SUPPORTING INFORMATION

An Initiation Kinetics Prediction Model Enables Rational Design of Ruthenium Olefin Metathesis Catalysts Bearing Modified Chelating Benzylidenes

Shao-Xiong Luo,[†] Keary M. Engle,[†] Xiaofei Dong,[‖] Andrew Hejl,[†] Michael K. Takase,[†] Lawrence M. Henling,[†] Peng Liu,*[,§] K. N. Houk,*[,‖] and Robert H. Grubbs*[,†]

† Arnold and Mabel Beckman Laboratories of Chemical Synthesis, California Institute of Technology, Pasadena, CA 91125
§ Department of Chemistry, University of Pittsburgh, Pittsburgh, PA 15260
‖ Department of Chemistry and Biochemistry, University of California, Los Angeles, CA 90095
**pengliu@pitt.edu*
**houk@chem.ucla.edu*
**rhg@caltech.edu*

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GENERAL INFORMATION

All reactions were carried out in a flask open to air, in dry glassware under an argon atmosphere using standard Schlenk techniques, or in a Vacuum Atmospheres Glovebox under a nitrogen atmosphere, as specified. Unless otherwise noted, all materials were used as received from commercial sources without further purification. Catalysts **2–5**, **33**, **36** and **39** were donated by Materia, Inc. All other chemicals were purchased from Aldrich. All bulk solvents were purchased from VWR and used as received. In air- or moisture-sensitive reactions, anhydrous, degassed solvents were used. All other non-deuterated solvents were purified by passage through solvent purification columns. ^{1}H and ^{13}C spectra were recorded on Varian Mercury (300 MHz and 75 MHz, respectively), Bruker Ascend 400 spectrometer (400 MHz and 101 MHz, respectively) and Varian Inova (500 MHz and 125 MHz, respectively) instruments. Solutions of catalysts for NMR analysis were prepared in a glovebox using freshly opened ampules of CD_2Cl_2 from Cambridge Isotope Laboratories. $CDCl_3$ was handled outside of the glovebox and used as received from Cambridge Isotope Laboratories. All NMR Spectra were internally referenced to $SiMe_4$, methylene chloride or chloroform signals. The following abbreviations (or combinations thereof) were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, and b = broad. High-resolution mass spectra (HRMS) were provided by the California Institute of Technology Mass Spectrometry Facility using a JEOL JMS-600H High Resolution Mass Spectrometer. All HRMS were ionized by EI or FAB.

EXPERIMENTAL PROCEDURES

UV/Vis Initiation Kinetics:

Septum-equipped screw-capped quartz cuvettes for UV/Vis were purchased from Starna Cells, Inc. (Item# 1-Q-10-GL14-S). All catalyst solutions were prepared and handled in a glovebox. Cuvettes were tightly sealed at removal and wrapped with additional parafilm. UV/Vis kinetics experiments were performed on an Agilent HP8452 UV/Vis spectrophotometer with temperature controller and magnetic stir plate. The solution was allowed to equilibrate to the desired temperature (10 °C) for at least 10 min prior to beginning the experiment. During the experiment, dry air was blown over the faces of the cuvette to prevent condensation.

General Procedure for UV/Vis Initiation kinetics with BVE:[1] In a glovebox, a $1 \cdot 10^{-3}$ M stock solution of the appropriate catalyst (0.01 mmol) in toluene (10.0 mL solution volume) was prepared. A 0.3 mL aliquot of the $1 \cdot 10^{-3}$ M catalyst stock solution was added to a UV/Vis cuvette, and additional toluene (2.7 mL) was added, to obtain 3.0 mL of a $1 \cdot 10^{-4}$ M solution of the catalyst in toluene. Separately, a 0.5 M stock solution of butyl vinyl ether (100.2 mg, 1.00 mmol) in toluene (2.0 mL solution volume) was prepared in a septum-topped vial; toluene was added in the glovebox, and butyl vinyl ether was added by syringe outside of the glovebox. Outside of the glovebox, the cuvette was placed in the UV/Vis spectrophotometer and allowed to equilibrate to the desired temperature (10 °C) for at least 10 min, prior to beginning the experiment. A spectrum was collected to determine λ_{max} for the catalyst. At a catalyst concentration of $1 \cdot 10^{-4}$ M, the absorbance was generally near 1.0 (± 0.2). An aliquot of the butyl vinyl ether stock solution (18 μL, $9 \cdot 10^{-3}$ mmol, 30 equiv, $3.0 \cdot 10^{-3}$ M in the reaction solution) was added, and data collection was initialized. Spectra were collected at regular intervals for at least three half-lives (Figure S1). The absorbance

value at λ_{max} was plotted against time, and the data were fit to a first-order exponential decay function, from which k_{obs} was determined (Figures S2 and S3). Other wavelengths ($\lambda_{max} \pm 4$ nm) gave very similar k_{obs} values. The experiments as repeated in triplicate for each catalyst. The results are summarized in Table S1.

