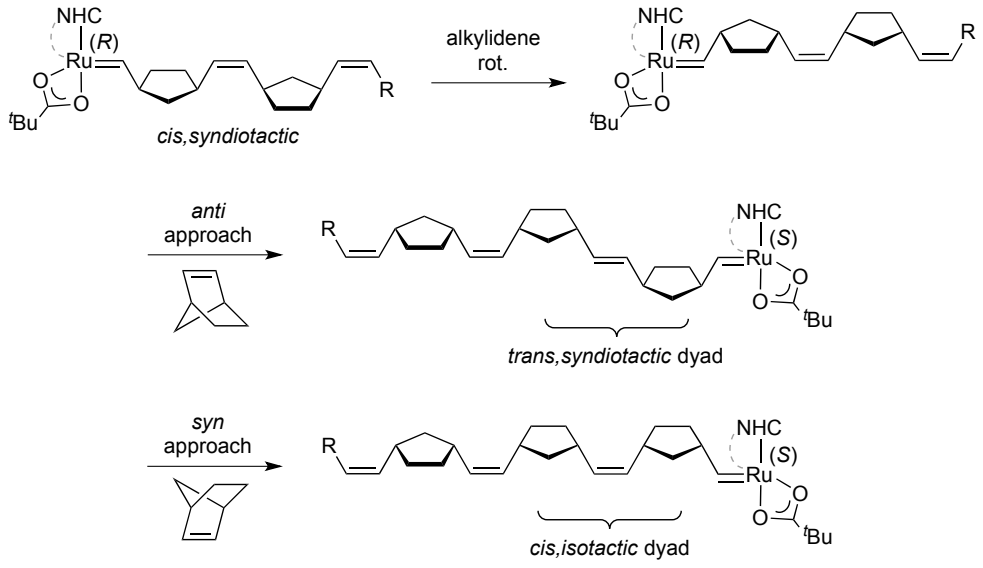


catalyst	alkylidene	$\Delta G^{\ddagger}_{rot}$ [a]	$\Delta G_{(syn\text{-}anti)}$ [b]
3.1		6.1	1.5
3.1	 E = CO_2Me	9.0	5.0
(*R*,*R*)-**3.4**	 E = CO_2Me	9.9	3.9
(*R*,*S*)-**3.4**	 E = CO_2Me	6.3	4.0

[a]Alkylidene rotational barrier with respect to the *anti* alkylidene. [b]Energy difference between *syn* and *anti* alkylidene isomers. All energies are in kcal/mol.

Given the high barrier and the unstable intermediates in the polytopal rearrangement process, we conclude that a nonmetathesis isomerization of the ruthenium alkylidene is highly unlikely to occur under the reaction conditions, and a pathway involving bond rotation about the Ru=C alkylidene is much more likely to be responsible for alkylidene isomerization. With this in mind, we can now complete our model for *cis*-selectivity and tacticity in catalysts **3.1**, **3.4**, and **3.8–3.13** by factoring in the effects of alkylidene rotation on the final polymer microstructure. In a predominantly *cis,syndiotactic* polymer resulting from stereogenic metal control, rotation of the alkylidene from *anti* to *syn* followed by monomer approach in either an *anti* or *syn*

fashion results in the formation of a *trans,syndiotactic* or *cis,isotactic* dyad, respectively (Scheme 3.5).



Scheme 3.5. Formation of a *trans,syndiotactic* or *cis,isotactic* dyad resulting from an *anti* or *syn* monomer approach, respectively, to a *syn* alkylidene following alkylidene rotation (*anti* to *syn*) in a predominantly *cis,syndiotactic* polymer. R = *o*-isopropoxyphenyl.

We next set out to explore the possible pathways leading to the formation of each type of dyad in more depth. We focused on the [2 + 2] cycloaddition step, as in reactions with norbornene and norbornadienc derivatives, the [2 +2] cycloaddition step requires a significantly higher barrier than the [2 +2] cycloelimination, and thus the [2 + 2] cycloaddition is effectively irreversible.[27b,29] Importantly, *cis*/*trans*-selectivity and tacticity are both determined in the [2 + 2] cycloaddition step. The four possible transition states derived for the [2 + 2] cycloaddition of monomer **3.6** at the *exo* face to ruthenium alkylidene **3.30**, a model of the propagating species of the *N*-^{t}Bu-cyclometalated catalyst **3.1**, are shown in Figure 3.11. Because isomerization between the *anti* and *syn* alkylidenes via rotation of the Ru=C bond occurs with a barrier comparable to that of propagation, monomer addition to both *anti* and *syn* alkylidenes was computed

(**3.31-TS-A/B** and **3.31-TS-C/D**, respectively). In these transition states, the olefin approaches the catalyst from the side, that is, *cis* to the NHC ligand, in line with previous computational studies of olefin cross-metathesis with cyclometalated *cis*-selective ruthenium catalysts.[24] The bottom-bound pathway, i.e., olefin approaching *trans* to the NHC, and the addition to the *endo* face of the norbornadiene both require much higher activation energies (15–21 kcal/mol, see the SI for details).

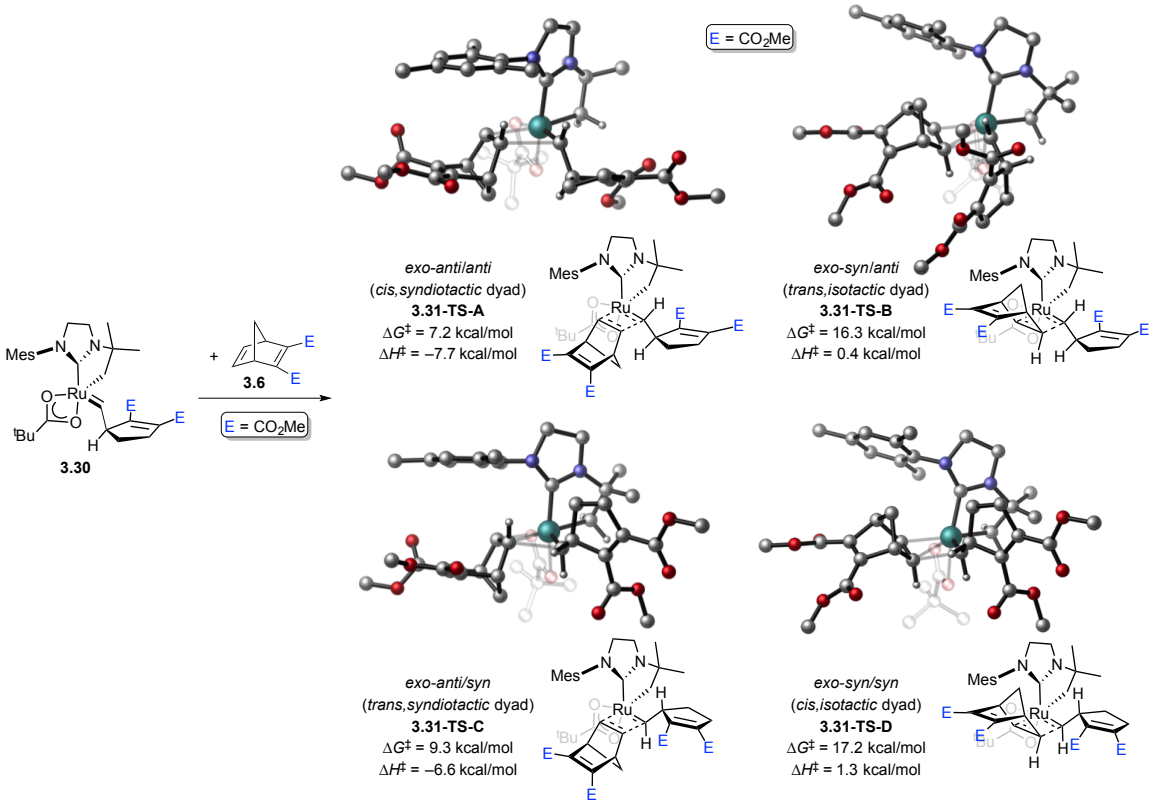


Figure 3.11. [2 + 2] cycloaddition transition states for the polymerization of monomer **3.6** with catalyst **3.30**. Energies are with respect to the separated ruthenium alkylidene and monomer **3.6**.

The most favorable [2 + 2] cycloaddition transition state is the one leading to the formation of a *cis,syndiotactic* dyad, **3.31-TS-A**, in which the *anti* alkylidene reacts with a monomer approaching in an *anti* fashion. The ligand–substrate steric repulsions in this *anti*/*anti* approach are minimized due to the bulk of the monomer and the alkylidene both

being directed away from the *N*-aryl group. The next lowest energy transition state leads to the formation of a *trans,syndiotactic* arrangement (**3.31-TS-C**), in which the *syn* alkylidene reacts with a monomer approaching in an *anti* fashion. This *anti*/*syn* approach (**3.31-TS-C**) is 2.1 kcal/mol higher in energy than the *anti*/*anti* approach (**3.31-TS-A**), which is consistent with the high *cis*-selectivity observed experimentally. Both *trans,isotactic* and *cis,isotactic* dyads result when the monomer approaches in a *syn* fashion (**3.31-TS-B** and **3.31-TS-D**, respectively), which requires much higher activation energies due to the repulsion of the methylene bridge with the *N*-aryl group. This is in agreement with the high syndiotacticity of both the *cis* and the *trans* regions observed experimentally.

Experimentally, the polymerization of monomer **3.6** with *N*-adamantyl cyclometalated ruthenium catalysts (**3.4**, **3.8–3.13**) is both less *cis*-selective and less syndioselective than that with the *N*-^{t}Bu cyclometalated catalyst **3.1** (Table 3.5). Interestingly, when the total content of *cis* double bonds in **poly(3.6)** is plotted against the percentage of *cis* double bonds in *cis, r* dyads for catalysts **3.1**, **3.4**, and **3.8–3.13**, a linear relationship is observed (Figure 3.12). Because the barriers to alkylidene rotation in catalysts **3.1** and **3.4** with monomer **3.6** are comparable (Table 3.11), this relationship is likely a result of the relative differences in the energetics of the propagation transition states for each catalyst (which also determine both *cis*- and syndioselectivity). Thus, the [2 + 2] cycloaddition transition states with monomer **3.6** and alkylidene **3.32**, a model of the propagating species of catalyst **3.4**, were calculated to further investigate the connection between *cis*-selectivity and tacticity in these systems.

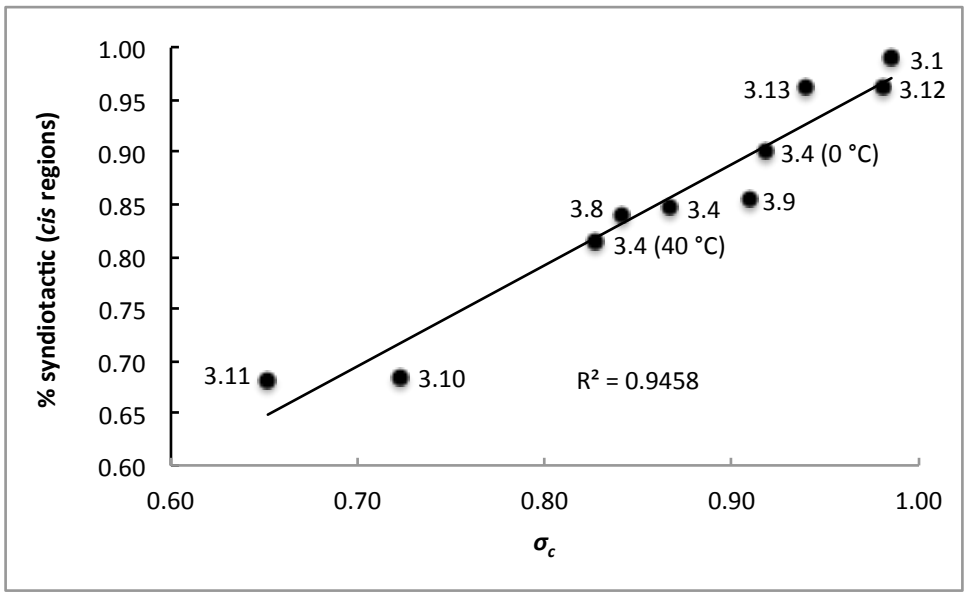


Figure 3.12. Linear relationship between *cis* content and tacticity of the *cis* regions in poly(DCMNBD) [**poly(3.6)**] for catalysts **3.1**, **3.4**, and **3.8–3.13** (data obtained from Table 3.5).

With the asymmetric *N*-adamantyl-cyclometalated group on catalyst **3.4**, an additional set of alkylidene diastereomers is possible, resulting in eight total propagation transition states (Figure 3.13). In the more stable alkylidene diastereomer (*R*,*R*)-**3.32**, the Ru=C bond is *anti* to the alpha C–H bond on the cyclometalated carbon atom. In (*R*,*S*)-**3.32**, the Ru=C bond is *syn* to the alpha C–H bond. As discussed above, direct isomerization between (*R*,*R*)-**3.32** and (*R*,*S*)-**3.32** via polytopal rearrangement is not possible. Instead, the configuration of ruthenium alternates between (*R*,*R*)-**3.32** and (*R*,*S*)-**3.32** after each monomer addition.

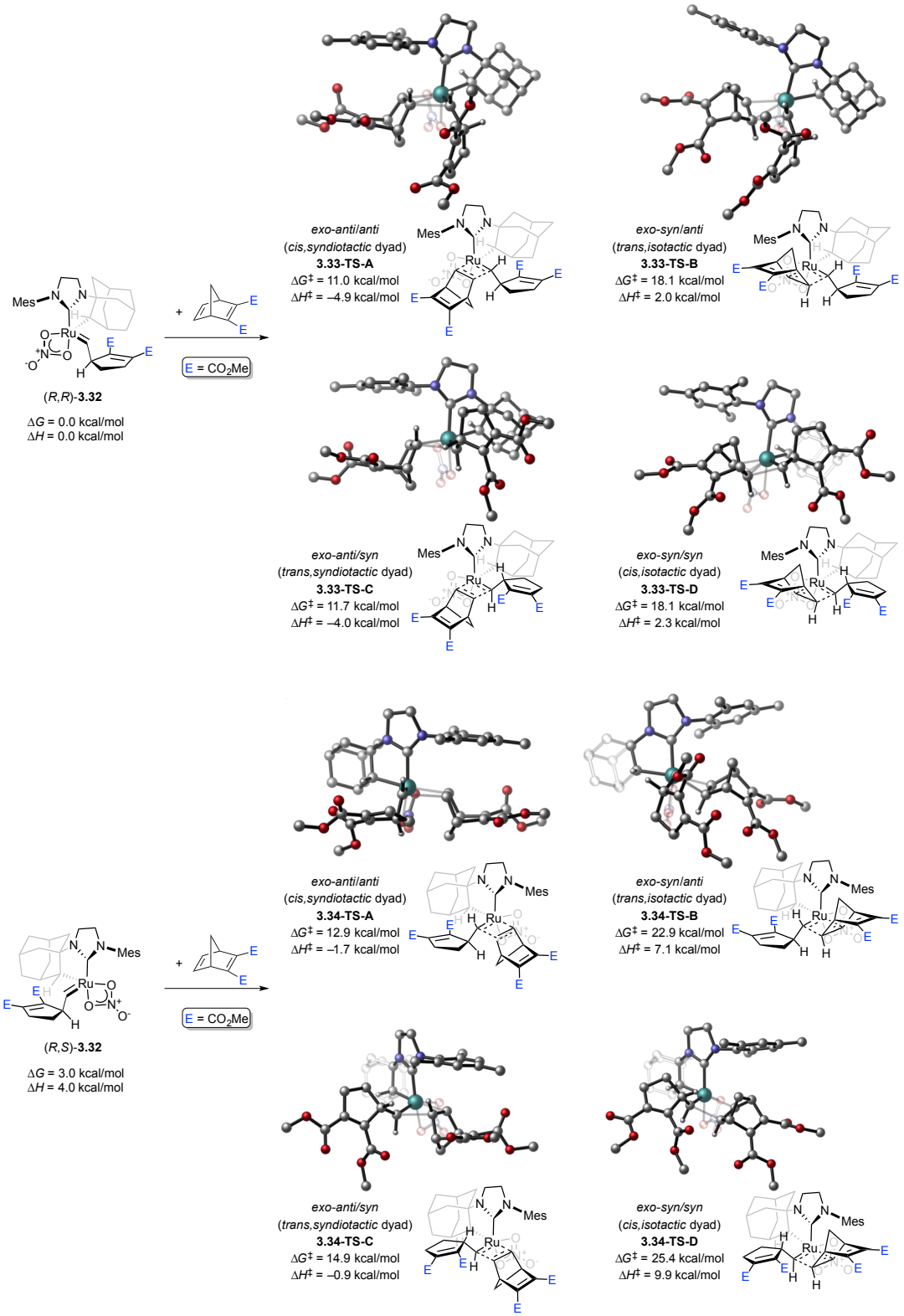


Figure 3.13. [2 + 2] cycloaddition transition states for the polymerization of monomer **3.6** with catalyst **3.32**. Energies are with respect to the separated ruthenium alkylidene and monomer **3.6**.

Similar to the reaction with catalyst **3.1**, the *cis,syndio*-selective *anti*/*anti* approach is the most favorable with catalyst **3.4** (**3.33-TS-A** and **3.34-TS-A** for the addition to alkylidenes (*R*,*R*)-**3.32** and (*R*,*S*)-**3.32**, respectively). However, the corresponding *trans,syndio*-selective transition states **3.33-TS-C** and **3.34-TS-C** are only 0.7 and 2.0 kcal/mol less stable, respectively. Similarly, the transition states leading to the formation of *trans,isotactic* and *cis,isotactic* dyads (**3.33-TS-B/D** and **3.34-TS-B/D**, respectively), while still highly unfavorable, are also less destabilized relative to *cis,syndio*-selective **3.33-TS-A** and **3.34-TS-A**. The lower selectivity for *cis,syndiotactic* dyads is attributed to the increased steric repulsion between the alkylidene R group and the bulkier cyclometalated *N*-adamantyl group in the *cis,syndio*-selective transition states, in particular in **3.33-TS-A** where the steric bulk of the adamantyl chelate is closer to the R group than in **3.34-TS-A**. These results likely extend to the other cyclometalated *N*-adamantyl initiators **3.8–3.13**.

Conclusions and Future Outlook

In spite of expectations to the contrary, we have demonstrated the ability of Ru-based olefin metathesis catalysts to generate norbornene- and norbornadiene-based polymers with singular microstructures via ROMP. Using the recently developed sodium pivalate method (detailed in *Chapter 2*), a series of ruthenium alkylidene initiators containing a cyclometalated *N*-^{t}Bu group were synthesized. All of these complexes yielded highly *cis,syndiotactic* ROMP polymers (>95% in some cases).

Using experimental and computational insights, a model was subsequently developed to explain the pattern of stereoselectivity exhibited in these and related

cyclometalated ruthenium metathesis catalysts. A series of Ru-based initiators containing differing cyclometalated groups, *N*-aryl substituents, and X-type ligands were evaluated in the ROMP of various norbornene- and norbornadiene-derived monomers. Highly *cis,syndiotactic* polymers were generated in many cases. In polymers with an imperfect microstructure, the major errors were in the form of *cis,isotactic* and *trans,syndiotactic* regions. Additionally, hypothetical reaction intermediates and propagation transition states were analyzed computationally. Combined experimental and computational data suggests that the near-perfect *cis,syndio*-selectivity of these systems arises from the inversion of configuration at the metal center that occurs with each propagation step (i.e., stereogenic metal control) in conjunction with an almost exclusive approach of the monomer in an *anti* fashion to the energetically preferred *anti* alkylidene. The majority of microstructural errors are likely a result of interconversion between *syn* and *anti* alkylidene isomers in the propagating catalytic species: Addition of the monomer in an *anti* or *syn* fashion to the higher energy *syn* alkylidene leads to the formation of a *trans,syndiotactic* or *cis,isotactic* dyad, respectively. Furthermore, the comparatively high *cis,syndio*-selectivity of the cyclometalated-*N*-^{t}Bu initiators was determined to originate from the decreased steric environment in these catalysts relative to the *N*-adamantyl-cyclometalated systems, as increased substitution close to the metal center was shown to minimize the differences in energy between transition states. The mechanistic insights gained in this study will not only aid in the development of new and improved *cis*-selective Ru-based catalysts, but also provide increased predictive power in synthetic transformations mediated by these systems.

Since the two papers comprising this chapter were published in the *Journal of the American Chemical Society*, an additional example of Ru-mediated stereoselective ROMP has been reported. Mikus et al. found that certain Ru catechothiolate systems generated all-*cis* polynorbornenes and –norbornadienes with controllable syndioselectivity, ranging from ~50% to >95%, also as a result of stereogenic metal control.[30] Higher syndioselectivities, resulting from lower rates of non-metathesis-based polytopal isomerization relative to monomer propagation, could be selected for by adjusting the monomer concentration and/or the catalyst's steric and electronic characteristics via substitution of the dithiolate ligand. Despite these recent advances in the area of Ru-mediated stereoselective ROMP, however, norbornene- and norbornadiene-based polymer architectures other than *cis,syndiotactic*, namely *cis,isotactic*, *trans,syndiotactic*, and *trans,isotactic*, remain elusive. Using the progress made in stereoselective ROMP mediated by W- and Mo-based complexes as a model, it is reasonable to expect that highly *cis,isotactic* polynorbornenes and –norbornadienes may be accessible through the design of a catalyst that operates via enantiomorphic site control, while the synthesis of a catalyst capable of generating *trans,syndiotactic* and *trans,isotactic* polymers will likely be significantly more challenging. Regardless, the insights gained in the studies presented in this chapter provide a platform for the development of new Ru-based systems capable of producing interesting and varied architectures via ring-opening metathesis polymerization.

References

1. (a) Hamilton, J. G. Stereoselectivity in Ring-Opening Metathesis Polymerization. In *Handbook of Metathesis*; Grubbs, R. H., Ed.; Wiley-VCH: Weinheim, Germany, 2003; pp 118–179. (b) Ivin, K. J.; Mol, J. C. Ring-Opening Metathesis Polymerization: General Aspects. *Olefin Metathesis and Metathesis Polymerization*; Academic Press: San Diego, CA, 1997; pp 224–259.

2. (a) Haas, F.; Theisen, D. *Kautsch. Gummi Kunstst.* **1970**, *23*, 502. (b) Edwards, J. H.; Feast, W. J.; Bott, D. C. *Polymer* **1984**, *25*, 395. (c) Park, L. Y.; Schrock, R. R.; Stieglitz, S. G.; Crowe, W. E. *Macromolecules* **1991**, *24*, 3489. (d) Dounis, P.; Feast, W. J.; Kenwright, A. M. *Polymer* **1995**, *36*, 2787. (e) Lee, C.; Wong, K.; Lam, W.; Tang, B. *Chem. Phys. Lett.* **1999**, *307*, 67. (f) Wong, K. S.; Lee, C. W.; Zang, B. Z. *Synth. Met.* **1999**, *101*, 505.

3. (a) Steinhausler, T.; Koros, W. *J. Polym. Sci., Part B: Polym. Phys.* **1997**, *35*, 91. (b) Esteruelas, M. A.; Gonzalez, F.; Herrero, J.; Lucio, P.; Olivan, M.; Ruiz-Labrador, B. *Polym. Bull.* **2007**, *58*, 923.

4. (a) Schrock, R. R. *Dalton Trans.* **2011**, *40*, 7484. (b) Schrock, R. R. *Acc. Chem. Res.* **2014**, *47*, 2457.

5. (a) McConville, D. H.; Wolf, J. R.; Schrock, R. R. *J. Am. Chem. Soc.* **1993**, *115*, 4413. (b) O'Dell, R.; McConville, D. H.; Hofmeister, G. E.; Schrock, R. R. *J. Am. Chem. Soc.* **1994**, *116*, 3414. (c) Schrock, R. R.; Lee, J. K.; O'Dell, R.; Oskam, J. H. *Macromolecules* **1995**, *28*, 5933. (d) Totland, K. M.; Boyd, T. J.; Lavoie, G. G.; Davis, W. M.; Schrock, R. R. *Macromolecules* **1996**, *29*, 6114.

6. (a) Flook, M. M.; Jiang, A. J.; Schrock, R. R.; Müller, P.; Hoveyda, A. H. *J. Am. Chem. Soc.* **2009**, *131*, 7962. (b) Flook, M. M.; Ng, V. W. L.; Schrock, R. R. *J. Am. Chem. Soc.* **2011**, *133*, 1784. (c) Flook, M. M.; Börner, J. Kilyanek, S. M.; Gerber, L. C. H.; Schrock, R. R. *Organometallics* **2012**, *31*, 6231. (d) Forrest, W. P.; Axtell, J. C.; Schrock, R. R. *Organometallics* **2014**, *33*, 2313. (e) Forrest, W. P.; Weis, J. G.; John, J. M.; Axtell, J. C.; Simpson, J. H.; Swager, T. M.; Schrock, R. R. *J. Am. Chem. Soc.* **2014**, *136*, 10910.

7. Bazan, G. C.; Khosravi, E.; Schrock, R. R.; Feast, W. J.; Gibson, V. C.; O'Regan, M. B.; Thomas, J. K.; Davis, W. M. *J. Am. Chem. Soc.* **1990**, *112*, 8378.

8. (a) Delaude, L.; Demonceau, A.; Noels, A. F. *Macromolecules* **1999**, *32*, 2091. (b) Delaude, L.; Demonceau, A.; Noels, A. F. *Macromolecules* **2003**, *36*, 1446. (c) Lee, J. C.; Parker, K. A.; Sampson, N. S. *J. Am. Chem. Soc.* **2006**, *128*, 4578. (d) Lin, W.-Y.; Wang, H.-W.; Liu, Z.-C.; Xu, J.; Chen, C.-W.; Yang, Y.-C.; Huang, S.-L.; Yang, H.-C.; Luh, T.-Y. *Chem. - Asian J.* **2007**, *2*, 764. (e) Song, A. R.; Lee, J. C.; Parker, K. A.; Sampson, N. S. *J. Am. Chem. Soc.* **2010**, *132*, 10513. (f) Leitgeb, A.; Wappel, J.; Slugovc, C. *Polymer* **2010**, *51*, 2927. (g) Kobayashi, S.; Pitet, L. M.; Hillmyer, M.

A. *J. Am. Chem. Soc.* **2011**, *133*, 5794. (h) Zhang, J.; Matta, M. E.; Martinez, H.; Hillmyer, M. A. *Macromolecules* **2013**, *46*, 2535.

9. Straub, B. F. *Adv. Synth. Catal.* **2007**, *349*, 204.
10. (a) Endo, K.; Grubbs, R. H. *J. Am. Chem. Soc.* **2011**, *133*, 8525. (b) Keitz, B. K.; Endo, K.; Patel, P. R.; Herbert, M. B.; Grubbs, R. H. *J. Am. Chem. Soc.* **2012**, *134*, 693.

11. Keitz, B. K.; Fedorov, A.; Grubbs, R. H. *J. Am. Chem. Soc.* **2012**, *134*, 2040.

12. Rosebrugh, L. E.; Herbert, M. B.; Marx, V. M.; Keitz, B. K.; Grubbs, R. H. *J. Am. Chem. Soc.* **2013**, *135*, 1276.

13. (a) Grutzner, J. B.; Jautelat, M.; Dence, J. B.; Smith, R. A.; Roberts, J. D. *J. Am. Chem. Soc.* **1970**, *92*, 7107. (b) Ivin, K. J.; Laverty, D. T.; Rooney, J. J. *Makromol. Chem.* **1977**, *178*, 1545.

14. Al-Samak, H.; Amir-Ebrahimi, V.; Corry, D. G.; Hamilton, J. G.; Rigby, S.; Rooney, J. J.; Thompson, J. M. *J. Mol. Catal. A: Chem.* **2000**, *160*, 13.

15. Amir-Ebrahimi, V.; Corry, D. A. K.; Hamilton, J. G.; Rooney, J. J. *J. Mol. Catal. A: Chem.* **1998**, *133*, 115.

16. For a discussion of initiation in ruthenium metathesis catalysts, see: (a) Sanford, M. S.; Love, J. A.; Grubbs, R. H. *J. Am. Chem. Soc.* **2001**, *123*, 6543. (b) Love, J. A.; Morgan, J. P.; Trnka, T. M.; Grubbs, R. H. *Angew. Chem., Int. Ed.* **2002**, *41*, 4035.

17. (a) Ivin, K. J.; Laverty, D. T.; Rooney, J. J. *Makromol. Chem.* **1978**, *179*, 253. (b) Ivin, K. J.; Laverty, D. T.; O'Donnell, J. H.; Rooney, J. J.; Stewart, C. D. *Makromol. Chem.* **1979**, *180*, 1989. (c) Gillan, E. M. D.; Hamilton, J. G.; Mackey, N. D.; Rooney, J. J. *J. Mol. Catal.* **1988**, *46*, 359.

18. Greene, R. M. E.; Hamilton, J. G.; Ivin, K. J.; Rooney, J. J. *Makromol. Chem*. **1986**, *187*, 619.

19. (a) Davies, G. R.; Feast, W. J.; Gibson, V. C.; Hubbard, H. V. S. A.; Ivin, K. J.; Kenwright, A. M.; Khosravi, E.; Marshall, E. L.; Mitchell, J. P.; Ward, I. M.; Wilson, B. *Makromol. Chem., Macromol. Symp.* **1993**, *66*, 289. (b) McConville, D. H.; Wolf, J. R.; Schrock, R. R. *J. Am. Chem. Soc.* **1993**, *115*, 4413.

20. (a) Hamilton, J. G.; Ivin, K. J.; Rooney, J. J. *J. Mol Catal.* **1985**, *28*, 255. (b) Feast, W. J.; Gibson, V. C.; Ivin, K. J.; Khosravi, E.; Kenwright, A. M.; Marshall, E. L.; Mitchell, J. P. *Makromol. Chem.* **1992**, *193*, 2103.

21. (a) Arnold, D. R.; Trecker, D. J. Whipple, E. B. *J. Am. Chem. Soc.* **1965**, *87*, 2596. (b) Gilliom, L. R.; Grubbs, R. H. *J. Am. Chem. Soc.* **1986**, *108*, 733.

22. (a) Ivin, K. J.; Lapienis, G.; Rooney, J. J.; Stewart, C. D. *J. Mol. Catal.* **1980**, *8*, 203. (b) Ivin, K. J.; Laverty, D. T.; Reddy, B. S. R.; Rooney, J. J. *Makromol. Chem., Rapid Commun.*, **1980**, *1*, 467.

23. Ho, H. T.; Ivin, K. J.; Rooney, J. J. *Makromol. Chem.* **1982**, *183*, 1629.

24. (a) Liu, P.; Xu, X.; Dong, X.; Keitz, B. K.; Herbert, M. H.; Grubbs, R. H.; Houk, K. N. *J. Am. Chem. Soc.* **2012**, *134*, 1464. (b) Dang, Y.; Wang, Z.-X.; Wang, X. *Organometallics* **2012**, *31*, 7222. (c) Dang, Y.; Wang, Z.-X.; Wang, X. *Organometallics* **2012**, *31*, 8654.

25. Hartung, J.; Grubbs, R. H. *J. Am. Chem. Soc.* **2013**, *135*, 10183.

26. (a) Khan, R. K. M.; Zhugralin, A. R.; Torker, S.; O'Brien, R. V.; Lombardi, P.J.; Hoveyda, A. H. *J. Am. Chem. Soc.* **2012**, *134*, 12438. (b) Torker, S.; Khan, R. K. M.; Hoveyda, A. H. *J. Am. Chem. Soc.* **2014**, *136*, 3439.

27. For computational studies on ROMP with non-cyclometalated ruthenium catalysts: (a) Song, A.; Chul-Lee, J.; Parker, K. A.; Sampson, N. S. *J. Am. Chem. Soc.*, **2010**, *132*, 10513. (b) Martinez, H.; Miro, P.; Charbonneau, P.; Hillmyer, M. A.; Cramer, C. J. *ACS Catal.* **2012**, *2*, 2547.

28. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, M. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09*, revision D.01; Gaussian, Inc.: Wallingford, CT, 2009.

29. (a) Chen, P.; Adlhart, C. *J. Am. Chem. Soc.* **2004**, *126*, 3496. (b) Naumov, S.; Buchmeiser, M. R. *J. Phys. Org. Chem.* **2008**, *21*, 963.

30. Mikus, M. S.; Torker, S.; Hoveyda, A. H. *Angew. Chem., Int. Ed.* **2016**, *55*, 4997.

31. Tabor, D. C.; White, F. H.; Collier, L. W.; Evans, S. A. *J. Org. Chem.* **1983**, *48*, 1638.

32. Maier, G.; Jung, W. A. *Chem. Ber.* **1982**, *125*, 804.

33. Alimuniar, A. B.; Blackmore, P. M.; Edwards, J. H.; Feast, W. J.; Wilson, B. *Polymer* **1986**, *27*, 1281.

34. Mühlebach, A.; Bernhard, P.; Bühler, N.; Karlen, T.; Ludi, A. *J. Mol. Catal.* **1994**, *90*, 143.

35. (a) Berson, J. A.; Walia, J. S.; Remanick, A.; Suzuki, S.; Reynolds-Warnhoff, P.; Willner, D. *J. Am. Chem. Soc.* **1961**, *83*, 3986. (b) Ishihara, K.; Hanaki, N.; Funahashi, M.; Miyata, M.; Yamamoto, H. *Bull. Chem. Soc. Jpn.* **1995**, *68*, 1721. (c) Evans, D. A.; Barnes, D. M.; Johnson, J. S.; Lectka, T.; von Matt, P.; Miller, S. J.; Murry, J. A.; Norcross, R. D.; Shaughnessy, E. A.; Campos, K. R. *J. Am. Chem. Soc.* **1999**, *121*, 7582.

36. Van Wingerden, M. M. PhD Dissertation, California Institute of Technology, 2012. It is worthy to note that although this procedure employs both NBu_4Cl and NH_4Cl, NBu_4Cl could be omitted, promoting ease of purification.

37. Ledoux, N.; Allaert, B.; Pattyn, S.; Vander Mierde, H.; Vercaemst, C.; Verpoort, F. *Chem. Eur. J.* **2006**, *12*, 4654.

Supporting Information

General Information: All reactions were carried out in dry glassware under an argon atmosphere using standard Schlenk techniques or in a Vacuum Atmospheres Glovebox under a nitrogen atmosphere, unless otherwise specified. All solvents were purified by passage through solvent purification columns and further degassed by bubbling argon. C_6D_6 was purified by passage through a solvent purification column. $CDCl_3$, CD_2Cl_2, THF-d_8, and $(CD_3)_2CO$ were used as received. Monomers **3.6**,[31] **3.7**,[5b,32] **3.14**,[33] **3.15**,[34] **3.16**,[13a] and **3.18**[35] were synthesized according to literature procedure, while monomers **3.5** and **3.17** were purchased from Sigma Aldrich and either used as received (**3.5**) or distilled over CaH_2 prior to use (**3.17**). Catalysts **3.4** and **3.9**, as well as $RuCl_2(PCy_3)(=CH\text{-}o\text{-}O^iPrC_6H_4)$ (**3.36**), were obtained from Materia, Inc. Catalysts **3.10**, **3.11**, **3.12**,[10b] and **3.13**,[36] as well as 2-bromo-*N*-(2-*iso*-propyl-6-methylphenyl)acetamide

(**3.38**)[12] and *N*-heterocyclic carbenes (NHCs) **3.35**[37] and **3.47**,[10b] were synthesized according to literature procedures.

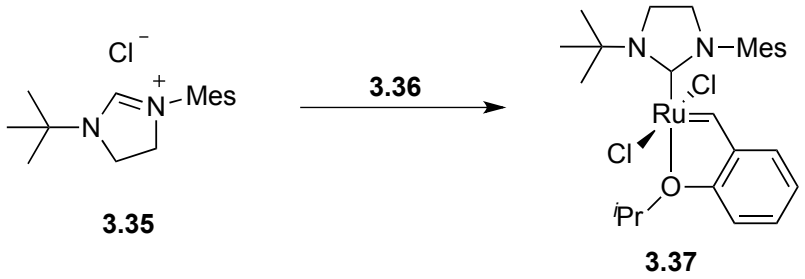
^{1}H NMR spectra were acquired at 500 MHz and ^{13}C NMR spectra at 100 or 126 MHz as $CDCl_3$ or C_6D_6 solutions unless otherwise noted. Chemical shifts are reported in ppm downfield from Me_4Si by using the residual solvent peak as an internal standard. Spectra were analyzed and processed using MestReNova Versions 7.1 and 9.0.

High-resolution mass spectra (HRMS) were provided by the California Institute of Technology Mass Spectrometry Facility using a JEOL JMS-600H High Resolution Mass Spectrometer. All HRMS were by FAB+ ionization, except where specified.

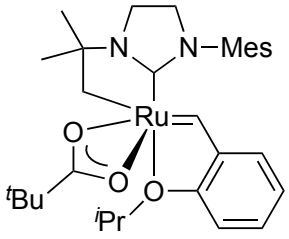
Polymer molecular weights were determined by multi-angle light scattering (MALS) gel permeation chromatography (GPC) using a miniDAWN TREOS light scattering detector, a Viscostar viscometer, and an OptilabRex refractive index detector, all from Wyatt Technology. An Agilent 1200 UV-Vis detector was also present in the detector stack. Absolute molecular weights were determined using d*n*/d*c* values calculated by assuming 100% mass recovery of the polymer sample injected into the GPC. No internal standards were used. DSC was performed using a Perkin Elmer DSC 7 at a nitrogen flow rate of 40 mL/min and a heating rate of 2 K/min from 0 °C to 200 °C. TGA was performed using a TA Instruments O5000 TGA at a nitrogen flow rate of 10 mL/min (sample) and 25 mL/min (balance).

Computational Details: Geometries were optimized with B3LYP and a mixed basis set of LANL2DZ for ruthenium and 6-31G(d) for other atoms. Single point calculations were performed with M06 and a mixed basis set of SDD for ruthenium and 6-311+G(d,p) for

other atoms. The SMD solvation model with THF as solvent was used in the single point energy calculations. This is the same level of theory used in the Houk group's previous calculations on ruthenium metathesis catalysts.

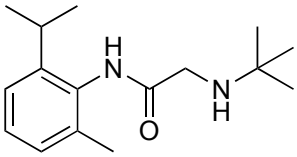


Preparation of 3.37: In a glovebox, a solution of **3.35** (0.19 g, 0.66 mmol) in hexanes (20 mL) was treated with $KCOMe_2Et$ (88 mg, 0.69 mmol), and the mixture was allowed to stir at r.t. for 2 h. To the reaction mixture was then added **3.36** (0.38 g, 0.64 mmol), upon which the mixture was removed from the glove box and allowed to stir at 65 °C overnight (12 h). The precipitated solids were filtered and washed well with warm hexanes and pentane and then collected with CH_2Cl_2 and concentrated. The crude mixture was further purified by flash column chromatography (SiO_2, eluent pentane to 20% Et_2O in pentane to CH_2Cl_2) to provide **3.37** (0.24 g, 68%) as a green powder. ^{1}H NMR (500 MHz, $CDCl_3$) δ 16.87 (s, 1H), 7.56 (m, 1H), 7.07 (s, 2H), 6.97–6.89 (m, 3H), 6.87 (m, 1H), 5.08 (hept, J = 6.2 Hz, 1H), 4.10–3.82 (m, 4H), 2.46 (s, 3H), 2.26–2.27 (m, 15H), 1.62 (d, J = 6.2 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 312.9, 207.5, 152.6, 145.7, 139.4, 138.6, 138.2, 130.9, 129.7, 124.0, 122.8, 113.3, 74.5, 56.3, 51.6, 46.1, 29.8, 22.5, 21.3, 18.4. HRMS (FAB+, (M)): Calculated—564.1249, Found—564.1268.



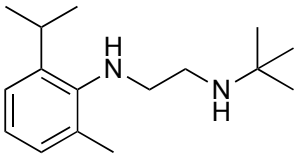
3.1

Preparation of 3.1: In a glovebox, a 20 mL scintillation vial was charged with **3.37** (0.11 g, 0.20 mmol), NaOPiv (0.25 g, 2.0 mmol), THF (4.0 mL), and MeOH (2.0 mL). The vial was capped, removed from the glovebox, and heated at 40 °C for 5 h during which a color change from green to brown to dark purple was observed. The vial was then returned to the box, where the solvent was removed *in vacuo* and the resulting solid dissolved in CH_2Cl_2 (30 mL), filtered through celite, and concentrated to a deep purple residue. The crude mixture was purified by pipette column (SiO_2, eluent 20% Et_2O in pentane) three times and subsequently recrystallized from pentane to provide **3.1** as a bright purple solid (59 mg, 22%). ^{1}H NMR (500 MHz, THF-d_8) δ 14.69 (s, 1H), 7.44–7.36 (m, 1H), 7.32 (m, 1H), 7.07 (m, 1H), 6.88 (m, 1H), 6.72 (s, 2H), 5.04 (hept, J = 6.2 Hz, 1H), 3.95–3.72 (m, 4H), 2.82 (d, J = 10 Hz, 1H), 2.38 (s, 3H), 2.38 (*overlapped*, 1H), 2.14 (s, 3H), 2.13 (s, 3H), 1.45 (d, J = 6.2 Hz, 3H), 1.44 (s, 3H), 1.38 (d, J = 6.2 Hz, 3H), 0.87 (s, 9H), 0.57 (s, 3H). ^{13}C NMR (126 MHz, CD_2Cl_2) δ 260.3, 211.4, 188.2, 155.0, 143.7, 137.9, 137.6, 137.0, 136.8, 129.9, 129.2, 126.2, 123.4, 122.7, 114.1, 75.8, 62.6, 51.1, 47.7, 43.9, 39.6, 29.4, 28.1, 23.2, 22.2, 22.0, 21.1, 18.8, 18.7. HRMS (FAB+, [(M+H)-H_2]): Calculated—593.2318, Found—593.2327.



3.39

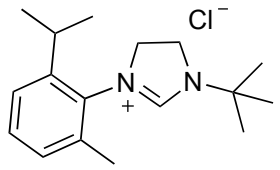
Preparation of 3.39: Compound **3.38** (7.2 g, 27 mmol) and $^{t}BuNH_2$ (4.2 mL, 39 mmol) were dissolved in MeCN (90 mL), K_2CO_3 (5.7 g, 42 mmol) was added, and the solution was refluxed for 24 h. After cooling to r.t., the mixture was filtered over celite and concentrated. The residue was then dissolved in CH_2Cl_2 and filtered over a pad of silica gel (eluent 10% MeOH in CH_2Cl_2). Removal of the solvent *in vacuo* provided **3.39** (6.7 g, 94%) as an off-white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.09 (br s, 1H), 7.18 (m, 1H), 7.16 (m, 1H), 7.09 (m, 1H), 3.41 (s, 2H), 3.03 (m, 1H), 2.22 (s, 3H), 1.71 (br s, 1H), 1.20 (d, J = 6.9 Hz, 6H), 1.17 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.6, 145.2, 135.6, 132.8, 128.2, 127.5, 123.4, 51.3, 46.1, 29.1, 28.7, 23.4, 18.8. HRMS (FAB+, (M+H)): Calculated—263.2123, Found—263.2111.



3.40

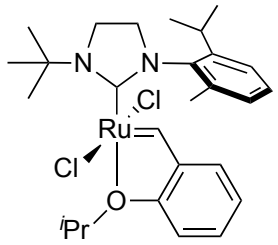
Preparation of 3.40: A solution of compound **3.39** (6.7 g, 26 mmol) in THF (10 mL) was added to a 0 °C solution of $LiAlH_4$ (3.0 g, 79 mmol) in THF (100 mL). The resulting solution was allowed to warm to r.t., then refluxed for 72 h. The mixture was then cooled to 0 °C and carefully quenched via the sequential, dropwise addition of H_2O (3.0 mL), 10% *aq.* NaOH (3.0 mL), and H_2O (3.0 mL). The solution was dried with $MgSO_4$, filtered, and concentrated. Flash chromatography of the residue (SiO_2, eluent 10% MeOH in CH_2Cl_2) provided **3.40** (3.7 g, 57%) as a pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$)

δ 7.09 (m, 1H), 6.98 (m, 1H), 6.91 (m, 1H), 3.29 (m, 1H), 3.00 (m, 2H), 2.80 (m, 2H), 2.33 (s, 3H), 1.24 (d, J = 6.9 Hz, 6H), 1.13 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 145.2, 140.7, 130.5, 128.4, 123.6, 122.4, 50.6, 50.3, 42.8, 29.2, 27.5, 24.0, 19.0. HRMS (FAB+, (M+H)): Calculated—249.2331, Found—249.2335.



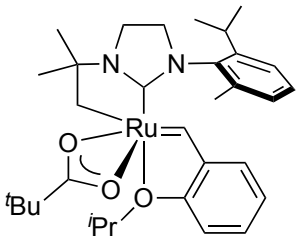
3.41

Preparation of 3.41: A solution of compound **3.40** (3.5 g, 14 mmol) in Et_2O (25 mL) was treated with HCl (14 mL, 2.0 M in Et_2O) and stirred for 15 minutes at r.t. The solid was then filtered, washed with Et_2O, dried, suspended in $CH(OEt)_3$ (25 mL), and refluxed for 2 h. After cooling the solution to r.t., the solvent was removed *in vacuo* and the resulting solid residue washed rigorously with Et_2O to provide **3.41** (1.5 g, 37%) as an off-white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.02 (br s, 1H), 7.31 (m, 1H), 7.22 (m, 1H), 7.12 (m, 1H), 4.49 (m, 1H), 4.38 (m, 2H), 4.22 (m, 1H), 2.91 (m, 1H), 2.40 (s, 3H), 1.61 (s, 9H), 1.27 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.0, 146.4, 135.9, 132.0, 130.5, 129.2, 124.8, 57.8, 52.4, 46.5, 28.6, 28.4, 24.8, 24.2, 18.6. HRMS (FAB+, (M-Cl)): Calculated—259.2174, Found—259.2172.



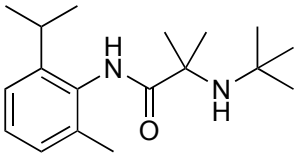
3.42

Preparation of 3.42: In a glovebox, $KCOMe_2Et$ (0.15 g, 1.2 mmol) was added to a suspension of compound **3.41** (0.29 g, 1.0 mmol) in hexanes (12 mL). After stirring at 35 °C for 30 minutes, compound **3.36** (0.60 g, 1.0 mmol) was added, and the reaction mixture was sealed and removed from the glovebox. The solution was stirred for 3 h at 65 °C and subsequently cooled to r.t. The resulting precipitate was filtered, washed with warm hexanes, and further purified by column chromatography (SiO_2, eluent pentane to 20% Et_2O in pentane to DCM) to provide **3.42** (0.55 g, 92%) as a green solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 16.86 (s, 1H), 7.54 (m, 1H), 7.49 (m, 1H), 7.41 (m, 1H), 7.23 (m, 1H), 6.94 (m, 1H), 6.88 (m, 1H), 6.85 (m, 1H), 5.07 (hept, J = 6.2 Hz, 1H), 4.02 (m, 2H), 3.91 (m, 2H), 3.17 (hept, J = 6.8 Hz, 1H), 2.33 (s, 3H), 2.28 (s, 9H), 1.67 (d, J = 6.2 Hz), 1.59 (d, J = 6.2 Hz, 3H), 1.19 (d, J = 6.8 Hz, 3H), 0.89 (d, J = 6.8 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 311.0, 207.8, 152.7, 148.8, 145.0, 140.4, 138.0, 130.7, 129.1, 129.0, 124.8, 123.9, 122.6, 113.2, 74.5, 56.3, 53.1, 46.0, 29.8, 27.6, 25.6, 23.8, 22.7, 22.3, 19.0. HRMS (FAB+, (M)): Calculated—578.1405, Found—578.1433.



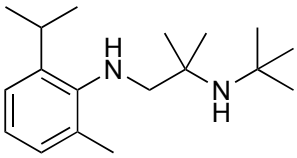
3.2

Preparation of 3.2: In a glovebox, a 20 mL scintillation vial was charged with **3.42** (0.10 g, 0.17 mmol), NaOPiv (0.22 g, 1.7 mmol), THF (6.0 mL) and MeOH (3.0 mL). The vial was capped, removed from the glovebox, and heated at 50 °C for 12 h during which a color change from green to brown to dark purple was observed. The vial was then returned to the glovebox, where the solvent was removed *in vacuo* and the resulting solid was dissolved in CH_2Cl_2 (30 mL), filtered over a pad of celite, and concentrated to a deep purple residue. Purification of the crude mixture by a silica gel plug (eluent pentane to 20% Et_2O in pentane) followed by recrystallized from hexanes provided **3.2** (65 mg, 65%) as a bright purple solid. ^{1}H NMR (500 MHz, CD_2Cl_2) δ 14.70 (s, 1H), 7.45 (m, 1H), 7.39 (m, 1H), 7.08 (m, 1H), 7.07 (m, 1H), 7.02 (m, 1H), 6.94 (m, 2H), 4.99 (hept, *J* = 6.4 Hz, 1H), 3.92–3.79 (m, 3H), 3.79–3.69 (m, 2H), 2.79 (d, *J* = 6.8 Hz, 1H), 2.45 (d, *J* = 6.8 Hz, 1H), 2.17 (s, 3H), 1.47 (s, 3H), 1.44 (d, *J* = 6.4 Hz, 3H), 1.40 (d, *J* = 6.4 Hz, 3H), 1.24 (d, *J* = 6.9 Hz, 3H), 1.10 (d, *J* = 6.9 Hz, 3H), 0.91 (s, 9H), 0.56 (s, 3H). ^{13}C NMR (126 MHz, CD_2Cl_2) δ 260.2, 210.9, 187.5, 154.5, 147.5, 143.2, 138.4, 137.5, 128.3, 127.5, 125.6, 123.8, 122.9, 122.3, 113.8, 75.5, 62.1, 51.8, 47.3, 43.4, 39.1, 28.8, 27.9, 27.7, 25.5, 23.7, 22.8, 21.8, 21.7, 18.7. HRMS (FAB+, (M)): Calculated—608.2552, Found—608.2536.



3.43

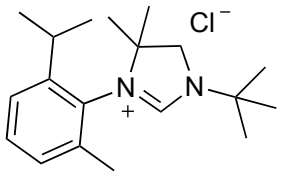
Preparation of 3.43: 2-Bromo-2-methylpropionyl bromide (4.1 g, 33 mmol) was dissolved in CH_2Cl_2 (60 mL), $^tBuNH_2$ (3.2 mL, 30 mmol) and then Et_3N (12 mL, 60 mmol) were added dropwise, and the mixture was stirred overnight at r.t. The solution was then washed with saturated NH_4Cl (*aq.*) (x2), dried with Na_2SO_4, and concentrated. The resulting residue was dissolved in THF (75 mL), cannulated into a solution of 2-isopropyl-6-methylaniline (5.0 g, 33 mmol) and NaH (1.4 g, 60 mmol) in THF (75 mL), and stirred overnight at r.t. The solution was then diluted with EtOAc, washed with saturated NH_4Cl (*aq.*) and brine, dried using Na_2SO_4, and concentrated. Purification by flash chromatography (SiO_2, eluent 10% MeOH in CH_2Cl_2) provided **3.43** (2.9 g, 33%) as a peach solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (br s, 1H), 7.10 (m, 1H), 6.98 (m, 2H), 3.17 (br s, 1H), 3.11 (m, 1H), 2.27 (s, 3H), 1.40 (s, 9H), 1.30 (s, 6H), 1.20 (d, J = 6.9 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 176.9, 143.4, 141.3, 132.7, 128.5, 124.1, 123.7, 60.3, 50.2, 28.5, 28.2, 27.1, 23.7, 20.7. HRMS (EI+, (M+H)): Calculated—291.2436, Found—291.2429.



3.44

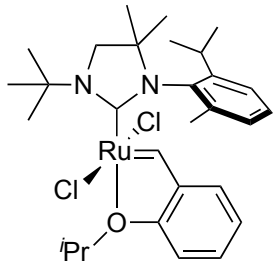
Preparation of 3.44: A solution of $BH_3{\cdot}THF$ (43 mL, 1.0 M in THF) was added dropwise to a 0 °C solution of compound **3.43** (2.5 g, 8.6 mmol) in THF (12 mL). The mixture was stirred overnight at r.t., then quenched via dropwise addition of MeOH at 0

°C and concentrated. The residue was then re-dissolved in MeOH and re-concentrated (x3). Purification by flash chromatography (SiO_2, eluent CH_2Cl_2 then 10% MeOH in CH_2Cl_2) provided **3.44** (1.2 g, 50%) as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.09 (m, 1H), 7.00 (m, 1H), 6.97 (m, 1H), 3.53 (m, 1H), 2.60 (2, 2H), 2.37 (s, 3H), 1.18 (d, *J* = 6.9 Hz, 6H), 1.15 (s, 9H), 1.06 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 145.5, 142.6, 135.2, 128.1, 123.4, 123.2, 56.0, 54.9, 49.9, 29.3, 27.5, 26.7, 24.1, 20.8. HRMS (EI+, (M+H)): Calculated—277.2644, Found—277.2636.



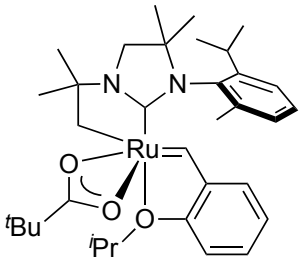
3.45

Preparation of 3.45: A solution of compound **3.44** (1.1 g, 4.0 mmol) in Et_2O (10 mL) was treated with HCl (4.0 mL, 2.0 M in Et_2O) and stirred for 15 minutes at r.t. The solid was then filtered, washed with Et_2O, dried, suspended in $CH(OEt)_3$ (10 mL), and refluxed for 2 h, at which point the solution was cooled to r.t. and concentrated. The resulting solid residue was washed rigorously with Et_2O to provide **3.45** (0.6 g, 46%) as an off-white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.26 (br s, 1H), 7.30 (m, 1H), 7.21 (m, 1H), 7.13 (m, 1H), 4.07 (d, *J* = 12 Hz, 1H), 4.02 (d, *J* = 12 Hz, 1H), 2.85 (m, 1H), 2.41 (s, 3H), 1.60 (s, 9H), 1.48 (s, 3H), 1.41 (s, 3H), 1.29 (d, *J* = 6.8 Hz, 3H), 1.16 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.7, 148.3, 137.8, 130.3, 129.7, 128.9, 124.7, 69.7, 58.7, 57.8, 29.2, 28.3, 26.9, 26.4, 25.9, 22.7, 20.5. HRMS (FAB+, (M-Cl)): Calculated—287.2487, Found—287.2499.



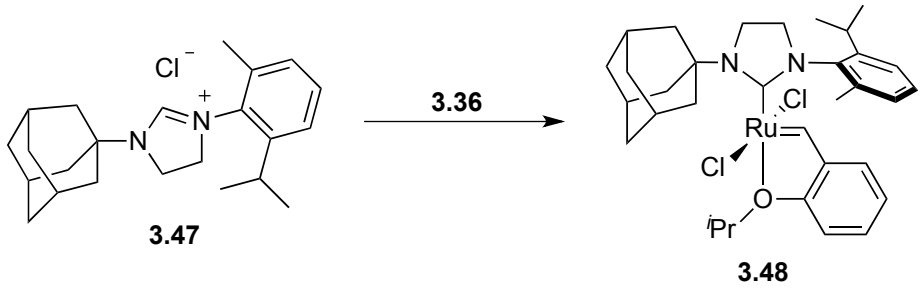
3.46

Preparation of 3.46: In a glovebox, $KCOMe_2Et$ (57 mg, 0.45 mmol) was added to a suspension of compound **3.45** (0.14 g, 0.43 mmol) in hexanes (13 mL). The solution was then stirred at r.t. for 2 h, at which point **3.36** (0.31 g, 0.52 mmol) was added and the reaction mixture subsequently sealed and removed from the glovebox. The solution was stirred for 3 h at 65 °C and then cooled to r.t. The resulting precipitate was filtered, washed thoroughly with warm hexanes, and further purified by flash chromatography (SiO_2, eluent pentane to 20% Et_2O in pentane to CH_2Cl_2) to provide **3.46** (0.21 g, 86%) as a green solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 16.66 (s, 1H), 7.57–7.42 (m, 3H), 7.24–7.20 (m, 1H), 6.93 (d, *J* = 8.4 Hz, 1H), 6.90–6.83 (m, 2H), 5.06 (hept, *J* = 6.3 Hz, 1H), 3.84 (d, *J* = 9.9 Hz, 1H), 3.65 (d, *J* = 9.8 Hz, 1H), 3.25 (hept, *J* = 6.7 Hz, 1H), 2.29 (*overlapped*, 12H), 1.68 (d, *J* = 6.2 Hz, 3H), 1.58 (d, *J* = 6.2 Hz, 3H), 1.40 (s, 3H), 1.24 (d, *J* = 6.8 Hz, 3H), 1.12 (s, 3H), 0.75 (d, *J* = 6.6 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 310.79, 207.99, 152.78, 150.31, 144.75, 140.38, 138.56, 130.61, 129.54, 128.67, 125.33, 124.12, 122.65, 113.34, 74.45, 65.40, 61.19, 56.32, 29.79, 28.33, 27.99, 25.63, 25.26, 23.92, 22.86, 22.29, 21.32. HRMS (FAB+, (M+H)-H_2): Calculated—605.1640, Found—605.1618.

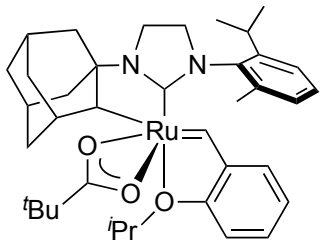


3.3

Preparation of 3.3: In a glovebox, a 20 mL scintillation vial was charged with **3.46** (60 mg, 0.10 mmol), NaOPiv (0.12 g, 1.0 mmol), THF (2.0 mL), and MeOH (2.0 mL). The vial was capped, removed from the glovebox, and heated at 40 °C for 21 h during which a color change from green to brown to dark purple was observed. The vial was returned to the box, where the solvent was removed *in vacuo* and the resulting solid dissolved in CH_2Cl_2 (15 mL), filtered through celite, and concentrated to a deep purple residue. The residue was purified by pipet column (SiO_2, eluent 20% Et_2O in pentane) and subsequently recrystallized from hexanes to provide **3.3** (25 mg, 40%) as a bright purple solid. ^{1}H NMR (500 MHz, C_6D_6) δ 14.98 (s, 1H), 7.47 (dd, *J* = 7.4, 1.7 Hz, 1H), 7.23 (td, *J* = 8.0, 1.7 Hz, 1H), 7.07 (*overlapped*, 2H), 6.97–6.99 (m, 1H), 6.88 (t, *J* = 7.4 Hz, 1H), 6.60 (d, *J* = 8.3 Hz, 1H), 4.63 (hept, *J* = 6.3 Hz, 1H), 3.98 (hept, *J* = 6.8 Hz, 1H), 3.35–3.21 (m, 2H), 2.80–2.69 (m, 2H), 2.32 (s, 3H), 1.46 (d, *J* = 6.4 Hz, 3H), 1.40 (s, 3H), 1.35 (s, 3H), 1.31 (d, *J* = 6.9 Hz, 3H), 1.24 (d, *J* = 6.1 Hz, 3H), 1.18 (s, 9H), 1.12 (d, *J* = 6.9 Hz, 3H), 0.76 (s, 3H), 0.61 (d, *J* = 9.0 Hz, 3H). ^{13}C NMR (126 MHz, C_6D_6) δ 260.95, 211.46, 187.86, 155.35, 149.68, 144.03, 139.68, 136.90, 128.69, 127.87, 127.57, 125.73, 124.69, 123.15, 122.70, 113.79, 75.07, 64.80, 62.12, 57.77, 47.76, 39.61, 30.87, 28.77, 28.69, 28.39, 25.63, 24.67, 24.12, 22.87, 22.01, 21.82, 20.68. HRMS (FAB+, (M+H)-H_2): Calculated—635.2787, Found—635.2788.

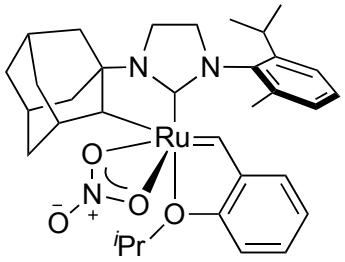


Preparation of 3.48: In a glovebox, a suspension of $KCOMe_2Et$ (75 mg, 0.57 mmol) in hexanes (6 mL) was added to **3.47** (0.19 g, 0.52 mmol), and the resulting solution was stirred in the glovebox at 30 °C for 30 minutes. Compound **3.36** (0.31 g, 0.52 mmol) was then added, and the vessel was sealed, taken out of the glovebox, and stirred for 2 h at 65 °C. After cooling the mixture to r.t., the precipitated solids were collected via filtration and washed thoroughly with warm hexanes, providing **3.48** (0.22 g, 65%) as a green powder. ^{1}H NMR ($CDCl_3$) d 16.89 (1H, s), 7.54 (1H, m), 7.50 (1H, m), 7.41 (1H, m), 7.23 (1H, m), 6.93 (1H, m), 6.85 (1H, m), 5.07 (1H, m), 4.05 (2H, m), 3.88 (2H, m), 3.15 (1H, m), 2.97 (4H, m), 2.42 (3H, m), 2.33 (3H, s), 1.95 (3H, m), 1.84 (3H, m), 1.69 (3H, d, J = 6.1 Hz), 1.60 (3H, d, J = 6.1 Hz), 1.19 (3H, d, J = 6.7 Hz), 0.89 (3H, d, J = 6.7 Hz); ^{13}C NMR ($CDCl_3$) d 208.6, 152.9, 149.0, 145.6, 141.0, 138.3, 131.0, 129.5, 129.3, 125.2, 124.2, 122.9, 113.6, 74.6, 57.6, 53.1, 44.9, 42.6 (2C), 36.5 (3C), 30.4 (3C), 28.0, 25.9, 24.2, 23.1, 22.6, 19.3; HRMS (FAB+, (M)): Calculated—656.1875, Found—656.1894.



3.49

Preparation of 3.49: In a glovebox, a 20 mL scintillation vial was charged with **3.48** (0.10 g, 0.15 mmol), NaOPiv (0.19 g, 1.5 mmol), THF (1.5 mL), and MeOH (1.5 mL). The solution was heated at 40 °C for 10 hours in the glovebox during which a color change from green to brown to dark purple was observed. The solvent was then removed *in vacuo*, and the resulting residue was dissolved in CH_2Cl_2, filtered over celite, and concentrated. Purification via a short plug of silica gel (eluent 20% Et_2O in pentane) provided **3.49** (52 mg, 52%) as a bright purple solid. ^{1}H NMR (CD_2Cl_2) d 14.66 (1H, s), 7.38 (2H, m), 7.11 (2H, m), 6.98 (1H, m), 6.94 (1H, m), 6.92 (1H, m), 5.00 (1H, m), 3.88 (3H, m), 3.76 (3H, m), 2.20 (2H, m), 2.16 (3H, s), 2.15 (1H, m), 1.97 (2H, m), 1.71 (1H, m), 1.54 (3H, d, J = 6.1 Hz), 1.52 (3H, m), 1.40 (3H, d, J = 6.1 Hz), 1.25 (3H, d, J = 6.7 Hz), 1.21 (3H, d, J = 6.7 Hz), 1.00 (9H, s), 0.98 (1H, m), 0.23 (1H, m); ^{13}C NMR (CD_2Cl_2) d 215.8, 154.2, 147.7, 143.4, 138.7, 138.1, 128.8, 128.1, 125.8, 124.3, 123.2, 123.0, 114.1, 74.9, 69.3, 63.0, 53.1, 43.5, 41.9, 40.6, 39.4, 38.2, 37.9, 37.1, 33.7, 31.2, 30.1, 28.5, 28.3 (3C), 26.3, 24.0, 21.9, 21.8, 19.5; HRMS (FAB+, (M+H)-H_2): Calculated—686.3022, Found—686.3039.



3.8

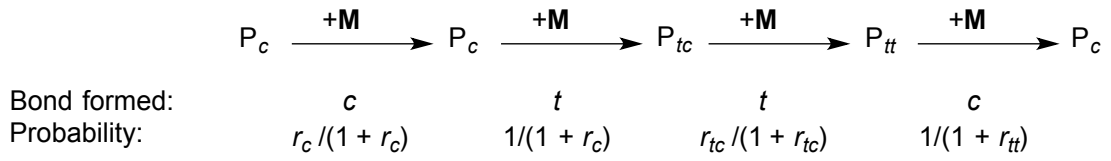
Preparation of 3.8: In a glovebox, complex **3.49** (0.11 g, 0.15 mmol) and NH_4NO_3 (0.12 g, 1.5 mmol) were dissolved in THF (8 mL), stirred for 3 h at r.t., and concentrated. The resulting solids were washed with Et_2O followed by THF to provide **3.8** (70 mg, 72%) as a bright purple solid. ^{1}H NMR (CD_2Cl_2) d 14.98 (1H, s), 7.48 (1H, m), 7.43 (1H, m), 7.13 (1H, m), 7.09 (1H, m), 6.98 (3H, m), 5.10 (1H, m), 3.90 (4H, m), 3.70 (2H, m), 2.23 (1H, m), 2.18 (3H, s), 2.07 (1H, m), 1.99 (1H, m), 1.93 (1H, m), 1.72 (1H, m), 1.65 (1H, m), 1.59 (1H, m), 1.55 (2H, m), 1.49 (3H, d, J = 6.1 Hz), 1.24 (3H, d, J = 6.1 Hz), 1.18 (3H, d, J = 6.7 Hz), 1.13 (3H, d, J = 6.7 Hz), 0.99 (2H, m), 0.25 (1H, m); ^{13}C NMR (CD_2Cl_2) d 213.2, 154.9, 147.8, 143.2, 138.1, 137.5, 128.8, 128.4, 127.3, 124.2, 123.6 (2C), 113.1, 74.6, 67.8, 63.6, 52.8, 43.4, 42.4, 40.5, 38.0, 37.9, 37.8, 33.4, 31.1, 29.9, 28.5, 26.4, 23.7, 21.5, 20.8, 17.7; HRMS (FAB+, (M+H)-H_2): Calculated—645.7706, Found—646.2040.

General Procedure for the Determination of Initiation Rates: In a glovebox, a 4 mL vial was charged with catalyst (12 μmol) and diluted with 1 mL C_6D_6 to create a stock solution (12 mM). A portion of the stock solution (0.25 mL, 3.0 μmol catalyst) was added to an NMR tube and diluted with C_6D_6 (0.35 mL). The NMR tube was sealed with a septum cap and placed in an NMR spectrometer heated to 30 °C. Butyl vinyl ether (12 μL, 0.090 mmol) was added and the disappearance of the benzylidene proton resonance was monitored by arraying the 'pad' function in VNMRj.

All reactions displayed clean first-order kinetics over a period of at least three half-lives. Spectra were baseline corrected and integrated with MestReNova Ver. 7.1.

General Polymerization Procedure: In a glovebox, an 8 mL vial with a septum cap was charged with catalyst (9.8 μmol) and THF (.84 mL) to make a stock solution (0.012 M). On a vacuum manifold, a Schlenk flask was flame-dried and charged with monomer (7.8 mmol) and THF (24 mL) to make a second stock solution (0.32 M). The monomer solution was degassed via freeze-pump-thaw (3x). An aliquot (2.0 mL, 0.64 mmol) of monomer stock solution was added via gas-tight syringe to an airtight vial with a septum cap under an argon balloon. An aliquot (0.55 mL, ca. 6.4 μmol, 1 mol %) of catalyst solution was then injected via gas-tight syringe. After stirring for 1 h at r.t., the polymerization was quenched with ethyl vinyl ether (0.1 mL) and precipitated into vigorously stirred MeOH. The precipitate was collected by vacuum filtration using either a medium or fine porosity frit and dried under vacuum.

General Method for Determining Bond Formation Probabilities: Bond formation probabilities in Scheme 2 were calculated as outlined in Reference 18.



Scheme 3.6. Probability formulas for the formation of *cis* or *trans* double bonds in the metal-catalyzed ROMP of norbornene (**3.5**). P_c refers to a propagating species that has just formed a *cis* double bond, while P_{tc} and P_{tt} describe species that have just formed a *trans* double bond but have different penultimate double bonds (*cis* and *trans*, respectively).

The probability of forming a *cis* double bond in a species in which the last-formed double bond is *cis* (P_c) is equivalent to the number of *cc* dyads present in the polymer divided by the total number of *cx* dyads ($x = c$ or t), or $(cc)/(cc + ct)$. Because $r_c = (cc)/(ct)$, this can also be written as $r_c/(1 + r_c)$. The probability of forming a *trans* double bond in P_c is equal to $1 - [r_c/(1 + r_c)]$, or $1/(1 + r_c)$. Dyad values can be determined by ^{13}C NMR.[13b]

Calculations that also take into account the identity of the penultimate double bond require triad-level NMR analysis (see reference 18 for peak assignments). For example, the probability of forming a *trans* double bond in a species in which the last-formed double bond is *trans* and the penultimate double bond is *cis* (P_{tc}) is equivalent to the proportion of *ctt* triads divided by all possible *ctx* triads, or $(ctt)/(ctt + ctc)$. If we define $r_{tc} = (ctt)/(ctc)$, this can also be written as $r_{tc}/(1 + r_{tc})$. Similarly, the probability of forming a *cis* double bond in P_{tt} is equal to $1/(1+r_{tt})$, where $r_{tt} = (ttt)/(ttc)$.

Preparation of Poly(3.5) Using Catalysts 3.1–3.4 and 3.8–3.13: Poly(3.5) was prepared according to the general procedure using catalysts **3.1–3.4** and **3.8–3.13**. NMR samples were prepared by stirring **poly(3.5)** in $CDCl_3$. ^{13}C NMR spectral assignments were consistent with the literature.[13]

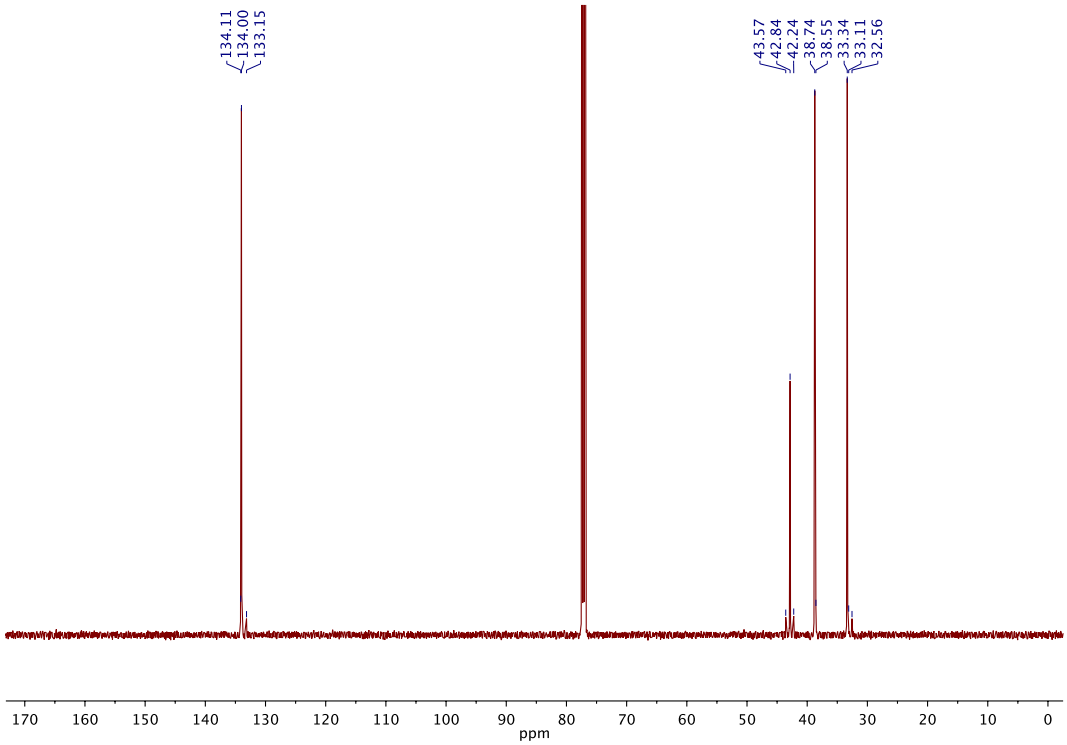


Figure 3.14. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly(3.5)/3.1**.

