SUPPORTING INFORMATION

Probing Stereoselectivity in Ring-Opening Metathesis Polymerization Mediated by Cyclometalated Ruthenium-Based Catalysts: A Combined Experimental and Computational Study

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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. $CDCl_3$, CD_2Cl_2, and $(CD_3)_2CO$ were used as received. Monomers **10**,[1] **11**,[2] **12**,[3] **13**,[4] and **15**[5] were synthesized according to literature procedure, while monomers **9** and **14** were purchased from Sigma Aldrich and either used as received (**9**) or distilled over CaH_2 prior to use (**14**). Catalysts **2** and **4**, as well as $RuCl_2(PCy_3)$(=CH-*o*-O*i*PrC_6H_4) (**S2**), were obtained from Materia, Inc. **1**,[6] **5**, **6**, **7**,[7] **8**[8] and *N*-heterocyclic carbene (NHC) **S1**[7] were synthesized according to literature procedures. Other commercially available reagents were used as received.

^{1}H NMR spectra were acquired at 500 MHz and ^{13}C spectra at 100 or 126 MHz as $CDCl_3$ 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 processed and analyzed using MestReNova Ver. 9.0.

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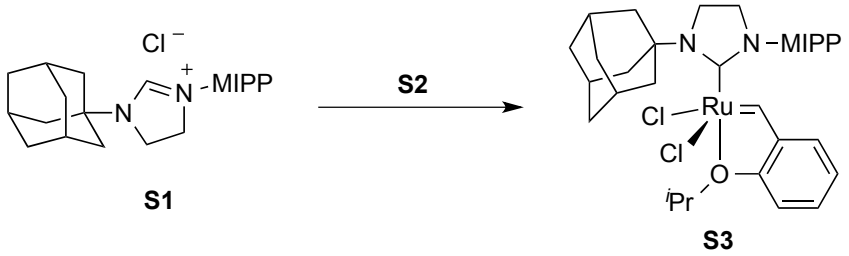
[1] Tabor, D.C.; White, F.H.; Collier, L.W.; Evans, S.A. *J. Org. Chem.* **1983**, *48*, 1638.
[2] Alimuniar, A. B.; Blackmore, P. M.; Edwards, J. H.; Feast, W. J.; Wilson, B. *Polymer* **1986**, *27*, 1281.
[3] Mühlebach, A.; Bernhard, P.; Bühler, N.; Karlen, T.; Ludi, A. *J. Mol. Catal.* **1994**, *90*, 143.
[4] Grutzner, J. B.; Jautelat, M.; Dence, J. B.; Smith, R. A.; Roberts, J. D. *J. Am. Chem. Soc.* **1970**, *92*, 7107.
[5] (a) Ishihara, K.; Hanaki, N.; Funahashi, M.; Miyata, M.; Yamamoto, H. *Bull. Chem. Soc. Jpn.* **1995**, *68*, 1721. (b) 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. (c) Berson, J. A.; Walia, J. S.; Remanick, A.; Suzuki, S.; Reynolds-Warnhoff, P.; Willner, D. *J. Am. Chem. Soc.* **1961**, *83*, 3986.
[6] Rosebrugh, L. R.; Marx, V. M.; Keitz, B. K.; Grubbs, R. H. *J. Am. Chem. Soc.* **2013**, *135*, 10032.
[7] Keitz, B. K.; Endo, K.; Patel, P. R.; Herbert, M. B.; Grubbs, R. H. *J. Am. Chem. Soc.* **2012**, *134*, 693.
[8] 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.

High-resolution mass spectra (HRMS) were provided by the California Institute of Technology Mass Spectrometry Facility using an IEOL JMS-600H High Resolution Mass Spectrometer. All HRMS were by FAB+ ionization.

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 our previous calculations on ruthenium metathesis catalysts.

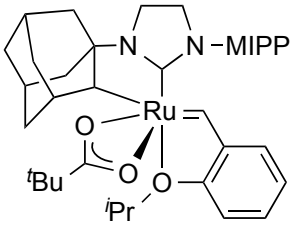
Preparation of Catalyst S3



In a glovebox, a suspension of potassium *tert*-amylate (0.075 g, 0.57 mmol) in hexanes (6mL) was added to NHC **S1** (0.19 g, 0.52 mmol), and the resulting solution was stirred in the glovebox box at 30 °C for 30 minutes. Then, **S2** (0.31 g, 0.52 mmol) was added, and the vessel was sealed, taken out of the glovebox, and stirred for 2 h at 65 °C. The mixture was then cooled to RT, and the resulting solids were collected via filtration. The solids were washed thoroughly with hexanes, yielding **S3** (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+) 656.1894, $[C_{33}H_{44}RuON_2Cl_2]^+$ requires 656.1875.

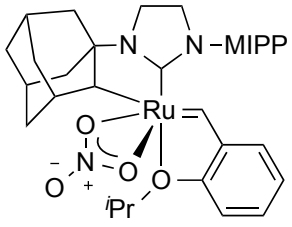
Preparation of Catalyst S4



S4

In a glovebox, sodium pivalate (0.19 g, 1.5 mmol) in MeOH (1.5 mL) was added to complex **S3** (0.10 g, 0.15 mmol) in THF (1.5 mL). The solution was heated at 40 °C for ten hours in the glovebox, then concentrated. The residue was dissolved in dichloromethane, filtered over celite, and then concentrated. Purification via a short plug of silica gel (eluant 4:1 pentane:diethyl ether) provided **S4** (0.052 g, 52%) as a 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+) 686.3039, $[C_{38}H_{52}RuO_3N_2]^+$ requires 686.3022.

Preparation of 3



3

In a glovebox, complex **S4** (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 room temperature, and then

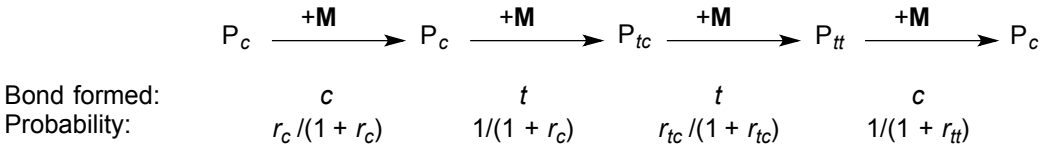
concentrated. The resulting solids were washed with Et_2O, followed by THF, to provide **3** (0.070 g, 72%) as a bright purple powder; ^{1}H NMR (CD_2Cl_2) d 14.98 (1H, s), 7.48 (1H, m), 7.43 (1H, m), 7.13 (1H, m), 7.09 (1H, m), 6.98 (3H, m), 5.10 (1H, m), 3.90 (4H, m), 3.70 (2H, m), 2.23 (1H, m), 2.18 (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+) 646.2040, $[C_{33}H_{43}RuO_4N_3\text{-}H]^+$ requires 645.7706.

General Polymerization Procedure

In a glovebox, a solution of catalyst was prepared from **1** (5.8 mg, 9.8 μmol) and THF (.84 mL) and added to an 8 mL vial with a septum cap. On a vacuum manifold, a Schlenk flask was flame-dried and charged with monomer (7.8 mmol) and THF (24 mL) to make a 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, 6.4 μmol) of catalyst solution was then injected via gas-tight syringe. After stirring for 1 h at room temperature, 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 9.[9]



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 $r_c/(1 + r_c)$. Dyad values can be determined by ^{13}C NMR.[10]

The probability of forming a *trans* double bond in P_c is equal to $1 - [r_c/(1 + r_c)]$, or $1/(1 + r_c)$.

Calculations that also take into account the identity of the penultimate double bond require triad-level NMR analysis (see reference 9 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*).

[9] Greene, R. M. E.; Hamilton, J. G.; Ivin, K. J.; Rooney, J. J. *Makromol. Chem*. **1986**, *187*, 619.
[10] Ivin, K. J.; Laverty, D. T.; Rooney, J. J. *Makromol. Chem.* **1977**, *178*, 1545.

Preparation of Poly-9 Using Catalysts 1-8:

Poly-9 was prepared according to the general procedure using catalysts **1**-**8**. NMR samples were prepared by stirring **poly-9** in $CDCl_3$. ^{13}C NMR spectral assignments were consistent with the literature.[4,10]

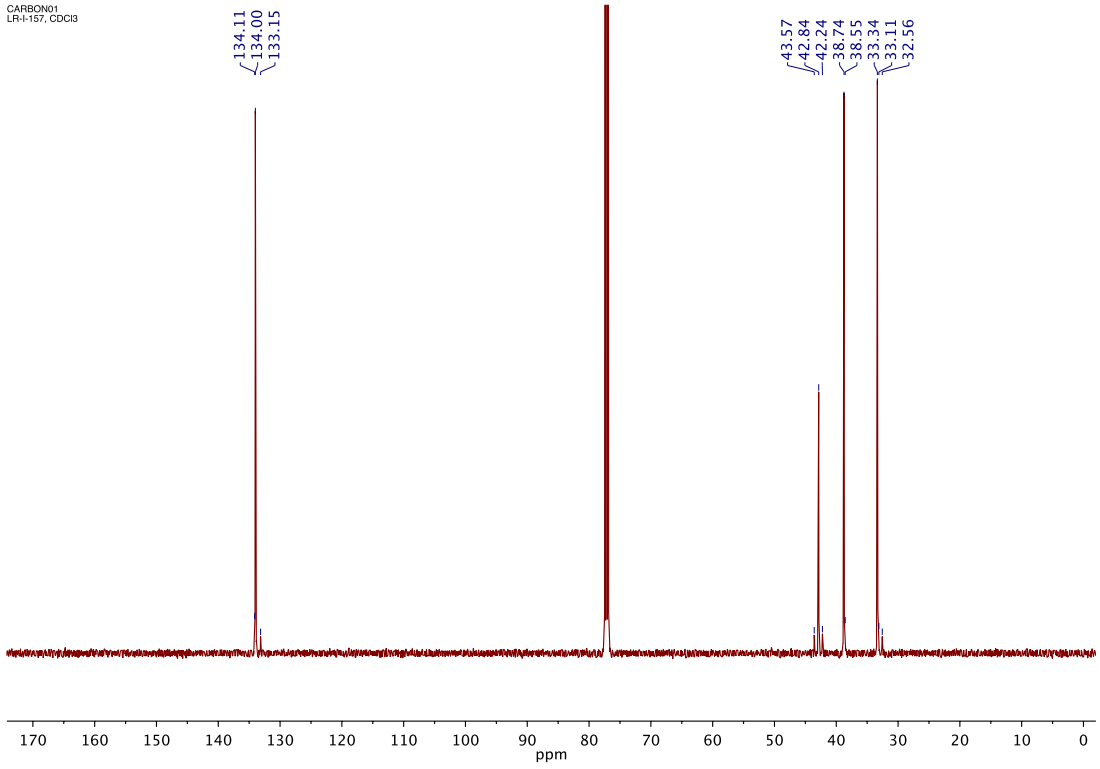


Figure S1. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly-9/1**.

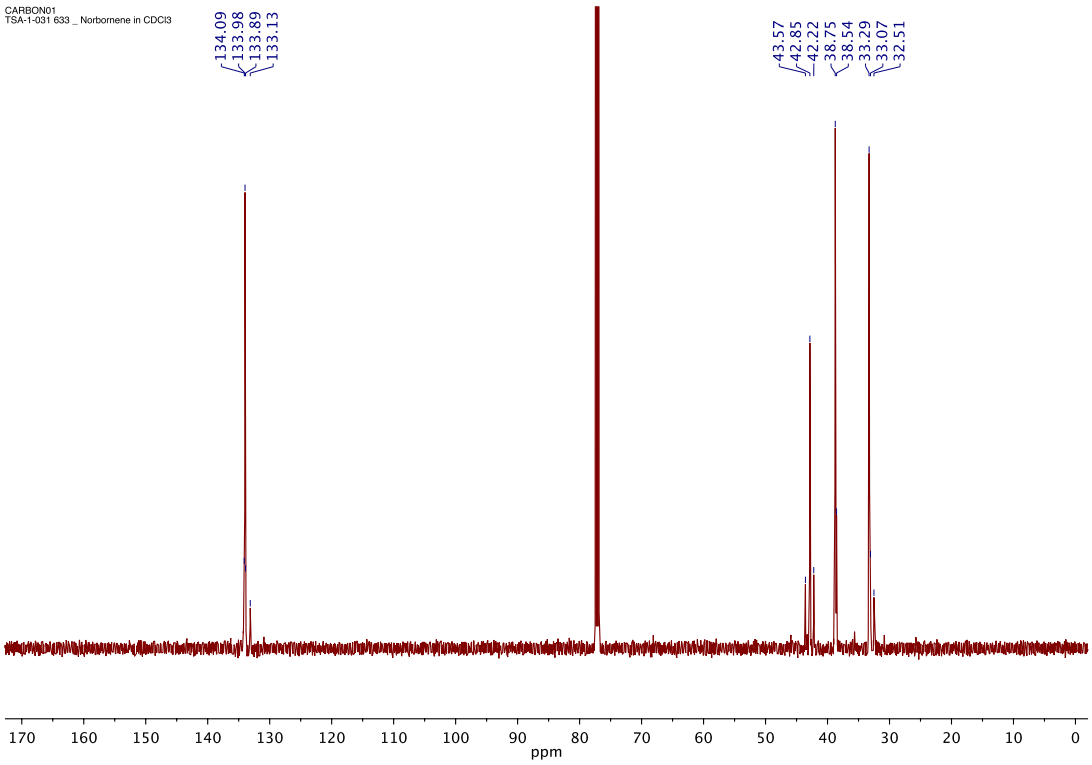


Figure S2. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly-9/2**.

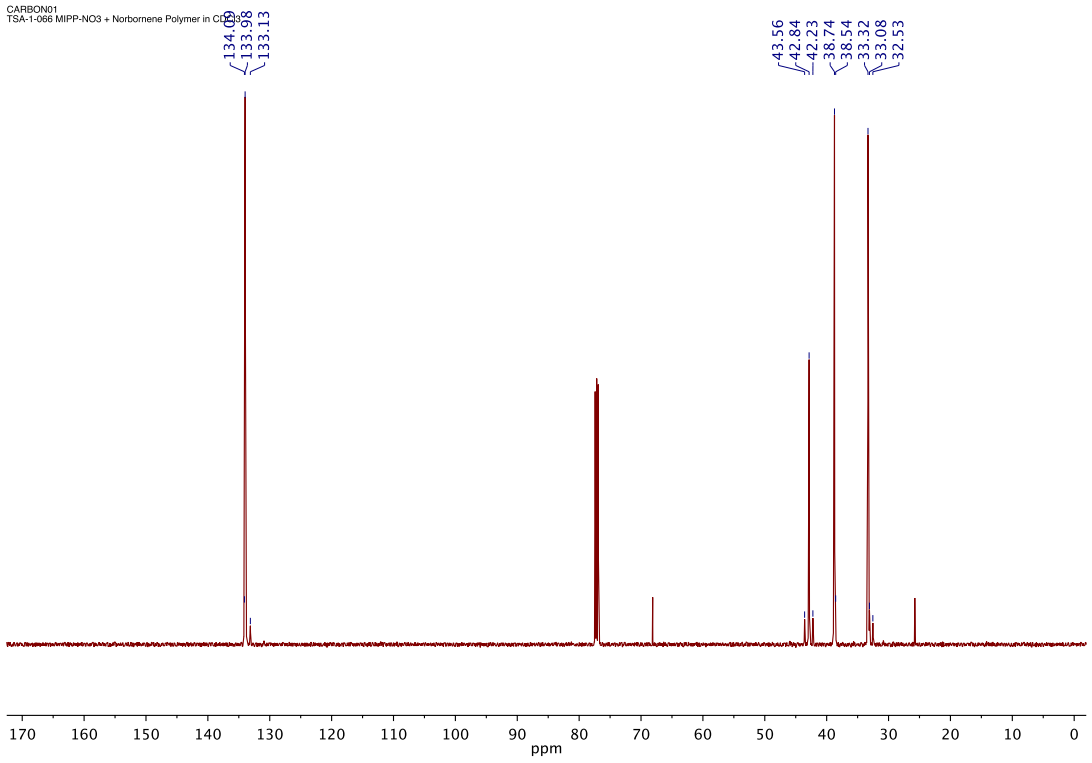


Figure S3. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly-9/3** (peaks at 25.76 and 68.11 ppm are residual THF).

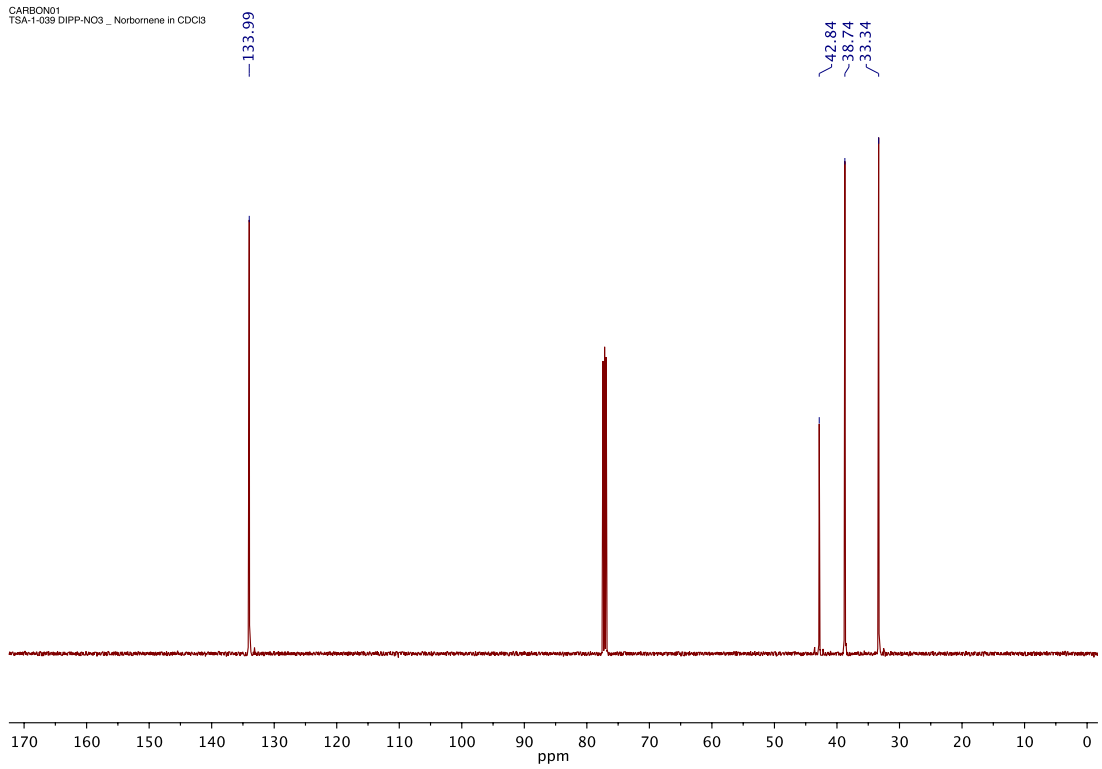


Figure S4. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly-9/4**.