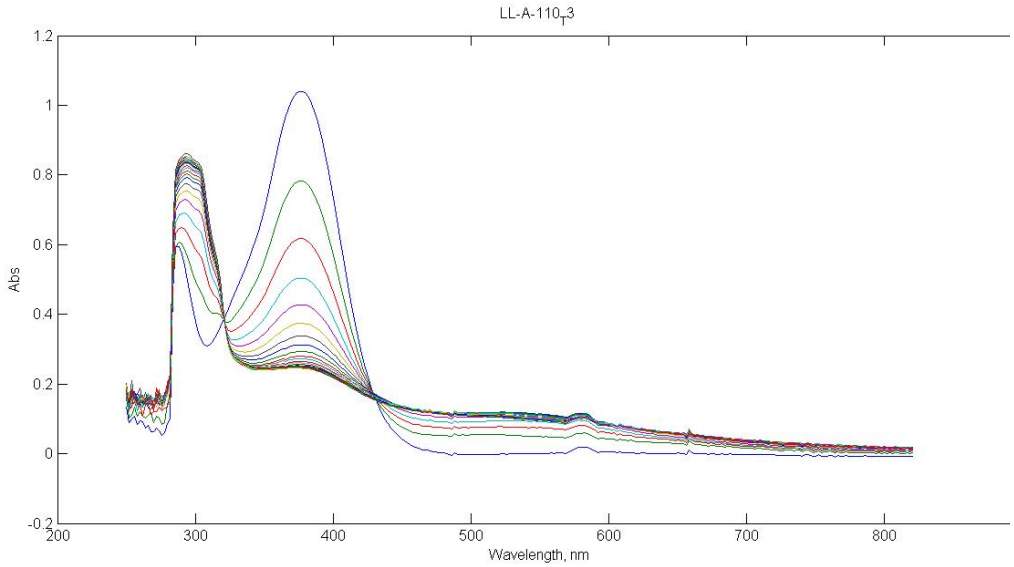


Figure S1: Representative data for a UV/Vis initiation kinetics experiment (catalyst **21**, trial 1).

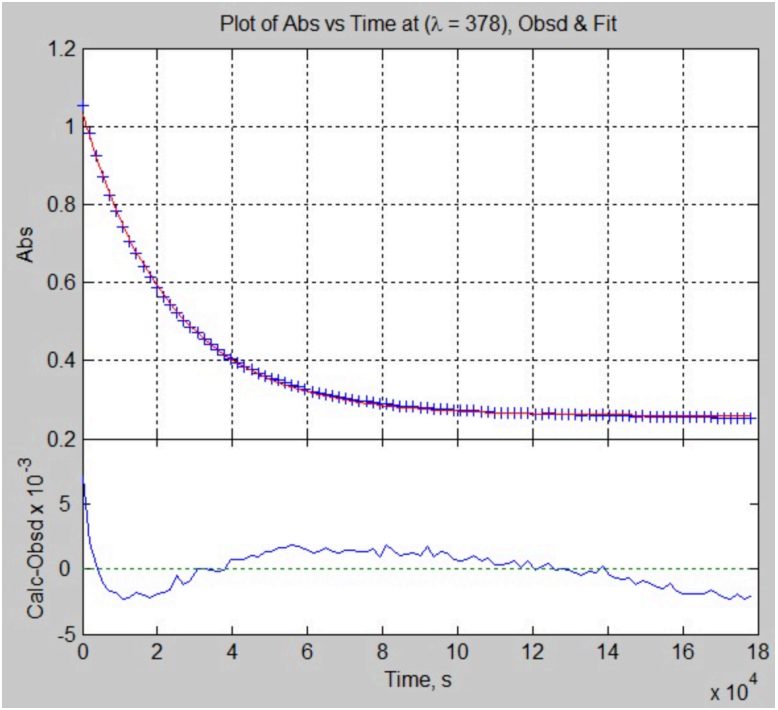


Figure S2: Representative plot of absorbance (λ_{max} = 376 nm) versus time for a UV/Vis initiation kinetics experiment (catalyst **21**, trial 1).

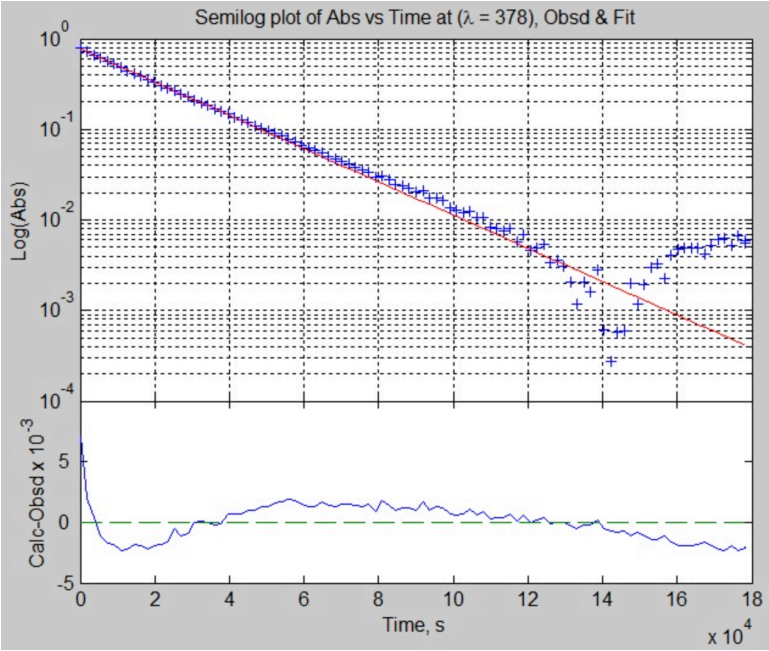


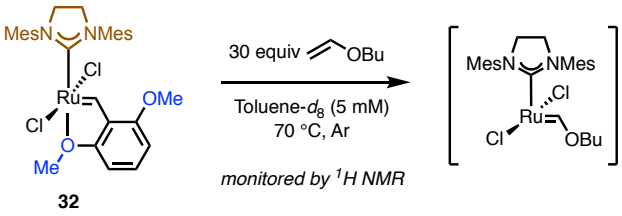
Figure S3: Representative semi-log plot of absorbance (λ_{max} = 376 nm) versus time for a UV/Vis initiation kinetics experiment (catalyst **21**, trial 1).