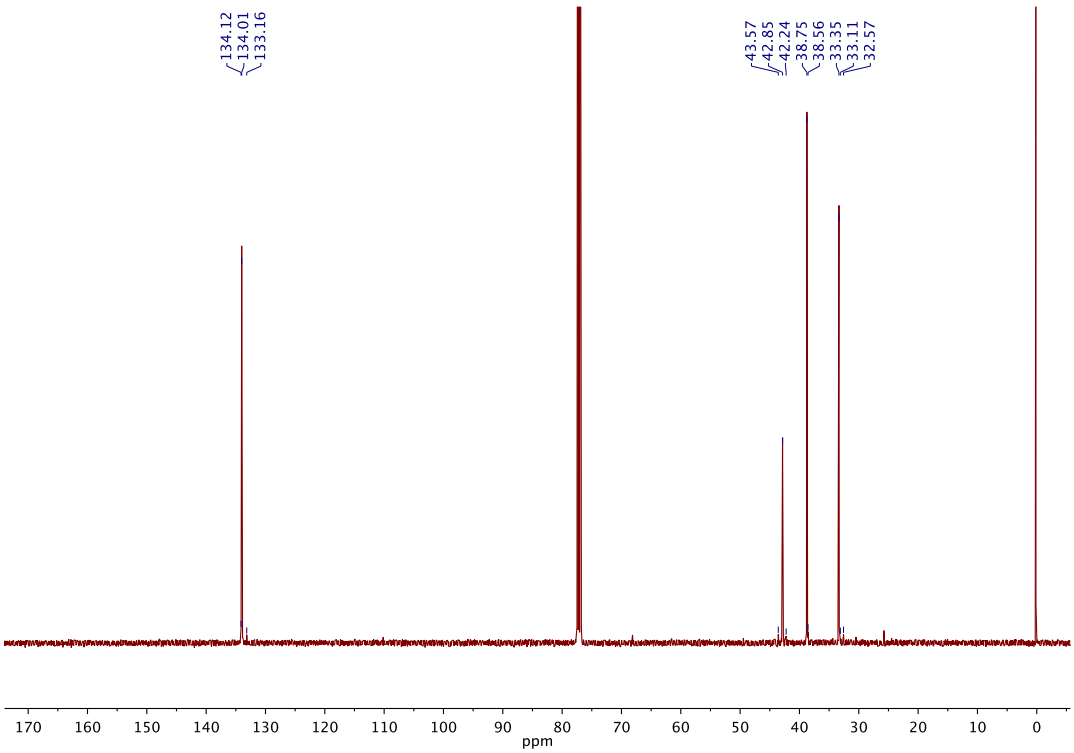


Figure 3.15. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly(3.5)/3.2**.

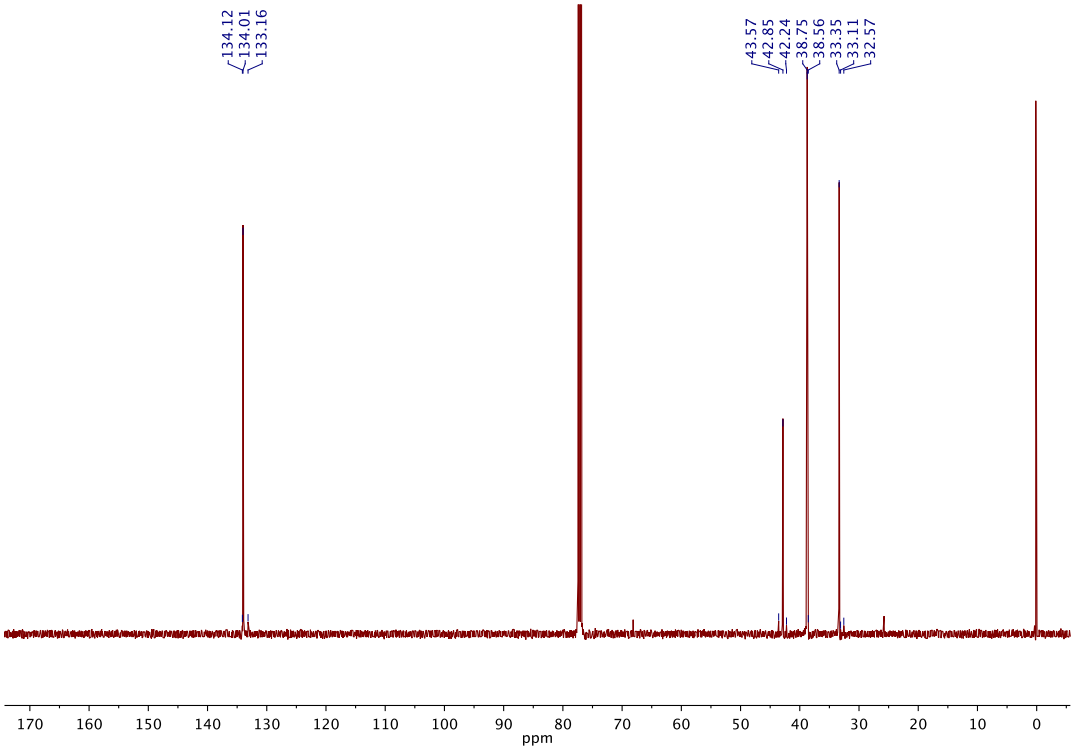


Figure 3.16. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly(3.5)/3.3** (peaks at 25.76 and 68.11 ppm are residual THF).

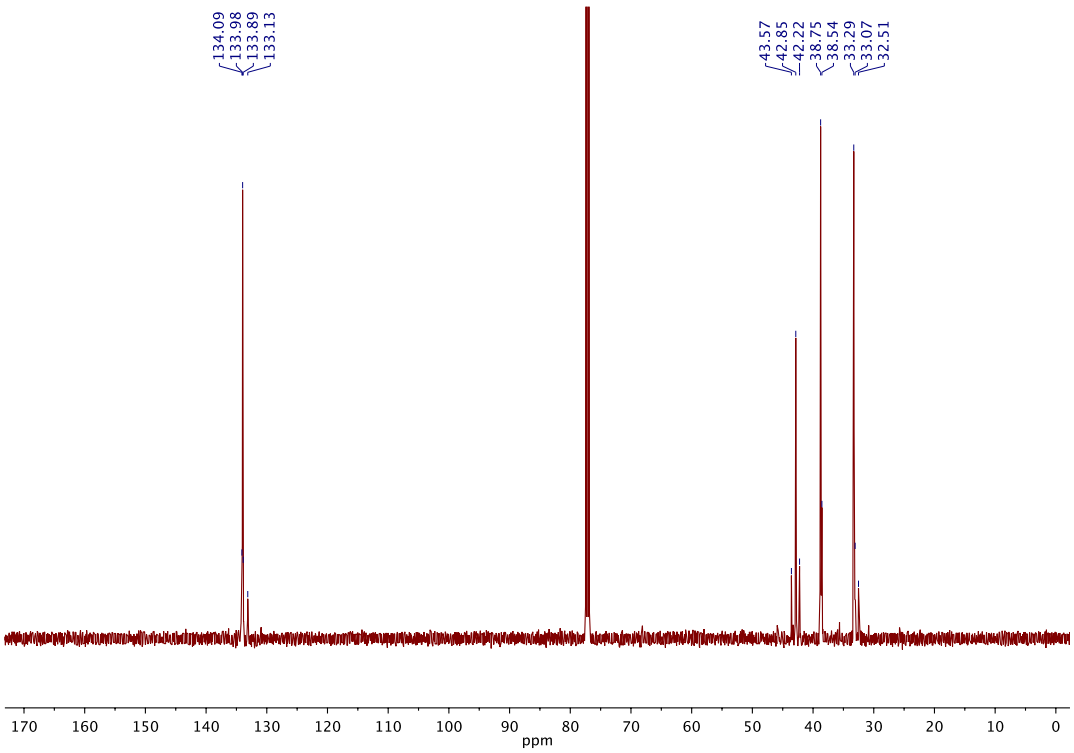


Figure 3.17. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly(3.5)/3.4**.

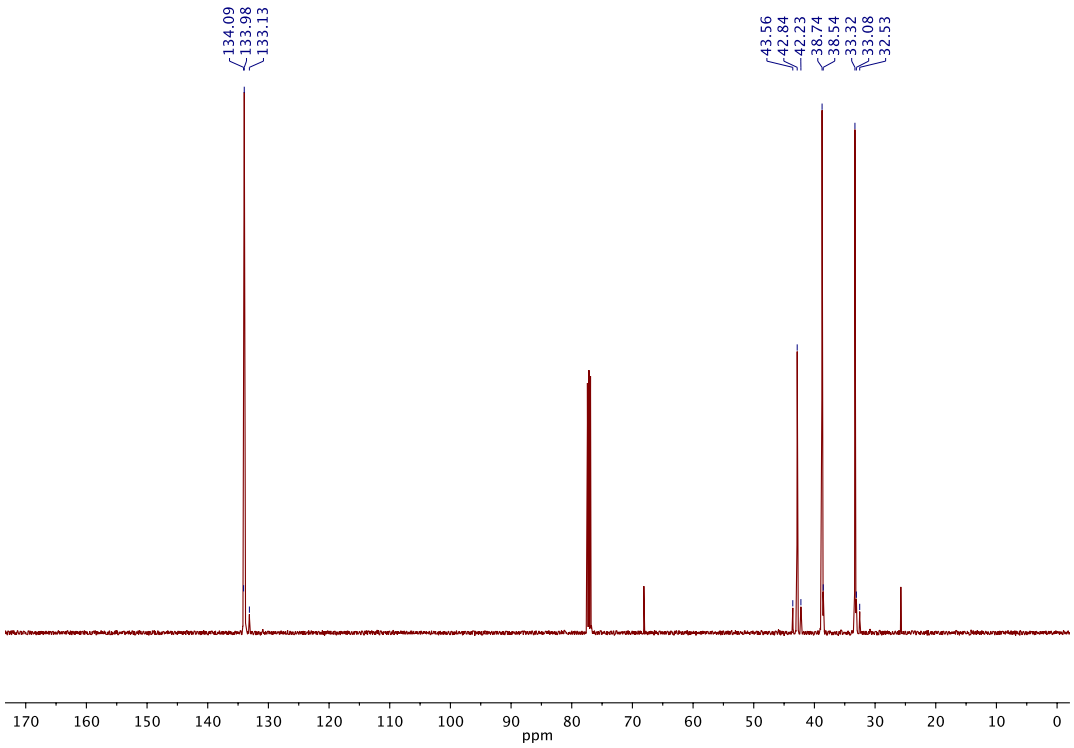


Figure 3.18. ^{13}C (126 MHz, $CDCl_3$) spectrum of **poly(3.5)/3.8** (peaks at 25.76 and 68.11 ppm are residual THF).

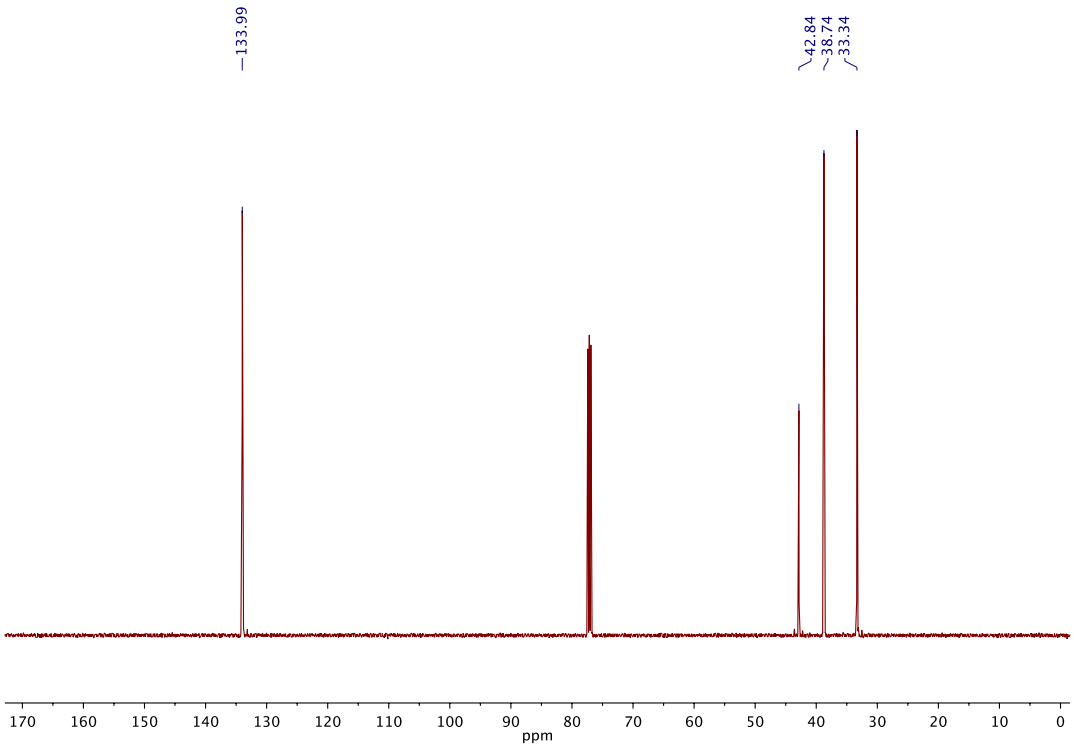


Figure 3.19. ^{13}C (126 MHz, $CDCl_3$) spectrum of **poly(3.5)/3.9**.

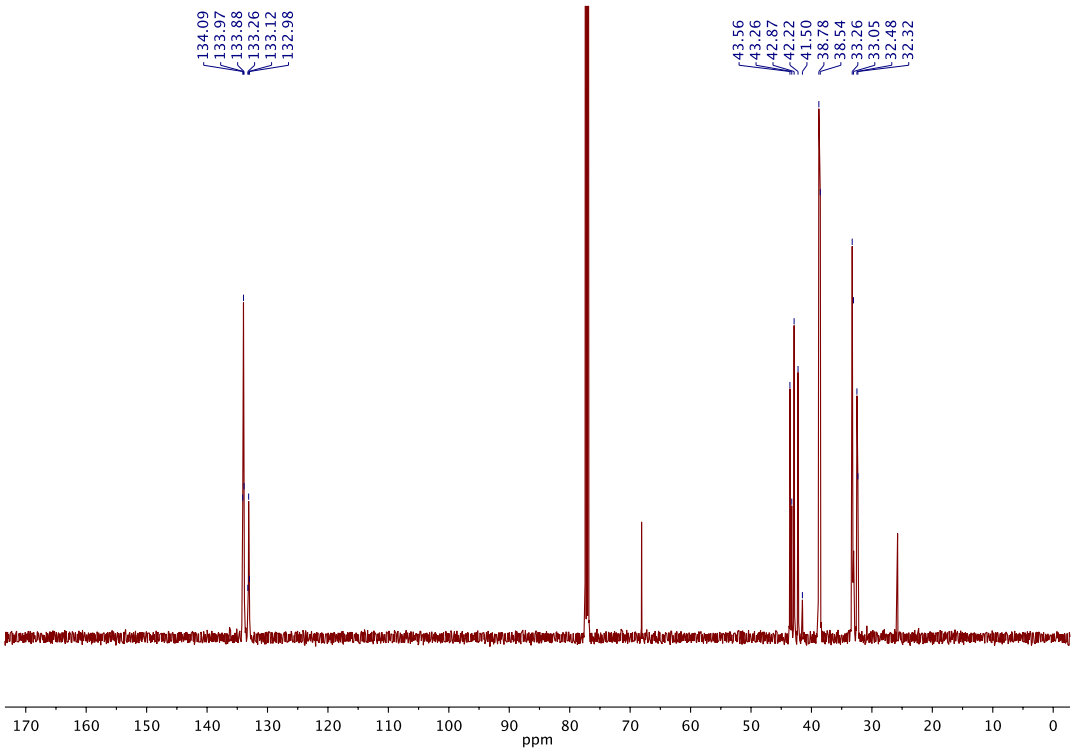


Figure 3.20. ^{13}C (126 MHz, $CDCl_3$) spectrum of **poly(3.5)/3.10** (peaks at 25.76 and 68.11 ppm are residual THF).

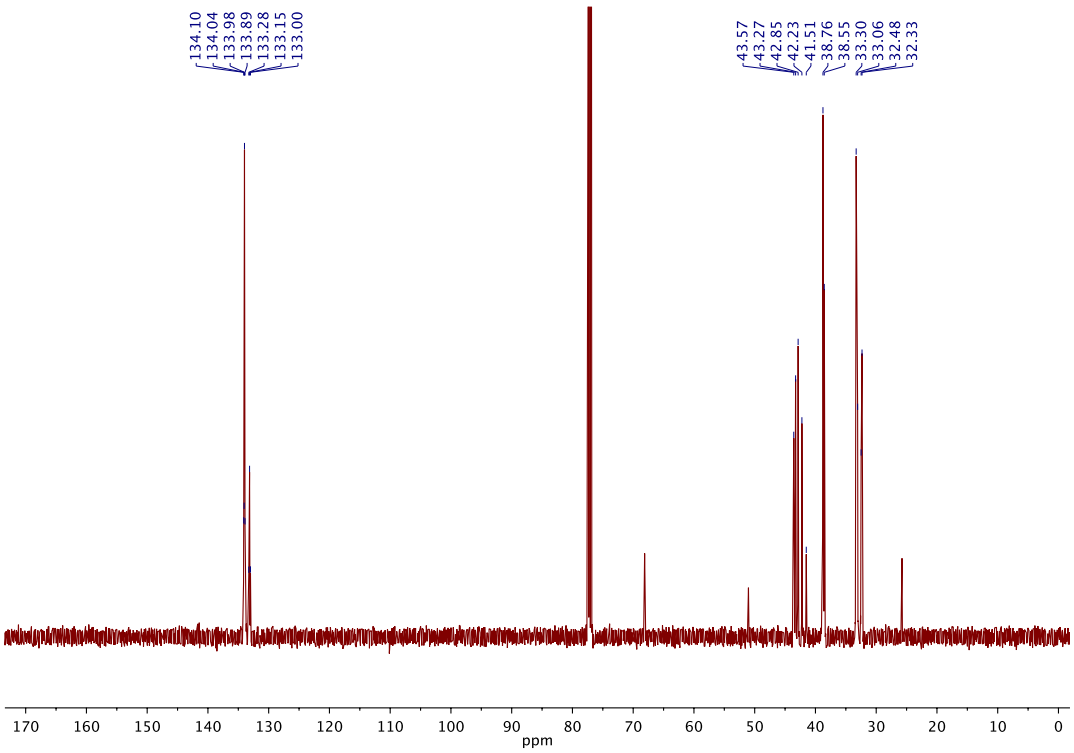


Figure 3.21. ^{13}C (126 MHz, $CDCl_3$) spectrum of **poly(3.5)/3.11** (peaks at 25.76 and 68.11 ppm are residual THF).

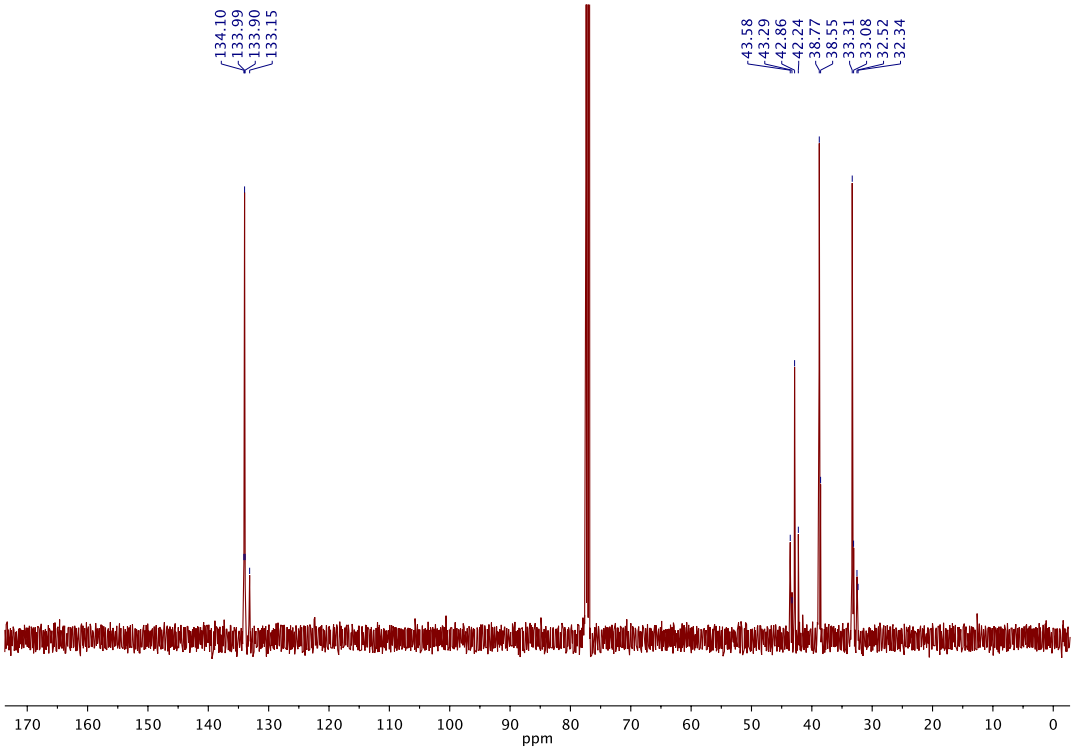


Figure 3.22. ^{13}C (126 MHz, $CDCl_3$) spectrum of **poly(3.5)/3.12**.

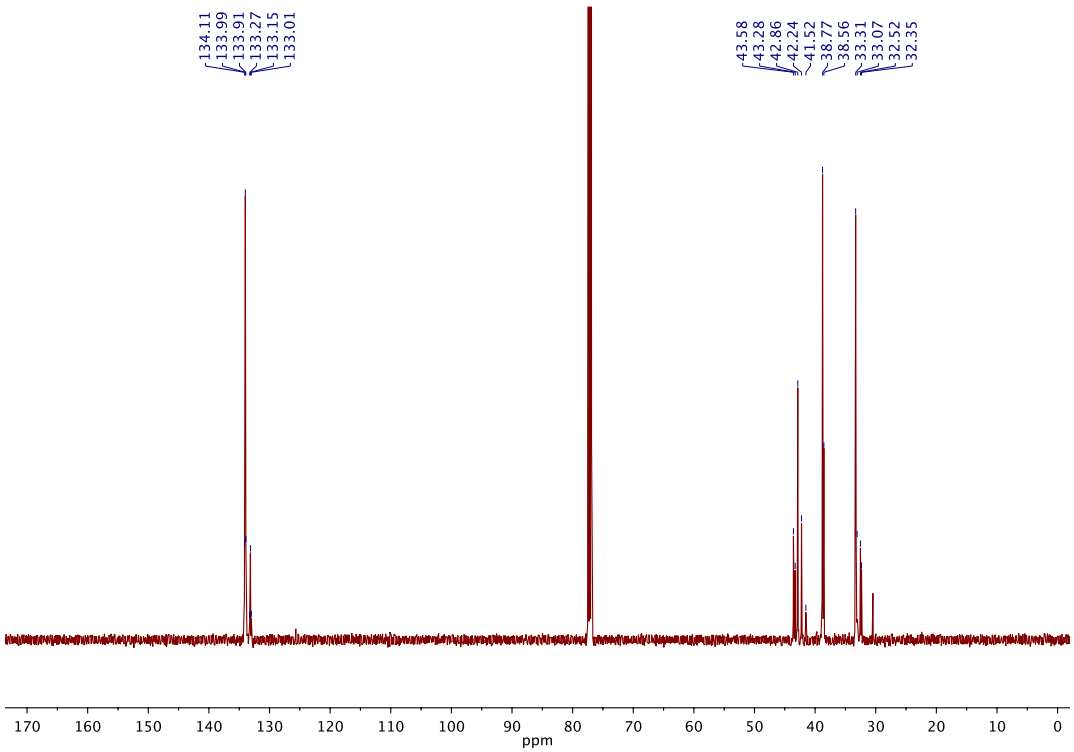


Figure 3.23. ^{13}C (126 MHz, $CDCl_3$) spectrum of **poly(3.5)/3.13**.

Preparation of Poly(3.6) Using Catalysts 3.1–3.4 and 3.8–3.13: Poly(3.6) was prepared according to the general procedure using catalysts **3.1–3.4** and **3.8–3.13**. NMR samples were prepared by stirring **poly(3.6)** in $CDCl_3$. ^{13}C NMR spectral assignments were consistent with the literature.[15] Samples of **poly(3.6)** prepared using catalysts **3.1–3.3** were virtually identical by ^{13}C NMR; thus, only the ^{13}C NMR spectrum of **poly(3.6)/3.1** is presented below.

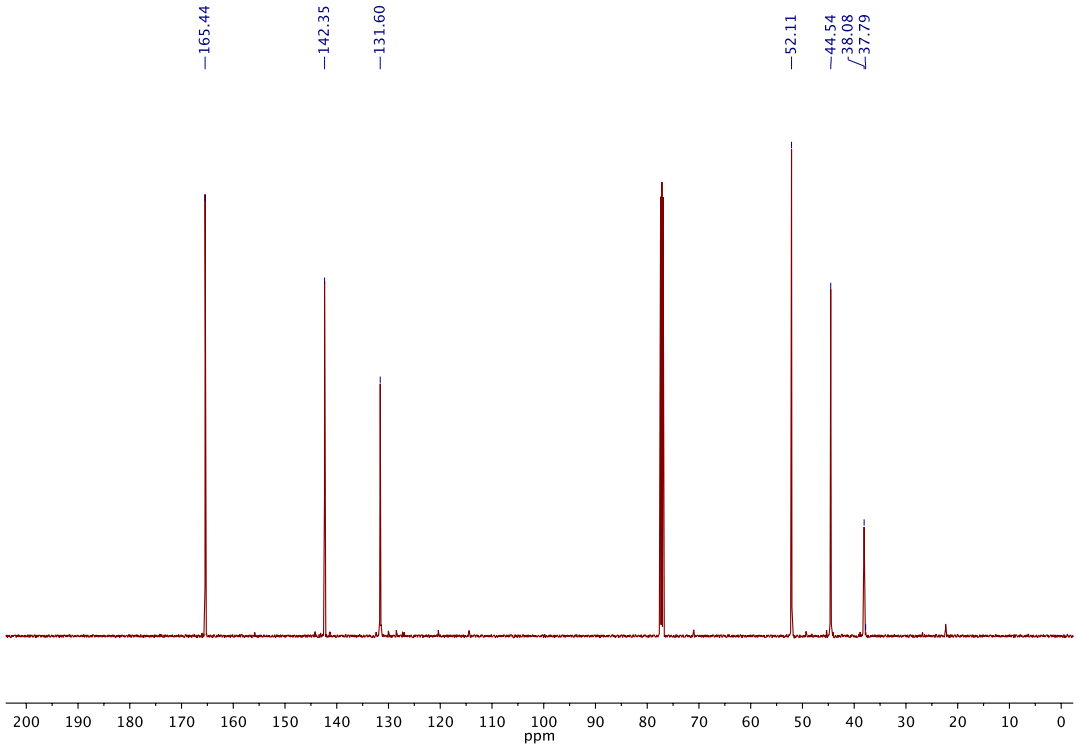


Figure 3.24. ^{13}C (126 MHz, $CDCl_3$) spectrum of **poly(3.6)/3.1**.

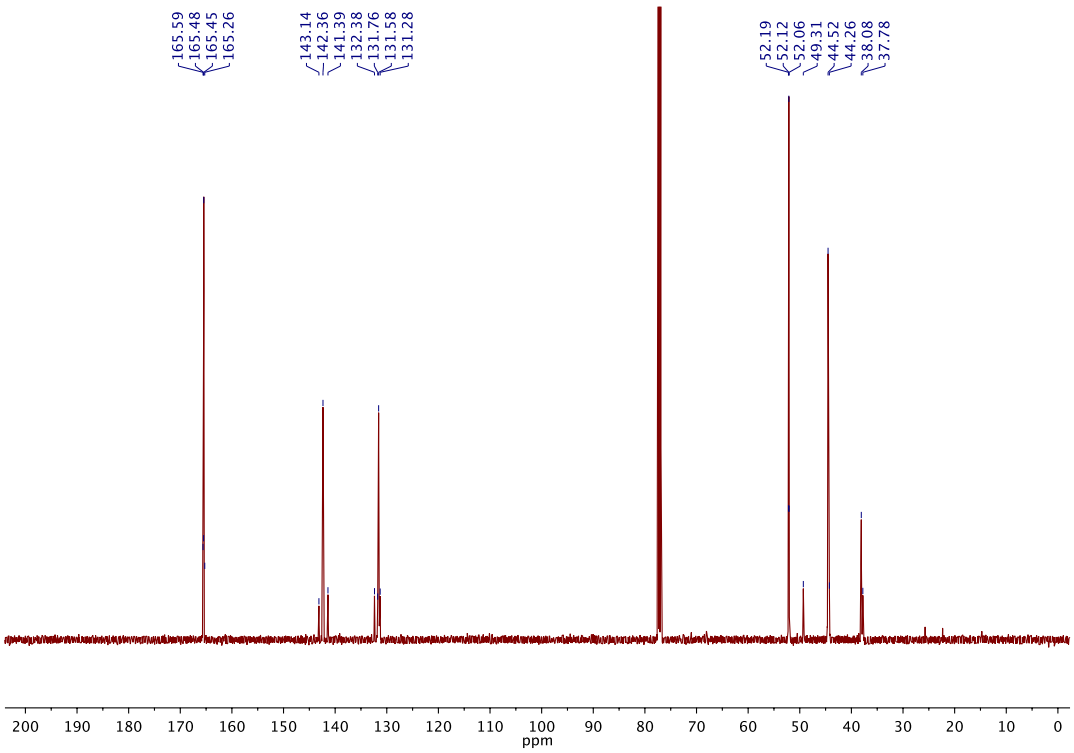


Figure 3.25. ^{13}C (126 MHz, $CDCl_3$) spectrum of **poly(3.6)/3.4**.

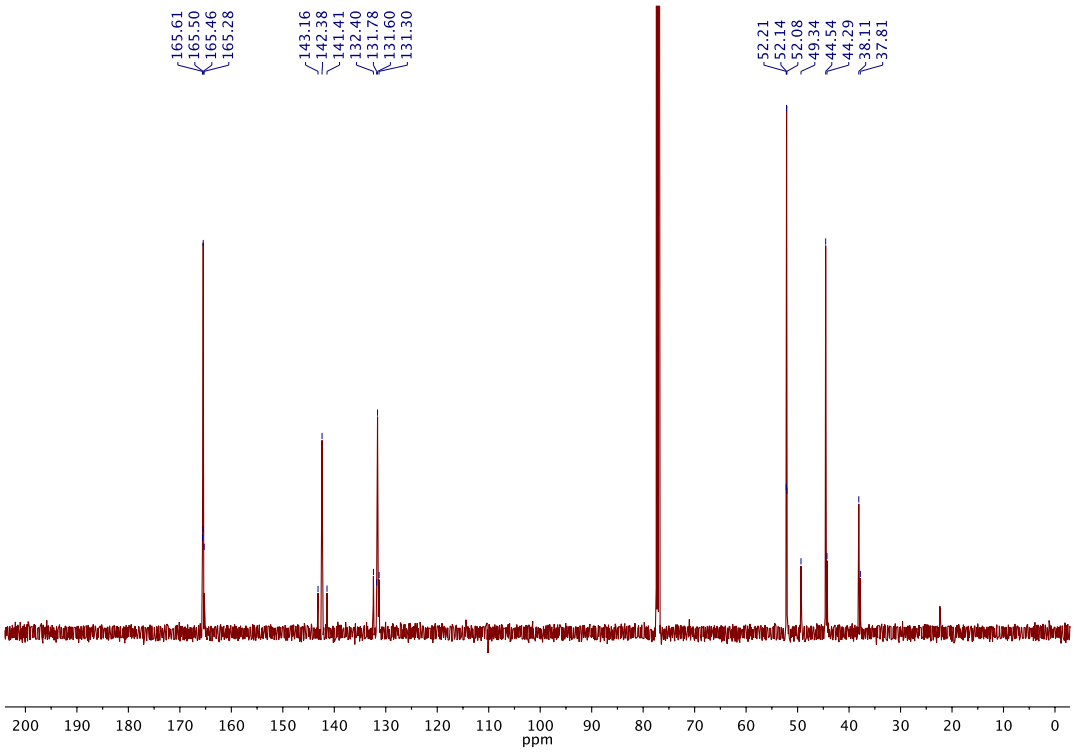


Figure 3.26. ^{13}C (126 MHz, $CDCl_3$) spectrum of **poly(3.6)/3.8**.

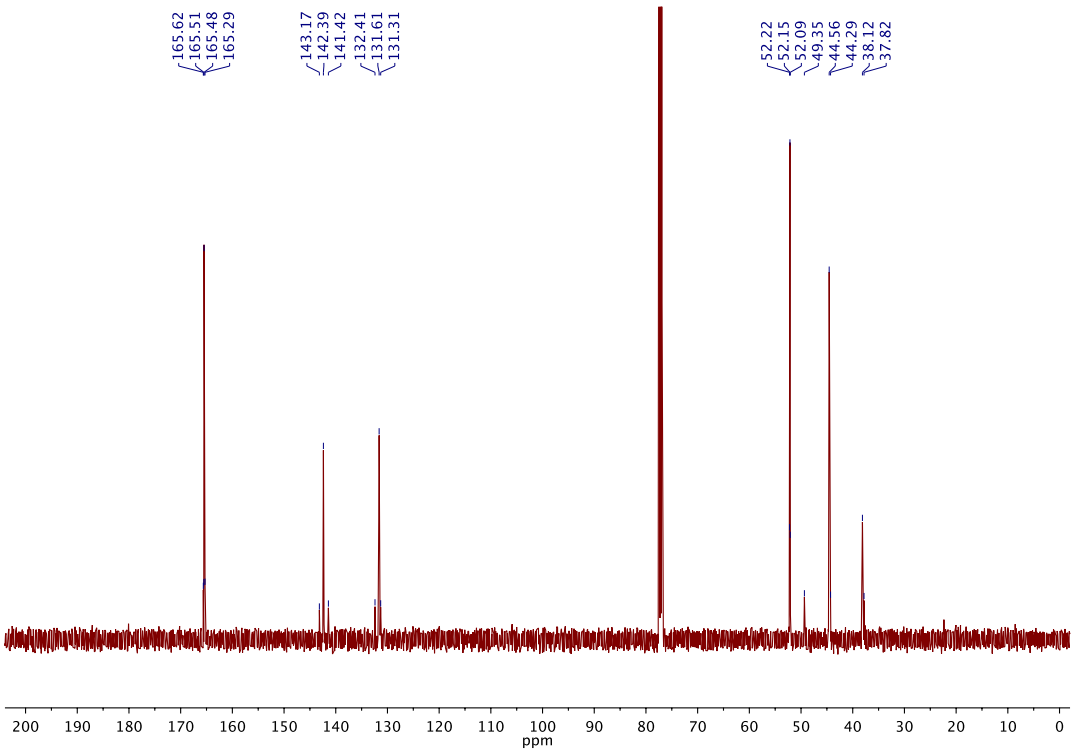


Figure 3.27. ^{13}C (126 MHz, $CDCl_3$) spectrum of **poly(3.6)/3.9**.

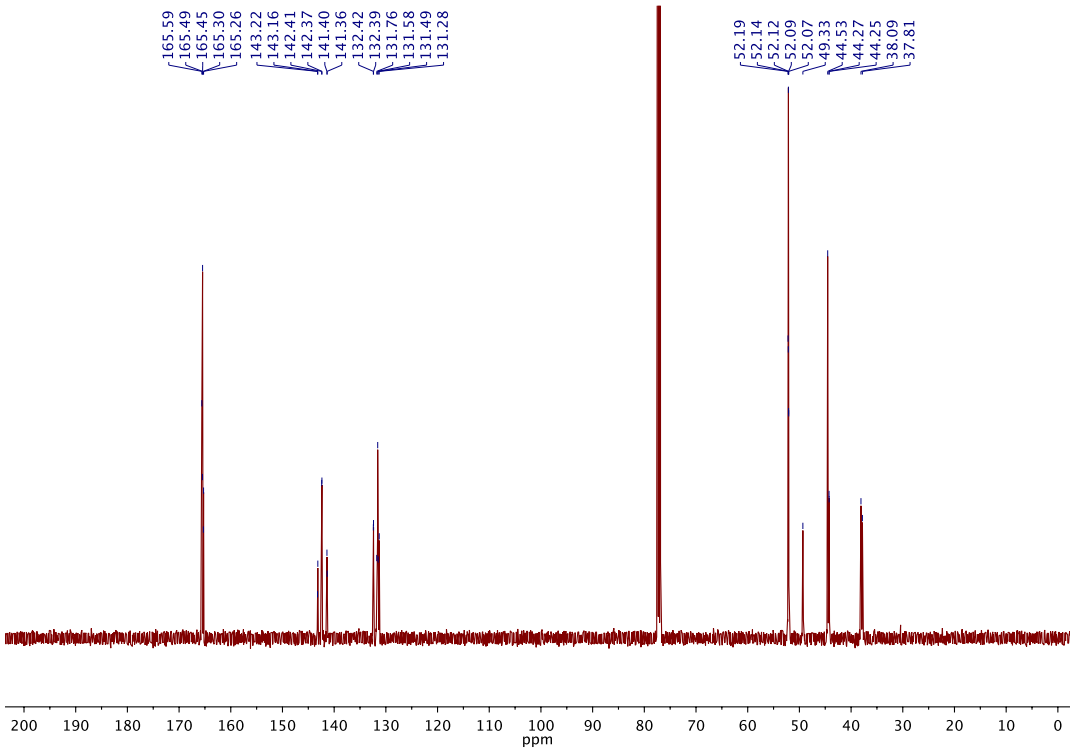


Figure 3.28. ^{13}C (126 MHz, $CDCl_3$) spectrum of **poly(3.6)/3.10**.

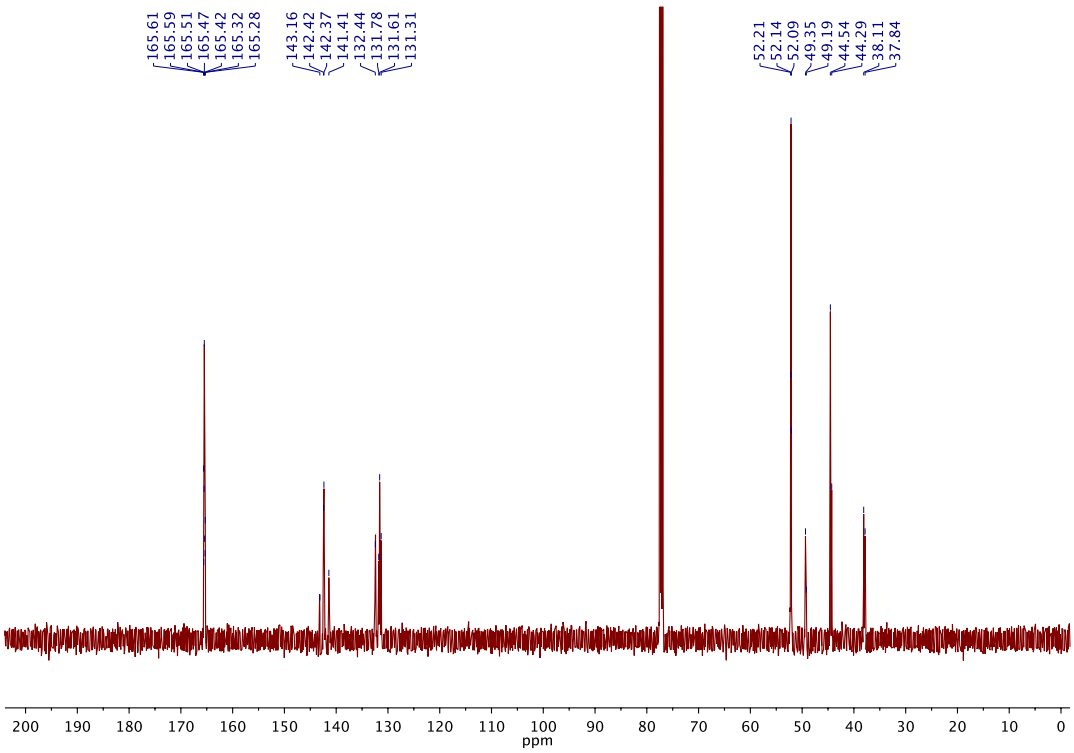


Figure 3.29. ^{13}C (126 MHz, $CDCl_3$) spectrum of **poly(3.6)/3.11**.

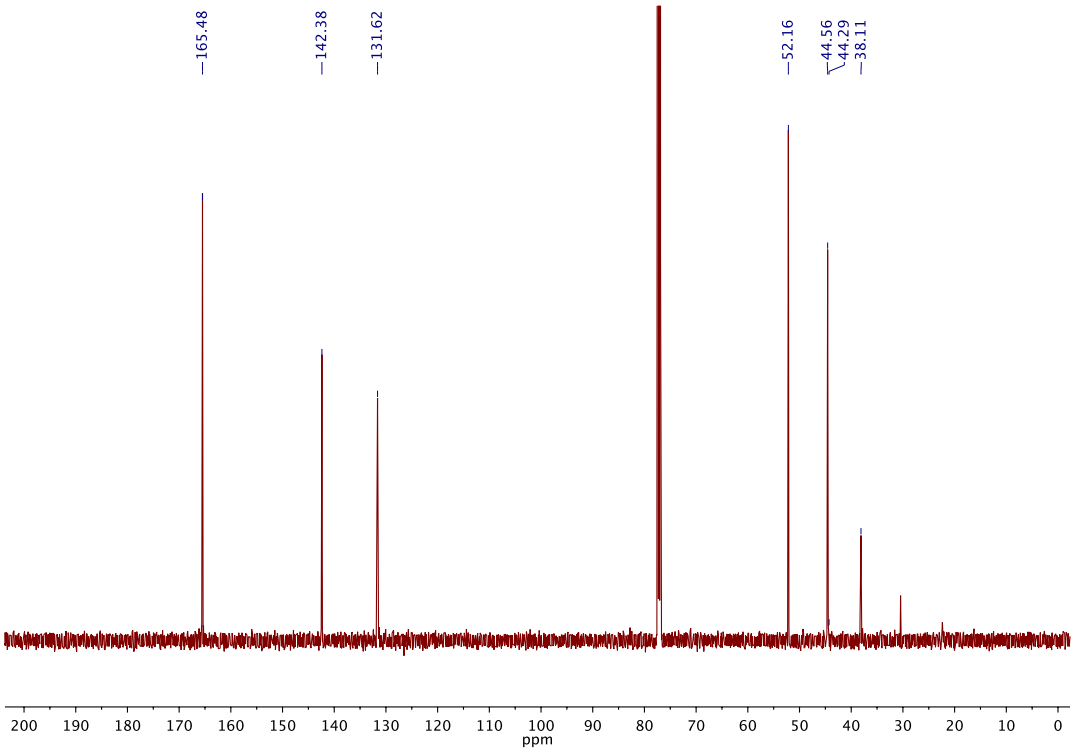


Figure 3.30. ^{13}C (126 MHz, $CDCl_3$) spectrum of **poly(3.6)/3.12**.

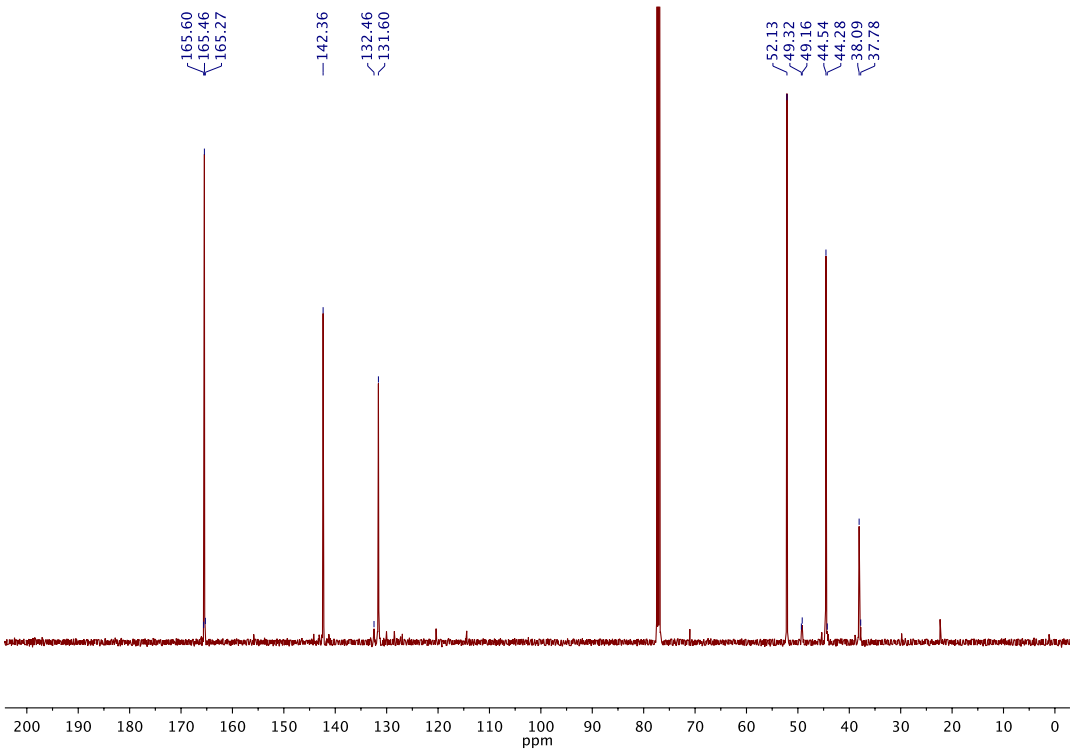


Figure 3.31. ^{13}C (126 MHz, $CDCl_3$) spectrum of **poly(3.6)/3.13**.

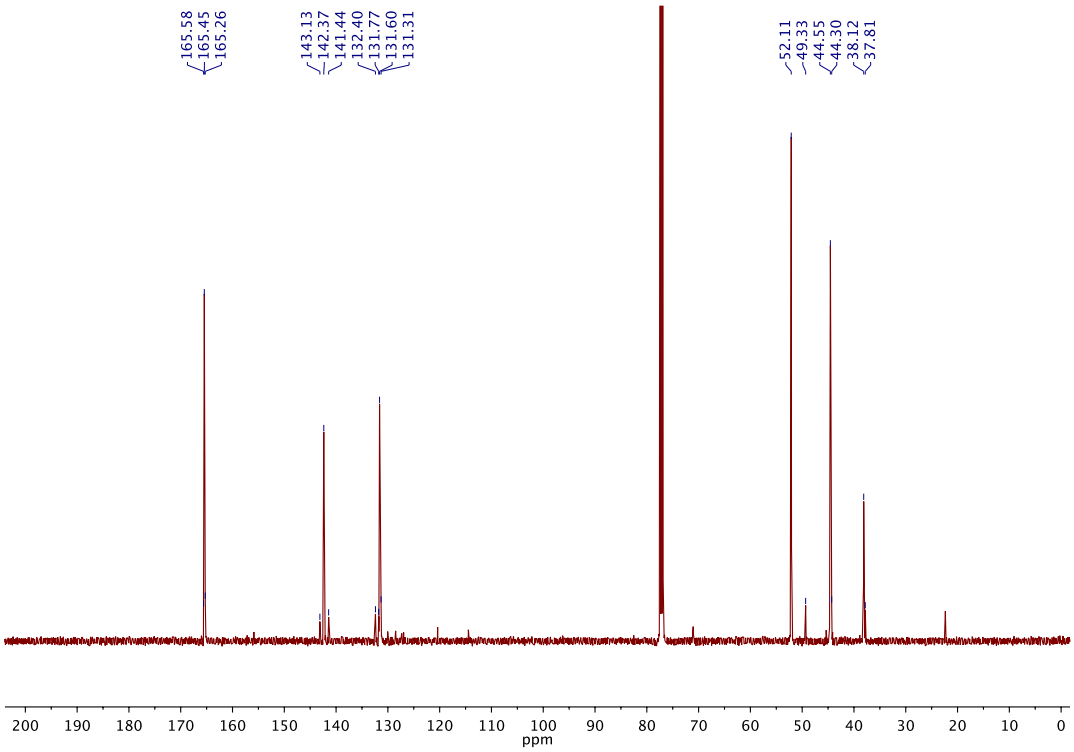


Figure 3.32. ^{13}C (126 MHz, $CDCl_3$) spectrum of **poly(3.6)/3.4** at 0 °C.

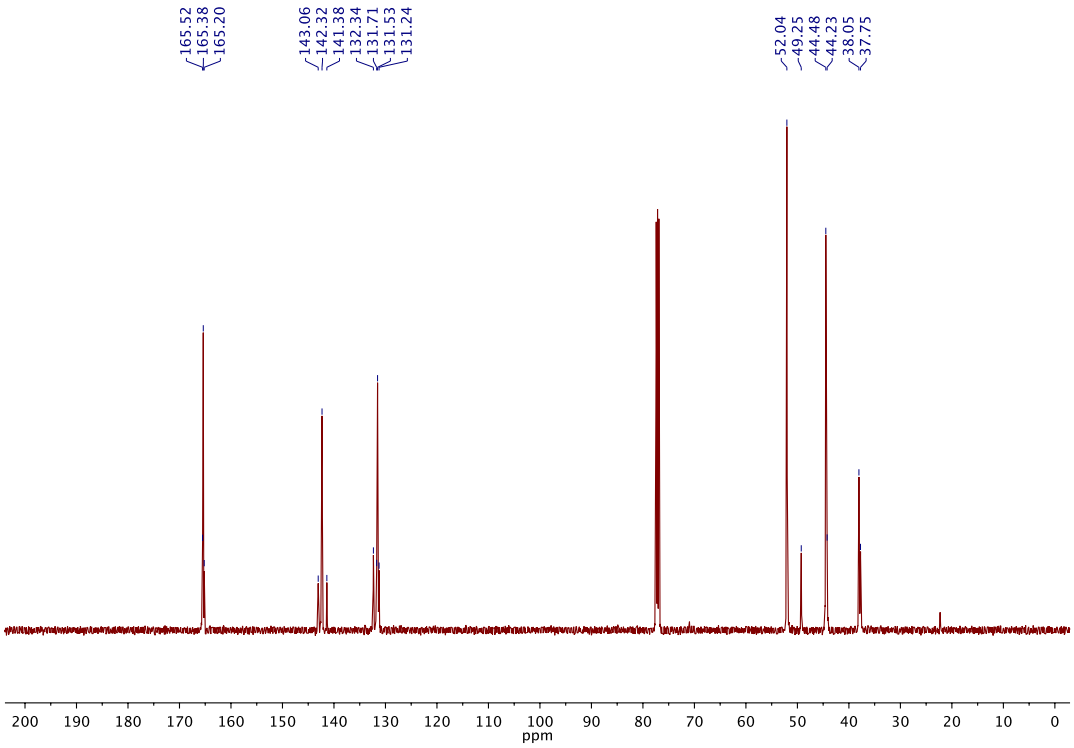


Figure 3.33. ^{13}C (126 MHz, $CDCl_3$) spectrum of **poly(3.6)/3.4** at 40 °C.

Preparation of Poly(3.7) Using Catalysts 3.1–3.3: Poly(3.7) was prepared according to the general procedure using catalysts **3.1–3.3**. NMR samples were prepared by stirring **poly(3.7)** in $CDCl_3$. Major ^{13}C NMR spectral assignments were consistent with the literature on *cis,syndiotactic* **poly(3.7)**,[6a] while the ^{13}C chemical shifts of the minor compound were consistent with those reported for the *trans,syndiotactic* **poly(3.7)**.[5b] Samples of **poly(3.7)** prepared using catalysts **3.1–3.3** were virtually identical by ^{13}C NMR; thus, only the ^{13}C NMR spectrum of **poly(3.7)/3.1** is presented below.

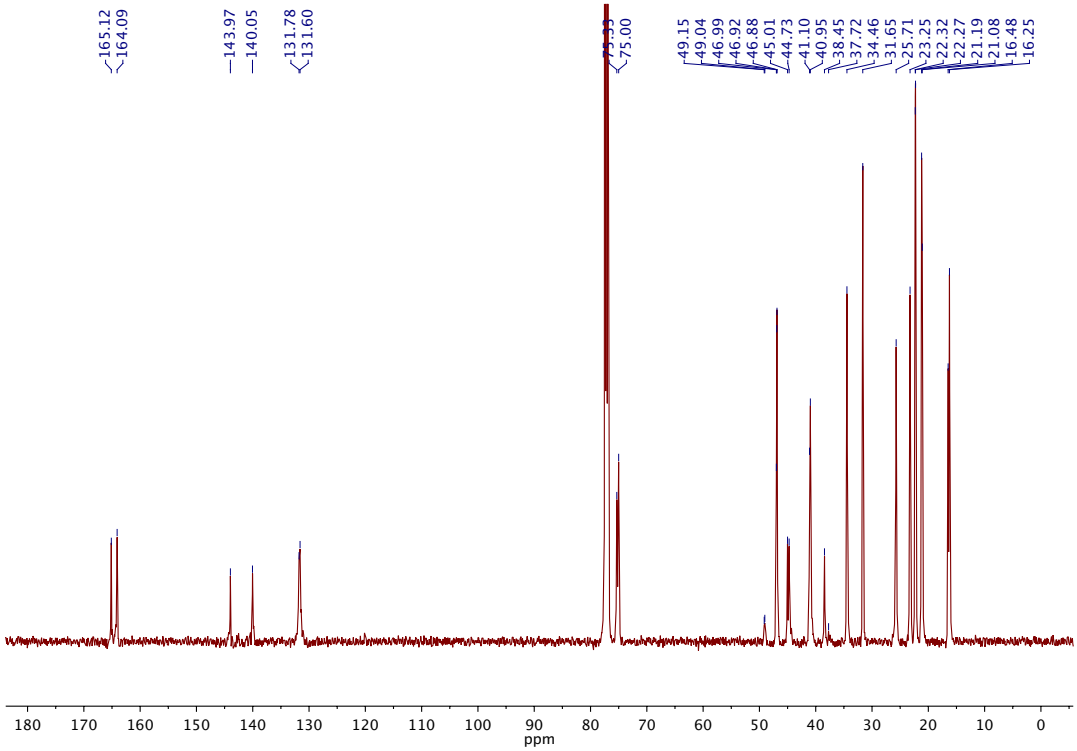


Figure 3.34. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly(3.7)/3.1**.

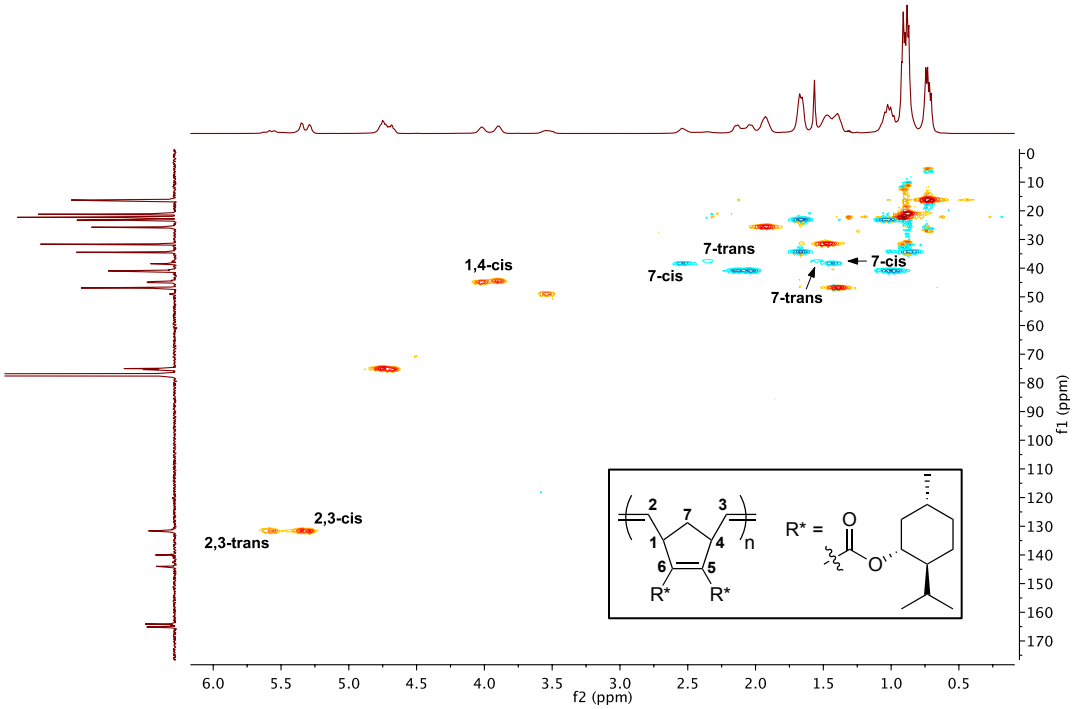


Figure 3.35. ^{1}H-^{13}C HSQC ($CDCl_3$) spectrum of **poly(3.7)/3.1**.

Preparation of Poly(3.14) Using Catalysts 3.1, 3.4, and 3.9: Poly(3.14) was prepared according to the general procedure using catalysts **3.1**, **3.4**, **3.9**. NMR samples were prepared by stirring **poly(3.14)** in $(CD_3)_2CO$. ^{13}C NMR spectral assignments were consistent with the literature.[19]

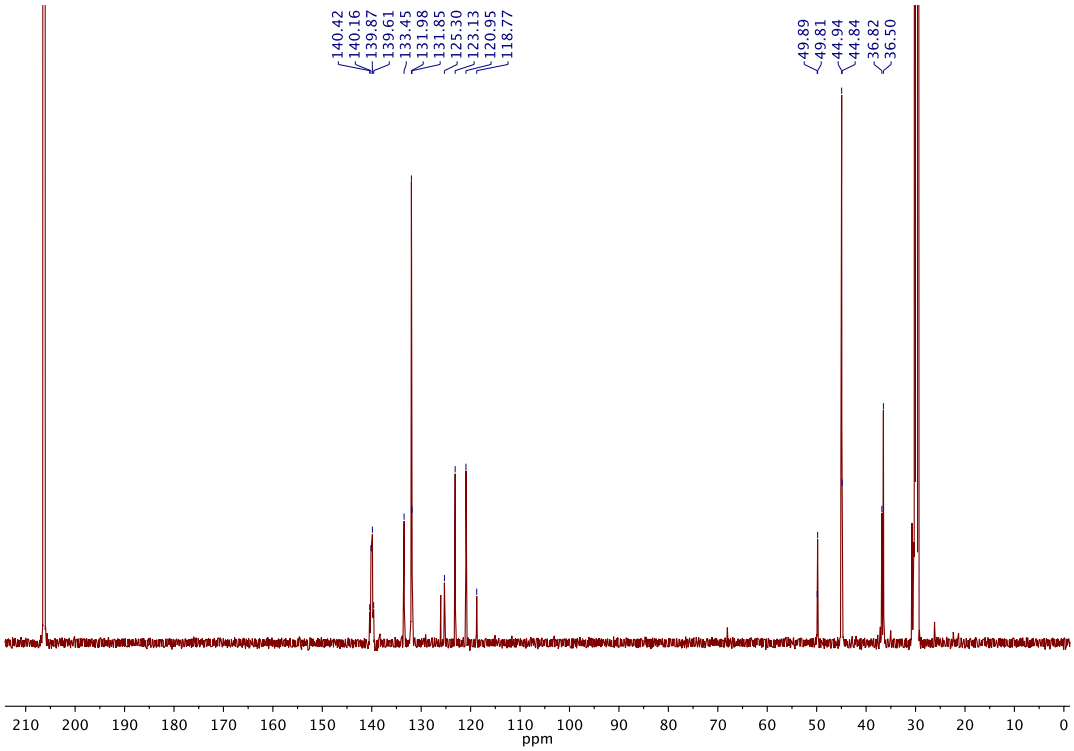


Figure 3.36. ^{13}C NMR (126 MHz, $(CD_3)_2CO$) spectrum of **poly(3.14)/3.1**.

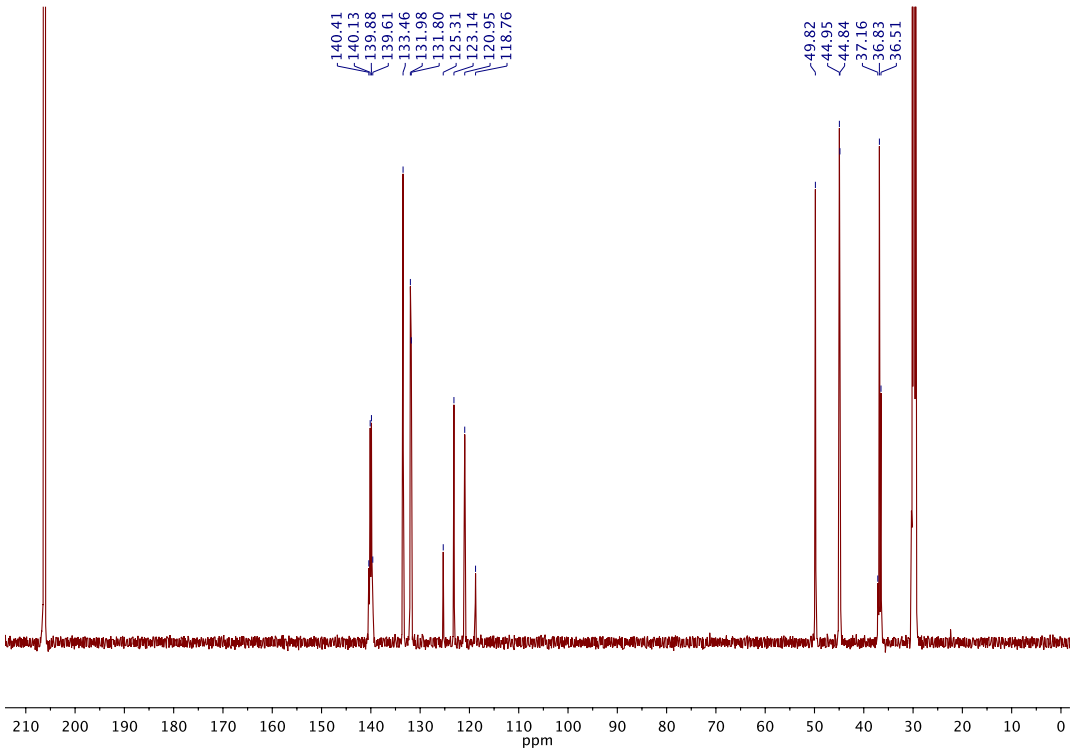


Figure 3.37. ^{13}C NMR (126 MHz, $(CD_3)_2CO$) spectrum of **poly(3.14)/3.4**.

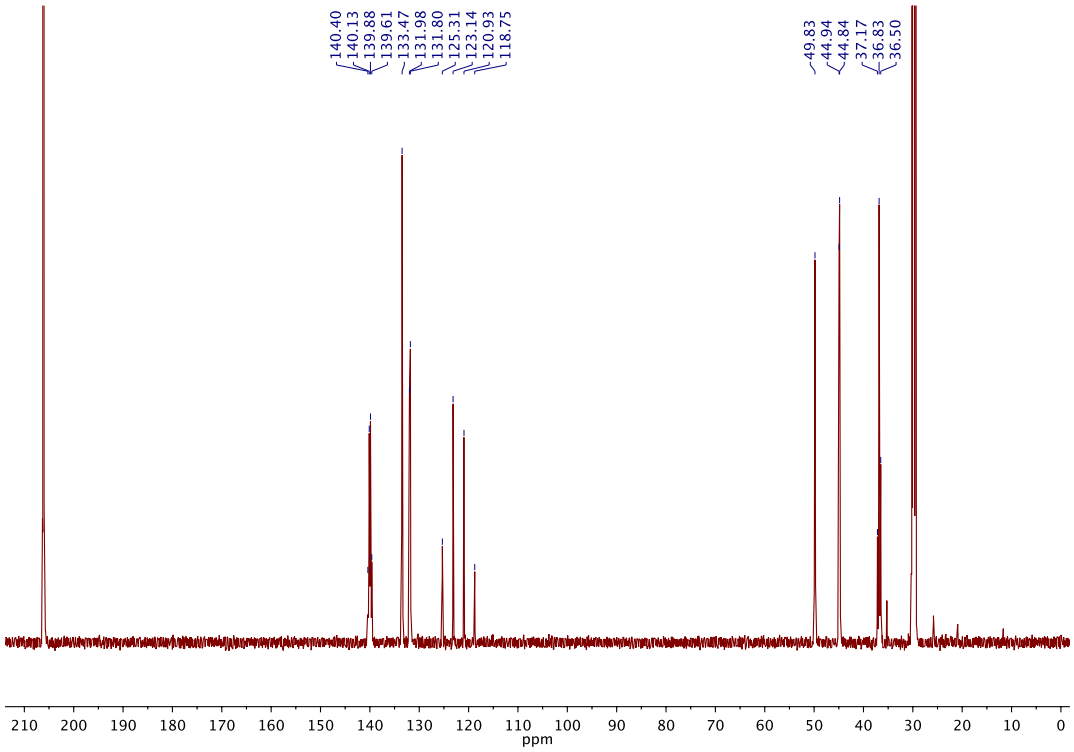


Figure 3.38. ^{13}C NMR (126 MHz, $(CD_3)_2CO$) spectrum of **poly(3.14)/3.9**.

Preparation of Poly(3.15) Using Catalysts 3.1, 3.4, and 3.9: Poly(3.15) was prepared according to the general procedure using catalysts **3.1**, **3.4**, and **3.9**. NMR samples were prepared by stirring **poly(3.15)** in CD_2Cl_2. ^{13}C NMR spectral assignments were consistent with the literature.[15]

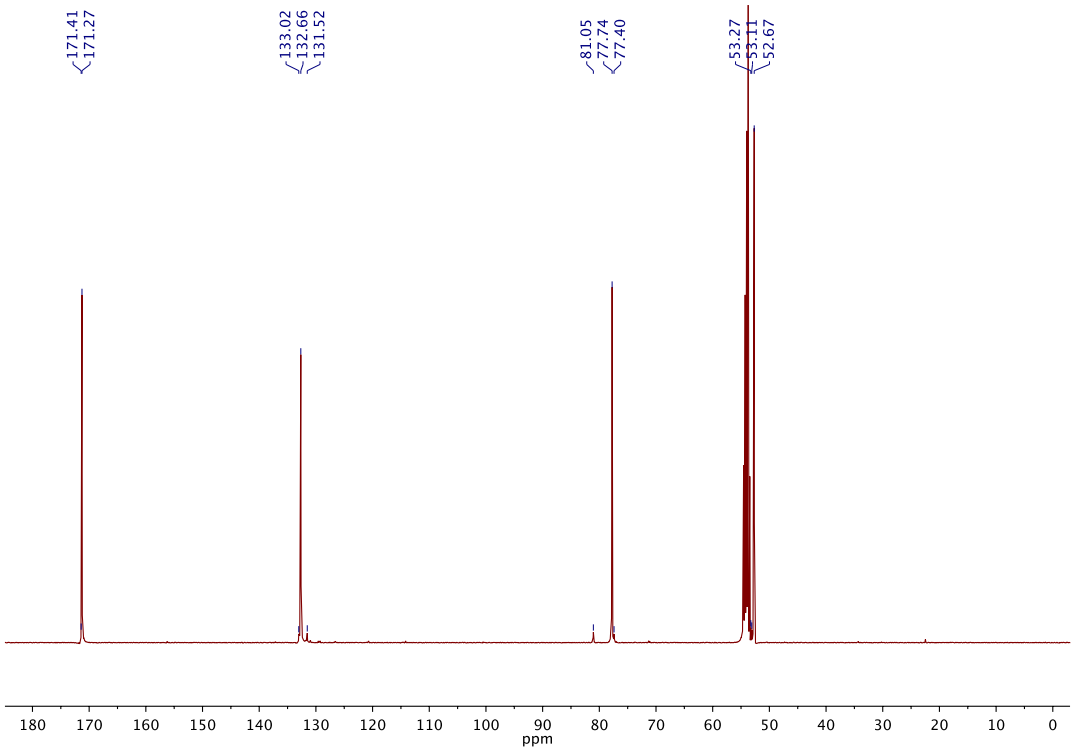


Figure 3.39. ^{13}C NMR (100 MHz, CD_2Cl_2) spectrum of **poly(3.15)/3.1**.

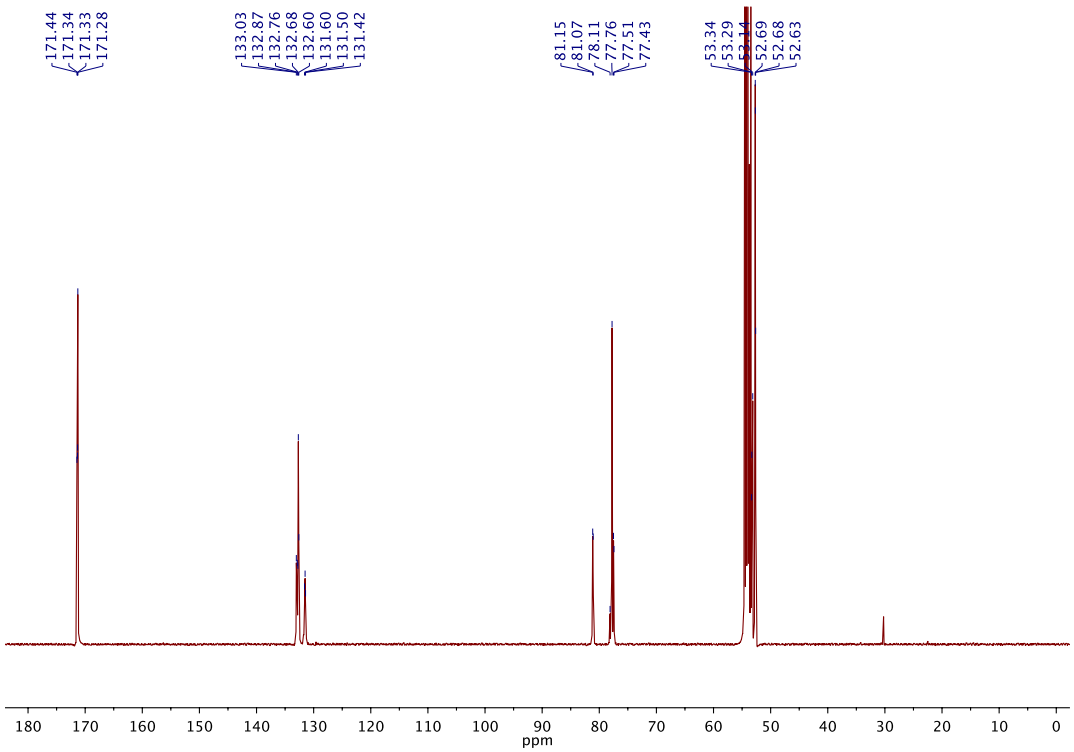


Figure 3.40. ^{13}C NMR (100 MHz, CD_2Cl_2) spectrum of **poly(3.15)/3.4**.