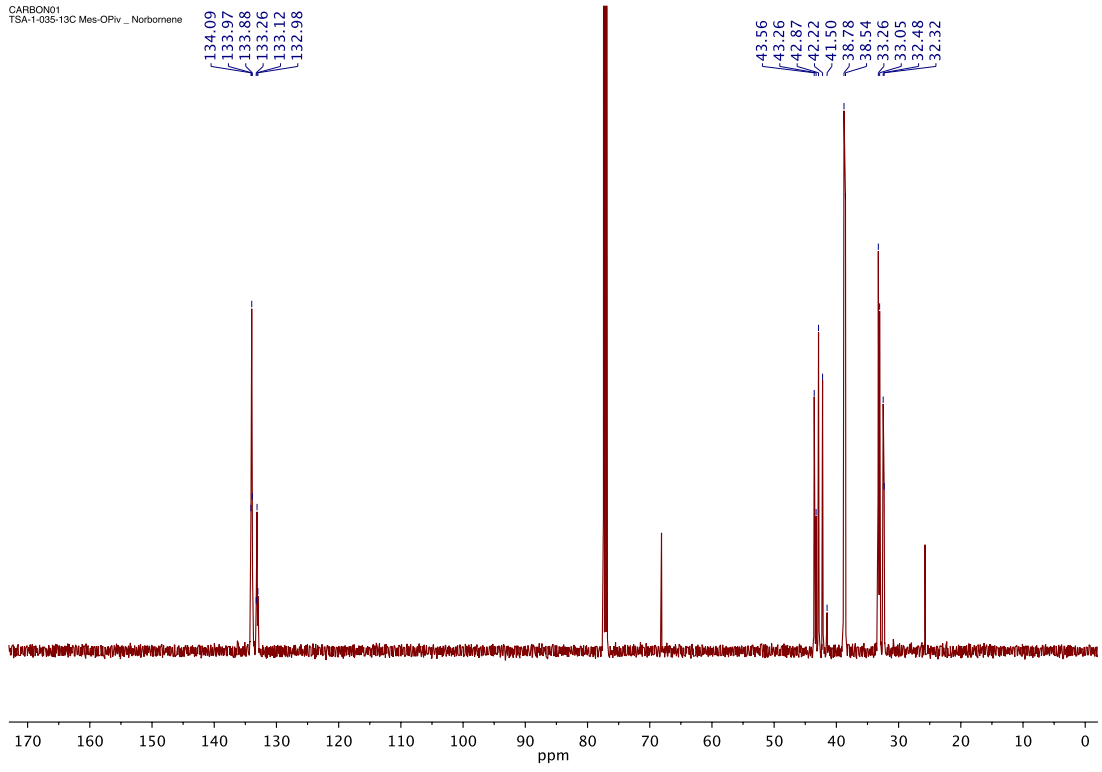


Figure S5. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly-9/5** (peaks at 25.76 and 68.11 ppm are residual THF).

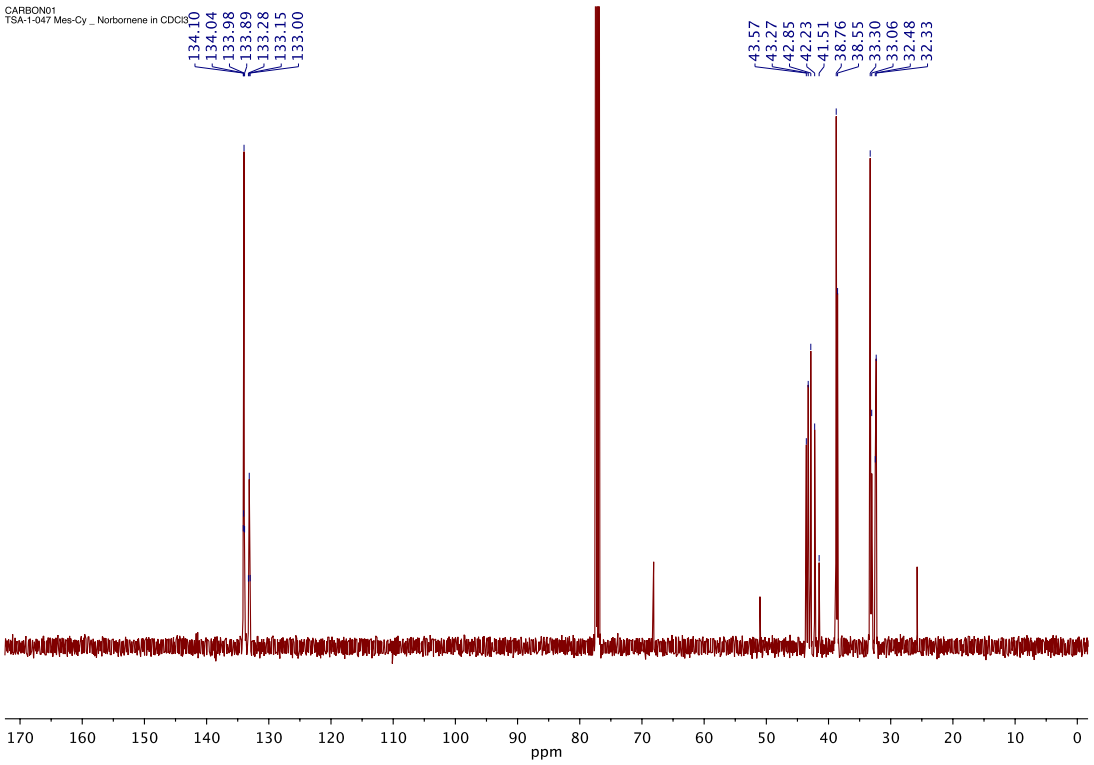


Figure S6. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly-9/6** (peaks at 25.76 and 68.11 ppm are residual THF; peak at 51.03 is residual MeOH).

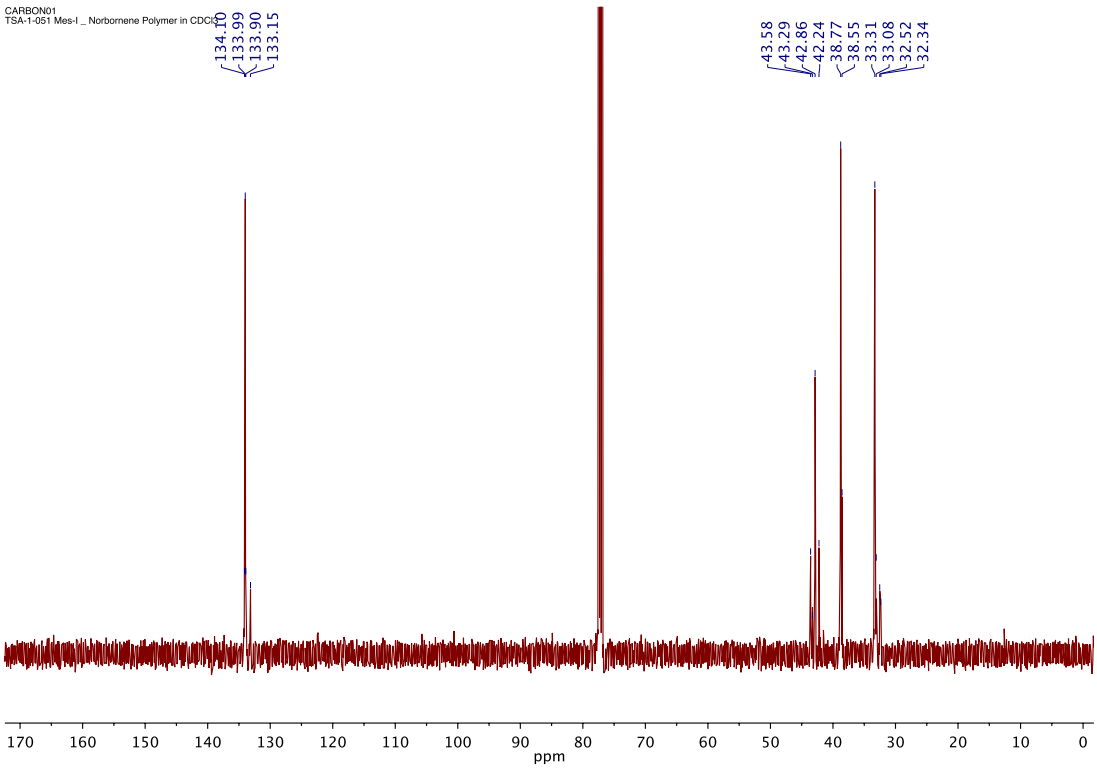


Figure S7. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly-9/7**.

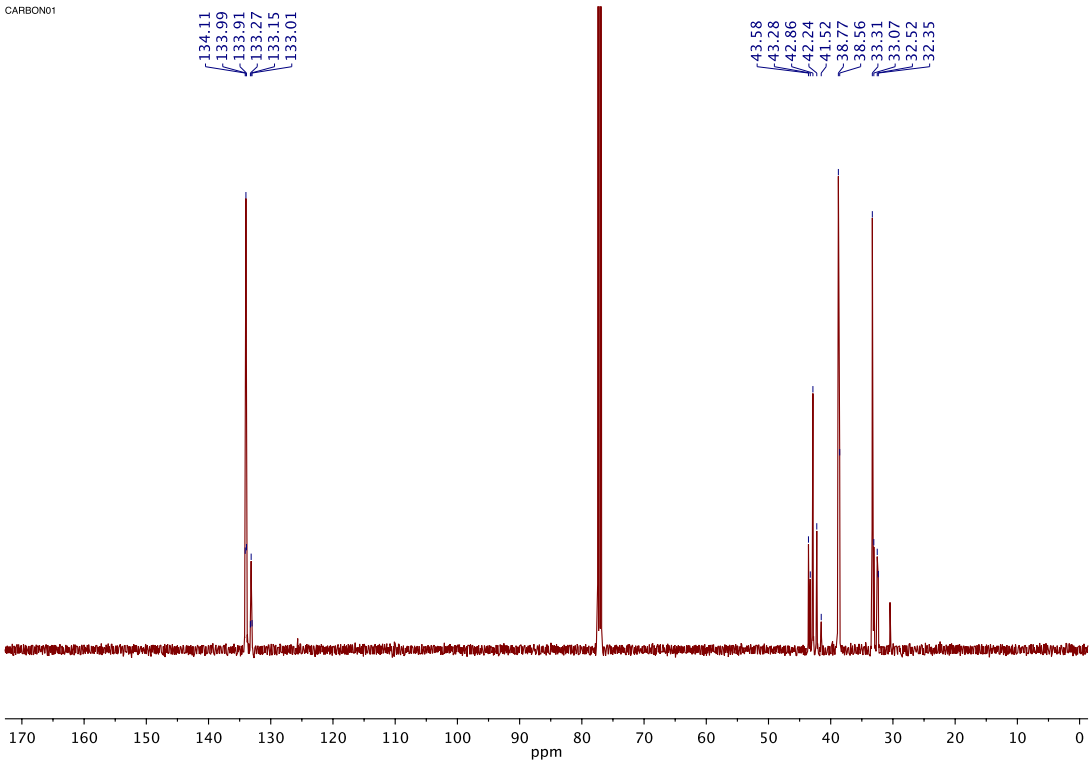


Figure S8. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly-9/8**.

Preparation of Poly-10 Using Catalysts 1-8:

Poly-10 was prepared according to the general procedure using catalysts **1-8**. NMR samples were prepared by stirring **poly-10** in $CDCl_3$. ^{13}C NMR spectral assignments were consistent with the literature.[11]

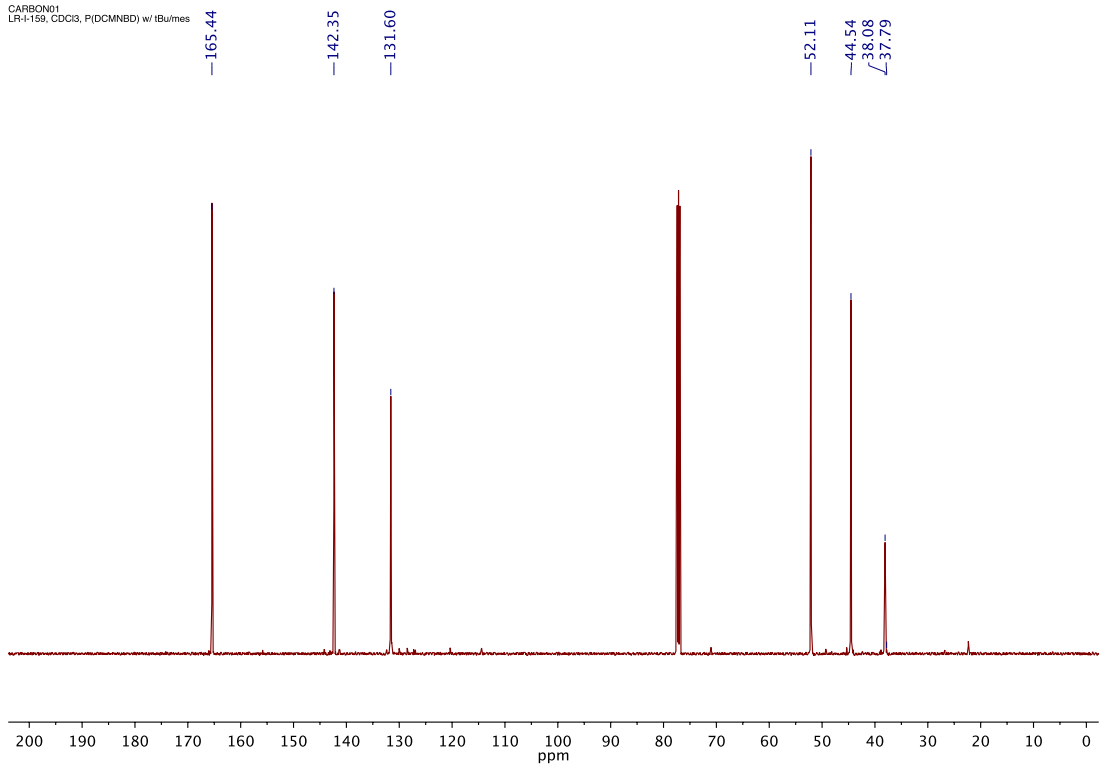


Figure S9. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly-10/1**.

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

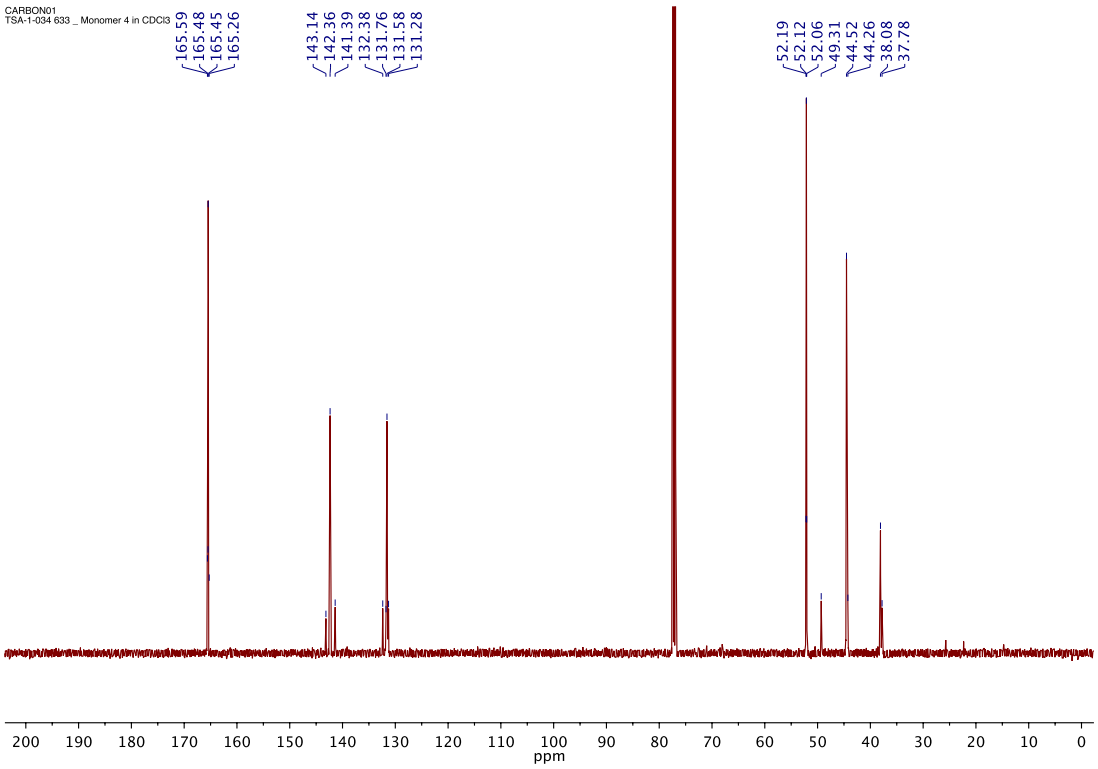


Figure S10. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly-10/2**.

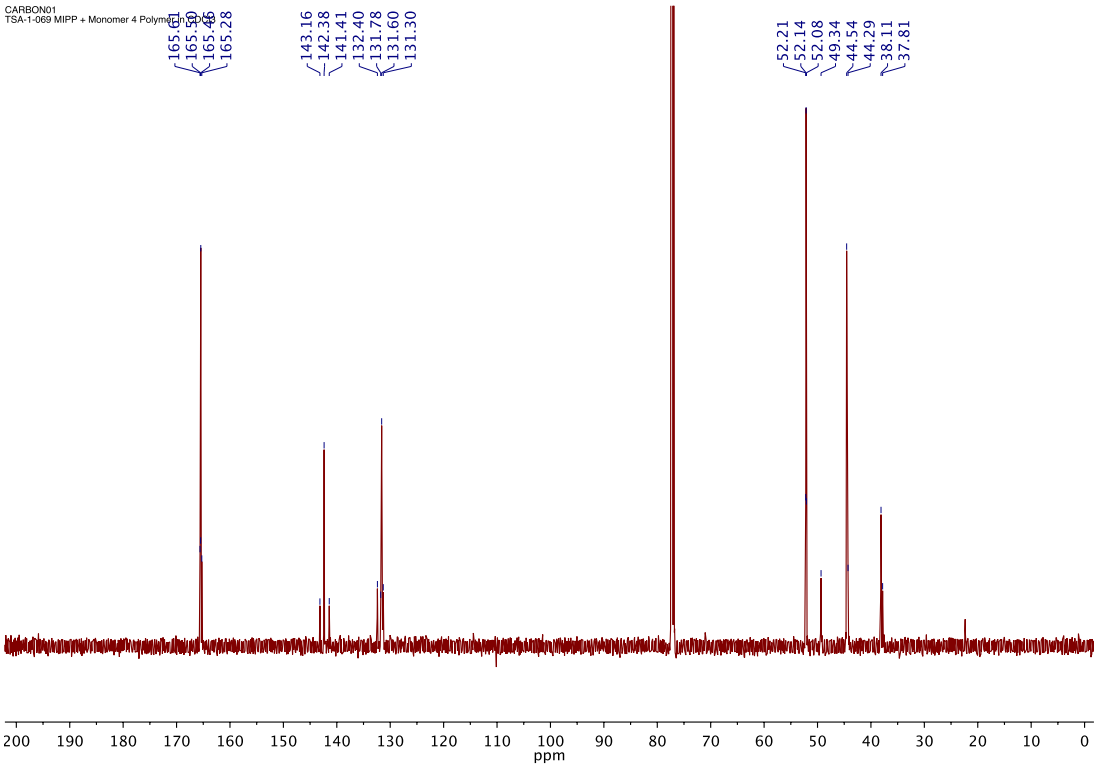


Figure S11. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly-10/3**.