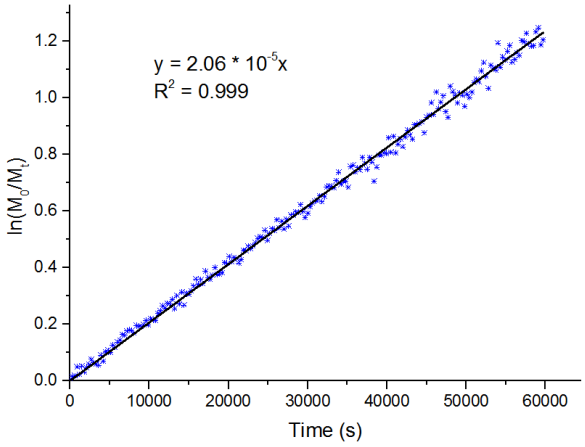
Table S1: Summary of UV/Vis initiation kinetics data.

					k_{init} (10^{-4} s^{-1})					
Catalyst	Ar =	R^1 =	R^2 =	λ_{max}	Trial 1	Trial 2	Trial 3	Average	Std. Dev.	k_{rel}
22	Mes	*c*-Butyl	H	378	0.2865	0.2795	0.2645	2.768E-05	1.12398E-06	0.69
16	Mes	Ethyl	H	376	0.3969	0.3772	0.4153	3.967E-05	1.90537E-06	1.0
25	Mes	*c*-Heptyl	H	380	0.3906	0.4186	0.417	4.083E-05	1.57243E-06	1.0
21	Mes	Phenethyl	H	376	0.4314	0.4489	0.4962	4.5883E-05	3.35226E-06	1.1
26	Mes	*c*-Octyl	H	380	0.4599	0.4622	0.4674	4.631E-05	3.84231E-07	1.2
24	Mes	*c*-Hexyl	H	380	0.4561	0.5109	0.4847	0.0000483	2.74088E-06	1.2
23	Mes	*c*-Pentyl	H	380	0.5879	0.5546	0.5873	0.0000576	1.90549E-06	1.4
17	Mes	*n*-Propyl	H	376	0.6923	0.7085	0.7129	7.0456E-05	1.08487E-06	1.8
18	Mes	*t*-Butyl	H	380	1.244	1.259	1.220	0.000124	1.96723E-06	3.1
19	Mes	*i*-Butyl	H	378	1.814	1.875	1.860	0.000184	3.17857E-06	4.6
20	Mes	Benzyl	H	370	5.429	4.939	4.849	0.000507	3.12143E-05	13
28	Mes	CH_2-1-Ada	H	374	5.29	5.61	5.604	0.000550	1.83045E-05	14
27	Mes	$CHCy_2$	H	376	137.4	133.5	136.9	0.0136	0.000212211	340
33	Dipp	*i*-Propyl	H	374	0.03695	-	-	0.03695	-	0.092
34	Dipp	1-Ada	H	378	0.09822	-	-	0.09822	-	0.25
35	Dipp	2-Ada	H	378	2.860	2.944	2.926	2.910E-04	4.423E-06	7.3
36	*o*-Tol	*i*-Propyl	H	374	0.2288	0.2152	0.1684	2.041E-05	3.168E-06	0.51
37	*o*-Tol	1-Ada	H	378	2.541	2.300	2.589	2.477E-04	1.549E-05	6.2
38	*o*-Tol	2-Ada	H	376	71.26	75.07	80.17	7.550E-03	4.471E-04	190

NMR Initiation Kinetics:[1c, 2]

An NMR tube with a screwcap septum top was charged with catalyst **32** solution in toluene-d_8 (5 mM). The sample was equilibrated at 70 °C in the NMR probe before butyl vinyl ether (30 equiv) was added via syringe. Reactions were monitored by measuring the decay of the benzylidene peak by ^{1}H NMR as a function of time using an array. Interchange rate k_I is approximated by k_{obs}/[BVE].[3]