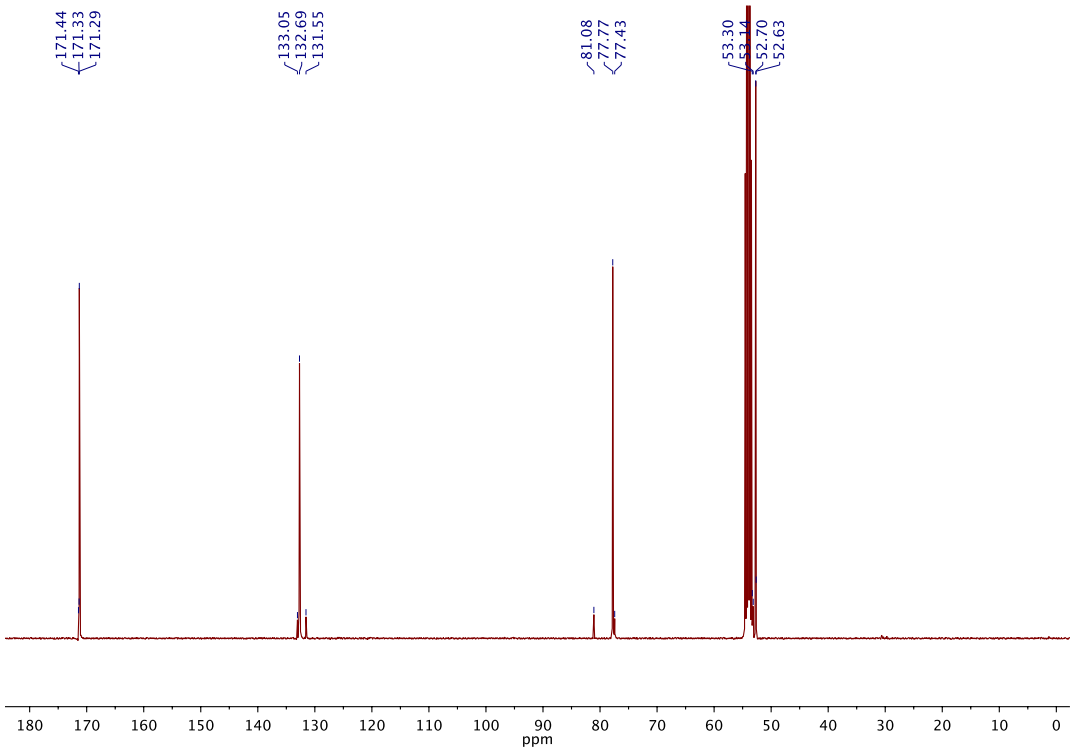


Figure 3.41. ^{13}C NMR (100 MHz, CD_2Cl_2) spectrum of **poly(3.15)/3.9**.

Preparation of Poly(3.16) Using Catalysts 3.1 and 3.4: Poly(3.16) was prepared according to the general procedure using catalysts **3.1** and **3.4**. NMR samples were prepared by stirring **poly(3.16)** in $CDCl_3$. ^{13}C NMR spectral assignments were consistent with the literature.[20]

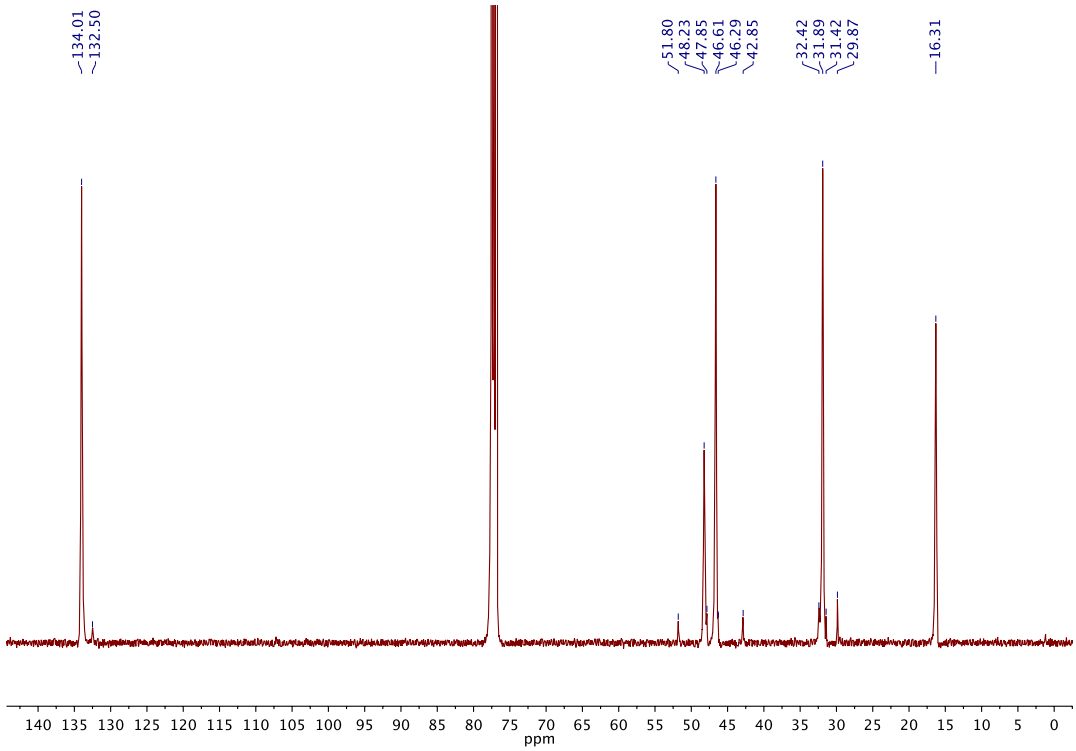


Figure 3.42. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **poly(3.16)/3.1**.

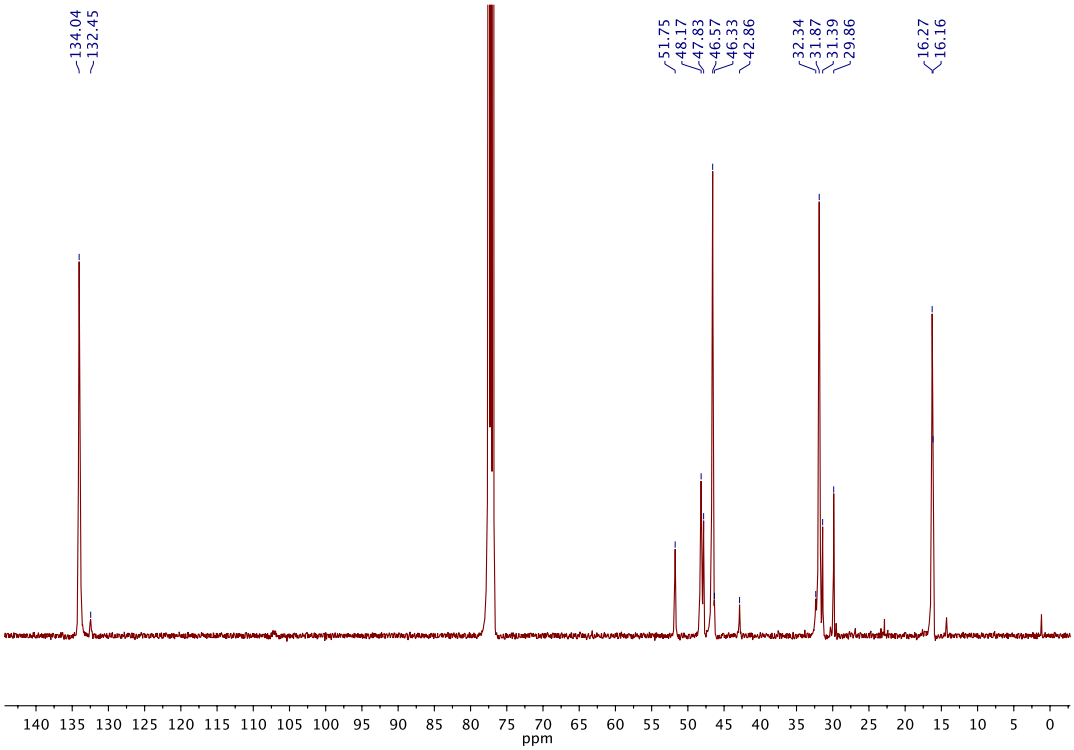


Figure 3.43. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **poly(3.16)/3.4**.

Preparation of Poly(3.17) Using Catalysts 3.1, 3.4, and 3.9: Poly(3.17) was prepared according to the general procedure using catalysts **3.1**, **3.4**, and **3.9**. NMR samples were prepared by stirring **poly(3.17)** in $CDCl_3$. ^{13}C NMR spectral assignments were consistent with the literature.[22]

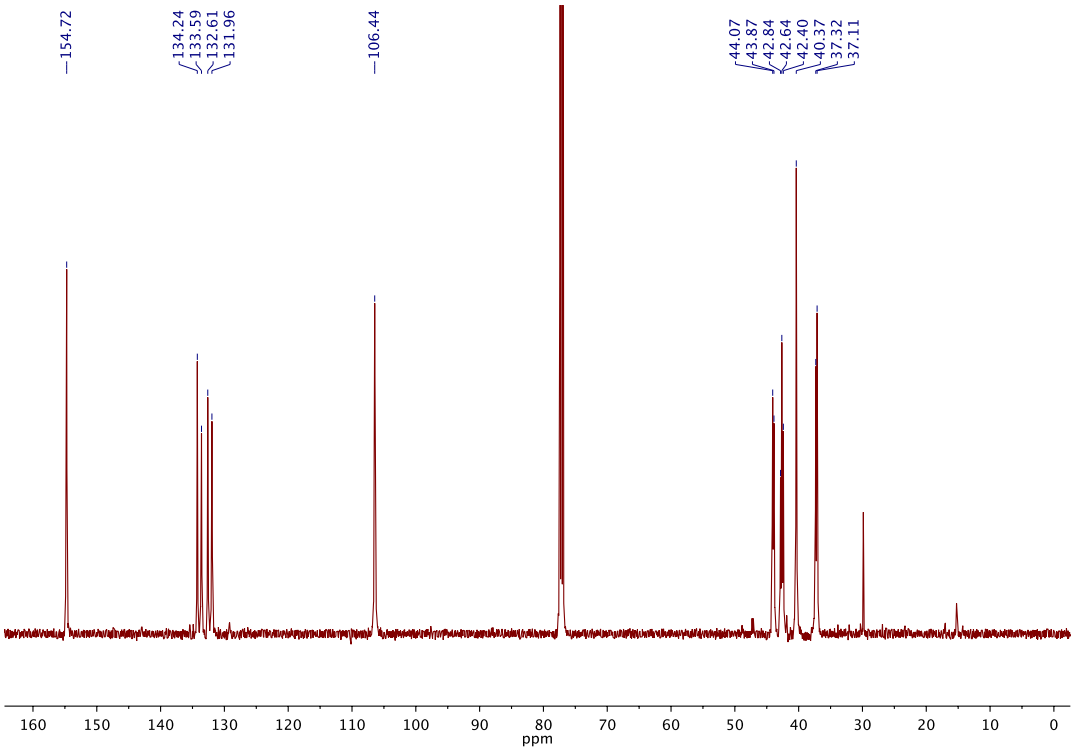


Figure 3.44. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly(3.17)/3.1** (peak at 29.86 is residual "grease").

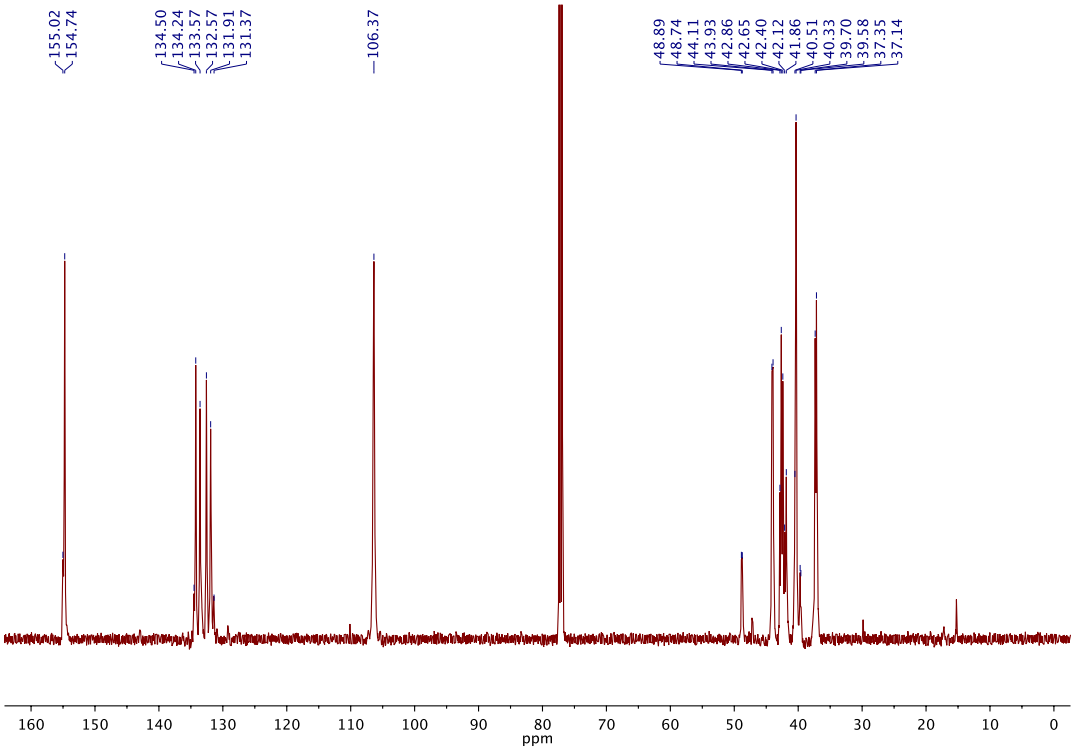


Figure 3.45. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly(3.17)/3.4**.

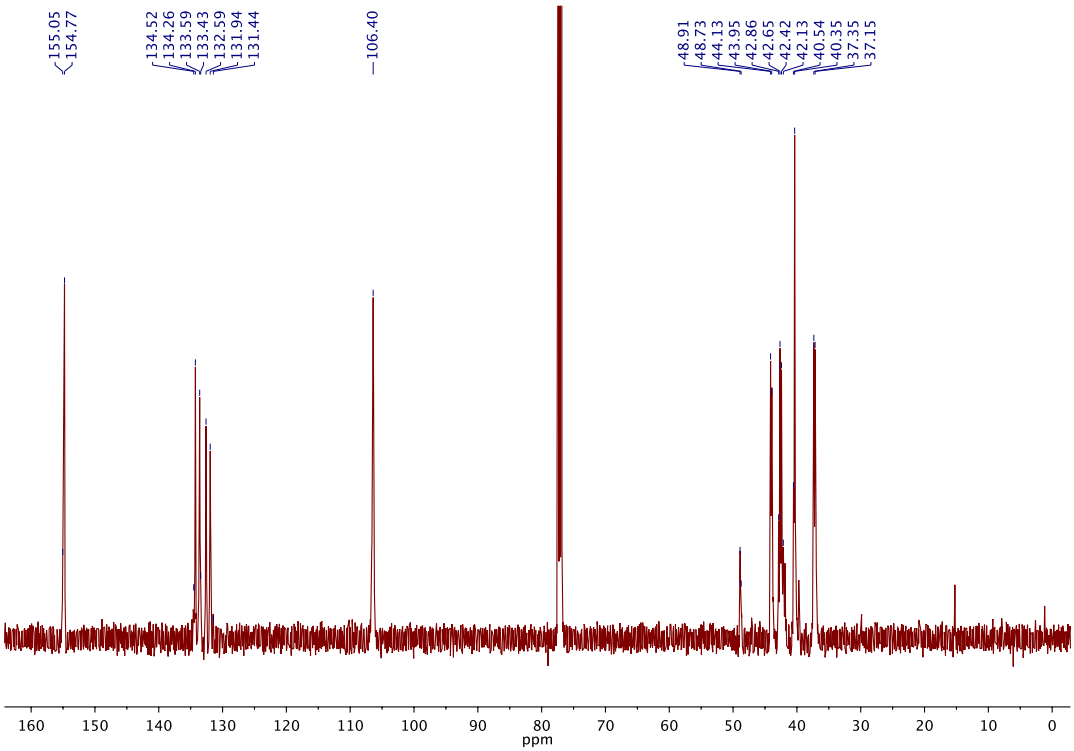


Figure 3.46. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly(3.17)/3.9**.

Preparation of Poly(3.18) Using Catalysts 3.1 and 3.4: Poly(3.18) was prepared according to the general procedure using catalysts **3.1** and **3.4**. NMR samples were prepared by stirring **poly(3.18)** in $CDCl_3$. ^{13}C NMR spectral assignments were consistent with the literature.[23]

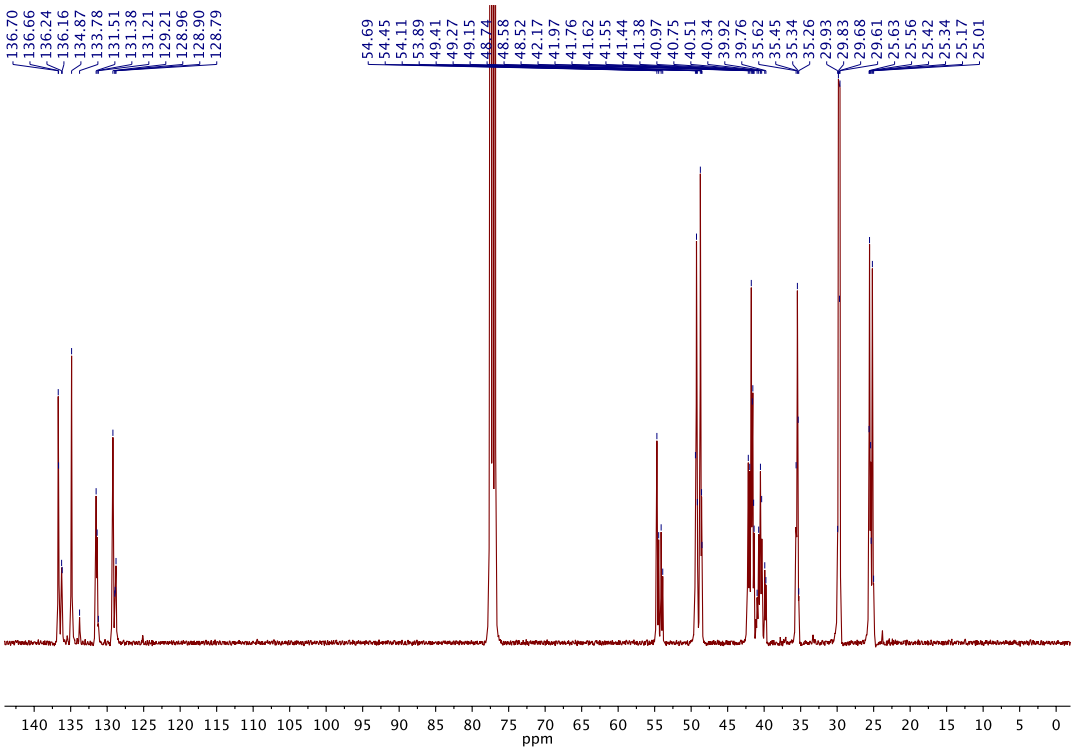


Figure 3.47. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **poly(3.18)/3.1**.

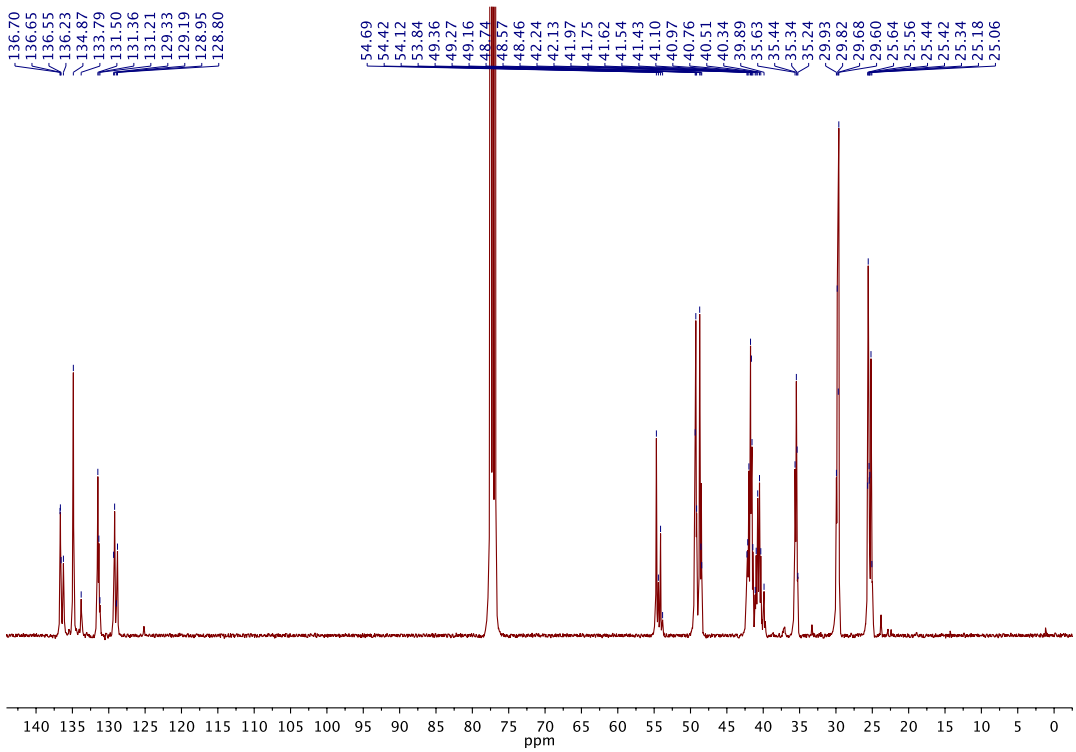


Figure 3.48. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **poly(3.18)/3.4**.

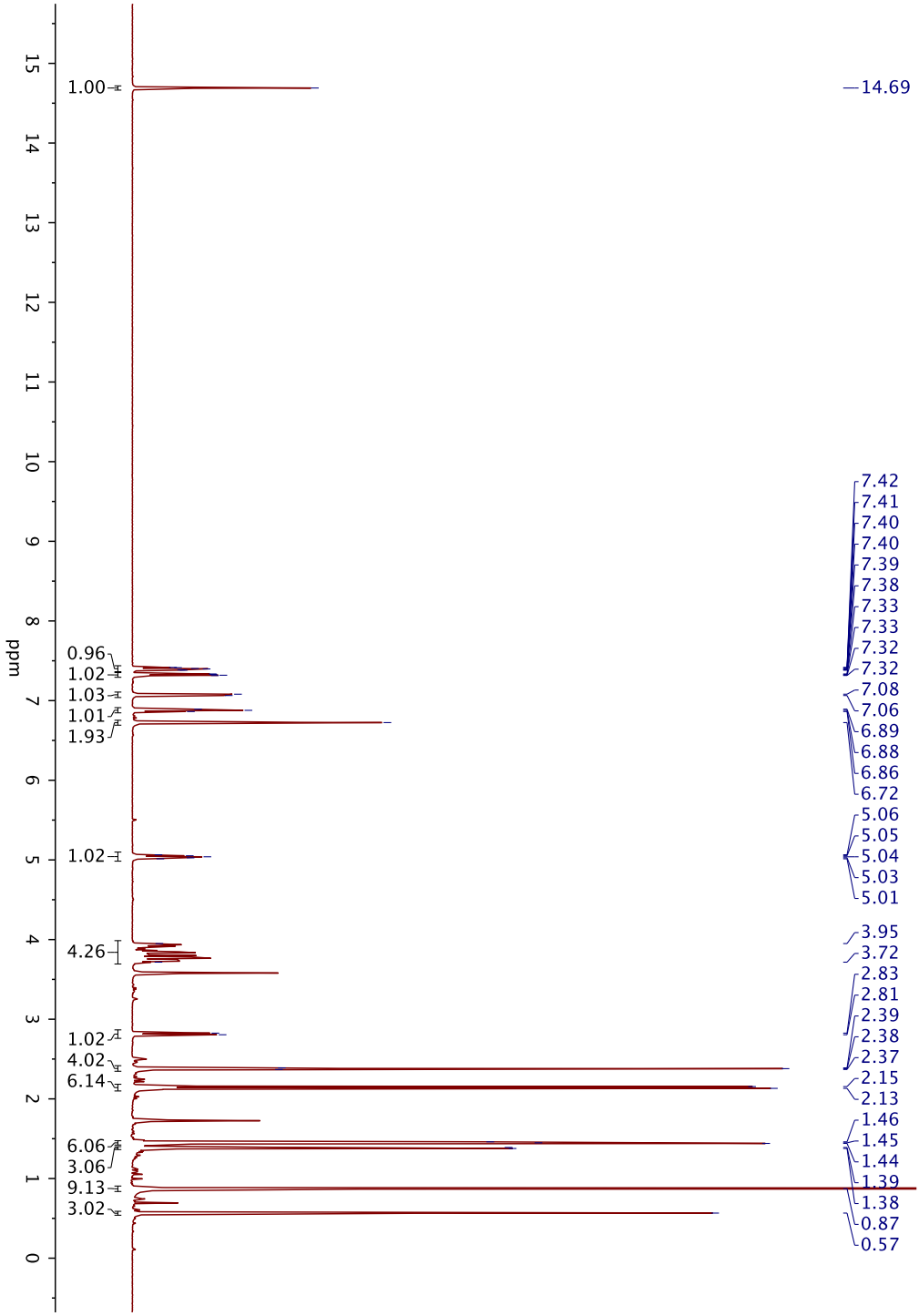


Figure 3.49. ^{1}H NMR (500 MHz, THF-d_8) spectrum of **3.1**.

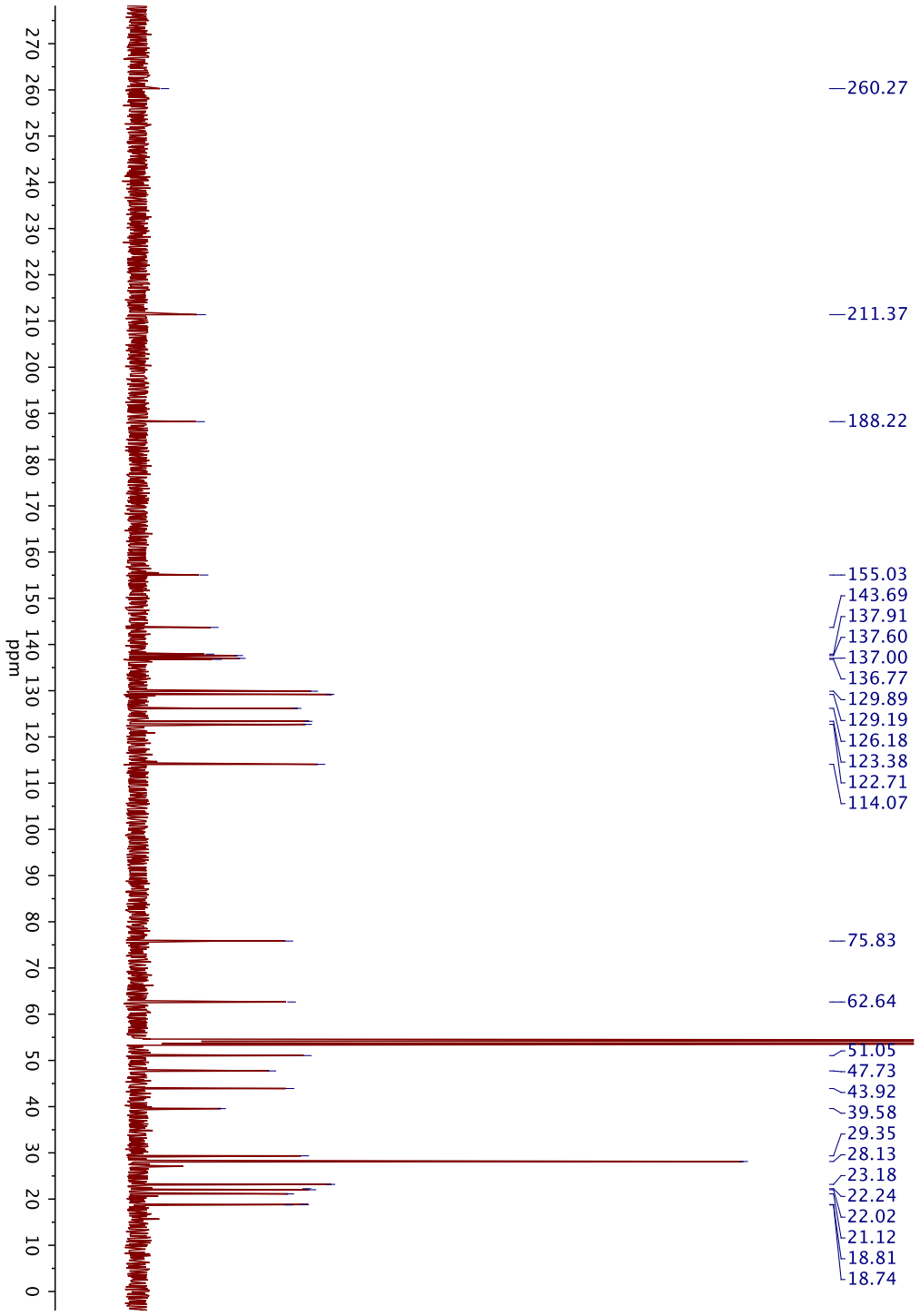


Figure 3.50. ^{13}C NMR (126 MHz, CD_2Cl_2) spectrum of **3.1**.

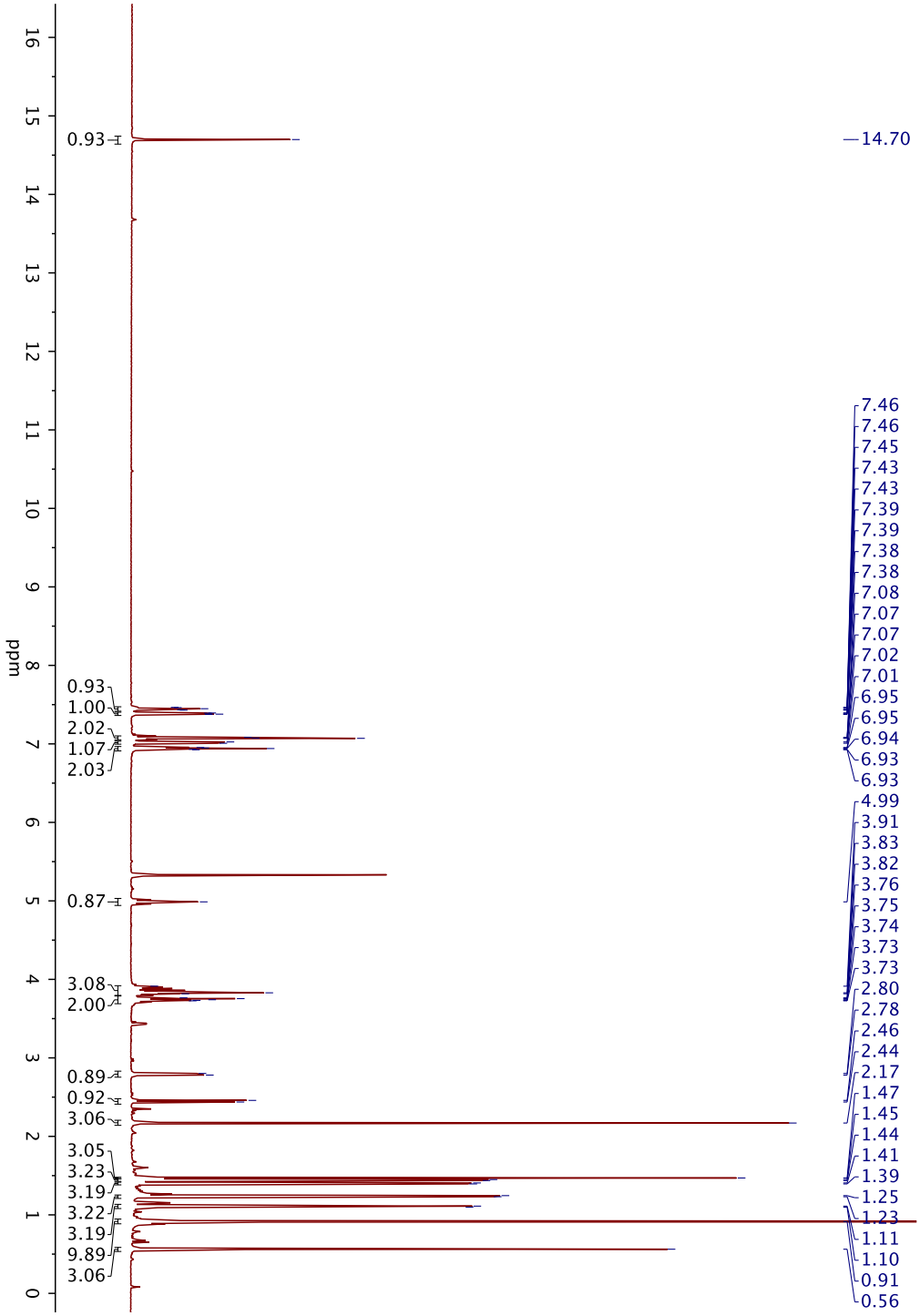


Figure 3.51. ^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of **3.2**.

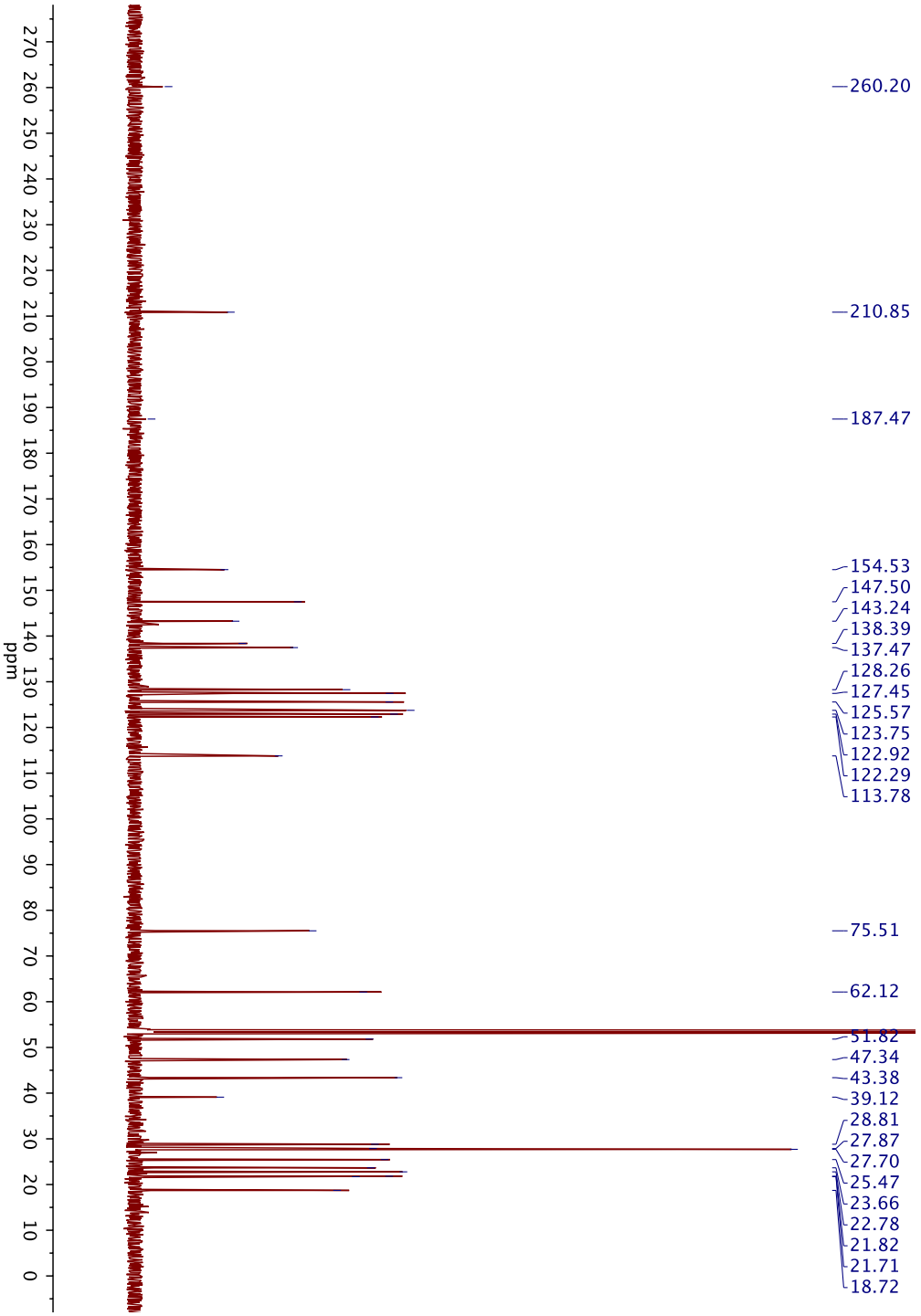


Figure 3.52. ^{13}C NMR (126 MHz, CD_2Cl_2) spectrum of **3.2**.

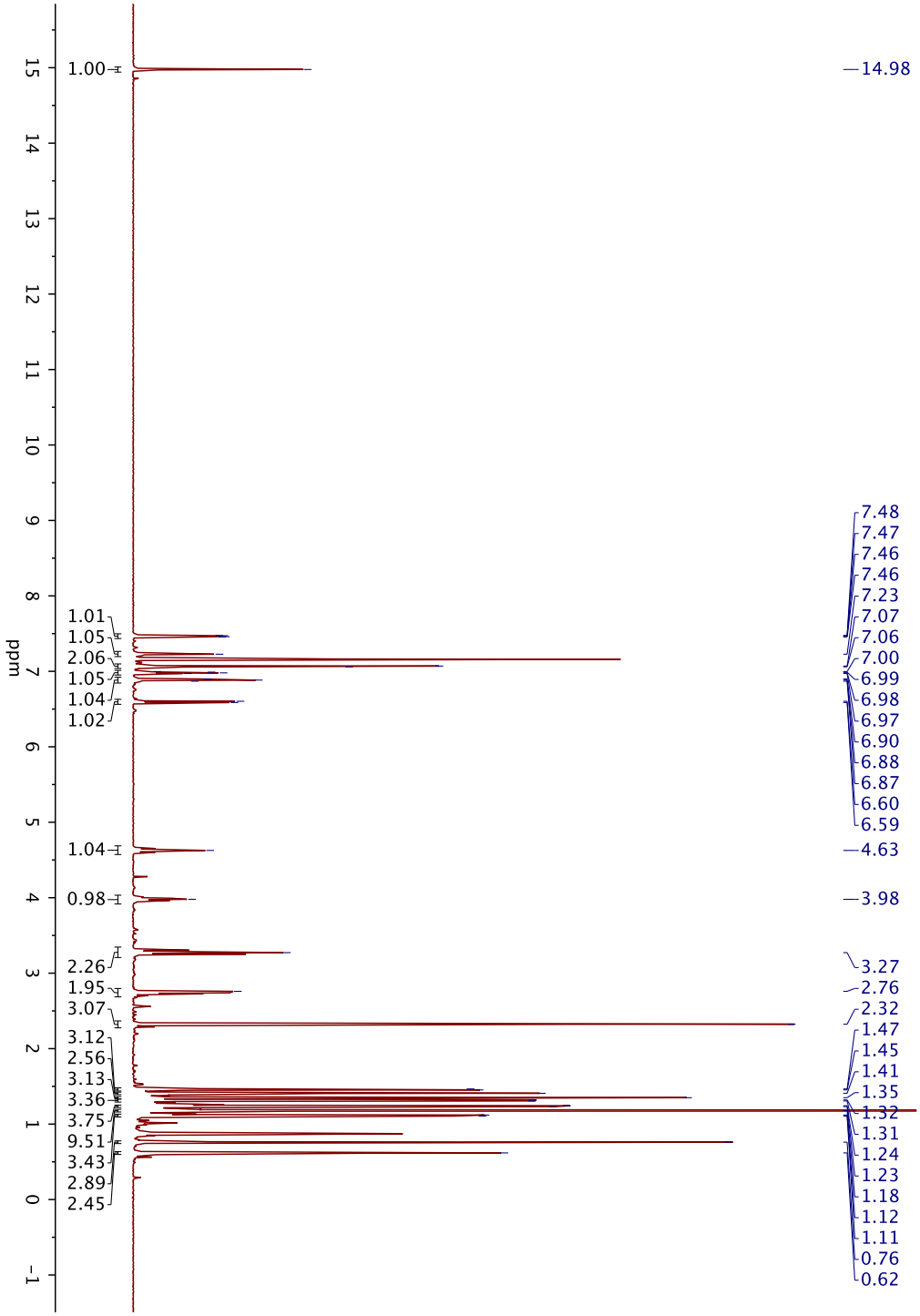


Figure 3.53. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **3.3**.

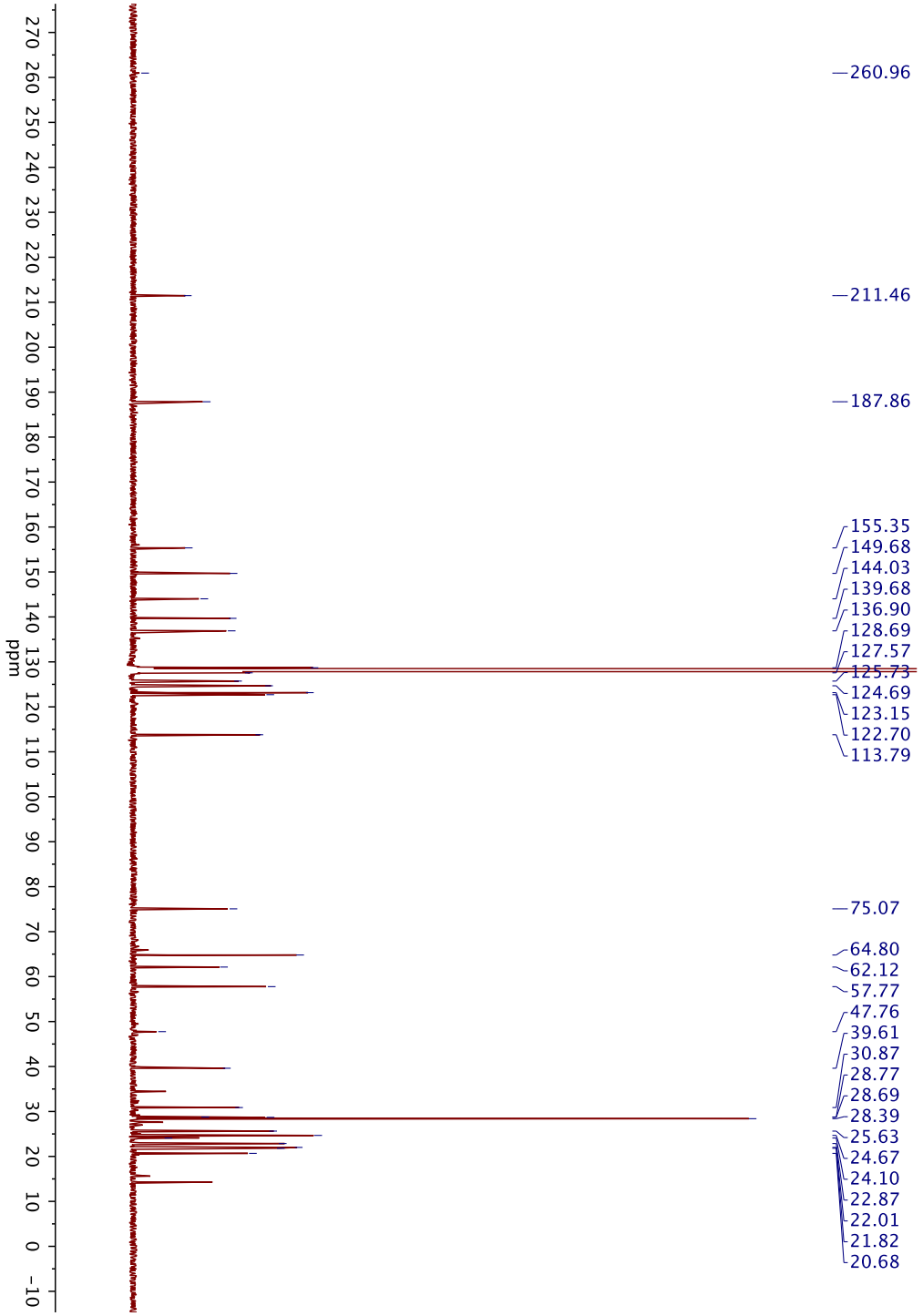


Figure 3.54. ^{13}C NMR (126 MHz, C_6D_6) spectrum of **3.3**.

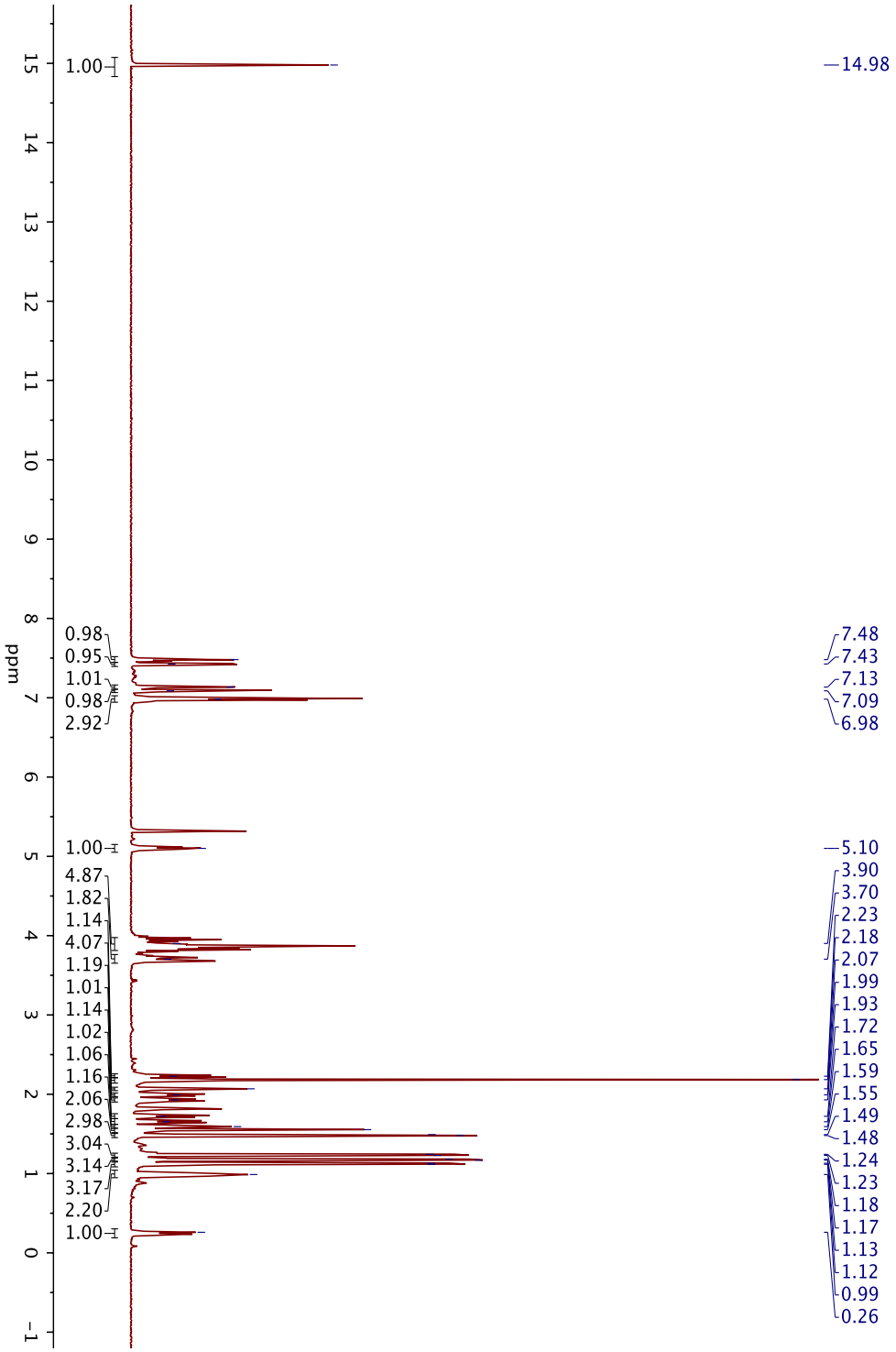


Figure 3.55. ^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of **3.8**.

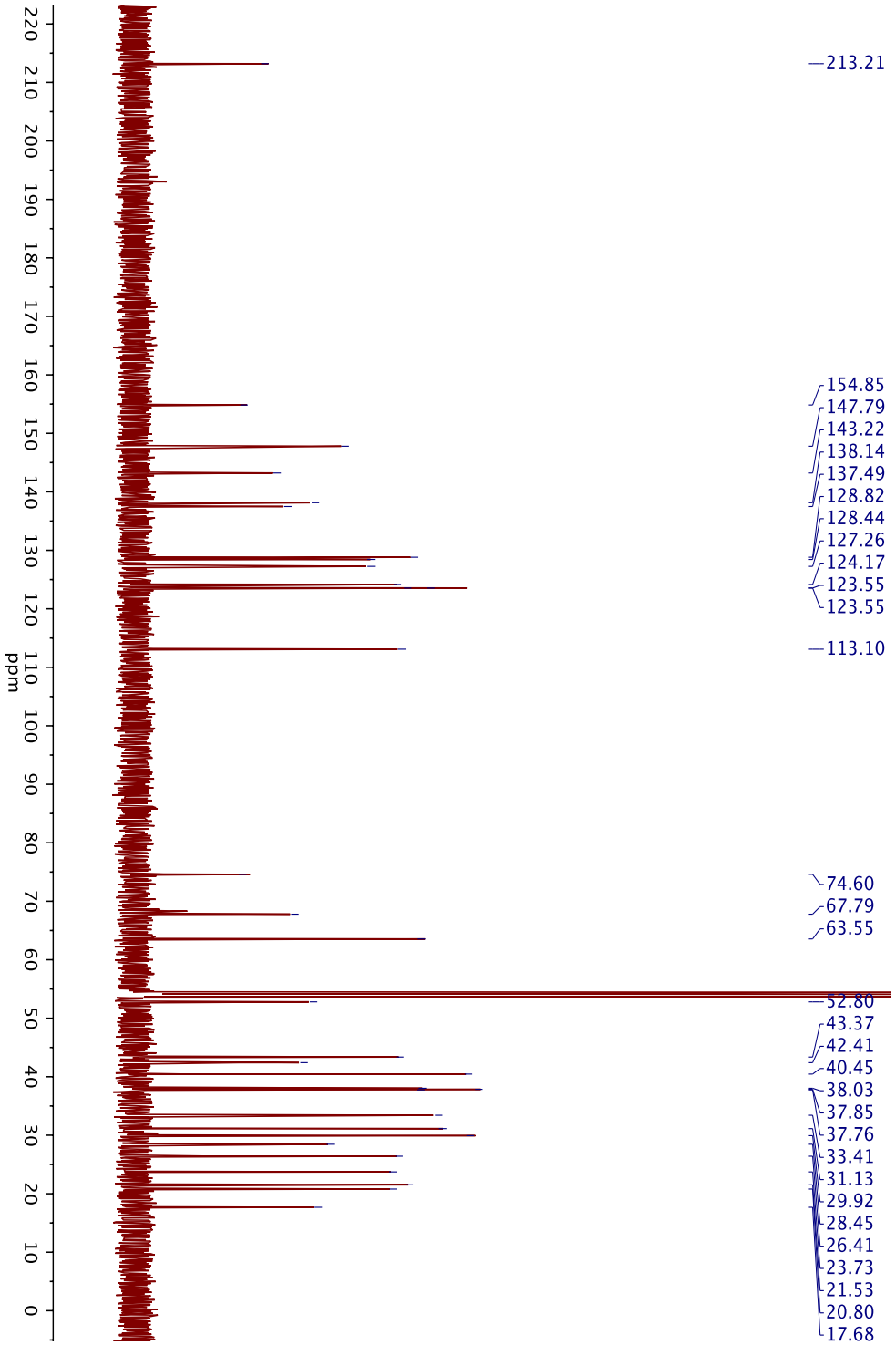


Figure 3.56. ^{13}C NMR (126 MHz, CD_2Cl_2) spectrum of **3.8**.

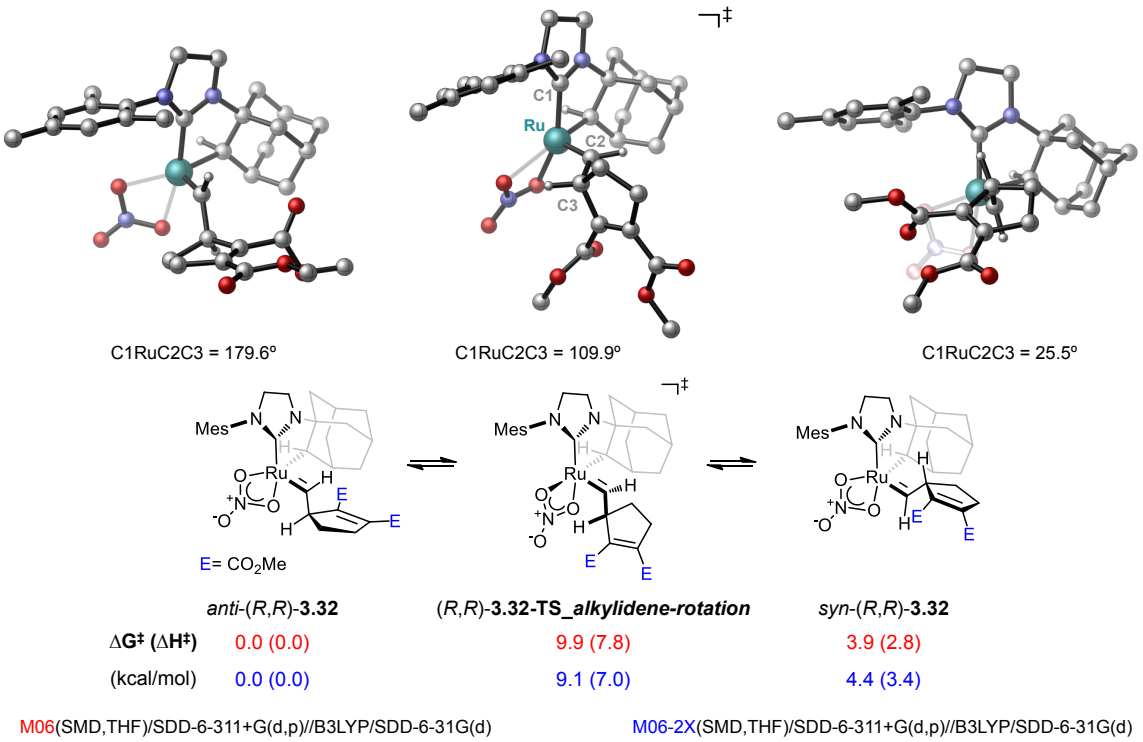


Figure 3.57. Free energies and enthalpies (in parentheses) for interconversion between ruthenium alkylidenes *anti*- and *syn*-(*R*,*R*)-**3.32** via alkylidene rotation. All energies are with respect to the ruthenium alkylidene complex *anti*-(*R*,*R*)-**3.4** and are given in kcal/mol.

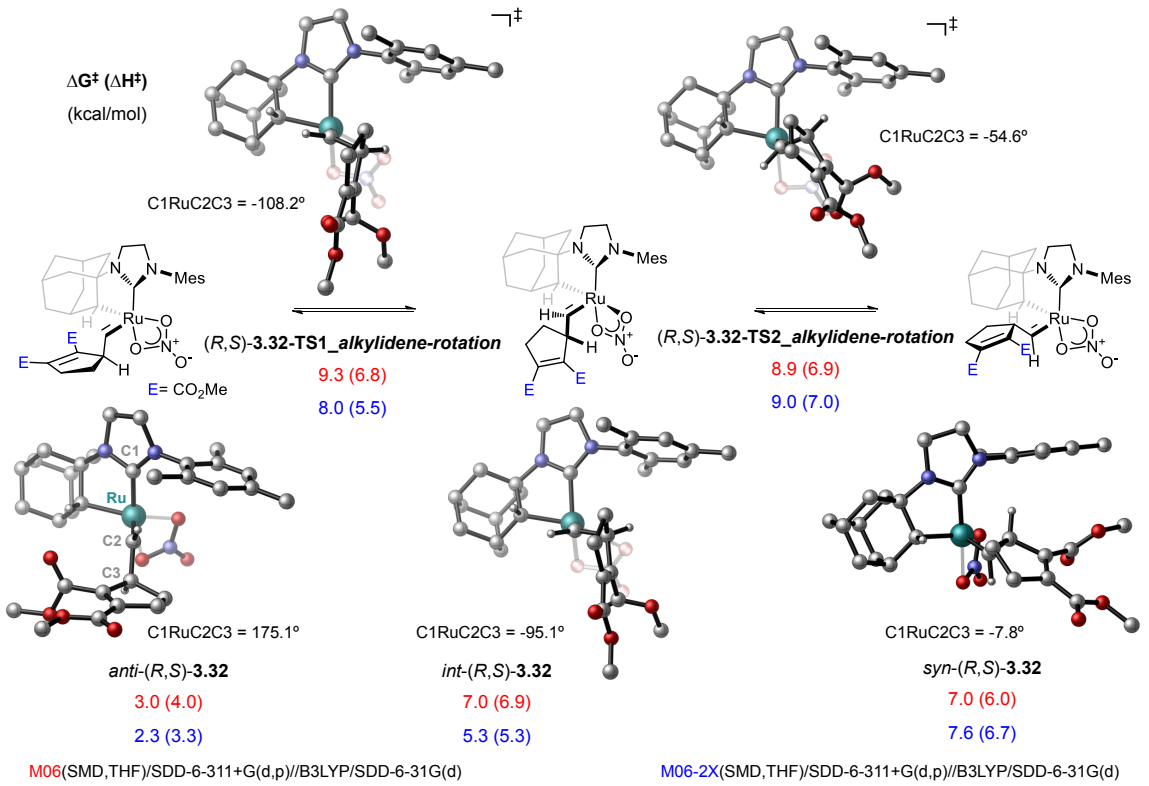


Figure 3.58. Free energies and enthalpies (in parentheses) for interconversion between ruthenium alkylidenes *anti*- and *syn*-(*R*,*S*)-**3.32** via alkylidene rotation. All energies are with respect to the ruthenium alkylidene complex *anti*-(*R*,*R*)-**3.4** and are given in kcal/mol.

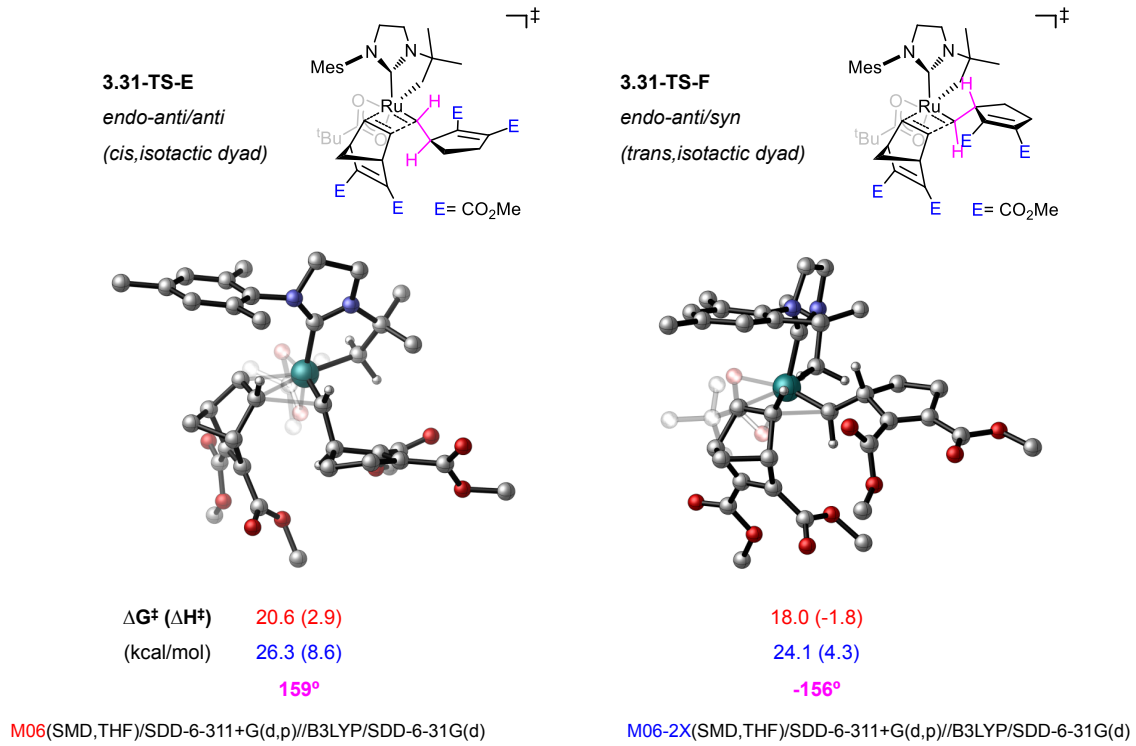


Figure 3.59. *Endo* transition states in the [2 + 2] cycloaddition for the polymerization of monomer **3.6** with catalyst **3.30**. Energies are with respect to the separated ruthenium alkylidene and monomer **3.6**.

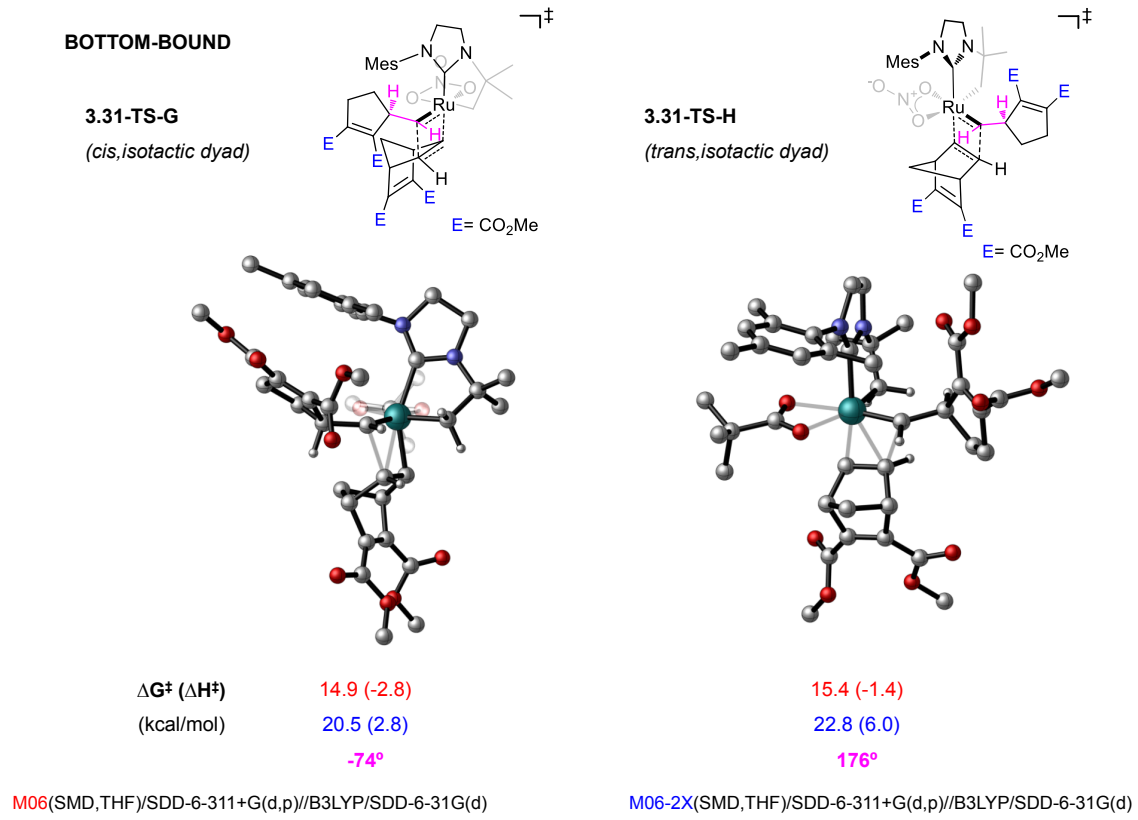


Figure 3.60. Bottom-bound transition states in the [2 + 2] cycloaddition for the polymerization of monomer **3.6** with catalyst **3.30**. Energies are with respect to the separated ruthenium alkylidene and monomer **3.6**.

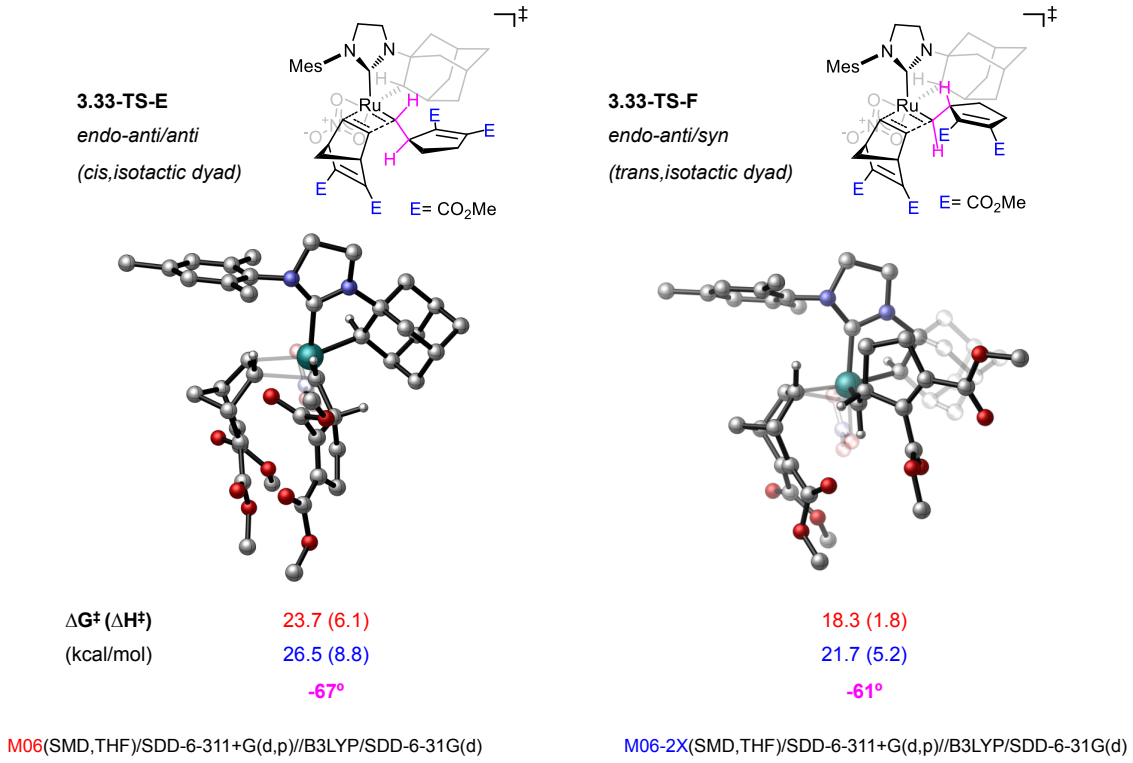


Figure 3.61. *Endo* transition states in the [2 + 2] cycloaddition for the polymerization of monomer **3.6** with catalyst (*R*,*R*)-**3.32**. Energies are with respect to the separated ruthenium alkylidene and monomer **3.6**.

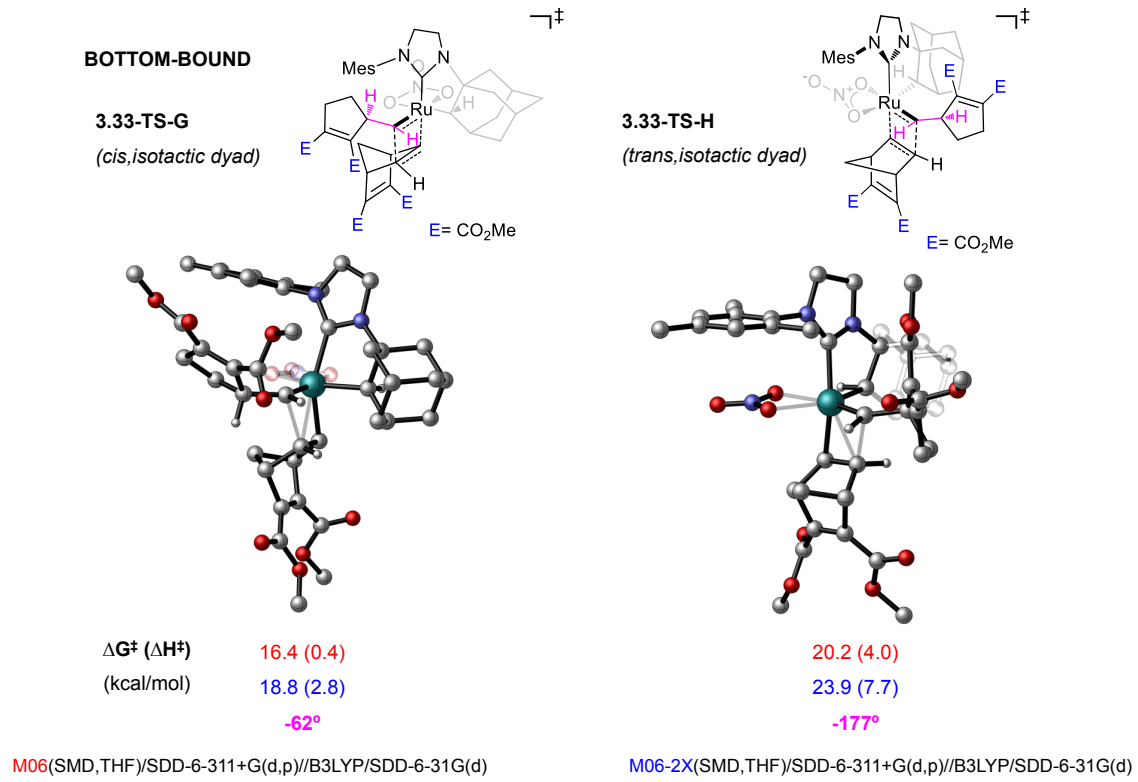


Figure 3.62. Bottom-bound transition states in the [2 + 2] cycloaddition for the polymerization of monomer **3.6** with catalyst (*R*,*R*)-**3.32**. Energies are with respect to the separated ruthenium alkylidene and monomer **3.6**.

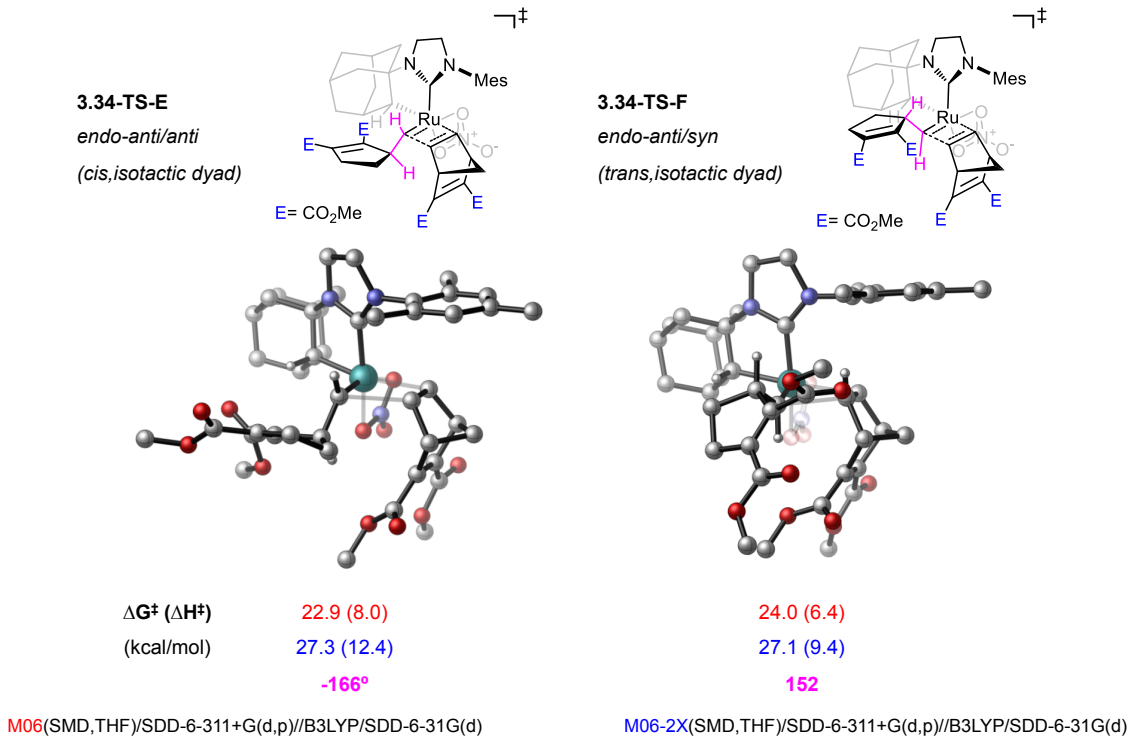


Figure 3.63. *Endo* transition states in the [2 + 2] cycloaddition for the polymerization of monomer **3.6** with catalyst (*R*,*S*)-**3.32**. Energies are with respect to the separated ruthenium alkylidene and monomer **3.6**.