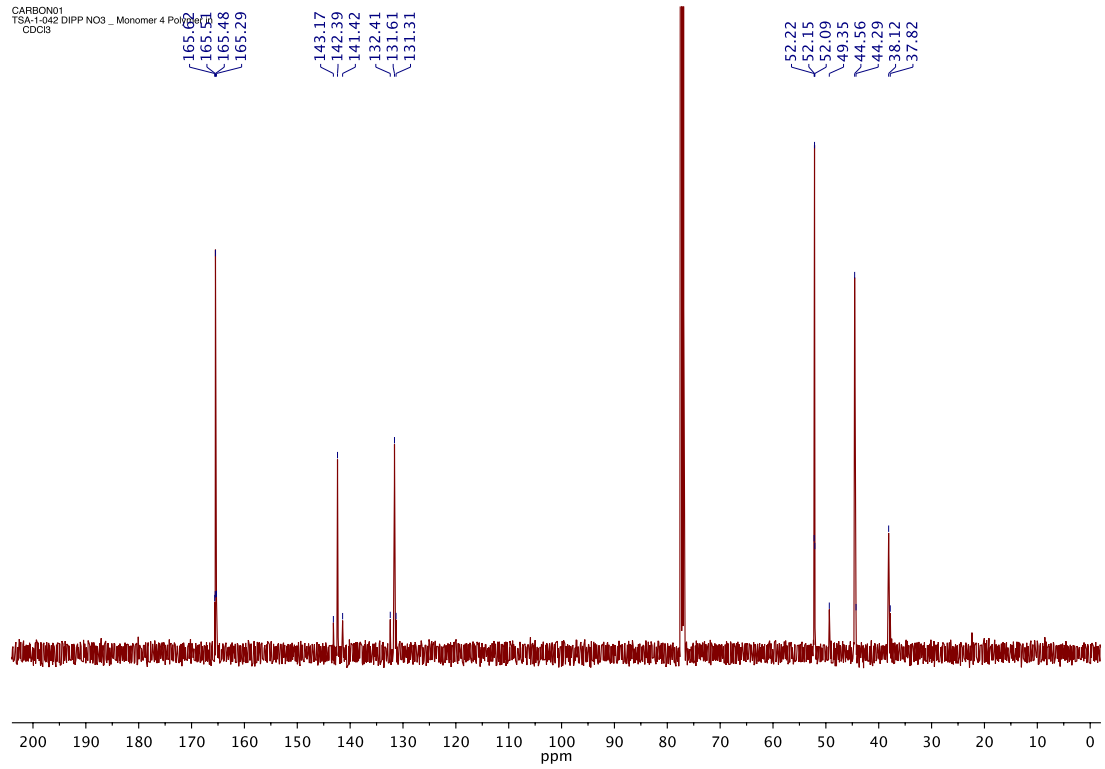


Figure S12. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly-10/4**.

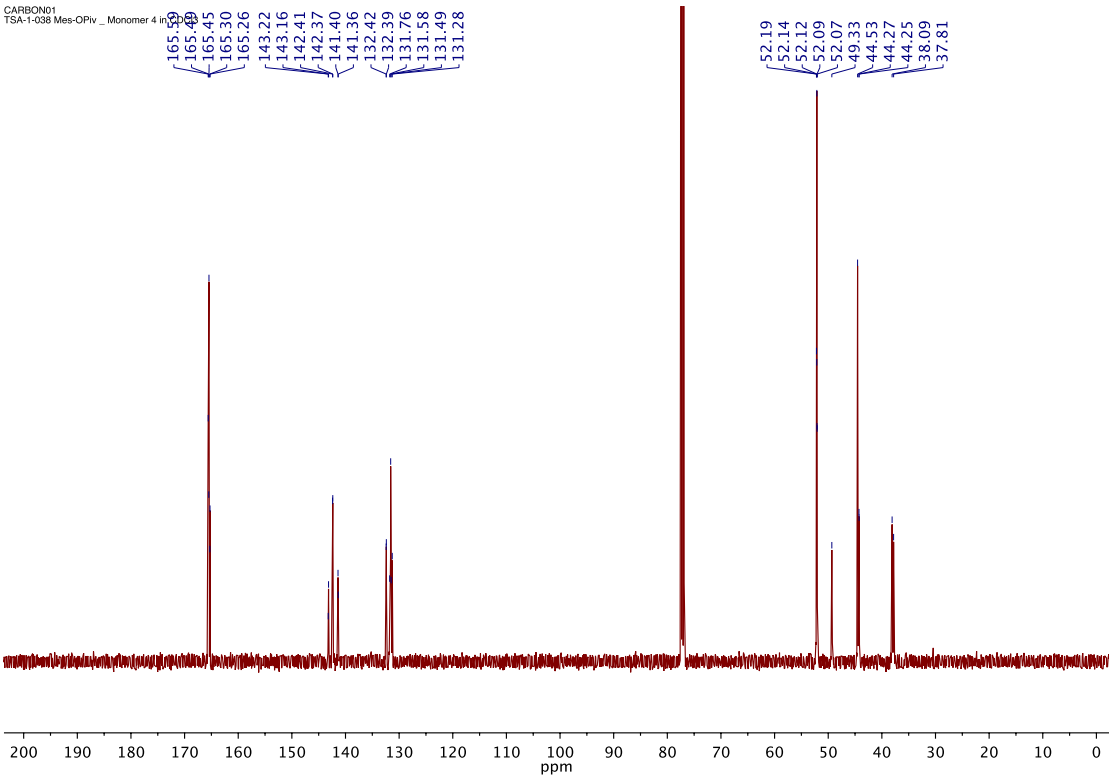


Figure S13. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly-10/5**.

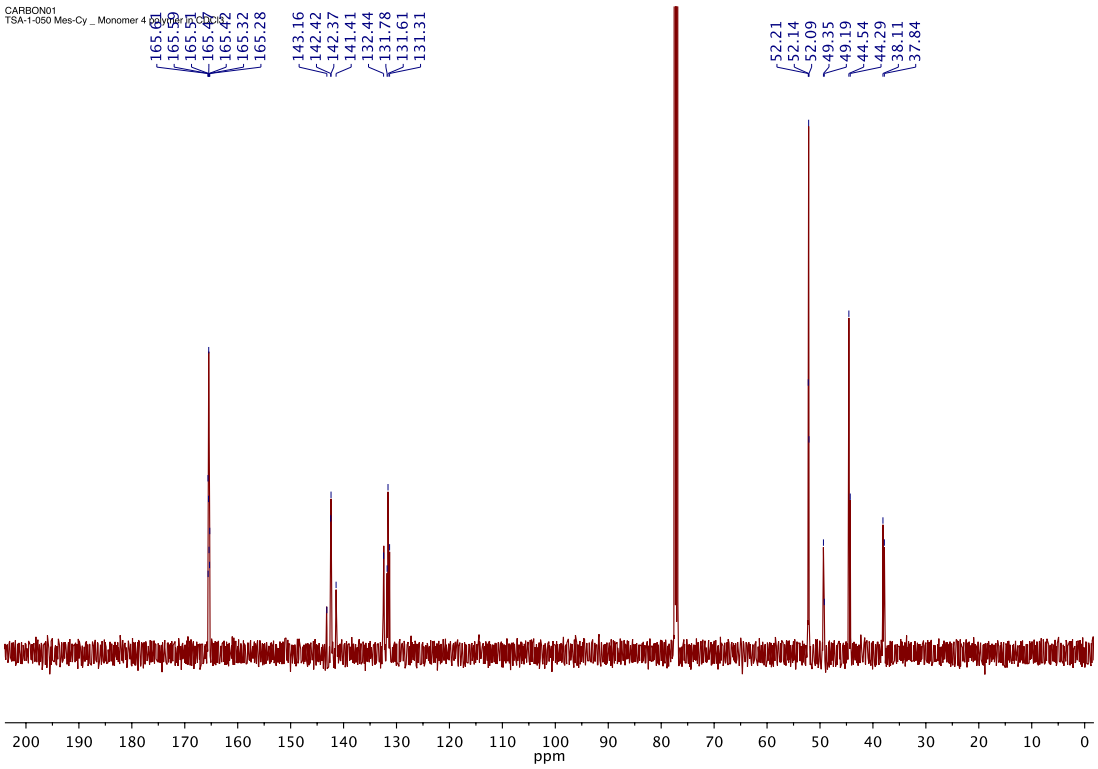


Figure S14. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly-10/6**.

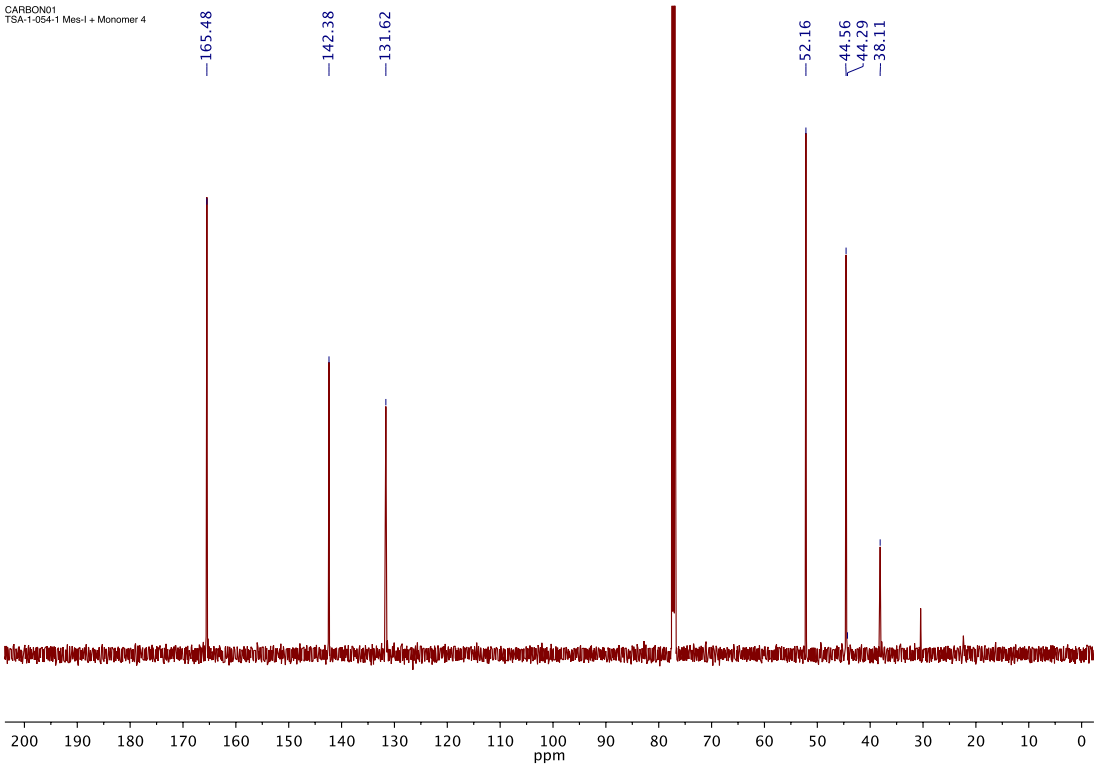


Figure S15. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly-10/7**.

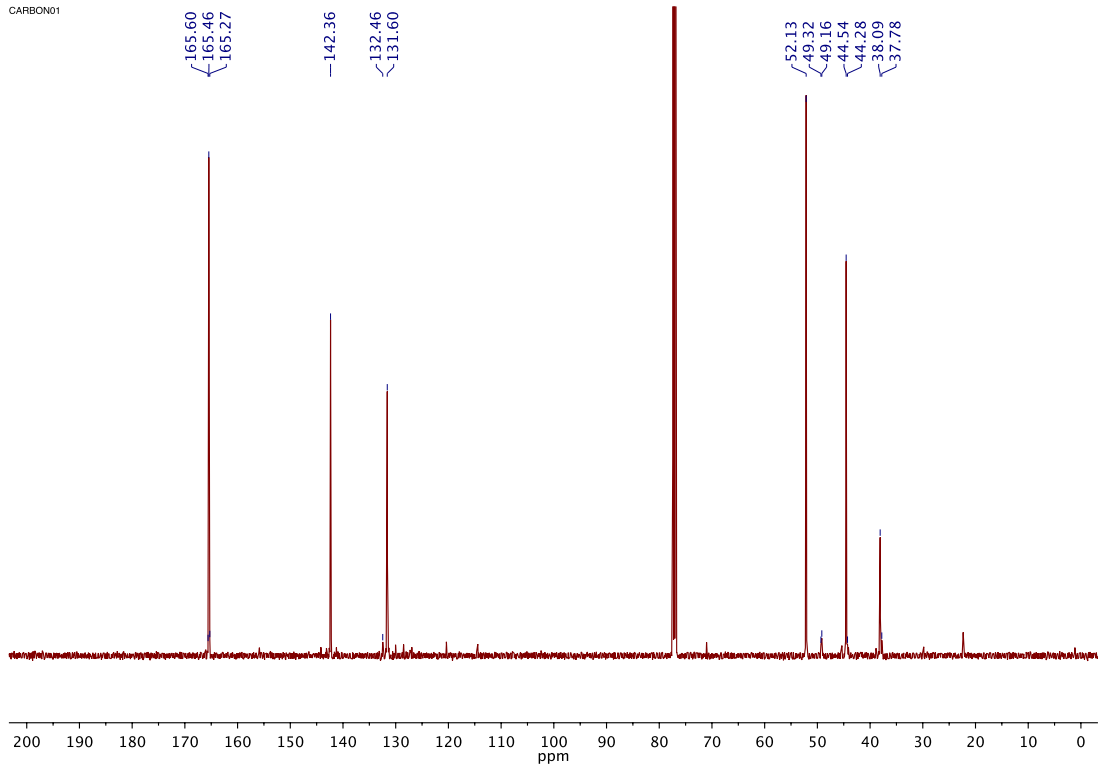


Figure S16. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly-10/8**.

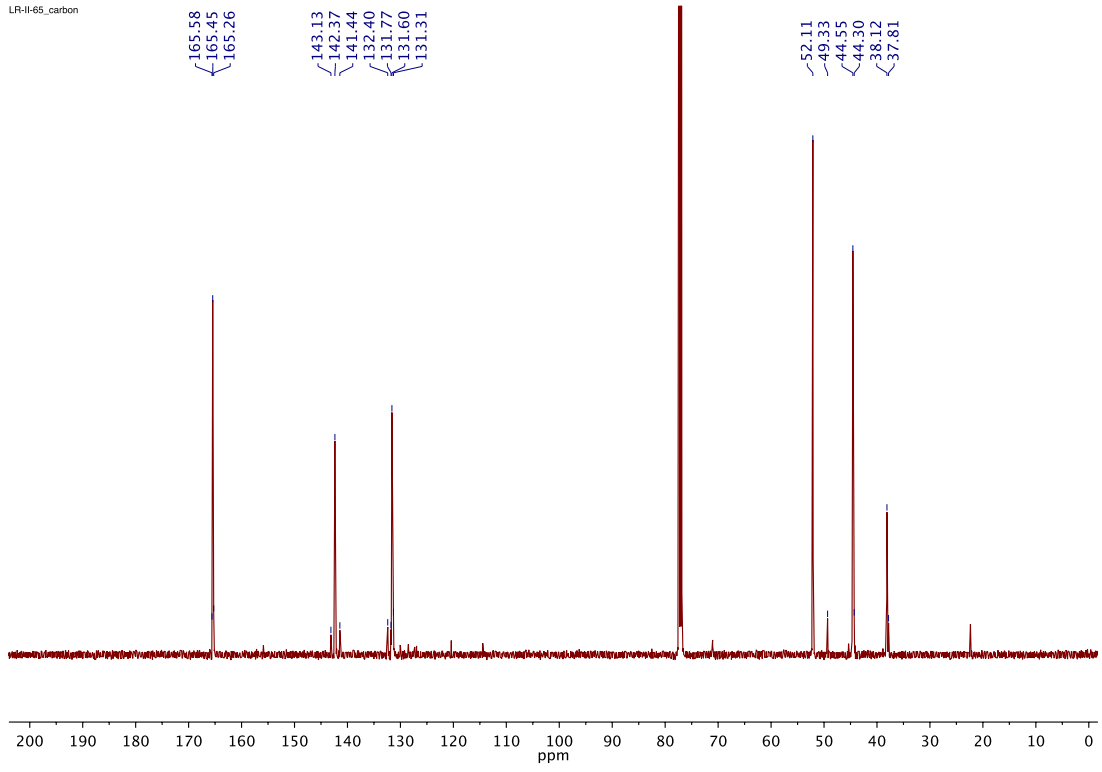


Figure S17. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly-10/2** at 0 °C.

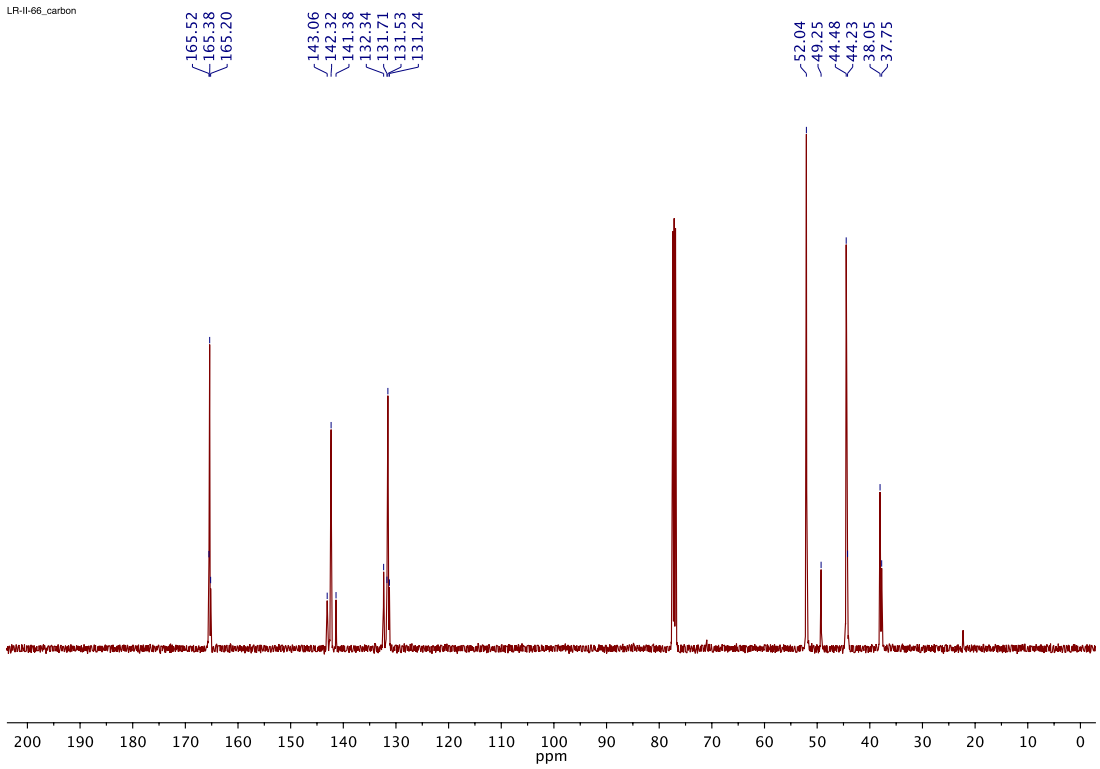


Figure S18. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly-10/2** at 40 °C.