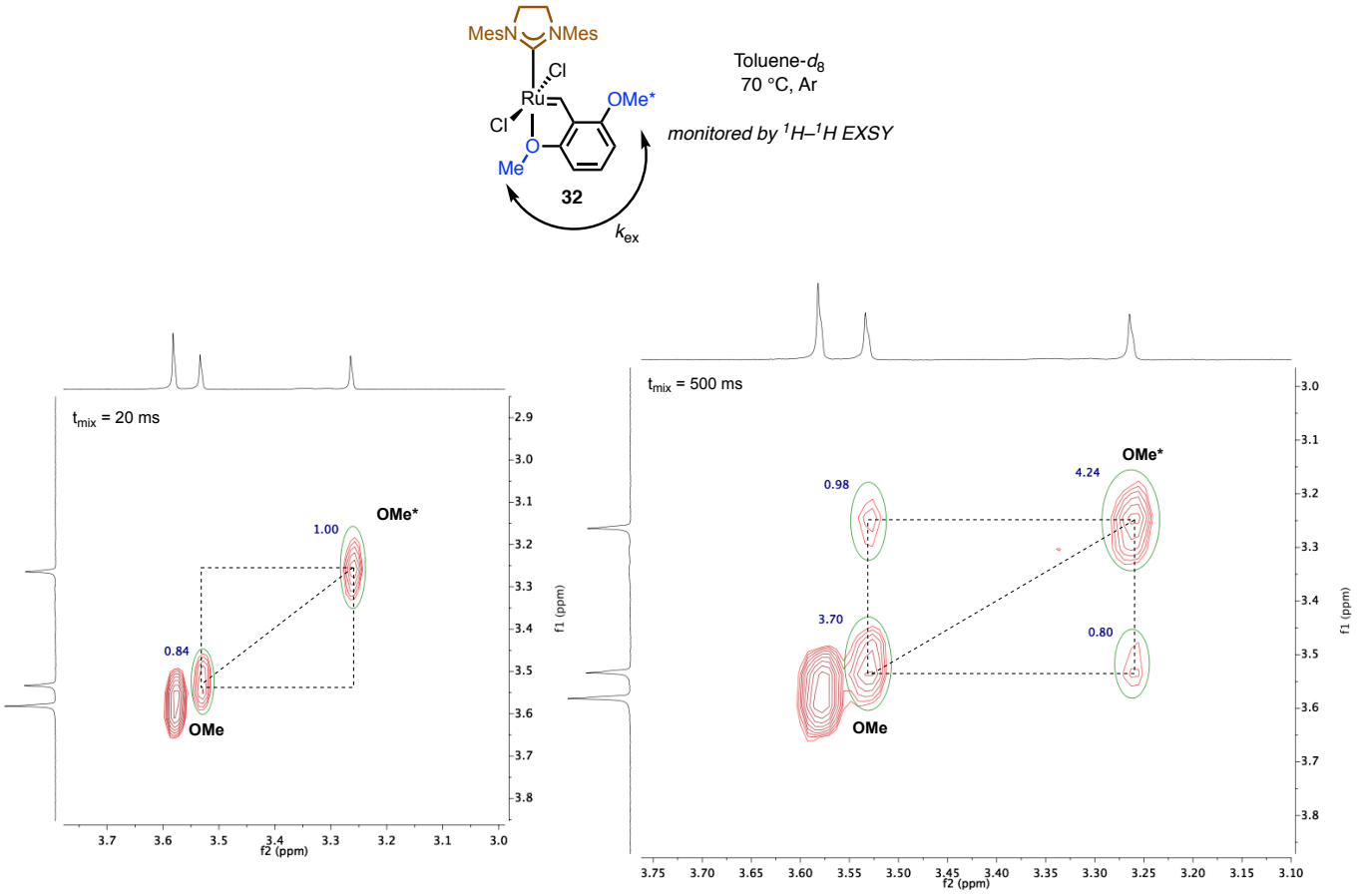


Temperature (°C)	[Ru] (mM)	[BVE] (mM)	k_{obs} (10^{-3} s^{-1})	k_I (10^{-3} s^{-1})
70	5.0	150	0.0206	0.137

Figure S4: Initiation kinetics of catalyst **32** approximately over the course of two half-lives of the initiation reaction

^{1}H–^{1}H EXSY NMR Study:[4]

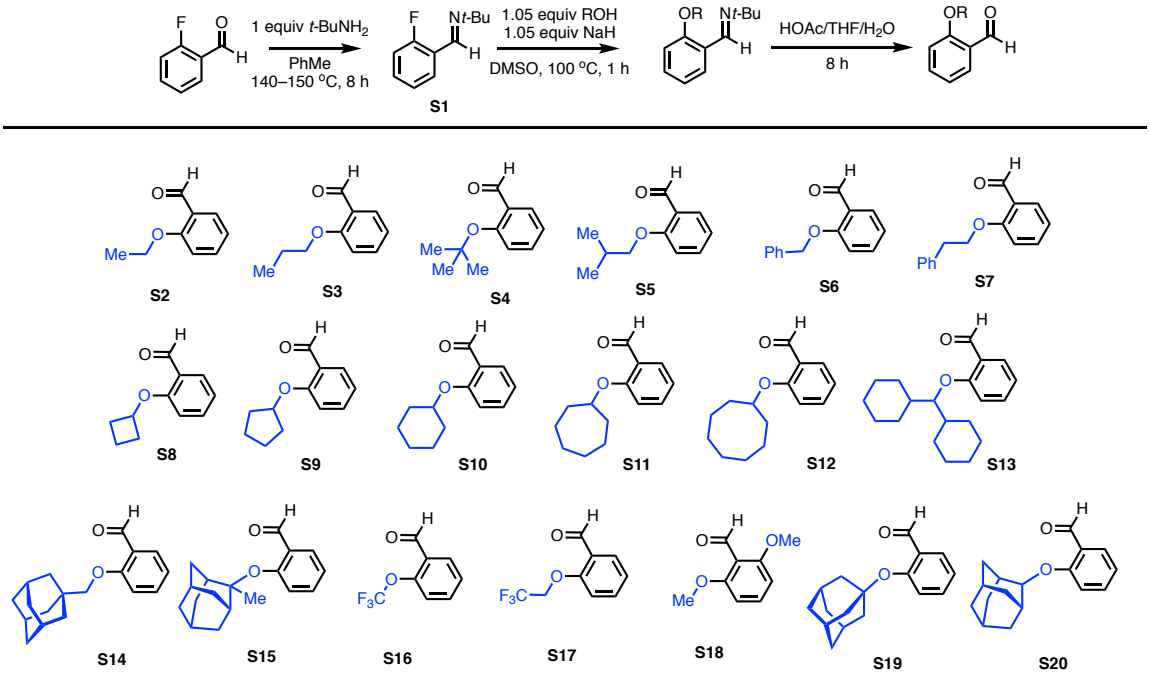
Solution of catalyst **32** in toluene-d_8 (5 mM) was equilibrated at 70 °C in the NMR probe before being subjected to ^{1}H–^{1}H NOESY pulse sequences with different mixing time (20 and 500 ms, respectively). The volume of the diagonal and cross-peaks were derived from the spectra. The rate exchange matrix was calculated with EXSYCalc and the methoxy exchange rate was determined.



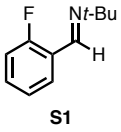
Temperature (°C)	Mixing time (ms)	$k_{OMe \rightarrow OMe*}$ (s^{-1})
70	500	0.448

Figure S5: ^{1}H–^{1}H EXSY studies for OMe exchange in **32**

General Three-Step S_NAr Procedure:



Scheme S1: General depiction of three-step S_NAr route for synthesizing 2-alkoxybenzaldehydes.