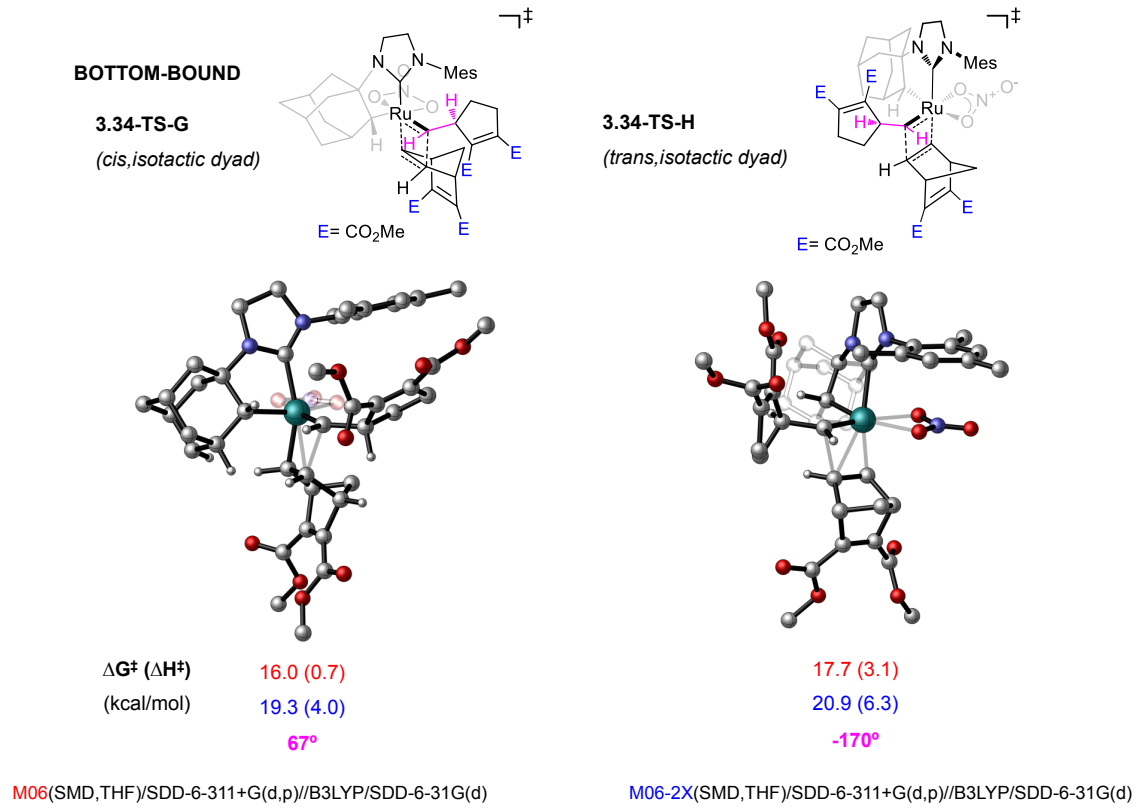


Figure 3.64. Bottom-bound transition states in the [2 + 2] cycloaddition for the polymerization of monomer **3.6** with catalyst (*R*,*S*)-**3.32**. Energies are with respect to the separated ruthenium alkylidene and monomer **3.6**.

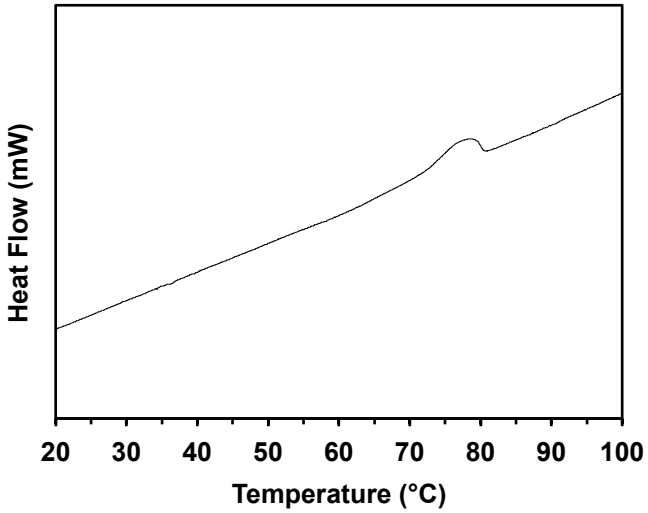


Figure 3.65. DSC curve for *cis,syndiotactic* **poly(3.5)** prepared with catalyst **3.1**.

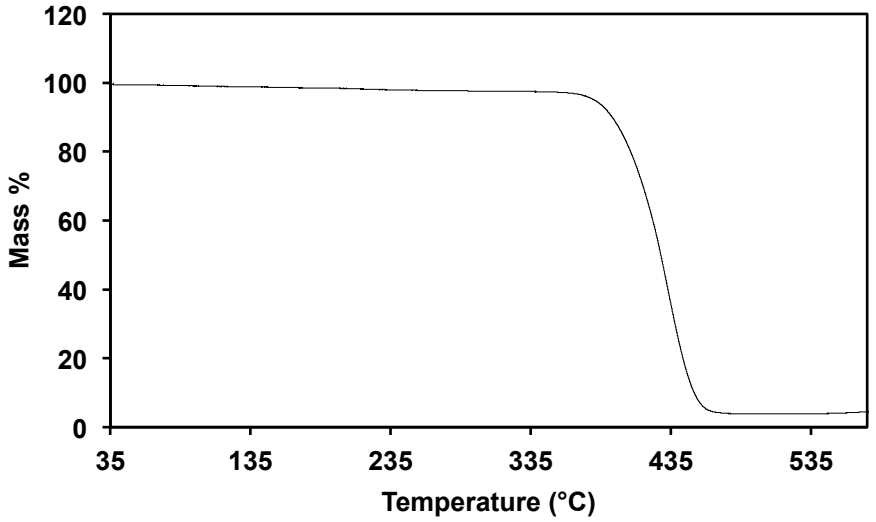


Figure 3.66. TGA curve for *cis,syndiotactic* **poly(3.5)** prepared with catalyst **3.1**.

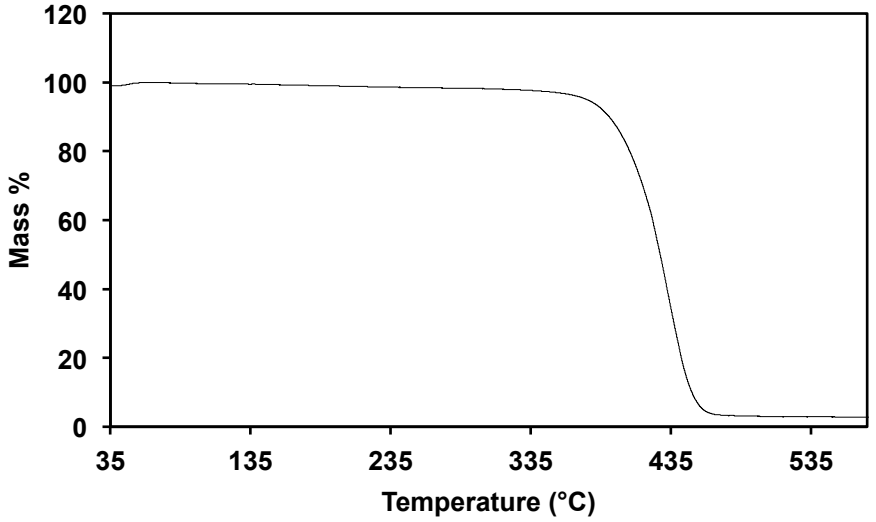


Figure 3.67. TGA curve for *trans,atactic* **poly(3.5)** prepared with (1,3-bis-(2,4,6-trimethylphenyl)-2-imidazolidinylidene)dichloro(*o*-isopropoxyphenylmethylene)-ruthenium.

Appendix A

Crystallographic Data (*Chapter 3*)

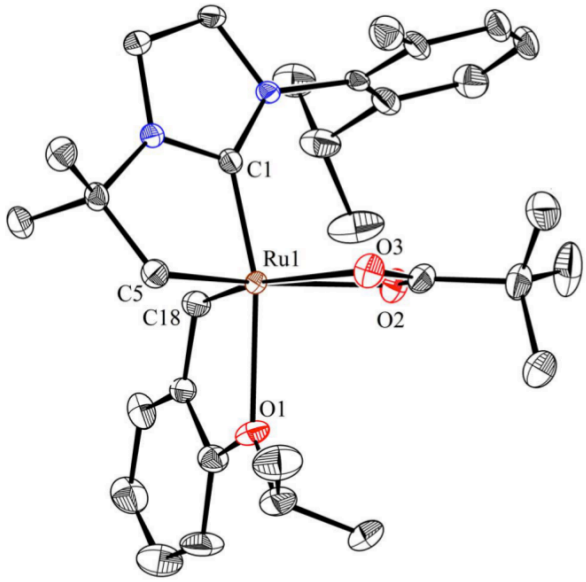


Table A1. Crystal Data and Structure Analysis Details for 3.2

Empirical Formula	$C_{32}H_{46}N_2O_3Ru$
Formula Weight	607.78
Crystallization Solvent	Hexanes
Crystal Shape	Plate
Crystal Color	Purple
Crystal Size	0.11 x 0.32 x 0.37 mm^3
Data Collection	
Preliminary Photograph(s)	Rotation
Type of Diffractometer	Bruker APEX-II CCD
Wavelength	0.71073 Å MoKa

Data Collection Temperature	100 K	
Theta Range for 9786 Reflections Used in Lattice Determination	2.39 to 31.77°	
Unit Cell Dimensions	a = 11.0782(5) Å	a= 90°
	b = 27.9893(11) Å	b= 103.793(2)°
	c = 10.2073(4) Å	g = 90°
Volume	3073.7(2) $Å^3$	
Z	4	
Crystal System	Monoclinic	
Space Group	$P2_1/c$	
Density (Calculated)	1.313 g/cm^3	
F(000)	1280	
Theta Range for Data Collection	2.0 to 39.1°	
Completeness to Theta = 25.000°	99.9%	
Index Ranges	$-19 \leq h \leq 18$, $-48 \leq k \leq 49$, $-17 \leq l \leq 17$	
Data Collection Scan Type	φ/ω scans	
Reflections Collected	191072	
Independent Reflections	17585 [R_{int} = 0.0616]	
Reflections > 2s(I)	13528	
Average s(I)/(net I)	0.0358	
Absorption Coefficient	0.54 mm^{-1}	
Absorption Correction	Semi-empirical from equivalents	
Max. and Min. Transmission	0.943 and 0.824	

Structure Solution and Refinement

Primary Solution Method	Dual
Hydrogen Placement	Mixed
Refinement method	Full-matrix least-squares on F^2
Data / Restraints / Parameters	17585 / 0 / 434
Treatment of Hydrogen Atoms	Mixed
Goodness-of-Fit on F^2	1.47
Final R Indices [I>2s(I), 13528 reflections]	R1 = 0.0435, *w*R2 = 0.1024
R Indices (All Data)	R1 = 0.0645, *w*R2 = 0.1085
Type of Weighting Scheme Used	Calc
Weighting Scheme Used	$w = 1/[\sigma^2(Fo^2) + (0.0400P)^2]$, where $P = (Fo^2 + 2Fc^2)/3$
Max Shift/Error	0.001
Average Shift/Error	0.000
Extinction Coefficient	N/A
Largest Diff. Peak and Hole	3.79 and -1.14 e/Å^3

Programs Used

Cell Refinement	SAINT V8.27B (Bruker-AXS, 2007)
Data Collection	APEX2 2012.10-0 (Bruker-AXS, 2007)
Data Reduction	SAINT V8.27B (Bruker-AXS, 2007)
Structure Solution	SHELXT (Sheldrick, 2012)
Structure Refinement	SHELXL-2013/2 (Sheldrick, 2013)
Graphics	DIAMOND 3 (Crystal Impact, 1999)

Special Refinement Details: The sample was multiple offset layered plates. In the unit cell determination 108 of 545 reflections were not indexed. Neither cell_now nor TwinRotMat (in Platon) detected any twinning. There are two orientations of the isopropyl group. This disorder is propagated through the molecule, resulting in most atoms being split. The ratio of components is 0.68:0.32; the minor component was modeled isotropically. Although the average bond precision is exemplary given the crystal problems, geometric parameters involving split and non-split atoms have larger errors.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles, and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table A2. Atomic Coordinates (x 10^4) and Equivalent Isotropic Displacement Parameters (Å^2 x 10^3) for 3.2. U(eq) is Defined as One Third of the Trace of the Orthogonalized U^{ij} Tensor

	x	y	z	U_{eq}
Ru(1)	8108(1)	8973(1)	7258(1)	11(1)
O(1)	9330(2)	8344(1)	6798(2)	22(1)
O(2)	6554(1)	8473(1)	7159(1)	23(1)
O(3)	6443(1)	8873(1)	5289(1)	24(1)
N(1)	8148(1)	9953(1)	7887(1)	16(1)
N(2)	6573(3)	9650(1)	8553(3)	14(1)
C(1)	7475(1)	9552(1)	7876(1)	15(1)
C(2)	7620(1)	10372(1)	8402(1)	19(1)
C(3)	6658(6)	10137(2)	9096(6)	18(1)
C(4)	9192(1)	9954(1)	7234(1)	18(1)
C(5)	9058(1)	9486(1)	6437(1)	20(1)
C(6)	10426(1)	9971(1)	8300(1)	23(1)
C(7)	9104(1)	10397(1)	6333(2)	26(1)

C(8)	5452(4)	9391(1)	8475(5)	16(1)
C(9)	5447(3)	9059(1)	9497(3)	21(1)
C(10)	4327(4)	8840(1)	9545(4)	28(1)
C(11)	3249(3)	8941(1)	8603(4)	25(1)
C(12)	3273(3)	9258(1)	7562(4)	23(1)
C(13)	4343(4)	9474(2)	7452(5)	22(1)
C(14)	6704(2)	8955(1)	10627(2)	30(1)
C(15)	7013(2)	8423(1)	10719(2)	48(1)
C(16)	6675(2)	9166(1)	11995(2)	36(1)
C(17)	4419(2)	9783(1)	6349(2)	30(1)
C(18)	9191(1)	8883(1)	8856(1)	19(1)
C(19)	10093(2)	8498(1)	9094(3)	16(1)
C(20)	10913(2)	8392(1)	10324(3)	24(1)
C(21)	11770(2)	8027(1)	10451(4)	33(1)
C(22)	11807(3)	7757(1)	9344(4)	42(1)
C(23)	11012(3)	7842(1)	8087(4)	35(1)
C(24)	10160(2)	8214(1)	7977(3)	21(1)
C(25)	9429(2)	8091(1)	5570(2)	30(1)
C(26)	8701(3)	7630(1)	5448(4)	44(1)
C(27)	8951(3)	8420(1)	4430(3)	43(1)
C(28)	6006(1)	8562(1)	5943(1)	22(1)
C(29)	4837(1)	8282(1)	5278(2)	30(1)
C(30)	4336(2)	8022(1)	6365(2)	50(1)
C(31)	3859(2)	8626(1)	4492(2)	43(1)
C(32)	5184(2)	7928(1)	4288(2)	44(1)
Ru(1A)	7983(1)	8976(1)	7052(1)	17(1)
O(1A)	8954(4)	8328(2)	6550(5)	24(1)
C(19A)	10003(7)	8454(3)	8776(6)	18(1)
C(20A)	10853(7)	8337(3)	9946(7)	27(2)
C(21A)	11665(6)	7944(2)	9956(6)	26(1)
C(22A)	11581(6)	7696(2)	8785(7)	32(1)
C(23A)	10691(6)	7811(2)	7613(6)	29(1)
C(24A)	9906(5)	8193(2)	7612(5)	16(1)
C(25A)	8922(4)	8217(2)	5155(4)	18(1)
C(26A)	8564(7)	7709(3)	4805(7)	38(1)
C(27A)	10089(4)	8372(2)	4738(5)	24(1)
N(2A)	6476(8)	9670(3)	8289(7)	19(2)
C(3A)	6602(14)	10161(5)	8894(13)	19(2)
C(8A)	5532(10)	9325(4)	8629(11)	19(2)
C(9A)	5656(6)	9047(2)	9745(6)	11(1)
C(10A)	4528(7)	8802(3)	9802(7)	17(1)
C(11A)	3453(7)	8880(3)	8896(7)	23(2)
C(12A)	3360(9)	9180(3)	7806(8)	23(2)
C(13A)	4482(10)	9444(4)	7661(10)	17(2)

Table A3. Bond Lengths [Å] and Angles [°] for 3.2

Ru(1)-C(18)	1.7978(15)	C(9)-C(10)	1.396(5)
Ru(1)-C(1)	1.9323(12)	C(9)-C(14)	1.610(4)
Ru(1)-C(5)	2.0709(13)	C(10)-C(11)	1.372(5)
Ru(1)-O(2)	2.2021(10)	C(10)-H(10)	0.9500
Ru(1)-O(1)	2.3336(18)	C(11)-C(12)	1.390(5)
Ru(1)-O(3)	2.3984(12)	C(11)-H(11)	0.9500
O(1)-C(24)	1.378(3)	C(12)-C(13)	1.359(6)
O(1)-C(25)	1.467(3)	C(12)-H(12)	0.9500
O(2)-C(28)	1.2699(17)	C(13)-C(17)	1.437(5)
O(2)-Ru(1A)	2.1402(14)	C(14)-C(9A)	1.315(6)
O(3)-C(28)	1.2624(18)	C(14)-C(15)	1.524(2)
O(3)-Ru(1A)	2.1838(17)	C(14)-C(16)	1.524(2)
N(1)-C(1)	1.3457(16)	C(14)-H(14)	1.0000
N(1)-C(2)	1.4631(16)	C(14)-H(14A)	0.81(7)
N(1)-C(4)	1.4660(16)	C(15)-H(15A)	0.9800
N(2)-C(1)	1.371(3)	C(15)-H(15B)	0.9800
N(2)-C(8)	1.424(5)	C(15)-H(15C)	0.9800
N(2)-C(3)	1.465(7)	C(16)-H(16A)	0.9800
C(1)-N(2A)	1.317(9)	C(16)-H(16B)	0.9800
C(1)-Ru(1A)	1.9640(16)	C(16)-H(16C)	0.9800
C(2)-C(3A)	1.463(15)	C(17)-C(13A)	1.630(10)
C(2)-C(3)	1.558(6)	C(17)-H(17A)	0.9804
C(2)-H(2AA)	0.9900	C(17)-H(17B)	0.9798
C(2)-H(2AB)	0.9900	C(17)-H(17C)	0.9796
C(2)-H(2BC)	0.9900	C(17)-H(17D)	0.8519
C(2)-H(2BD)	0.9900	C(17)-H(17E)	0.9743
C(3)-H(3A)	0.9900	C(17)-H(17F)	1.0594
C(3)-H(3B)	0.9900	C(18)-C(19)	1.449(3)
C(4)-C(6)	1.5310(18)	C(18)-C(19A)	1.513(7)
C(4)-C(5)	1.5318(18)	C(18)-Ru(1A)	2.0186(19)
C(4)-C(7)	1.5336(19)	C(18)-H(18)	0.9500
C(5)-Ru(1A)	2.0508(16)	C(19)-C(20)	1.395(4)
C(5)-H(5A)	0.9900	C(19)-C(24)	1.406(4)
C(5)-H(5B)	0.9900	C(20)-C(21)	1.379(4)
C(5)-H(5C)	0.9900	C(20)-H(20)	0.9500
C(5)-H(5D)	0.9900	C(21)-C(22)	1.368(5)
C(6)-H(6A)	0.9800	C(21)-H(21)	0.9500
C(6)-H(6B)	0.9800	C(22)-C(23)	1.392(4)
C(6)-H(6C)	0.9800	C(22)-H(22)	0.9500
C(7)-H(7A)	0.9800	C(23)-C(24)	1.392(3)
C(7)-H(7B)	0.9800	C(23)-H(23)	0.9500
C(7)-H(7C)	0.9800	C(25)-C(27)	1.479(4)
C(8)-C(9)	1.398(5)	C(25)-C(26)	1.511(4)
C(8)-C(13)	1.429(6)	C(25)-H(25)	1.0000

C(26)-H(26A)	0.9800	C(8A)-C(9A)	1.360(11)
C(26)-H(26B)	0.9800	C(8A)-C(13A)	1.375(14)
C(26)-H(26C)	0.9800	C(9A)-C(10A)	1.439(11)
C(27)-H(27A)	0.9800	C(10A)-C(11A)	1.340(9)
C(27)-H(27B)	0.9800	C(10A)-H(10A)	0.9500
C(27)-H(27C)	0.9800	C(11A)-C(12A)	1.378(10)
C(28)-C(29)	1.528(2)	C(11A)-H(11A)	0.9500
C(28)-Ru(1A)	2.4975(18)	C(12A)-C(13A)	1.483(15)
C(29)-C(31)	1.526(3)	C(12A)-H(12A)	0.9500
C(29)-C(32)	1.528(2)	C(18)-Ru(1)-C(1)	92.11(6)
C(29)-C(30)	1.536(3)	C(18)-Ru(1)-C(5)	99.85(6)
C(30)-H(30A)	0.9800	C(1)-Ru(1)-C(5)	79.03(5)
C(30)-H(30B)	0.9800	C(18)-Ru(1)-O(2)	107.30(5)
C(30)-H(30C)	0.9800	C(1)-Ru(1)-O(2)	101.97(5)
C(31)-H(31A)	0.9800	C(5)-Ru(1)-O(2)	152.74(6)
C(31)-H(31B)	0.9800	C(18)-Ru(1)-O(1)	77.49(7)
C(31)-H(31C)	0.9800	C(1)-Ru(1)-O(1)	166.27(7)
C(32)-H(32A)	0.9800	C(5)-Ru(1)-O(1)	93.79(6)
C(32)-H(32B)	0.9800	O(2)-Ru(1)-O(1)	89.79(6)
C(32)-H(32C)	0.9800	C(18)-Ru(1)-O(3)	163.29(5)
Ru(1A)-O(1A)	2.227(5)	C(1)-Ru(1)-O(3)	96.01(5)
O(1A)-C(24A)	1.373(6)	C(5)-Ru(1)-O(3)	96.03(5)
O(1A)-C(25A)	1.449(7)	O(2)-Ru(1)-O(3)	56.71(4)
C(19A)-C(20A)	1.372(9)	O(1)-Ru(1)-O(3)	96.38(6)
C(19A)-C(24A)	1.377(8)	C(24)-O(1)-C(25)	116.6(2)
C(20A)-C(21A)	1.421(10)	C(24)-O(1)-Ru(1)	108.78(14)
C(20A)-H(20A)	0.9500	C(25)-O(1)-Ru(1)	134.49(16)
C(21A)-C(22A)	1.365(8)	C(28)-O(2)-Ru(1A)	90.47(9)
C(21A)-H(21A)	0.9500	C(28)-O(2)-Ru(1)	96.11(8)
C(22A)-C(23A)	1.394(8)	C(28)-O(3)-Ru(1A)	88.70(9)
C(22A)-H(22A)	0.9500	C(28)-O(3)-Ru(1)	87.26(8)
C(23A)-C(24A)	1.379(9)	C(1)-N(1)-C(2)	113.73(10)
C(23A)-H(23A)	0.9500	C(1)-N(1)-C(4)	119.57(10)
C(25A)-C(26A)	1.496(8)	C(2)-N(1)-C(4)	126.07(10)
C(25A)-C(27A)	1.517(6)	C(1)-N(2)-C(8)	126.9(3)
C(25A)-H(25A)	1.0000	C(1)-N(2)-C(3)	112.9(3)
C(26A)-H(26D)	0.9800	C(8)-N(2)-C(3)	118.1(3)
C(26A)-H(26E)	0.9800	N(2A)-C(1)-N(1)	107.2(4)
C(26A)-H(26F)	0.9800	N(1)-C(1)-N(2)	107.32(16)
C(27A)-H(27D)	0.9800	N(1)-C(1)-Ru(1)	117.30(8)
C(27A)-H(27E)	0.9800	N(2)-C(1)-Ru(1)	134.28(15)
C(27A)-H(27F)	0.9800	N(2A)-C(1)-Ru(1A)	133.8(4)
N(2A)-C(3A)	1.499(18)	N(1)-C(1)-Ru(1A)	118.27(9)
N(2A)-C(8A)	1.522(14)	N(1)-C(2)-C(3A)	101.9(6)
C(3A)-H(3AC)	0.9900	N(1)-C(2)-C(3)	101.6(2)
C(3A)-H(3AD)	0.9900	N(1)-C(2)-H(2AA)	111.5

C(3)-C(2)-H(2AA)	111.5	C(9)-C(8)-C(13)	119.8(4)
N(1)-C(2)-H(2AB)	111.5	N(2)-C(8)-C(13)	123.0(4)
C(3)-C(2)-H(2AB)	111.5	C(10)-C(9)-C(8)	118.7(3)
H(2AA)-C(2)-H(2AB)	109.3	C(10)-C(9)-C(14)	121.3(3)
N(1)-C(2)-H(2BC)	111.4	C(8)-C(9)-C(14)	119.9(3)
C(3A)-C(2)-H(2BC)	111.4	C(11)-C(10)-C(9)	121.1(3)
N(1)-C(2)-H(2BD)	111.4	C(11)-C(10)-H(10)	119.4
C(3A)-C(2)-H(2BD)	111.4	C(9)-C(10)-H(10)	119.4
H(2BC)-C(2)-H(2BD)	109.2	C(10)-C(11)-C(12)	119.7(3)
N(2)-C(3)-C(2)	102.1(4)	C(10)-C(11)-H(11)	120.2
N(2)-C(3)-H(3A)	111.4	C(12)-C(11)-H(11)	120.2
C(2)-C(3)-H(3A)	111.4	C(13)-C(12)-C(11)	121.6(4)
N(2)-C(3)-H(3B)	111.4	C(13)-C(12)-H(12)	119.2
C(2)-C(3)-H(3B)	111.4	C(11)-C(12)-H(12)	119.2
H(3A)-C(3)-H(3B)	109.2	C(12)-C(13)-C(8)	118.8(4)
N(1)-C(4)-C(6)	110.15(10)	C(12)-C(13)-C(17)	123.2(3)
N(1)-C(4)-C(5)	104.65(10)	C(8)-C(13)-C(17)	118.0(4)
C(6)-C(4)-C(5)	111.19(11)	C(9A)-C(14)-C(15)	112.5(3)
N(1)-C(4)-C(7)	109.26(11)	C(9A)-C(14)-C(16)	110.0(3)
C(6)-C(4)-C(7)	108.61(11)	C(15)-C(14)-C(16)	112.16(15)
C(5)-C(4)-C(7)	112.91(11)	C(15)-C(14)-C(9)	111.40(19)
C(4)-C(5)-Ru(1A)	115.02(9)	C(16)-C(14)-C(9)	112.44(16)
C(4)-C(5)-Ru(1)	111.87(8)	C(15)-C(14)-H(14)	106.8
C(4)-C(5)-H(5A)	109.2	C(16)-C(14)-H(14)	106.8
Ru(1)-C(5)-H(5A)	109.2	C(9)-C(14)-H(14)	106.8
C(4)-C(5)-H(5B)	109.2	C(9A)-C(14)-H(14A)	103(5)
Ru(1)-C(5)-H(5B)	109.2	C(15)-C(14)-H(14A)	109(5)
H(5A)-C(5)-H(5B)	107.9	C(16)-C(14)-H(14A)	110(5)
C(4)-C(5)-H(5C)	108.5	C(14)-C(15)-H(15A)	109.5
Ru(1A)-C(5)-H(5C)	108.5	C(14)-C(15)-H(15B)	109.5
C(4)-C(5)-H(5D)	108.5	H(15A)-C(15)-H(15B)	109.5
Ru(1A)-C(5)-H(5D)	108.5	C(14)-C(15)-H(15C)	109.5
H(5C)-C(5)-H(5D)	107.5	H(15A)-C(15)-H(15C)	109.5
C(4)-C(6)-H(6A)	109.5	H(15B)-C(15)-H(15C)	109.5
C(4)-C(6)-H(6B)	109.5	C(14)-C(16)-H(16A)	109.5
H(6A)-C(6)-H(6B)	109.5	C(14)-C(16)-H(16B)	109.5
C(4)-C(6)-H(6C)	109.5	H(16A)-C(16)-H(16B)	109.5
H(6A)-C(6)-H(6C)	109.5	C(14)-C(16)-H(16C)	109.5
H(6B)-C(6)-H(6C)	109.5	H(16A)-C(16)-H(16C)	109.5
C(4)-C(7)-H(7A)	109.5	H(16B)-C(16)-H(16C)	109.5
C(4)-C(7)-H(7B)	109.5	C(13)-C(17)-H(17A)	109.4
H(7A)-C(7)-H(7B)	109.5	C(13)-C(17)-H(17B)	109.5
C(4)-C(7)-H(7C)	109.5	H(17A)-C(17)-H(17B)	109.5
H(7A)-C(7)-H(7C)	109.5	C(13)-C(17)-H(17C)	109.5
H(7B)-C(7)-H(7C)	109.5	H(17A)-C(17)-H(17C)	109.5
C(9)-C(8)-N(2)	117.1(4)	H(17B)-C(17)-H(17C)	109.5

C(13A)-C(17)-H(17D)	106.0
C(13A)-C(17)-H(17E)	105.0
H(17D)-C(17)-H(17E)	110.4
C(13A)-C(17)-H(17F)	110.3
H(17D)-C(17)-H(17F)	114.7
H(17E)-C(17)-H(17F)	109.9
C(19)-C(18)-Ru(1)	122.71(15)
C(19A)-C(18)-Ru(1A)	109.0(2)
C(19)-C(18)-H(18)	118.6
Ru(1)-C(18)-H(18)	118.6
C(20)-C(19)-C(24)	117.4(2)
C(20)-C(19)-C(18)	125.8(3)
C(24)-C(19)-C(18)	116.8(2)
C(21)-C(20)-C(19)	121.9(3)
C(21)-C(20)-H(20)	119.0
C(19)-C(20)-H(20)	119.0
C(22)-C(21)-C(20)	119.1(3)
C(22)-C(21)-H(21)	120.4
C(20)-C(21)-H(21)	120.4
C(21)-C(22)-C(23)	121.9(2)
C(21)-C(22)-H(22)	119.0
C(23)-C(22)-H(22)	119.0
C(22)-C(23)-C(24)	118.1(3)
C(22)-C(23)-H(23)	121.0
C(24)-C(23)-H(23)	121.0
O(1)-C(24)-C(23)	124.5(3)
O(1)-C(24)-C(19)	113.9(2)
C(23)-C(24)-C(19)	121.6(3)
O(1)-C(25)-C(27)	106.6(2)
O(1)-C(25)-C(26)	109.6(2)
C(27)-C(25)-C(26)	112.5(3)
O(1)-C(25)-H(25)	109.3
C(27)-C(25)-H(25)	109.3
C(26)-C(25)-H(25)	109.3
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5

O(3)-C(28)-O(2)	119.89(13)
O(3)-C(28)-C(29)	120.69(13)
O(2)-C(28)-C(29)	119.40(13)
O(3)-C(28)-Ru(1A)	60.95(8)
O(2)-C(28)-Ru(1A)	58.97(7)
C(29)-C(28)-Ru(1A)	176.70(11)
C(31)-C(29)-C(32)	108.65(15)
C(31)-C(29)-C(28)	109.30(13)
C(32)-C(29)-C(28)	107.84(13)
C(31)-C(29)-C(30)	110.17(16)
C(32)-C(29)-C(30)	111.21(16)
C(28)-C(29)-C(30)	109.62(14)
C(29)-C(30)-H(30A)	109.5
C(29)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(29)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(29)-C(31)-H(31A)	109.5
C(29)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(29)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(29)-C(32)-H(32A)	109.5
C(29)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(29)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(1)-Ru(1A)-C(18)	84.86(7)
C(1)-Ru(1A)-C(5)	78.81(6)
C(18)-Ru(1A)-C(5)	93.56(7)
C(1)-Ru(1A)-O(2)	103.14(6)
C(18)-Ru(1A)-O(2)	101.89(7)
C(5)-Ru(1A)-O(2)	164.52(8)
C(1)-Ru(1A)-O(3)	102.32(6)
C(18)-Ru(1A)-O(3)	162.32(7)
C(5)-Ru(1A)-O(3)	103.62(7)
O(2)-Ru(1A)-O(3)	60.90(5)
C(1)-Ru(1A)-O(1A)	166.01(12)
C(18)-Ru(1A)-O(1A)	81.59(12)
C(5)-Ru(1A)-O(1A)	98.51(14)
O(2)-Ru(1A)-O(1A)	83.15(13)
O(3)-Ru(1A)-O(1A)	91.66(11)
C(1)-Ru(1A)-C(28)	105.35(6)

C(18)-Ru(1A)-C(28)	132.28(7)	H(26D)-C(26A)-H(26F)	109.5
C(5)-Ru(1A)-C(28)	133.97(8)	H(26E)-C(26A)-H(26F)	109.5
O(2)-Ru(1A)-C(28)	30.56(4)	C(25A)-C(27A)-H(27D)	109.5
O(3)-Ru(1A)-C(28)	30.35(5)	C(25A)-C(27A)-H(27E)	109.5
O(1A)-Ru(1A)-C(28)	86.48(12)	H(27D)-C(27A)-H(27E)	109.5
C(24A)-O(1A)-C(25A)	123.4(5)	C(25A)-C(27A)-H(27F)	109.5
C(24A)-O(1A)-Ru(1A)	111.4(4)	H(27D)-C(27A)-H(27F)	109.5
C(25A)-O(1A)-Ru(1A)	120.0(3)	H(27E)-C(27A)-H(27F)	109.5
C(20A)-C(19A)-C(24A)	121.4(6)	C(1)-N(2A)-C(3A)	111.0(8)
C(20A)-C(19A)-C(18)	115.8(5)	C(1)-N(2A)-C(8A)	126.1(8)
C(24A)-C(19A)-C(18)	122.8(5)	C(3A)-N(2A)-C(8A)	119.3(9)
C(19A)-C(20A)-C(21A)	119.5(6)	C(2)-C(3A)-N(2A)	103.5(10)
C(19A)-C(20A)-H(20A)	120.2	C(2)-C(3A)-H(3AC)	111.1
C(21A)-C(20A)-H(20A)	120.2	N(2A)-C(3A)-H(3AC)	111.1
C(22A)-C(21A)-C(20A)	118.5(6)	C(2)-C(3A)-H(3AD)	111.1
C(22A)-C(21A)-H(21A)	120.8	N(2A)-C(3A)-H(3AD)	111.1
C(20A)-C(21A)-H(21A)	120.8	H(3AC)-C(3A)-H(3AD)	109.0
C(21A)-C(22A)-C(23A)	121.4(6)	C(9A)-C(8A)-C(13A)	129.7(10)
C(21A)-C(22A)-H(22A)	119.3	C(9A)-C(8A)-N(2A)	128.1(9)
C(23A)-C(22A)-H(22A)	119.3	C(13A)-C(8A)-N(2A)	101.1(8)
C(24A)-C(23A)-C(22A)	119.8(6)	C(14)-C(9A)-C(8A)	125.6(7)
C(24A)-C(23A)-H(23A)	120.1	C(14)-C(9A)-C(10A)	120.9(5)
C(22A)-C(23A)-H(23A)	120.1	C(8A)-C(9A)-C(10A)	113.1(7)
O(1A)-C(24A)-C(19A)	115.0(5)	C(11A)-C(10A)-C(9A)	122.2(7)
O(1A)-C(24A)-C(23A)	125.5(5)	C(11A)-C(10A)-H(10A)	118.9
C(19A)-C(24A)-C(23A)	119.4(5)	C(9A)-C(10A)-H(10A)	118.9
O(1A)-C(25A)-C(26A)	112.5(4)	C(10A)-C(11A)-C(12A)	122.6(8)
O(1A)-C(25A)-C(27A)	113.1(4)	C(10A)-C(11A)-H(11A)	118.7
C(26A)-C(25A)-C(27A)	113.4(4)	C(12A)-C(11A)-H(11A)	118.7
O(1A)-C(25A)-H(25A)	105.7	C(11A)-C(12A)-C(13A)	118.7(8)
C(26A)-C(25A)-H(25A)	105.7	C(11A)-C(12A)-H(12A)	120.6
C(27A)-C(25A)-H(25A)	105.7	C(13A)-C(12A)-H(12A)	120.6
C(25A)-C(26A)-H(26D)	109.5	C(8A)-C(13A)-C(12A)	113.2(9)
C(25A)-C(26A)-H(26E)	109.5	C(8A)-C(13A)-C(17)	126.4(9)
H(26D)-C(26A)-H(26E)	109.5	C(12A)-C(13A)-C(17)	120.0(6)
C(25A)-C(26A)-H(26F)	109.5		

Table A4. Anistropic Displacement Parameters (Å^2 x 10^4) for 3.2. The Anistropic Displacement Factor Exponent Takes the Form: -2p^2[h^{2}a*^{2}U^{11} + … + 2 h k a* b* U^{12}]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	127(1)	119(1)	85(1)	-4(1)	20(1)	-6(1)
O(1)	311(11)	161(7)	216(8)	-35(6)	106(8)	27(7)
O(2)	267(5)	207(5)	224(4)	3(3)	69(4)	-63(4)

O(3)	268(5)	242(5)	214(4)	9(4)	48(4)	-34(4)
N(1)	150(4)	140(4)	219(5)	-7(3)	81(4)	-13(3)
N(2)	143(9)	139(9)	155(11)	-6(8)	77(9)	0(6)
C(1)	131(5)	153(5)	171(5)	14(4)	38(4)	0(4)
C(2)	193(5)	145(5)	232(5)	-5(4)	54(4)	13(4)
C(3)	175(13)	165(13)	204(19)	-17(13)	76(13)	24(8)
C(4)	163(5)	197(6)	183(5)	-4(4)	72(4)	-35(4)
C(5)	204(5)	207(6)	195(5)	3(4)	90(4)	-20(4)
C(6)	160(5)	276(7)	246(6)	-11(5)	45(4)	-24(5)
C(7)	285(7)	237(7)	261(6)	35(5)	104(5)	-39(5)
C(8)	140(10)	121(12)	259(14)	13(11)	129(10)	6(9)
C(9)	150(11)	254(12)	211(13)	-8(9)	32(10)	31(9)
C(10)	303(17)	275(13)	291(17)	62(12)	159(14)	-3(12)
C(11)	170(11)	309(14)	313(15)	-43(12)	122(11)	-68(10)
C(12)	162(10)	281(16)	263(14)	-9(12)	80(10)	-36(9)
C(13)	126(12)	288(15)	229(17)	-30(13)	40(12)	12(10)
C(14)	352(8)	273(8)	335(8)	48(6)	186(6)	85(6)
C(15)	721(14)	323(9)	425(10)	50(8)	197(10)	221(9)
C(16)	401(9)	375(9)	351(8)	-17(7)	154(7)	68(7)
C(17)	277(7)	338(8)	282(7)	-19(6)	54(6)	9(6)
C(18)	189(5)	168(5)	230(6)	18(4)	83(4)	14(4)
C(19)	175(9)	146(9)	190(12)	20(9)	73(9)	3(6)
C(20)	185(10)	243(12)	279(13)	129(11)	13(9)	-11(7)
C(21)	266(11)	293(13)	412(16)	144(12)	21(11)	73(9)
C(22)	386(15)	310(14)	530(20)	101(14)	40(14)	193(11)
C(23)	360(14)	265(12)	429(16)	-7(11)	84(13)	179(10)
C(24)	208(10)	185(9)	252(12)	39(8)	57(9)	31(8)
C(25)	341(12)	277(11)	292(11)	-81(9)	111(9)	31(9)
C(26)	380(14)	183(11)	750(20)	-139(13)	109(15)	-2(10)
C(27)	568(17)	431(15)	290(12)	-42(11)	122(11)	122(13)
C(28)	236(6)	197(6)	241(6)	-54(5)	64(5)	-34(5)
C(29)	256(7)	288(8)	337(8)	-93(6)	46(6)	-91(6)
C(30)	455(11)	527(12)	528(12)	-62(9)	118(9)	-303(9)
C(31)	262(8)	472(11)	500(11)	-155(9)	-21(7)	-6(7)
C(32)	343(9)	408(10)	531(11)	-258(9)	34(8)	-64(7)

Table A5. Hydrogen Coordinates (x 10^3) and Isotropic Displacement Parameters (Å^2 x 10^3) for 3.2

	x	y	z	U_{iso}
H(2AA)	721	1059	766	23
H(2AB)	826	1055	906	23
H(2BC)	731	1061	768	23
H(2BD)	824	1053	914	23
H(3A)	696	1014	1009	21

H(3B)	585	1030	885	21
H(5A)	989	936	643	23
H(5B)	861	955	549	23
H(5C)	990	935	650	23
H(5D)	870	956	547	23
H(6A)	1042	1024	891	34
H(6B)	1111	1001	786	34
H(6C)	1054	967	881	34
H(7A)	828	1041	571	38
H(7B)	974	1038	582	38
H(7C)	923	1068	690	38
H(10)	431	862	1024	33
H(11)	249	879	866	30
H(12)	252	933	691	28
H(14)	739	912	1033	36
H(14A)	721(7)	909(2)	1031(7)	36
H(15A)	639	825	1108	72
H(15B)	784	838	1132	72
H(15C)	701	830	982	72
H(16A)	649	951	1190	55
H(16B)	748	912	1263	55
H(16C)	603	901	1234	55
H(17A)	527	990	647	45
H(17B)	386	1006	632	45
H(17C)	418	960	550	45
H(17D)	368	976	587	45
H(17E)	500	964	588	45
H(17F)	471	1013	666	45
H(18)	917	910	958	23
H(20)	1088	858	1110	29
H(21)	1233	796	1130	40
H(22)	1239	750	943	50
H(23)	1105	765	733	42
H(25)	1032	802	562	36
H(26A)	904	743	624	66
H(26B)	877	746	463	66
H(26C)	783	770	540	66
H(27A)	813	854	448	64
H(27B)	887	825	358	64
H(27C)	953	869	447	64
H(30A)	357	785	594	75
H(30B)	416	826	701	75
H(30C)	496	779	684	75
H(31A)	421	880	384	65
H(31B)	361	885	512	65
H(31C)	313	844	401	65

H(32A)	443	776	378	66
H(32B)	577	769	479	66
H(32C)	557	810	366	66
H(20A)	1090	852	1074	33
H(21A)	1225	786	1076	31
H(22A)	1214	744	877	38
H(23A)	1063	763	682	35
H(25A)	823	842	460	22
H(26D)	931	751	500	56
H(26E)	815	769	384	56
H(26F)	800	760	534	56
H(27D)	1020	872	486	37
H(27E)	1001	829	379	37
H(27F)	1081	821	530	37
H(3AC)	583	1035	858	22
H(3AD)	681	1015	989	22
H(10A)	454	858	1051	20
H(11A)	273	872	901	27
H(12A)	259	922	716	27

Appendix B

The Cartesian Coordinates (Å), SCF Energies, Enthalpies at 298 K, and Gibbs Free Energies at 298 K for Optimized Structures (*Chapter 3*)

3.19

B3LYP SCF energy:	-1407.85446090	a.u.
B3LYP enthalpy:	-1407.19555300	a.u.
B3LYP free energy:	-1407.30347300	a.u.
M06 SCF energy in solution:	-1407.21835495	a.u.
M06 enthalpy in solution:	-1406.55944705	a.u.
M06 free energy in solution:	-1406.66736705	a.u.
M06-2X SCF energy in solution:	-1407.51112942	a.u.
M06-2X enthalpy in solution:	-1406.85222152	a.u.
M06-2X free energy in solution:	-1406.96014152	a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.85192700	0.24653500	-0.58862200
O	-1.11942300	2.52201900	-0.86708700
O	0.84026600	1.52962900	-1.04151100
N	-1.13189200	-2.53572600	-1.21611200
N	0.79056700	-2.31474400	-0.16871100
C	-0.29695300	-1.63484300	-0.62895300
C	-0.69715200	-3.92186200	-1.02734300
H	-0.78046800	-4.50526200	-1.94928500
H	-1.29882800	-4.41860500	-0.25338600
C	0.76250700	-3.73366400	-0.57732300
H	1.04322500	-4.38908300	0.25169500
H	1.47117900	-3.90258200	-1.39972500
C	-2.50594100	-2.11114300	-1.55619200
C	-3.48631100	-2.55342500	-0.45233100
H	-3.22599700	-2.08261500	0.50056500
H	-3.48959400	-3.64175600	-0.31721200
C	-2.91677800	-2.73364700	-2.90296600
H	-2.19822600	-2.46901900	-3.68678800
H	-2.98483800	-3.82837200	-2.85200100
C	-2.43637700	-0.57005300	-1.63280700
H	-2.12394300	-0.26529200	-2.65195000
C	2.00756600	-1.73948200	0.33111200
C	2.28683200	-1.84057200	1.70814300
C	3.49709600	-1.32889100	2.18339300
H	3.71574900	-1.40268500	3.24683700
C	4.43154400	-0.72989600	1.33192800
C	4.13330000	-0.66467100	-0.03086000
H	4.85398900	-0.21719400	-0.71250600
C	2.93428200	-1.16097500	-0.55543600
C	1.31321200	-2.48622100	2.66592700
H	1.67660800	-2.40860600	3.69515200
H	1.16589800	-3.55221000	2.44948900
H	0.32824800	-2.01090100	2.61638700
C	5.71946500	-0.15615600	1.87600300
H	6.08291200	-0.72926900	2.73607400
H	5.57983000	0.87992300	2.21212300
H	6.50758500	-0.14768100	1.11558300
C	2.66250200	-1.04432000	-2.03634000
H	2.04229000	-0.16346600	-2.23556700
H	2.13730300	-1.91805500	-2.43585100
H	3.59958600	-0.93132500	-2.59120800
C	-1.47114500	0.08937900	1.11986200
H	-1.28904800	-0.79168100	1.75635000
C	-2.21677200	1.18499500	1.85215600
C	-1.45856700	1.67985500	3.12807800
C	-3.53961800	0.70589400	2.43613300
H	-2.39627600	2.02160100	1.16453200
C	-2.54430300	1.91017000	4.21134400
C	-3.70860800	1.09044400	3.70408300
H	-3.41991600	-0.12354000	-1.44990900
H	-4.50595300	-2.25315200	-0.71830700
H	-3.90113000	-2.35646000	-3.20040700
C	0.11925400	2.60012700	-1.09581700
C	0.80115000	3.92830600	-1.43895500
H	-0.77191700	0.89252600	3.46317400
H	-2.82650800	2.97155900	4.28778600
H	-2.20865700	1.60900500	5.21232100
H	-0.85583900	2.56930500	2.92160400
H	-4.59697200	0.89741500	4.30072100
H	-4.26420500	0.15382100	1.84373400
C	1.86549400	4.21273000	-0.35529000
H	2.59421500	3.39899300	-0.29981000
H	2.39612500	5.14424300	-0.58711500
H	1.40238400	4.32595700	0.63222200
C	1.49221600	3.77758400	-2.81217300
H	0.76099700	3.56888900	-3.60263100
H	2.01312500	4.70657900	-3.07359400
H	2.22166400	2.96274300	-2.79592100
C	-0.22887200	5.06755300	-1.48512700
H	-0.99987300	4.87645700	-2.23803900
H	-0.73246200	5.18725200	-0.52102200
H	0.27092100	6.01182100	-1.73367500

3.20

B3LYP SCF energy:	-1407.85459910	a.u.
B3LYP enthalpy:	-1407.19565000	a.u.
B3LYP free energy:	-1407.30341400	a.u.
M06 SCF energy in solution:	-1407.21792376	a.u.

M06 enthalpy in solution:	-1406.55897466	a.u.
M06 free energy in solution:	-1406.66673866	a.u.
M06-2X SCF energy in solution:	-1407.51084159	a.u.
M06-2X enthalpy in solution:	-1406.85189249	a.u.
M06-2X free energy in solution:	-1406.95965649	a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.85412500	0.23052700	-0.58258100
O	1.16221900	2.49939500	-0.86869800
O	-0.81822000	1.54419600	-1.01684600
N	1.07333500	-2.55381500	-1.22261000
N	-0.83885900	-2.29607600	-0.16488400
C	0.26130300	-1.63826400	-0.62643900
C	0.60805300	-3.93099400	-1.04167900
H	0.67281100	-4.50907300	-1.96846700
H	1.20226000	-4.44775900	-0.27504400
C	-0.84475300	-3.71273600	-0.58210200
H	-1.13580500	-4.36640800	0.24487400
H	-1.56166700	-3.86137300	-1.40124800
C	2.45238600	-2.15564900	-1.57380000
C	3.43413200	-2.62093600	-0.48084200
H	3.19681400	-2.14129200	0.47349500
H	3.41140600	-3.70884100	-0.34397700
C	2.83810400	-2.78143800	-2.92646500
H	2.11739500	-2.50048600	-3.70260200
H	2.88544600	-3.87743500	-2.87937600
C	2.41343100	-0.61309200	-1.64408800
H	2.09976600	-0.29734400	-2.65944900
C	-2.04175600	-1.69593600	0.34030700
C	-2.31278700	-1.78359600	1.71972400
C	-3.51239100	-1.25133000	2.19951500
H	-3.72551200	-1.31616600	3.26464400
C	-4.44282300	-0.64252400	1.35062600
C	-4.15184800	-0.58824300	-0.01424600
H	-4.86940000	-0.13242900	-0.69369600
C	-2.96419500	-1.10632000	-0.54344100
C	-1.33649100	-2.42559500	2.67735100
H	-1.74558700	-2.43990800	3.69218700
H	-1.10069600	-3.46034800	2.40044400
H	-0.38836400	-1.87743300	2.70400700
C	-5.71897800	-0.04720300	1.89929400
H	-6.08238400	-0.60712800	2.76798500
H	-5.56372100	0.99037100	2.22377700
H	-6.51321400	-0.03635500	1.14525900
C	-2.69808400	-0.99724000	-2.02601500
H	-2.06790600	-0.12445500	-2.23007700
H	-2.18527300	-1.87783400	-2.42632100
H	-3.63613800	-0.87378400	-2.57700300
C	1.48583900	0.05179800	1.11938300
H	1.31004400	-0.83683500	1.74681800
C	2.22757800	1.14480200	1.85956900
C	1.48049000	1.63957200	3.09159200
C	3.57602300	0.64529100	2.47534600
H	2.40106900	1.98706600	1.17711700
C	2.26963400	1.73310400	4.16508000
C	3.69539600	1.33409200	3.86009900
H	3.40694200	-0.18774500	-1.46563900
H	4.45774200	-2.34606800	-0.75844700
H	3.82671900	-2.42252100	-3.23225700
C	-0.07659200	2.59982300	-1.08820200
C	-0.73397400	3.93678300	-1.44458700
H	4.34351200	2.22300800	3.81748700
H	4.42549900	0.84958500	1.81684500
C	-1.80550900	4.24530900	-0.37504800
H	-2.54764500	3.44365200	-0.32233400
H	-2.31863300	5.18349300	-0.61901200
H	-1.35158900	4.35831200	0.61672200
C	-1.41203000	3.78747500	-2.82470100
H	-0.67540100	3.56155300	-3.60535500
H	-1.91495000	4.72280200	-3.09841700
H	-2.15473200	2.98457100	-2.81090500
C	0.31469700	5.05899400	-1.48685800
H	1.09000700	4.85101000	-2.23072200
H	0.81022400	5.17632500	-0.51823100
H	-0.16741800	6.00965200	-1.74575000
H	0.43016500	1.91572100	3.05149600
H	1.95764100	2.10303900	5.13874300
H	4.13060700	0.67271300	4.62069100
H	3.52600700	-0.44220000	2.61588800

3.21-TS

B3LYP SCF energy:	-1407.83706050	a.u.
B3LYP enthalpy:	-1407.17960400	a.u.
B3LYP free energy:	-1407.28775400	a.u.
M06 SCF energy in solution:	-1407.20696736	a.u.
M06 enthalpy in solution:	-1406.54951086	a.u.
M06 free energy in solution:	-1406.65766086	a.u.
M06-2X SCF energy in solution:	-1407.50037914	a.u.
M06-2X enthalpy in solution:	-1406.84292264	a.u.
M06-2X free energy in solution:	-1406.95107264	a.u.
Imaginary frequency:	-34.3888	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.36753700	-1.06046100	-0.34669800
O	-2.35929800	-1.29832000	-0.99224700
O	-2.03292600	0.74851800	-0.21814800
N	2.37816000	-1.63211100	-1.08758800
N	2.32225900	0.52140700	-0.66054300
C	1.59071000	-0.62133200	-0.66989200
C	3.78314200	-1.22796400	-1.22828200
H	4.22724500	-1.62044100	-2.14688400
H	4.37543400	-1.59169700	-0.37760600
C	3.66834700	0.30639300	-1.23191900
H	4.43893500	0.79543500	-0.63102200
H	3.71060800	0.72208800	-2.24801700
C	1.88884700	-3.03091800	-0.98872800

C	2.48369000	-3.68265000	0.27565600
H	2.17747500	-3.13391300	1.17171800
H	3.58022500	-3.71949000	0.24729200
C	2.33822200	-3.80930500	-2.23722400
H	1.97340200	-3.32276400	-3.14879500
H	3.43023100	-3.90458000	-2.30683700
C	0.34265300	-2.92423600	-0.89821200
H	-0.08820300	-3.11290200	-1.89737600
C	1.82474900	1.84859400	-0.43928300
C	2.22715000	2.53258500	0.72401900
C	1.77871600	3.84228000	0.91648000
H	2.08337500	4.37310400	1.81620900
C	0.95066700	4.48349800	-0.00999900
C	0.58264500	3.78187300	-1.16077800
H	-0.05385900	4.26637700	-1.89825500
C	1.00411600	2.46991100	-1.39897800
C	3.12811300	1.88458400	1.74953200
H	3.10212000	2.44006300	2.69185300
H	4.17555300	1.86171100	1.41809500
H	2.82913300	0.85182900	1.95268500
C	0.44867500	5.88705600	0.23709800
H	1.14982600	6.46289100	0.85069300
H	-0.51353500	5.87356200	0.76590100
H	0.29426500	6.42895500	-0.70222700
C	0.55592200	1.75825200	-2.65302600
H	-0.31728400	1.12901700	-2.44082100
H	1.33517400	1.11187600	-3.07027200
H	0.26500200	2.47954900	-3.42339900
C	-0.18185000	-1.27627600	1.45222900
H	0.13980000	-2.24874200	1.86817900
C	-0.58082400	-0.28516600	2.52916200
C	0.42239100	-0.26078900	3.73015000
C	-1.86336500	-0.76642700	3.19292300
H	-0.71039200	0.70494200	2.08017600
C	-0.21519700	-1.12156200	4.85549300
C	-1.66107500	-1.22901200	4.42967800
H	-0.04357500	-3.71581500	-0.24018500
H	2.12221100	-4.71233200	0.36636200
H	1.92093700	-4.82120000	-2.20367900
C	-2.79263400	-0.10045800	-0.74116100
C	-4.25153700	0.21383600	-1.10316900
C	-5.16224800	-0.71199000	-0.26567500
H	-6.21483900	-0.53067000	-0.51579800
H	-4.93369800	-1.76411300	-0.45810400
H	-5.03649200	-0.52355700	0.80766500
C	-4.57483800	1.68546100	-0.80293800
H	-3.93724600	2.35866600	-1.38485000
H	-5.62137200	1.89737800	-1.05465100
H	-4.41946200	1.91811700	0.25489100
C	-4.45976100	-0.08341500	-2.60411100
H	-5.50325900	0.10647700	-2.88440900
H	-3.82433400	0.55908800	-3.22628100
H	-4.22075200	-1.12554900	-2.83357000
H	0.53628000	0.77428000	4.07061600
H	0.24748500	-2.11708100	4.92838000
H	-0.09883500	-0.65901200	5.84465600
H	1.41828900	-0.61806300	3.44563600
H	-2.43075000	-1.65415200	5.06897500
H	-2.81119700	-0.76263100	2.66357000

3.22

B3LYP SCF energy:	-1407.85065680	a.u.
B3LYP enthalpy:	-1407.19172400	a.u.
B3LYP free energy:	-1407.29781800	a.u.
M06 SCF energy in solution:	-1407.21782597	a.u.
M06 enthalpy in solution:	-1406.55889317	a.u.
M06 free energy in solution:	-1406.66498717	a.u.
M06-2X SCF energy in solution:	-1407.50981344	a.u.
M06-2X enthalpy in solution:	-1406.85088064	a.u.
M06-2X free energy in solution:	-1406.95697464	a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.20555900	-1.25313700	-0.19094200
O	-1.30204700	-2.83335000	0.48079900
O	-1.93616100	-0.89515500	-0.35496100
N	2.35071700	-0.11254700	-1.72001100
N	1.05498900	1.56949200	-1.14741600
C	1.22182400	0.21513700	-1.03246000
C	3.09888900	1.05291300	-2.19129900
H	3.45048000	0.92485300	-3.21937800
H	3.97427000	1.24123600	-1.55289400
C	2.04867300	2.16821000	-2.06119900
H	2.45785300	3.09442300	-1.64837300
H	1.57696800	2.40367400	-3.02555200
C	2.87382100	-1.48990600	-1.63513900
C	4.02472300	-1.56311400	-0.61379500
H	3.66401000	-1.31229600	0.38733400
H	4.84574100	-0.88374100	-0.87437200
C	3.37870600	-1.93371400	-3.02108700
H	2.59077200	-1.82318800	-3.77467900
H	4.25566600	-1.36083600	-3.34999700
C	1.67167500	-2.33619400	-1.16692600
H	1.07457500	-2.64600600	-2.04865700
C	-0.12243500	2.31614300	-0.80734100
C	-0.04640300	3.27577800	0.22229800
C	-1.19087900	4.01666800	0.53340700
H	-1.13705600	4.75047300	1.33538600
C	-2.39212900	3.84845400	-0.16079700
C	-2.41940100	2.92857500	-1.21198700
H	-3.33452300	2.80683200	-1.78829800
C	-1.30389400	2.15967300	-1.55954500
C	1.24313100	3.56106500	0.95665400
H	1.04450400	3.94578900	1.96151900
H	1.83689600	4.32233900	0.43055500
H	1.86495800	2.66894100	1.05186400
C	-3.62682800	4.63354300	0.21707800
H	-3.36815100	5.59446700	0.67478300
H	-4.23977500	4.08172700	0.94220600
H	-4.25869900	4.83183200	-0.65555100
C	-1.40245100	1.20364000	-2.72500200
H	-1.72348600	0.21581700	-2.37850800
H	-0.44809300	1.08217600	-3.24678700

H	-2.14050900	1.56312700	-3.45011800
C	0.92737300	-1.09821700	1.47052100
H	0.58656300	-1.92576500	2.12112600
C	1.73230600	-0.06628900	2.21986000
C	2.77398700	-0.68797300	3.20721900
C	0.86049300	0.76283300	3.15681800
H	2.23152400	0.59812800	1.50092800
C	2.71839300	0.17256000	4.49704200
C	1.38851700	0.87919500	4.37799500
H	2.00497000	-3.25043400	-0.66506600
H	4.43444600	-2.57890800	-0.58524300
H	3.67006600	-2.98886600	-2.98518900
C	-3.70924500	-2.42594900	0.29813100
C	-2.23261900	-2.05159200	0.13833400
H	2.47090000	-1.71557100	3.44122800
H	3.54211300	0.90205900	4.53871900
H	-0.06733900	1.21333100	2.81681300
H	0.95111900	1.45004300	5.19339900
H	3.77686900	-0.73844400	2.77167700
H	2.80165700	-0.43509100	5.40725600
C	-3.84723400	-3.85768300	0.83835900
H	-4.90820300	-4.11236600	0.95084400
H	-3.38800400	-4.58427500	0.16069500
H	-3.36098600	-3.96262700	1.81278900
C	-4.34809500	-1.41940900	1.28201100
H	-4.24179600	-0.39397400	0.91626200
H	-5.41572800	-1.64015600	1.40220600
H	-3.87744500	-1.48160500	2.27041100
C	-4.39663000	-2.30592900	-1.07959600
H	-3.96110200	-3.00723900	-1.80178100
H	-5.46417600	-2.53943300	-0.98712800
H	-4.29633900	-1.29348500	-1.48104600

3.23-TS

B3LYP SCF energy:	-1407.79353680	a.u.
B3LYP enthalpy:	-1407.13613500	a.u.
B3LYP free energy:	-1407.24384000	a.u.
M06 SCF energy in solution:	-1407.16478981	a.u.
M06 enthalpy in solution:	-1406.50738801	a.u.
M06 free energy in solution:	-1406.61509301	a.u.
M06-2X SCF energy in solution:	-1407.45461519	a.u.
M06-2X enthalpy in solution:	-1406.79721339	a.u.
M06-2X free energy in solution:	-1406.90491839	a.u.
Imaginary frequency:	-28.1822	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	1.06393700	-0.13821600	-0.35185200
O	0.46303800	-1.37620500	-1.90617600
O	-0.66942200	-1.58719900	-0.04571500
N	0.42644900	2.79933200	-0.69073200
N	-1.38923900	2.05842600	0.26501500
C	-0.19638800	1.68884900	-0.25953500
C	-0.28776400	4.04448600	-0.36673700
H	-0.40545400	4.67692100	-1.25153700
H	0.25895600	4.62180300	0.39027000
C	-1.63434000	3.51562600	0.16494200
H	-1.90125200	3.92743800	1.14375400
H	-2.46084800	3.72136100	-0.52481300
C	1.81546700	2.72670400	-1.19338700
C	2.79068800	3.12832600	-0.06755700
H	2.71493700	2.43038100	0.77400100
H	2.59683600	4.14215600	0.30455900
C	1.98081300	3.68393000	-2.38887700
H	1.24397800	3.46078800	-3.16833500
H	1.87771000	4.73912400	-2.10250500
C	2.03362700	1.26112100	-1.61411700
H	1.54492200	1.08559300	-2.58288100
C	-2.38881800	1.19285300	0.81958100
C	-2.25714700	0.75270700	2.15055700
C	-3.27022500	-0.03936900	2.69400000
H	-3.17112600	-0.38342100	3.72179700
C	-4.40275600	-0.40209900	1.95598100
C	-4.50074200	0.04671700	0.63745500
H	-5.36887700	-0.23198400	0.04350700
C	-3.50926400	0.84106900	0.04832800
C	-1.04078400	1.10072000	2.97423000
H	-1.19612300	0.84167000	4.02609400
H	-0.79520500	2.16761200	2.91834500
H	-0.16172300	0.54836500	2.61845300
C	-5.48314200	-1.25931100	2.57423200
H	-5.92004700	-0.77750300	3.45808900
H	-5.08511500	-2.22797300	2.90072600
H	-6.29419600	-1.45372000	1.86532300
C	-3.65511000	1.28700100	-1.38821500
H	-2.70268800	1.22839200	-1.92482700
H	-4.01135200	2.32361400	-1.46336900
H	-4.38180900	0.66030400	-1.91401600
C	2.67712300	-1.01107700	-0.14008100
H	3.33452800	-1.41145800	-0.93209300
C	3.31815100	-1.04282600	1.22994600
C	4.76818100	-0.46114500	1.29383200
C	3.51703300	-2.46345100	1.74726400
H	2.66378300	-0.50335000	1.94403100
C	5.55793500	-1.38107500	2.26145500
C	4.72348300	-2.64112900	2.29085900
H	3.10851500	1.10411700	-1.75716200
H	3.82190700	3.10258700	-0.43643500
H	2.97885700	3.55691500	-2.82098800
C	-1.29827900	-3.07180900	-1.88266900
C	-0.46590600	-1.96069200	-1.23986000
H	5.21248400	-0.51594700	0.29272800
H	5.63530900	-0.94591500	3.26995600
H	2.72631500	-3.20583700	1.69104200
H	5.06828600	-3.56363700	2.75143700
H	4.77786200	0.59049300	1.59716300
H	6.58759200	-1.55596200	1.92354900
C	-0.74271600	-3.44239600	-3.26740300
H	-1.35415800	-4.23737200	-3.71161900
H	-0.75081000	-2.58235900	-3.94385700
H	0.28959200	-3.80025100	-3.19950600
C	-1.26295600	-4.29794100	-0.94493200
H	-1.63587500	-4.03887600	0.04978700
H	-1.88616900	-5.10126000	-1.35626200

H	-0.24215900	-4.68340000	-0.83779600
C	-2.75166800	-2.56329300	-2.01140200
H	-2.80775800	-1.69987600	-2.68508500
H	-3.38863900	-3.35491100	-2.42477000
H	-3.15061000	-2.26514900	-1.03748800

3.24

B3LYP SCF energy:	-1407.79494940	a.u.
B3LYP enthalpy:	-1407.13654600	a.u.
B3LYP free energy:	-1407.24659200	a.u.
M06 SCF energy in solution:	-1407.16598773	a.u.
M06 enthalpy in solution:	-1406.50758433	a.u.
M06 free energy in solution:	-1406.61763033	a.u.
M06-2X SCF energy in solution:	-1407.45618224	a.u.
M06-2X enthalpy in solution:	-1406.79777884	a.u.
M06-2X free energy in solution:	-1406.90782484	a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	1.13898700	0.01137400	-0.17859200
O	0.41240800	-1.05457900	-1.79339800
O	-0.49106200	-1.56695500	0.13247800
N	0.21451500	2.86874800	-0.46673500
N	-1.61341600	1.91371200	0.23782800
C	-0.32835100	1.68619400	-0.13040100
C	-0.69486400	4.01555900	-0.31727600
H	-0.87238200	4.50024000	-1.28391600
H	-0.27790300	4.76791500	0.36224400
C	-1.96563300	3.35275900	0.24857900
H	-2.19368600	3.67566400	1.27201900
H	-2.84924300	3.54500700	-0.36735900
C	1.65138500	2.97727500	-0.79779900
C	2.42154900	3.44133400	0.45720500
H	2.34410700	2.69223200	1.25456900
H	2.04080300	4.39448200	0.84531900
C	1.84315600	4.00163700	-1.93212300
H	1.24514500	3.72669600	-2.80800000
H	1.57209100	5.02232100	-1.63079000
C	2.11561900	1.57151500	-1.23149700
H	1.83299800	1.40222900	-2.28022800
C	-2.56013700	0.95077200	0.71763600
C	-2.45365500	0.45728500	2.03116200
C	-3.43385400	-0.42514300	2.49264900
H	-3.35539800	-0.80871900	3.50801500
C	-4.50697500	-0.82691100	1.69133500
C	-4.58566600	-0.31735300	0.39222100
H	-5.41340800	-0.61640300	-0.24805200
C	-3.62752800	0.56753300	-0.11481500
C	-1.30322800	0.84452900	2.92850000
H	-1.50838600	0.56309800	3.96611800
H	-1.10094600	1.92142800	2.90111100
H	-0.38331700	0.33415300	2.61601000
C	-5.53578300	-1.80602400	2.20791400
H	-5.72940700	-1.65812500	3.27615300
H	-5.19404000	-2.84186200	2.08129200
H	-6.48704100	-1.70846500	1.67401500
C	-3.75163200	1.08573400	-1.52937300
H	-2.78240300	1.10000500	-2.03797600
H	-4.15098300	2.10883100	-1.55968500
H	-4.43529200	0.45976800	-2.11124700
C	2.66890300	-1.05017000	-0.13692300
H	3.00536300	-1.73046900	-0.94032000
C	3.65557300	-1.00097000	1.00461600
C	5.12101100	-0.66850300	0.56837400
C	3.82575000	-2.34707700	1.69995700
H	3.31084200	-0.26084200	1.75282500
C	6.04026800	-1.55050100	1.45354000
C	5.10791000	-2.63927700	1.93224600
H	3.21016300	1.55255200	-1.18505400
H	3.48315000	3.57871400	0.22301000
H	2.89564900	4.01591500	-2.23367400
C	-1.18433300	-2.88674100	-1.82151200
C	-0.40207300	-1.78056900	-1.10979500
H	5.24699300	-0.95083100	-0.48378000
H	6.44899700	-0.98886900	2.30779800
H	2.97201900	-2.95225100	1.99119500
H	5.45882800	-3.52934600	2.44863200
H	5.34180000	0.40016600	0.64845600
H	6.90450300	-1.93771800	0.89869500
C	-0.16635400	-3.96450400	-2.26366600
H	-0.68571600	-4.77536200	-2.78896100
H	0.58600700	-3.54126600	-2.93617200
H	0.35019700	-4.39776600	-1.39921100
C	-2.22194200	-3.49967000	-0.86793100
H	-2.93706800	-2.74619300	-0.52348200
H	-2.77483800	-4.29469000	-1.38354700
H	-1.74124100	-3.92903600	0.01601600
C	-1.87879300	-2.29579100	-3.06610100
H	-1.15247800	-1.83077300	-3.73863800
H	-2.40328000	-3.08844500	-3.61345600
H	-2.61702900	-1.53694900	-2.78250500

3.25-TS

B3LYP SCF energy:	-1407.79368580	a.u.
B3LYP enthalpy:	-1407.13606000	a.u.
B3LYP free energy:	-1407.24154700	a.u.
M06 SCF energy in solution:	-1407.16244359	a.u.
M06 enthalpy in solution:	-1406.50481779	a.u.
M06 free energy in solution:	-1406.61030479	a.u.
M06-2X SCF energy in solution:	-1407.45280205	a.u.
M06-2X enthalpy in solution:	-1406.79517625	a.u.
M06-2X free energy in solution:	-1406.90066325	a.u.
Imaginary frequency:	-71.9696	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	-1.12656300	0.09936600	0.08168100
O	-0.54259200	-0.80892200	1.84257600
O	0.43878400	-1.58215000	0.04659900
N	-0.03938700	2.89148100	0.33163200
N	1.73733300	1.78006000	-0.27670600
C	0.41756100	1.66439600	0.03009200
C	1.01445700	3.92005800	0.35189600
H	1.26032200	4.19727400	1.38520600
H	0.70733500	4.82585900	-0.17861900
C	2.17572700	3.19278900	-0.33885500
H	2.29764300	3.49952500	-1.38719900
H	3.13237300	3.33693600	0.16933700
C	-1.44375000	3.14073700	0.72994500
C	-2.08583700	4.07168300	-0.32007600
H	-2.10826900	3.58316000	-1.30118600
H	-1.54778400	5.02262700	-0.42163800
C	-1.46109100	3.82554400	2.11099400
H	-0.97621500	3.18876300	2.85947000
H	-0.95877900	4.80163400	2.10416600
C	-2.20070600	1.78136500	0.78453900
H	-2.47696500	1.56216100	1.82327000
C	2.59258800	0.75363200	-0.79575200
C	2.38685400	0.24418700	-2.09180300
C	3.28107600	-0.71170100	-2.58176900
H	3.12455900	-1.10812200	-3.58314100
C	4.36506500	-1.17031400	-1.82776700
C	4.54753900	-0.63873900	-0.54821500
H	5.38686500	-0.97934400	0.05525500
C	3.67823900	0.31815800	-0.01352100
C	1.22363000	0.68928400	-2.94487200
H	1.37710600	0.40177500	-3.98982500
H	1.07185300	1.77380500	-2.90802200
H	0.29244400	0.22035600	-2.59984800
C	5.29474100	-2.23030600	-2.37159400
H	5.42120800	-2.13535100	-3.45575400
H	4.90146700	-3.23719700	-2.17829100
H	6.28540700	-2.17278400	-1.90815100
C	3.91610800	0.85595000	1.37860300
H	2.97707000	0.97354800	1.92838700
H	4.40859700	1.83821200	1.36263600
H	4.56627700	0.18314300	1.94647900
C	-2.67099100	-0.95938200	0.05712200
H	-2.99083400	-1.61980000	0.88418400
C	-3.66858200	-0.97803100	-1.07415700
C	-5.13459000	-0.65431600	-0.63096900
C	-3.82249700	-2.35810200	-1.70393000
H	-3.34830100	-0.26587600	-1.85789600
C	-6.04853600	-1.59391000	-1.46092600
C	-5.10179600	-2.68525500	-1.90311300
H	-3.14358400	1.89731000	0.23235400
H	-3.11628800	4.30608600	-0.03191400
H	-2.49703400	3.99001100	2.42516000
C	0.95895200	-2.69002700	2.17790300
C	0.27163600	-1.64472400	1.29627500
H	-5.24009800	-0.89014400	0.43476100
H	-6.48097500	-1.08049100	-2.33362600
H	-2.96166100	-2.96034800	-1.98004900
H	-5.44204500	-3.60473100	-2.37302900
H	-5.37775200	0.40500800	-0.75623500
H	-6.89666400	-1.97152800	-0.87541200
C	-0.12848400	-3.67921600	2.65963300
H	0.32239000	-4.44689700	3.30055300
H	-0.90427700	-3.16132700	3.23183200
H	-0.60544200	-4.18438100	1.81168600
C	2.03202800	-3.43957100	1.37233200
H	2.79830100	-2.75499200	0.99526300
H	2.51726300	-4.18848300	2.01025500
H	1.59382600	-3.95033500	0.50987800
C	1.59100900	-1.98880800	3.39824200
H	0.83822100	-1.43697500	3.96821200
H	2.05364300	-2.73219300	4.05881100
H	2.37032200	-1.28249400	3.08926600