Preparation of Poly-11 Using Catalysts 1, **2**, and **4:**

Poly-11 was prepared according to the general procedure using catalysts **1**, **2**, and **4**. NMR samples were prepared by stirring **poly-11** in $(CD_3)_2CO$. ^{13}C NMR spectral assignments were consistent with the literature.[12]

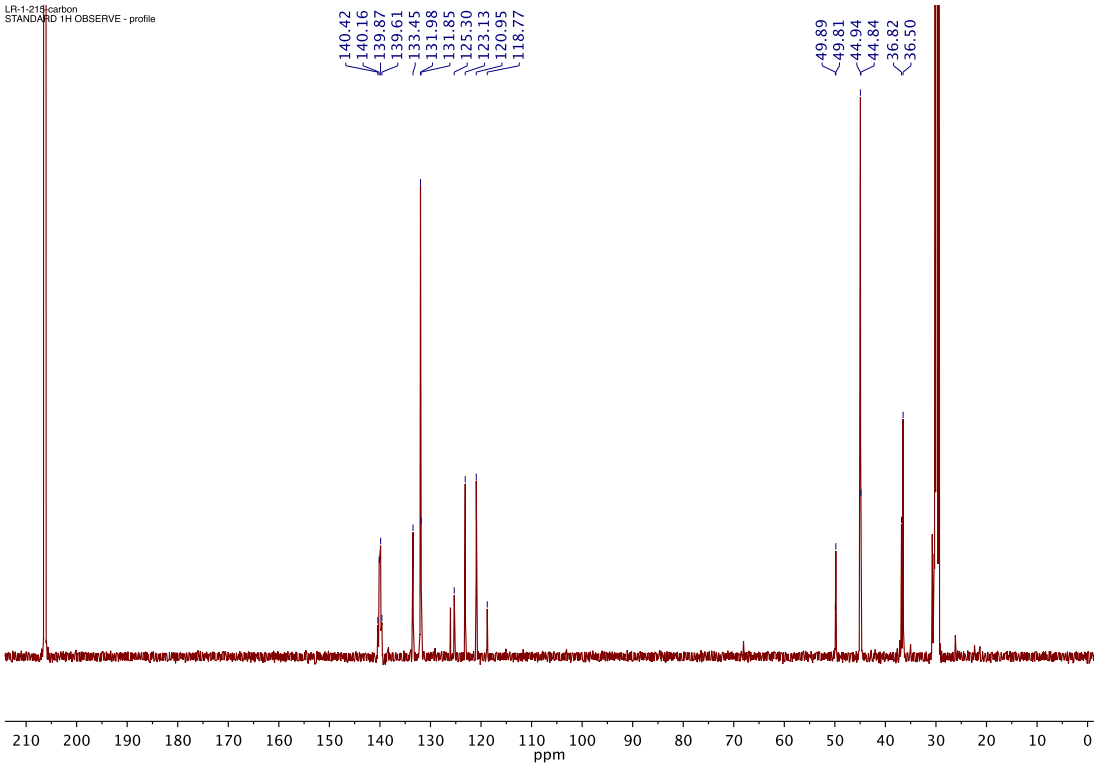


Figure S19. ^{13}C NMR (126 MHz, $(CD_3)_2CO$) spectrum of **poly-11/1**.

[12] (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.

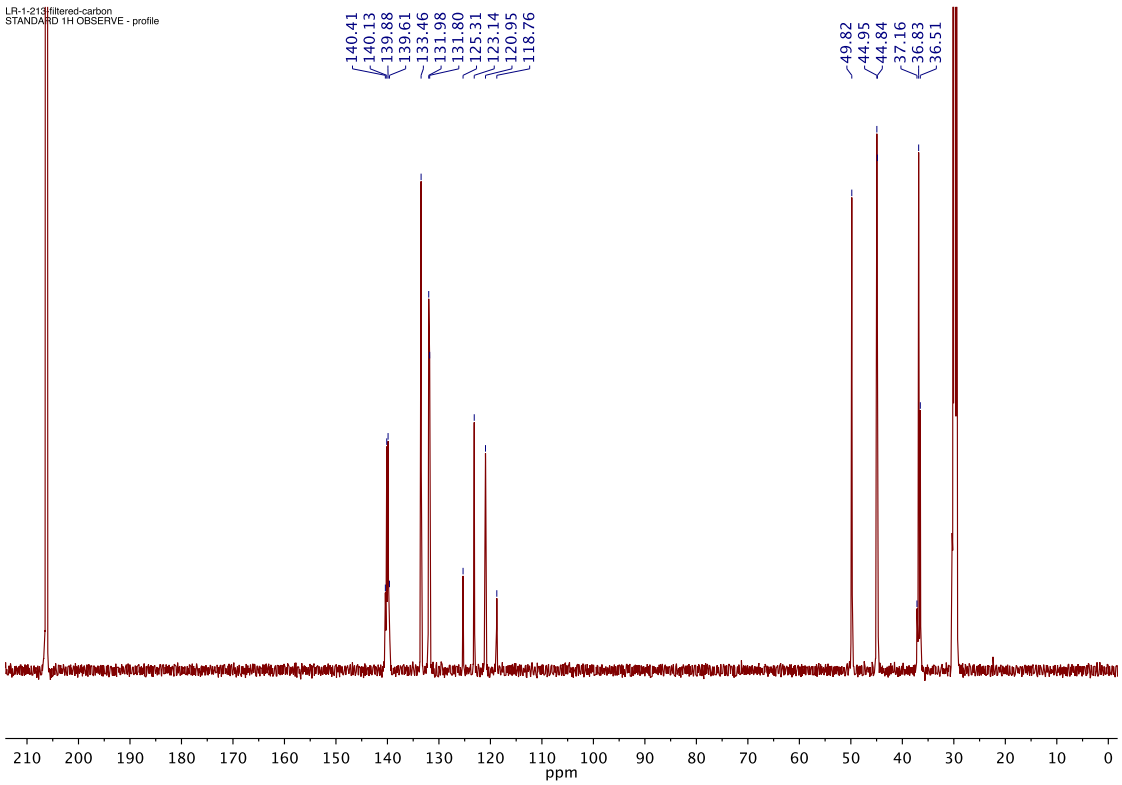


Figure S20. ^{13}C NMR (126 MHz, $(CD_3)_2CO$) spectrum of **poly-11/2**.

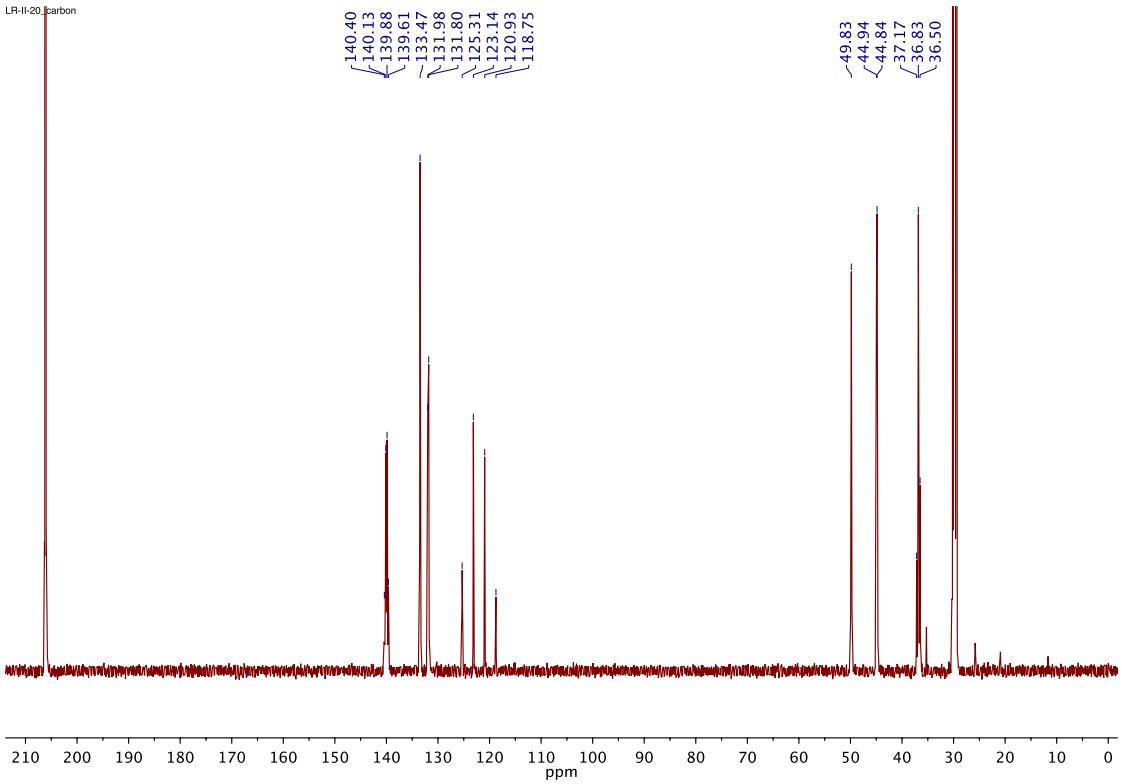


Figure S21. ^{13}C NMR (126 MHz, $(CD_3)_2CO$) spectrum of **poly-11/4**.

Preparation of Poly-12 Using Catalysts 1, 2, and 4:

Poly-12 was prepared according to the general procedure using catalysts **1**, **2**, and **4**. NMR samples were prepared by stirring **poly-12** in CD_2Cl_2. ^{13}C NMR spectral assignments were consistent with the literature.[11]

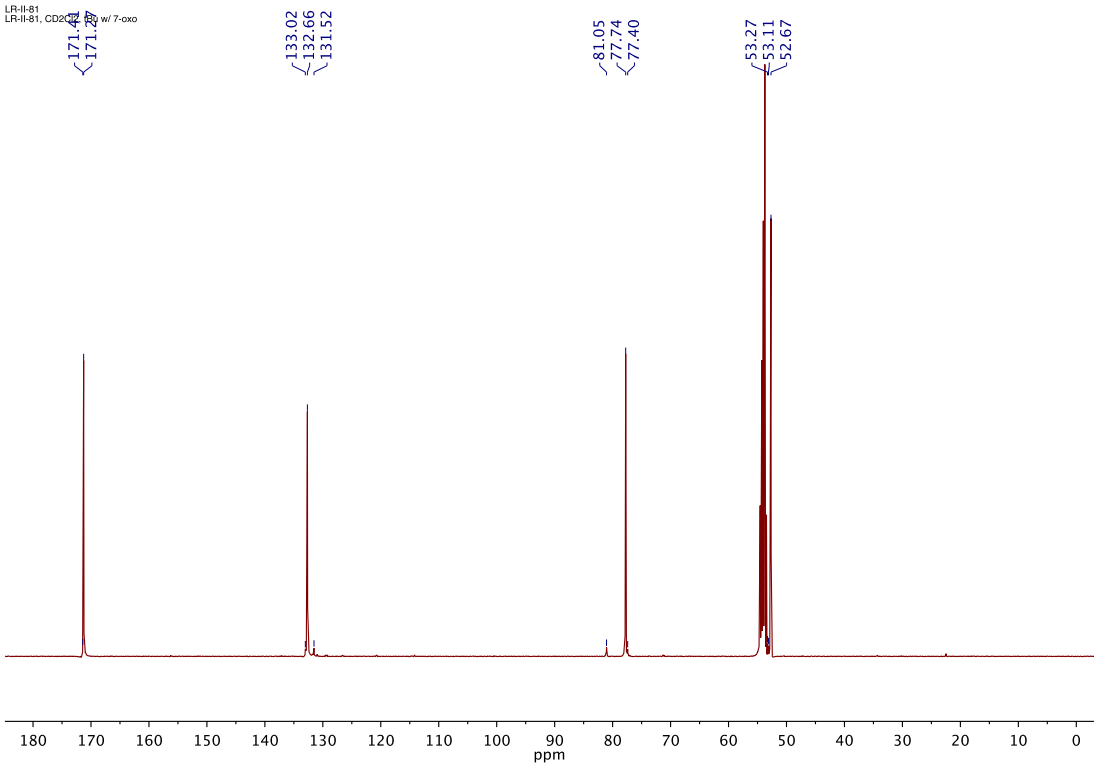


Figure S22. ^{13}C NMR (100 MHz, CD_2Cl_2) spectrum of **poly-12/1**.

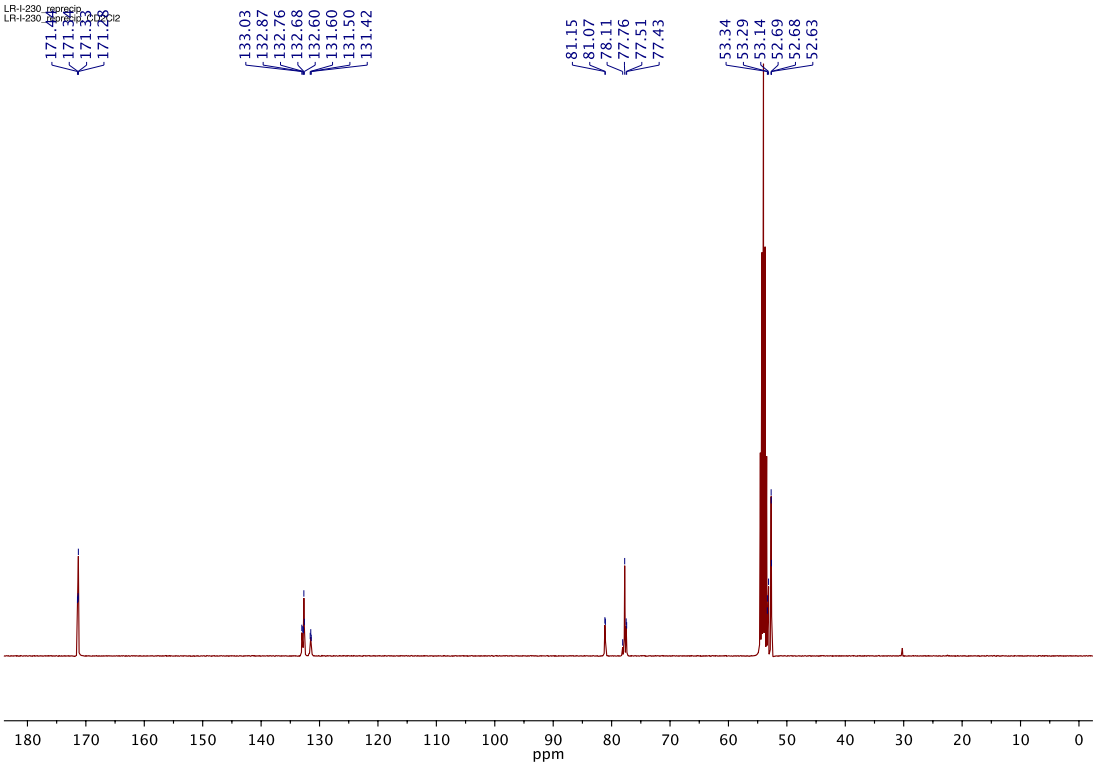


Figure S23. ^{13}C NMR (100 MHz, CD_2Cl_2) spectrum of **poly-12/2**.

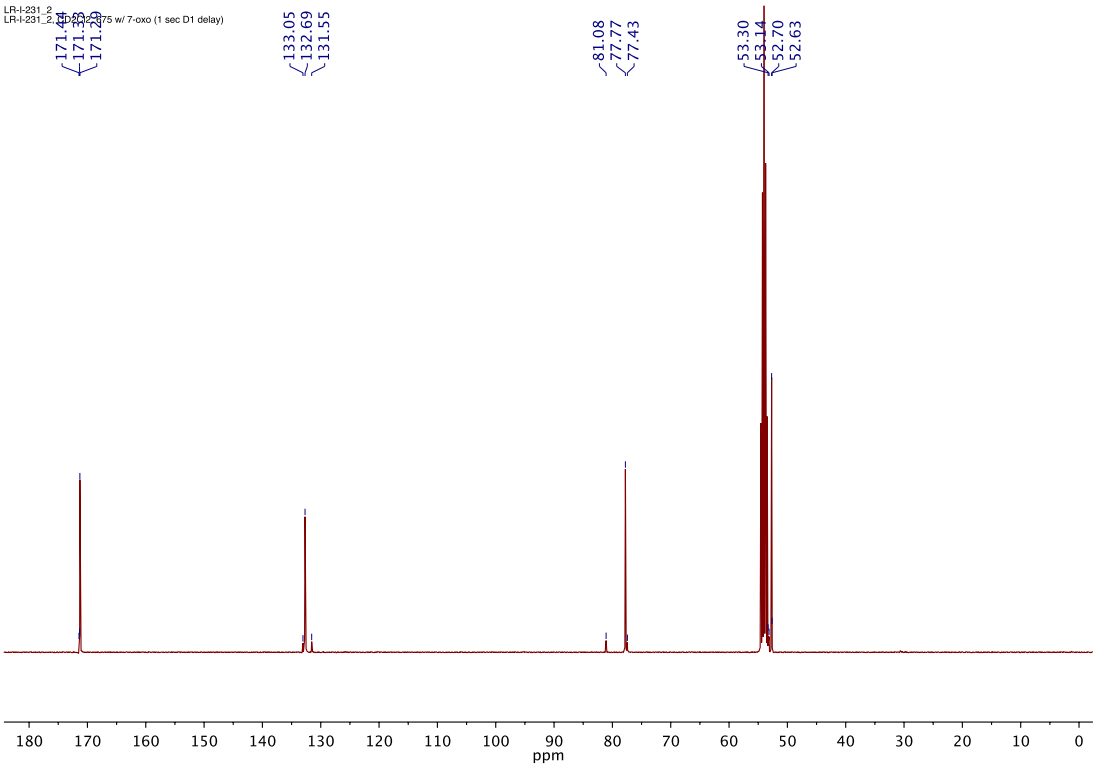


Figure S24. ^{13}C NMR (100 MHz, CD_2Cl_2) spectrum of **poly-12/4**.