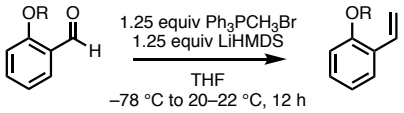
***N-tert*-butyl-1-(2-fluorophenyl)methanimine (S1):**[5] To a 100-mL round-bottom flask equipped with a Teflon-coated magnetic stir bar were added *tert*-butylamine (1.04 mL, 10.0 mmol), 2-fluorobenzaldehyde (1.05 mL, 10.0 mmol), and toluene (50 mL). The flask was equipped with a Dean–Stark apparatus wrapped in aluminum foil and a reflux condenser. The reaction was allowed to stir at vigorous reflux (140–150 °C) for 8 h. During the course of the reaction, water accumulated at the bottom of the Dean–Stark apparatus. The reaction was allowed to cool to room temperature. A small aliquot was taken, concentrated *in vacuo*, and analyzed by ^{1}H NMR to monitor reaction progress. (2-Fluorobenzaldehyde has a characteristic ^{1}H NMR peak at 10.35 ppm (s) in $CDCl_3$, and the product (**S1**) has a ^{1}H NMR peak at 8.57 ppm (s); comparison of these two peaks provides a convenient means of monitoring reaction progress.) In cases where the reaction had not proceeded to >95% conversion, an additional portion of *tert*-butylamine commensurate with the amount of starting material remaining was added, and the reaction was heated for an additional 2–4 h. Upon completion, the reaction mixture was allowed to cool to room temperature, and the solvent was removed *in vacuo*. The crude imine product (**S1**) was obtained as a yellow oil and was used in the subsequent step without further purification. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.57 (s, 1H), 8.00 (td, J_1 = 7.7 Hz, J_2 = 1.8 Hz, 1H), 7.41–7.31 (m, 1H), 7.16 (t, J = 7.5 Hz, 1H), 7.10–7.02 (m, 1H), 1.30 (s, 9H).

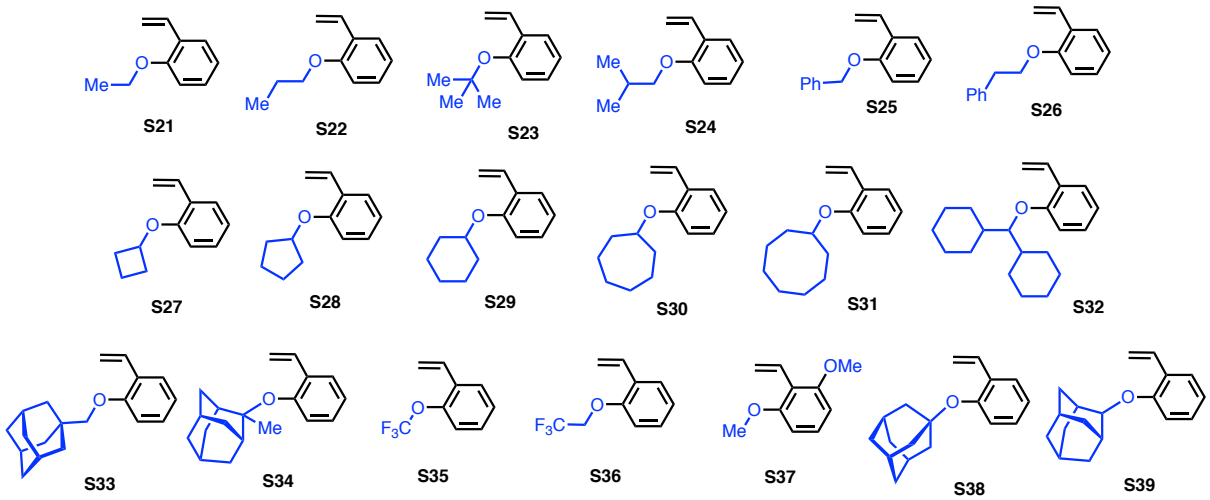
General S_NAr procedure:[5a, 6] To a 100-mL Schlenk flask equipped with a Teflon-coated magnetic stir bar under Ar, were added dry NaH (252 mg, 10.5 mmol), DMSO (20 mL), and the appropriate alcohol (10.0 mmol). Upon addition of the alcohol, vigorous bubbling was observed.

The solution was allowed to stir at room temperature, at which point it was a white suspension. A solution of crude *N*-*tert*-butyl-1-(2-fluorophenyl)methanimine (**S1**) (assumed to be 10.0 mmol) in DMSO (10 mL) was added. The reaction mixture was heated to 100 °C for 1 h, during which time it changed color from yellow to red to brown. After 1 h, a small aliquot of the reaction mixture was removed with a syringe and quenched with H_2O. The resulting mixture was extracted with Et_2O, and the organic phase was concentrated *in vacuo* and examined by ^1H NMR spectroscopy to monitor reaction progress. In instances where the reaction had not proceeded to completion (*i.e.*, >95% conversion) an additional portion of NaH and alcohol commensurate with the amount of starting material remaining was added, and the reaction mixture was heated at 100 °C for an additional 1 h. Upon completion of the reaction, the flask was allowed to cool to room temperature. The reaction mixture was carefully poured into a separatory funnel containing 100 mL of H_2O to quench residual NaH and sodium alkoxide salts. The mixture was extracted with Et_2O (3 × 100 mL). The organic layers were combined and concentrated *in vacuo*. The crude product was obtained as a pink oil or off-white solid and was used in the next step without further purification.

General acidic hydrolysis procedure:[5a, 6] To a 500-mL round-bottom flask equipped with a Teflon-coated magnetic stir bar, were added crude S_NAr product (assumed to be 10.0 mmol). A 50:15:1 H_2O:THF:HOAc solution was added, and the reaction was stirred at room temperature overnight (approximately 12 h). THF was removed *in vacuo*, and the resulting aqueous solution was extracted with Et_2O (3 × 50 mL). The combined organic layers were washed with brine (100 mL), dried over Na_2SO_4, filtered, and concentrated *in vacuo*. Purification by silica gel column chromatography using a gradient solvent system (100:1 hexane:Et_2O → 40:1 hexane:Et_2O) as the eluent, gave the pure product as white or off-white solid. The final yield was calculated for the combined three steps.