3.26

B3LYP SCF energy:	-1407.79965980	a.u.
B3LYP enthalpy:	-1407.14136300	a.u.
B3LYP free energy:	-1407.24908400	a.u.
M06 SCF energy in solution:	-1407.16865257	a.u.
M06 enthalpy in solution:	-1406.51035577	a.u.
M06 free energy in solution:	-1406.61807677	a.u.
M06-2X SCF energy in solution:	-1407.45875404	a.u.
M06-2X enthalpy in solution:	-1406.80045724	a.u.
M06-2X free energy in solution:	-1406.90817824	a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-1.12339900	0.18286200	-0.04522700
O	-0.71415500	-0.54847900	1.84621400
O	0.31271700	-1.60247200	0.22797900
N	0.17157900	2.88673700	0.17519700
N	1.88848800	1.64789000	-0.35848900
C	0.55603600	1.62604300	-0.10230100
C	1.30167300	3.82027500	0.29815200
H	1.52594800	4.02061500	1.35547600
H	1.09594700	4.77399600	-0.19441500
C	2.42478500	3.02907700	-0.38649000
H	2.57876000	3.34655800	-1.42735300
H	3.38160300	3.09787000	0.13629600
C	-1.18789400	3.13430700	0.70755300
C	-1.65566600	4.53686700	0.27826300
H	-1.60136000	4.65222400	-0.81046600
H	-1.06473700	5.33711400	0.74281200
C	-1.16530100	3.03297100	2.24738600
H	-0.88047300	2.02275600	2.55523100
H	-0.46609700	3.75392000	2.69000500
C	-2.08879500	2.03420500	0.11440800
H	-3.03957400	2.03523500	0.65694800
C	2.67569300	0.56285700	-0.86588400
C	2.44306900	0.05829200	-2.15941700
C	3.26428500	-0.97058500	-2.63024800
H	3.08744400	-1.36317000	-3.62972100
C	4.30242100	-1.50409300	-1.86163000
C	4.51544800	-0.97323300	-0.58656600

H	5.32037100	-1.37116900	0.02845600
C	3.71863600	0.05334500	-0.06967000
C	1.33289100	0.58877500	-3.03498300
H	1.48939000	0.29436300	-4.07755700
H	1.25871500	1.68104200	-2.99615000
H	0.36105400	0.18901600	-2.71629800
C	5.15186100	-2.63922300	-2.38454200
H	5.26481100	-2.58763800	-3.47299700
H	4.69847800	-3.61176300	-2.15109700
H	6.15232700	-2.63123600	-1.93877800
C	3.98952800	0.58666200	1.31814900
H	3.05961900	0.81083000	1.84996900
H	4.58237500	1.51179200	1.29490400
H	4.55715800	-0.14025400	1.90736600
C	-2.72755700	-0.78318000	-0.05227200
H	-3.07895900	-1.37271000	0.81504300
C	-3.71634000	-0.85753100	-1.18922400
C	-5.17521900	-0.46260700	-0.78165300
C	-3.90401900	-2.27838300	-1.70999400
H	-3.37193200	-0.21704100	-2.02096600
C	-6.11092000	-1.44286300	-1.53717100
C	-5.19057400	-2.58820900	-1.88919800
H	-2.31697400	2.29301900	-0.94120400
H	-2.69750100	4.68025600	0.58271000
H	-2.16052900	3.24916500	2.65203000
C	0.64755700	-2.45283400	2.50706600
C	0.07465600	-1.49329000	1.46100400
H	-5.29079100	-0.60817100	0.29916700
H	-6.53056400	-0.98988100	-2.44874000
H	-3.05801700	-2.92187600	-1.93422600
H	-5.55244100	-3.53278300	-2.28785000
H	-5.38947800	0.58886800	-0.99443100
H	-6.96844700	-1.75306400	-0.92615900
C	-0.51492800	-3.34432400	3.00443800
H	-0.14995200	-4.04656300	3.76394100
H	-1.31221500	-2.73931300	3.44720000
H	-0.94283700	-3.92841600	2.18145300
C	1.74574400	-3.32347200	1.87573100
H	2.56381600	-2.71036000	1.48403300
H	2.15455400	-4.00972700	2.62761900
H	1.35164700	-3.91392600	1.04371500
C	1.21413800	-1.64097900	3.69001500
H	0.44563300	-1.00084500	4.13241600
H	1.59013900	-2.31984200	4.46510700
H	2.04644100	-1.00285700	3.37045900

3.27-TS

B3LYP SCF energy:	-1407.77345110	a.u.
B3LYP enthalpy:	-1407.11649800	a.u.
B3LYP free energy:	-1407.22339100	a.u.
M06 SCF energy in solution:	-1407.14177747	a.u.
M06 enthalpy in solution:	-1406.48482437	a.u.
M06 free energy in solution:	-1406.59171737	a.u.
M06-2X SCF energy in solution:	-1407.42986674	a.u.
M06-2X enthalpy in solution:	-1406.77291364	a.u.
M06-2X free energy in solution:	-1406.87980664	a.u.
Imaginary frequency:	-189.4792	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	1.16855700	0.27838500	-0.26111900
O	0.10512800	-1.32131300	0.67303700
O	-0.07863300	-0.99354300	-1.45775200
N	0.06503000	3.07108600	0.05262500
N	-1.74139000	1.85165000	0.08115700
C	-0.38645200	1.79821000	0.00085800
C	-1.00534500	4.07811400	0.00707200
H	-0.85085700	4.86644100	0.74901500
H	-1.05344700	4.54880600	-0.98442500
C	-2.24695600	3.22683300	0.29690100
H	-3.08695800	3.44407200	-0.36935800
H	-2.59781800	3.34030300	1.33142600
C	1.48240300	3.37954700	-0.22487500
C	1.65026900	3.75756200	-1.71242600
H	1.33825000	2.92462400	-2.35096700
H	1.06511700	4.64624300	-1.97965200
C	1.92943400	4.55892800	0.66232800
H	1.75215600	4.33595600	1.72058100
H	1.41344700	5.49578500	0.41371100
C	2.27630300	2.10402000	0.09228400
H	2.44680600	2.03018600	1.17925700
C	-2.66746000	0.77382900	0.27308500
C	-3.47147400	0.37540200	-0.81009900
C	-4.48991200	-0.55562600	-0.57722700
H	-5.12349900	-0.85869600	-1.40851400
C	-4.71750300	-1.09955300	0.69140000
C	-3.88289000	-0.70058600	1.74081800
H	-4.03963900	-1.11765000	2.73370200
C	-2.85321500	0.22925200	1.55759800
C	-3.22900200	0.91673900	-2.19898000
H	-3.94926500	0.49835500	-2.90884700
H	-3.31534100	2.00932900	-2.24096500
H	-2.22003200	0.65798500	-2.53931300
C	-5.81381100	-2.11572800	0.91581400
H	-6.63583900	-1.98222700	0.20452200
H	-5.43781400	-3.14000500	0.79035900
H	-6.22546100	-2.04414500	1.92839000
C	-1.95780900	0.61524900	2.71037000
H	-0.93794000	0.25462000	2.53660400
H	-1.90006100	1.70168300	2.84599600
H	-2.32190400	0.17924300	3.64579600
C	2.80962700	-0.66011500	-0.46714000
H	3.32418500	-0.67804600	-1.44848500
C	3.69274100	-1.32201900	0.56099900
C	4.20457000	-2.69220200	0.13292200
C	5.03217500	-0.53600300	0.77982900
H	3.14890400	-1.41268500	1.51260800
C	5.51237300	-2.84348500	0.35836800
C	6.13007600	-1.61284500	0.97938400
H	3.26469500	2.16208500	-0.37276200
H	2.70124100	3.98044900	-1.92758500
H	3.00243400	4.72961400	0.52606000
C	-0.86660200	-3.16082000	-0.62778300

C	-0.29844200	-1.75659100	-0.45821200
H	4.95693900	0.16838700	1.61312300
H	6.34756100	-1.78416200	2.04499600
C	0.34070800	-4.08116700	-0.94119500
H	-0.00856100	-5.11073100	-1.08369400
H	1.06220400	-4.07679000	-0.11693000
H	0.85260000	-3.76214500	-1.85528000
C	-1.85608700	-3.19288900	-1.80626800
H	-2.72218900	-2.55229200	-1.61240900
H	-2.21486700	-4.21795000	-1.95813900
H	-1.37981700	-2.85279500	-2.73022300
C	-1.54432600	-3.62447700	0.67317500
H	-0.84327400	-3.60388000	1.51258100
H	-1.90960000	-4.65147000	0.55242000
H	-2.39413300	-2.98373200	0.92761100
H	5.25695100	0.04636600	-0.12219200
H	7.08158800	-1.32655300	0.51305900
H	3.54375500	-3.45676400	-0.26582800
H	6.07518100	-3.75454100	0.17022700

3.28

B3LYP SCF energy:	-1407.79578130	a.u.
B3LYP enthalpy:	-1407.13756800	a.u.
B3LYP free energy:	-1407.24706100	a.u.
M06 SCF energy in solution:	-1407.16766169	a.u.
M06 enthalpy in solution:	-1406.50944839	a.u.
M06 free energy in solution:	-1406.61894139	a.u.
M06-2X SCF energy in solution:	-1407.45767233	a.u.
M06-2X enthalpy in solution:	-1406.79945903	a.u.
M06-2X free energy in solution:	-1406.90895203	a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	1.04103600	0.31469800	-0.34033900
O	0.90001700	-1.06418800	1.19806600
O	-0.36185400	-1.47460800	-0.53988500
N	-0.19738300	2.92873200	0.52590700
N	-1.97252100	1.75716600	0.04474800
C	-0.62161000	1.70640100	0.15151400
C	-1.26044800	3.94406300	0.56227300
H	-1.26073500	4.48764400	1.51182900
H	-1.12900800	4.67743600	-0.24456300
C	-2.52846900	3.09074000	0.37076200
H	-3.16815300	3.44747300	-0.44342700
H	-3.13641700	3.04450600	1.28113600
C	1.24921100	3.22962200	0.55886300
C	1.67469400	3.86037200	-0.78443900
H	1.49452600	3.16259400	-1.61145200
H	1.13155500	4.78985300	-0.99619000
C	1.54727000	4.20694900	1.71079200
H	1.19121400	3.80088600	2.66401000
H	1.08750000	5.19244700	1.55782500
C	1.95433200	1.87810500	0.76944000
H	1.83032300	1.56213400	1.81506000
C	-2.85287000	0.68244200	-0.30911500
C	-2.99163600	0.31989900	-1.66240100
C	-3.90692400	-0.68133400	-1.99391100
H	-4.01645400	-0.96468500	-3.03885400
C	-4.68084800	-1.32871500	-1.02502600
C	-4.51865900	-0.94786000	0.30921600
H	-5.10915800	-1.44081700	1.07924500
C	-3.61324800	0.04990400	0.69050500
C	-2.15924900	0.97296100	-2.73828300
H	-2.52744700	0.70301300	-3.73287700
H	-2.16362600	2.06620100	-2.65694900
H	-1.11438800	0.64656000	-2.66362100
C	-5.64289900	-2.42810800	-1.41213100
H	-6.39372800	-2.59781700	-0.63333200
H	-6.16887000	-2.19129200	-2.34401700
H	-5.11492400	-3.37745800	-1.57188400
C	-3.47175800	0.41744400	2.14999200
H	-2.43039600	0.62787900	2.41331600
H	-4.06318700	1.30654100	2.40883200
H	-3.82714900	-0.39713400	2.78882800
C	2.70540900	-0.28283100	-0.90205700
H	2.96615100	0.05866700	-1.93318300
C	3.87078100	-0.97736800	-0.25340700
C	5.20825700	-0.16817000	-0.29608100
C	4.25748400	-2.26210700	-0.97840000
H	3.59421300	-1.21642400	0.78403100
C	6.33081300	-1.20765600	-0.55307200
C	5.57809300	-2.37829200	-1.14108300
H	3.02540600	2.02488500	0.59609900
H	2.74428500	4.09738600	-0.76998800
H	2.62894900	4.35791900	1.78999700
C	-0.37917700	-3.12968600	1.27840300
C	0.05387600	-1.82854500	0.60011000
H	5.36324200	0.41572400	0.61609700
H	7.11458600	-0.82065400	-1.21716500
H	3.51649100	-2.99857700	-1.27612800
H	6.07624500	-3.23335900	-1.59139700
H	5.17032500	0.53798000	-1.13529000
H	6.83595800	-1.50319300	0.37960100
C	0.85981500	-4.05084500	1.36436400
H	0.59070700	-4.99393200	1.85537700
H	1.66283500	-3.57830900	1.93787300
H	1.24456500	-4.28915000	0.36573300
C	-1.48813300	-3.81025400	0.46063300
H	-2.36554000	-3.16306800	0.36755300
H	-1.79196900	-4.74183100	0.95380000
H	-1.14430500	-4.04991500	-0.55001100
C	-0.88026000	-2.80848700	2.70253700
H	-0.10649300	-2.30287000	3.28729600
H	-1.15758000	-3.73554500	3.21901700
H	-1.76414800	-2.16117800	2.67264400

3.29-TS

B3LYP SCF energy:	-1407.79544030	a.u.
B3LYP enthalpy:	-1407.13844900	a.u.
B3LYP free energy:	-1407.24662900	a.u.
M06 SCF energy in solution:	-1407.16687943	a.u.

M06 enthalpy in solution:	-1406.50988813	a.u.
M06 free energy in solution:	-1406.61806813	a.u.
M06-2X SCF energy in solution:	-1407.45606532	a.u.
M06-2X enthalpy in solution:	-1406.79907402	a.u.
M06-2X free energy in solution:	-1406.90725402	a.u.
Imaginary frequency:	-23.6890	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.96397400	0.08566500	-0.20726200
O	0.86427100	-1.41330900	1.22812400
O	-0.62789000	-1.53501600	-0.36610300
N	0.05657400	2.82204600	0.68705100
N	-1.81147400	1.91271200	0.02034900
C	-0.49302300	1.68296400	0.23098500
C	-0.86854900	3.96531000	0.69142000
H	-0.86094900	4.48077100	1.65623600
H	-0.59239100	4.69355400	-0.08272700
C	-2.21984700	3.28601000	0.39452600
H	-2.76869100	3.76084000	-0.42521000
H	-2.87545100	3.26741200	1.27309700
C	1.51934800	2.90874700	0.88053900
C	2.16336900	3.58071400	-0.34989900
H	1.97720700	2.99047400	-1.25410600
H	1.77780000	4.59499300	-0.51251200
C	1.82446400	3.73732400	2.14263800
H	1.31314500	3.31645700	3.01539900
H	1.52803900	4.78950100	2.03780800
C	2.00130700	1.45367800	1.03503600
H	1.75490000	1.09635600	2.04499500
C	-2.78797300	0.95580200	-0.41246200
C	-2.96231400	0.72763100	-1.78868000
C	-3.95767500	-0.16528500	-2.19533200
H	-4.09687900	-0.34565900	-3.25936400
C	-4.77269700	-0.83251800	-1.27614600
C	-4.57329500	-0.58362500	0.08508000
H	-5.19745700	-1.09344800	0.81664200
C	-3.58881100	0.30017200	0.53939400
C	-2.08504300	1.40793400	-2.81201300
H	-2.46013100	1.23122200	-3.82472900
H	-2.02963900	2.49155900	-2.65456100
H	-1.05893100	1.02274400	-2.76109200
C	-5.81821300	-1.81984300	-1.74070100
H	-6.65361200	-1.88329600	-1.03506400
H	-6.22190800	-1.54526300	-2.72128400
H	-5.39371300	-2.82819200	-1.83488600
C	-3.39873700	0.52500500	2.02190400
H	-2.33901900	0.51357700	2.29769800
H	-3.81006100	1.48948800	2.34934700
H	-3.90960200	-0.25264600	2.59811100
C	2.58703000	-0.41270500	-0.91419400
H	2.58906100	-0.17458300	-2.00778700
C	3.93489000	-0.85662500	-0.41735600
C	5.13322500	0.04377300	-0.86255200
C	4.33188900	-2.21458200	-0.98600600
H	3.88646200	-0.92992400	0.67985800
C	6.30190200	-0.92189800	-1.19133500
C	5.59911300	-2.24204400	-1.40656700
H	3.09235000	1.44599100	0.94127300
H	3.24772600	3.65654700	-0.21323900
H	2.90145500	3.71777200	2.33961400
C	-0.65404700	-3.30692400	1.33991500
C	-0.13108300	-2.02521900	0.68985000
H	5.39330200	0.78788700	-0.10336300
H	6.88241300	-0.59477300	-2.06385000
H	3.64332100	-3.05439000	-0.99272900
H	6.10218100	-3.11842400	-1.80768700
H	4.84658900	0.58980300	-1.77009500
H	7.01683800	-0.99724200	-0.35733800
C	0.48442700	-4.35208900	1.31825400
H	0.14714700	-5.28200600	1.79204300
H	1.36313800	-3.98631500	1.85765400
H	0.78502700	-4.58735000	0.29045000
C	-1.87428200	-3.83396400	0.56836000
H	-2.68442300	-3.09839200	0.55407400
H	-2.24395100	-4.75147900	1.04254900
H	-1.61760300	-4.06154300	-0.47077200
C	-1.03648100	-2.99396100	2.80319600
H	-0.17868400	-2.60315600	3.35813000
H	-1.38794500	-3.90571700	3.30134200
H	-1.84203600	-2.25182000	2.85051900

*anti-(R,R)-***3.32**

B3LYP SCF energy:	-2029.73476550	a.u.
B3LYP enthalpy:	-2028.99241700	a.u.
B3LYP free energy:	-2029.11567400	a.u.
M06 SCF energy in solution:	-2028.98306278	a.u.
M06 enthalpy in solution:	-2028.24071428	a.u.
M06 free energy in solution:	-2028.36397128	a.u.
M06-2X SCF energy in solution:	-2029.38668153	a.u.
M06-2X enthalpy in solution:	-2028.64433303	a.u.
M06-2X free energy in solution:	-2028.76759003	a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.83352500	0.78331000	0.96842400
O	0.45726000	0.58023600	3.18916500
O	2.37418400	0.05392600	2.31188200
N	1.17128700	2.13573700	-1.55075100
N	2.34359700	0.27751800	-1.67486300
C	1.53506100	1.01643900	-0.87029300
C	1.58689700	2.09949900	-2.95625800
H	1.98712800	3.06218300	-3.28696600
H	0.73992600	1.83648800	-3.60423800
C	2.65245500	0.98922300	-2.93366600
H	2.59120900	0.31632300	-3.79275200
H	3.67113300	1.39815900	-2.89078600
C	0.06036700	2.92706700	-1.00745400

C	-1.28888400	2.48743100	-1.62793500
H	-1.42148800	1.40935200	-1.50066300
H	-1.28974200	2.70109200	-2.70656700
C	-2.44899000	3.24101600	-0.94863400
H	-3.39391200	2.91251800	-1.39868900
C	-2.26160700	4.75751700	-1.15310400
H	-2.28259300	5.00189400	-2.22472700
H	-3.08674500	5.31049900	-0.68347900
C	-0.91807500	5.19555100	-0.53256100
H	-0.77867900	6.27531200	-0.67478900
C	0.24279600	4.44572900	-1.23032700
H	1.21033600	4.76566700	-0.82020300
H	0.24607500	4.68690100	-2.30376800
C	-0.93184100	4.87035600	0.97728600
H	0.00228400	5.20669700	1.44809200
H	-1.75016800	5.41734400	1.46639400
C	-1.11240300	3.34208900	1.18559000
H	-1.10982800	3.11431400	2.25890000
C	0.06880800	2.63464900	0.50705500
H	1.00592800	3.08890100	0.92126200
C	-2.45012600	2.90933100	0.55705600
H	-2.60052500	1.83446400	0.69752300
H	-3.28082400	3.42738200	1.05730100
C	3.12238200	-0.86157900	-1.27440900
C	2.75125400	-2.13459100	-1.75092700
C	3.52860700	-3.23593800	-1.38286900
H	3.24452600	-4.22200300	-1.74460400
C	4.65814200	-3.10517100	-0.56776800
C	5.01498200	-1.82538200	-0.13750900
H	5.90073200	-1.69967200	0.48178200
C	4.26966400	-0.69048900	-0.47755000
C	1.54996200	-2.32616200	-2.64746700
H	1.37631200	-3.38978800	-2.83608600
H	1.68218400	-1.83907300	-3.62244200
H	0.64062800	-1.90766100	-2.20392700
C	5.46038600	-4.31679700	-0.15370200
H	5.41934200	-5.10474300	-0.91343800
H	5.07375700	-4.74462200	0.78074700
H	6.51188300	-4.06255000	0.01702700
C	4.71012900	0.66417100	0.02708100
H	4.21186000	0.90447100	0.97306800
H	4.48328500	1.46873700	-0.67925200
H	5.78925700	0.67081700	0.21143800
C	-0.40012300	-0.44435700	0.40834800
H	-0.40673500	-0.85370300	-0.61004700
N	1.64676100	0.15427600	3.39730500
O	2.08248000	-0.13199000	4.48843200
C	-1.38739000	-1.14081400	1.34602200
C	-0.77764200	-2.41865900	2.01881700
C	-2.56622900	-1.73450800	0.57693600
H	-1.71696200	-0.43247000	2.11373400
C	-1.23874000	-3.61187800	1.15505000
H	-1.19379100	-2.50725900	3.02835500
H	0.30882500	-2.35154300	2.11201500
C	-2.46290900	-3.07131200	0.44958100
H	-0.47934800	-3.91572500	0.42121900
H	-1.47118200	-4.50516800	1.74364700
C	-3.34536500	-3.98923300	-0.30365000
O	-3.19432900	-5.19615400	-0.32908300
C	-3.60116800	-0.84803600	-0.03134700
O	-3.40413500	-0.13969000	-0.99907500
O	-4.33220600	-3.35146000	-0.97667100
O	-4.75228300	-0.87375700	0.66162700
C	-5.21265000	-4.20239000	-1.72468300
H	-5.92976300	-3.53386000	-2.20209400
H	-4.65470200	-4.76690600	-2.47673300
H	-5.72376000	-4.90555600	-1.06144800
C	-5.80336700	-0.04088400	0.14379500
H	-6.65102200	-0.19447000	0.81187900
H	-5.49865100	1.00898500	0.14416500
H	-6.05688500	-0.34029900	-0.87661000

(R,R)-3.32-TS_alkylidene-rotation

B3LYP SCF energy:	-2029.71721871	a.u.
B3LYP enthalpy:	-2028.97589800	a.u.
B3LYP free energy:	-2029.09579600	a.u.
M06 SCF energy in solution:	-2028.96964356	a.u.
M06 enthalpy in solution:	-2028.22832285	a.u.
M06 free energy in solution:	-2028.34822085	a.u.
M06-2X SCF energy in solution:	-2029.37448305	a.u.
M06-2X enthalpy in solution:	-2028.63316234	a.u.
M06-2X free energy in solution:	-2028.75306034	a.u.
Imaginary frequency:	-28.9637	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.61284900	-0.32149600	0.87108900
O	0.34014700	-0.60882700	2.72270900
O	0.30106600	1.50652100	2.20271500
N	-2.94403200	-1.19036600	-0.65339600
N	-2.92693200	0.99896000	-0.81577700
C	-2.25991600	-0.07421500	-0.32615600
C	-4.05670400	-0.92036700	-1.57135300
H	-4.95512400	-1.47545600	-1.28931900
H	-3.78531900	-1.20106100	-2.59824500
C	-4.22068600	0.60215300	-1.41555700
H	-4.39228900	1.11522700	-2.36450400
H	-5.03884700	0.86241700	-0.73053000
C	-2.28451800	-2.48914500	-0.44489400
C	-1.50288800	-2.90533400	-1.71634800
H	-0.83506800	-2.09130300	-2.01685700
H	-2.20320900	-3.07663300	-2.54721200
C	-0.69706900	-4.18904700	-1.43632400
H	-0.14315400	-4.47125600	-2.34171000
C	-1.67491900	-5.31825000	-1.05189300
H	-2.36463300	-5.52260800	-1.88359400
H	-1.12245700	-6.24772100	-0.85955700
C	-2.46281700	-4.90616400	0.20877900
H	-3.16170800	-5.70681300	0.48443500
C	-3.27471900	-3.61955600	-0.08875000
H	-3.86984300	-3.32914900	0.78735100
H	-3.97650600	-3.81140900	-0.91490000
C	-1.46580000	-4.66484500	1.36444600
H	-2.00502200	-4.41228200	2.28741400

H	-0.90788800	-5.59068300	1.56449300
C	-0.49072500	-3.51736800	0.98794800
H	0.20962100	-3.33793500	1.81159000
C	-1.33275300	-2.25092600	0.74697300
H	-1.99754200	-2.14626500	1.63865400
C	0.28801700	-3.92491000	-0.27863600
H	0.99846400	-3.13641300	-0.55224600
H	0.87811900	-4.82999700	-0.07904000
C	-2.62487100	2.37808600	-0.56085700
C	-2.21647200	3.18835500	-1.63790700
C	-1.94533200	4.53796600	-1.39173400
H	-1.62293200	5.16598600	-2.21977800
C	-2.07568900	5.09859700	-0.11820600
C	-2.50891200	4.27258400	0.92323000
H	-2.63155300	4.69225800	1.91941000
C	-2.79309900	2.91750700	0.72985400
C	-2.08672600	2.64359800	-3.04183400
H	-1.38564300	3.24559000	-3.62782300
H	-3.04812200	2.66476700	-3.57402000
H	-1.73452100	1.60808000	-3.04528900
C	-1.74218600	6.55059300	0.13280100
H	-2.42705900	6.99915500	0.86081200
H	-1.79223200	7.13933700	-0.78898800
H	-0.72674000	6.65664000	0.53640600
C	-3.25696300	2.08180600	1.89972700
H	-2.40786500	1.56691600	2.36620900
H	-3.98623800	1.31976600	1.60621300
H	-3.71716800	2.71450800	2.66516100
C	0.58668900	-0.13946000	-0.49135800
H	0.73275900	-0.93254000	-1.24113300
N	0.63029000	0.62870700	3.05570500
O	1.17563900	0.87350900	4.11517600
C	1.53042700	1.03552300	-0.71022000
C	1.52995500	1.52677400	-2.19518700
C	2.98071200	0.59377100	-0.51865800
H	1.27901900	1.84153300	-0.01401200
C	2.78054700	0.90761800	-2.86284700
H	1.60101500	2.61975000	-2.19766300
H	0.60326700	1.26153000	-2.71230700
C	3.64597300	0.51736900	-1.68567000
H	2.54082100	0.02409300	-3.46990100
H	3.29538300	1.60467000	-3.53255000
C	5.04144900	0.08472800	-1.91119800
O	5.54846300	0.00538300	-3.01509900
C	3.46814600	0.21151400	0.84348700
O	3.28443400	-0.88029100	1.33784700
O	5.69694800	-0.21335500	-0.76722400
O	4.05710800	1.24494700	1.46496600
C	7.05178600	-0.65568500	-0.93045900
H	7.41508400	-0.86068400	0.07683800
H	7.08924200	-1.56006200	-1.54379100
H	7.65502000	0.12193200	-1.40720500
C	4.49417600	0.98683300	2.81554400
H	4.98792600	1.90425600	3.13640600
H	3.63660300	0.76756700	3.45561800
H	5.19126700	0.14528500	2.83237900

syn-(R,R)-**3.32**

B3LYP SCF energy: -2029.72841918 a.u.

B3LYP enthalpy: -2028.98602700 a.u.

B3LYP free energy: -2029.10758100 a.u.

M06 SCF energy in solution: -2028.97857922 a.u.

M06 enthalpy in solution: -2028.23618704 a.u.

M06 free energy in solution: -2028.35774104 a.u.

M06-2X SCF energy in solution: -2029.38135356 a.u.

M06-2X enthalpy in solution: -2028.63896138 a.u.

M06-2X free energy in solution: -2028.76051538 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.96744700	-0.13724600	1.01224200
O	0.65656000	0.62945200	3.10620600
O	0.02765300	-1.37095500	2.53482400
N	2.49790400	-1.08857900	-1.23376200
N	0.55483100	-2.10595400	-1.38090500
C	1.26999900	-1.19725000	-0.65315800
C	2.59307300	-1.78608000	-2.51692400
H	3.54028900	-2.32356100	-2.61836700
H	2.50938000	-1.07787400	-3.35363600
C	1.38014300	-2.72627200	-2.44117400
H	0.82463700	-2.79094100	-3.38077500
H	1.66579500	-3.74411100	-2.14301900
C	3.39604000	-0.02891500	-0.76950500
C	3.25108400	1.23817200	-1.64590600
H	2.19490800	1.51689100	-1.69050500
H	3.58219000	1.01951600	-2.67153000
C	4.08971800	2.38826400	-1.05582800
H	3.97351200	3.28044500	-1.68578100
C	5.57196800	1.96538100	-1.02409800
H	5.93323300	1.77399000	-2.04458200
H	6.18904500	2.77608400	-0.61373100
C	5.72395200	0.69974600	-0.15492700
H	6.77768600	0.39270900	-0.13064900
C	4.88366800	-0.45180000	-0.76291100
H	5.00502200	-1.37013200	-0.17294100
H	5.23737100	-0.66748400	-1.78213000
C	5.24465400	1.02099000	1.27826100
H	5.38191400	0.14873000	1.93173100
H	5.85564600	1.83263200	1.69754500
C	3.74835900	1.43366800	1.25353100
H	3.40762300	1.64681200	2.27364200
C	2.95571500	0.24984500	0.68206400
H	3.23570200	-0.65373100	1.27574900
C	3.59088700	2.68900300	0.37300200
H	2.53918200	2.99899900	0.34726000
H	4.16425100	3.52103300	0.80418200
C	-0.63733600	-2.79294100	-0.96475500
C	-1.83002600	-2.59417400	-1.68245600
C	-2.96178000	-3.33507600	-1.31626900
H	-3.88371000	-3.18834900	-1.87617200
C	-2.93688900	-4.25809600	-0.27036300
C	-1.72684500	-4.45383800	0.40498200
H	-1.67862700	-5.18682500	1.20762500
C	-0.56826800	-3.74965700	0.07287400

C	-1.93766300	-1.63333400	-2.84589600
H	-2.69507800	-0.86686200	-2.64498600
H	-2.24400000	-2.15896200	-3.75913000
H	-0.99213100	-1.12637900	-3.04905900
C	-4.17546800	-5.02693900	0.12754300
H	-3.94658500	-6.08017100	0.32622100
H	-4.94085900	-4.98877600	-0.65455200
H	-4.61785700	-4.61663600	1.04481600
C	0.71212200	-4.03971000	0.82152600
H	0.85381800	-3.32507500	1.63884900
H	1.59514100	-3.98605300	0.17657100
H	0.67678400	-5.04187900	1.26042500
C	0.09969700	1.29217800	0.28355200
H	0.03228700	2.13685600	0.99316100
N	0.09526300	-0.46001500	3.47508200
O	-0.32809200	-0.65992400	4.58871900
C	-0.73730800	1.51611500	-0.95847200
C	-0.33062000	2.79184200	-1.77531200
C	-2.17916500	1.84240400	-0.55812000
H	-0.69978200	0.62170400	-1.58674800
C	-1.35107500	3.89556800	-1.41605700
H	-0.39064500	2.55798800	-2.84409900
H	0.69742000	3.09852000	-1.56716700
C	-2.49089000	3.13294000	-0.78306700
H	-0.94392000	4.62753400	-0.70543100
H	-1.68515900	4.47081900	-2.28594200
C	-3.74320600	3.85192300	-0.45306200
O	-3.98498500	4.97968600	-0.84120300
C	-3.02913100	0.82532100	0.13017800
O	-2.80007600	0.39337600	1.23892200
O	-4.57911200	3.14363600	0.33798300
O	-4.05658500	0.41698400	-0.64344600
C	-5.80122000	3.80897300	0.69046000
H	-6.33040400	3.11829800	1.34745500
H	-5.59027200	4.74761600	1.20943000
H	-6.39434700	4.02277200	-0.20312800
C	-4.96471000	-0.50016100	-0.00643200
H	-5.73569500	-0.70711000	-0.74964200
H	-4.44514900	-1.41712900	0.27933000
H	-5.40202500	-0.03783800	0.88242500

anti-(R,S)-**3.32**

B3LYP SCF energy:	-2029.73039654	a.u.
B3LYP enthalpy:	-2028.98765300	a.u.
B3LYP free energy:	-2029.11252800	a.u.
M06 SCF energy in solution:	-2028.97703498	a.u.
M06 enthalpy in solution:	-2028.23429144	a.u.
M06 free energy in solution:	-2028.35916644	a.u.
M06-2X SCF energy in solution:	-2029.38181193	a.u.
M06-2X enthalpy in solution:	-2028.63906839	a.u.
M06-2X free energy in solution:	-2028.76394339	a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.96928400	-0.10506600	0.80170200
O	-0.85079500	0.54981000	2.98350700
O	-1.76965600	-1.33030500	2.39978800
N	-2.22382100	-0.11141000	-1.75410700
N	-1.33654900	-2.11018100	-1.54495400
C	-1.47482000	-0.90153800	-0.94004100
C	-2.85593600	-0.86118400	-2.84062400
H	-3.90473600	-1.09363000	-2.60372700
H	-2.83087400	-0.30772100	-3.78311800
C	-1.98291900	-2.13135300	-2.87494100
H	-1.22801200	-2.08284600	-3.66977300
H	-2.56310800	-3.04895900	-3.00679400
C	-2.64363300	1.18157600	-1.19830100
C	-2.90448200	2.24948400	-2.27890100
H	-2.01715700	2.34849200	-2.91751600
H	-3.74803000	1.96211300	-2.92518800
C	-3.22247900	3.59409000	-1.57989300
H	-3.38669700	4.36174800	-2.34746600
C	-4.49570100	3.43780800	-0.72194500
H	-5.35032500	3.15978200	-1.35508100
H	-4.74808800	4.39612000	-0.24831100
C	-4.26091200	2.36130700	0.35748100
H	-5.16995800	2.23782000	0.96073900
C	-3.92197100	1.02464600	-0.33126100
H	-3.76392200	0.23939900	0.42414600
H	-4.76407300	0.69347200	-0.95647000
C	-3.08282800	2.77470200	1.26337500
H	-2.92636500	2.02869500	2.05334700
H	-3.31532600	3.72276400	1.76804400
C	-1.80456300	2.92848100	0.41316300
H	-0.96950600	3.23253300	1.05698600
C	-1.44102700	1.62342200	-0.32007400
C	-2.04841900	4.01534200	-0.66725800
H	-1.13604100	4.15750500	-1.26129800
H	-2.28165400	4.97975800	-0.19284900
C	-0.54366600	-3.21147600	-1.07943300
C	0.75254700	-3.40600500	-1.59150900
C	1.49416900	-4.49959400	-1.12807400
H	2.50052800	-4.64978400	-1.51382700
C	0.98022900	-5.39816100	-0.19063400
C	-0.32287500	-5.19164200	0.27626100
H	-0.74821000	-5.89066400	0.99358500
C	-1.10343000	-4.11541800	-0.15353000
C	1.35146500	-2.49071300	-2.63626700
H	2.44472500	-2.50861500	-2.58593400
H	1.07340600	-2.80698200	-3.65110200
H	1.02494700	-1.45344300	-2.51699600
C	1.80456700	-6.56049900	0.31279300
H	2.71168900	-6.69685200	-0.28435400
H	2.11367900	-6.40577500	1.35452100
H	1.23565700	-7.49725100	0.28286000
C	-2.50942400	-3.94422800	0.37132600
H	-2.55916200	-3.14964400	1.12343600
H	-3.21267100	-3.68390300	-0.42775000
H	-2.85758400	-4.86946600	0.84095400
C	0.81772900	-0.18189400	0.47423300
H	1.24263900	-0.73886100	-0.37059200
N	-1.44742200	-0.51116400	3.37327900
O	-1.71027400	-0.75834500	4.52744600
C	1.88183700	0.39003000	1.39992400

C	2.79472000	-0.71830200	2.02068600
C	2.88542700	1.20811600	0.59064700
H	1.41004600	0.99573700	2.18009700
C	4.04850200	-0.79019400	1.11954300
H	3.07921500	-0.40587900	3.03163500
H	2.27295600	-1.67586500	2.10564300
C	4.05080500	0.55506900	0.42531700
H	3.98642600	-1.59992500	0.37969800
H	4.97256800	-0.95995700	1.68179000
C	5.23171400	0.98384800	-0.35333600
O	6.23285200	0.30489100	-0.48563100
C	2.47702300	2.51742500	-0.00301000
O	1.82653700	2.63168100	-1.02160100
O	5.08698800	2.20999000	-0.90860000
O	2.85392400	3.54863800	0.77311000
C	6.20458100	2.66854800	-1.68255400
H	5.91638200	3.65045900	-2.05904100
H	6.40575400	1.98357200	-2.51066300
H	7.09956000	2.74279200	-1.05862800
C	2.47434900	4.85084200	0.29625500
H	2.85985900	5.55404700	1.03469700
H	1.38660000	4.93009000	0.22022800
H	2.91748400	5.03986300	-0.68507600
H	-0.60968000	1.83535800	-0.99590600

(R,S)-3.32-TS1_alkylidene-rotation

B3LYP SCF energy:	-2029.71966860	a.u.
B3LYP enthalpy:	-2028.97811800	a.u.
B3LYP free energy:	-2029.09745500	a.u.
M06 SCF energy in solution:	-2028.97135449	a.u.
M06 enthalpy in solution:	-2028.22980389	a.u.
M06 free energy in solution:	-2028.34914089	a.u.
M06-2X SCF energy in solution:	-2029.37710195	a.u.
M06-2X enthalpy in solution:	-2028.63555135	a.u.
M06-2X free energy in solution:	-2028.75488835	a.u.
Imaginary frequency:	-14.8333	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.71533900	-0.33197600	0.51227300
O	0.28469000	-1.53497000	2.19450200
O	-0.55276300	0.46533400	2.40251600
N	3.11559900	0.37168700	-0.90842000
N	2.08798100	2.28673500	-0.60068300
C	1.99078700	0.94469000	-0.43751200
C	4.15355600	1.34594800	-1.26022900
H	4.95632500	1.34349200	-0.51075900
H	4.59637100	1.12285100	-2.23468300
C	3.35827200	2.66952700	-1.25814300
H	3.17172900	3.03541000	-2.27406000
H	3.85233400	3.46583700	-0.69388300
C	3.28923200	-1.07794500	-0.71959200
C	4.07127000	-1.74024500	-1.87252200
H	3.58009000	-1.51479600	-2.82856700
H	5.10094600	-1.35500300	-1.93190900
C	4.10498000	-3.26873600	-1.62643300
H	4.63624500	-3.74839900	-2.45912100
C	4.84814200	-3.55340200	-0.30477900
H	5.87990700	-3.17700800	-0.35933100
H	4.91145500	-4.63686900	-0.13727600
C	4.09391200	-2.88414000	0.86214000
H	4.62667500	-3.07211500	1.80378700
C	4.02757200	-1.36379000	0.61365000
H	3.49507300	-0.87073500	1.44041000
H	5.04127700	-0.93733000	0.58378100
C	2.65791500	-3.43889400	0.94925300
H	2.12736600	-2.99525500	1.79792900
H	2.69008900	-4.52335100	1.12480100
C	1.90753800	-3.14533000	-0.36639700
H	0.88869200	-3.54643800	-0.30415500
C	1.84205700	-1.63329300	-0.67273200
C	2.66842100	-3.83141000	-1.53162500
H	2.13530900	-3.66895000	-2.47838400
H	2.71175900	-4.91831400	-1.37218700
C	1.11495100	3.26793600	-0.21933100
C	0.34717600	3.90364300	-1.21347100
C	-0.57661100	4.87868400	-0.82103900
H	-1.17706100	5.36792100	-1.58540000
C	-0.74957100	5.23782200	0.51807300
C	0.04783300	4.60588000	1.47770300
H	-0.05828300	4.88383700	2.52418100
C	0.98717900	3.62816700	1.13774900
C	0.50688400	3.57500200	-2.68036200
H	-0.40571300	3.81830100	-3.23275100
H	1.32030900	4.15478700	-3.13777200
H	0.72898900	2.51527200	-2.83996600
C	-1.77664200	6.26896900	0.92422800
H	-2.67911500	5.79020800	1.32616700
H	-1.39012700	6.93314200	1.70543500
H	-2.08320200	6.88718800	0.07429900
C	1.82689200	2.99092200	2.21918500
H	1.39960800	2.02893800	2.52516000
H	2.85483400	2.80866400	1.88791900
H	1.86284100	3.63293000	3.10480100
C	-0.62071100	-0.20266500	-0.71419400
H	-0.55347600	-0.73481600	-1.67997400
N	-0.39066100	-0.67926200	2.92703100
O	-0.81169300	-0.99488200	4.02215400
C	-1.95077700	0.51146300	-0.52770600
C	-2.36355400	1.33719600	-1.79054700
C	-3.09111800	-0.50172500	-0.41882000
H	-1.90596300	1.13513300	0.37084000
C	-3.40632100	0.48629400	-2.55352500
H	-2.80855800	2.28085300	-1.45851300
H	-1.49831000	1.58827100	-2.40901000
C	-3.86395400	-0.51713800	-1.51974000
H	-2.97505100	-0.02990500	-3.42178800
H	-4.24229600	1.08009500	-2.93843200
H	1.44311400	-1.53305700	-1.69684200
C	-5.02408700	-1.38841000	-1.80572000
O	-5.66536900	-1.33253100	-2.83883900
C	-3.18517300	-1.39142200	0.77961100
O	-2.50238300	-2.38204500	0.93195700
O	-5.29743300	-2.25584400	-0.80575300

O	-4.05561900	-0.91527400	1.68385100
C	-6.40590300	-3.13611400	-1.03943000
H	-7.32874000	-2.56486000	-1.17330200
H	-6.23187900	-3.74362900	-1.93162200
H	-6.46938400	-3.76700800	-0.15252900
C	-4.15974200	-1.67998200	2.90241400
H	-4.45497700	-2.70831100	2.67872800
H	-3.20506500	-1.68004600	3.43331300
H	-4.92737000	-1.17739400	3.49114400

*int-(R,S)-***3.32**

B3LYP SCF energy:	-2029.71983315	a.u.
B3LYP enthalpy:	-2028.97736500	a.u.
B3LYP free energy:	-2029.10047100	a.u.
M06 SCF energy in solution:	-2028.97215987	a.u.
M06 enthalpy in solution:	-2028.22969172	a.u.
M06 free energy in solution:	-2028.35279772	a.u.
M06-2X SCF energy in solution:	-2029.37843408	a.u.
M06-2X enthalpy in solution:	-2028.63596593	a.u.
M06-2X free energy in solution:	-2028.75907193	a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.79533500	-0.37281600	0.45275100
O	0.56182200	-1.66290400	2.10410000
O	-0.68059600	0.11515400	2.30068500
N	3.10827500	0.82966100	-0.72581300
N	1.73387300	2.51766800	-0.44143700
C	1.86646200	1.17357600	-0.33268200
C	3.97781600	1.98528900	-0.96878900
H	4.72399900	2.08431700	-0.16934600
H	4.50927500	1.88926000	-1.91960700
C	2.96397200	3.15043700	-0.96917100
H	2.79251600	3.54449100	-1.97693700
H	3.26750500	3.98143700	-0.32552600
C	3.52001400	-0.58001600	-0.61202200
C	4.49397000	-1.00565900	-1.72982200
H	4.04489300	-0.79738200	-2.71010000
H	5.43900600	-0.44385000	-1.67268500
C	4.78450700	-2.51857900	-1.57651500
H	5.45531100	-2.83257400	-2.38709700
C	5.46466200	-2.76828700	-0.21455300
H	6.41167000	-2.21245800	-0.15593200
H	5.71168900	-3.83304000	-0.10899700
C	4.51573400	-2.33323200	0.92073800
H	5.00078600	-2.49613400	1.89223300
C	4.19350200	-0.83396600	0.76144800
H	3.51918700	-0.50657100	1.56648600
H	5.11196100	-0.23442300	0.84733700
C	3.20254800	-3.13828300	0.84583400
H	2.53903200	-2.86402800	1.67184100
H	3.41962200	-4.21041900	0.95202900
C	2.51287000	-2.87820900	-0.50951100
H	1.58241200	-3.45717200	-0.56281000
C	2.19545900	-1.38215800	-0.72411800
C	3.46978500	-3.32833300	-1.64522100
H	2.98914700	-3.18714400	-2.62307100
H	3.69537300	-4.40026300	-1.55199400
C	0.56992800	3.29614200	-0.13212200
C	-0.21230800	3.81336700	-1.18306200
C	-1.32650000	4.59602900	-0.86216100
H	-1.93629400	4.99390400	-1.67087900
C	-1.67547900	4.87908000	0.46142300
C	-0.86161300	4.37301000	1.47950100
H	-1.10420300	4.59853100	2.51579000
C	0.26492500	3.58850100	1.21234800
C	0.12992500	3.56297200	-2.63436300
H	-0.75915200	3.66414000	-3.26392200
H	0.86826700	4.28685500	-3.00576700
H	0.54384900	2.56206600	-2.78999000
C	-2.90470200	5.69538700	0.78631400
H	-3.75939800	5.04587400	1.01684600
H	-2.74092300	6.33527600	1.66024900
H	-3.19631100	6.33446400	-0.05357500
C	1.11124600	3.08264600	2.35614900
H	0.83435400	2.05528300	2.61878900
H	2.17852000	3.08626000	2.11062700
H	0.96378800	3.70360300	3.24528900
C	-0.52333000	-0.41762700	-0.79602000
H	-0.40629000	-1.06707300	-1.68222100
N	-0.29949000	-0.97651300	2.82193300
O	-0.67212500	-1.38595600	3.90219700
C	-1.88560900	0.25450400	-0.73079900
C	-2.29623300	0.87928400	-2.10429100
C	-2.98844600	-0.78237100	-0.51167400
H	-1.89007100	0.99722200	0.07321500
C	-3.24907500	-0.13434600	-2.77923100
H	-2.81880900	1.82219800	-1.91237100
H	-1.42440200	1.11019500	-2.72247000
C	-3.71255600	-0.99478400	-1.62550400
H	-2.74221700	-0.74924500	-3.53517500
H	-4.08968500	0.34546900	-3.29165500
H	1.85400800	-1.27177300	-1.76756700
C	-4.82377700	-1.95051700	-1.82004800
O	-5.40606400	-2.09501700	-2.87924600
C	-3.10105200	-1.48850000	0.80182600
O	-2.41900800	-2.44315800	1.10921800
O	-5.12632600	-2.64807000	-0.70250000
O	-3.99288800	-0.89259600	1.60744200
C	-6.18530500	-3.60573600	-0.84072800
H	-7.11871100	-3.10910300	-1.12011300
H	-5.93507600	-4.34704500	-1.60441300
H	-6.27933600	-4.07959200	0.13666500
C	-4.11063900	-1.46488000	2.92640600
H	-4.41025000	-2.51379300	2.85649400
H	-3.15980800	-1.39062000	3.45829800
H	-4.88131400	-0.87701000	3.42557700

*(R,S)-***3.32-TS2_alkylidene-rotation**

B3LYP SCF energy:	-2029.71577434	a.u.
B3LYP enthalpy:	-2028.97447700	a.u.
B3LYP free energy:	-2029.09441100	a.u.

M06 SCF energy in solution:	-2028.97108924	a.u.
M06 enthalpy in solution:	-2028.22979190	a.u.
M06 free energy in solution:	-2028.34972590	a.u.
M06-2X SCF energy in solution:	-2029.37455152	a.u.
M06-2X enthalpy in solution:	-2028.63325418	a.u.
M06-2X free energy in solution:	-2028.75318818	a.u.
Imaginary frequency:	-71.0276	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.96284200	-0.44489600	0.46743500
O	0.71370800	-1.74889300	2.23187100
O	-0.35457700	0.14293300	2.27731700
N	2.86993800	1.10920100	-0.97297900
N	1.14201900	2.45226800	-0.78048900
C	1.58555500	1.19037100	-0.53392300
C	3.43501200	2.41316400	-1.32975700
H	4.09689400	2.78376400	-0.53423800
H	4.01158900	2.36114900	-2.25710700
C	2.16451300	3.27089900	-1.46947700
H	1.89076000	3.42275300	-2.52042900
H	2.25142700	4.25125100	-0.99250400
C	3.64460700	-0.08981500	-0.61316200
C	4.75240600	-0.41838600	-1.63479200
H	4.31146300	-0.51302900	-2.63599900
H	5.50516400	0.38351200	-1.67963700
C	5.43586200	-1.74296800	-1.21465800
H	6.20795600	-1.99197800	-1.95437200
C	6.08607900	-1.56218000	0.17266700
H	6.84379600	-0.76627500	0.13718700
H	6.60499500	-2.48428300	0.46638800
C	4.99760200	-1.21829400	1.21019700
H	5.45840500	-1.07521400	2.19650900
C	4.29255400	0.08461800	0.78637700
H	3.51515600	0.34879700	1.52090600
H	5.00990500	0.91836500	0.77205500
C	3.95593400	-2.35349300	1.27612300
H	3.19500200	-2.13171800	2.03331800
H	4.44507700	-3.28921600	1.58035800
C	3.29745900	-2.53090400	-0.10761100
H	2.56251600	-3.34487700	-0.06085100
C	2.60219100	-1.23813300	-0.58190400
C	4.39735000	-2.88557000	-1.14153300
H	3.94666200	-3.05035500	-2.12978900
H	4.90123300	-3.82107000	-0.85946700
C	-0.12458100	3.02118600	-0.42401600
C	-1.08415100	3.25965800	-1.42837600
C	-2.29997600	3.84622900	-1.06500600
H	-3.04823600	4.02083200	-1.83560800
C	-2.57863000	4.21145500	0.25555500
C	-1.58845600	4.00266000	1.21914700
H	-1.77371800	4.30852700	2.24662300
C	-0.35498600	3.42066200	0.90713700
C	-0.81994500	2.92272400	-2.87821600
H	-1.75964900	2.78734000	-3.42245800
H	-0.27248600	3.72981900	-3.38411200
H	-0.22784300	2.00908900	-2.98477100
C	-3.91736400	4.80256400	0.63049100
H	-4.64754400	4.01203500	0.84883800
H	-3.84182400	5.43300700	1.52270700
H	-4.33121100	5.40996500	-0.18175800
C	0.68775600	3.25341000	1.98632300
H	0.68141900	2.23110900	2.37894600
H	1.69686300	3.46188900	1.61446300
H	0.48620400	3.93272800	2.82059000
C	-0.34295000	-1.05817500	-0.62861000
H	-0.30135400	-2.15063600	-0.80639500
N	-0.09552900	-0.96664100	2.87604600
O	-0.55480900	-1.25361200	3.95929600
C	-1.57991100	-0.41361900	-1.20987100
C	-1.71470800	-0.65841600	-2.75086800
C	-2.81993800	-1.11683300	-0.65739200
H	-1.59226700	0.65126200	-0.96119700
C	-2.71776800	-1.82287800	-2.92206000
H	-2.11561800	0.24961400	-3.21161400
H	-0.74644900	-0.86124500	-3.22003700
C	-3.43238900	-1.86816200	-1.59008500
H	-2.22050900	-2.78339900	-3.11191000
H	-3.40883500	-1.66830000	-3.75768700
H	2.28709700	-1.39336400	-1.62287800
C	-4.62658500	-2.72657900	-1.42703800
O	-4.98630600	-3.53538000	-2.26224500
C	-3.11747300	-1.05622200	0.80897400
O	-2.85728700	-1.95460300	1.57997200
O	-5.28207800	-2.50658600	-0.26750800
O	-3.62559600	0.13381600	1.16581100
C	-6.41559000	-3.35389700	-0.02983500
H	-7.17127300	-3.21093600	-0.80728600
H	-6.11256300	-4.40419200	-0.01660900
H	-6.80339300	-3.05530500	0.94429700
C	-3.81997800	0.31130900	2.58494600
H	-4.54331500	-0.41729100	2.96024500
H	-2.87007200	0.19182600	3.10902500
H	-4.20290600	1.32598300	2.69647400

syn-(R,S)-**3.32**

B3LYP SCF energy:	-2029.72204601	a.u.
B3LYP enthalpy:	-2028.97932800	a.u.
B3LYP free energy:	-2029.10110200	a.u.
M06 SCF energy in solution:	-2028.97383352	a.u.
M06 enthalpy in solution:	-2028.23111551	a.u.
M06 free energy in solution:	-2028.35288951	a.u.
M06-2X SCF energy in solution:	-2029.37635457	a.u.
M06-2X enthalpy in solution:	-2028.63363656	a.u.
M06-2X free energy in solution:	-2028.75541056	a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	1.05151300	-0.18088900	0.79759300
O	1.00930400	-0.91980200	2.92491400
O	0.83479800	1.19784200	2.46627700
N	2.37263800	0.52642200	-1.65208800
N	0.68035900	1.92582300	-1.48225300
C	1.28066500	0.85215300	-0.89430600
C	2.69439800	1.54760800	-2.65253300
H	3.53868400	2.17107100	-2.32499200
H	2.95670200	1.09901700	-3.61484700
C	1.38165500	2.35023900	-2.71360900
H	0.78702800	2.09781000	-3.60050500
H	1.53871900	3.43282000	-2.70809000
C	3.36167600	-0.34984200	-1.00184000
C	4.24631700	-1.13152800	-1.99481900
H	3.60904300	-1.69837500	-2.68642100
H	4.86268000	-0.44983500	-2.60019900
C	5.16506600	-2.08826500	-1.19190400
H	5.78001200	-2.66202900	-1.89750300
C	6.07808200	-1.26190200	-0.26215900
H	6.70788700	-0.58099600	-0.85224400
H	6.75621400	-1.92969800	0.28576600
C	5.21171000	-0.45867200	0.72930300
H	5.85775100	0.14100200	1.38391000
C	4.28033200	0.47749700	-0.06311400
H	3.66206500	1.06893700	0.62847000
H	4.87507300	1.19361100	-0.64828500
C	4.35165800	-1.41746500	1.57734400
H	3.74666900	-0.85138400	2.29775500
H	4.99887700	-2.08361300	2.16377400
C	3.43692100	-2.24929900	0.65428900
H	2.83481000	-2.93918700	1.25843700
C	2.50938600	-1.35137800	-0.18679600
C	4.32111800	-3.05608700	-0.33172400
H	3.68996900	-3.68458900	-0.97476500
H	4.98889300	-3.73323900	0.21973600
C	-0.37818600	2.73440400	-0.94499300
C	-1.65957200	2.69793300	-1.52328300
C	-2.65350400	3.53648100	-1.00015500
H	-3.64485400	3.51024000	-1.44890500
C	-2.40673000	4.40598600	0.06231900
C	-1.10820200	4.45594600	0.58162300
H	-0.88365000	5.15375800	1.38547900
C	-0.08008100	3.65013000	0.08972800
C	-2.00505600	1.82681300	-2.71141900
H	-2.91267800	1.24512900	-2.51508700
H	-2.20058300	2.44165300	-3.59978600
H	-1.20384800	1.12885200	-2.96223500
C	-3.50161700	5.27267800	0.63937200
H	-3.89251200	4.84453500	1.57184700
H	-3.13393000	6.27702400	0.87798700
H	-4.34207900	5.37567000	-0.05498900
C	1.31506900	3.80605800	0.64775600
H	1.54037000	3.02597800	1.38083700
H	2.07721500	3.75716100	-0.13796100
H	1.41452500	4.77190100	1.15288500
C	-0.35792000	-1.22446100	0.32754200
H	-0.58588700	-1.98179300	1.09846900
N	0.87291000	0.26493300	3.38815500
O	0.79879700	0.52854700	4.56475200
C	-1.28563800	-1.27116400	-0.86260400
C	-1.00205600	-2.50788700	-1.78470800
C	-2.73292300	-1.51304100	-0.44132400
H	-1.18703300	-0.34123200	-1.42352000
C	-2.06389500	-3.56903700	-1.41974700
H	-1.12669200	-2.19762700	-2.82830500
H	0.02162800	-2.87585100	-1.67400300
C	-3.13915700	-2.76551800	-0.72281300
H	-1.66945400	-4.33948200	-0.74323200
H	-2.45724500	-4.10092800	-2.29217700
H	2.00680400	-1.98809900	-0.92204000
C	-4.43277800	-3.40944400	-0.39936800
O	-4.75796200	-4.50295100	-0.82261900
C	-3.47403400	-0.46026000	0.31353200
O	-3.17136400	-0.09663200	1.42926500
O	-5.20771900	-2.67145400	0.42636100
O	-4.47677200	0.07672600	-0.41216600
C	-6.47085200	-3.26019000	0.77036000
H	-7.08540700	-3.40133600	-0.12315600
H	-6.32273400	-4.22840700	1.25566600
H	-6.94414000	-2.55629400	1.45539700
C	-5.25913900	1.06623600	0.27969200
H	-5.73531900	0.62302400	1.15833000
H	-4.62924000	1.90158100	0.59383200
H	-6.01120000	1.39555000	-0.43822900

3.31-TS-A-rotamer1

exo-anti/anti
(cis,syndiotactic dyad)

B3LYP SCF energy:	-2590.80648930	a.u.
B3LYP enthalpy:	-2589.81905000	a.u.
B3LYP free energy:	-2589.98089500	a.u.
M06 SCF energy in solution:	-2589.87850255	a.u.
M06 enthalpy in solution:	-2588.89106325	a.u.
M06 free energy in solution:	-2589.05290825	a.u.
M06-2X SCF energy in solution:	-2590.41196591	a.u.
M06-2X enthalpy in solution:	-2589.42452661	a.u.
M06-2X free energy in solution:	-2589.58637161	a.u.
Imaginary frequency:	-68.1442	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.68001000	0.77366800	0.41479100
O	0.96359700	2.26267200	-1.29022900
O	0.04323900	2.99207800	0.57499500
N	1.63350900	0.44946900	3.11412000
N	-0.16020000	-0.80947300	3.02957700
C	0.62196500	0.05640200	2.29923100
C	1.50127200	-0.01327400	4.49762200
H	1.22365500	0.81512800	5.16343800
H	2.43856800	-0.44162900	4.86323900
C	0.38704000	-1.06164500	4.37966300
H	0.77484300	-2.08572800	4.44737000

H	-0.39387600	-0.94375900	5.13698500
C	2.53822200	1.54791500	2.71059500
C	3.96424600	1.24931500	3.20905700
H	4.31088400	0.27771700	2.83999100
H	4.04043100	1.25674700	4.30469800
C	2.03207300	2.87247100	3.32028400
H	1.04626100	3.12346000	2.91908800
H	1.97933000	2.82978000	4.41567700
C	2.47517700	1.59065400	1.17366400
C	-1.50239600	-1.22704000	2.75631800
C	-1.76815200	-2.56658300	2.41668000
C	-3.09274500	-2.93696700	2.15078200
H	-3.30030500	-3.96566900	1.86303100
C	-4.14578200	-2.02211200	2.22830700
C	-3.85805500	-0.71537100	2.63831800
H	-4.66747100	0.00548500	2.72519200
C	-2.55467100	-0.30123600	2.92325200
C	-0.66809900	-3.60025900	2.33918300
H	-0.97520900	-4.45196200	1.72432500
H	-0.41790900	-3.99279600	3.33417100
H	0.25282100	-3.18500400	1.91892900
C	-5.55519700	-2.41525300	1.85352300
H	-5.68474500	-3.50267100	1.85650400
H	-5.79723200	-2.05011900	0.84699100
H	-6.29068200	-1.98232800	2.54088500
C	-2.29727000	1.10466000	3.42012000
H	-1.62026000	1.66607300	2.76726000
H	-1.84032000	1.09513000	4.41838100
H	-3.23537800	1.66276500	3.48983700
C	1.24256500	-0.92308300	-0.21965300
H	1.24089100	-1.81679200	0.42605700
C	-1.51471900	0.64194100	-0.13922900
H	-1.98097500	0.90319600	0.79856400
C	-1.13162000	-0.66700300	-0.47106200
H	-1.20250400	-1.50053900	0.21116400
C	-1.47987400	-0.85082000	-1.96564700
H	-1.04495000	-1.70617600	-2.47647400
C	-2.10304500	1.24025200	-1.43960700
H	-2.22089700	2.32356000	-1.45605100
C	-1.21762600	0.56786800	-2.51825100
C	-3.02444300	-0.83155800	-1.97631500
C	-3.40024700	0.42931400	-1.67366900
H	-1.61240700	0.69628000	-3.53052900
H	-0.18121000	0.89461400	-2.46787500
C	1.79497700	-1.31052800	-1.58973700
C	1.42569800	-2.77150600	-1.99250600
C	3.32130900	-1.39898900	-1.49280800
H	1.50477800	-0.57129500	-2.34044900
C	2.58764600	-3.65200900	-1.47965000
H	1.37182000	-2.83757600	-3.08545300
H	0.45762600	-3.08896400	-1.59531100
C	3.74285700	-2.67589700	-1.42182400
H	2.39791800	-4.07229600	-0.48287000
H	2.79614200	-4.50410800	-2.13656100
C	-3.80638200	-2.06311200	-2.16380500
O	-3.31309100	-3.13523500	-2.46596600
C	-4.73953300	0.99718700	-1.38042500
O	-5.03912200	1.44272600	-0.28979800
C	5.12936500	-3.17778700	-1.23271300
O	5.39730200	-4.10230800	-0.49010000
C	4.19800900	-0.19407300	-1.43467500
O	5.16520700	-0.05912900	-0.71216400
O	-5.54656600	1.01839300	-2.45460800
O	-5.13576500	-1.89257400	-1.96081600
O	6.03010100	-2.53862500	-2.00005200
O	3.76744500	0.74121100	-2.30181600
C	-6.85656200	1.56453900	-2.22624400
H	-7.35316000	1.54383100	-3.19655200
H	-7.40254800	0.95424000	-1.50164600
H	-6.78704700	2.58827900	-1.84923600
C	-5.93932800	-3.05964500	-2.19133600
H	-5.82436200	-3.40768200	-3.22145500
H	-5.65313200	-3.86619400	-1.51101500
H	-6.96751500	-2.74770900	-2.00497300
C	7.39787700	-2.92417100	-1.79342500
H	7.97632000	-2.33848300	-2.50820200
H	7.70601700	-2.69199800	-0.77053800
H	7.52770300	-3.99454700	-1.97411500
C	4.49028500	1.98176800	-2.29113000
H	3.99389000	2.61147900	-3.02869200
H	4.43707700	2.43876500	-1.30035600
H	5.53716500	1.81579700	-2.56043300
C	0.47455700	3.21419500	-0.60077700
C	0.45302300	4.64711800	-1.16303000
C	0.49080900	4.62553300	-2.70066000
H	0.50335700	5.65066200	-3.09122700
H	1.37704600	4.10121800	-3.06810500
H	-0.38896500	4.11780000	-3.11262800
C	1.71075100	5.36708500	-0.62229500
H	1.74210000	6.40016100	-0.99023100
H	1.70734000	5.39279300	0.47254000
H	2.62607100	4.86195300	-0.95169500
C	-0.80753100	5.38339200	-0.67209100
H	-0.85848400	5.39073700	0.41958100
H	-0.80309400	6.41998400	-1.03144400
H	-1.71987400	4.90324000	-1.04638500
H	4.64773800	2.01547700	2.82820200
H	2.72150900	3.68318700	3.05890100
H	2.59416300	2.61883800	0.81982500
H	3.29997900	1.00248200	0.76319400

3.31-TS-A-rotamer2

exo-anti/anti
(cis,syndiotactic dyad)

B3LYP SCF energy:	-2590.80126164	a.u.
B3LYP enthalpy:	-2589.81386900	a.u.
B3LYP free energy:	-2589.97408800	a.u.
M06 SCF energy in solution:	-2589.87577538	a.u.
M06 enthalpy in solution:	-2588.88838274	a.u.
M06 free energy in solution:	-2589.04860174	a.u.
M06-2X SCF energy in solution:	-2590.40927854	a.u.
M06-2X enthalpy in solution:	-2589.42188590	a.u.
M06-2X free energy in solution:	-2589.58210490	a.u.
Imaginary frequency:	-143.3008	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	1.57750200	-0.81187700	-0.14373500
O	1.84347000	-1.12537100	-2.40686600
O	3.24721100	0.22007600	-1.37406000
N	3.13805200	-1.29012100	2.22674500
N	1.69337100	0.24288000	2.84051100
C	2.11692600	-0.51458300	1.77632200
C	3.55881900	-0.98293500	3.59619700
H	4.52902000	-0.46792500	3.60257600
H	3.65683200	-1.89318600	4.19463200
C	2.41882100	-0.08045800	4.08696700
H	1.75341200	-0.59907200	4.78878000
H	2.77431800	0.83433600	4.57040600
C	3.96770000	-2.07300100	1.28367600
C	4.34582300	-3.41883700	1.93052400
H	3.44869700	-3.96508500	2.24453400
H	5.00304700	-3.29953400	2.80217300
C	5.24467100	-1.27515200	0.94365800
H	4.98508000	-0.34848500	0.42451800
H	5.83472600	-1.03814400	1.83790800
C	3.10090300	-2.26316700	0.03021000
C	0.89020700	1.43062700	2.81908600
C	-0.41142400	1.41315800	3.34952000
C	-1.16365800	2.59488800	3.30890600
H	-2.18350900	2.57764800	3.68767200
C	-0.64917200	3.77992400	2.78002900
C	0.67587400	3.78299500	2.32808900
H	1.09665200	4.69979600	1.92385700
C	1.46463100	2.63168400	2.34846500
C	-1.00755800	0.16929100	3.96789700
H	-2.10051900	0.19313300	3.91096900
H	-0.73989300	0.08839600	5.03069300
H	-0.65796500	-0.74258800	3.47561400
C	-1.49842200	5.02277900	2.66060600
H	-1.76836100	5.19585700	1.61123300
H	-0.96118000	5.91328300	3.00716200
H	-2.42342200	4.93661000	3.24031900
C	2.89960100	2.68535700	1.87289200
H	3.07337000	2.04478600	1.00108800
H	3.59482500	2.35514400	2.65553000
H	3.17151200	3.70825900	1.59688900
C	0.00713300	-1.74223500	0.44476600
H	-0.35573200	-1.66541800	1.47484000
C	0.57308300	1.07159400	-0.52412000
H	1.05002300	1.82027900	0.09276500
C	-0.52329000	0.28707000	-0.00345600
H	-0.82491200	0.42116900	1.02671300
C	-1.63192900	0.37019800	-1.08590000
H	-2.46066200	-0.32901400	-0.99710800
C	0.08967600	1.55931000	-1.91555200
H	0.86539500	1.93017100	-2.58636700
C	-0.79623000	0.38207800	-2.38407100
C	-2.05313600	1.85447200	-1.05724400
C	-1.03199400	2.56704100	-1.57631000
H	-1.39951500	0.63019900	-3.26222800
H	-0.21681800	-0.52006600	-2.56083900
C	-0.67632400	-2.94942100	-0.19623100
C	-0.46899300	-3.26867600	-1.70453900
C	-2.19304800	-3.03155700	-0.03265300
H	-0.21656700	-3.74815800	0.41428500
C	-1.85007800	-3.08920300	-2.37968800
H	-0.15947400	-4.31526900	-1.80031400
H	0.31285100	-2.66007800	-2.15677600
C	-2.81932500	-3.10959000	-1.22156700
H	-1.94911700	-2.14119200	-2.92456300
H	-2.07009800	-3.88293000	-3.10459200
C	-3.27059200	2.31095400	-0.37067500
O	-4.01024200	1.57922400	0.25992800
C	-0.82906400	4.03747300	-1.64401000
O	-0.06873100	4.64530300	-0.91536200
C	-4.29048000	-3.08718400	-1.47453800
O	-4.83722400	-2.16791300	-2.04760700
C	-2.91754000	-3.03613800	1.26016200
O	-4.10641100	-2.83120700	1.40481600
O	-1.52591500	4.60237100	-2.64484300
O	-3.47932400	3.64700700	-0.49572500
O	-4.90393000	-4.21186700	-1.07175500
O	-2.08985900	-3.32955000	2.29762300
C	-1.36073900	6.02330800	-2.78299500
H	-1.96078900	6.30268900	-3.64926800
H	-1.71795100	6.53708400	-1.88628900
H	-0.30913500	6.27554900	-2.94320900
C	-4.66131100	4.13757300	0.15204300
H	-5.54989500	3.63138600	-0.23453100
H	-4.60508000	3.97691500	1.23237600
H	-4.69797100	5.20388500	-0.07434700
C	-6.33357700	-4.21454100	-1.22226500
H	-6.65832400	-5.20390200	-0.89892400
H	-6.77535600	-3.43962700	-0.59055200
H	-6.61329600	-4.03613300	-2.26379300
C	-2.73141100	-3.40792700	3.57948700
H	-1.93817500	-3.64247500	4.29014900
H	-3.20750600	-2.45650400	3.83100900
H	-3.49171500	-4.19369800	3.57916600
C	2.86527600	-0.36402100	-2.43367700
C	3.64528400	-0.19957800	-3.75001100
C	4.67476000	0.93617400	-3.63560100
H	5.22808500	1.03592900	-4.57772200
H	4.18854000	1.89400600	-3.42162000
H	5.39105600	0.74371200	-2.83187400
C	4.36749900	-1.53717900	-4.03150200
H	3.65021800	-2.36049400	-4.10585800
H	4.92398700	-1.47455200	-4.97488300
H	5.08235100	-1.77526200	-3.23473300
C	2.65533100	0.09502100	-4.89505100
H	2.12911700	1.04355400	-4.73137200
H	3.19251500	0.17237000	-5.84839300
H	1.90709200	-0.69763300	-4.98078600
H	5.88269000	-1.86952100	0.27999100
H	4.87976800	-4.03474100	1.19929600
H	3.72306100	-2.31228100	-0.86716200
H	2.54592700	-3.21003800	0.09822400

3.31-TS-A-rotamer3

exo-anti/anti
(cis,syndiotactic dyad)

B3LYP SCF energy:	-2590.79816299	a.u.
B3LYP enthalpy:	-2589.81099200	a.u.
B3LYP free energy:	-2589.96865100	a.u.
M06 SCF energy in solution:	-2589.86848317	a.u.