Preparation of Poly-13 Using Catalysts 1 and **2:**

Poly-13 was prepared according to the general procedure using catalysts **1** and **2**. NMR samples were prepared by stirring **poly-13** in $CDCl_3$. ^{13}C NMR spectral assignments were consistent with the literature.[13]

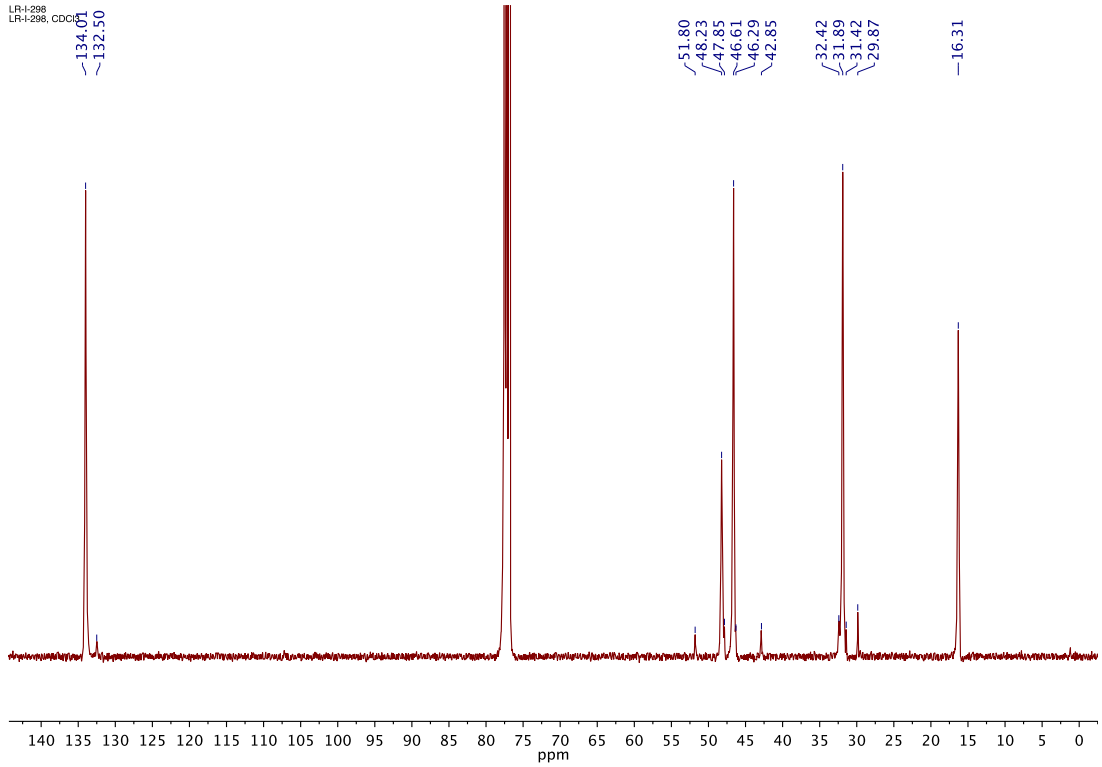


Figure S25. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **poly-13/1**.

[13] (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.

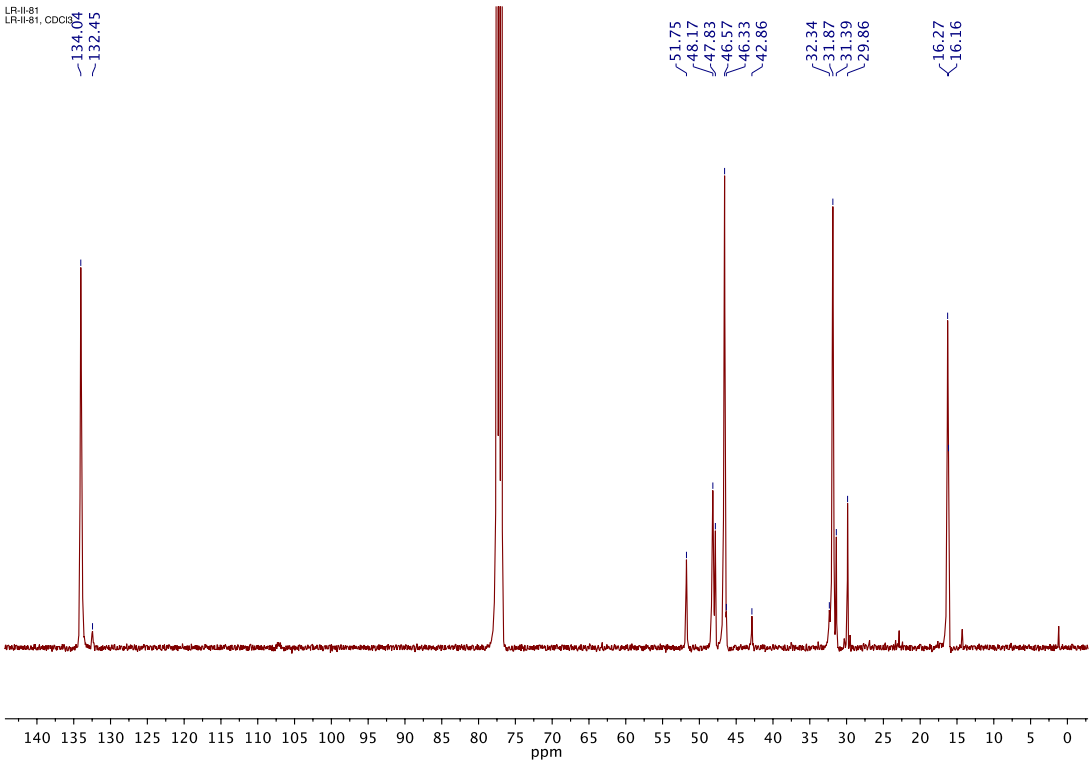


Figure S26. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **poly-13/2**.

Preparation of Poly-14 Using Catalysts 1, 2, and 4:

Poly-14 was prepared according to the general procedure using catalysts **1**, **2**, and **4**. NMR samples were prepared by stirring **poly-14** in $CDCl_3$. ^{13}C NMR spectral assignments were consistent with the literature.[14]

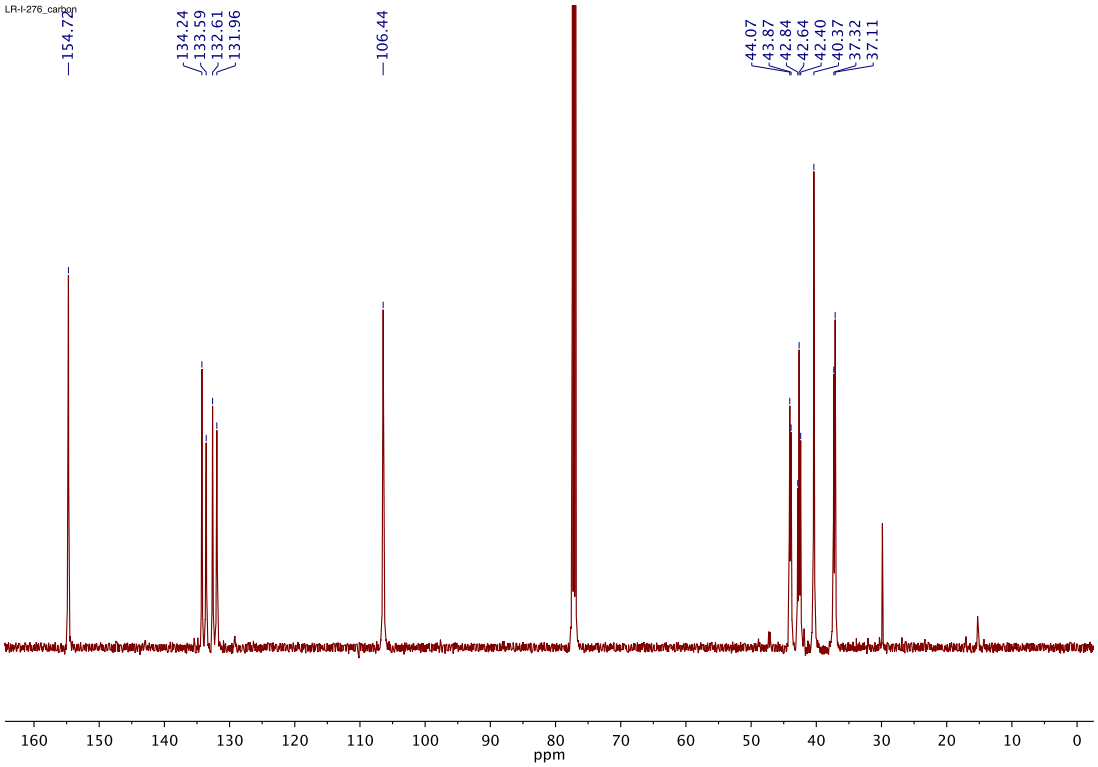


Figure S27. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly-14/1** (peak at 29.86 is residual "grease").

[14] (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.

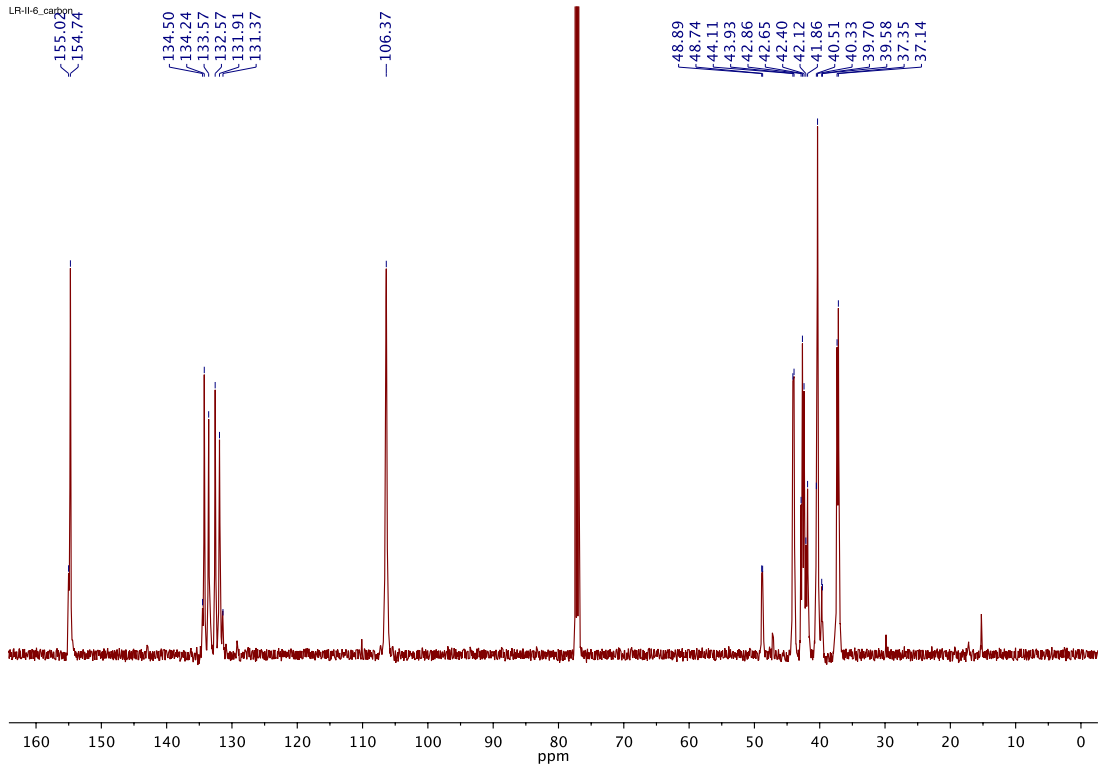


Figure S28. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly-14/2**.

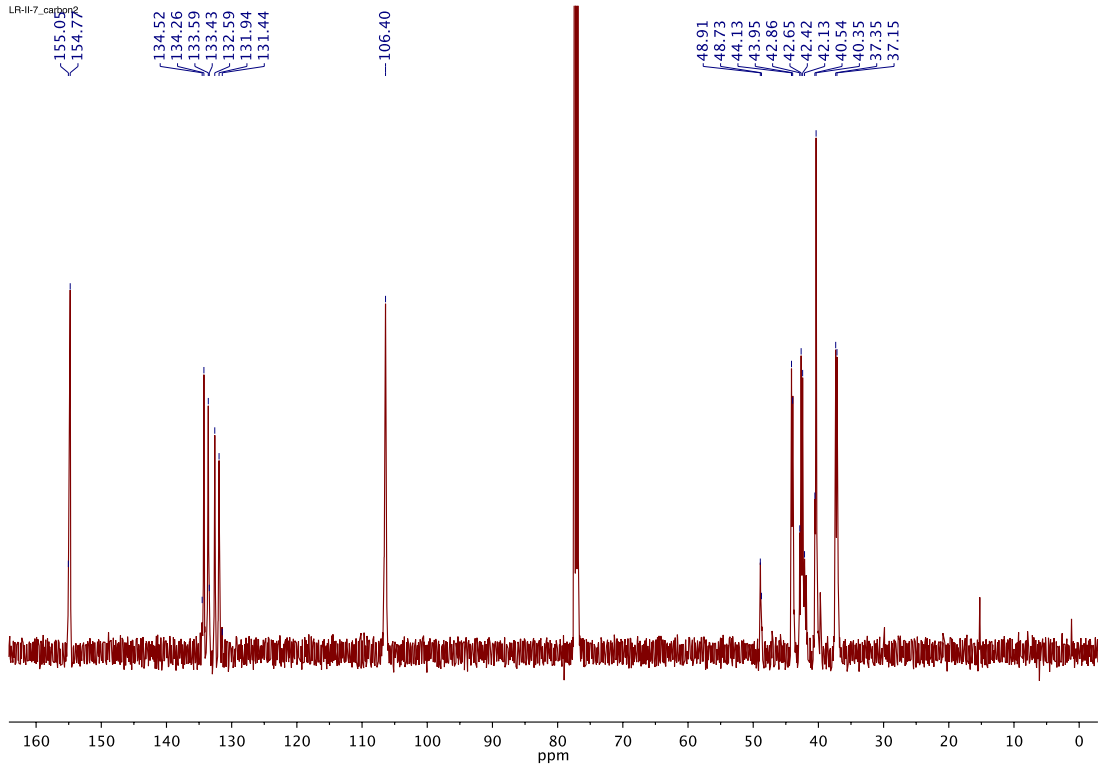


Figure S29. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **poly-14/4**.

Preparation of Poly-15 Using Catalysts 1 and **2:**

Poly-15 was prepared according to the general procedure using catalysts **1** and **2**. NMR samples were prepared by stirring **poly-15** in $CDCl_3$. ^{13}C NMR spectral assignments were consistent with the literature.[15]

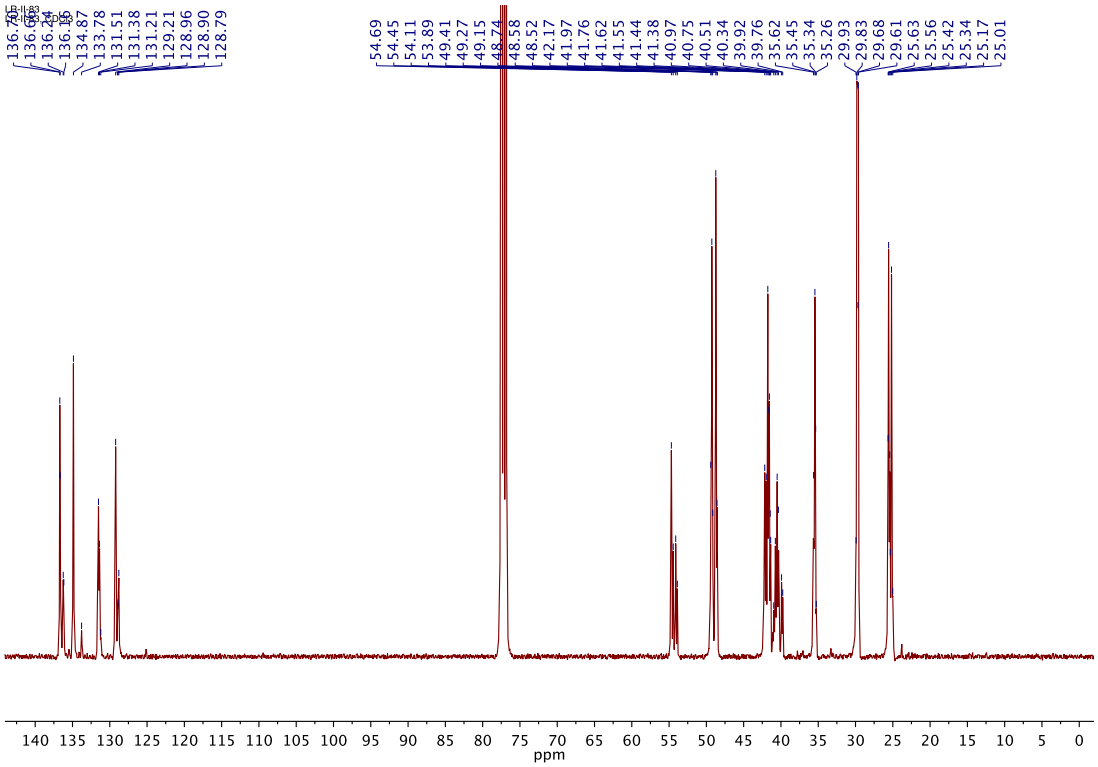


Figure S30. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **poly-15/1**.

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

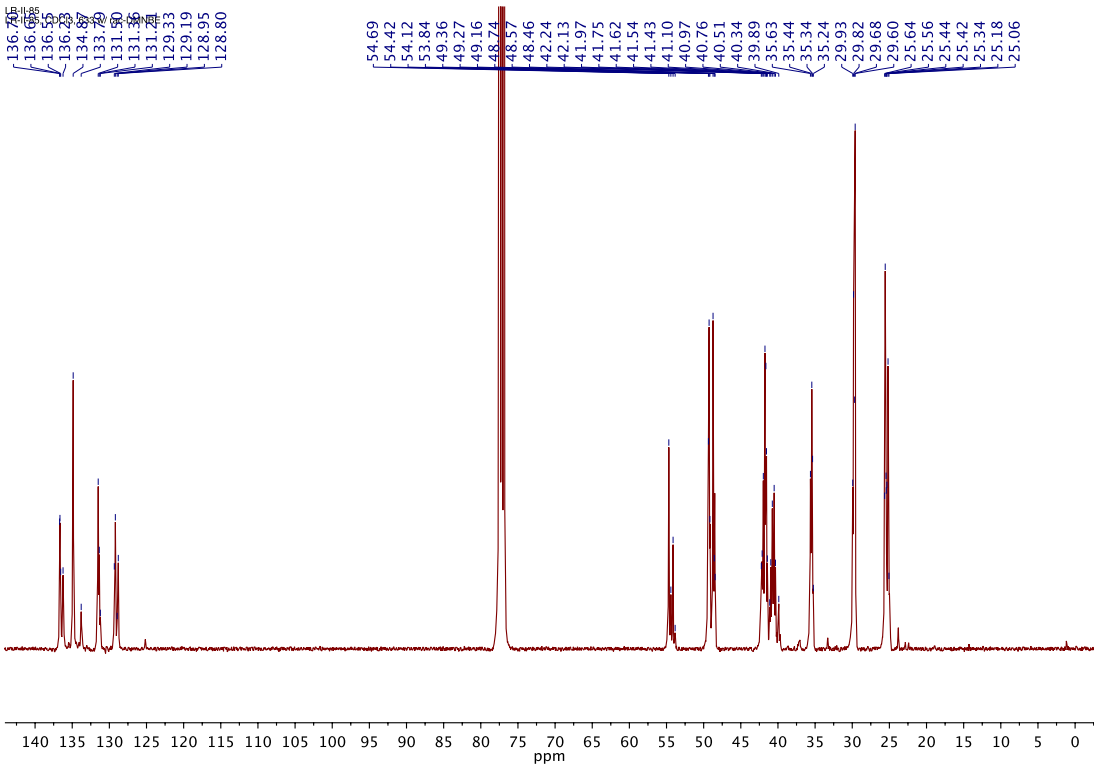


Figure S31. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **poly-15/2**.