General Wittig Olefination Procedure:

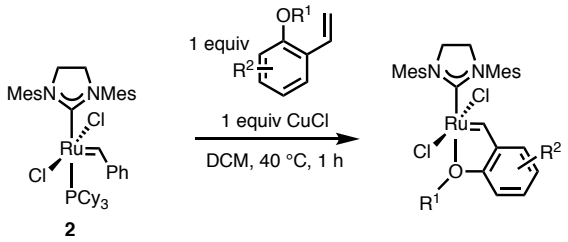




Scheme S2: General depiction of Wittig olefination reaction.

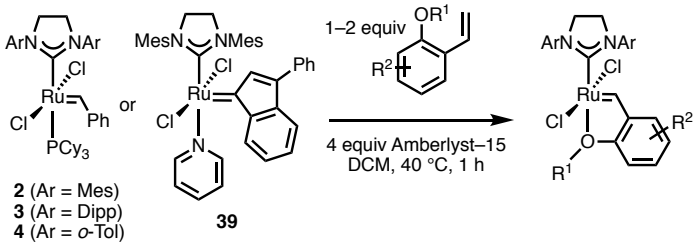
General Wittig olefination procedure:[5a, 7] To a flame-dried 100-mL Schlenk flask equipped with a magnetic stir bar under Ar, were added methyltriphenylphosphonium bromide (1.34 g, 3.75 mmol) and anhydrous THF (20 mL). LiHMDS solution (1.0 M in THF) (3.75 mL, 3.75 mmol) was added at 0 °C. The resulting yellow solution was allowed to warm to room temperature are stir until it became homogeneous (approximately 1 h). The solution was cooled to –78 °C in a dry ice/acetone bath, and the appropriate 2-alkoxybenzaldehyde was added (3.0 mmol). The solution was allowed to warm to room temperature are stir overnight (approximately 12 h). Et_2O (30 mL) was added, and the resulting heterogeneous solution was cooled to –20 °C for 30 min. The solution was filtered through a pad of Celite to remove the triphenylphosphine oxide precipitate, and the Celite was washed twice with Et_2O that had been cooled to 0 °C. The filtrate was concentrated *in vacuo*, and the resulting yellow oil was purified by silica gel column chromatography using a gradient solvent system (100:1 hexane:Et_2O → 40:1 hexane:Et_2O) as the eluent. The pure product was thus obtained as a white solid or colorless oil. To prevent polymerization during prolonged storage, all styrenes were kept under an Ar atmosphere at –20 °C.

Styrene Chelation:



Scheme S3: General depiction of styrene chelation reaction using CuCl procedure.

General chelation procedure with CuCl (Method A):[8] To a flame-dried 20-mL Schlenk flask equipped with a magnetic stir bar under Ar, were added Grubbs 2nd generation catalyst (**2**) (170 mg, 0.2 mmol), CuCl (19.8 mg, 0.2 mmol), the appropriate styrene (0.2 mmol) and DCM (5 mL). The reaction was stirred at 40 °C for 1 h, during which time a color change from maroon to brown or green was observed. The reaction vessel was allowed to cool to room temperature, and the volatiles were removed *in vacuo* to give a green or brown residue. The crude product was dissolved in a minimal amount of 1:1 hexane:DCM, at which point a white precipitate, CuCl•PCy_3, was observed. The suspension was filtered through a pad of cotton in a glass pipette to remove CuCl•PCy_3, and the solution was loaded directly onto a silica gel column. The column was performed first using 4:1 hexane:Et_2O as the eluent to remove organic byproducts. Next, DCM was used as the eluent, at which point the product eluted rapidly. The fractions containing the product were combined, concentrated *in vacuo*, and dried under high vacuum to give the analytically pure product as a green microcrystalline solid.

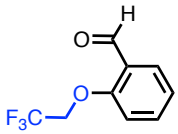


Scheme S4: General depiction of styrene chelation reaction using Amberlyst-15 procedure.

General chelation procedure with Amberlyst 15 resin (Methods B and C):[9] To a flame-dried 20-mL Schlenk flask equipped with a magnetic stir bar under Ar, were added Grubbs catalyst (**2**, **3**, or **4**) (170 mg, 0.2 mmol) or Umicore M31 (**39**) (149 mg, 0.2 mmol), dry Amberlyst-15 hydrogen form (dry, acidic) (4.7 mmol H^+/g) (170 mg, 0.8 mmol H^+), the appropriate styrene (0.2 or 0.4 mmol), and DCM (5 mL). The reaction was stirred at 40 °C for 1 h, during which time a color change from maroon to brown or green was observed. The reaction vessel was allowed to cool to room temperature, and the reaction mixture was filtered through a pad of cotton in a glass pipette to remove the Amberlyst-15 resin. The resulting filtrate was concentrated *in vacuo* to give a brown residue. Pentane (10 mL) was added, and the resulting suspension was sonicated for 1 min, during which time the pentane phase became dark brown, and a green precipitate was observed. The suspension was filtered through a fritted Buchner filter funnel. The green precipitate was washed sequentially with methanol (2 × 5 mL) and pentane (2 × 5 mL) and then dried under high vacuum to give the analytically pure product as a green solid.

Characterization of New Compounds

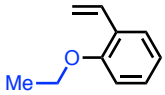
Known 2-alkoxybenzaldehydes **S2–S16, S18–S20** were prepared according to previously reported procedures.[5a, 10] Analytical data were in agreement with previously reported data.[5a, 10-11]