M06 enthalpy in solution:	-2588.88131218	a.u.
M06 free energy in solution:	-2589.03897118	a.u.
M06-2X SCF energy in solution:	-2590.40269967	a.u.
M06-2X enthalpy in solution:	-2589.41552868	a.u.
M06-2X free energy in solution:	-2589.57318768	a.u.
Imaginary frequency:	-27.4463	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.64395700	0.52356200	0.76876500
O	1.31442400	2.08745500	-0.78473700
O	0.20563300	2.77509000	0.98912000
N	0.95030100	0.35042800	3.62131300
N	-0.93516300	-0.69727800	3.24051900
C	0.12355400	-0.06840800	2.62722900
C	0.38094100	0.19557300	4.96275200
H	0.02427500	1.16122400	5.34519500
H	1.11635800	-0.19936000	5.66915600
C	-0.77472900	-0.77503500	4.70521300
H	-0.52806700	-1.80156300	5.00721900
H	-1.70177200	-0.48580600	5.20935800
C	2.13875900	1.18796600	3.34377900
C	3.34132700	0.62550000	4.12791900
H	3.51400100	-0.42580700	3.87027900
H	3.21266000	0.70106500	5.21588000
C	1.86557200	2.64093300	3.78393900
H	1.03149000	3.05984700	3.21581500
H	1.65089300	2.71434600	4.85777900
C	2.37506000	1.10008300	1.82360400
C	-1.97605000	-1.48116400	2.64463200
C	-1.76380500	-2.85909900	2.41254000
C	-2.78219700	-3.59940300	1.80765900
H	-2.61202600	-4.65444700	1.60193100
C	-4.00814700	-3.02346700	1.45438000
C	-4.21403800	-1.67772900	1.76404600
H	-5.16750300	-1.21423500	1.51900700
C	-3.22437100	-0.89097100	2.36790400
C	-0.48886800	-3.56142700	2.82736900
H	-0.27852500	-4.40822700	2.16620300
H	-0.57925600	-3.96573200	3.84510300
H	0.37882600	-2.89756300	2.81553300
C	-5.05705300	-3.83219700	0.72862000
H	-4.83121500	-3.86981700	-0.34509300
H	-6.05414700	-3.39494800	0.84839600
H	-5.09274500	-4.86511200	1.09271200
C	-3.54011100	0.54896800	2.70644400
H	-2.64115200	1.12351400	2.94001000
H	-4.20536200	0.59994200	3.57920500
H	-4.05865200	1.04069300	1.87592300
C	1.03012700	-1.24682300	0.19415600
H	0.58550700	-2.08160000	0.75036200
C	-1.42272000	0.73819200	-0.15424000
H	-1.95716300	1.12374300	0.70221000
C	-1.23429000	-0.62115200	-0.41927700
H	-1.53559500	-1.42201700	0.23706100
C	-1.34283000	-0.79139700	-1.94807600
H	-0.99015500	-1.73437800	-2.36506400
C	-1.64548800	1.39480100	-1.53954600
H	-1.55221100	2.47956900	-1.58025000
C	-0.72348900	0.53576300	-2.44290000
C	-2.82968300	-0.48567500	-2.23699000
C	-3.00972800	0.83002100	-1.99720100
H	-0.90258200	0.70451300	-3.50858900
H	0.33355400	0.66318500	-2.21759800
C	1.82033700	-1.88282200	-0.95669600
C	2.12921400	-3.38024400	-0.63840800
C	3.19199000	-1.34850200	-1.36577000
H	1.18648900	-1.81317900	-1.85707100
C	3.46503200	-3.71341300	-1.32685500
H	1.30875100	-4.03866300	-0.94067400
H	2.24657900	-3.48415900	0.44720000
C	4.07480100	-2.34953600	-1.56341500
H	4.10562500	-4.36820200	-0.72743300
H	3.31563800	-4.22212800	-2.28989100
C	-3.81707900	-1.53709300	-2.51510200
O	-3.56574900	-2.73047500	-2.50443800
C	-4.26174000	1.62081800	-1.87906700
O	-4.72835100	1.95082100	-0.80553800
C	5.44046500	-2.16513200	-2.10740600
O	5.91703000	-1.12734600	-2.52582300
C	3.43301600	0.05940200	-1.80897400
O	2.92709800	0.49715300	-2.82138300
O	-4.76881100	1.98276200	-3.06739300
O	-5.04874100	-1.04012400	-2.78034900
O	6.12279700	-3.33879800	-2.10356800
O	4.26836800	0.72563600	-1.00610600
C	-5.96617900	2.77756900	-3.00856300
H	-6.21617100	3.00227800	-4.04554700
H	-6.77306800	2.21548700	-2.53083700
H	-5.78960700	3.69744300	-2.44504700
C	-6.06038300	-2.01498800	-3.06727700
H	-5.74775000	-2.66546800	-3.88823300
H	-6.26669400	-2.62927000	-2.18593200
H	-6.94621500	-1.44315300	-3.34597000
C	7.45420400	-3.27023600	-2.63197900
H	7.84813700	-4.28520600	-2.56660600
H	7.43945200	-2.92878600	-3.67072700
H	8.06695900	-2.58132700	-2.04381800
C	4.66272100	2.02369300	-1.48118200
H	5.29942600	2.43725900	-0.69839900
H	5.22293300	1.91690800	-2.41404400
H	3.78036800	2.64470800	-1.63814600
H	3.14363500	0.35294900	1.60207600
H	2.73621500	2.05702700	1.43816200
H	4.24170100	1.19090900	3.86475200
H	2.75439600	3.25150500	3.58883300
C	0.80564600	3.03110700	-0.10373200
C	0.94013800	4.49178600	-0.57610500
C	-0.28705400	5.30519100	-0.12417300
H	-0.41116800	5.26251100	0.96079600
H	-0.17425600	6.35428300	-0.42483300
H	-1.20818700	4.92285900	-0.58019500
C	2.21015300	5.07538900	0.08654300
H	3.10459100	4.51611200	-0.20867100
H	2.34795700	6.12040200	-0.21752100
H	2.13235500	5.04505800	1.17881000
C	1.07738900	4.55084000	-2.10772400

H	0.18190300	4.15570100	-2.60146200
H	1.20972900	5.59012700	-2.43340100
H	1.92870700	3.96272300	-2.45909200

3.31-TS-B

exo-syn/anti
(trans,isotactic dyad)

B3LYP SCF energy:	-2590.79604787	a.u.
B3LYP enthalpy:	-2589.80876900	a.u.
B3LYP free energy:	-2589.96901800	a.u.
M06 SCF energy in solution:	-2589.86542794	a.u.
M06 enthalpy in solution:	-2588.87814907	a.u.
M06 free energy in solution:	-2589.03839807	a.u.
M06-2X SCF energy in solution:	-2590.40300043	a.u.
M06-2X enthalpy in solution:	-2589.41572156	a.u.
M06-2X free energy in solution:	-2589.57597056	a.u.
Imaginary frequency:	-177.7790	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	-1.22045100	-1.14411600	0.59555500
O	-0.40101500	-1.37344400	2.67473800
O	-2.34995000	-0.36935400	2.50290900
N	-3.19590800	-2.24843400	-1.20314800
N	-2.98871000	-0.19142200	-1.93135400
C	-2.52959800	-1.08524800	-0.98129100
C	-3.96800100	-2.26819800	-2.44438900
H	-4.94199900	-2.74509200	-2.31108400
H	-3.42450000	-2.81174500	-3.23041100
C	-4.07934400	-0.77644600	-2.74866600
H	-3.94292800	-0.54106000	-3.80672400
H	-5.04321300	-0.35958000	-2.42610400
C	-3.02135700	1.24349200	-1.86335200
C	-2.51457000	1.98147900	-2.95070500
C	-2.62751300	3.37698100	-2.92842000
H	-2.21924100	3.94756000	-3.76039200
C	-3.25321200	4.05133100	-1.87846300
C	-3.79870900	3.28677100	-0.84079900
H	-4.32247400	3.78892300	-0.02989100
C	-3.71129000	1.89142000	-0.81338900
C	-1.88357500	1.31525900	-4.15300800
H	-1.09606200	1.94573600	-4.57846300
H	-2.62404700	1.15055700	-4.94806900
H	-1.44956700	0.34380300	-3.90340500
C	-3.34714200	5.55944500	-1.85852600
H	-2.67361100	5.98899900	-1.10563600
H	-4.36082800	5.89413600	-1.60888300
H	-3.07791400	5.99095200	-2.82797200
C	-4.37859800	1.13163300	0.30880500
H	-3.66067400	0.77428100	1.05306000
H	-4.91763800	0.25160500	-0.06031900
H	-5.10121600	1.77556300	0.82019900
C	0.21872500	-1.77369800	-0.49023100
C	0.80209900	0.08885100	0.41771400
H	1.38738200	-0.36891800	1.20604400
C	-0.32186400	0.91678200	0.73897700
H	-0.56733700	1.15792500	1.76664800
C	-0.25025400	2.09114500	-0.26381000
H	-1.14661400	2.69701300	-0.36590700
C	1.52792400	0.79996200	-0.75320300
H	2.26412200	0.22097100	-1.30353900
C	0.32387400	1.38688000	-1.51328400
C	1.01408300	2.87423800	0.15989200
C	2.07904300	2.08930000	-0.11520400
H	0.61922400	2.08357300	-2.30242400
H	-0.34264600	0.62411100	-1.91248100
H	0.25246700	-1.51824700	-1.55998800
C	1.31948400	-2.80318800	-0.20691600
C	1.80964800	-3.06863400	1.24484700
C	2.61471000	-2.50867300	-0.95362000
H	0.88377100	-3.72031600	-0.63646200
C	3.22931100	-2.45334100	1.33317300
H	1.88221200	-4.15214600	1.39142500
H	1.12655700	-2.67608800	1.99628600
C	3.64786900	-2.31148400	-0.11541200
H	3.24345900	-1.47362600	1.83027500
H	3.92324900	-3.08616400	1.89755800
C	0.90027400	4.15584800	0.89556400
O	0.15904100	4.30009900	1.84841900
C	3.51059600	2.22375500	0.21023800
O	4.36733500	1.45261000	-0.18699800
C	5.02567100	-1.97305300	-0.54821800
O	5.47501800	-2.12228500	-1.66808300
C	2.64376400	-2.54541700	-2.44555000
O	2.31458500	-3.52644500	-3.08192800
O	1.64494600	5.14221300	0.36334400
O	3.77933100	3.27494900	1.01636100
O	3.00980100	-1.37563600	-2.99853400
O	5.73842900	-1.47259300	0.48523200
C	1.57779100	6.39846100	1.05661300
H	0.54871800	6.76631300	1.09154600
H	1.95058200	6.29089400	2.07888800
H	2.21089500	7.07937800	0.48699700
C	5.16176600	3.44716700	1.35631200
H	5.54109200	2.56799000	1.88455600
H	5.76348100	3.60756800	0.45720600
H	5.19642500	4.32553800	2.00165100
C	3.17909100	-1.39168600	-4.42501200
H	3.99283900	-2.07012300	-4.69320900
H	2.25929900	-1.71305300	-4.92084000
H	3.43071900	-0.36705900	-4.69895800
C	7.04756200	-0.99244000	0.14983300
H	7.63142000	-1.77201600	-0.34627800
H	6.96543100	-0.12370300	-0.50864600
H	7.50759000	-0.71031400	1.09778100
C	-3.04242000	-3.40815900	-0.30254900
C	-2.14686200	-4.47564400	-0.95721000
C	-4.42972300	-4.01955900	-0.01468500
C	-2.43177200	-2.81536100	0.97725200
H	-2.57823800	-4.84249800	-1.89694900
H	-1.15517800	-4.07218300	-1.17301900
H	-4.87825200	-4.50005300	-0.89375800
H	-5.12037300	-3.25538900	0.35925600
H	-3.22778900	-2.50346500	1.66191700

C	-1.41448000	-0.82217800	3.22640300
C	-1.46543100	-0.72221500	4.75843500
C	-2.74781800	-0.00804800	5.21328300
H	-2.77139500	0.05620500	6.30818400
H	-2.80213000	1.00715800	4.80789000
H	-3.64105400	-0.54551400	4.88003400
C	-0.22424600	0.06411800	5.23427800
H	-0.22047300	0.13618900	6.32879800
H	0.69815300	-0.43043700	4.91602900
H	-0.22304300	1.08423300	4.83123500
C	-1.42089400	-2.15344300	5.33719800
H	-1.42690400	-2.11689600	6.43351400
H	-2.29160800	-2.73757700	5.01532600
H	-0.51835500	-2.67894200	5.01158100
H	-1.80871600	-3.55267700	1.49990100
H	-4.32587200	-4.78708100	0.75957500
H	-2.03284500	-5.33528600	-0.28754600

3.31-TS-C-rotamer1

exo-anti/syn

(trans,syndiotactic dyad)

B3LYP SCF energy:	-2590.80997560	a.u.
B3LYP enthalpy:	-2589.82265700	a.u.
B3LYP free energy:	-2589.98026800	a.u.
M06 SCF energy in solution:	-2589.87808347	a.u.
M06 enthalpy in solution:	-2588.89076487	a.u.
M06 free energy in solution:	-2589.04837587	a.u.
M06-2X SCF energy in solution:	-2590.41252293	a.u.
M06-2X enthalpy in solution:	-2589.42520433	a.u.
M06-2X free energy in solution:	-2589.58281533	a.u.
Imaginary frequency:	-77.8796	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.63588000	-1.63507200	-0.38970400
O	1.66353400	-1.82152900	-2.40366300
O	2.89179900	-2.10297600	-0.59648100
N	0.11754500	-3.37087400	1.85270500
N	0.02667600	-1.34797700	2.70652100
C	0.21968300	-2.05103700	1.53765500
C	-0.11363400	-3.64080900	3.27343700
H	0.69098300	-4.25194200	3.69843500
H	-1.05504600	-4.18323100	3.41872000
C	-0.15593800	-2.22897500	3.87978900
H	-1.10778700	-2.01267500	4.37741200
H	0.64472900	-2.05735000	4.60837000
C	0.57245100	-4.40871500	0.90095300
C	-0.35669800	-5.63374800	0.98946600
H	-1.39741200	-5.35422200	0.79008000
H	-0.31290700	-6.12461200	1.97076200
C	2.01608000	-4.82550900	1.25848400
H	2.69699200	-3.97936900	1.13337100
H	2.09623800	-5.20796600	2.28405900
C	0.53224500	-3.74850000	-0.48743300
H	1.33899300	-4.13650300	-1.11487600
C	0.40730300	0.01060600	2.97577400
C	-0.57771700	0.98323000	3.22435900
C	-0.16392600	2.29406400	3.49751600
H	-0.92430400	3.05340400	3.67052000
C	1.18396800	2.65224000	3.54290100
C	2.14088200	1.64565800	3.36748400
H	3.19687500	1.89812600	3.42925500
C	1.78026700	0.32273800	3.10183000
C	-2.05861100	0.67732300	3.19594700
H	-2.56119100	1.15303600	4.04619100
H	-2.25937000	-0.39565400	3.24221500
H	-2.52552900	1.06717800	2.28350700
C	1.60122300	4.08925100	3.74755000
H	2.57457500	4.16015700	4.24454500
H	0.86888500	4.64077000	4.34735100
H	1.68832300	4.59956100	2.77924700
C	2.85285800	-0.73521500	2.95669600
H	2.88887300	-1.16168500	1.94796700
H	2.69336100	-1.57074100	3.64975900
H	3.83712500	-0.30983200	3.17365600
C	-1.12970900	-1.14297000	-0.86403700
C	1.47094700	0.44188900	-0.24982300
H	2.02005400	0.41432200	0.67961100
C	0.09797000	0.76155200	-0.30737300
H	-0.51924700	0.91349200	0.56627500
C	-0.07019400	1.68384900	-1.54228500
H	-1.08201900	1.84267000	-1.90651700
C	2.11340400	1.16553200	-1.45604500
H	3.11305900	0.83519800	-1.73557300
C	0.97938800	1.09164700	-2.50960700
C	0.68139300	2.97419000	-1.13560600
C	1.99517100	2.66277000	-1.09951500
H	1.15967100	1.74440400	-3.36882400
H	0.77329000	0.07687700	-2.84304000
H	-1.26180100	-0.90117500	-1.93358700
C	-2.45539600	-1.23180400	-0.14072400
C	-3.02359800	-2.67435700	-0.36090500
C	-3.62914700	-0.36535900	-0.60757100
H	-2.29720500	-1.05275800	0.92941300
C	-4.55731300	-2.53079000	-0.34046100
C	-4.77257500	-1.07520100	-0.68456500
H	-0.41115000	-3.98819300	-0.99069300
H	2.34337100	-5.62683700	0.58632200
H	-0.05663400	-6.37241800	0.23868500
C	2.78521700	-2.09096500	-1.86399800
C	3.98683700	-2.45008100	-2.75504500
C	4.02718600	-1.50824600	-3.97393100
H	4.85448100	-1.78696300	-4.63816100
H	3.09283700	-1.55805600	-4.53913400
H	4.18288200	-0.46695600	-3.66653000
C	5.30006200	-2.34931100	-1.96155700
H	5.29118700	-3.01377100	-1.09323300
H	6.14680600	-2.62450700	-2.60271200
H	5.46720700	-1.32998300	-1.59612200
C	3.77812400	-3.90398200	-3.23977100
H	4.60477300	-4.20476700	-3.89534600
H	3.74734500	-4.60106500	-2.39412900
H	2.84169600	-3.99976900	-3.79892400
H	-2.70378000	-3.03728200	-1.34504200

H	-4.97785100	-2.74527500	0.65328500
H	-5.06838600	-3.19590800	-1.04338300
H	-2.63488700	-3.36999400	0.38493800
C	-3.50360500	1.11176400	-0.76393800
O	-3.10384000	1.84209300	0.12493500
C	-6.14896500	-0.60758200	-0.98585500
O	-7.04110900	-1.35547900	-1.33804700
C	3.17087000	3.45155700	-0.66836900
O	4.00609400	3.01944700	0.10278900
C	-0.01011800	4.23994100	-0.83258300
O	-1.07120300	4.57022000	-1.33243800
O	-3.84928900	1.53073900	-1.98867500
O	-6.32622500	0.71685700	-0.78704900
O	0.64937800	5.00803200	0.06295800
O	3.24116800	4.66298700	-1.25359700
C	4.36067500	5.46910400	-0.85367700
H	4.30870400	5.69309800	0.21548800
H	5.30127400	4.95268700	-1.06269200
H	4.28539700	6.38442000	-1.44144300
C	0.04561300	6.28321500	0.33221000
H	-0.00210600	6.88546200	-0.57924700
H	-0.96576700	6.15344300	0.72601800
H	0.68828700	6.75966100	1.07306600
C	-3.90863100	2.96313900	-2.17300900
H	-4.67132200	3.38349500	-1.51146700
H	-2.94450900	3.42855400	-1.96240100
H	-4.19108100	3.10171800	-3.21692500
C	-7.64448500	1.20706900	-1.07826800
H	-7.88700900	1.05328600	-2.13329500
H	-8.38869000	0.69257100	-0.46472200
H	-7.61935500	2.27086600	-0.84055200

3.31-TS-C-rotamer2

exo-anti/syn

(trans,syndiotactic dyad)

B3LYP SCF energy:	-2590.80476680	a.u.
B3LYP enthalpy:	-2589.81749200	a.u.
B3LYP free energy:	-2589.97763300	a.u.
M06 SCF energy in solution:	-2589.87672237	a.u.
M06 enthalpy in solution:	-2588.88944757	a.u.
M06 free energy in solution:	-2589.04958857	a.u.
M06-2X SCF energy in solution:	-2590.41053463	a.u.
M06-2X enthalpy in solution:	-2589.42325983	a.u.
M06-2X free energy in solution:	-2589.58340083	a.u.
Imaginary frequency:	-123.6175	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.38494700	1.20985000	0.08278000
O	0.18994400	2.43966700	-1.80888300
O	-0.91816800	3.13906800	-0.03827300
N	1.65580600	1.33777200	2.66161000
N	-0.08876500	0.03300800	2.97194600
C	0.60072500	0.76560200	2.02427100
C	1.83707400	0.88255100	4.03901000
H	2.03675500	1.71569900	4.71853000
H	2.67869700	0.17847200	4.11043300
C	0.49305100	0.19950500	4.32290100
H	0.60134100	-0.76928400	4.82005700
H	-0.16511800	0.82317300	4.94182900
C	-1.48531800	-0.31389000	2.93014500
C	-1.87135400	-1.66539600	2.92831400
C	-3.23854800	-1.97463200	2.92218200
H	-3.53608700	-3.02168000	2.90848600
C	-4.22173800	-0.98636700	2.92896500
C	-3.80737000	0.34961100	2.99156500
H	-4.55827800	1.13595600	3.02356200
C	-2.45923000	0.71132300	3.00412600
C	-0.87294700	-2.80116700	2.93035000
H	-1.18255900	-3.58429500	3.63172200
H	0.12901100	-2.46848800	3.20614600
H	-0.80248200	-3.27341100	1.94111500
C	-5.68859800	-1.33256800	2.84729500
H	-6.28353500	-0.73214900	3.54538100
H	-5.86592100	-2.38977000	3.07140500
H	-6.06368800	-1.12963400	1.83675300
C	-2.08512800	2.17554300	3.06091000
H	-1.73284200	2.54339500	2.09074600
H	-1.28981200	2.37342300	3.78807800
H	-2.95440400	2.77501100	3.34887000
C	1.36237800	-0.22844900	-0.67132700
C	-1.61350000	0.31297800	-0.33436900
H	-2.16859400	0.50271400	0.57372300
C	-0.77011300	-0.81846200	-0.48382200
H	-0.57509200	-1.51085400	0.32526800
C	-1.05162400	-1.36698900	-1.90540500
H	-0.34032000	-2.09134200	-2.30099000
C	-2.36779700	0.44102600	-1.68369600
H	-2.85675200	1.39759600	-1.86815300
C	-1.30624000	-0.06169200	-2.69306800
C	-2.50355100	-1.88138600	-1.81881800
C	-3.29854900	-0.79460500	-1.70924000
H	-1.72640600	-0.25711200	-3.68371600
H	-0.45060400	0.60496700	-2.77237500
H	1.41782200	-0.05068000	-1.75840100
C	2.12885300	-1.50855700	-0.37909700
C	2.38546200	-1.94926700	1.08143700
C	3.54301300	-1.47106100	-0.96482800
H	1.60623400	-2.31389100	-0.92767000
C	3.76137900	-2.65708900	1.07303300
C	4.42287600	-2.11258100	-0.17490600
H	2.43035400	-1.06073000	1.71392000
H	3.66064900	-3.74934700	0.99699800
H	4.34918900	-2.46370700	1.97636100
H	1.58840200	-2.59002600	1.46312600
C	3.79086500	-0.92048900	-2.33177400
O	3.28978200	-1.39789100	-3.32917500
C	5.83583700	-2.35539800	-0.54633000
O	6.34331800	-2.09056600	-1.61940700
C	-4.75770300	-0.68044300	-1.46196400
O	-5.22329200	-0.16852400	-0.46181400
C	-2.80044000	-3.31701400	-1.69272400
O	-1.94151800	-4.18173400	-1.68282100
O	4.55139500	0.18324900	-2.30889400

O	6.51422400	-2.93707800	0.47228100
O	-4.12055400	-3.58323600	-1.56492100
O	-5.49459600	-1.13657300	-2.48866500
C	-6.91775400	-1.04202900	-2.31351300
H	-7.24025000	-1.66574900	-1.47516100
H	-7.21541700	-0.00741300	-2.12386400
H	-7.34987500	-1.40281900	-3.24710800
C	-4.45229800	-4.97293700	-1.43634700
H	-4.11457100	-5.53247200	-2.31293100
H	-3.98705100	-5.40072300	-0.54378200
H	-5.53929900	-5.00749000	-1.35543000
C	4.85514900	0.74676900	-3.59784100
H	5.43981500	0.03518200	-4.18625500
H	3.93554400	0.99649200	-4.13283000
H	5.43705000	1.64461100	-3.39056000
C	7.89296100	-3.22725900	0.19900900
H	7.98105000	-3.90468800	-0.65474000
H	8.44243400	-2.30796600	-0.02168000
H	8.27839600	-3.69709000	1.10450700
C	2.57209100	2.25069500	1.94523600
C	1.82073700	2.64967600	0.66102500
C	3.90604100	1.54775300	1.63239100
C	2.84371200	3.48612700	2.82794600
H	3.76399300	0.73497600	0.91640100
H	4.37583700	1.14119500	2.53742400
H	1.90338000	3.95614900	3.13730200
H	3.43034500	3.24894300	3.72536500
H	1.26527500	3.57805500	0.82792800
C	-0.56441000	3.29964800	-1.24853500
C	-0.99412800	4.55253000	-2.03022300
C	0.22945500	5.49736800	-2.08152900
H	1.07801200	5.01048300	-2.57275200
H	-0.01967800	6.40762200	-2.64092700
H	0.54017000	5.79408100	-1.07291200
C	-1.39295200	4.15548500	-3.46484000
H	-2.26280400	3.48717800	-3.46489700
H	-1.65831400	5.04874200	-4.04367300
H	-0.57226200	3.64182900	-3.97247800
C	-2.16661100	5.25582200	-1.32728700
H	-1.90091200	5.54470400	-0.30674200
H	-2.45000600	6.15826000	-1.88317900
H	-3.04451500	4.60282100	-1.26801900
H	2.52236000	2.81545700	-0.16394600
H	4.60754300	2.26394000	1.19030300
H	3.41401000	4.22007500	2.24905200

3.31-TS-C-rotamer3

exo-anti/syn

(trans,syndiotactic dyad)

B3LYP SCF energy:	-2590.79267052	a.u.
B3LYP enthalpy:	-2589.80544700	a.u.
B3LYP free energy:	-2589.96190000	a.u.
M06 SCF energy in solution:	-2589.86412018	a.u.
M06 enthalpy in solution:	-2588.87689666	a.u.
M06 free energy in solution:	-2589.03334966	a.u.
M06-2X SCF energy in solution:	-2590.39601063	a.u.
M06-2X enthalpy in solution:	-2589.40878711	a.u.
M06-2X free energy in solution:	-2589.56524011	a.u.
Imaginary frequency:	-111.2221	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.07303400	1.58017500	-0.46156500
O	-1.15968300	2.77875600	-1.95934700
O	-1.48880800	3.14017500	0.18837400
N	1.94804800	2.19743400	1.63786900
N	1.09250500	0.26110700	2.22531500
C	1.08485900	1.22254200	1.24640500
C	2.58161100	1.95339500	2.93526900
H	2.30073000	2.72566100	3.66251600
H	3.67058300	1.94781700	2.83727100
C	2.04305800	0.56529600	3.31493300
H	2.83524700	-0.18815600	3.33850500
H	1.52456200	0.55782800	4.28004900
C	0.10590300	-0.74737500	2.48612200
C	0.38148800	-2.10280200	2.24213800
C	-0.61369300	-3.04973000	2.53046700
H	-0.40894700	-4.09849400	2.32137900
C	-1.84759300	-2.68837400	3.06824600
C	-2.06598900	-1.33734800	3.36931300
H	-3.01679300	-1.03711400	3.80219300
C	-1.10854300	-0.35924500	3.10214000
C	1.70940800	-2.57447400	1.69664100
H	2.20243000	-3.24019400	2.41719900
H	2.38590200	-1.74658000	1.48228200
H	1.57435700	-3.15528900	0.77548300
C	-2.93671700	-3.70885800	3.29846600
H	-3.71872800	-3.60779500	2.53520500
H	-3.41829800	-3.57168100	4.27362400
H	-2.54727700	-4.73141700	3.25232100
C	-1.38935300	1.08530500	3.45372500
H	-1.43551200	1.72747200	2.56670800
H	-0.61421900	1.50212700	4.10845300
H	-2.34650000	1.16961600	3.97705700
C	0.98183100	0.45334600	-1.70214300
C	-1.66642900	0.24670900	-0.15445700
H	-1.79824300	0.22793700	0.91696400
C	-0.78090900	-0.65585900	-0.80650700
H	-0.14878700	-1.33689200	-0.25226400
C	-1.56515400	-1.17356900	-2.04262900
H	-0.99727300	-1.69164900	-2.81129700
C	-2.95387000	0.26292600	-1.02028200
H	-3.64096200	1.08879300	-0.83580500
C	-2.38069800	0.07329700	-2.44530900
C	-2.69897000	-2.01540400	-1.42315400
C	-3.54862700	-1.15093700	-0.82773800
H	-3.15339200	-0.16469100	-3.18236000
H	-1.79070700	0.92443500	-2.77768000
H	0.48139300	0.62320800	-2.67333300
C	2.16993200	-0.43331300	-2.05617000
C	1.76582300	-1.79597800	-2.70856200
C	3.33112600	-0.85001200	-1.15190400
H	2.65238400	0.18453900	-2.84121700

C	3.01559700	-2.68764500	-2.63328600
C	3.80183400	-2.06526500	-1.50357100
H	0.97358800	-2.25467300	-2.11376800
H	3.61056400	-2.64781500	-3.55742600
H	2.77591500	-3.74150500	-2.46136800
H	1.38572700	-1.66556500	-3.72578900
C	4.09510700	0.01700200	-0.19511200
O	3.99465500	-0.00449900	1.01194800
C	5.04946800	-2.65600500	-0.96488100
O	5.83085700	-2.10788000	-0.20857900
C	-4.73261300	-1.40194000	0.03224100
O	-4.77277900	-1.11505700	1.21291500
C	-2.63765900	-3.48364500	-1.39487200
O	-1.74435500	-4.13092500	-1.91410300
O	4.96408600	0.79242300	-0.87107200
O	5.23552500	-3.91071600	-1.43551000
O	-3.66401300	-4.04982900	-0.71710900
O	-5.76755500	-1.91574400	-0.65525100
C	-6.95224900	-2.16870000	0.11808200
H	-6.75328300	-2.92386600	0.88354200
H	-7.29891900	-1.25255500	0.60331500
H	-7.69270000	-2.53188600	-0.59493300
C	-3.64487000	-5.48352000	-0.66734500
H	-3.68173000	-5.90466900	-1.67578000
H	-2.74002100	-5.84030400	-0.16769000
H	-4.53228300	-5.76807700	-0.10102300
C	5.99591800	1.40553500	-0.07487700
H	5.56940900	2.05929600	0.68723100
H	6.59261100	0.62267500	0.39984000
H	6.59961100	1.98073000	-0.77728700
C	6.42784900	-4.56707600	-0.97917400
H	7.31569700	-4.00527100	-1.28206600
H	6.42184400	-4.65879400	0.11031400
H	6.41716000	-5.55135700	-1.44814700
C	1.90907200	3.52893400	0.99715300
C	1.30747400	3.29687100	-0.39657700
C	3.32825200	4.11759700	0.91113000
C	1.01395900	4.47028500	1.83348700
H	3.98033500	3.46859700	0.31935100
H	3.78352300	4.26737100	1.89920800
H	-0.01181700	4.09564800	1.85752800
H	1.38459800	4.58446200	2.85991500
H	0.75893600	4.18124700	-0.73348100
C	-1.74493400	3.41712700	-1.02673200
C	-2.72138500	4.55149800	-1.38240000
C	-1.87752600	5.73344800	-1.91390200
H	-1.29613100	5.43479700	-2.79180400
H	-2.53199500	6.56709700	-2.19711600
H	-1.18151700	6.09651600	-1.14841400
C	-3.67979700	4.07235600	-2.49078000
H	-4.30894300	3.24385900	-2.14238100
H	-4.34494500	4.89018600	-2.79402400
H	-3.12414700	3.73098800	-3.36834100
C	-3.51964500	4.99419800	-0.14566400
H	-2.85711400	5.34435600	0.65071500
H	-4.20276500	5.80979400	-0.41394200
H	-4.11585400	4.16941800	0.25974000
H	2.10903200	3.11364700	-1.12295100
H	3.28712300	5.09401200	0.41608600
H	1.00165000	5.46747700	1.37852600

3.31-TS-D

exo-syn/syn

(cis,isotactic dyad)

B3LYP SCF energy:	-2590.79085462	a.u.
B3LYP enthalpy:	-2589.80316700	a.u.
B3LYP free energy:	-2589.96336300	a.u.
M06 SCF energy in solution:	-2589.86453254	a.u.
M06 enthalpy in solution:	-2588.87684492	a.u.
M06 free energy in solution:	-2589.03704092	a.u.
M06-2X SCF energy in solution:	-2590.40078980	a.u.
M06-2X enthalpy in solution:	-2589.41310218	a.u.
M06-2X free energy in solution:	-2589.57329818	a.u.
Imaginary frequency:	-179.6176	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.30517700	-0.38050200	1.14928000
O	0.11491900	1.21141300	2.68294500
O	-1.04087400	-0.61446000	3.11188000
N	1.70789600	-2.85233900	0.59912300
N	-0.05488700	-3.00813300	-0.69706500
C	0.58666600	-2.18129200	0.21240100
C	1.99826400	-4.04329100	-0.19406300
H	2.34178300	-4.87455400	0.42601600
H	2.77609900	-3.83292500	-0.94309900
C	0.63928800	-4.31094300	-0.83743200
H	0.71069800	-4.60398400	-1.88788900
H	0.07621200	-5.08797000	-0.30254500
C	-1.45864300	-3.06569200	-0.99929800
C	-1.86324800	-3.04414200	-2.34771900
C	-3.22505100	-3.18011700	-2.64533400
H	-3.53845900	-3.14357500	-3.68698000
C	-4.18469300	-3.36644200	-1.64906100
C	-3.74493300	-3.44672600	-0.32269500
H	-4.47113100	-3.62411700	0.46783100
C	-2.39821900	-3.31429200	0.02798300
C	-0.87359000	-2.91444000	-3.48320200
H	-1.30647800	-2.35321900	-4.31794500
H	-0.59291300	-3.90177500	-3.87587600
H	0.04471200	-2.41359800	-3.16926300
C	-5.65436600	-3.47639900	-1.98188800
H	-5.81375500	-3.61581300	-3.05598300
H	-6.19478900	-2.57020100	-1.67904700
H	-6.12180600	-4.31818000	-1.45770300
C	-1.99700000	-3.45822600	1.47717300
H	-1.77861000	-2.49228200	1.94303400
H	-1.10128500	-4.07904800	1.59320400
H	-2.80503700	-3.92881200	2.04616100
C	1.32099200	0.79681500	0.04317700
C	-0.69543600	1.41904300	-0.06058600
H	-0.50458000	2.28862200	0.55830000
C	-1.61894200	0.40824300	0.40799500

H	-2.15766900	0.55042300	1.33824000
C	-2.46573100	0.04054900	-0.83171300
H	-3.04608100	-0.87387200	-0.76390300
C	-1.04232500	1.62334000	-1.55324900
H	-0.32656700	2.18010600	-2.15578700
C	-1.42192600	0.18487700	-1.96145500
C	-3.30233300	1.30485500	-1.11976200
C	-2.44456900	2.26280300	-1.53128400
H	-1.85831700	0.12927400	-2.96248900
H	-0.59897700	-0.52018600	-1.86272000
H	1.58900100	1.66510900	0.66345500
C	2.06161300	0.91168900	-1.28579300
C	2.17893800	-0.32459200	-2.21290600
C	3.52307700	1.31864300	-1.08642900
H	1.60745300	1.75428300	-1.83279900
C	3.58322200	-0.24903800	-2.86133500
H	1.38297500	-0.35361800	-2.96094600
H	2.09232500	-1.22577500	-1.60331100
C	4.34015600	0.69610800	-1.95456600
H	4.07012300	-1.22655600	-2.94582600
H	3.54299300	0.16278800	-3.87971200
C	-4.75273000	1.33582200	-0.82801300
O	-5.23924800	0.79491800	0.14699900
C	-2.63064000	3.69002100	-1.86214700
O	-1.85007100	4.31913900	-2.55312700
C	3.88427000	2.42763700	-0.15124500
O	3.49248300	3.56523700	-0.30947200
C	5.78439000	0.99606600	-2.08372900
O	6.38285800	1.87661700	-1.49564900
O	-5.47358000	1.96750100	-1.77441400
O	-3.73182600	4.23021900	-1.29995000
O	4.61312600	2.00604700	0.89256500
O	6.37790100	0.16058000	-2.97065500
C	-6.88434300	2.04128300	-1.51736100
H	-7.31094300	1.03959200	-1.41566200
H	-7.07784200	2.60325900	-0.59954200
H	-7.31101000	2.55524900	-2.37919300
C	-3.96321800	5.61126600	-1.61654900
H	-3.11875500	6.22633400	-1.29437300
H	-4.10573000	5.74086400	-2.69308000
H	-4.86799600	5.88662000	-1.07379000
C	5.03421500	3.03835900	1.80254600
H	5.70151600	3.73528400	1.28921800
H	4.17012400	3.58059200	2.19433000
H	5.56153900	2.52051700	2.60355500
C	7.77965200	0.38840700	-3.17808400
H	7.95350400	1.40288100	-3.54710500
H	8.33316500	0.25275100	-2.24483100
H	8.08977000	-0.34902900	-3.91920700
C	2.53649600	-2.36472700	1.71897000
C	1.61068400	-1.38538200	2.45359000
C	3.82617100	-1.70240900	1.20726500
C	2.90910400	-3.54894800	2.63640000
H	0.99482400	-1.92378500	3.18095800
H	3.60895200	-0.80696300	0.62298100
H	4.40873000	-2.39225500	0.58294100
H	2.01580700	-4.10949100	2.93441500
H	3.62183600	-4.24248600	2.17185100
C	-0.65750600	0.54232200	3.45432600
C	-1.11002900	1.17618700	4.77895800
C	0.14520400	1.55133900	5.59563800
H	0.78733200	2.23513600	5.03322000
H	-0.14719300	2.03837500	6.53417600
H	0.73260400	0.66018300	5.84841900
C	-1.90921400	2.45648100	4.44803900
H	-2.80390500	2.22362600	3.85759500
H	-2.23690200	2.94589800	5.37340000
H	-1.29764200	3.16363600	3.87971600
C	-1.98842700	0.19966600	5.57648900
H	-1.44420800	-0.71946100	5.81588400
H	-2.30732700	0.66656800	6.51669100
H	-2.88164000	-0.08349000	5.01127100
H	2.17971500	-0.61704400	2.99112000
H	3.37911000	-3.15789600	3.54483200
H	4.45856600	-1.40665800	2.05178800

3.31-TS-E

endo-anti/anti

(cis,isotactic dyad)

B3LYP SCF energy:	-2590.78947898	a.u.
B3LYP enthalpy:	-2589.80206100	a.u.
B3LYP free energy:	-2589.95938100	a.u.
M06 SCF energy in solution:	-2589.86167792	a.u.
M06 enthalpy in solution:	-2588.87425994	a.u.
M06 free energy in solution:	-2589.03157994	a.u.
M06-2X SCF energy in solution:	-2590.39577871	a.u.
M06-2X enthalpy in solution:	-2589.40836073	a.u.
M06-2X free energy in solution:	-2589.56568073	a.u.
Imaginary frequency:	-164.0073	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.45141900	-0.28783300	0.64357800
O	0.38650600	1.73758300	1.38504400
O	-1.46946800	0.94845700	2.27216600
N	-0.84329300	-2.94033200	1.70850500
N	-2.42869000	-2.72525700	0.20853600
C	-1.36657900	-2.07634900	0.80688200
C	-1.41619300	-4.28581900	1.64937900
H	-1.63060300	-4.67721900	2.64776000
H	-0.72367800	-4.97894900	1.15311800
C	-2.68187200	-4.04890300	0.82194900
H	-2.84173500	-4.80900300	0.05207700
H	-3.58282200	-4.00483200	1.44769200
C	-3.54673100	-2.14159000	-0.47749600
C	-3.74456700	-2.44362200	-1.83697200
C	-4.87498500	-1.92546700	-2.48155100
H	-5.02532700	-2.14883000	-3.53588900
C	-5.81587500	-1.14334300	-1.80764400
C	-5.61132300	-0.89388400	-0.44528300
H	-6.34396000	-0.30473600	0.10271600
C	-4.49674600	-1.38300200	0.24247700
C	-2.78884000	-3.33268500	-2.60032100

H	-2.89846100	-3.18579800	-3.67942100
H	-2.98349200	-4.39469600	-2.39793700
H	-1.74554400	-3.14614900	-2.32828700
C	-7.01877100	-0.57499300	-2.52460900
H	-7.20285200	-1.09215900	-3.47179800
H	-6.87881100	0.48978400	-2.75280500
H	-7.92430200	-0.65567700	-1.91265700
C	-4.32623500	-1.08257100	1.71499000
H	-3.47101700	-0.42422300	1.90628200
H	-4.16260500	-1.99407600	2.30202900
H	-5.22229100	-0.59288900	2.10833800
C	0.62352900	-0.95724400	-0.79405900
H	0.42460600	-1.94233700	-1.24694500
C	-1.94592000	0.74077100	-0.60717800
H	-2.86779100	0.31363400	-0.24045800
C	-1.17247800	0.06864100	-1.60263000
H	-1.48354100	-0.89326500	-1.99003300
C	-0.84294300	1.16169600	-2.66816700
C	-2.07890100	2.20754500	-1.10837400
C	-2.23441000	1.88352600	-2.63240500
C	0.01434700	2.29315200	-2.10099900
C	-0.73942300	2.93390200	-1.17859100
C	1.88733600	-0.37728100	-1.43033400
C	3.12963900	-0.98438600	-0.77245600
C	2.06754100	-0.83273800	-2.91020600
H	1.90743100	0.70350800	-1.29478000
C	3.68554000	-1.93743000	-1.54436100
C	2.92874100	-2.11521600	-2.84420300
H	2.59819300	-0.05539800	-3.46921100
H	3.60171600	-2.21806100	-3.70324500
H	-2.86629000	2.77735400	-0.61698800
H	-3.07778700	1.22022400	-2.85426100
H	-2.27458500	2.76937200	-3.27820300
H	-0.48937400	0.77841600	-3.62447700
H	1.11151000	-0.99772200	-3.41565600
H	2.32963900	-3.03542100	-2.81210500
C	-0.56656600	4.22307800	-0.47447200
O	-1.30853900	4.59880500	0.41602800
C	1.32531500	2.61904900	-2.71455000
O	1.54956000	2.43523800	-3.89899500
C	4.84347400	-2.81605000	-1.22830600
O	4.82884900	-4.01513300	-1.42674100
C	3.64744700	-0.53653600	0.55289600
O	4.14161800	-1.25136900	1.40253500
O	0.41255100	4.99300500	-0.98732000
O	2.23728000	3.09428700	-1.85157700
O	5.90417000	-2.13998400	-0.75356700
O	3.50944900	0.79597000	0.67914100
C	7.01597900	-2.95128900	-0.34257300
H	6.72092400	-3.60550000	0.48200100
H	7.37671000	-3.56119000	-1.17506600
H	7.78359300	-2.24916200	-0.01657000
C	3.92509400	1.35518100	1.93391500
H	3.72991500	2.42344600	1.85132800
H	3.33912600	0.92647500	2.75003200
H	4.98756100	1.16017000	2.10558200
C	3.50331800	3.45248300	-2.42426300
H	3.97359200	2.58496100	-2.89505100
H	3.37643700	4.23906600	-3.17327100
H	4.10745800	3.80761700	-1.58963900
C	0.55924800	6.28686100	-0.38517400
H	-0.38279700	6.84042500	-0.42473900
H	0.87360900	6.19276000	0.65761100
H	1.32829000	6.79327500	-0.96963200
C	0.39269900	-2.60875100	2.44722900
C	1.58564300	-3.34096200	1.80632600
C	0.24427700	-3.05953000	3.91434900
C	0.51118700	-1.07519400	2.35962300
H	1.46705400	-4.43047200	1.86258700
H	1.69493000	-3.06240700	0.75469900
H	0.19001100	-4.15097400	4.02105900
H	-0.65040700	-2.61757200	4.36704100
H	0.01488300	-0.62526700	3.22339300
C	-0.52144600	1.80207100	2.27290100
C	-0.45996400	2.82601100	3.42287500
C	-1.83550600	3.50665900	3.57756100
H	-1.81496300	4.20154500	4.42704200
H	-2.09384400	4.06990900	2.67662200
H	-2.61644700	2.76232600	3.75862500
C	0.63186300	3.87978400	3.18211800
H	0.68487500	4.56144200	4.04057600
H	1.61289700	3.41337100	3.05113000
H	0.41254100	4.47111100	2.29016000
C	-0.13531600	2.03896300	4.71487100
H	-0.08999600	2.72637200	5.56875200
H	-0.90305900	1.28604300	4.91768300
H	0.83347900	1.53006700	4.64047400
H	2.51539900	-3.07599300	2.31629600
H	1.11640200	-2.71878000	4.48210900
H	1.56236800	-0.77224300	2.37490900

3.31-TS-F

endo-anti/syn
(trans,isotactic dyad)

B3LYP SCF energy:	-2590.79817274	a.u.
B3LYP enthalpy:	-2589.81051200	a.u.
B3LYP free energy:	-2589.96451700	a.u.
M06 SCF energy in solution:	-2589.86934453	a.u.
M06 enthalpy in solution:	-2588.88168379	a.u.
M06 free energy in solution:	-2589.03568879	a.u.
M06-2X SCF energy in solution:	-2590.40277336	a.u.
M06-2X enthalpy in solution:	-2589.41511262	a.u.
M06-2X free energy in solution:	-2589.56911762	a.u.
Imaginary frequency:	-159.0560	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	1.05914300	-0.23080500	-0.72007800
O	2.25914400	1.74670800	-0.95450400
O	3.34074600	-0.15599700	-0.71327600
N	0.94224900	-2.68782900	-2.21447000
N	0.44881400	-3.27440100	-0.15201000
C	0.77015900	-2.20033200	-0.95620800
C	0.77588500	-4.13740100	-2.33295100

H	1.68348600	-4.61213600	-2.72272100
H	-0.04612200	-4.38006200	-3.01668200
C	0.47257300	-4.55879200	-0.88684100
H	-0.48940200	-5.07368300	-0.78993800
H	1.24321400	-5.21654800	-0.46868300
C	0.57581900	-3.37043800	1.27672300
C	-0.56761700	-3.57530900	2.07013900
C	-0.40060900	-3.73722600	3.45285700
H	-1.28477100	-3.88825600	4.06902700
C	0.85712000	-3.71769600	4.05597500
C	1.97989200	-3.56351700	3.23254700
H	2.97258400	-3.58450500	3.67795700
C	1.86905400	-3.40518400	1.84936200
C	-1.96578600	-3.62278200	1.49526500
H	-1.96252000	-3.82079100	0.42084000
H	-2.50056400	-2.67838500	1.65706600
H	-2.55118100	-4.40985000	1.98389500
C	1.01045000	-3.86349700	5.55233500
H	1.87249100	-4.48998300	5.80800200
H	0.11941200	-4.31038300	6.00494700
H	1.16758700	-2.88818400	6.03161400
C	3.11880600	-3.30338700	1.00210000
H	3.20548000	-2.33976200	0.48876000
H	3.14410200	-4.07972200	0.22692800
H	4.00979700	-3.43411300	1.62399400
C	-0.79074800	0.21028000	-0.68577900
H	-1.00407900	1.28814100	-0.64492600
C	1.38007800	0.00417900	1.46033000
H	1.99943800	-0.85850900	1.66843300
C	-0.03647900	-0.08736200	1.43199300
H	-0.56817900	-1.02109900	1.54374800
C	-0.54731000	1.13338900	2.25524400
C	1.69515100	1.30404300	2.25964300
C	0.57926700	1.14130700	3.34315400
C	-0.19985000	2.44305600	1.55086400
C	1.14375400	2.54635900	1.56082600
C	-2.04050700	-0.60302300	-0.95796900
C	-3.39481400	-0.08978400	-0.46573800
C	-2.26853300	-0.63882500	-2.50590600
H	-1.90379400	-1.62354700	-0.57940000
C	-4.34643000	-0.18740800	-1.41527800
C	-3.79415600	-0.73772300	-2.71089400
H	-1.70802600	-1.45274700	-2.96824800
H	-4.12409000	-1.77786600	-2.84907100
H	2.72777600	1.39898200	2.59241000
H	0.64420600	0.20197800	3.90348900
H	0.50155500	1.98835800	4.03488000
H	-1.57735100	1.04033900	2.59190100
H	-1.90151000	0.29888300	-2.93989300
H	-4.14522600	-0.18243900	-3.58648600
C	1.98301300	3.70682600	1.21382000
O	3.17093000	3.79023900	1.47032600
C	-1.25215900	3.41917100	1.15565300
O	-1.98461600	3.94953000	1.96869900
C	-3.65591200	0.28054600	0.95585800
O	-3.52707400	-0.50565900	1.87626800
C	-5.78562500	0.08497000	-1.18451300
O	-6.30590600	0.30601600	-0.10684300
O	1.26968900	4.71679900	0.67093000
O	-1.34935300	3.60030100	-0.17183700
O	-3.99618400	1.56925700	1.09043900
O	-6.48102000	0.03725300	-2.34515900
C	2.00153600	5.91886000	0.39639200
H	2.51871300	6.26987900	1.29344100
H	2.73358800	5.74818600	-0.39705600
H	1.25574800	6.64593600	0.07270200
C	-2.39811900	4.48626300	-0.59968600
H	-3.37315600	4.05557300	-0.35650600
H	-2.29776700	5.46019300	-0.11472200
H	-2.27578300	4.57768000	-1.67905400
C	-4.49725900	1.98227500	2.37968300
H	-5.56007600	1.73011200	2.42614300
H	-3.95887700	1.47916400	3.18388100
H	-4.33722700	3.05749700	2.42571700
C	-7.89269800	0.26800700	-2.22300000
H	-8.34827800	-0.47829000	-1.56648600
H	-8.08468300	1.26340700	-1.81335200
H	-8.29104800	0.18544900	-3.23463700
C	1.59709300	-1.86410500	-3.25601300
C	1.41779000	-0.40438100	-2.80489800
C	0.94052700	-2.13557600	-4.62247400
C	3.09456200	-2.23431400	-3.31846500
H	-0.13414300	-1.92395600	-4.59455000
H	1.07988400	-3.17173800	-4.95855400
H	3.58208400	-1.98646600	-2.37252700
H	3.24963500	-3.29748700	-3.54287800
C	3.35268500	1.10073500	-0.93902800
C	4.70500600	1.77948200	-1.22627000
C	4.51591000	3.24005100	-1.66461000
H	5.48977700	3.67910700	-1.91616000
H	3.86963700	3.31089800	-2.54602100
H	4.07080600	3.83259900	-0.86307000
C	5.56161900	1.71887700	0.05871900
H	5.70827100	0.68207800	0.37883900
H	6.54730400	2.16357000	-0.12868600
H	5.08418700	2.27619400	0.87048900
C	5.41197400	0.98970500	-2.34900200
H	6.38936200	1.43979100	-2.56268600
H	5.56426300	-0.05387200	-2.06089800
H	4.82624500	1.00594000	-3.27661000
H	1.39199800	-1.48226700	-5.37659600
H	3.58236200	-1.65937500	-4.11343900
H	2.28637100	0.19200100	-3.09427200
H	0.54523600	0.03761800	-3.29960000

3.31-TS-G

(cis,isotactic dyad)

B3LYP SCF energy:	-2590.79517164	a.u.
B3LYP enthalpy:	-2589.80712400	a.u.
B3LYP free energy:	-2589.96442100	a.u.
M06 SCF energy in solution:	-2589.87143329	a.u.
M06 enthalpy in solution:	-2588.88338565	a.u.
M06 free energy in solution:	-2589.04068265	a.u.
M06-2X SCF energy in solution:	-2590.40562778	a.u.
M06-2X enthalpy in solution:	-2589.41758014	a.u.

M06-2X free energy in solution: -2589.57487714 a.u.

Imaginary frequency: -91.8233 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.49804000	-0.70995300	0.59114200
N	0.68818300	-2.44395900	2.58968700
N	2.15542200	-2.55071300	0.95899000
C	0.99586200	-1.97085900	1.37498900
C	1.53313900	-3.57251600	2.99601800
C	2.69522800	-3.46707400	1.99456600
C	-0.48066900	-1.92254400	3.34001200
C	-1.65085500	-2.92279400	3.27781100
C	-0.07162800	-1.70430400	4.81033600
C	-0.81274700	-0.57432900	2.65569600
C	3.09751700	-2.00372200	0.01549800
C	3.30781100	-2.65218700	-1.21200600
C	4.30205400	-2.16096100	-2.06723900
C	5.09253100	-1.06118600	-1.72833300
C	4.86900000	-0.44650300	-0.49100300
C	3.89032200	-0.90002500	0.39714300
C	2.47018600	-3.83277800	-1.62758000
C	6.16606400	-0.54482600	-2.65836800
C	3.72372900	-0.21798200	1.73503700
C	0.16759700	1.09140900	0.60099100
C	0.83807700	1.90185300	-0.50637900
C	2.09438300	2.64394500	-0.04847400
C	1.32557400	1.14929300	-1.77228100
C	3.04066600	2.65178200	-1.00703200
C	2.59837200	1.89268600	-2.23965500
H	1.85893100	-3.47866700	4.03500100
H	0.98232400	-4.51581300	2.88997700
H	2.96554800	-4.42909000	1.55054800
H	3.59552800	-3.03480100	2.44733800
H	-1.96446500	-3.09107100	2.24676600
H	-1.37107000	-3.88717800	3.72178300
H	0.82469000	-1.07744500	4.88229600
H	0.11499700	-2.64621000	5.34224000
H	-0.17227000	0.20575100	3.09966900
H	4.45896000	-2.65645400	-3.02287200
H	5.47284000	0.41248800	-0.20706500
H	2.88685800	-4.31269800	-2.51863000
H	2.39726400	-4.58744900	-0.83671200
H	1.45465000	-3.49975400	-1.85705900
H	6.06438200	0.53603700	-2.81045200
H	7.16854700	-0.72211100	-2.24726400
H	6.11804100	-1.03357000	-3.63662900
H	2.67449400	-0.00806800	1.95948000
H	4.11633500	-0.83525100	2.55491300
H	4.25807700	0.73427500	1.75352300
H	0.20806500	1.66942900	1.53784400
H	0.13494500	2.70350100	-0.78502200
H	1.56530000	0.11758700	-1.50388600
H	3.36961500	1.21450000	-2.61456600
O	-0.44470900	-1.80417800	-1.63150500
O	-1.30522100	-2.80074200	0.14273300
C	-2.53669700	-0.18010100	0.35089700
C	-1.89429300	1.12387400	0.43729000
C	-2.33524800	1.85668200	-0.86004000
C	-3.29792400	-0.16746700	-0.99504900
C	-2.36343400	0.69213500	-1.87648300
C	-3.85060000	2.06910400	-0.67596800
C	-4.43278600	0.85536700	-0.77910700
H	-3.08335000	-0.57629900	1.20207100
H	-1.95818600	1.67099400	1.37411500
H	-1.80373800	2.77244700	-1.11374300
H	-3.61892800	-1.14047000	-1.36163200
H	-2.82184400	0.98420700	-2.82599600
H	-1.40212000	0.21085700	-2.05064100
H	0.56164600	1.10895600	-2.55164900
H	2.38368400	2.60479700	-3.05004500
H	-1.85006500	-0.30801600	2.90624500
H	-0.88550900	-1.19088100	5.33301800
H	-2.49849700	-2.53229300	3.85288500
C	-1.58716500	-3.95422700	-1.96718400
C	-1.06392300	-2.77442000	-1.11230700
C	-3.13254200	-3.92756800	-1.93312000
H	-3.52575900	-3.03808200	-2.43885200
H	-3.53348300	-4.80565300	-2.45443200
H	-3.50429400	-3.93523300	-0.90428000
C	-1.11074000	-3.84083600	-3.42404600
H	-0.02077100	-3.89968100	-3.50265100
H	-1.53698000	-4.65727600	-4.02057300
H	-1.42130800	-2.88996500	-3.86693900
C	-1.10864100	-5.28294200	-1.34415600
H	-1.50723600	-6.13066800	-1.91533500
H	-0.01597500	-5.36064100	-1.35066000
H	-1.45034100	-5.37026000	-0.30896500
C	-4.40187800	3.40039200	-0.36183900
O	-3.78551300	4.43668300	-0.53176100
C	-5.83204900	0.41571400	-0.56818900
O	-6.12512300	-0.49022000	0.18792600
C	2.09091300	3.43833600	1.21503700
O	1.24983500	4.28177700	1.45059900
C	4.29424600	3.43935100	-0.92954300
O	4.54752300	4.30305400	-0.11178300
O	-6.71757900	1.07540900	-1.33611600
O	-5.65055500	3.35340500	0.15254800
O	3.06970200	3.08718500	2.06728400
O	5.15379300	3.09421400	-1.92294600
C	-6.23603600	4.63019300	0.44711600
H	-5.62409700	5.17682700	1.16968000
H	-6.32981600	5.23010800	-0.46247300
H	-7.21923200	4.41077900	0.86465600
C	-8.08916400	0.68660600	-1.15682500
H	-8.21698200	-0.37981400	-1.36076900
H	-8.41443300	0.89441000	-0.13377500
H	-8.65671300	1.28594500	-1.86919100
C	3.17625100	3.90458600	3.24556000
H	3.43590800	4.92831900	2.96438200
H	2.23475100	3.90732900	3.80047900
H	3.97386300	3.45687800	3.83876500
C	6.37781000	3.84430100	-1.95442400
H	6.17068000	4.91116800	-2.07327100
H	6.94461900	3.69604000	-1.03117900
H	6.93337200	3.46243400	-2.81149300

3.31-TS-H

(trans,isotactic dyad)

B3LYP SCF energy: -2590.79235039 a.u.

B3LYP enthalpy: -2589.80444600 a.u.

B3LYP free energy:	-2589.96319000	a.u.
M06 SCF energy in solution:	-2589.86899602	a.u.
M06 enthalpy in solution:	-2588.88109163	a.u.
M06 free energy in solution:	-2589.03983563	a.u.
M06-2X SCF energy in solution:	-2590.40038138	a.u.
M06-2X enthalpy in solution:	-2589.41247699	a.u.
M06-2X free energy in solution:	-2589.57122099	a.u.
Imaginary frequency:	-64.0617	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.28759800	-0.52024900	0.69711200
N	1.81889100	-0.70237100	2.70781500
N	2.83391300	-1.29760000	0.85929900
C	1.63834700	-0.93929800	1.40358900
C	3.18698500	-0.95636200	3.17051900
C	3.93382900	-1.15825400	1.84343200
C	0.66070400	-0.47533000	3.59909700
C	0.25118000	-1.82868100	4.21888800
C	1.04984100	0.52041000	4.70564400
C	-0.46936700	0.08313900	2.70374400
C	3.09741400	-1.99441600	-0.37199000
C	3.22546700	-3.39810400	-0.32063000
C	3.60170300	-4.07934200	-1.48245200
C	3.83607300	-3.41160400	-2.68853000
C	3.69784200	-2.02224200	-2.70582900
C	3.34188800	-1.29381300	-1.56527500
C	2.96034100	-4.17182900	0.95115000
C	4.19948900	-4.17465900	-3.94105600
C	3.24411000	0.20733800	-1.63697600
C	0.05071500	1.24635500	0.06727400
C	0.43539800	2.60188800	0.68027600
C	1.81269600	3.04016500	0.17681100
C	-0.43780600	3.78243900	0.14847700
C	1.71020800	3.89655500	-0.86041100
C	0.26447600	4.24749200	-1.14582900
H	3.57143400	-0.09968700	3.72778700
H	3.22130500	-1.84351700	3.81750700
H	4.57917400	-2.03934900	1.83916200
H	4.54072400	-0.28322200	1.58771600
H	-0.08120100	-2.51785000	3.43636900
H	1.08054400	-2.29136600	4.76940300
H	1.45155800	1.44186300	4.27112900
H	1.79436400	0.10898800	5.40013100
H	-0.49440600	1.17607600	2.81055700
H	3.70662200	-5.16194500	-1.44346100
H	3.88137300	-1.48068800	-3.63146500
H	3.71189800	-3.97479600	1.72644800
H	1.98132100	-3.92008800	1.37113400
H	2.98084800	-5.24800100	0.75493900
H	4.80916500	-5.05612000	-3.71315800
H	3.29995000	-4.52830500	-4.46239900
H	4.75781600	-3.54796700	-4.64461000
H	3.92785300	0.69241900	-0.93221700
H	3.49015400	0.57349900	-2.63775300
H	2.23367700	0.54668100	-1.39457300
H	-0.00298600	1.35540000	-1.03149000
H	0.42249700	2.54671200	1.76885400
H	-1.49172600	3.54353900	0.00229100
H	-0.09364200	3.71768000	-2.04019700
O	-0.23581900	-1.96137300	-1.19627400
O	-0.54065700	-2.78147100	0.82934400
C	-2.48553100	-0.47505400	0.56049300
C	-2.12254700	0.89101400	0.38217300
C	-2.71574900	1.29479800	-0.99488600
C	-3.31379800	-0.84587200	-0.69519300
C	-2.58821300	-0.02494400	-1.78655600
C	-4.23441000	1.29467600	-0.74291100
C	-4.59933900	0.00410100	-0.57821800
H	-2.82009300	-0.85359300	1.52133000
H	-2.14782500	1.60474200	1.19917800
H	-2.34141300	2.21019100	-1.44858400
H	-3.47876300	-1.90751900	-0.86197900
H	-3.14013800	0.01011500	-2.73070300
H	-1.56723100	-0.36655400	-1.95460900
H	-0.38677700	4.59287600	0.88581100
H	0.13576400	5.31818000	-1.34310700
H	-1.42751600	-0.28295100	3.10178500
H	0.15956100	0.77235500	5.29188000
H	-0.57284500	-1.68188900	4.92654800
C	-0.83017400	-4.32583600	-1.04117500
C	-0.49261300	-2.94157800	-0.43928800
C	-2.36018500	-4.37950300	-1.26304700
H	-2.67899400	-3.62690400	-1.99206800
H	-2.64418200	-5.36451800	-1.65397400
H	-2.90400200	-4.21716200	-0.32571300
C	-0.12328400	-4.50945100	-2.39551400
H	0.96492500	-4.49460100	-2.28055300
H	-0.41003100	-5.47166000	-2.83902800
H	-0.39509400	-3.70985700	-3.08978400
C	-0.43757700	-5.45485700	-0.07196100
H	-0.74988900	-6.42347500	-0.48236200
H	0.64498600	-5.49106400	0.08140900
H	-0.91307600	-5.31997700	0.90319400
C	-5.88267800	-0.60173100	-0.14503100
O	-5.98084800	-1.27142200	0.86427800
C	-4.96058000	2.55615300	-0.53258900
O	-4.42988800	3.65271500	-0.60931400
C	3.06369300	2.65586200	0.86356900
O	3.11969600	2.05235600	1.92001100
C	2.80143800	4.45059700	-1.71865100
O	3.19950200	3.91421100	-2.72947100
O	-6.88697200	-0.38658700	-1.01215700
O	-6.26426100	2.38590000	-0.22368200
O	3.20981100	5.65728500	-1.28338300
O	4.16583100	3.11136800	0.22076900
C	-8.14891500	-0.96583100	-0.64109200
H	-8.05403500	-2.04754300	-0.51427600
H	-8.50955900	-0.52842300	0.29388000
H	-8.82821000	-0.73196300	-1.46120600
C	-7.00165100	3.59469300	0.00769700
H	-6.57470600	4.15259400	0.84575000
H	-6.99077100	4.22962100	-0.88251600
H	-8.01865400	3.27593300	0.23831300
C	4.22104400	6.28862100	-2.08854600
H	5.12696100	5.67701600	-2.11043200

H	3.86388200	6.43215500	-3.11164800
H	4.41677700	7.24850900	-1.61018600
C	5.41812400	2.88617400	0.88206800
H	5.64631400	1.81722600	0.92169300
H	6.16346800	3.40586800	0.27948900
H	5.39485800	3.28593000	1.89909400

3.33-TS-A-rotamer1

exo-anti/anti

(cis,syndiotactic dyad)

B3LYP SCF energy:	-2756.93657380	a.u.
B3LYP enthalpy:	-2755.96070800	a.u.
B3LYP free energy:	-2756.11338300	a.u.
M06 SCF energy in solution:	-2755.98400148	a.u.
M06 enthalpy in solution:	-2755.00813568	a.u.
M06 free energy in solution:	-2755.16081068	a.u.
M06-2X SCF energy in solution:	-2756.55640344	a.u.
M06-2X enthalpy in solution:	-2755.58053764	a.u.
M06-2X free energy in solution:	-2755.73321264	a.u.
Imaginary frequency:	-110.3878	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.38512000	-0.77632700	0.55778700
O	0.78824700	-0.11629100	2.62285400
O	-0.24548800	-2.02227300	2.50580500
N	1.38703700	-2.48398400	-1.56273200
N	-0.59249400	-1.89159500	-2.28515700
C	0.27620700	-1.79204600	-1.22362700
C	1.40118600	-2.95430800	-2.94907700
H	1.74199300	-3.99067700	-3.02069600
H	2.06960500	-2.33172100	-3.55900000
C	-0.06954800	-2.78360500	-3.34593300
H	-0.19904300	-2.33137700	-4.33278900
H	-0.61510700	-3.73615800	-3.33351800
C	2.53596000	-2.52642700	-0.65346000
C	3.62565300	-1.50250400	-1.05058900
H	3.18407200	-0.50183000	-1.10687900
H	4.02684200	-1.74256800	-2.04595300
C	4.75836000	-1.52480100	-0.00357200
H	5.51660400	-0.78179900	-0.27944800
C	5.38710300	-2.93163200	0.04341300
H	5.82512900	-3.18705700	-0.93217300
H	6.20463200	-2.95501400	0.77665800
C	4.30504500	-3.96169800	0.42872300
H	4.74399300	-4.96807100	0.45541100
C	3.18038200	-3.93653300	-0.63051700
H	2.41259000	-4.68576500	-0.39455800
H	3.60106200	-4.19287900	-1.61436200
C	3.72777000	-3.60675400	1.81510400
H	2.97879500	-4.35090900	2.11786200
H	4.52909900	-3.63436700	2.56739400
C	3.08775400	-2.19474000	1.76985700
H	2.69817100	-1.94944900	2.76322800
C	1.94620900	-2.22099600	0.73628600
H	1.30018100	-3.07535200	0.99036100
C	4.17150600	-1.17689000	1.37845300
H	3.73434300	-0.17817600	1.36020400
H	4.97439300	-1.16964500	2.12923200
C	-2.01075600	-1.66903500	-2.27050500
C	-2.54983300	-0.63712100	-3.06053400
C	-3.93406800	-0.42763600	-3.03109100
H	-4.35175000	0.38578000	-3.62078500
C	-4.78526200	-1.22124000	-2.25894100
C	-4.22546000	-2.28168500	-1.53776900
H	-4.87470600	-2.91876100	-0.94266200
C	-2.85116700	-2.53321100	-1.53616100
C	-1.67641100	0.23970900	-3.92944800
H	-2.20727300	1.15196600	-4.21792100
H	-1.38642700	-0.27376500	-4.85622900
H	-0.74931800	0.52609100	-3.42260800
C	-6.26433100	-0.93168800	-2.16974200
H	-6.59108000	-0.25214700	-2.96383500
H	-6.49971600	-0.46738900	-1.20394800
H	-6.85915700	-1.84947900	-2.24072500
C	-2.30221600	-3.70316400	-0.74844500
H	-1.69687200	-3.38277800	0.10714700
H	-1.66245300	-4.34642300	-1.36404500
H	-3.12018500	-4.31833400	-0.36276900
C	0.88134100	0.76342300	-0.44984000
H	0.88916700	0.70488300	-1.55036000
C	-1.78094500	-0.31229500	0.81219500
H	-2.22123700	-1.23828200	0.46961500
C	-1.47315000	0.74925700	-0.05956000
H	-1.57124200	0.67945700	-1.13202600
C	-1.90092900	2.04004600	0.67172200
H	-1.53813400	2.98267100	0.26853800
C	-2.39016700	0.35228700	2.07437500
H	-2.44605300	-0.27330600	2.96488400
N	0.27746500	-1.12448200	3.25004300
O	0.30217300	-1.19909400	4.46845400
C	-1.59719000	1.68260500	2.14442700
C	-3.44173300	1.92396300	0.71550700
C	-3.73684300	0.92397000	1.57118500
H	-2.04035400	2.39847400	2.84222400
H	-0.54417200	1.53592900	2.37459700
C	1.24172700	2.20364000	-0.05633500
C	0.75163000	3.19322200	-1.16144200
C	2.74986300	2.46505500	-0.09925300
H	0.84859000	2.44184400	0.93280200
C	1.93286300	3.31010400	-2.15309300
H	0.56768300	4.17389200	-0.70696100
H	-0.17522300	2.87253900	-1.64499700
C	3.12326800	3.03661300	-1.25914800
H	1.88273300	2.57546600	-2.96871000
H	1.99127800	4.29727100	-2.62659900
C	-4.30808500	2.70330300	-0.18010000
O	-3.89195000	3.50939700	-0.99325200
C	-5.03976700	0.27682300	1.87660400
O	-5.34506700	-0.82521900	1.46478100
C	4.51424300	3.34178800	-1.70880600
O	5.06222900	2.73045200	-2.60221300
C	3.68837800	2.25214300	1.03016300
O	4.90138100	2.21879000	0.93437700

O	-5.79743700	1.01523800	2.70215600
O	-5.62368900	2.42441000	-0.01672100
O	5.03803500	4.39955400	-1.06988800
O	3.02098600	2.15992800	2.19671200
C	-7.06072300	0.43132800	3.06662200
H	-7.51302000	1.13311100	3.76736900
H	-7.69231900	0.30941800	2.18249900
H	-6.91140200	-0.54386000	3.53701500
C	-6.51440500	3.16619300	-0.86283700
H	-6.39458300	4.24053200	-0.69971900
H	-6.31990100	2.94362500	-1.91569300
H	-7.51831800	2.84538400	-0.58309100
C	6.40638700	4.69756200	-1.39645900
H	6.64965000	5.59936900	-0.83421900
H	7.04959900	3.86893200	-1.08942700
H	6.51974200	4.86739400	-2.47024600
C	3.82259500	1.99750600	3.37757700
H	3.11152900	1.84000000	4.18757500
H	4.48424800	1.13520400	3.27308900
H	4.42399100	2.89461200	3.55143200

3.33-TS-A-rotamer2

exo-anti/anti

(cis,syndiotactic dyad)

B3LYP SCF energy:	-2756.93847010	a.u.
B3LYP enthalpy:	-2755.96233600	a.u.
B3LYP free energy:	-2756.11490000	a.u.
M06 SCF energy in solution:	-2755.98542780	a.u.
M06 enthalpy in solution:	-2755.00929370	a.u.
M06 free energy in solution:	-2755.16185770	a.u.
M06-2X SCF energy in solution:	-2756.55886790	a.u.
M06-2X enthalpy in solution:	-2755.58273380	a.u.
M06-2X free energy in solution:	-2755.73529780	a.u.
Imaginary frequency:	-129.4449	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	-1.30343600	-0.59931400	-0.65090500
O	-1.38729000	-0.12114100	-2.83780200
O	-1.40117100	-2.23383800	-2.35194800
N	-2.96261800	-1.51021600	1.54221000
N	-0.92147400	-1.88352200	2.24393100
C	-1.65788600	-1.42829500	1.18007700
C	-3.16643600	-1.85157500	2.95083100
H	-3.95793200	-2.59570400	3.07471500
H	-3.44249800	-0.95833100	3.52822500
C	-1.78275000	-2.38257500	3.34046400
H	-1.43279500	-2.00974500	4.30686500
H	-1.75283800	-3.47960600	3.36778200
C	-3.99793600	-0.96155000	0.66261500
C	-4.36485200	0.48727300	1.06789400
H	-3.45414100	1.09284800	1.10967100
H	-4.80902500	0.49412000	2.07422100
C	-5.36022800	1.07722700	0.05027600
H	-5.60498300	2.10852900	0.33907900
C	-6.64351100	0.22285400	0.04424500
H	-7.11884600	0.24646100	1.03545300
H	-7.36985000	0.63650700	-0.66833100
C	-6.29039400	-1.22731400	-0.34667100
H	-7.20043300	-1.84179900	-0.34542600
C	-5.29525800	-1.80830400	0.68697700
H	-5.05684500	-2.85267400	0.44634300
H	-5.75861900	-1.79677300	1.68522100
C	-5.66208600	-1.22754800	-1.75735100
H	-5.43977800	-2.25434600	-2.07632200
H	-6.38200800	-0.81699000	-2.47994100
C	-4.36121100	-0.38308200	-1.75322400
H	-3.92774300	-0.38311000	-2.75816200
C	-3.38701700	-1.03533700	-0.75122800
C	-4.71357900	1.06337100	-1.35033500
H	-3.81141300	1.68506500	-1.35720300
H	-5.40732900	1.49722400	-2.08415400
C	0.43895700	-2.34565500	2.23626600
C	1.40626600	-1.63987900	2.97286100
C	2.72387900	-2.11554900	2.96924000
H	3.48202700	-1.55679600	3.51371000
C	3.08977500	-3.27231700	2.27884200
C	2.09076900	-3.98334000	1.60356100
H	2.35741900	-4.88918700	1.06517600
C	0.76435200	-3.54905100	1.57280200
C	1.06010900	-0.40081700	3.76775800
H	1.95864400	0.18872400	3.97341700
H	0.61026800	-0.66026500	4.73640300
H	0.34331000	0.23907700	3.24400000
C	4.52433800	-3.73987200	2.22837000
H	4.91806600	-3.63499800	1.21027700
H	4.61239700	-4.79784600	2.50339600
H	5.16075900	-3.16069400	2.90545100
C	-0.27455300	-4.35131600	0.82047500
H	-0.62380900	-3.83202400	-0.07951200
H	-1.16061100	-4.55463100	1.43309900
H	0.14160700	-5.31307200	0.50703300
C	-0.94572900	1.06645500	0.23191900
H	-0.77865400	1.08688100	1.31399900
C	0.79183500	-1.15993300	-0.87496800
H	0.86876000	-2.13217000	-0.40737100
C	0.96627900	0.04322100	-0.11380000
H	1.10781100	-0.00680300	0.95668600
C	1.95229400	0.90923500	-0.93585000
H	2.05801500	1.95128000	-0.64368400
C	1.63772200	-0.95495700	-2.16106100
H	1.41519600	-1.62308800	-2.99347000
C	1.53046500	0.57266100	-2.38332200
C	3.26878600	0.10365000	-0.88399000
C	3.09304200	-0.99868900	-1.63979400
H	2.24965000	0.94059100	-3.12019100
H	0.52539800	0.88636800	-2.65030300
C	-1.14991000	2.51695100	-0.21734700
C	-1.25826700	2.88570700	-1.72590400
C	-0.11829300	3.51601600	0.30724800
H	-2.11121600	2.73440200	0.27889300
C	-0.03848900	3.78298400	-2.04939500
H	-2.17615600	3.46190400	-1.88225300
H	-1.32236300	2.00955800	-2.36843700