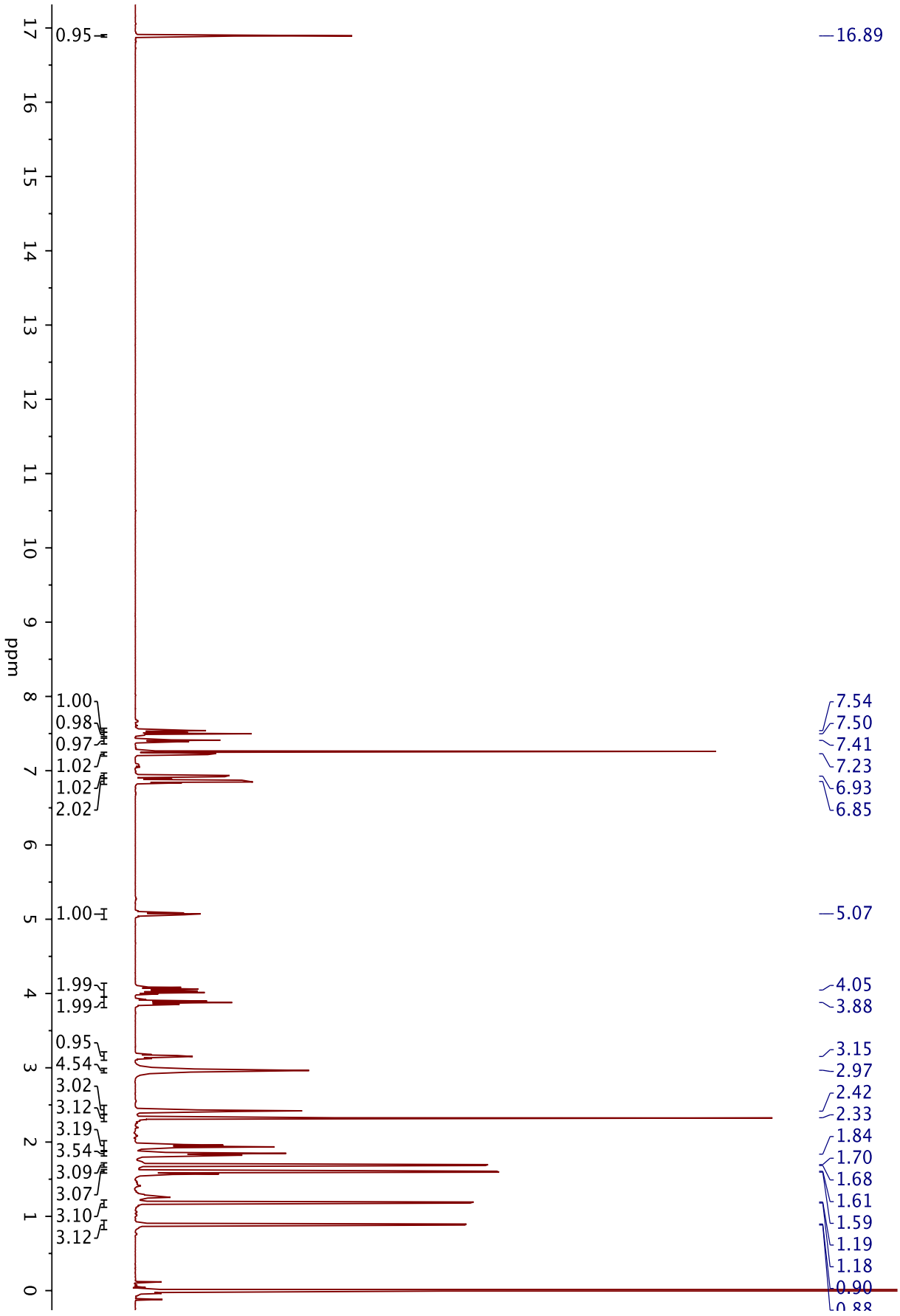


Figure S32. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **S3**.

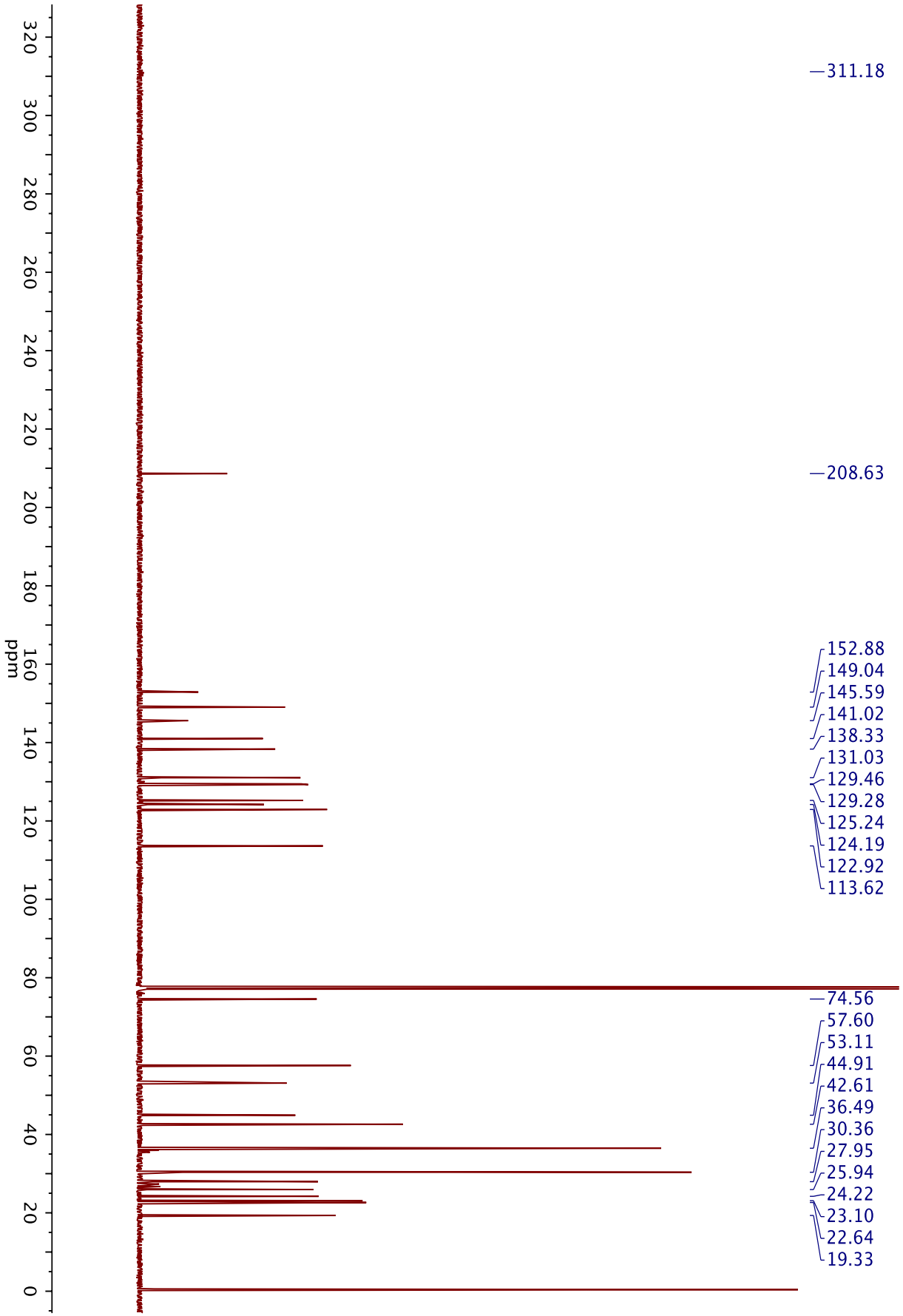


Figure S33. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **S3**.

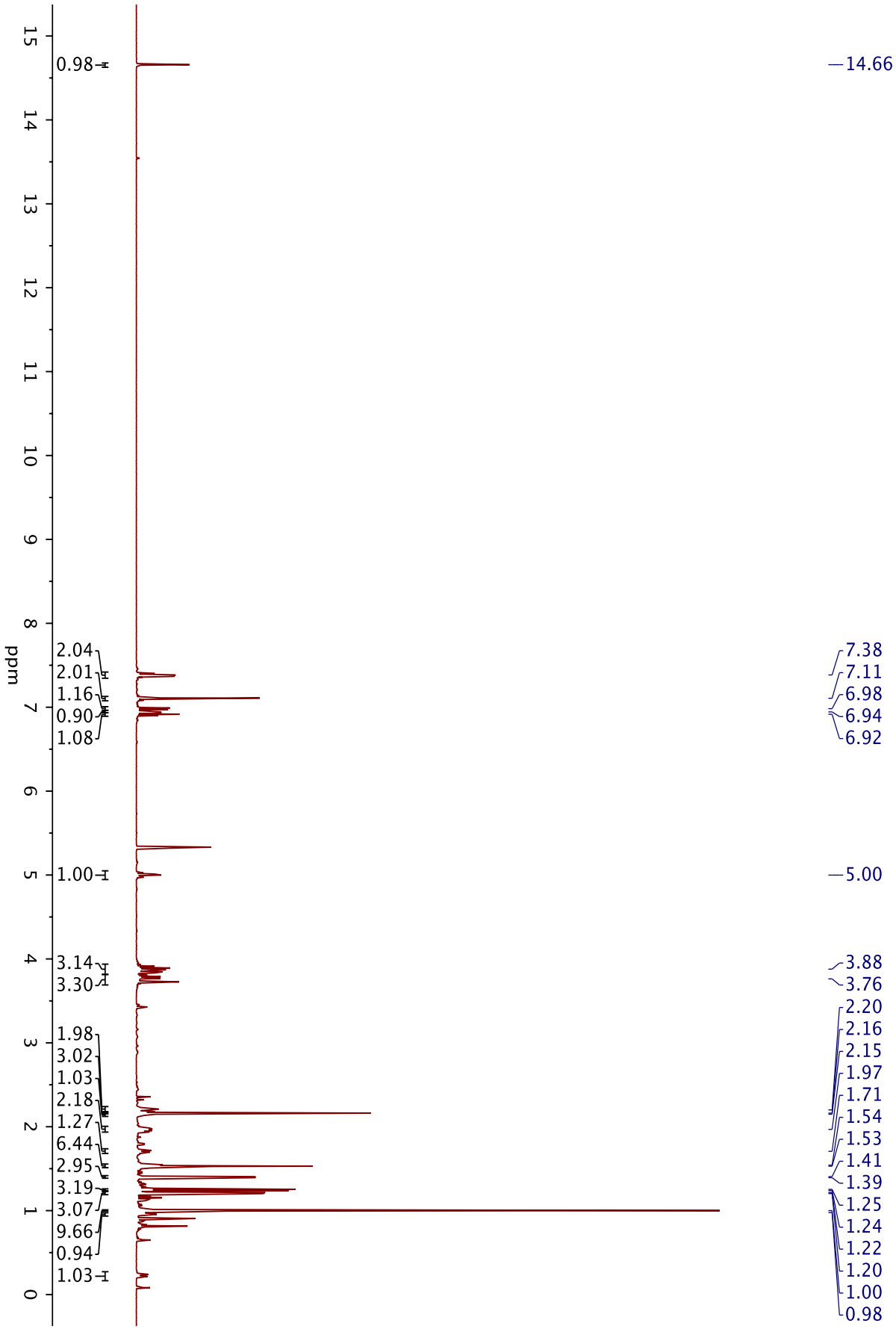


Figure S34. ^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of **S4**.

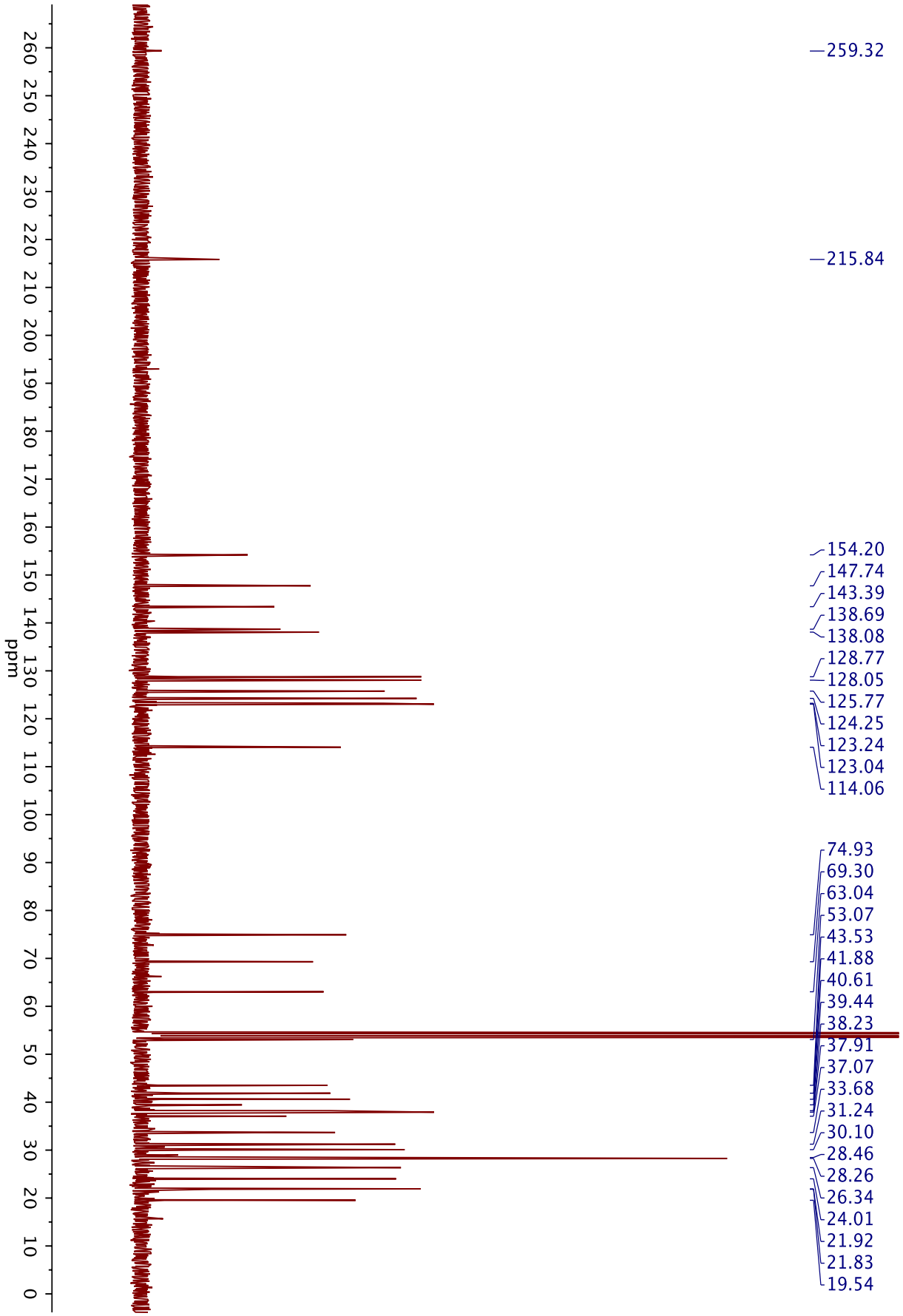


Figure S35. ^{13}C NMR (126 MHz, CD_2Cl_2) spectrum of **S4**.

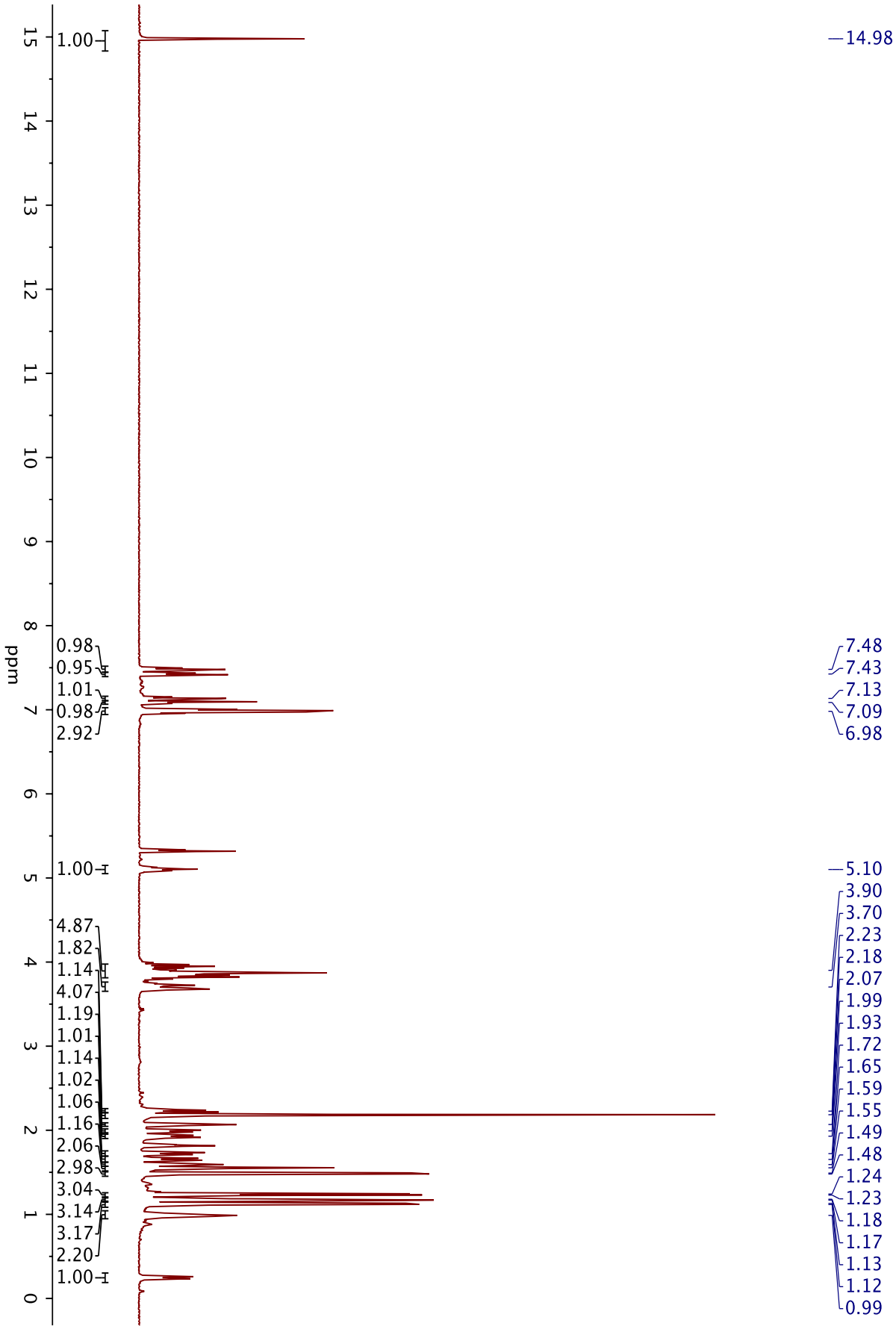


Figure S36. ^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of **3**.