S17

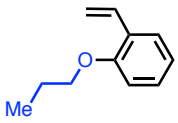
2-(2,2,2-trifluoroethoxy)benzaldehyde (S17): To a flame-dried 250 mL Schlenk flask equipped with a magnetic stir bar under Ar, were added salicylaldehyde (10 mmol), Cs_2CO_3 (45 mmol) and dry DMF (40 mL). Reaction mixture was cooled in ice bath and 2,2,2-trifluoroethyl trifluoromethanesulfonate (12 mmol) was added slowly. The reaction mixture was allowed to warm to room temperature and stir for 3 hours. The reaction mixture was quenched with water and extracted three times with ethyl ether. The ethereal solution was washed with brine and dried over Na_2SO_4 before being concentrated *in vacuo*. The crude product was purified by column chromatography with 4:1 pentane:Et_2O as the eluent to yield a white solid (98% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 10.49 (d, J = 0.8 Hz, 1H), 7.89 (dd, J = 7.7, 1.8 Hz, 1H), 7.59 (ddd, J = 8.4, 7.4, 1.8 Hz, 1H), 7.19–7.07 (m, 1H), 6.96 (d, J = 8.4 Hz, 1H), 4.49 (q, J = 7.9 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 188.96, 159.47, 136.03, 128.96, 125.69, 123.16 (q, J_{CF} = 278.0 Hz), 122.92, 112.92, 66.31 (q, J_{CF} = 36.2 Hz); **HRMS** (EI+) *m/z* Calcd for $C_9H_7F_3O_2$ $[M]^+$204.0398, found 204.0372.

Known styrenes **S25**, **S32**, **S35**, and **S37–S39** were prepared according to previously reported procedures.[1a, 7] Analytical data were in agreement with previously reported data.[1a, 12]



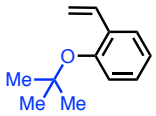
S21

1-ethoxy-2-vinylbenzene (S21): The title compound was prepared on a 3.0-mmol scale from commercially available 2-ethoxybenzaldehyde (**S2**) according to the general Wittig procedure and was obtained as a colorless oil (430 mg, 97% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.48 (dd, J_1 = 7.6 Hz, J_2 = 1.7 Hz, 1H), 7.22 (ddd, J_1 = 8.0 Hz, J_2 = 7.3 Hz, J_3 = 1.7 Hz, 1H), 7.08 (dd, J_1 = 17.8 Hz, J_2 = 11.2 Hz, 1H), 6.97–6.89 (m, 1H), 6.86 (dd, J_1 = 8.2 Hz, J_2 = 1.1 Hz, 1H), 5.76 (dd, J_1 = 17.8 Hz, J_2 = 1.6 Hz, 1H), 5.26 (dd, J_1 = 11.2 Hz, J_2 = 1.6 Hz, 1H), 4.06 (q, J = 7.0 Hz, 2H), 1.45 (t, J = 7.0 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 156.31, 131.96, 128.91, 126.91, 126.66, 120.63, 114.36, 112.09, 63.99, 15.04; **HRMS** (FAB+) *m/z* Calcd for $C_{10}H_{13}O$ $[M+H]^+$ 149.0966, found 149.0986.



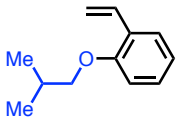
S22

1-*n*-propoxy-2-vinylbenzene (S22): The title compound was prepared on a 3.0-mmol scale from commercially available 2-*n*-propoxybenzaldehyde (**S3**) according to the general Wittig procedure and was obtained as a colorless oil (372 mg, 76% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.48 (dd, J_1 = 7.6 Hz, J_2 = 1.7 Hz, 1H), 7.21 (ddd, J_1 = 8.1 Hz, J_2 = 7.3 Hz, J_3 = 1.7 Hz, 1H), 7.08 (dd, J_1 = 17.8 Hz, J_2 = 11.2 Hz, 1H), 6.94–6.89 (m, 1H), 6.86 (dd, J_1 = 8.2 Hz, J_2 = 0.8 Hz, 1H), 5.76 (dd, J_1 = 17.8 Hz, J_2 = 1.6 Hz, 1H), 5.25 (dd, J_1 = 11.2 Hz, J_2 = 1.6 Hz, 1H), 3.95 (t, J = 6.4 Hz, 2H), 1.90–1.79 (m, 2H), 1.07 (t, J = 7.4 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 156.50, 132.01, 128.89, 127.05, 126.67, 120.60, 114.25, 112.16, 70.02, 22.84, 10.79; **HRMS** (EI+) *m/z* Calcd for $C_{11}H_{14}O$ $[M]^+$ 162.1045, found 162.1064.



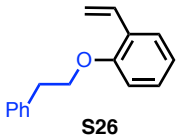
S23

1-(*tert*-butoxy)-2-vinylbenzene (S23): The title compound was prepared on a 2.0-mmol scale from 2-(*tert*-butoxy)benzaldehyde (**S4**) according to the general Wittig procedure and was obtained as a colorless oil (322 mg, 91% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.54 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.17 (ddd, J_1 = 8.3 Hz, J_2 = 7.2 Hz, J_3 = 1.8 Hz, 1H), 7.10 (dd, J_1 = 18.0 Hz, J_2 = 11.1 Hz, 1H), 7.06–7.01 (m, 2H), 5.70 (dd, J_1 = 17.9 Hz, J_2 = 1.4 Hz, 1H), 5.22 (dd, J_1 = 11.1 Hz, J_1 = 1.4 Hz, 1H), 1.37 (s, 9H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 153.51, 133.01, 132.64, 128.21, 125.93, 123.45, 123.23, 113.69, 79.93, 29.27; **HRMS** (EI+) *m/z* Calcd for $C_{12}H_{16}O$ $[M]^+$ 176.1201, found 176.1238.



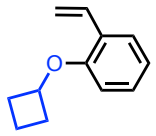
S24

1-*iso*-butoxy-2-vinylbenzene (S24): The title compound was prepared on a 2.0-mmol scale from commercially available 2-*iso*-butoxybenzaldehyde (**S5**) according to the general Wittig procedure and was obtained as a colorless oil (3% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.51 (dd, J = 7.6, 1.7 Hz, 1H), 7.23 (ddd, J = 8.2, 7.4, 1.7 Hz, 1H), 7.13 (dd, J = 17.8, 11.2 Hz, 1H), 6.98–6.91 (m, 1H), 6.87 (dd, J = 8.3, 0.9 Hz, 1H), 5.79 (dd, J = 17.8, 1.6 Hz, 1H), 5.28 (dd, J = 11.2, 1.6 Hz, 1H), 3.78 (d, J = 6.4 Hz, 2H), 2.16 (dh, J = 13.3, 6.7 Hz, 1H), 1.08 (d, J = 6.7 Hz, 6H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 156.59, 132.01, 128.89, 127.10, 126.64, 120.58, 114.20, 112.15, 74.94, 28.60, 19.50; **HRMS** (FAB+) *m/z* Calcd for $C_{12}H_{17}O$ $[M+H]^+$ 177.1279, found 177.1285.