C	0.47128400	4.19917200	-0.69108500
H	0.75633200	3.25923500	-2.59624400
H	-0.30916200	4.65193900	-2.66206500
C	4.36501000	0.44887100	0.03390900
O	4.27549400	1.28830300	0.91014900
C	3.97618100	-2.18074800	-1.82540200
O	3.79877600	-3.24805200	-1.27070500
C	1.60195800	5.16834800	-0.57895100
O	2.70778400	4.92487800	-1.01527700
C	0.20989400	3.74581500	1.73427100
O	1.18824300	4.33743600	2.14527500
O	4.94429800	-1.94976100	-2.72636900
O	5.48272500	-0.28615900	-0.18337700
O	1.23528700	6.33341200	-0.02339000
O	-0.73975000	3.23186500	2.55989100
C	5.82320800	-3.05796100	-2.98504300
H	6.50767400	-2.71068900	-3.75908200
H	6.37256100	-3.32665500	-2.07859900
H	5.25626700	-3.92625300	-3.33065100
C	6.57566100	-0.00765900	0.70309600
H	6.86364800	1.04499700	0.63949900
H	6.30298000	-0.23775700	1.73714300
H	7.39234100	-0.64982900	0.37138000
C	2.30212700	7.27700900	0.17694500
H	1.82866400	8.16698300	0.59215700
H	3.03338800	6.86733100	0.87832900
H	2.79702200	7.50742700	-0.76999600
C	-0.51309000	3.46179900	3.95954400
H	-1.35707800	2.99959600	4.47257300
H	0.42928500	3.00683800	4.27605900
H	-0.47602900	4.53394000	4.16981800
N	-1.43725400	-1.33964600	-3.26513500
O	-1.51331500	-1.60195700	-4.45336800
H	-3.33165600	-2.10415300	-1.00111100

3.33-TS-A-rotamer3

exo-anti/anti
(cis,syndiotactic dyad)

B3LYP SCF energy:	-2756.93536519	a.u.
B3LYP enthalpy:	-2755.95953700	a.u.
B3LYP free energy:	-2756.11146300	a.u.
M06 SCF energy in solution:	-2755.97888241	a.u.
M06 enthalpy in solution:	-2755.00305422	a.u.
M06 free energy in solution:	-2755.15498022	a.u.
M06-2X SCF energy in solution:	-2756.55102256	a.u.
M06-2X enthalpy in solution:	-2755.57519437	a.u.
M06-2X free energy in solution:	-2755.72712037	a.u.
Imaginary frequency:	-118.6992	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.41006700	0.64693500	0.51221100
O	-1.08706300	-0.72662300	2.09940900
O	-0.00063800	1.00104200	2.82819700
N	-0.97885300	3.21677300	-0.71826300
N	1.07466800	2.79629100	-1.34931300
C	0.02845400	2.32059300	-0.59770200
C	-0.72804600	4.27033300	-1.70341100
H	-1.00961700	5.25472100	-1.32009600
H	-1.30192200	4.08431800	-2.62146100
C	0.78099600	4.12866000	-1.92711200
H	1.06666800	4.16450300	-2.98188200
H	1.35261200	4.89885400	-1.39358000
C	-2.28228000	2.94706800	-0.10676300
C	-3.26857800	2.34110000	-1.13291000
H	-2.81695200	1.44917000	-1.57962700
H	-3.45448900	3.06061100	-1.94412100
C	-4.59007300	1.97452200	-0.43008700
H	-5.27986500	1.53621500	-1.16408200
C	-5.21746100	3.24505300	0.17644300
H	-5.44896600	3.97310000	-0.61467900
H	-6.16687400	2.99778800	0.67033500
C	-4.23727300	3.85900400	1.19670600
H	-4.67478500	4.76880200	1.62899400
C	-2.92251000	4.23443700	0.47354200
H	-2.22007400	4.70952500	1.17103100
H	-3.14182600	4.96219300	-0.32239000
C	-3.96003700	2.83121000	2.31520400
H	-3.29657600	3.26415000	3.07579300
H	-4.90267900	2.57586100	2.82033700
C	-3.31294000	1.55763900	1.70918300
H	-3.13015000	0.82982500	2.50571700
C	-1.98125600	1.98174400	1.05697600
C	-4.28858300	0.95110400	0.68187300
H	-3.86304000	0.04091900	0.25252800
H	-5.22144000	0.65764100	1.18312900
C	2.46372200	2.44525800	-1.24178100
C	3.10250300	1.83483700	-2.33527400
C	4.46288300	1.52013500	-2.22110400
H	4.95661300	1.02621300	-3.05543900
C	5.19487600	1.81292100	-1.06905800
C	4.54268900	2.47369700	-0.02139800
H	5.09924100	2.71638100	0.88021600
C	3.18884900	2.80847000	-0.08564500
C	2.36496700	1.52468000	-3.61821200
H	2.28629500	2.41331000	-4.25971300
H	1.34452300	1.17634300	-3.43107100
H	2.89057800	0.75630500	-4.19317600
C	6.64330000	1.41028500	-0.93130400
H	6.74637300	0.63282900	-0.16485300
H	7.26800800	2.25662900	-0.62149200
H	7.04428700	1.02046200	-1.87256400
C	2.53408900	3.52663600	1.07425400
H	1.78288900	2.90545300	1.57515300
H	2.02540500	4.44375100	0.75401900
H	3.28379300	3.80570700	1.82004500
C	-0.74516400	-0.31227000	-1.11228000
H	-0.38759100	0.13116100	-2.05156400
C	1.64607300	-0.10400000	0.76793100
H	2.22969000	0.79936300	0.87441500
C	1.36347900	-0.65734600	-0.51492800
H	1.67393000	-0.14883600	-1.41683100
C	1.63984900	-2.17132200	-0.38491300
H	1.27274200	-2.81122500	-1.18632400

C	2.06257500	-1.31148300	1.64862300
H	2.05927600	-1.14370800	2.72590200
C	1.19218900	-2.45108100	1.06617000
C	3.16846800	-2.23778700	-0.18124000
C	3.42304200	-1.74217100	1.04771800
H	1.50843300	-3.43999400	1.40821400
H	0.13010300	-2.33009500	1.24712200
C	-1.50188700	-1.58124200	-1.54696800
C	-2.12517400	-1.30254400	-2.95551400
C	-2.67961700	-2.19934500	-0.78470000
H	-0.75111900	-2.38266000	-1.63830200
C	-3.39307300	-2.16680600	-3.06061200
H	-1.40444000	-1.49224200	-3.75679900
H	-2.40302100	-0.24390800	-3.01341900
C	-3.68738900	-2.52521200	-1.62197500
H	-4.22589300	-1.64933700	-3.54714600
H	-3.21776400	-3.08504600	-3.63901900
C	4.07988900	-2.63301500	-1.26497200
O	3.70588100	-2.96072100	-2.37740000
C	4.71928100	-1.45327100	1.71363800
O	5.12838500	-0.32691900	1.92017300
C	-4.89318900	-3.30440600	-1.24067600
O	-5.04551700	-3.94781000	-0.22173200
C	-2.58600500	-2.71886000	0.61741200
O	-1.75940100	-3.55754300	0.91963900
O	5.34730200	-2.57070700	2.11351400
O	5.38514400	-2.58172300	-0.90716000
O	-5.83381800	-3.23402400	-2.21643400
O	-3.49718000	-2.20212800	1.43944400
C	6.60159600	-2.36596700	2.78548500
H	6.93814800	-3.35988800	3.08067400
H	7.32379900	-1.90120500	2.10849300
H	6.46909900	-1.72578400	3.66139000
C	6.31306900	-2.96704900	-1.93090800
H	6.12205000	-3.99265800	-2.25815000
H	6.23404800	-2.30048500	-2.79441200
H	7.30075100	-2.88807400	-1.47542600
C	-7.03640700	-3.97216700	-1.95642100
H	-7.67262700	-3.81164600	-2.82754900
H	-6.81562000	-5.03577000	-1.83088000
H	-7.52465700	-3.60405300	-1.04993500
C	-3.50393000	-2.73560600	2.77838700
H	-4.38763300	-2.30621500	3.25092400
H	-3.57595200	-3.82489900	2.74481000
H	-2.59790300	-2.42532100	3.30176500
N	-0.63388100	-0.07134100	3.11295800
O	-0.80977800	-0.46249800	4.25707800
H	-1.42880500	2.57233100	1.80214700

3.33-TS-B

exo-syn/anti

(trans,isotactic dyad)

B3LYP SCF energy:	-2756.92952487	a.u.
B3LYP enthalpy:	-2755.95356800	a.u.
B3LYP free energy:	-2756.10578400	a.u.
M06 SCF energy in solution:	-2755.97435967	a.u.
M06 enthalpy in solution:	-2754.99840280	a.u.
M06 free energy in solution:	-2755.15061880	a.u.
M06-2X SCF energy in solution:	-2756.54964309	a.u.
M06-2X enthalpy in solution:	-2755.57368622	a.u.
M06-2X free energy in solution:	-2755.72590222	a.u.
Imaginary frequency:	-152.4310	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	1.32098900	0.08315800	-0.75000600
O	0.92566000	-0.77931600	-2.75556200
O	1.68917100	1.25005000	-2.77305500
N	3.41802600	0.68852300	1.16649000
N	1.86093400	2.12568700	1.71875400
C	2.16786400	1.10358200	0.84224100
C	3.94325200	1.26202800	2.40436900
H	4.99307100	1.54745000	2.30499800
H	3.85940400	0.54124500	3.22977400
C	3.01745800	2.46220300	2.58776400
H	2.69889000	2.60658300	3.62235400
H	3.47633700	3.39607800	2.23598000
C	0.93701100	3.21252800	1.54308100
C	0.01981000	3.48801200	2.57662900
C	-0.81522200	4.60477700	2.45484000
H	-1.53459500	4.80742400	3.24587300
C	-0.74381500	5.46682600	1.35861000
C	0.21428700	5.19755900	0.37503400
H	0.31025000	5.87288900	-0.47264800
C	1.06940500	4.09311700	0.44595000
C	-0.06971100	2.63666800	3.82321400
H	-1.09400600	2.61922100	4.20947700
H	0.56536400	3.03916800	4.62443400
H	0.24674900	1.60663100	3.64053200
C	-1.66870700	6.65496500	1.23259900
H	-2.14992700	6.89161900	2.18697300
H	-2.46344300	6.46266700	0.50005100
H	-1.12996000	7.54708800	0.89349800
C	2.10768000	3.89644800	-0.63361800
H	1.80841500	3.12830900	-1.35268300
H	3.07523800	3.58824400	-0.22260900
H	2.25928400	4.82865200	-1.18643100
C	0.61327500	-1.26876000	0.38960300
C	-1.06630600	-0.29152800	-0.68165100
H	-1.14425600	-1.08321500	-1.41551500
C	-0.73719300	1.03705000	-1.06021100
H	-0.62780700	1.33038200	-2.09798200
C	-1.60104500	1.93823600	-0.14788000
H	-1.32267700	2.98703000	-0.09792000
C	-2.12547400	-0.16979800	0.43938900
H	-2.32576000	-1.05746800	1.03192000
C	-1.63390600	1.10389400	1.15235000
C	-3.05139000	1.67919100	-0.62150200
C	-3.35701300	0.40635600	-0.28709500
H	-2.35063700	1.48145000	1.88635700
H	-0.65313300	0.98731800	1.60997900
H	0.39128500	-1.01229500	1.43637800
C	0.40153000	-2.77823600	0.21004100
C	0.15841500	-3.40269200	-1.19631800

C	-0.77193300	-3.31451300	1.02247500
H	1.32314400	-3.19126100	0.65216600
C	-1.32120900	-3.86401300	-1.21508600
H	0.80430100	-4.28088700	-1.30081200
H	0.40521300	-2.72507100	-2.01159000
C	-1.69995200	-3.90478800	0.24906700
H	-1.98341900	-3.17560200	-1.75762600
H	-1.44368600	-4.84011000	-1.69665300
C	-3.76241500	2.68778800	-1.44240600
O	-3.22960300	3.26086900	-2.37278400
C	-4.50788900	-0.45711100	-0.61319900
O	-4.65440400	-1.57749600	-0.15474200
C	-2.95210200	-4.51043900	0.76432500
O	-3.19087900	-4.75591000	1.93155100
C	-0.75403600	-3.23172900	2.51321800
O	0.10885100	-3.75438300	3.18901000
O	-5.01233100	2.94102400	-1.01524600
O	-5.36625100	0.10160700	-1.49210700
O	-1.74685100	-2.47181900	3.00914400
O	-3.80775600	-4.77082600	-0.24697900
C	-5.73988000	3.90173500	-1.79795000
H	-5.20977400	4.85753900	-1.82586200
H	-5.87128700	3.53931400	-2.82108600
H	-6.70477500	4.01022200	-1.30198300
C	-6.49752200	-0.70834000	-1.84276800
H	-6.17164900	-1.64793900	-2.29719000
H	-7.10066000	-0.93170700	-0.95827800
H	-7.06985200	-0.11568000	-2.55697800
C	-1.86275200	-2.46461100	4.44157800
H	-2.10671800	-3.46893800	4.79669000
H	-0.93032900	-2.13094600	4.90448300
H	-2.67600100	-1.77358800	4.66386400
C	-5.09440800	-5.26508800	0.14986300
H	-4.99108100	-6.16497000	0.76176200
H	-5.62854200	-4.49917400	0.71832500
H	-5.62122300	-5.48762200	-0.77873500
C	4.11439200	-0.29832000	0.33821500
C	4.04626500	-1.71621700	0.95012300
C	5.61096300	0.05982500	0.14055800
C	3.40508700	-0.20305200	-1.02633400
H	4.58440200	-1.73303900	1.90927700
H	3.00493700	-1.97230900	1.16221600
C	4.67074800	-2.73339600	-0.02595600
H	6.16040400	0.01812000	1.09278100
H	5.69712900	1.08393100	-0.24704400
C	6.23993200	-0.94872700	-0.85088300
H	3.67550400	0.77938300	-1.44032200
C	3.99347600	-1.26917300	-1.97394000
H	4.60083200	-3.74020400	0.40708900
C	6.15087100	-2.36947300	-0.25658300
C	3.90848800	-2.68464800	-1.36729800
H	7.29278000	-0.67895700	-1.00731500
C	5.48734900	-0.91771200	-2.19891400
H	3.47345300	-1.25541500	-2.93707300
H	6.61589100	-3.09142400	-0.94137600
H	6.70685100	-2.42280600	0.69032000
H	2.86203900	-2.96943500	-1.22050300
H	4.34179500	-3.41449000	-2.06545900
H	5.57297600	0.07417200	-2.66215100
H	5.94706600	-1.63583900	-2.89294800
N	1.32552400	0.23346000	-3.45796600
O	1.35129600	0.20033300	-4.67357000

3.33-TS-C-rotamer1

exo-anti/syn

(trans,syndiotactic dyad)

B3LYP SCF energy:	-2756.94007810	a.u.
B3LYP enthalpy:	-2755.96433700	a.u.
B3LYP free energy:	-2756.11512100	a.u.
M06 SCF energy in solution:	-2755.97988011	a.u.
M06 enthalpy in solution:	-2755.00413901	a.u.
M06 free energy in solution:	-2755.15492301	a.u.
M06-2X SCF energy in solution:	-2756.55315559	a.u.
M06-2X enthalpy in solution:	-2755.57741449	a.u.
M06-2X free energy in solution:	-2755.72819849	a.u.
Imaginary frequency:	-99.1720	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	-1.41307000	-0.55174500	-0.62972000
O	-1.53540100	-0.41436900	-2.84073500
O	-1.61287300	-2.44543500	-2.07802500
N	-3.07397600	-1.11118900	1.69122200
N	-1.05013500	-1.58584700	2.37954300
C	-1.76930100	-1.11238800	1.30603300
C	-3.27751800	-1.37827100	3.11362100
H	-4.11403000	-2.06241400	3.28011500
H	-3.48494200	-0.44690700	3.66015400
C	-1.92655800	-1.98472400	3.50368100
H	-1.53902800	-1.60063200	4.45090300
H	-1.96874200	-3.07992600	3.57128400
C	0.26017500	-2.17442600	2.36374200
C	1.28637400	-1.58245700	3.12065500
C	2.55810500	-2.17058000	3.09099600
H	3.36290800	-1.69750900	3.65008200
C	2.81915600	-3.33559500	2.36891500
C	1.75232900	-3.95204300	1.70395800
H	1.92866000	-4.87655600	1.15972700
C	0.46794900	-3.40468900	1.69806700
C	1.03890900	-0.38139900	4.00203900
H	0.71887600	-0.70068800	5.00461000
H	0.26809900	0.27320000	3.59249700
H	1.94744400	0.21380800	4.11723300
C	4.20779300	-3.92326200	2.29008400
H	4.90653200	-3.39401400	2.94627900
H	4.58640200	-3.86242100	1.26253300
H	4.21279200	-4.98264100	2.57450300
C	-0.65062300	-4.13457100	0.98532700
H	-0.93383100	-3.65335700	0.04273900
H	-1.55856600	-4.19137700	1.59642200
H	-0.34248700	-5.15788100	0.75091500
C	-0.97790600	1.27166800	-0.36391000
C	0.70755000	-1.24162100	-0.87644600
H	0.69818100	-2.14938000	-0.29137400
C	0.97274600	0.01651000	-0.30039300

H	1.06798000	0.18598900	0.76254200
C	1.91396900	0.74789000	-1.29320300
H	2.05089100	1.81941300	-1.15938400
C	1.47137300	-1.25296800	-2.22580900
H	1.17976400	-2.02277800	-2.94030100
C	1.38952500	0.23540200	-2.65395700
C	3.21720400	-0.08074500	-1.22349800
C	2.95677400	-1.27434100	-1.79806800
H	2.07374700	0.47284800	-3.47304200
H	0.38188000	0.55465000	-2.90907700
H	-0.81444900	1.75052500	-1.34611000
C	-0.92406400	2.34567200	0.72228700
C	-2.01383700	3.41667700	0.36566400
C	0.33276600	3.22651900	0.67970500
H	-1.08032600	1.90491700	1.71044400
C	-1.29417600	4.45592400	-0.52039800
C	0.14207400	4.33143300	-0.06832800
H	-2.88878700	2.99353700	-0.12719400
H	-1.67089000	5.47545900	-0.37834200
H	-1.39074100	4.23154200	-1.59234800
H	-2.34672000	3.89387100	1.29486000
C	1.55253700	2.91571200	1.45972800
O	1.72457200	1.88098700	2.08147500
C	1.16771300	5.32071700	-0.51972100
O	2.01646600	5.08713300	-1.35159600
C	3.78777500	-2.50201000	-1.88778900
O	3.51482400	-3.53161800	-1.30171800
C	4.42534000	0.39575800	-0.53539800
O	4.56481500	1.52804300	-0.10594600
O	2.42737500	3.93669000	1.46945200
O	0.96189300	6.52906500	0.04048700
O	5.37782100	-0.55855600	-0.41975300
O	4.82437500	-2.36341300	-2.73077200
C	5.66063400	-3.52409400	-2.87197500
H	6.14063600	-3.76465500	-1.91927400
H	5.07329300	-4.38427600	-3.20332400
H	6.40683800	-3.25511900	-3.61981300
C	6.58867500	-0.14176100	0.22541100
H	7.05102400	0.68637400	-0.31874900
H	6.38789400	0.17603200	1.25245000
H	7.23991300	-1.01638100	0.21751800
C	3.65644000	3.70860100	2.18429400
H	3.44538600	3.45758600	3.22733200
H	4.21683000	2.90378700	1.70687000
H	4.20157300	4.65083800	2.12012500
C	1.86927800	7.56164900	-0.38348900
H	2.89799700	7.29078600	-0.13231900
H	1.79559600	7.71741900	-1.46304400
H	1.56410200	8.45782300	0.15718200
C	-4.11135100	-0.64857100	0.77054700
C	-3.51639000	-0.88019400	-0.63145600
C	-4.45887600	0.83398000	1.03014900
C	-5.42039600	-1.46919100	0.89050800
H	-3.48984400	-1.97084200	-0.76765000
C	-4.48577000	-0.32087000	-1.69217100
H	-3.53699400	1.41677700	1.02918800
H	-4.91087600	0.94052600	2.02770100
C	-5.44066300	1.33936000	-0.04497500
H	-5.20196800	-2.53653700	0.75350700
H	-5.87585900	-1.35005300	1.88523400
C	-6.41512800	-0.97754900	-0.18954600
H	-4.05879800	-0.43534500	-2.69333500
C	-4.80892200	1.16477700	-1.44281700
C	-5.80175100	-1.13757800	-1.59691100
H	-5.66530200	2.39988700	0.13545600
C	-6.73978500	0.51270700	0.04703900
H	-7.33650300	-1.57051500	-0.11681600
H	-5.50321200	1.53243000	-2.21136100
H	-3.89328800	1.76211300	-1.53056900
H	-5.59980800	-2.19605100	-1.80773500
H	-6.52185400	-0.79277700	-2.35300000
H	-7.20650500	0.65055600	1.03298100
H	-7.46483100	0.85964800	-0.70164400
N	-1.63897700	-1.67556100	-3.09913800
O	-1.75265100	-2.08936200	-4.24092900

3.33-TS-C-rotamer2

exo-anti/syn

(trans,syndiotactic dyad)

B3LYP SCF energy:	-2756.93835310	a.u.
B3LYP enthalpy:	-2755.96287700	a.u.
B3LYP free energy:	-2756.11582900	a.u.
M06 SCF energy in solution:	-2755.98336767	a.u.
M06 enthalpy in solution:	-2755.00789157	a.u.
M06 free energy in solution:	-2755.16084357	a.u.
M06-2X SCF energy in solution:	-2756.55575053	a.u.
M06-2X enthalpy in solution:	-2755.58027443	a.u.
M06-2X free energy in solution:	-2755.73322643	a.u.
Imaginary frequency:	-136.1503	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.22794400	-1.00086600	-0.70127000
O	-0.17361900	-1.00621100	-2.93577000
O	0.79730400	-2.68826800	-1.97077500
N	-1.55068800	-2.22469900	1.55304000
N	0.39729300	-1.58831500	2.35243700
C	-0.39355000	-1.59916100	1.22189800
C	-1.68360500	-2.51976800	2.97818600
H	-2.05468900	-3.53417300	3.14788500
H	-2.38080800	-1.81832800	3.45853900
C	-0.24167200	-2.32456100	3.46931400
H	-0.17934900	-1.74957100	4.39792100
H	0.27368800	-3.28006800	3.63068100
C	1.83540800	-1.51667800	2.38245300
C	2.46996100	-0.45335600	3.04824500
C	3.87064700	-0.42516000	3.08863600
H	4.36062500	0.40513700	3.59400200
C	4.64962500	-1.42124900	2.50140500
C	3.98912600	-2.49830500	1.89816200
H	4.57686200	-3.29982300	1.45631100
C	2.59694300	-2.57710700	1.83456500
C	1.70457400	0.66425400	3.72034900
H	2.15394000	0.90920000	4.68925200

H	0.65670000	0.40690400	3.88269200
H	1.72872100	1.58363400	3.11960800
C	6.15650500	-1.34148000	2.49029700
H	6.61223200	-2.31194000	2.71848000
H	6.52706600	-0.61198100	3.21810900
H	6.50542600	-1.03979100	1.49532400
C	1.95586400	-3.77093000	1.16218400
H	1.58933700	-3.52481900	0.15961100
H	1.10411800	-4.16200600	1.72872200
H	2.68479600	-4.58004800	1.05579200
C	-0.94923300	0.74843300	-0.52197300
C	1.90062200	-0.32978000	-0.73658800
H	2.38918200	-1.06345500	-0.10990000
C	1.27944200	0.82685100	-0.20876900
H	1.17685000	0.99985800	0.85453500
C	1.69244100	1.99166300	-1.14041200
H	1.13791000	2.92398200	-1.03600100
C	2.65216500	0.15241200	-2.00683000
H	2.96377000	-0.62321100	-2.70645000
C	1.73042400	1.28969200	-2.51665500
C	3.21140900	2.12849200	-0.90351100
C	3.79222900	1.03531200	-1.44336300
H	2.21264600	1.90669600	-3.27973300
H	0.77053700	0.93167900	-2.88081100
H	-1.05459800	1.16530800	-1.53587300
C	-1.41903300	1.80240700	0.47688000
C	-1.62327300	1.41568200	1.96600100
C	-2.76029200	2.44025700	0.10601100
H	-0.68150200	2.62375100	0.41041900
C	-2.84754900	2.22183400	2.46548000
C	-3.52762300	2.65761600	1.18784400
H	-1.83080200	0.34751100	2.02824900
H	-2.55149000	3.10498500	3.04853100
H	-3.50825100	1.63447600	3.11226700
H	-0.72920700	1.61325000	2.55974100
C	-3.10941900	2.82044200	-1.29943000
O	-3.45828300	2.02981100	-2.15004800
C	-4.85220700	3.31411000	1.12235800
O	-5.43730700	3.62230400	0.10083500
C	5.19992400	0.56382700	-1.40238600
O	5.53736100	-0.46249000	-0.84461200
C	3.76081000	3.20727600	-0.06739100
O	3.07289200	4.07011600	0.45072000
O	-2.91615500	4.13271100	-1.51221200
O	-5.35222900	3.53182300	2.36129800
O	5.10150600	3.13392400	0.08844800
O	6.03031000	1.35385700	-2.10121100
C	7.40604100	0.93625200	-2.12080900
H	7.82549200	0.96088700	-1.11129000
H	7.49463100	-0.07720800	-2.52047700
H	7.91700200	1.65149400	-2.76546600
C	5.67982300	4.16532300	0.90140400
H	5.48525700	5.15072500	0.46940300
H	5.26774300	4.13556400	1.91393700
H	6.75036400	3.95858700	0.91694700
C	-3.29360100	4.60343900	-2.81966000
H	-2.74959900	4.06110500	-3.59696000
H	-4.36813100	4.46707800	-2.96464900
H	-3.03444400	5.66220800	-2.83199100
C	-6.64072600	4.16415000	2.39817300
H	-6.59834500	5.14926700	1.92565900
H	-7.38262700	3.55345100	1.87661500
H	-6.89156100	4.25566300	3.45540400
C	-2.56826900	-2.46440900	0.52073000
C	-1.77336900	-2.46486500	-0.80061800
C	-3.67624600	-1.38524000	0.53070000
C	-3.24300200	-3.84948400	0.68527800
C	-2.75135700	-2.61484000	-1.98188700
H	-3.22161900	-0.39674100	0.43685700
H	-4.21895100	-1.41607300	1.48787500
C	-4.64496900	-1.61710000	-0.64596500
H	-2.47279700	-4.63167400	0.72392700
H	-3.81688900	-3.90343700	1.62293600
C	-4.19614900	-4.08696700	-0.51092700
H	-2.20924200	-2.56802500	-2.93185000
C	-3.84907600	-1.53309300	-1.96515200
C	-3.42120000	-4.00816700	-1.84432700
H	-5.41876600	-0.83869900	-0.63101600
C	-5.29678700	-3.00631800	-0.50498900
H	-4.65188500	-5.08061500	-0.40495000
H	-4.52806400	-1.68120800	-2.81657800
H	-3.41359000	-0.53503700	-2.07575500
H	-2.65913000	-4.79792200	-1.88999500
H	-4.11314400	-4.18211400	-2.68066400
H	-5.88001600	-3.06205000	0.42589300
H	-5.99744000	-3.18153700	-1.33249800
N	0.47626900	-2.11061800	-3.07054400
O	0.76334200	-2.56596200	-4.16397200
H	-1.15019800	-3.37051000	-0.77896500

3.33-TS-C-rotamer3

exo-anti/syn

(trans,syndiotactic dyad)

B3LYP SCF energy:	-2756.92614001	a.u.
B3LYP enthalpy:	-2755.95069800	a.u.
B3LYP free energy:	-2756.10071200	a.u.
M06 SCF energy in solution:	-2755.96889982	a.u.
M06 enthalpy in solution:	-2754.99345781	a.u.
M06 free energy in solution:	-2755.14347181	a.u.
M06-2X SCF energy in solution:	-2756.54088606	a.u.
M06-2X enthalpy in solution:	-2755.56544405	a.u.
M06-2X free energy in solution:	-2755.71545805	a.u.
Imaginary frequency:	-148.9354	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.57983500	-1.36176300	-0.56248300
O	-0.27592800	-2.70566200	-2.33076700
O	0.20608200	-3.58035600	-0.40470700
N	-2.41143200	-0.94010700	1.63082000
N	-0.49737800	-0.17414800	2.37685800
C	-1.11981000	-0.71361500	1.28577700
C	-2.76639400	-0.50601600	2.98201200
H	-3.15692000	-1.34224600	3.57265700

H	-3.52230400	0.28440500	2.95383700
C	-1.42169600	0.01973900	3.51607300
H	-1.46890300	1.07943400	3.77973100
H	-1.06370800	-0.54182700	4.38660900
C	0.90792900	-0.10938800	2.66259500
C	1.58507000	1.12080000	2.63707900
C	2.94827800	1.13825200	2.97014500
H	3.47869900	2.08847600	2.93632500
C	3.63831100	-0.01397800	3.34041700
C	2.92488100	-1.21882400	3.39904400
H	3.44405700	-2.12892000	3.69024700
C	1.57073300	-1.29126600	3.07567500
C	0.90051000	2.41982000	2.27946200
H	0.87517900	3.09276300	3.14693100
H	-0.12651500	2.26950300	1.94504600
H	1.45217800	2.94842700	1.49143400
C	5.11518600	0.01456800	3.65225600
H	5.33225900	-0.46738300	4.61331700
H	5.49691700	1.04001000	3.69542200
H	5.67363200	-0.52840500	2.88053500
C	0.85464600	-2.62173400	3.13586500
H	0.61459100	-3.00039300	2.13537600
H	-0.08953000	-2.55821000	3.68911800
H	1.48208100	-3.36984800	3.62958500
C	-0.88825500	0.21763100	-1.59693400
C	1.60689000	-1.09223400	-0.38881500
H	1.77675000	-1.24183800	0.66790800
C	1.28359200	0.18571700	-0.92155600
H	1.11128700	1.04386300	-0.28341600
C	2.17198400	0.32741000	-2.18858500
H	1.93496700	1.12616800	-2.88447400
C	2.64986600	-1.70369400	-1.36324100
H	2.81054000	-2.77787000	-1.27509500
C	2.20178900	-1.11764600	-2.72574100
C	3.60547800	0.40335700	-1.62477000
C	3.90802700	-0.82687100	-1.15670400
H	2.95749000	-1.24770600	-3.50548400
H	1.24315000	-1.49765300	-3.06991500
H	-0.72268000	-0.10589000	-2.64143600
C	-1.38555300	1.66151500	-1.76526200
C	-0.42276800	2.51773400	-2.65246700
C	-1.80500200	2.68630900	-0.70111600
H	-2.30950500	1.48189900	-2.35146800
C	-0.82161200	3.98358000	-2.43974200
C	-1.49212200	3.94179900	-1.08944300
H	0.59427200	2.39389400	-2.28215600
H	-1.54573100	4.33491300	-3.18929100
H	0.03217400	4.66648100	-2.48221300
H	-0.44287700	2.20176000	-3.69951700
C	-2.72171500	2.47938500	0.46958600
O	-2.39393300	2.14908500	1.58828900
C	-1.89516900	5.15886800	-0.34497500
O	-2.44893800	5.18069900	0.73960500
C	5.10351400	-1.32919200	-0.43437900
O	5.05200000	-1.82433400	0.67494900
C	4.31261300	1.69132500	-1.53827900
O	3.84683300	2.73701800	-1.95940000
O	-3.98868400	2.75403100	0.10603800
O	-1.56201800	6.27696200	-1.02744500
O	5.51393200	1.60823400	-0.92690100
O	6.22421600	-1.23892600	-1.17024600
C	7.41730300	-1.72927300	-0.53651700
H	7.66172900	-1.11985400	0.33809900
H	7.28791900	-2.76840600	-0.22332200
H	8.20084300	-1.64757800	-1.29007700
C	6.23196300	2.84589800	-0.81884700
H	6.42944100	3.26466700	-1.80941100
H	5.66120300	3.57293600	-0.23445900
H	7.16642600	2.59785200	-0.31459000
C	-4.93592900	2.85764000	1.18288700
H	-5.03422400	1.90669600	1.71152200
H	-4.61183300	3.63673700	1.87694000
H	-5.88107700	3.12773200	0.71124400
C	-1.90948500	7.51458500	-0.38762000
H	-2.99087600	7.57924800	-0.23947100
H	-1.41323100	7.59639000	0.58309600
H	-1.56636000	8.29863700	-1.06298600
C	-3.30488000	-1.62022200	0.68816200
C	-2.36414300	-2.45976000	-0.19341100
C	-4.12618500	-0.61515000	-0.15210400
C	-4.30190400	-2.57332500	1.39510400
C	-3.17907000	-3.15478500	-1.30170000
H	-3.44464300	0.09150200	-0.62916800
H	-4.79485400	-0.04320700	0.50499200
C	-4.94556600	-1.35709000	-1.22481600
H	-3.75193600	-3.28338500	2.02684000
H	-4.98855300	-2.01490300	2.04894800
C	-5.11613100	-3.33360100	0.31974200
H	-2.51880000	-3.72559600	-1.96140600
C	-3.98126100	-2.14055400	-2.13941600
C	-4.17025200	-4.12619600	-0.60771800
H	-5.51232600	-0.62560400	-1.81721400
C	-5.92011900	-2.32823200	-0.52982600
H	-5.80521400	-4.02434700	0.82385000
H	-4.54872700	-2.66438000	-2.92123300
H	-3.29589700	-1.45009000	-2.64789200
H	-3.61396800	-4.87894200	-0.03325000
H	-4.76133700	-4.66962600	-1.35890300
H	-6.62417200	-1.76930000	0.10352600
H	-6.52005200	-2.86589800	-1.27676900
N	0.12805700	-3.73910000	-1.67371900
O	0.41155500	-4.78763200	-2.22814400
H	-1.95523900	-3.24668000	0.45544900

3.33-TS-D

exo-syn/syn
(cis,isotactic dyad)

B3LYP SCF energy:	-2756.92526100	a.u.
B3LYP enthalpy:	-2755.94940000	a.u.
B3LYP free energy:	-2756.10218000	a.u.
M06 SCF energy in solution:	-2755.97372380	a.u.
M06 enthalpy in solution:	-2754.99786280	a.u.
M06 free energy in solution:	-2755.15064280	a.u.
M06-2X SCF energy in solution:	-2756.54928131	a.u.
M06-2X enthalpy in solution:	-2755.57342031	a.u.

M06-2X free energy
in solution: -2755.72620031 a.u.

Imaginary frequency: -192.0472 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.16419100	-0.67972900	-0.90064200
O	-0.22784900	0.17813200	-2.92876300
O	0.75747100	-1.75558900	-2.86179400
N	-1.46963700	-2.56659100	0.87707300
N	0.52753600	-2.39003900	1.76333100
C	-0.27831100	-1.92471000	0.74080100
C	-1.60759400	-3.33086600	2.11392900
H	-2.07921200	-4.30098800	1.94068500
H	-2.21680900	-2.78056500	2.84543100
C	-0.14729300	-3.45051000	2.55297400
H	-0.00600700	-3.28701400	3.62413400
H	0.28289700	-4.42765300	2.29565600
C	1.96254000	-2.46622000	1.78445800
C	2.65448100	-1.94956600	2.89657600
C	4.04888300	-2.07229900	2.93752200
H	4.58621300	-1.64795800	3.78347000
C	4.76482500	-2.71507800	1.92593100
C	4.04157500	-3.28754300	0.87357400
H	4.57652200	-3.82240200	0.09187400
C	2.65032300	-3.19048700	0.78372200
C	1.93968400	-1.28835400	4.05331300
H	2.54273500	-0.47679900	4.47359100
H	1.75890800	-2.00459300	4.86683600
H	0.97166900	-0.88001000	3.75441200
C	6.27375700	-2.77449600	1.94221400
H	6.67799900	-2.49875000	2.92161200
H	6.69127600	-2.08365500	1.19823100
H	6.63992100	-3.77710600	1.69288300
C	1.94260800	-3.86536700	-0.36869200
H	1.70053000	-3.16060100	-1.17033700
H	1.00256300	-4.33398200	-0.05882400
H	2.58053800	-4.64471500	-0.79694400
C	-0.89425300	0.93998300	-0.20128200
C	1.12397800	1.34488200	-0.73170600
H	0.82600400	1.90896400	-1.60841800
C	1.89605400	0.13344200	-0.89241100
H	2.23655900	-0.16982000	-1.87741600
C	2.96592600	0.19628100	0.22030200
H	3.49180700	-0.72625300	0.43657800
C	1.77778100	2.08907500	0.45161800
H	1.22425700	2.92301300	0.88051900
C	2.18387300	0.90093200	1.35113600
C	3.89145400	1.36212700	-0.18656600
C	3.16878300	2.49706000	-0.07777100
H	2.81740800	1.20265500	2.18935400
H	1.33563000	0.31799100	1.70560200
H	-1.26312000	1.53407100	-1.04991900
C	-1.32178100	1.62585800	1.09486600
C	-1.35448600	0.81085300	2.41355700
C	-2.74519200	2.19576200	1.01703900
H	-0.67311300	2.50773100	1.21428700
C	-2.56250200	1.34208000	3.21930500
H	-0.41931500	0.89669200	2.97168600
H	-1.49861900	-0.24262800	2.17035200
C	-3.40109800	2.05452500	2.18338200
H	-3.12864900	0.55624500	3.73010300
H	-2.25637400	2.05466100	3.99855100
N	0.35167500	-0.78173200	-3.58000200
O	0.48189900	-0.74165900	-4.78997200
C	5.28239500	1.10347400	-0.61377600
O	5.64644800	0.03638000	-1.07419100
C	3.47513200	3.91872700	-0.35710600
O	3.01382200	4.83066700	0.30360700
C	-3.17062400	2.95614300	-0.19449600
O	-2.53263600	3.89056100	-0.63576900
C	-4.74543100	2.55261100	2.56353200
O	-5.35414200	2.14207700	3.53372700
O	6.11229500	2.14162200	-0.38958200
O	4.26960900	4.09405300	-1.42871500
O	-4.27896100	2.45782000	-0.76866300
O	-5.20878000	3.52563400	1.75098000
C	7.47125800	1.93698300	-0.80461800
H	7.90911900	1.08262100	-0.28097600
H	7.52101400	1.75553200	-1.88167000
H	7.99666600	2.85646200	-0.54499400
C	4.60405000	5.45988800	-1.72383100
H	3.69921000	6.04562000	-1.90595300
H	5.15595600	5.90716600	-0.89250800
H	5.22354600	5.41985200	-2.61999400
C	-4.72548900	3.15799600	-1.94494900
H	-4.97770900	4.19206500	-1.69610900
H	-3.94708600	3.15169000	-2.71188100
H	-5.60712800	2.61629800	-2.28678000
C	-6.51576300	4.02465700	2.07499700
H	-7.25830400	3.22431900	2.01461000
H	-6.52636200	4.44338500	3.08476500
H	-6.72368700	4.79890800	1.33611800
C	-2.48141100	-2.46099900	-0.17790700
C	-1.66390000	-2.08869900	-1.42890100
C	-3.56527200	-1.41057900	0.15132900
C	-3.19277900	-3.81369000	-0.44251000
H	-1.04690800	-2.96502500	-1.67286800
C	-2.62574600	-1.85380900	-2.61201300
H	-3.08991200	-0.45554100	0.38279300
H	-4.12752700	-1.72297700	1.04384100
C	-4.51665100	-1.24494100	-1.04968800
H	-2.44362000	-4.59319800	-0.63697000
H	-3.78265700	-4.13084900	0.43004600
C	-4.13316100	-3.65381400	-1.66122200
H	-2.07596000	-1.54560600	-3.50591400
C	-3.69748500	-0.79653800	-2.27783500
C	-3.33339100	-3.20411400	-2.90173300
H	-5.26808000	-0.48264600	-0.80791200
C	-5.20583100	-2.59211100	-1.34157200
H	-4.61619200	-4.61940200	-1.86149700
H	-4.36398600	-0.66025300	-3.14123000
H	-3.22651900	0.17298900	-2.08137300
H	-2.58984400	-3.96462300	-3.17460200
H	-4.01290900	-3.09893300	-3.75940800
H	-5.80794800	-2.90588900	-0.47684500
H	-5.89492000	-2.49075300	-2.19110100

3.33-TS-E

endo-anti/anti
(cis,isotactic dyad)

B3LYP SCF energy: -2756.92475530 a.u.

B3LYP enthalpy:	-2755.94910100	a.u.
B3LYP free energy:	-2756.09896600	a.u.
M06 SCF energy in solution:	-2755.96744326	a.u.
M06 enthalpy in solution:	-2754.99178896	a.u.
M06 free energy in solution:	-2755.14165396	a.u.
M06-2X SCF energy in solution:	-2756.54136029	a.u.
M06-2X enthalpy in solution:	-2755.56570599	a.u.
M06-2X free energy in solution:	-2755.71557099	a.u.
Imaginary frequency:	-186.4235	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	-1.12201200	-0.49218200	0.41536100
O	0.02950600	-1.73360900	1.85136500
O	-1.86046400	-0.97725000	2.59785900
N	-3.45155400	-0.55049000	-1.31271300
N	-3.05698200	1.58870600	-1.06069600
C	-2.63506300	0.33433100	-0.68802700
C	-4.35331100	0.05859300	-2.29124800
H	-5.36239900	-0.35655100	-2.22383800
H	-3.98261400	-0.10518600	-3.31279400
C	-4.28717500	1.53270900	-1.88598900
H	-4.21361300	2.21494900	-2.73703600
H	-5.15372800	1.83460500	-1.28336200
C	-2.81642500	2.84101300	-0.39576000
C	-2.09528800	3.84655500	-1.06438200
C	-1.93319000	5.08391000	-0.42591400
H	-1.36908200	5.86269300	-0.93469800
C	-2.47622200	5.34694000	0.83312600
C	-3.21788800	4.33537100	1.45596500
H	-3.66462900	4.52580900	2.42975500
C	-3.41479900	3.08688700	0.86095200
C	-1.48586500	3.63410600	-2.43294700
H	-0.49150600	3.17318900	-2.37834300
H	-1.36534900	4.59371100	-2.94602400
H	-2.10144000	2.98712900	-3.06447900
C	-2.30740200	6.69601100	1.49308800
H	-3.24020600	7.27399600	1.45771600
H	-1.53226500	7.28977800	0.99869400
H	-2.03303800	6.59320900	2.54913200
C	-4.23857500	2.03680100	1.57456100
H	-3.62619900	1.19884400	1.92790700
H	-5.01226500	1.60972300	0.92668800
H	-4.73824100	2.47204600	2.44504600
C	0.05277400	-0.20676700	-1.06952800
H	-0.24559300	0.44791900	-1.89662200
C	-0.53964000	1.30671000	1.48111300
H	-1.49229000	1.80786400	1.58319300
C	0.26056200	1.50350000	0.30940700
H	-0.11202500	2.09359600	-0.51461000
C	1.66808100	1.92622900	0.83102200
C	0.42458500	1.55860500	2.67443600
C	1.16266800	2.79147400	2.03960200
C	2.37759000	0.84292100	1.64000900
C	1.60309600	0.58634400	2.72293900
C	1.28421100	-0.98703700	-1.49908300
C	2.40751900	-0.19789400	-2.17150300
C	2.04423900	-1.88735800	-0.49284200
H	0.85263800	-1.62953700	-2.29446300
C	3.61273500	-0.71776900	-1.88580700
C	3.49948500	-1.94765300	-1.01144600
H	1.58672500	-2.87399400	-0.39756800
H	3.68493700	-2.84822900	-1.61530400
H	-0.06825100	1.69050200	3.63672600
H	0.48693600	3.60540800	1.75390500
H	1.97767100	3.18362000	2.65945000
H	2.28928400	2.39738000	0.07256400
H	2.01517700	-1.43890500	0.50020700
H	4.23419600	-1.96367300	-0.20211000
N	-0.83575600	-1.71377300	2.80713100
O	-0.68180300	-2.35984500	3.83286200
C	1.81874400	-0.23360200	3.94975800
O	1.50244300	0.18667200	5.04826300
C	3.79393300	0.53796000	1.34105400
O	4.40651400	1.07773900	0.43436800
C	4.88317100	-0.13902400	-2.37725500
O	4.98561800	0.87321900	-3.04373600
C	2.14574200	0.98108100	-3.04899300
O	1.74084100	2.05615600	-2.64747000
O	2.35484700	-1.43631400	3.72860900
O	4.37544500	-0.32035800	2.20204800
O	5.94747100	-0.88199600	-1.98895300
O	2.33529600	0.68864500	-4.34596200
C	7.22465100	-0.36500800	-2.39004700
H	7.28831800	-0.29868000	-3.47963200
H	7.38315600	0.62926000	-1.96396800
H	7.96100500	-1.07169600	-2.00539300
C	2.21855300	1.79803000	-5.25256200
H	2.38209300	1.37966900	-6.24593600
H	1.22724300	2.25382200	-5.18396400
H	2.98097500	2.54572100	-5.02009900
C	5.78475000	-0.51600500	2.01147900
H	5.99509800	-0.87156000	0.99952000
H	6.32664500	0.41993700	2.17726900
H	6.07516300	-1.26158000	2.75236000
C	2.49602200	-2.26817000	4.89193400
H	3.13129700	-1.78200200	5.63738700
H	1.51301600	-2.47393900	5.31981400
H	2.95678500	-3.18810600	4.53142100
C	-3.19518600	-1.98830800	-1.20712000
C	-2.39193900	-2.50618100	-2.42545700
C	-4.50856600	-2.80606300	-1.11636900
C	-2.42607100	-2.15213800	0.11953500
H	-2.98304900	-2.38010600	-3.34457100
H	-1.47982100	-1.91027200	-2.54098200
C	-2.04324100	-3.99383200	-2.22382400
H	-5.10204000	-2.70796100	-2.03792400
H	-5.12046400	-2.42516600	-0.28820200
C	-4.15693300	-4.29645100	-0.89273900
H	-3.15274000	-1.93624300	0.91473700
C	-2.01189100	-3.63018800	0.27756400
H	-1.46505200	-4.35070500	-3.08700100
C	-3.34538000	-4.81053300	-2.09922100
C	-1.20747400	-4.13829900	-0.93608000
H	-5.08875800	-4.87031900	-0.80314400

C	-3.31338300	-4.46656000	0.39008300
H	-1.41834000	-3.76415000	1.18754900
H	-3.11128800	-5.87552900	-1.96770000
H	-3.93634700	-4.72384500	-3.02233500
H	-0.27421000	-3.57341800	-1.03112100
H	-0.93111000	-5.19151000	-0.78650100
H	-3.88760500	-4.14835200	1.27004700
H	-3.07316700	-5.53017600	0.53176900

3.33-TS-F

endo-anti/syn
(trans,isotactic dyad)

B3LYP SCF energy:	-2756.92910690	a.u.
B3LYP enthalpy:	-2755.95383600	a.u.
B3LYP free energy:	-2756.10553200	a.u.
M06 SCF energy in solution:	-2755.97389661	a.u.
M06 enthalpy in solution:	-2754.99862571	a.u.
M06 free energy in solution:	-2755.15032171	a.u.
M06-2X SCF energy in solution:	-2756.54672346	a.u.
M06-2X enthalpy in solution:	-2755.57145256	a.u.
M06-2X free energy in solution:	-2755.72314856	a.u.
Imaginary frequency:	-200.0201	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.73715700	-0.17004600	0.68243600
O	-0.60637600	1.64115000	1.99916200
O	-2.21685000	0.25888700	2.44676800
N	-0.28203400	-3.02537900	0.72433000
N	-1.87720300	-2.75909500	-0.76492000
C	-1.03731800	-2.08536300	0.10466600
C	-0.42457300	-4.37030000	0.17167800
H	-0.51473700	-5.12319500	0.95951600
H	0.44477800	-4.63039100	-0.44869900
C	-1.70519300	-4.22762900	-0.66243200
H	-1.62091500	-4.67689500	-1.65629500
H	-2.57557800	-4.67173200	-0.16225700
C	-3.15612900	-2.31284000	-1.24905400
C	-3.36351300	-2.18385800	-2.63460000
C	-4.62707000	-1.78842100	-3.09328100
H	-4.78113400	-1.67300000	-4.16431700
C	-5.69040400	-1.55206700	-2.22118100
C	-5.46955500	-1.74004400	-0.85137800
H	-6.29126000	-1.58661600	-0.15457800
C	-4.22699400	-2.12797700	-0.34250800
C	-2.28161600	-2.50113100	-3.64015500
H	-2.40225100	-1.90153300	-4.54859100
H	-2.32711100	-3.55585000	-3.94591400
H	-1.28391600	-2.32585300	-3.23532100
C	-7.04892900	-1.13218500	-2.73269800
H	-7.38536200	-0.20372900	-2.25606000
H	-7.80780300	-1.89541900	-2.51863300
H	-7.03660200	-0.96915100	-3.81487700
C	-4.06726700	-2.32449800	1.14833100
H	-3.58050800	-1.46680500	1.62458200
H	-3.46334400	-3.20581200	1.38759800
H	-5.04669900	-2.45135000	1.61967100
C	0.60283400	0.37182700	-0.55595100
H	0.93202700	1.36976000	-0.23520800
C	-2.38416600	0.83215800	-0.41435300
H	-3.16481700	0.08958900	-0.31642700
C	-1.40254000	0.75259100	-1.43547300
H	-1.33278900	-0.09328300	-2.10768500
C	-1.33747100	2.17904400	-2.06361000
C	-2.85567700	2.31972800	-0.41211100
C	-2.86206700	2.51556100	-1.96534100
C	-0.81889900	3.21652200	-1.06775700
C	-1.72038200	3.27871300	-0.06247000
C	1.40402400	-0.01289300	-1.80082900
C	2.91377000	0.09179700	-1.57991900
C	1.22706200	-1.43562000	-2.40447100
H	1.15694800	0.75929000	-2.54684800
C	3.56250800	-1.02793000	-1.94454800
C	2.63455800	-2.08445000	-2.49455600
H	0.76761100	-1.37290900	-3.39546500
H	2.91098300	-2.33844800	-3.52504700
H	-3.77447300	2.50525100	0.14134400
H	-3.50250400	1.79901300	-2.49103400
H	-3.10281900	3.53708400	-2.28220700
H	-0.85982000	2.21317100	-3.04365800
H	0.56220100	-2.02530300	-1.77432400
H	2.70671700	-3.01712000	-1.92187900
N	-1.56858500	1.31084600	2.78939800
O	-1.83242600	1.95124700	3.79331300
C	-1.78909400	4.07881700	1.18891000
O	-2.83992600	4.23321400	1.78438800
C	0.43972300	3.94187400	-1.33566200
O	1.38475900	3.44094000	-1.92627700
C	3.55332100	1.34263900	-1.06265100
O	3.41125800	1.76283500	0.06687000
C	5.02685300	-1.20888300	-1.81463800
O	5.78669700	-0.46308100	-1.22710200
O	-0.61677600	4.58756500	1.58632300
O	0.40378800	5.22565300	-0.94556100
O	4.25629200	1.95748100	-2.02400400
O	5.43215700	-2.34749900	-2.42883500
C	-0.63803100	5.22143000	2.87739300
H	-1.33856900	6.06086200	2.88405500
H	-0.92958400	4.49129500	3.63575500
H	0.38221400	5.56820000	3.04402300
C	1.61120300	5.97466100	-1.14014400
H	2.40972500	5.57600600	-0.50779400
H	1.92555700	5.93867400	-2.18660300
H	1.36966400	6.99614000	-0.84509300
C	4.90889800	3.17193000	-1.62168800
H	4.16435300	3.90770000	-1.31043800
H	5.60216700	2.97408000	-0.80040100
H	5.44715200	3.51782700	-2.50474400
C	6.83853000	-2.61940000	-2.34011300
H	7.41514300	-1.81858500	-2.81114900
H	7.14725700	-2.70847800	-1.29494000
H	6.98868600	-3.56194400	-2.86768600
C	0.68671100	-2.61670500	1.74855400
C	0.13177300	-1.28229500	2.28498500

C	2.10792500	-2.46592000	1.16209300
C	0.75376500	-3.62566700	2.92229700
H	-0.78230200	-1.53777700	2.83862700
C	1.13025200	-0.69372100	3.30246000
H	2.07551300	-1.78347000	0.31122500
H	2.46517100	-3.44129900	0.79726300
C	3.06468600	-1.91399500	2.23695400
H	-0.25320600	-3.78446500	3.33109500
H	1.13271800	-4.60285100	2.58594500
C	1.69776000	-3.05957800	4.01129000
H	0.77917800	0.27954300	3.65983300
C	2.54358700	-0.54022400	2.70735400
C	1.19644500	-1.68256400	4.49769400
H	4.06690500	-1.80114900	1.80302400
C	3.11467800	-2.89812400	3.42252200
H	1.72474700	-3.76373900	4.85372500
H	3.22187500	-0.13004100	3.46870900
H	2.53893100	0.16981500	1.87431700
H	0.20537300	-1.77885500	4.96123900
H	1.87579400	-1.29843300	5.27199200
H	3.50416800	-3.87303900	3.09414200
H	3.79955500	-2.52456200	4.19564900

3.33-TS-G

(cis,isotactic dyad)

B3LYP SCF energy:	-2756.92962010	a.u.
B3LYP enthalpy:	-2755.95364000	a.u.
B3LYP free energy:	-2756.10614000	a.u.
M06 SCF energy in solution:	-2755.97686498	a.u.
M06 enthalpy in solution:	-2755.00088488	a.u.
M06 free energy in solution:	-2755.15338488	a.u.
M06-2X SCF energy in solution:	-2756.55131826	a.u.
M06-2X enthalpy in solution:	-2755.57533816	a.u.
M06-2X free energy in solution:	-2755.72783816	a.u.
Imaginary frequency:	-64.9887	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.28579100	0.55472900	0.56638700
N	-1.42884100	0.13588200	2.93448100
N	-2.60144600	1.52637700	1.72209700
C	-1.45236600	0.81164600	1.77377700
C	-2.67714500	0.25304500	3.70206500
C	-3.39395900	1.39367400	2.96533000
C	-3.07891700	2.41185300	0.69579300
C	-2.87249000	3.79859000	0.80852500
C	-3.38880700	4.62322800	-0.19746000
C	-4.11378200	4.11480800	-1.27739600
C	-4.35465400	2.73722000	-1.32168000
C	-3.85962800	1.87147400	-0.34322900
C	-2.16277700	4.41878700	1.99119700
C	-4.61570300	5.02678100	-2.37235200
C	-4.20616200	0.40183500	-0.37620800
C	-0.01408400	-1.03873900	-0.44151300
C	-0.59484100	-1.26599700	-1.83643800
C	-1.77949800	-2.23469900	-1.80916000
C	-1.15458600	-0.06197100	-2.63701000
C	-2.73958900	-1.86973800	-2.67875500
C	-2.38300300	-0.59518400	-3.41086400
H	-3.23992400	-0.68846500	3.66170900
H	-2.47799000	0.48830600	4.75035100
H	-3.36417200	2.33461500	3.52702300
H	-4.43784400	1.16783900	2.73042400
H	-3.21089400	5.69432000	-0.13214900
H	-4.95321700	2.32610200	-2.13227000
H	-2.86673000	4.60416200	2.81501600
H	-1.35702300	3.78609800	2.36965400
H	-1.72289500	5.37954500	1.71287300
H	-3.84973700	5.16954700	-3.14604300
H	-5.50355900	4.61441000	-2.86376500
H	-4.87108700	6.01852300	-1.98363200
H	-3.32053300	-0.23447300	-0.30883500
H	-4.86000300	0.12789000	0.46324800
H	-4.73655200	0.14524300	-1.29813100
H	0.18599800	-2.02861000	-0.01408800
H	0.19067800	-1.78558500	-2.41291300
H	-1.45636300	0.72667400	-1.94393500
H	-3.21209800	0.11869100	-3.43727100
O	-0.18440800	2.45212000	-0.72922800
O	0.61005500	2.70618400	1.27637700
C	2.38239500	0.75977300	0.12085100
C	2.07415400	-0.47873100	-0.53766000
C	2.50070800	-0.26597100	-2.01390000
C	2.97474700	1.67344600	-0.98132600
C	2.17557100	1.22894700	-2.22843900
C	4.03850900	-0.16881500	-1.92959100
C	4.32481900	1.00368400	-1.32427900
H	2.87808100	0.78141700	1.08635500
H	2.31270900	-1.42727000	-0.07104100
H	2.14633100	-0.99874900	-2.73707100
H	3.02598900	2.73586300	-0.74190900
H	2.60153200	1.61285100	-3.15978300
H	1.12193100	1.48665100	-2.16455600
H	-0.40704800	0.36764400	-3.30743000
H	-2.14145400	-0.82671000	-4.45834500
C	4.90056500	-1.28631900	-2.35088900
O	4.48287300	-2.27512600	-2.92680000
C	5.60814900	1.55840000	-0.82615700
O	5.80075600	1.79098500	0.35081000
C	-1.72800600	-3.50131800	-1.02299700
O	-0.83596100	-4.31595800	-1.14269900
C	-3.95141000	-2.67477300	-2.96903000
O	-4.11348700	-3.84727600	-2.69208600
O	6.48477700	1.82601800	-1.80747100
O	6.19916500	-1.11038400	-2.02073000
O	-2.73987500	-3.60471400	-0.14235400
O	-4.88314700	-1.92941500	-3.61246100
C	7.08021700	-2.16996200	-2.42219000
H	6.78338100	-3.11440700	-1.95801100
H	7.06747200	-2.29021800	-3.50894800
H	8.07141100	-1.86967900	-2.08110100
C	7.74157100	2.37257100	-1.37194900
H	7.58532400	3.30285000	-0.81960800
H	8.26428800	1.65940200	-0.72897300

H	8.30973500	2.55605200	-2.28408100
C	-2.82830600	-4.86660500	0.54222600
H	-3.02736100	-5.66354300	-0.17871200
H	-1.90073500	-5.08166600	1.07839200
H	-3.66179000	-4.76239400	1.23701700
C	-6.09051900	-2.62574900	-3.95752200
H	-5.87059100	-3.47226800	-4.61356500
H	-6.59064000	-2.99597700	-3.05844000
H	-6.71431800	-1.89316900	-4.47051800
C	-0.36166700	-0.82543700	3.23841900
C	0.86089100	-0.40543400	2.38830600
C	-0.82986800	-2.26687800	2.91454600
C	0.01836700	-0.76771500	4.74018000
H	1.23578000	0.51990400	2.86037400
C	1.97371900	-1.46172300	2.62454800
H	-1.14536300	-2.32648300	1.86793300
H	-1.70544700	-2.52105600	3.52991500
C	0.30929200	-3.26637900	3.19912800
H	0.31109800	0.25721600	5.00303500
H	-0.83920900	-1.03750600	5.37450500
C	1.17710100	-1.75230600	5.01000200
H	2.85816100	-1.22310000	2.02189200
C	1.52311300	-2.90786200	2.32103700
C	2.38644400	-1.40118700	4.11973200
H	-0.03271700	-4.28327000	2.96300500
C	0.70576200	-3.18492500	4.68679400
H	1.46244200	-1.68640000	6.06822300
H	2.34952100	-3.60202500	2.53020300
H	1.27039600	-3.04051300	1.26328500
H	2.76090700	-0.39877700	4.36536700
H	3.20728600	-2.10625900	4.31555000
H	-0.14787200	-3.45767500	5.32373400
H	1.50813800	-3.90326500	4.90231400
N	0.25348000	3.25414500	0.16316500
O	0.33343500	4.46040700	-0.01489500

3.33-TS-H

(trans,isotactic dyad)

B3LYP SCF energy:	-2756.92422761	a.u.
B3LYP enthalpy:	-2755.94806300	a.u.
B3LYP free energy:	-2756.10013800	a.u.
M06 SCF energy in solution:	-2755.97131550	a.u.
M06 enthalpy in solution:	-2754.99515089	a.u.
M06 free energy in solution:	-2755.14722589	a.u.
M06-2X SCF energy in solution:	-2756.54375306	a.u.
M06-2X enthalpy in solution:	-2755.56758845	a.u.
M06-2X free energy in solution:	-2755.71966345	a.u.
Imaginary frequency:	-78.2443	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.16531600	-0.81304200	0.19128000
N	1.81025500	-1.46706600	2.29338100
N	2.83810500	-1.93120200	0.41268300
C	1.68334700	-1.47455200	0.95802300
C	3.18353900	-1.73980600	2.73937800
C	3.83365100	-2.27744700	1.45318000
C	3.06290400	-2.39327100	-0.93386000
C	2.91297400	-3.76306800	-1.23009200
C	3.19926200	-4.19551700	-2.52942600
C	3.62973900	-3.32022800	-3.52778300
C	3.78588800	-1.97192200	-3.19556900
C	3.51026200	-1.48907500	-1.91407300
C	2.45899300	-4.77942400	-0.20540400
C	3.88653300	-3.81091600	-4.93340600
C	3.67765700	-0.02219500	-1.61540200
C	0.12389700	1.03460800	-0.19135700
C	0.43623500	2.34273100	0.54381300
C	1.76365700	2.91629100	0.03437800
C	-0.52893900	3.52106700	0.19522400
C	1.56485900	3.90364100	-0.86282400
C	0.09266000	4.20687200	-1.03936600
H	3.65624600	-0.81093700	3.07820800
H	3.20105800	-2.46316200	3.55928300
H	3.98518100	-3.36183500	1.48589300
H	4.79436600	-1.80444800	1.22962400
H	3.06417100	-5.24866700	-2.76653100
H	4.12745900	-1.27113000	-3.95480400
H	1.90115400	-5.58216600	-0.69560000
H	3.31340900	-5.24093400	0.30969500
H	1.80003000	-4.34118000	0.54702100
H	4.25819400	-4.84144000	-4.93827300
H	2.96340100	-3.79565900	-5.52765800
H	4.61878000	-3.18201200	-5.45134400
H	4.11720700	0.13983400	-0.62750100
H	4.30862900	0.46147800	-2.36743700
H	2.70760700	0.48894600	-1.61941200
H	0.15170700	1.23529900	-1.27911000
H	0.46773800	2.16880300	1.61668400
H	-1.56891600	3.23176200	0.04408600
H	-0.27089500	3.78969500	-1.98959300
O	0.12820700	-1.86351100	-1.88465000
O	-0.39413700	-3.05990400	-0.14838600
C	-2.29326100	-0.82559800	-0.18547500
C	-2.01060200	0.57671000	-0.12107100
C	-2.51795800	1.14526500	-1.47719900
C	-2.94925200	-1.05667100	-1.57185100
C	-2.21047000	-0.01545600	-2.44494600
C	-4.04673500	0.98852300	-1.37805100
C	-4.31080700	-0.33460900	-1.45345800
H	-2.72469500	-1.35326500	0.65945100
H	-2.18444700	1.14850200	0.78242900
H	-2.18926100	2.14680600	-1.74638000
H	-2.99250500	-2.09087800	-1.91423300
H	-2.68312800	0.12821400	-3.42064500
H	-1.15382400	-0.24214900	-2.57343900
H	-0.50565200	4.22497500	1.03569600
H	-0.10437800	5.28473400	-1.07564000
C	-5.56587500	-1.08998600	-1.20934400
O	-5.69202700	-1.85096000	-0.27058400
C	-4.89973600	2.13542300	-1.03246700
O	-4.46055000	3.25548500	-0.82716900
C	3.07215100	2.45852800	0.54898200
O	3.21974400	1.66996300	1.46597800

C	2.57535600	4.63082100	-1.69093800
O	2.86421100	4.31062400	-2.82293500
O	-6.49677100	-0.88827000	-2.15527900
O	-6.21065000	1.82505000	-0.94294900
O	3.03642600	5.72927900	-1.06568000
O	4.11085900	3.05061900	-0.08259400
C	-7.72482500	-1.61327000	-1.96846200
H	-7.53393300	-2.68887500	-1.92949200
H	-8.21191900	-1.30356300	-1.03998600
H	-8.34382500	-1.36206800	-2.82992800
C	-7.07539100	2.91283000	-0.58387100
H	-6.80460100	3.31291600	0.39713700
H	-7.01189100	3.71505200	-1.32404300
H	-8.08039900	2.49053600	-0.56141600
C	3.97230000	6.51612300	-1.82395800
H	4.86412100	5.92765800	-2.05510800
H	3.51926400	6.85776700	-2.75827400
H	4.22487900	7.36294700	-1.18557700
C	5.41530600	2.74677200	0.43188400
H	5.64111900	1.68487200	0.30660000
H	6.10693800	3.35181800	-0.15478000
H	5.47957700	3.00589800	1.49206000
N	-0.18491100	-3.01183300	-1.42156300
O	-0.28313600	-4.00553900	-2.12537500
C	0.73507400	-0.96910200	3.15925500
C	0.49239800	-1.91604100	4.36605500
C	1.10204900	0.42152900	3.72935200
C	-0.54772100	-0.95986800	2.28972200
H	1.38740300	-1.98003400	5.00307200
H	0.27442900	-2.92868400	4.00281900
C	-0.69026300	-1.37241700	5.20356500
H	1.37721900	1.09334900	2.91617000
H	1.99355000	0.32959400	4.36667300
C	-0.06581500	0.97720100	4.56494100
H	-0.83274400	-2.02328500	2.20093600
C	-1.68289600	-0.31992700	3.12763400
H	-0.87621200	-2.05849400	6.04059300
C	-0.33499500	0.02631500	5.74816300
C	-1.95905800	-1.25778700	4.33308000
H	0.20114000	1.97305900	4.94445800
C	-1.32278600	1.07523600	3.67735600
H	-2.60257200	-0.24818200	2.53416000
H	0.55184100	-0.02952900	6.39535000
H	-1.15893300	0.40860000	6.36637400
H	-2.26684100	-2.24790800	3.97222900
H	-2.78801600	-0.86600300	4.94056300
H	-2.16442800	1.47144200	4.26351400
H	-1.15127300	1.78377700	2.85858600

3.34-TS-A-rotamer1

exo-anti/anti

(cis,syndiotactic dyad)

B3LYP SCF energy:	-2756.93733610	a.u.
B3LYP enthalpy:	-2755.96170800	a.u.
B3LYP free energy:	-2756.11640800	a.u.
M06 SCF energy in solution:	-2755.97983464	a.u.
M06 enthalpy in solution:	-2755.00420654	a.u.
M06 free energy in solution:	-2755.15890654	a.u.
M06-2X SCF energy in solution:	-2756.55046860	a.u.
M06-2X enthalpy in solution:	-2755.57484050	a.u.
M06-2X free energy in solution:	-2755.72954050	a.u.
Imaginary frequency:	-76.4220	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.52668300	-0.63414100	-0.35018200
O	0.85225700	-0.48828600	-2.54209600
O	0.09372300	-2.38434800	-1.81049900
N	1.64407100	-1.87334200	2.02258600
N	-0.30854100	-1.13201500	2.68626700
C	0.51706400	-1.25069200	1.59314800
C	1.56672300	-2.36330900	3.40150000
H	1.44671700	-3.45497100	3.42237300
H	2.47091900	-2.11062800	3.96148600
C	0.32584800	-1.63105600	3.92637100
H	0.59156900	-0.79122000	4.58037200
H	-0.36161900	-2.28376900	4.47209600
C	2.58496300	-2.41383100	1.03447200
C	4.03954100	-2.42303400	1.55910800
H	4.32661200	-1.40634100	1.85771000
H	4.13917600	-3.06894500	2.44501900
C	4.96927100	-2.94664200	0.43942400
H	6.00694700	-2.91603000	0.79766900
C	4.57641600	-4.39922700	0.10395600
H	4.67622800	-5.03665200	0.99491800
H	5.25467400	-4.80706100	-0.65786500
C	3.12592500	-4.42453100	-0.41532700
H	2.83392300	-5.45694500	-0.65023400
C	2.17811300	-3.86474500	0.66270900
H	1.14689600	-3.86381500	0.29023100
H	2.21052100	-4.50547200	1.55602600
C	3.00031800	-3.54798100	-1.67488200
H	1.98961900	-3.62996800	-2.07838000
H	3.68921700	-3.91107000	-2.45093500
C	3.35915100	-2.08592700	-1.32432200
H	3.27342000	-1.46417500	-2.22254400
C	2.50467200	-1.47430600	-0.18307900
C	4.83357700	-2.07371600	-0.82905700
H	5.15447700	-1.04650100	-0.62303500
H	5.49569300	-2.47080900	-1.61310000
C	-1.71317600	-0.85059400	2.71202600
C	-2.18079000	0.36019700	3.25593000
C	-3.56153100	0.59862400	3.26365000
H	-3.92611800	1.54400800	3.66015900
C	-4.47574200	-0.33221600	2.76482800
C	-3.98382300	-1.55501500	2.29382400
H	-4.68079500	-2.29949100	1.91698300
C	-2.61750700	-1.84335400	2.27612300
C	-1.23817800	1.39260100	3.83060200
H	-1.70116900	2.38425100	3.83566000
H	-0.97206200	1.15518100	4.86946700
H	-0.30332800	1.45134700	3.26534800
C	-5.95402900	-0.02826300	2.70710600
H	-6.21365300	0.82866700	3.33738600