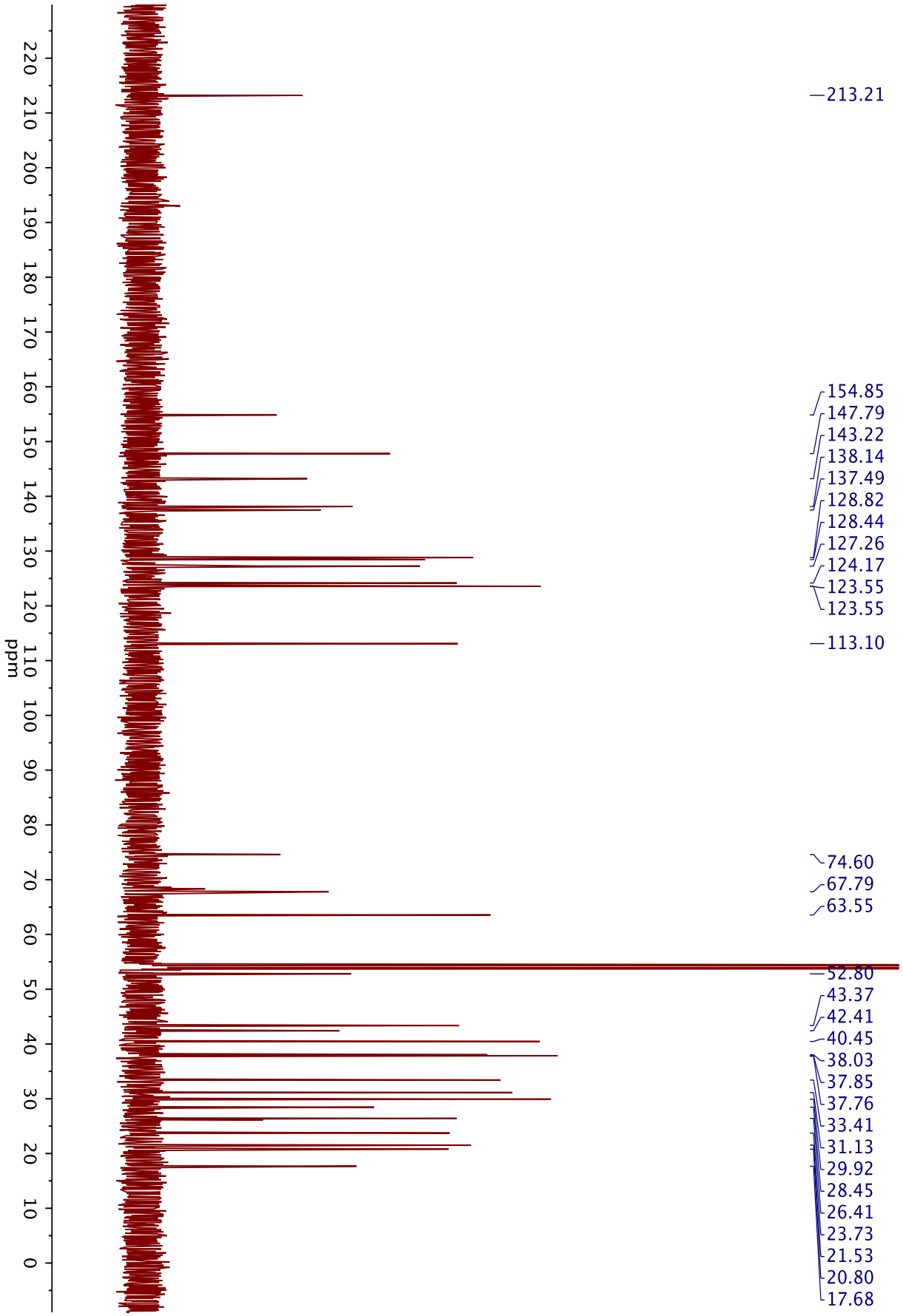


Figure S37. ^{13}C NMR (126 MHz, CD_2Cl_2) spectrum of **3**.

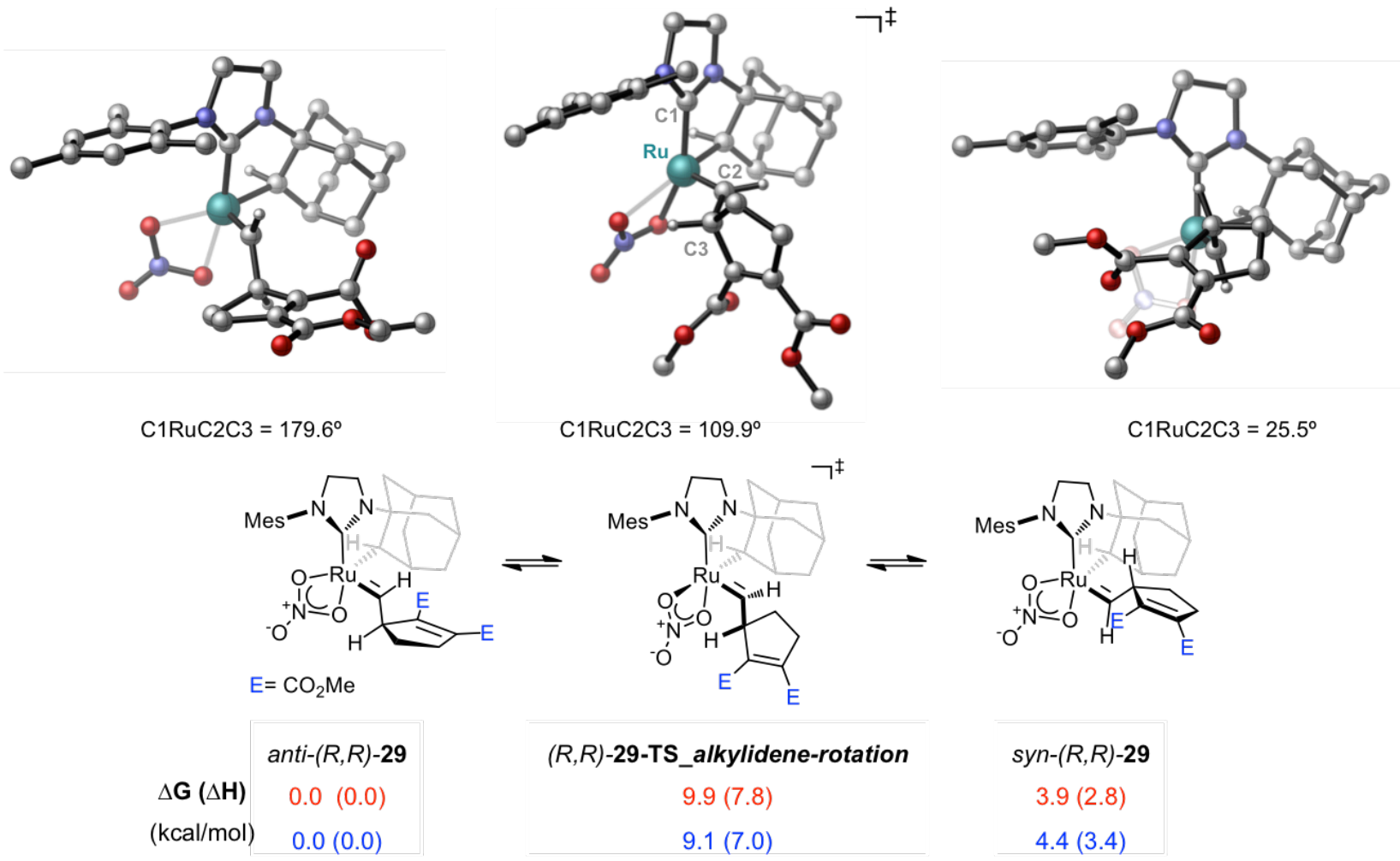


Figure S38. Free energies and enthalpies (in parentheses) for interconversion between ruthenium alkylidenes *anti-* and *syn-(R,R)*-**29** via "*alkylidene rotation*." All energies are with respect to the ruthenium alkylidene complex *anti-(R,R)*-**2** and are given in kcal/mol.

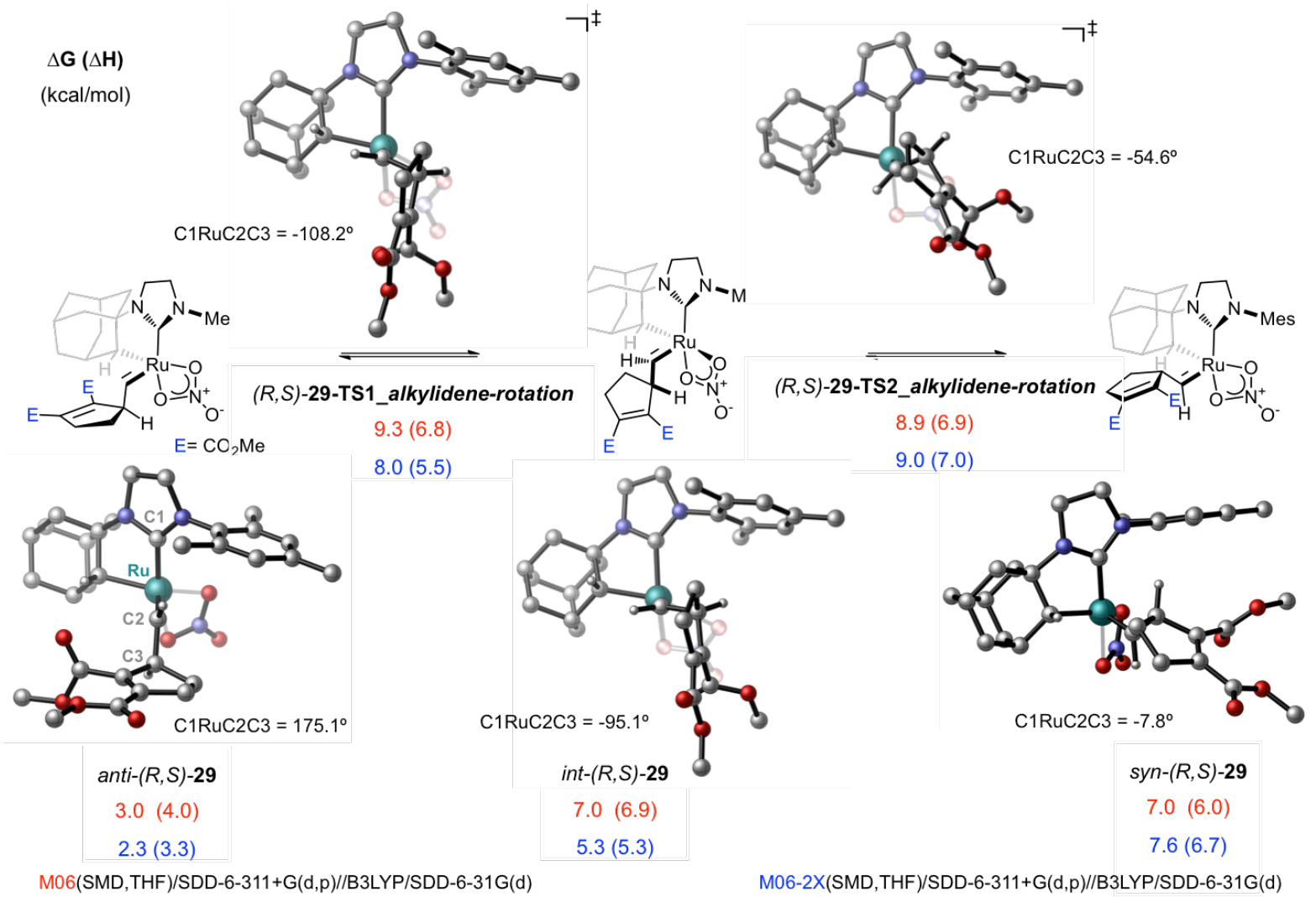


Figure S39. Free energies and enthalpies (in parentheses) for interconversion between ruthenium alkylidenes *anti-* and *syn-(R,S)*-**29** via "*alkylidene rotation*." All energies are with respect to the ruthenium alkylidene complex *anti-(R,R)*-**2** and are given in kcal/mol.

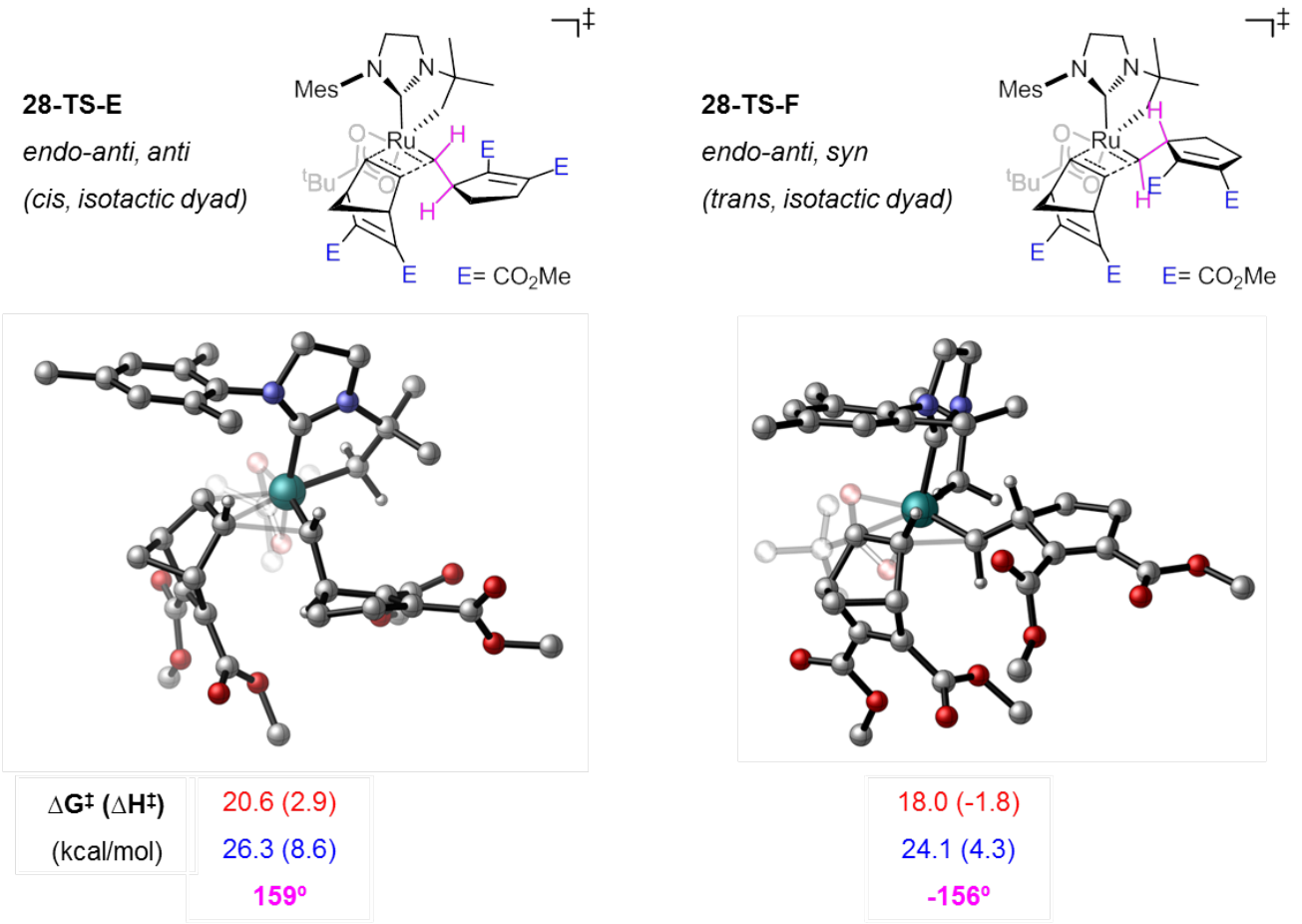


Figure S40. *Endo* transition states in the [2+2] cycloaddition for the polymerization of monomer **10** with catalyst **27**. Energies are with respect to the separated ruthenium alkylidene and monomer **10**.