H	-6.25547200	0.20554600	1.67805300
H	-6.55406700	-0.88528700	3.03348300
C	-2.14030100	-3.20557400	1.82265600
H	-1.42657800	-3.15081300	0.99402100
H	-1.63689600	-3.74094300	2.63841500
H	-2.98572000	-3.81771200	1.49629600
C	0.82314600	1.12915600	0.24884100
H	0.77557800	1.40266000	1.31586400
C	-1.77320600	-0.52961900	-0.71155000
H	-2.03098700	-1.40819900	-0.14014700
C	-1.63237400	0.74245400	-0.17107700
H	-1.67600800	0.97031700	0.88199300
C	-2.16832500	1.73144500	-1.22631800
H	-1.92123500	2.78218100	-1.09522000
C	-2.41570100	-0.32161400	-2.10396300
H	-2.37381600	-1.17132000	-2.78502400
N	0.47176300	-1.68841100	-2.82061000
O	0.47669200	-2.12496900	-3.95880200
C	-1.77749200	1.02240700	-2.54316400
C	-3.68629300	1.43476100	-1.24487000
C	-3.83707000	0.20593000	-1.78115600
H	-2.27699300	1.46024700	-3.41180300
H	-0.70701000	0.94866300	-2.72287600
C	1.14655300	2.37952800	-0.56618000
C	0.47433400	3.65588400	0.02911200
C	2.63201700	2.71750100	-0.39998300
H	0.90867600	2.22476500	-1.62238900
C	1.50479200	4.24648100	1.01658000
H	0.29177000	4.37103900	-0.78144100
H	-0.48674400	3.44432000	0.50516200
C	2.81845000	3.72546300	0.47383700
H	1.35320100	3.90081500	2.04787800
H	1.47962800	5.34089300	1.05473600
C	-4.65740900	2.35801200	-0.63852400
O	-4.35909600	3.44928700	-0.18738000
C	-5.03583900	-0.66537800	-1.87971100
O	-5.15102200	-1.69072900	-1.23720600
C	4.09384100	4.30814700	0.95938700
O	4.21246900	4.80075500	2.06532800
C	3.70232500	1.97275900	-1.12939100
O	4.66022700	1.43057000	-0.61847300
O	-5.92785600	-0.22931500	-2.78227800
O	-5.92214900	1.87189100	-0.62721300
O	5.08059700	4.26721500	0.04445300
O	3.45085100	1.98508300	-2.45142600
C	-7.10279600	-1.04605000	-2.92948900
H	-7.68641400	-0.57455900	-3.72023900
H	-7.66895900	-1.06931900	-1.99444900
H	-6.82860000	-2.06704200	-3.20707500
C	-6.91266000	2.76688500	-0.09760900
H	-6.94267500	3.69246700	-0.67874200
H	-6.69488800	3.00987600	0.94574600
H	-7.86028200	2.23342900	-0.17760600
C	6.35694700	4.74859900	0.49269500
H	7.02279400	4.64925600	-0.36470100
H	6.71857400	4.14628700	1.33033400
H	6.28437300	5.79297400	0.80795200
C	4.41599800	1.31639800	-3.28247500
H	4.05993300	1.45069300	-4.30349700
H	4.46381000	0.25534900	-3.03076300
H	5.40370100	1.76658400	-3.15161900
H	3.03033700	-0.56076700	0.11137000

3.34-TS-A-rotamer2

exo-anti/anti

(cis,syndiotactic dyad)

B3LYP SCF energy:	-2756.93288875	a.u.
B3LYP enthalpy:	-2755.95738800	a.u.
B3LYP free energy:	-2756.11094200	a.u.
M06 SCF energy in solution:	-2755.97846786	a.u.
M06 enthalpy in solution:	-2755.00296711	a.u.
M06 free energy in solution:	-2755.15652111	a.u.
M06-2X SCF energy in solution:	-2756.54911679	a.u.
M06-2X enthalpy in solution:	-2755.57361604	a.u.
M06-2X free energy in solution:	-2755.72717004	a.u.
Imaginary frequency:	-101.9317	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	1.37959600	-0.08839800	-0.49622300
O	1.45513300	0.26270200	-2.72218200
O	2.09063900	-1.67895800	-2.00433300
N	3.17015100	-0.56692400	1.72876800
N	1.22832200	-1.30161900	2.43809800
C	1.87487600	-0.75290700	1.35945500
C	3.50110600	-1.14782100	3.03368700
H	4.08559700	-2.06980300	2.91328200
H	4.08606800	-0.45131100	3.64021000
C	2.11012700	-1.41532700	3.62039900
H	1.82926700	-0.66740200	4.37259800
H	2.01603000	-2.40652400	4.07291300
C	4.18358400	-0.27135000	0.70647500
C	5.32405800	0.61648400	1.25942500
H	4.89812200	1.53874300	1.67787000
H	5.86926900	0.10949100	2.07024200
C	6.30588100	0.93937400	0.10887600
H	7.09510900	1.60096800	0.49054100
C	6.93049400	-0.37707600	-0.39711900
H	7.47116800	-0.87771200	0.41935200
H	7.66578400	-0.16609500	-1.18539400
C	5.81650400	-1.28973600	-0.94573900
H	6.25187000	-2.23352100	-1.30009100
C	4.79629300	-1.59267500	0.16938700
H	3.99311200	-2.22792100	-0.22045400
H	5.28999600	-2.13795700	0.98668300
C	5.08553100	-0.58578300	-2.10371700
H	4.34837300	-1.26381600	-2.53691000
H	5.80166900	-0.33712300	-2.89956900
C	4.42852400	0.71460400	-1.58659100
H	3.91004300	1.21900700	-2.40980700
C	3.44959300	0.49033700	-0.40953300
C	5.56477800	1.63358300	-1.05638900
H	5.14990800	2.59429800	-0.72093000
H	6.27889300	1.85783100	-1.86182200
C	-0.03059600	-1.98876000	2.46558200

C	-1.13096000	-1.42230900	3.13283400
C	-2.34446300	-2.12276000	3.12927300
H	-3.20806000	-1.67207300	3.61367200
C	-2.47975000	-3.36407000	2.50447200
C	-1.34536200	-3.93588700	1.91653600
H	-1.42807400	-4.90859100	1.43897500
C	-0.11415600	-3.27848000	1.89630100
C	-1.03728400	-0.09413600	3.84879900
H	-2.02287300	0.37611600	3.92332100
H	-0.65916500	-0.22050300	4.87279100
H	-0.36363100	0.60105300	3.33908800
C	-3.81460100	-4.06503300	2.42608800
H	-4.21588000	-3.99592500	1.40713800
H	-3.72505200	-5.13073600	2.66637500
H	-4.54427300	-3.62151900	3.11156000
C	1.09129500	-3.94807000	1.27469500
H	1.44336800	-3.42472700	0.37865100
H	1.93600400	-3.98512900	1.97388700
H	0.85073300	-4.97531800	0.98641700
C	0.54610800	1.42991500	0.30453700
H	0.26394100	1.42965500	1.36296100
C	-0.47707900	-1.25770800	-0.80270900
H	-0.28758100	-2.19479100	-0.29866400
C	-1.02764500	-0.14017000	-0.11510400
H	-1.19605500	-0.16688000	0.95108000
C	-2.14557800	0.41457500	-1.02933600
H	-2.54015100	1.40057600	-0.79133700
C	-1.25722300	-1.33107000	-2.14280500
H	-0.80920900	-1.93805800	-2.93033100
C	-1.54964900	0.16196500	-2.43173200
C	-3.20186500	-0.71259100	-1.01994200
C	-2.68139600	-1.75101700	-1.70485500
H	-2.28832600	0.29827800	-3.22636900
H	-0.65068500	0.73045600	-2.65420900
C	0.46367500	2.86693900	-0.19654900
C	0.60381200	3.19608500	-1.70957300
C	-0.80390200	3.61976900	0.20309200
H	1.32120800	3.29613100	0.35604400
C	-0.77773200	3.72358100	-2.16732700
H	1.34756800	3.99117400	-1.82831800
H	0.94862700	2.34592800	-2.29601100
C	-1.47230900	4.07479900	-0.87284400
H	-1.37013200	2.97692000	-2.71168400
H	-0.69539700	4.59261000	-2.83171100
C	-4.42851000	-0.63193200	-0.21291800
O	-4.67992300	0.28008700	0.55181100
C	-3.19572300	-3.13572000	-1.87500000
O	-2.77110600	-4.08982400	-1.25276100
C	-2.81326800	4.73109300	-0.89317600
O	-3.78318700	4.20465200	-1.39788200
C	-1.27235400	3.82848300	1.59386700
O	-2.39852800	4.14697100	1.91970200
O	-4.12887200	-3.21520400	-2.83698100
O	-5.25132500	-1.69515600	-0.39797200
O	-2.79722900	5.96485900	-0.36561700
O	-0.26988700	3.64208300	2.49231900
C	-4.65385300	-4.53187100	-3.07905800
H	-5.36236700	-4.41519700	-3.89921800
H	-5.15811800	-4.91026900	-2.18578200
H	-3.85172900	-5.22097500	-3.35587500
C	-6.47008900	-1.65727100	0.35846400
H	-7.04232500	-0.75695800	0.11951300
H	-6.25948700	-1.66817400	1.43151200
H	-7.02263100	-2.55155700	0.06800900
C	-4.07917300	6.61189200	-0.28522800
H	-3.87844900	7.60563800	0.11579100
H	-4.73597600	6.05201100	0.38540100
H	-4.54101000	6.67864100	-1.27357600
C	-0.63046200	3.88205300	3.86149000
H	0.27457400	3.69273000	4.43961200
H	-1.43530300	3.21007000	4.17099900
H	-0.96211200	4.91532700	3.99403800
H	3.24872900	1.49527800	-0.00638600
N	1.89991400	-0.91069300	-3.01296900
O	2.12685400	-1.25624300	-4.15966700

3.34-TS-A-rotamer3

exo-anti/anti

(cis,syndiotactic dyad)

B3LYP SCF energy:	-2756.93300723	a.u.
B3LYP enthalpy:	-2755.95692200	a.u.
B3LYP free energy:	-2756.10607400	a.u.
M06 SCF energy in solution:	-2755.97309524	a.u.
M06 enthalpy in solution:	-2754.99701001	a.u.
M06 free energy in solution:	-2755.14616201	a.u.
M06-2X SCF energy in solution:	-2756.54534686	a.u.
M06-2X enthalpy in solution:	-2755.56926163	a.u.
M06-2X free energy in solution:	-2755.71841363	a.u.
Imaginary frequency:	-89.4678	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.52622600	0.55915200	-0.29615100
O	-1.22645600	-0.62984500	-2.02997000
O	-0.45106800	1.33635100	-2.48877100
N	-1.06664000	3.15852800	0.87693100
N	0.93877000	2.68316600	1.61016400
C	-0.11004900	2.19468800	0.87013000
C	-0.62174200	4.42977400	1.45603200
H	-0.40973200	5.16022900	0.66393100
H	-1.38070100	4.85548700	2.11758800
C	0.64722900	4.00598900	2.19975400
H	0.48128700	3.90905500	3.28056500
H	1.48873600	4.68751000	2.04468500
C	-2.27688700	3.03331900	0.05659100
C	-3.52995500	3.52979500	0.82194300
H	-3.61394100	2.98743200	1.77366800
H	-3.45389100	4.60161300	1.05993300
C	-4.78099100	3.29185700	-0.05496000
H	-5.67169700	3.60984300	0.50367200
C	-4.64916200	4.12738300	-1.34475400
H	-4.57256500	5.19621100	-1.09738500
H	-5.54748200	4.00580000	-1.96500800

C	-3.40393200	3.66273800	-2.12338100
H	-3.29741200	4.25730600	-3.04030700
C	-2.14470100	3.85362500	-1.25231000
H	-1.25446300	3.52971600	-1.80028800
H	-2.02325500	4.91993000	-1.01129300
C	-3.54567800	2.17131800	-2.48295100
H	-2.71244400	1.86738700	-3.11693400
H	-4.46113700	2.02005000	-3.07261600
C	-3.63465200	1.32926900	-1.18932200
H	-3.73266100	0.26775000	-1.43836500
C	-2.43764100	1.52888400	-0.22918300
C	-4.90424600	1.79584200	-0.42332000
H	-5.04188800	1.19222700	0.48442100
H	-5.79830600	1.64420700	-1.04520100
C	2.08698700	1.98418800	2.11145900
C	1.98534200	1.25104700	3.31551700
C	3.10974600	0.55869900	3.77126700
H	3.02910700	-0.02901700	4.68369900
C	4.33298700	0.60133500	3.09176800
C	4.42303700	1.40389200	1.95276600
H	5.37118400	1.47602100	1.42392100
C	3.32452900	2.11541600	1.45254600
C	0.72366700	1.23712300	4.15196900
H	0.62857100	0.29371500	4.69925100
H	0.74922300	2.03893600	4.90287800
H	-0.18082500	1.37642000	3.55567500
C	5.50695000	-0.22005300	3.56886800
H	5.42880100	-1.24815200	3.19214200
H	6.45667700	0.19651600	3.21622100
H	5.54401700	-0.27238900	4.66267500
C	3.51798700	3.00407300	0.24421500
H	2.56923100	3.38231400	-0.14335100
H	4.14100700	3.86971900	0.50642300
H	4.03215000	2.46698200	-0.56014300
C	-0.51607300	-0.64260600	1.18402500
H	0.00134100	-0.35219400	2.10374500
C	1.59014600	0.20894700	-0.89635900
H	1.99678300	1.21050100	-0.85181300
C	1.56505600	-0.65490800	0.22549500
H	1.89735800	-0.33721600	1.20227400
C	1.98766800	-2.04688300	-0.29016500
H	1.79238400	-2.89527500	0.36466600
C	2.03119100	-0.68845500	-2.08272000
H	1.86640700	-0.28246200	-3.08113300
C	1.39456400	-2.05339700	-1.71491900
C	3.47493900	-1.84252900	-0.66026800
C	3.50112800	-1.03528000	-1.74096300
H	1.79097800	-2.87399100	-2.31886000
H	0.31096500	-2.06576900	-1.75051200
C	-1.19585700	-1.97052300	1.51847900
C	-1.80268200	-1.80481700	2.95407100
C	-2.37310000	-2.55515600	0.73600800
H	-0.41105000	-2.74658100	1.53967700
C	-3.03043400	-2.72901900	3.01932400
H	-1.06184300	-2.01185300	3.73204300
H	-2.12500000	-0.76351300	3.07730600
C	-3.34829800	-2.98552300	1.56347900
H	-3.87174500	-2.28736400	3.56246600
H	-2.80067600	-3.68059400	3.52039000
C	4.58379500	-2.33787900	0.16629600
O	4.44229400	-2.87905700	1.24964000
C	4.64756900	-0.36509200	-2.40817000
O	4.94173900	0.79913100	-2.21345900
C	-4.53458700	-3.78511200	1.15694300
O	-4.64574500	-4.44867200	0.14644100
C	-2.30088500	-2.90630700	-0.71392800
O	-1.38219400	-3.56513800	-1.16206600
O	5.26485000	-1.16022300	-3.29387500
O	5.79282500	-2.12638800	-0.40694100
O	-5.50224500	-3.71594600	2.10570200
O	-3.34298700	-2.45614700	-1.41541900
C	6.35807400	-0.55673400	-4.00870900
H	6.71696800	-1.32646000	-4.69193900
H	7.14786800	-0.25841400	-3.31424600
H	6.01634100	0.32225300	-4.56131400
C	6.92292600	-2.60513300	0.33500400
H	6.80693600	-3.66585100	0.57193000
H	7.04080400	-2.04355300	1.26618900
H	7.78559300	-2.44825600	-0.31348000
C	-6.68552000	-4.47732800	1.82387600
H	-7.34666500	-4.31721600	2.67628700
H	-6.44394000	-5.53844200	1.71689100
H	-7.15606000	-4.12787500	0.90084300
C	-3.38143700	-2.84965700	-2.80066000
H	-4.35642900	-2.52282300	-3.16275600
H	-3.28419200	-3.93442300	-2.88301100
H	-2.58025900	-2.34929600	-3.34718100
N	-0.94792800	0.24288100	-2.93073700
O	-1.15499500	0.03669800	-4.11751900
H	-2.74613300	1.07215700	0.72244400

3.34-TS-B

exo-syn/anti
(trans,isotactic dyad)

B3LYP SCF energy:	-2756.92296531	a.u.
B3LYP enthalpy:	-2755.94734400	a.u.
B3LYP free energy:	-2756.10010300	a.u.
M06 SCF energy in solution:	-2755.96586452	a.u.
M06 enthalpy in solution:	-2754.99024321	a.u.
M06 free energy in solution:	-2755.14300221	a.u.
M06-2X SCF energy in solution:	-2756.53764173	a.u.
M06-2X enthalpy in solution:	-2755.56202042	a.u.
M06-2X free energy in solution:	-2755.71477942	a.u.
Imaginary frequency:	-180.0304	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	-1.28047400	-0.25269600	-0.56140100
O	-0.80355600	-1.07796500	-2.59813500
O	-1.99189900	0.73229200	-2.52060600
N	-3.50185700	0.14741800	1.26532000
N	-2.01598800	1.61237900	1.95606400
C	-2.26147600	0.65021700	0.99823400
C	-4.21455400	0.85533700	2.33055400

H	-4.98234500	1.52086700	1.91275700
H	-4.70372500	0.15564800	3.01303600
C	-3.07620500	1.62365900	2.99589700
H	-2.72052900	1.11351400	3.89841800
H	-3.34078300	2.65027800	3.25875800
C	-1.19797100	2.78948600	1.88746900
C	-0.30987500	3.06105900	2.94885400
C	0.37929800	4.27819800	2.95443500
H	1.07177400	4.48084800	3.76912600
C	0.20118400	5.23651200	1.95322700
C	-0.70825400	4.95163400	0.93028000
H	-0.88272200	5.69257700	0.15281500
C	-1.42254800	3.74905700	0.87589700
C	-0.09239400	2.08162800	4.08008700
H	0.88656000	2.23848200	4.54320100
H	-0.84557300	2.20517800	4.86990200
H	-0.14210700	1.04257700	3.74079100
C	0.97494100	6.53431300	1.96925900
H	1.19724200	6.85628500	2.99232700
H	1.93491500	6.43150300	1.44578100
H	0.41980500	7.33748000	1.47308500
C	-2.42051100	3.53231300	-0.23617300
H	-2.08630900	2.76368300	-0.94044800
H	-3.39387000	3.20899900	0.15148200
H	-2.57458900	4.45936700	-0.79648200
C	-0.24909900	-1.31200600	0.63377200
C	1.13104600	-0.19993300	-0.65802400
H	1.26399400	-0.99438700	-1.38192700
C	0.56213900	1.05120900	-1.03207700
H	0.32895900	1.28829200	-2.06398000
C	1.36845900	2.10538600	-0.23473200
H	0.93495600	3.09966700	-0.16517900
C	2.28216600	0.12687500	0.32384100
H	2.68239900	-0.69594000	0.90882800
C	1.68837800	1.33488900	1.06560700
C	2.77453500	2.05423800	-0.87983400
C	3.31192100	0.85543000	-0.56266200
H	2.41796100	1.84535700	1.69933100
H	0.80576000	1.08350000	1.64690000
H	0.04577700	-0.92604900	1.61435100
C	0.08448500	-2.80122800	0.56448300
C	0.19321100	-3.52490900	-0.80887900
C	1.41931700	-3.14727600	1.22217300
H	-0.74968300	-3.23022500	1.15250900
C	1.70708400	-3.74561200	-1.05400500
H	-0.30332600	-4.49805000	-0.72846800
H	-0.29295000	-2.97435700	-1.61341400
C	2.31267200	-3.59864800	0.32337700
H	2.14258600	-3.01338600	-1.74650100
H	1.92099700	-4.73001400	-1.48439000
C	3.19953200	3.10921700	-1.83210100
O	2.50184600	3.46153400	-2.76293600
C	4.50660400	0.15634000	-1.06638300
O	4.77902000	-0.99830400	-0.78020900
C	3.75337400	-3.78413200	0.62623600
O	4.28701600	-3.50511000	1.68395000
C	1.67870800	-2.88340100	2.66811100
O	1.62567700	-1.78071500	3.18273500
O	4.38081400	3.66885400	-1.51850200
O	5.25718900	0.90739400	-1.89989500
O	1.90210600	-4.01876000	3.34712700
O	4.41531700	-4.27331300	-0.44176400
C	4.82515100	4.69685500	-2.41942100
H	4.08826800	5.50225800	-2.47946500
H	4.98254100	4.28494600	-3.41989800
H	5.76394100	5.06268400	-2.00276500
C	6.41557700	0.25629700	-2.43992800
H	6.12769800	-0.62665000	-3.01727200
H	7.09516500	-0.04785300	-1.63892100
H	6.89133500	0.99613700	-3.08435700
C	2.26795100	-3.85121300	4.72688300
H	1.49852200	-3.29418100	5.26772900
H	3.21977400	-3.31812500	4.79423400
H	2.36586400	-4.86112900	5.12569200
C	5.84398000	-4.31838500	-0.30650900
H	6.13182000	-4.91687800	0.56164500
H	6.23215300	-3.30273100	-0.19731400
H	6.20957800	-4.77454500	-1.22728900
C	-4.21680200	-0.60770000	0.22962500
C	-5.17929500	-1.66225100	0.82282100
C	-5.03837500	0.36690600	-0.65973500
C	-3.13541300	-1.31500500	-0.59134600
H	-5.96754700	-1.19009800	1.42848400
H	-4.61983300	-2.33859300	1.48345300
C	-5.83114500	-2.44870500	-0.33943900
H	-5.79369200	0.88536500	-0.05209100
H	-4.36748700	1.12539300	-1.07764900
C	-5.73152600	-0.40517400	-1.79894200
C	-3.79843300	-2.01698800	-1.80015400
H	-6.48518100	-3.22465000	0.08027500
C	-6.66250400	-1.47797500	-1.20246000
C	-4.74473300	-3.10606700	-1.22034200
H	-6.31766800	0.29938800	-2.40384600
C	-4.65036900	-1.06910400	-2.67204800
H	-3.03254400	-2.49935600	-2.41735200
H	-7.16749200	-2.02868700	-2.00743800
H	-7.44927500	-1.00848400	-0.59419400
H	-4.16883300	-3.83349500	-0.63152400
H	-5.22296800	-3.66448600	-2.03784000
H	-4.03460100	-0.29986300	-3.14297500
H	-5.12352500	-1.64423400	-3.48027600
N	-1.45575400	-0.17429100	-3.25198500
O	-1.55601000	-0.19495800	-4.46403000
H	-2.75667600	-2.12943300	0.04671900

3.34-TS-C-rotamer1

exo-anti/syn

(trans,syndiotactic dyad)

B3LYP SCF energy:	-2756.93931559	a.u.
B3LYP enthalpy:	-2755.96385500	a.u.
B3LYP free energy:	-2756.11574300	a.u.
M06 SCF energy in solution:	-2755.97738875	a.u.
M06 enthalpy in solution:	-2755.00192816	a.u.
M06 free energy in solution:	-2755.15381616	a.u.
M06-2X SCF energy in solution:	-2756.54876022	a.u.
M06-2X enthalpy in solution:	-2755.57329963	a.u.

M06-2X free energy
in solution: -2755.72518763 a.u.

Imaginary frequency: -72.8159 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	1.31365000	-0.42245900	-0.56579500
O	1.43247600	-0.62345000	-2.77722800
O	1.75018700	-2.43489400	-1.62795800
N	3.02598100	-0.56211300	1.77433400
N	1.00593700	-0.87102100	2.57663400
C	1.71217300	-0.63594400	1.42125200
C	3.28844100	-0.81303100	3.19407700
H	3.91183600	-1.70459800	3.32752200
H	3.81425200	0.03383100	3.64791200
C	1.87494900	-0.99992300	3.76658000
H	1.61782000	-0.23789700	4.51058600
H	1.73036800	-1.98043200	4.23350700
C	-0.34119000	-1.35219100	2.70587800
C	-1.33906800	-0.52491000	3.24970200
C	-2.63926000	-1.03828600	3.36252000
H	-3.41870100	-0.39240400	3.76235300
C	-2.96022300	-2.33827400	2.97229000
C	-1.92658400	-3.16403700	2.51188300
H	-2.15012600	-4.18964100	2.22862800
C	-0.61477900	-2.70351900	2.39056600
C	-1.07089900	0.88802500	3.71775900
H	-1.45588600	1.03070200	4.73481400
H	-0.00421200	1.12303500	3.72582100
H	-1.57035900	1.61885000	3.07216500
C	-4.38287400	-2.84229200	3.02124900
H	-4.99020500	-2.26609400	3.72739400
H	-4.84956000	-2.75717400	2.03126000
H	-4.42703000	-3.89738400	3.31296900
C	0.47684700	-3.65154100	1.94284600
H	0.95746600	-3.33356000	1.01143100
H	1.27048300	-3.73549200	2.69627400
H	0.06828400	-4.65286600	1.78005200
C	0.73964400	1.37026900	-0.47668100
C	-0.74787300	-1.39016800	-0.69159300
H	-0.60294800	-2.19553900	0.01206800
C	-1.18974900	-0.11618500	-0.32090200
H	-1.30518400	0.22112700	0.69857200
C	-2.17451900	0.34038300	-1.42370900
H	-2.44206700	1.39429500	-1.44694100
C	-1.45055700	-1.69899300	-2.03558900
H	-1.03812300	-2.52162300	-2.61919700
C	-1.53635600	-0.29051900	-2.68182500
C	-3.37162500	-0.63014100	-1.26165900
C	-2.93671700	-1.85082400	-1.64049300
H	-2.20994900	-0.26574300	-3.54282700
H	-0.56754100	0.12072500	-2.95495600
H	0.55507100	1.79677300	-1.47964100
C	0.60799300	2.41944400	0.61580200
C	1.97219800	3.17302600	0.79392800
C	-0.32681700	3.57506800	0.26156700
H	0.31215900	1.93579000	1.54863000
C	1.85060700	4.45169100	-0.05746400
C	0.35437300	4.67988800	-0.10216800
H	2.83327700	2.55874000	0.52671700
H	2.39033300	5.30305500	0.37230400
H	2.23776800	4.32162000	-1.07752300
H	2.07490300	3.44589700	1.85077900
C	-1.80270900	3.42749500	0.35159400
O	-2.35850400	2.77760300	1.22073500
C	-0.16208600	5.99573100	-0.56720600
O	0.31660500	6.59462500	-1.50904100
C	-3.58680300	-3.18198000	-1.56242400
O	-3.11721800	-4.10101000	-0.92038900
C	-4.68276800	-0.20762000	-0.74461100
O	-5.07061500	0.94750600	-0.72661100
O	-2.45495000	4.07105100	-0.62948900
O	-1.15480300	6.47802400	0.20682400
O	-5.43318800	-1.23854800	-0.29194800
O	-4.69809400	-3.27083600	-2.31278400
C	-5.35989200	-4.54691200	-2.27750500
H	-5.71533600	-4.76380700	-1.26640600
H	-4.67953800	-5.34146900	-2.59440900
H	-6.19834300	-4.45852200	-2.96861400
C	-6.75470600	-0.88496100	0.14631900
H	-7.32582600	-0.44379900	-0.67506300
H	-6.70700400	-0.16948300	0.97127100
H	-7.21274900	-1.81874700	0.47337500
C	-3.89606300	4.08415800	-0.52456900
H	-4.19487600	4.55668700	0.41513100
H	-4.29354800	3.06932400	-0.57234400
H	-4.23520200	4.67588100	-1.37533000
C	-1.68871000	7.74600500	-0.20845500
H	-2.13769100	7.66464200	-1.20209800
H	-0.90150500	8.50398300	-0.23552600
H	-2.44420100	8.00156800	0.53499900
C	4.06321200	-0.70902700	0.74468300
C	3.45059000	-0.15880300	-0.55354300
C	5.33860300	0.10122900	1.07924400
C	4.45437200	-2.20433300	0.59163300
C	4.43595100	-0.41839500	-1.71958100
H	5.07472800	1.15697600	1.22999000
H	5.80270100	-0.25489900	2.01158600
C	6.34587500	-0.04827500	-0.08548500
H	3.55820700	-2.79011500	0.35830800
H	4.86578200	-2.58485300	1.53785200
C	5.49712100	-2.37113600	-0.53138400
H	3.99439100	-0.07294200	-2.66078400
C	5.71017200	0.41800100	-1.41607700
C	4.87158600	-1.89496000	-1.85596100
H	7.23419600	0.55975600	0.13245000
C	6.74810900	-1.53182400	-0.20914900
H	5.77279500	-3.43115200	-0.61030000
H	6.44109200	0.30479400	-2.22956800
H	5.45898000	1.48641600	-1.36176900
H	4.03067700	-2.53999700	-2.11593500
H	5.60735400	-1.98121400	-2.66788500
H	7.21305300	-1.87784200	0.72549500
H	7.49698100	-1.65385400	-1.00337600
N	1.68040700	-1.88755900	-2.78740400
O	1.84124400	-2.51224900	-3.82152100
H	3.44079900	0.93066000	-0.43646500

3.34-TS-C-rotamer2

exo-anti/syn

(trans,syndiotactic dyad)

B3LYP SCF energy: -2756.93449100 a.u.

B3LYP enthalpy:	-2755.95909700	a.u.
B3LYP free energy:	-2756.11182900	a.u.
M06 SCF energy in solution:	-2755.97841046	a.u.
M06 enthalpy in solution:	-2755.00301646	a.u.
M06 free energy in solution:	-2755.15574846	a.u.
M06-2X SCF energy in solution:	-2756.54915311	a.u.
M06-2X enthalpy in solution:	-2755.57375911	a.u.
M06-2X free energy in solution:	-2755.72649111	a.u.
Imaginary frequency:	-92.3973	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.62456300	-0.96321800	-0.58018400
O	0.54978900	-1.16683300	-2.80281500
O	-0.02160800	-2.90311800	-1.63573700
N	2.02629300	-2.04835800	1.71655000
N	0.14272600	-1.27418500	2.54325800
C	0.86818000	-1.41427000	1.38120900
C	2.07406400	-2.50252600	3.10920800
H	1.96335400	-3.59322200	3.16937100
H	3.02349000	-2.23283200	3.58079300
C	0.88017200	-1.76392100	3.72788700
H	1.19598700	-0.91886500	4.35286200
H	0.24116400	-2.41247700	4.33424400
C	-1.26834800	-1.04891300	2.68043300
C	-1.74460900	0.15144000	3.23658200
C	-3.12989700	0.33574200	3.34370800
H	-3.50126700	1.27762300	3.74218900
C	-4.03914300	-0.64262600	2.93918600
C	-3.53246500	-1.85929600	2.46661300
H	-4.22497700	-2.64116500	2.16570500
C	-2.16151400	-2.09063600	2.34264400
C	-0.81103500	1.23153700	3.73168600
H	-1.27772700	2.21883000	3.65576800
H	-0.55285800	1.07679800	4.78846500
H	0.12561700	1.24845400	3.16957300
C	-5.52899600	-0.40237100	2.98174700
H	-6.05803900	-1.23941600	3.45235100
H	-5.77464900	0.50916800	3.53640700
H	-5.92428000	-0.30190600	1.96338700
C	-1.66594600	-3.43659100	1.86078300
H	-1.15863600	-3.37549200	0.89148300
H	-0.95186900	-3.87910400	2.56654700
H	-2.50236800	-4.13312700	1.75329600
C	1.01726400	0.88128700	-0.48083700
C	-1.61810400	-0.71495100	-0.68745300
H	-1.94718000	-1.50683700	-0.03040600
C	-1.28153500	0.56769100	-0.21854300
H	-1.21979300	0.81824200	0.82987700
C	-1.88859800	1.57598200	-1.21967100
H	-1.53684100	2.60402900	-1.15260400
C	-2.40865700	-0.47342900	-2.00160000
H	-2.52350600	-1.33106800	-2.66512300
C	-1.73076000	0.80803800	-2.55178200
C	-3.41052100	1.38896700	-1.02325000
C	-3.72650100	0.17032700	-1.50773300
H	-2.30200100	1.26652300	-3.36351400
H	-0.70253700	0.64444500	-2.86861600
H	0.99028200	1.31539000	-1.49427100
C	1.44540400	1.91719400	0.54565000
C	2.59338100	1.48610900	1.50636400
C	2.00621200	3.21133900	-0.04432800
H	0.55833800	2.19886800	1.13680300
C	3.34745400	2.78747200	1.85673000
C	3.03270000	3.68920800	0.68199200
H	3.26298300	0.80679000	0.97151900
H	2.97274600	3.23859700	2.78739900
H	4.42270100	2.63649400	1.99444600
H	2.22353500	0.95114800	2.38372500
C	1.34833900	3.87950200	-1.20623800
O	0.20917600	4.29989100	-1.16778400
C	3.69176700	4.99063300	0.42416400
O	3.33758100	5.81312200	-0.39888000
C	-4.99736200	-0.59551300	-1.41646700
O	-5.16722200	-1.50846000	-0.63169000
C	-4.23012700	2.34137100	-0.25884000
O	-3.78813600	3.33059200	0.29452400
O	2.12952600	3.89048800	-2.29574500
O	4.75456200	5.17012300	1.24393700
O	-5.54068200	1.99175800	-0.22011000
O	-5.89610000	-0.21020200	-2.33558500
C	-7.13958400	-0.93286400	-2.32169300
H	-7.65529300	-0.78394800	-1.36917200
H	-6.96468600	-2.00153200	-2.47050200
H	-7.72446700	-0.51937700	-3.14336400
C	-6.38786200	2.88960900	0.51104900
H	-6.33516300	3.89706400	0.08983600
H	-6.09116000	2.93010800	1.56289200
H	-7.39600400	2.48527700	0.41359300
C	1.59419200	4.59235700	-3.43256300
H	1.48386900	5.65278000	-3.19234700
H	0.62377400	4.17953000	-3.71896400
H	2.32433600	4.45210000	-4.22935100
C	5.45279300	6.41304000	1.07461900
H	4.78166600	7.25773300	1.25221900
H	5.85778500	6.49027200	0.06192300
H	6.25764400	6.39912000	1.81016900
C	2.85156700	-2.65139700	0.65939100
C	2.61279000	-1.79837600	-0.59794700
C	4.35823000	-2.61807700	1.00979900
C	2.43171300	-4.12665200	0.42139500
C	3.34528700	-2.45130500	-1.79429900
H	4.66319000	-1.58398700	1.22008400
H	4.57131000	-3.21167300	1.91192900
C	5.16168800	-3.19234400	-0.18074700
H	1.36450000	-4.16413300	0.17754000
H	2.58887400	-4.71535400	1.33676700
C	3.25607500	-4.73459900	-0.73181300
H	3.14826800	-1.87760900	-2.70686400
C	4.86485200	-2.39375900	-1.47085600
C	2.97494700	-3.93463400	-2.01785800
H	6.23340500	-3.13201700	0.05195400
C	4.75698000	-4.66548500	-0.39030800
H	2.95615200	-5.78152200	-0.87250400
H	5.44644600	-2.81483000	-2.30353000

H	5.18752700	-1.34991900	-1.35311900
H	1.92730400	-4.05172900	-2.29944500
H	3.57645400	-4.33726700	-2.84510200
H	4.97304500	-5.25034300	0.51565600
H	5.34810100	-5.10629000	-1.20437800
N	0.12991600	-2.38340000	-2.80163100
O	-0.10105100	-2.99678300	-3.82906000
H	3.14452700	-0.85562900	-0.42325700

3.34-TS-C-rotamer3

exo-anti/syn

(trans,syndiotactic dyad)

B3LYP SCF energy:	-2756.92406664	a.u.
B3LYP enthalpy:	-2755.94842100	a.u.
B3LYP free energy:	-2756.09835700	a.u.
M06 SCF energy in solution:	-2755.96707507	a.u.
M06 enthalpy in solution:	-2754.99142943	a.u.
M06 free energy in solution:	-2755.14136543	a.u.
M06-2X SCF energy in solution:	-2756.53688444	a.u.
M06-2X enthalpy in solution:	-2755.56123880	a.u.
M06-2X free energy in solution:	-2755.71117480	a.u.
Imaginary frequency:	-111.2185	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.64667900	-1.14395700	-0.67097700
O	0.34711400	-2.61624800	-2.34159600
O	0.26018700	-3.37475000	-0.31216100
N	2.46186400	-0.70930600	1.54469900
N	0.58932200	0.23861900	2.18689100
C	1.19446800	-0.42430800	1.14979700
C	2.78069100	-0.27960700	2.90758800
H	2.98880000	-1.14388400	3.55090500
H	3.65574700	0.37540400	2.90940500
C	1.50755500	0.47244100	3.32302500
H	1.68582300	1.54478200	3.43933300
H	1.06594100	0.08770300	4.24842700
C	-0.81271600	0.40645400	2.44427000
C	-1.42099100	1.66659700	2.32121300
C	-2.79199100	1.77602200	2.60203100
H	-3.26956500	2.74743400	2.48551000
C	-3.55372000	0.68610200	3.01912700
C	-2.90292400	-0.54090500	3.20551600
H	-3.47566300	-1.40004100	3.54471900
C	-1.54309400	-0.70016300	2.94163500
C	-0.65514200	2.90340400	1.91107400
H	-0.69485400	3.65677400	2.70854000
H	0.39304600	2.69235000	1.69691800
H	-1.10054400	3.36632900	1.02134100
C	-5.04230400	0.80370300	3.24380900
H	-5.34868100	0.31678900	4.17687200
H	-5.36187900	1.85036600	3.28555900
H	-5.58887900	0.31330500	2.42843300
C	-0.88478600	-2.04156900	3.18008400
H	-0.51245800	-2.49471200	2.25435000
H	-0.02813800	-1.95852300	3.85996600
H	-1.59760400	-2.74052700	3.62700100
C	0.68306100	0.42972900	-1.74063800
C	-1.56281100	-1.18805700	-0.38403900
H	-1.65743600	-1.40775900	0.66897500
C	-1.43161500	0.13855400	-0.86129800
H	-1.32188800	0.98394400	-0.19644500
C	-2.37840500	0.23358200	-2.08558200
H	-2.26093700	1.09311700	-2.74012700
C	-2.56814600	-1.87890800	-1.34523900
H	-2.59553400	-2.96832200	-1.31372000
C	-2.25803000	-1.18011900	-2.69281100
C	-3.78305300	0.10454100	-1.45992300
C	-3.90900100	-1.17098700	-1.03615500
H	-3.02565400	-1.36897400	-3.44840700
H	-1.27760800	-1.43024500	-3.09139500
H	0.38710900	0.10251900	-2.75424200
C	1.08561600	1.88403400	-1.93716200
C	-0.05964900	2.77725400	-2.51570800
C	1.74008600	2.82814600	-0.92765900
H	1.85336100	1.76839900	-2.73042200
C	0.39469200	4.22991500	-2.30417800
C	1.38088600	4.10711500	-1.16647000
H	-0.96858200	2.60716300	-1.93471600
H	0.90607200	4.63733800	-3.18844800
H	-0.43597700	4.90727400	-2.08363300
H	-0.27945200	2.53664400	-3.55979400
C	2.85990600	2.50879500	0.01794200
O	2.74767800	2.33201800	1.21124400
C	2.00895700	5.27719200	-0.50869000
O	2.93571600	5.23868300	0.28030200
C	-4.98188700	-1.82298700	-0.24204200
O	-4.82013000	-2.21325400	0.89760800
C	-4.64465300	1.27898600	-1.26064600
O	-4.34234700	2.40404200	-1.61949200
O	4.03081000	2.49658000	-0.64586600
O	1.42648900	6.42978600	-0.90969800
O	-5.80275500	0.98982700	-0.62300900
O	-6.11485800	-1.98653000	-0.94448800
C	-7.18683700	-2.63425200	-0.23780700
H	-7.50086400	-2.02748700	0.61594100
H	-6.87254000	-3.61810400	0.11986100
H	-7.99701300	-2.72688600	-0.96119800
C	-6.67995200	2.10632400	-0.41350100
H	-6.95523500	2.56342000	-1.36772000
H	-6.19991300	2.86063300	0.21595800
H	-7.55986700	1.69687500	0.08355300
C	5.21185700	2.54251900	0.17770500
H	5.25590600	1.68398800	0.84937900
H	5.20612000	3.46850100	0.75805700
H	6.05052600	2.52663600	-0.51859900
C	1.97809100	7.62790500	-0.34223200
H	3.03572400	7.72386400	-0.60241200
H	1.88068500	7.61642500	0.74665500
H	1.40046800	8.44686400	-0.77161900
C	3.25405500	-1.70360100	0.81364400
C	2.73891000	-1.66695300	-0.63391300
C	4.76309300	-1.36337900	0.81673700
C	3.06788300	-3.11294400	1.43868400

C	3.44148200	-2.78236900	-1.44481900
H	4.90529300	-0.35909800	0.40105000
H	5.16859600	-1.35844700	1.83983400
C	5.52049300	-2.40695900	-0.03479600
H	2.00288000	-3.36528000	1.44802900
H	3.42245900	-3.11023600	2.47963400
C	3.85235700	-4.16364700	0.62539600
H	3.05306200	-2.79727100	-2.46958100
C	4.95627400	-2.43089700	-1.47392500
C	3.31029800	-4.18823200	-0.81671000
H	6.58580200	-2.13979200	-0.06125600
C	5.34867600	-3.79700800	0.60860100
H	3.71779600	-5.14994800	1.08899800
H	5.50554700	-3.17284000	-2.07133300
H	5.10991500	-1.45534700	-1.95608700
H	2.27871400	-4.54120700	-0.81301400
H	3.88744400	-4.90600800	-1.41702700
H	5.75592600	-3.79316300	1.63012900
H	5.91418900	-4.54840000	0.04084100
N	0.15851700	-3.62624000	-1.56884200
O	-0.09064000	-4.74081900	-1.99568200
H	3.10778200	-0.72318300	-1.05813000

3.34-TS-D

exo-syn/syn
(cis,isotactic dyad)

B3LYP SCF energy:	-2756.91724130	a.u.
B3LYP enthalpy:	-2755.94141600	a.u.
B3LYP free energy:	-2756.09450700	a.u.
M06 SCF energy in solution:	-2755.96164216	a.u.
M06 enthalpy in solution:	-2754.98581686	a.u.
M06 free energy in solution:	-2755.13890786	a.u.
M06-2X SCF energy in solution:	-2756.53189749	a.u.
M06-2X enthalpy in solution:	-2755.55607219	a.u.
M06-2X free energy in solution:	-2755.70916319	a.u.
Imaginary frequency:	-176.7248	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.82065100	-0.57336800	-0.73850700
O	0.67488900	0.00604100	-2.86962100
O	0.62080000	-2.12503200	-2.45977900
N	2.65637100	-1.84255300	1.13446900
N	0.71914100	-2.06842700	2.13624200
C	1.32521300	-1.56885400	1.00187300
C	3.03498000	-2.49596600	2.38721500
H	3.58719300	-3.42287200	2.20167900
H	3.67677900	-1.83707100	2.98414800
C	1.67714700	-2.74464100	3.04701900
H	1.61069200	-2.31988800	4.05292100
H	1.42822600	-3.81038900	3.11471200
C	-0.63711600	-2.49313500	2.34945100
C	-1.35504200	-1.95444500	3.43390800
C	-2.61285200	-2.48747000	3.73944800
H	-3.17415500	-2.06041700	4.56831900
C	-3.15786600	-3.55459200	3.02232800
C	-2.40330600	-4.09603600	1.97518100
H	-2.79973200	-4.94144200	1.41663600
C	-1.14714900	-3.59211800	1.62276800
C	-0.79841200	-0.83406100	4.28270100
H	-1.59770100	-0.16672000	4.62122600
H	-0.30503900	-1.22474700	5.18323900
H	-0.06072200	-0.23970800	3.73724200
C	-4.52642500	-4.10126200	3.35576800
H	-4.57819800	-5.18225700	3.18626800
H	-4.79234200	-3.90731400	4.40014100
H	-5.30124800	-3.63806200	2.73040600
C	-0.37679300	-4.23428900	0.49328000
H	-0.30862400	-3.57440300	-0.37842800
H	0.65044600	-4.48071100	0.78681100
H	-0.86475700	-5.16078000	0.17648000
C	0.76662600	1.21322900	-0.08682000
C	-1.21967800	0.73546700	-0.89383500
H	-1.01865400	1.29202300	-1.80169400
C	-1.42094100	-0.68534600	-0.93589200
H	-1.49699900	-1.20649400	-1.88401800
C	-2.55902800	-0.94741600	0.08025200
H	-2.69366100	-1.97452300	0.40463000
C	-2.25553600	1.28239100	0.11249000
H	-2.12305200	2.30130600	0.46736900
C	-2.28249200	0.13860400	1.14197100
C	-3.80113400	-0.31280000	-0.58182100
C	-3.60834400	1.02383200	-0.58615500
H	-3.08663800	0.24172100	1.87482800
H	-1.33008200	-0.00452100	1.64748900
H	0.94459900	1.92039100	-0.91243300
C	0.81043800	1.92124600	1.26856400
C	2.11586200	1.60849500	2.07592300
C	0.90405700	3.43959700	1.11635500
H	-0.07102500	1.64497500	1.85578200
C	3.07921700	2.77590100	1.77898700
H	1.86758200	1.60749500	3.14399800
H	2.53032200	0.63337700	1.82240500
C	2.14224400	3.89577800	1.38221600
H	3.77033700	2.54997300	0.95458000
H	3.70201900	3.04542100	2.63827600
N	0.61511100	-1.19628200	-3.34445800
O	0.56828000	-1.41870600	-4.53904200
C	-4.82319500	-1.16838100	-1.23386600
O	-4.52858600	-2.03326600	-2.03497600
C	-4.34863900	2.10535000	-1.25843400
O	-4.01380300	3.27762800	-1.22356000
C	-0.30156400	4.23591700	0.73880700
O	-1.25490400	4.36573500	1.48144800
C	2.64971000	5.28386900	1.30613000
O	3.83240500	5.56472500	1.36010400
O	-6.07177900	-0.93565700	-0.79480700
O	-5.42617100	1.66868200	-1.94278100
O	-0.23677900	4.71188000	-0.51193500
O	1.66845300	6.20647900	1.19693800
C	-7.09238000	-1.74557200	-1.40262500
H	-6.88608600	-2.80761800	-1.24548100
H	-7.14510100	-1.54933500	-2.47684500

H	-8.02263200	-1.45616100	-0.91324200
C	-6.16992200	2.68491200	-2.63179400
H	-5.54066300	3.18604100	-3.37230500
H	-6.55031700	3.42848300	-1.92620600
H	-6.99300600	2.16217300	-3.11965700
C	-1.38512600	5.47573100	-0.94549800
H	-1.52855200	6.33635400	-0.28710700
H	-2.28059200	4.85138300	-0.94138100
H	-1.14230600	5.80167900	-1.95705900
C	2.11350600	7.56802300	1.10614200
H	2.72949700	7.71186400	0.21420300
H	2.69825000	7.84010300	1.98892100
H	1.20543700	8.16855000	1.04682300
C	3.52513000	-1.87103500	-0.04486200
C	2.92764900	-0.86427300	-1.02653700
C	4.98123900	-1.45549500	0.27458000
C	3.53740600	-3.30226300	-0.64897500
C	3.68781800	-0.95193800	-2.37102700
H	4.98714300	-0.45881400	0.73614200
H	5.44725000	-2.15008300	0.98968400
C	5.79474800	-1.45028000	-1.04144400
H	2.50803300	-3.60318600	-0.87440200
H	3.94205700	-4.01573200	0.08383500
C	4.38620800	-3.33174100	-1.93453600
H	3.24252700	-0.26500700	-3.09870800
C	5.14686300	-0.50175400	-2.07563900
C	3.74470900	-2.37857000	-2.96003900
H	6.81783800	-1.11588800	-0.82425600
C	5.82530800	-2.88044100	-1.61766900
H	4.39809000	-4.35467600	-2.33359100
H	5.73888300	-0.51023600	-3.00172500
H	5.15686100	0.53138700	-1.70191400
H	2.74707900	-2.73677600	-3.22354400
H	4.34016200	-2.36666700	-3.88360300
H	6.29440900	-3.56889100	-0.89973700
H	6.43620200	-2.90539000	-2.53001500
H	3.16971400	0.12801500	-0.62253800

3.34-TS-E

endo-anti/anti
(cis,isotactic dyad)

B3LYP SCF energy:	-2756.92091800	a.u.
B3LYP enthalpy:	-2755.94535400	a.u.
B3LYP free energy:	-2756.09954100	a.u.
M06 SCF energy in solution:	-2755.96428006	a.u.
M06 enthalpy in solution:	-2754.98871606	a.u.
M06 free energy in solution:	-2755.14290306	a.u.
M06-2X SCF energy in solution:	-2756.53552410	a.u.
M06-2X enthalpy in solution:	-2755.55996010	a.u.
M06-2X free energy in solution:	-2755.71414710	a.u.
Imaginary frequency:	-148.3357	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.37189600	-0.33695200	-0.57397200
O	0.57455500	1.20146600	-1.85461000
O	-0.85078000	-0.11821000	-2.81988800
N	-0.38796100	-3.20663000	-0.12556600
N	-2.08534400	-2.49211000	1.05844100
C	-1.09822600	-2.09396900	0.18242300
C	-0.95802700	-4.45052700	0.39794500
H	-1.43192800	-5.03122000	-0.40511300
H	-0.18803000	-5.07403800	0.85917100
C	-1.97523300	-3.92480300	1.41524700
H	-1.61913400	-4.03049000	2.44767800
H	-2.95102200	-4.41349100	1.34086400
C	-3.29081800	-1.81710400	1.43701100
C	-3.46175400	-1.36784000	2.75981600
C	-4.67337200	-0.75561800	3.10807600
H	-4.80118300	-0.39240900	4.12579400
C	-5.71777400	-0.60560100	2.19382500
C	-5.53960700	-1.11627800	0.90156600
H	-6.35512400	-1.04444800	0.18472000
C	-4.35149000	-1.73605000	0.50705400
C	-2.39446600	-1.55563100	3.81397500
H	-2.44640300	-0.76546400	4.57000200
H	-2.52421000	-2.51109800	4.34019400
H	-1.38944900	-1.55796000	3.38423700
C	-7.00750400	0.07935700	2.58246200
H	-7.88038900	-0.48320000	2.23178100
H	-7.09052200	0.19092400	3.66809100
H	-7.07365800	1.08249100	2.14158900
C	-4.24021800	-2.34936500	-0.87167300
H	-3.41462800	-1.93347500	-1.45870000
H	-4.06613000	-3.43131800	-0.81034100
H	-5.16436500	-2.19519200	-1.43639000
C	0.24241500	0.09803800	1.16724100
H	-0.05678100	-0.48626800	2.05112400
C	-2.32391300	0.85077600	-0.50557300
H	-2.96577100	0.02391700	-0.77200400
C	-1.90384700	1.10717400	0.80572400
H	-2.14264600	0.47468500	1.64678500
C	-1.97808400	2.64831300	0.98691500
C	-2.68271900	2.24300400	-1.10519300
C	-3.30872700	2.86204200	0.18805200
C	-1.01676700	3.37598400	0.04278100
C	-1.45826900	3.14890600	-1.21603000
C	1.20900700	1.19351100	1.60843900
C	2.56435700	0.55910000	1.94040800
C	0.81280500	1.80023500	2.99178400
H	1.32649900	1.94044500	0.81999900
C	2.73663200	0.41542100	3.26864100
C	1.55245100	0.94836500	4.04608300
H	1.15686300	2.83814100	3.04150400
H	1.86358500	1.52931600	4.92111200
H	-3.28411400	2.20332700	-2.01109000
H	-4.15481100	2.28902900	0.58344300
H	-3.58409700	3.91849500	0.08748100
H	-1.93590600	2.99673100	2.01767900
H	-0.26881500	1.81287200	3.14792000
H	0.94278800	0.11959200	4.43082700
N	0.03303700	0.80211200	-2.95573200
O	0.35567000	1.25538900	-4.04008200
C	-1.10423800	3.69459000	-2.55041500

O	-1.72160500	3.38020100	-3.55185500
C	0.03922400	4.24954300	0.61176300
O	-0.10930200	4.83394600	1.67243200
C	3.87211000	-0.20362000	3.99487200
O	3.74718000	-0.73418800	5.08255400
C	3.53446900	0.16017000	0.87684000
O	4.00287200	-0.94924900	0.72584400
O	-0.10547000	4.59018000	-2.54586600
O	1.16688100	4.30482100	-0.11216400
O	5.04708800	-0.08807300	3.34640700
O	3.81636300	1.21771900	0.09345200
C	6.16237300	-0.74116800	3.97153500
H	5.97581800	-1.81482300	4.05860400
H	6.34054600	-0.32737700	4.96779700
H	7.01383300	-0.55306400	3.31729500
C	4.74214700	0.97861600	-0.98133100
H	4.90283200	1.95137300	-1.44565500
H	4.31294600	0.28017500	-1.70231000
H	5.67947900	0.57242200	-0.59244400
C	2.19132100	5.16999900	0.39999400
H	2.52266000	4.83415300	1.38644800
H	1.82322200	6.19653100	0.47784700
H	3.00786900	5.10526800	-0.31883400
C	0.28063000	5.06525600	-3.84615700
H	-0.55101100	5.58413100	-4.33104100
H	0.59565100	4.22543100	-4.47002200
H	1.11000200	5.75076700	-3.66838900
C	0.57142300	-3.17366400	-1.23434200
C	1.75778400	-4.14006800	-1.00044700
C	-0.14063700	-3.56720400	-2.55557100
C	1.11087700	-1.73254800	-1.28647600
H	1.41335700	-5.18364300	-0.93513100
H	2.24906700	-3.89315000	-0.05041200
C	2.74886000	-4.00565700	-2.17891000
H	-0.54556100	-4.58658600	-2.47303900
H	-0.98210000	-2.88550900	-2.72663700
C	0.84713900	-3.49110700	-3.73597800
C	2.01443300	-1.60195000	-2.54142800
H	3.61004200	-4.66144500	-1.99336700
C	2.03903700	-4.43277600	-3.47858900
C	3.23211100	-2.54395000	-2.31149000
H	0.32976000	-3.79007400	-4.65748100
C	1.34120500	-2.03891700	-3.86362700
H	2.37027800	-0.56958900	-2.63758700
H	2.74039000	-4.38911600	-4.32301000
H	1.69686100	-5.47536600	-3.40071700
H	3.78074700	-2.24512400	-1.41135700
H	3.92853400	-2.46874200	-3.16007700
H	0.50573600	-1.38934700	-4.12667800
H	2.07517100	-1.96702000	-4.67877100
H	1.78822000	-1.63781900	-0.43184200

3.34-TS-F

endo-anti/syn
(trans,isotactic dyad)

B3LYP SCF energy:	-2756.92865980	a.u.
B3LYP enthalpy:	-2755.95324300	a.u.
B3LYP free energy:	-2756.10310400	a.u.
M06 SCF energy in solution:	-2755.96677116	a.u.
M06 enthalpy in solution:	-2754.99135436	a.u.
M06 free energy in solution:	-2755.14121536	a.u.
M06-2X SCF energy in solution:	-2756.54016862	a.u.
M06-2X enthalpy in solution:	-2755.56475182	a.u.
M06-2X free energy in solution:	-2755.71461282	a.u.
Imaginary frequency:	-129.4321	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	-1.07794700	0.07666200	-0.14241000
O	-1.71305600	1.91364600	-1.24968600
O	-3.15200500	1.03069700	0.11159800
N	-1.79829800	-2.72533100	0.04762400
N	-0.82019800	-2.27968500	1.96686800
C	-1.19544400	-1.73090000	0.75934100
C	-1.96961600	-3.97852600	0.78747300
H	-3.03029100	-4.17453000	0.98668000
H	-1.57369300	-4.82668900	0.21990200
C	-1.17557600	-3.71261900	2.07405500
H	-0.26840000	-4.32505600	2.13913500
H	-1.76145700	-3.89049800	2.98142600
C	-0.52455900	-1.60434300	3.20156300
C	0.76684000	-1.66607900	3.75481600
C	0.98998500	-1.05516200	4.99742700
H	1.99078700	-1.09531300	5.42269200
C	-0.02541100	-0.40900800	5.70230800
C	-1.31250000	-0.40921400	5.14933200
H	-2.12789400	0.05709200	5.69863200
C	-1.58861400	-1.00835800	3.91875500
C	1.92597600	-2.35329000	3.06797000
H	2.57484900	-1.63086500	2.55655600
H	2.54625500	-2.87718200	3.80362700
H	1.59526500	-3.08386800	2.32578100
C	0.24703400	0.26681700	7.02608600
H	-0.56558300	0.09183800	7.74017500
H	1.17793000	-0.09328100	7.47562700
H	0.34007600	1.35402100	6.90437000
C	-3.00760000	-1.02570400	3.39406500
H	-3.11594500	-0.46252500	2.46078600
H	-3.35187200	-2.04713800	3.18979900
H	-3.69105300	-0.58824300	4.12783400
C	0.73431200	-0.13685700	-0.66945200
H	1.15165900	0.69470000	-1.25635500
C	-0.69212100	1.41079900	1.65509600
H	-1.34372900	0.90816100	2.35618800
C	0.62406600	0.99105600	1.40662500
H	1.07450100	0.10545400	1.82704900
C	1.47971700	2.28543900	1.33619700
C	-0.62414300	2.96990900	1.74080800
C	0.74949800	3.06021700	2.48402500
C	1.06381900	3.18597800	0.16988700
C	-0.19966700	3.59284600	0.41346100
C	1.67116100	-1.32575800	-0.60260200
C	3.18912200	-1.14100000	-0.73040200
C	1.38443600	-2.27615800	-1.81170200

H	1.48210800	-1.87400700	0.32874900
C	3.74401900	-2.11453000	-1.48063800
C	2.69784200	-3.04314300	-2.05385300
H	0.52933200	-2.92448700	-1.61636700
H	2.71304400	-4.00482500	-1.51859700
H	-1.49623900	3.43980700	2.19250600
H	0.76408400	2.52917900	3.44184600
H	1.11414800	4.08566200	2.61723300
H	2.54759500	2.10322900	1.43166100
H	1.15098100	-1.66913900	-2.69477600
H	2.87501400	-3.27088500	-3.10941100
N	-2.90723000	1.93172900	-0.77013200
O	-3.74706500	2.73492900	-1.14037100
C	-1.11206400	4.50668200	-0.31704800
O	-2.08048100	5.00963700	0.22217500
C	1.97778600	3.44681200	-0.96202600
O	2.64332400	2.57534300	-1.49850800
C	3.94671700	-0.12318200	0.04668600
O	3.77792400	0.06236500	1.24166500
C	5.20210500	-2.36810400	-1.62683600
O	6.07466200	-1.98902700	-0.87145100
O	-0.76541300	4.72739700	-1.59456100
O	2.05748900	4.74646600	-1.29237800
O	4.80926000	0.55930500	-0.70742000
O	5.44718200	-3.13496500	-2.71629900
C	-1.70586600	5.51196800	-2.34673200
H	-1.82728400	6.50275600	-1.90043200
H	-2.67121900	5.00120200	-2.37275200
H	-1.28116200	5.59026200	-3.34821500
C	2.88811200	5.04539200	-2.42460700
H	2.50262300	4.55169300	-3.32077400
H	3.91531300	4.71429300	-2.24930000
H	2.84682400	6.12912600	-2.53656500
C	5.64373200	1.50044500	-0.01806700
H	6.20100600	1.00099700	0.77820400
H	5.03920600	2.30759900	0.40268700
H	6.32266400	1.89198700	-0.77552000
C	6.82742600	-3.46290000	-2.93485400
H	7.23277700	-4.00936300	-2.07885700
H	7.41784400	-2.55519500	-3.08637800
H	6.84211000	-4.08425300	-3.83078100
C	-2.63434900	-2.37823100	-1.11229300
C	-2.03425700	-1.08666800	-1.69484400
C	-2.60841600	-3.47997300	-2.19911000
C	-4.10492100	-2.16256600	-0.66456200
C	-2.95774200	-0.58273300	-2.83394900
H	-1.57102400	-3.67564100	-2.50210600
H	-3.02078700	-4.42704500	-1.81825300
C	-3.44667100	-3.00870600	-3.41108100
H	-4.13611100	-1.38312500	0.10426700
H	-4.50579300	-3.08716000	-0.22433800
C	-4.97382000	-1.74576000	-1.86833700
H	-2.57189100	0.36282000	-3.23111500
C	-2.90935800	-1.66338400	-3.95075300
C	-4.43862300	-0.41333800	-2.42370800
H	-3.39109800	-3.77153800	-4.19939800
C	-4.91041400	-2.82989200	-2.96116400
H	-6.01186200	-1.61855300	-1.53330000
H	-3.51647900	-1.34703600	-4.81128600
H	-1.88016100	-1.78627400	-4.31572400
H	-4.56938900	0.37267000	-1.67939700
H	-5.02432700	-0.11679900	-3.30554600
H	-5.30976700	-3.78258800	-2.58363700
H	-5.53505200	-2.53750900	-3.81604300
H	-1.11500000	-1.39002200	-2.20490800

3.34-TS-G

(cis,isotactic dyad)

B3LYP SCF energy:	-2756.93055129	a.u.
B3LYP enthalpy:	-2755.95446600	a.u.
B3LYP free energy:	-2756.10798500	a.u.
M06 SCF energy in solution:	-2755.97653933	a.u.
M06 enthalpy in solution:	-2755.00045404	a.u.
M06 free energy in solution:	-2755.15397304	a.u.
M06-2X SCF energy in solution:	-2756.54956302	a.u.
M06-2X enthalpy in solution:	-2755.57347773	a.u.
M06-2X free energy in solution:	-2755.72699673	a.u.
Imaginary frequency:	-75.5281	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.38656300	0.70610900	-0.28069600
N	0.90456300	3.17480100	0.64872300
N	2.31947700	2.41797900	-0.83924400
C	1.16059800	2.15868400	-0.18485300
C	1.82913500	4.30676700	0.49126900
C	2.91601400	3.70694700	-0.41575100
C	3.14578700	1.51758500	-1.59745100
C	3.15178300	1.58141900	-2.99957400
C	4.02467300	0.73302500	-3.69676700
C	4.89302100	-0.13941700	-3.04310600
C	4.89150900	-0.14759700	-1.64106700
C	4.04125200	0.67525000	-0.90097100
C	2.28415200	2.53963700	-3.77873000
C	5.83607200	-1.03285700	-3.81592700
C	4.12492000	0.68510500	0.60775000
C	0.20935900	-0.75128200	0.80255900
C	0.96113900	-2.03816400	0.48303600
C	2.17721800	-2.25467200	1.38627700
C	1.55087100	-2.23219500	-0.93671400
C	3.19805100	-2.81538700	0.71186500
C	2.85545200	-3.03933700	-0.74483500
H	2.21705900	4.63894200	1.45795800
H	1.31594600	5.15224700	0.01827200
H	3.13433300	4.32530100	-1.29134600
H	3.85583800	3.53004400	0.11888000
H	4.02200800	0.76674600	-4.78440900
H	5.56894700	-0.81365700	-1.11021600
H	2.90293300	3.18742300	-4.41236800
H	1.68152000	3.17479500	-3.12638300
H	1.59342300	2.00191200	-4.43536900
H	5.79329700	-2.06731300	-3.45496500
H	6.87674500	-0.69905000	-3.71060800
H	5.59669900	-1.03849900	-4.88383200

H	3.14634100	0.58717000	1.08361000
H	4.57356900	1.61753800	0.97671300
H	4.74853200	-0.13573800	0.96956500
H	0.07755700	-0.70016800	1.89609800
H	0.27645100	-2.86568300	0.73704000
H	1.77301300	-1.25192400	-1.36731300
H	3.65432000	-2.71652400	-1.41773100
O	0.02683400	0.36345400	-2.59241900
O	-1.01808200	2.14867200	-1.92993200
C	-2.40776000	0.01351500	-0.54026700
C	-1.87911600	-0.99740400	0.33218500
C	-2.10730100	-2.33483800	-0.42237400
C	-2.91570100	-0.74702500	-1.79075000
C	-1.89965800	-1.90798400	-1.89252900
C	-3.64244800	-2.48906900	-0.42844600
C	-4.12835300	-1.54784400	-1.26556700
H	-3.04815200	0.79677800	-0.15971900
H	-2.08279400	-0.96932200	1.39731900
H	-1.58567600	-3.21116300	-0.04167100
H	-3.10597200	-0.13728300	-2.67432100
H	-2.21448200	-2.68453600	-2.59535500
H	-0.89656100	-1.56709600	-2.13553800
H	0.85435900	-2.73549800	-1.61034100
H	2.70421100	-4.11342600	-0.92667300
C	-4.31607500	-3.45495100	0.45710800
O	-3.72278700	-4.31102200	1.08859700
C	-5.51742500	-1.11344400	-1.55385500
O	-5.89624200	0.02306300	-1.34951800
C	2.08330200	-2.04309700	2.86122800
O	1.26673100	-2.61699700	3.55194700
C	4.45676500	-3.27108800	1.34801700
O	4.65593100	-3.37232500	2.54350800
O	-6.27003000	-2.07650200	-2.11026700
O	-5.65530700	-3.28514000	0.50953700
O	2.94745800	-1.11873100	3.31382900
O	5.39007500	-3.58210300	0.41425300
C	-6.35669500	-4.21832900	1.34479900
H	-6.00476500	-4.15055900	2.37772100
H	-6.20958300	-5.24108400	0.98687300
H	-7.40783200	-3.93618200	1.27793800
C	-7.62377800	-1.69645300	-2.41126000
H	-7.64057100	-0.84292600	-3.09402800
H	-8.15721600	-1.43065100	-1.49471200
H	-8.07412500	-2.57270100	-2.87800300
C	2.97566700	-0.95546400	4.74280200
H	3.31113400	-1.88255300	5.21434000
H	1.98498400	-0.69180200	5.12150300
H	3.68795900	-0.15152600	4.92894200
C	6.63701100	-4.06646100	0.93618700
H	6.47903200	-4.97255700	1.52727700
H	7.10917900	-3.31016500	1.56918100
H	7.25620000	-4.27904400	0.06417400
C	-0.35561600	3.23424200	1.40314800
C	-0.86670700	1.76919100	1.52329200
C	-0.11357100	3.79803500	2.82537300
C	-1.36527400	4.16044100	0.67726000
C	-2.26011600	1.84048300	2.21535700
H	0.63679200	3.18339700	3.34054900
H	0.27707100	4.82576100	2.78188300
C	-1.44787600	3.80039300	3.60372200
H	-1.53702700	3.79398100	-0.33916300
H	-0.94376100	5.17293000	0.59524600
C	-2.69010400	4.21190700	1.46005700
H	-2.70272500	0.83879200	2.28641500
C	-2.04070300	2.37579500	3.65671900
C	-3.26541100	2.78667700	1.51710600
H	-1.26553600	4.16333300	4.62403800
C	-2.44132600	4.73637100	2.88683300
H	-3.39258700	4.87463700	0.93796900
H	-2.99428100	2.39578000	4.20409000
H	-1.36912900	1.70444600	4.20851200
H	-3.49928200	2.45917800	0.49926300
H	-4.21374400	2.78265000	2.07277300
H	-2.04212900	5.76031800	2.85315100
H	-3.38710800	4.78073500	3.44380000
N	-0.61586700	1.41737100	-2.91473800
O	-0.84380300	1.72662000	-4.07556100
H	-0.20550200	1.29934900	2.26970400

3.34-TS-H

(trans,isotactic dyad)

B3LYP SCF energy:	-2756.93065880	a.u.
B3LYP enthalpy:	-2755.95522200	a.u.
B3LYP free energy:	-2756.11074700	a.u.
M06 SCF energy in solution:	-2755.97575183	a.u.
M06 enthalpy in solution:	-2755.00031503	a.u.
M06 free energy in solution:	-2755.15584003	a.u.
M06-2X SCF energy in solution:	-2756.54821529	a.u.
M06-2X enthalpy in solution:	-2755.57277849	a.u.
M06-2X free energy in solution:	-2755.72830349	a.u.
Imaginary frequency:	-33.1144	cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.24765700	-0.65654200	0.05383100
N	-1.78900000	-1.86338400	1.78810500
N	-2.69178600	-1.92927900	-0.20780400
C	-1.59299700	-1.56726800	0.49973900
C	-3.06496100	-2.53625600	2.05004400
C	-3.75972700	-2.45004600	0.67629900
C	-2.84826400	-2.02593300	-1.63553500
C	-2.58725000	-3.25966000	-2.26406500
C	-2.78564100	-3.35414400	-3.64487400
C	-3.23716100	-2.27283700	-4.40585000
C	-3.51356600	-1.07261400	-3.74558900
C	-3.33427700	-0.92843900	-2.36653200
C	-2.12107800	-4.47406800	-1.49218500
C	-3.39921100	-2.39308300	-5.90329300
C	-3.66548000	0.37806800	-1.69264200
C	-0.28450500	1.16426700	-0.03585500
C	-0.67501600	2.28840600	0.93084800
C	-2.15144000	2.64782200	0.74617900
C	-0.00553300	3.65382300	0.58385700
C	-2.30193400	3.73940000	-0.03063200

C	-0.96356500	4.33343200	-0.41872500
H	-3.62190800	-2.01318200	2.83177200
H	-2.89926500	-3.57157800	2.37361700
H	-4.12046000	-3.41735900	0.31636300
H	-4.60646100	-1.75319900	0.68368000
H	-2.56834800	-4.29907100	-4.13807600
H	-3.88162900	-0.22178900	-4.31526200
H	-1.70101000	-5.21969300	-2.17216000
H	-2.95173300	-4.95262400	-0.95412000
H	-1.35086800	-4.22606100	-0.75733400
H	-3.74038400	-3.39353900	-6.19174400
H	-2.44539900	-2.21556900	-6.41742200
H	-4.11935000	-1.66352700	-6.28896700
H	-4.46403300	0.26293700	-0.94911300
H	-3.99426600	1.13105900	-2.41403800
H	-2.79576700	0.78066000	-1.16775500
H	-0.33422700	1.55435800	-1.07106900
H	-0.47488100	1.99620300	1.96256100
H	1.01706100	3.57055900	0.21362200
H	-0.72850600	4.09526500	-1.46591500
O	0.24559000	-1.47721600	-2.16369500
O	0.79598600	-2.78510700	-0.51948800
C	2.44547800	-0.40202000	-0.16865300
C	2.05152200	0.92876200	0.05890100
C	2.52637000	1.72498300	-1.18391600
C	3.15525400	-0.39924500	-1.54714500
C	2.34833400	0.68253300	-2.30771600
C	4.06345300	1.69166900	-1.06324900
C	4.44559200	0.41772300	-1.29923200
H	2.82429000	-1.04548400	0.61495600
H	2.04497400	1.39678800	1.03565200
H	2.11309300	2.72065400	-1.32837800
H	3.29889900	-1.37240400	-2.01621800
H	2.83449300	0.99311200	-3.23669000
H	1.31866300	0.39129500	-2.50563200
H	0.03030300	4.25397000	1.50098000
H	-0.96156600	5.42684900	-0.33840500
C	5.76172900	-0.25179600	-1.14637700
O	5.94567100	-1.14313100	-0.34162400
C	4.80732500	2.86641800	-0.58255700
O	4.27432500	3.93082100	-0.31661300
C	-3.22872600	1.90128700	1.43201800
O	-3.04679300	1.03022700	2.26213100
C	-3.56629800	4.33407000	-0.56301900
O	-4.03824000	4.04800600	-1.64213300
O	6.68239000	0.18587800	-2.02018600
O	6.13231200	2.64456500	-0.44642900
O	-4.05094200	5.28670000	0.25335400
O	-4.46236400	2.32744700	1.07149400
C	7.96969100	-0.44746500	-1.91944100
H	7.87891700	-1.52729900	-2.06315100
H	8.41338200	-0.25413600	-0.93912800
H	8.57438000	-0.00257400	-2.70992600
C	6.89484100	3.76289900	0.03056500
H	6.54932300	4.07061200	1.02134600
H	6.80541200	4.60998100	-0.65500900
H	7.92674900	3.41360200	0.07591400
C	-5.23924900	5.94947900	-0.21510200
H	-6.05581700	5.23145100	-0.32742200
H	-5.05516000	6.43329900	-1.17786500
H	-5.47974100	6.68930600	0.54855700
C	-5.55889100	1.71742000	1.76573300
H	-5.59486700	0.64375900	1.56088700
H	-6.45509900	2.20604200	1.38280100
H	-5.46566000	1.87151000	2.84408900
N	0.65199000	-2.62691300	-1.79710400
O	0.89071100	-3.53176600	-2.58212900
C	-0.65159900	-1.81274100	2.71681100
C	0.05653400	-3.19372400	2.72894400
C	-1.08986000	-1.47661100	4.16120800
C	0.26735600	-0.67425300	2.19524900
H	-0.64269100	-3.96270500	3.09018700
H	0.34828200	-3.46726100	1.71030000
C	1.29509000	-3.14107500	3.64013600
H	-1.63486300	-0.52523000	4.16655100
H	-1.76686400	-2.24882500	4.55782000
C	0.16834800	-1.39830400	5.05905600
C	1.55711700	-0.69806100	3.05943100
H	1.78855500	-4.12200800	3.63996900
C	0.87038700	-2.77134400	5.07449600
C	2.25587700	-2.07643800	3.07855100
H	-0.13829500	-1.12753900	6.07836300
C	1.15411600	-0.34198600	4.51559300
H	2.27051700	0.05804600	2.70601900
H	0.19565400	-3.53902700	5.47971000
H	1.74897900	-2.73757200	5.73346500
H	2.57242800	-2.37746000	2.07309400
H	3.16408200	-2.02198000	3.69540200
H	2.04389600	-0.30343600	5.16140700
H	0.69555700	0.65594100	4.54405800
H	-0.26237800	0.24005200	2.48041100