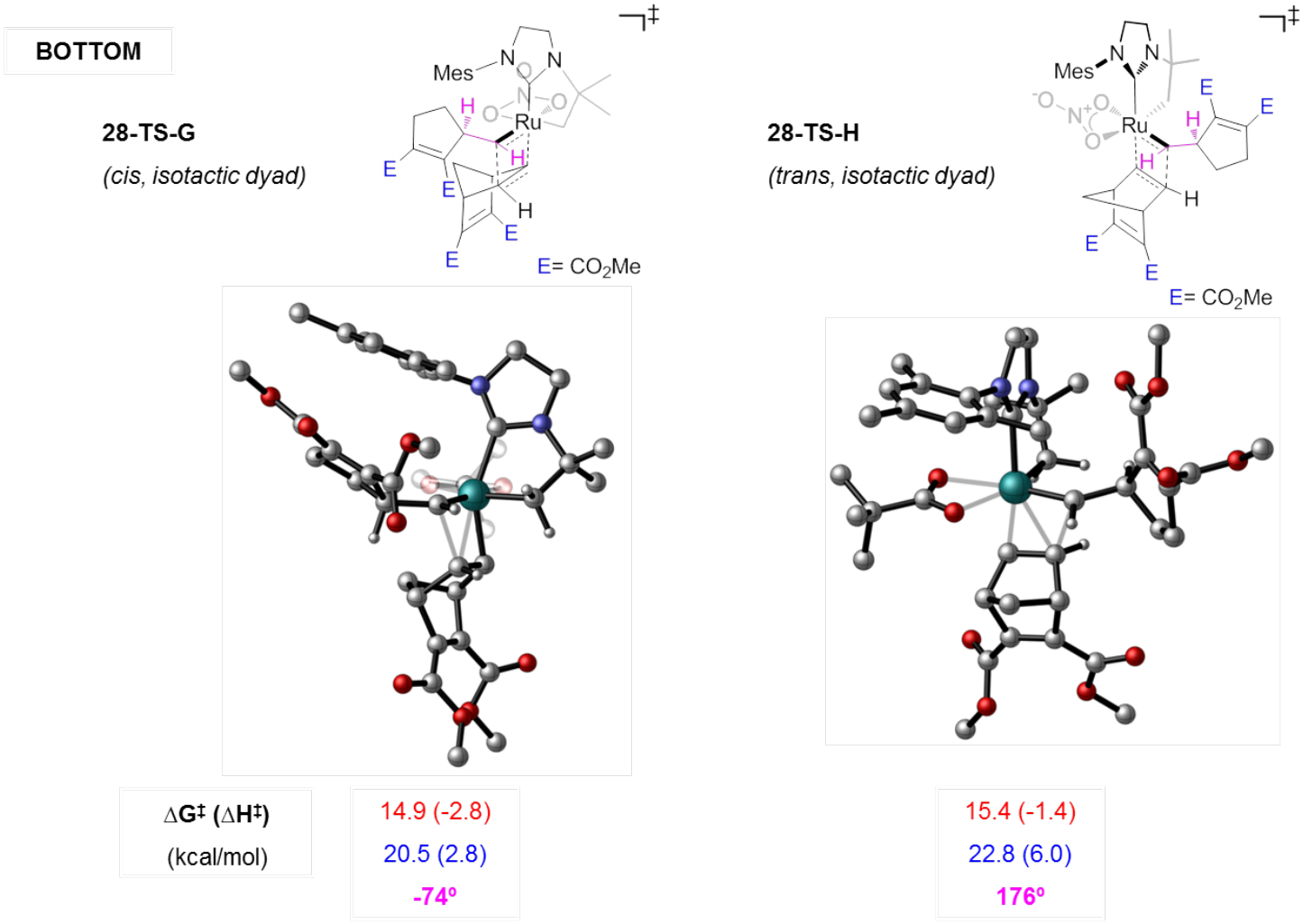


Figure S41. Bottom bound transition states in the [2+2] cycloaddition for the polymerization of monomer **10** with catalyst **27**. Energies are with respect to the separated ruthenium alkylidene and monomer **10**.

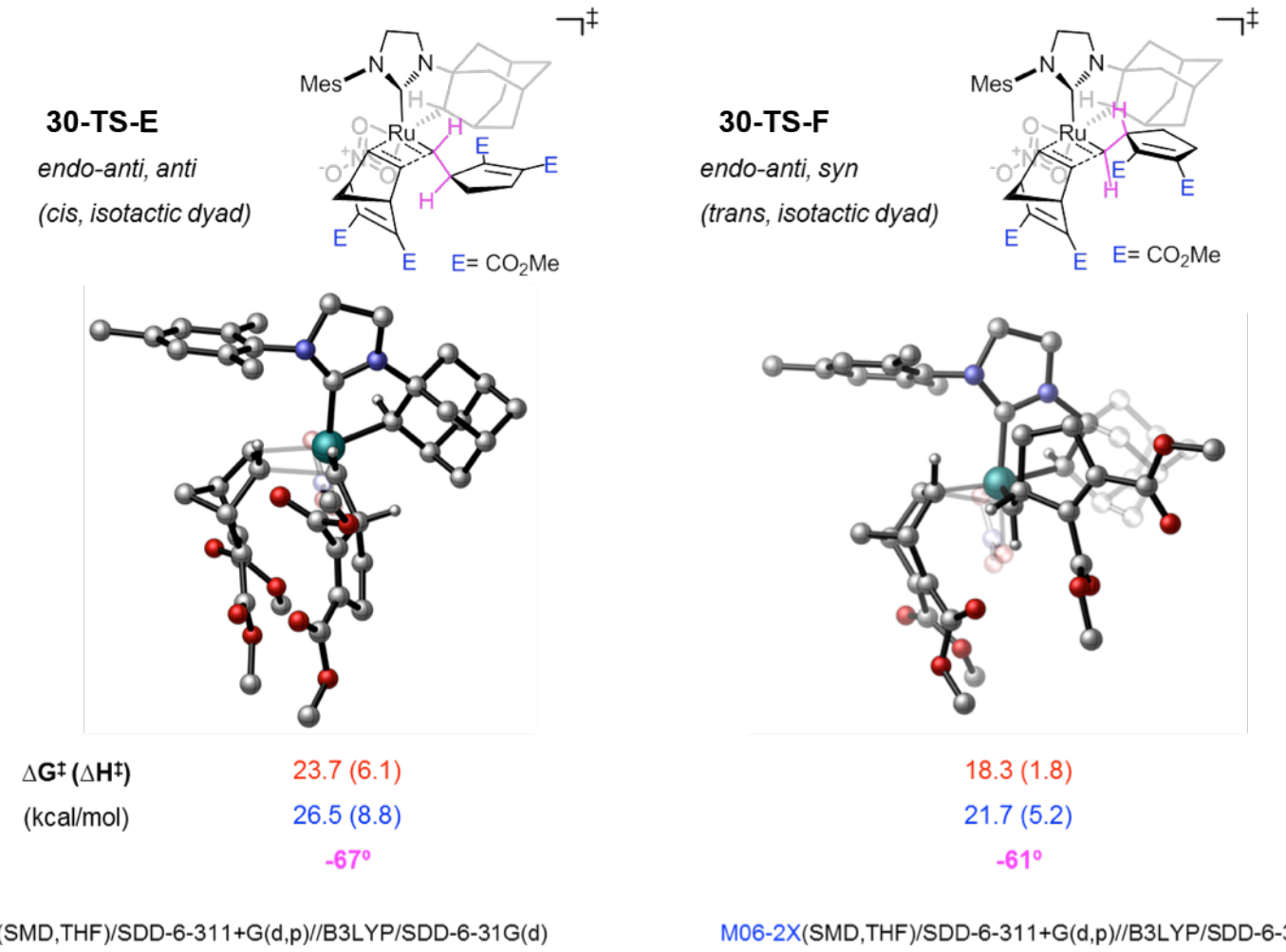


Figure S42. *Endo* transition states in the [2+2] cycloaddition for the polymerization of monomer **10** with catalyst *(R,R)*-**29**. Energies are with respect to the separated ruthenium alkylidene and monomer **10**.

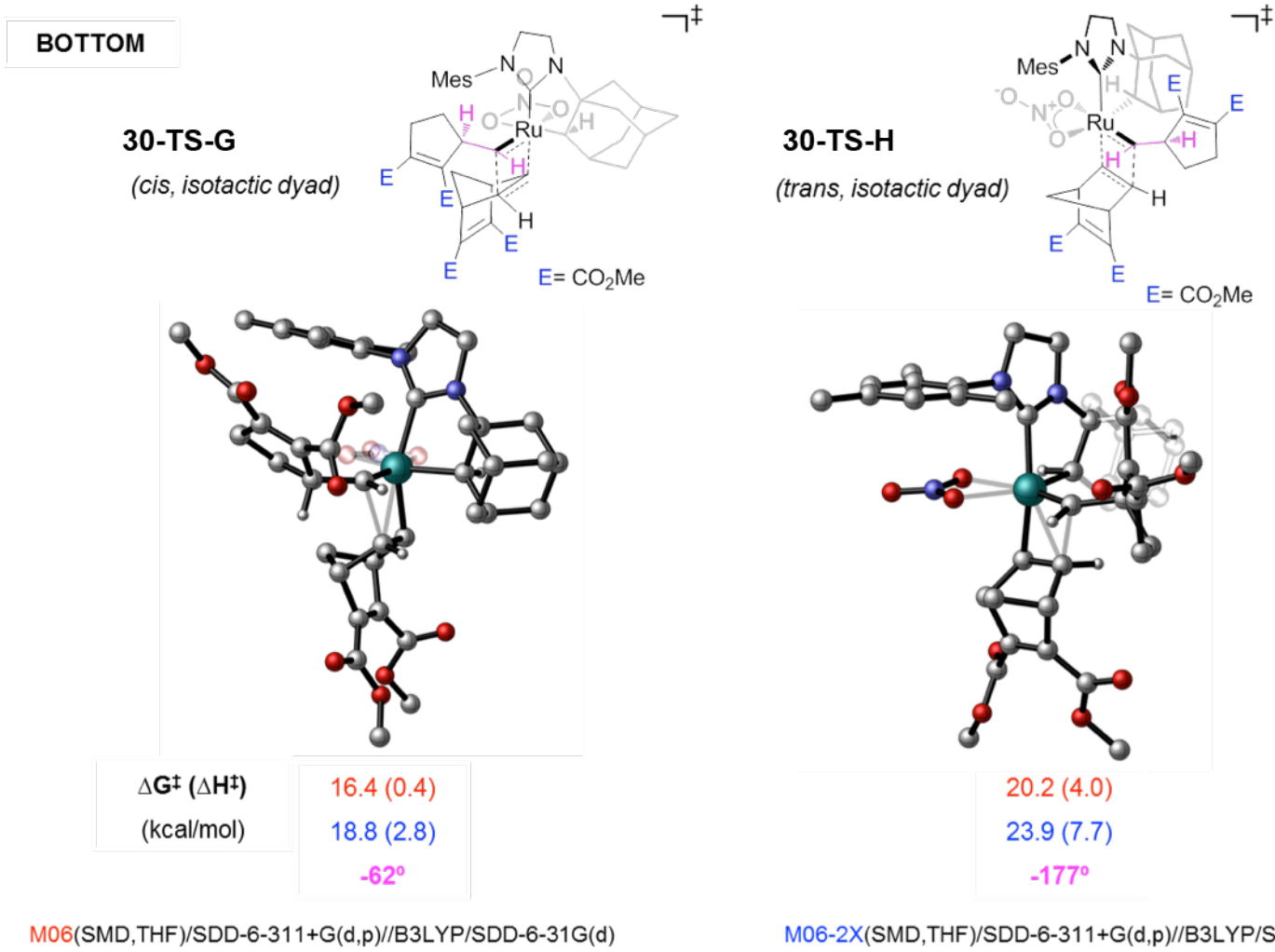


Figure S43. Bottom bound transition states in the [2+2] cycloaddition for the polymerization of monomer **10** with catalyst *(R,R)*-**29**. Energies are with respect to the separated ruthenium alkylidene and monomer **10**.

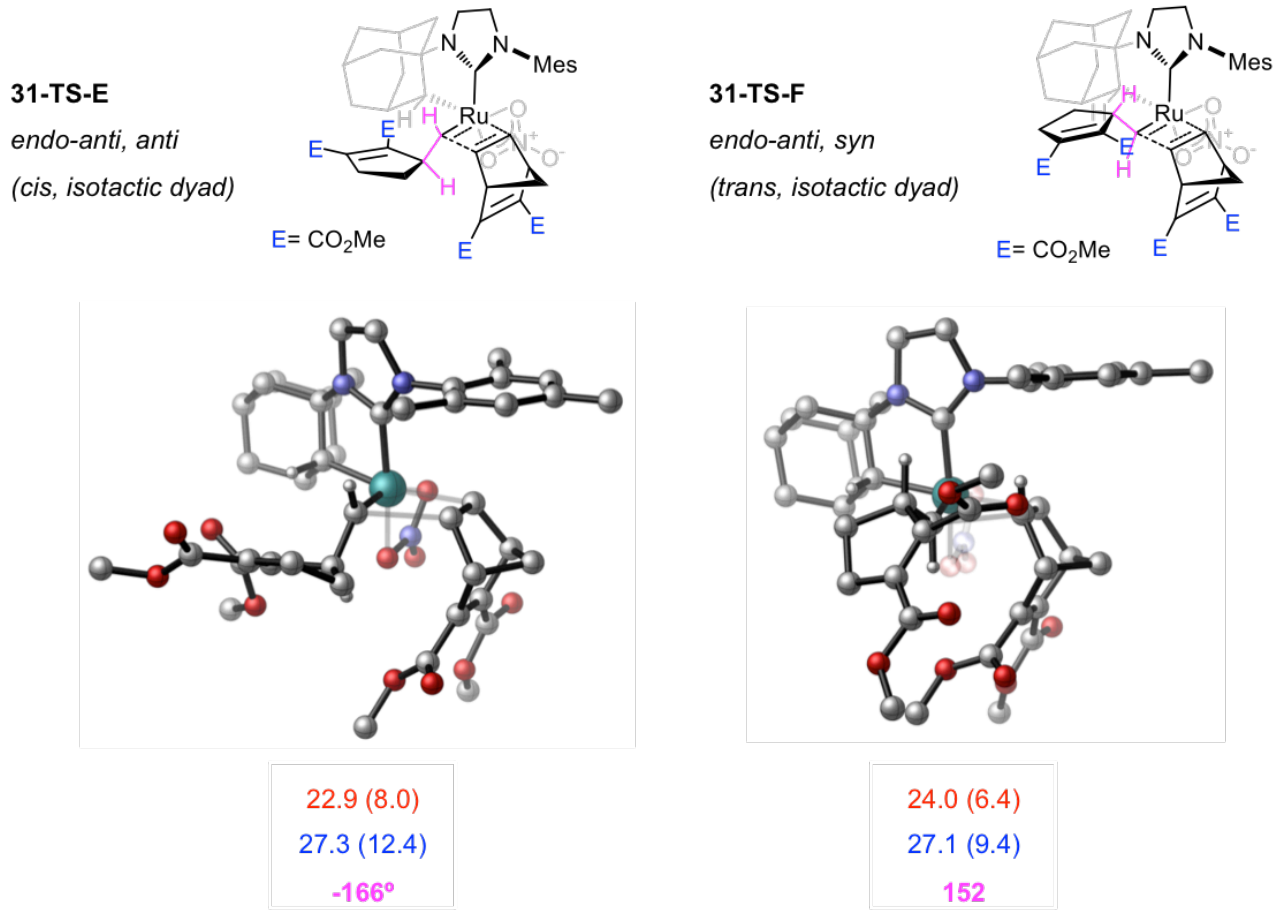


Figure S44. *Endo* transition states in the [2+2] cycloaddition for the polymerization of monomer **10** with catalyst *(R,S)*-**29**. Energies are with respect to the separated ruthenium alkylidene and monomer **10**.

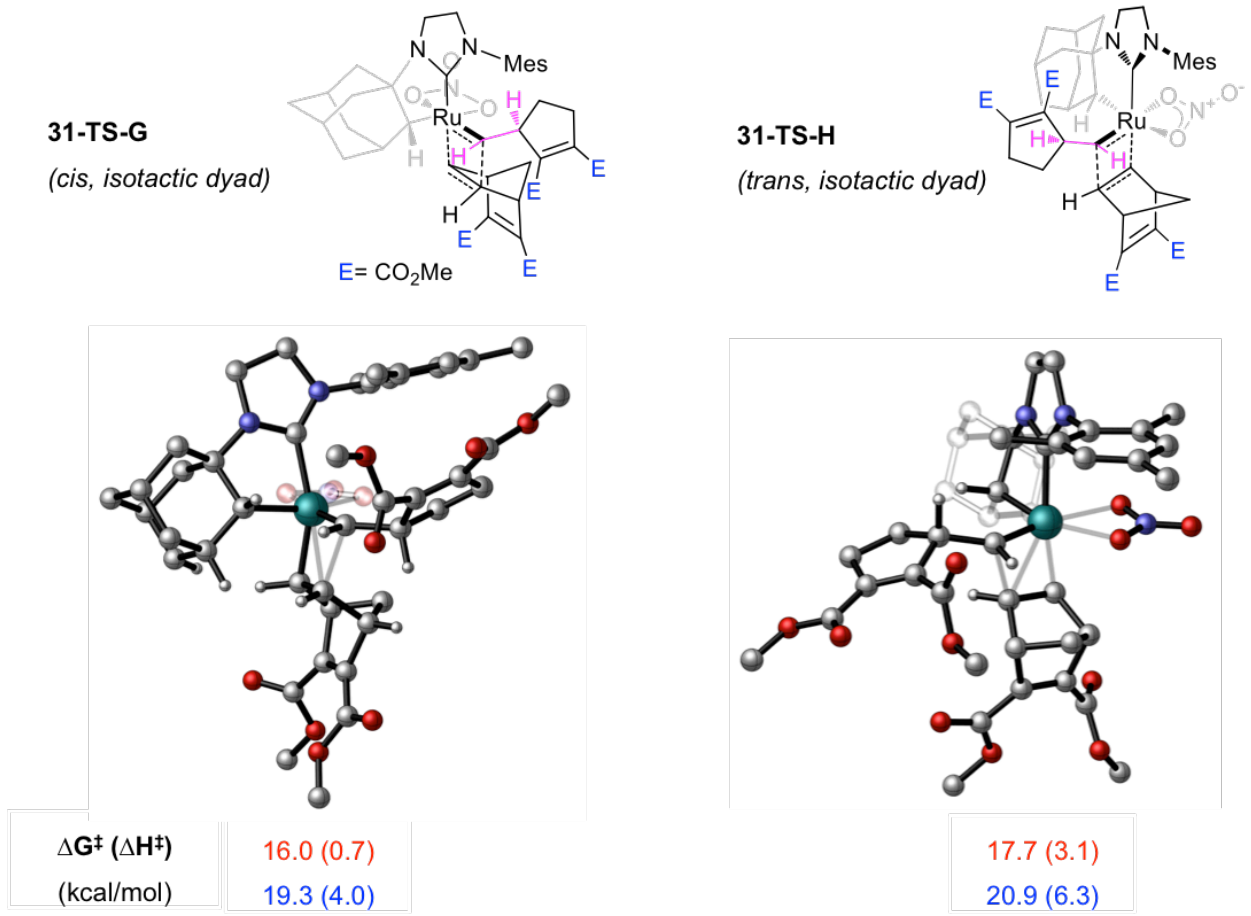


Figure S45. Bottom bound transition states in the [2+2] cycloaddition for the polymerization of monomer **10** with catalyst *(R,S)*-**29**. Energies are with respect to the separated ruthenium alkylidene and monomer **10**.

Cartesian Coordinates and Energies of All Optimized Geometries

16

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

17

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

18-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

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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

20-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

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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

22-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

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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

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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

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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

26-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)-**29**

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)-29-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)-**29**

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)-**29**

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)-29-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)-**29**

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)-29-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)-**29**

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

28-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

28-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

28-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

28-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

28-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

28-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

28-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

28-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

28-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

28-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

28-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

28-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

30-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

30-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

30-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

30-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

30-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

30-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

30-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

30-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

30-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

30-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

30-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

30-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

31-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

31-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

31-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

31-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

31-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

31-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

31-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

31-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

31-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

31-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

31-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	-2755.00045404	a.u.

in solution:

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

31-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	3.16408200	-2.02198000	3.69540200
H	0.19565400	-3.53902700	5.47971000	H	2.04389600	-0.30343600	5.16140700
H	1.74897900	-2.73757200	5.73346500	H	0.69555700	0.65594100	4.54405800
H	2.57242800	-2.37746000	2.07309400	H	-0.26237800	0.24005200	2.48041100