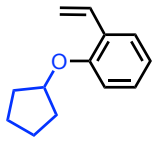


S26

1-phenethoxy-2-vinylbenzene (S26): The title compound was prepared on a 2.0-mmol scale from 2-phenethoxybenzaldehyde (**S7**) according to the general Wittig procedure and was obtained as a colorless oil (96% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.46 (ddt, J = 7.6, 1.7, 0.5 Hz, 1H), 7.33–7.26 (m, 4H), 7.24–7.20 (m, 1H), 7.18 (ddd, J = 8.2, 7.4, 1.7 Hz, 1H), 7.03 (ddt, J = 17.7, 11.1, 0.6 Hz, 1H), 6.94–6.87 (m, 1H), 6.83 (dd, J = 8.3, 1.1 Hz, 1H), 5.71 (dd, J = 17.8, 1.6 Hz, 1H), 5.23 (dd, J = 11.1, 1.6 Hz, 1H), 4.18 (t, J = 7.0 Hz, 2H), 3.12 (t, J = 7.0 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 156.17, 138.53, 131.95, 129.16, 128.90, 128.62, 127.26, 126.71, 126.62, 120.92, 114.39, 112.29, 69.34, 36.09; **HRMS** (FAB+) *m/z* Calcd for $C_{16}H_{16}O$ $[M]^+$ 224.1201, found 224.1205.

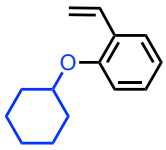

S27

1-cyclobutoxy-2-vinylbenzene (S27): The title compound was prepared on a 3.0-mmol scale from 2-cyclobutoxybenzaldehyde (**S8**) according to the general Wittig procedure and was obtained as a colorless oil (499 mg, 95% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.50 (d, J = 7.6 Hz, 1H), 7.20 (t, J = 7.8 Hz, 1H), 7.15–7.05 (m, 1H), 6.94 (t, J = 7.5 Hz, 1H), 6.74 (d, J = 8.2 Hz, 1H), 5.81–5.77 (m, 1H), 5.30–5.27 (m, 1H), 4.68 (p, J = 7.2 Hz, 1H), 2.52–2.44 (m, 2H), 2.28–2.18 (m, 2H), 1.93–1.83 (m, 1H), 1.77–1.64 (m, 1H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 154.93, 131.98, 128.81, 126.85, 126.68, 120.61, 114.30, 112.85, 71.89, 30.89, 13.43; **HRMS** (EI+) *m/z* Calcd for $C_{12}H_{14}O$ $[M]^+$ 174.1045, found 174.1052.


S28

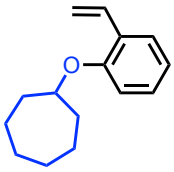
1-(cyclopentyloxy)-2-vinylbenzene (S28): The title compound was prepared on a 3.0-mmol scale from 2-(cyclopentyloxy)benzaldehyde (**S9**) according to the general Wittig procedure and was obtained as a colorless oil (500 mg, 87% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.49–7.45 (m, 1H), 7.23–7.17 (m, 1H), 7.03 (ddd, J_1 = 17.6 Hz, J_2 = 11.2 Hz, J_3 = 3.8 Hz, 1H), 6.93–6.85 (m, 2H), 5.78–5.71 (m, 1H), 5.26–5.20 (m, 1H), 4.83–4.78 (m, 1H), 1.93–1.87 (m, 4H), 1.87–1.78 (m, 2H), 1.68–1.59 (m, 2H); **^{13}C NMR**

(125 MHz, $CDCl_3$) δ 155.39, 132.15, 128.73, 127.44, 126.71, 120.31, 114.06, 113.51, 79.74, 33.05, 24.18; **HRMS** (EI+) *m/z* Calcd for $C_{13}H_{16}O$ $[M]^+$ 188.1201, found 188.1205.



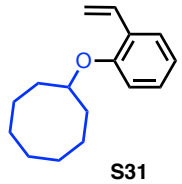
S29

1-(cyclohexyloxy)-2-vinylbenzene (S29): The title compound was prepared on a 2.0-mmol scale from 2-(cyclohexyloxy)benzaldehyde **(S10)** according to the general Wittig procedure and was obtained as a colorless oil (>99% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.49 (dd, J_1 = 7.6 Hz, J_2 = 1.7 Hz, 1H), 7.19 (ddd, J_1 = 8.2 Hz, J_2 = 7.4 Hz, J_3 = 1.7 Hz, 1H), 7.09 (dd, J_1 = 17.8 Hz, J_2 = 11.2 Hz, 1H), 6.93–6.88 (m, 2H), 5.74 (dd, J_1 = 17.8 Hz, J_2 = 1.6 Hz, 1H), 5.24 (dd, J_1 = 11.1 Hz, J_2 = 1.6 Hz, 1H), 4.28 (tt, J_1 = 8.4 Hz, J_2 = 3.6 Hz, 1H), 2.00–1.93 (m, 2H), 1.83–1.76 (m, 2H), 1.64–1.52 (m, 3H), 1.42–1.33 (m, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 155.12, 132.08, 128.75, 128.06, 126.61, 120.68, 114.45, 114.01, 76.05, 31.95, 25.82, 23.77; **HRMS** (EI+) *m/z* Calcd for $C_{14}H_{18}O$ $[M]^+$ 202.1358, found 202.1383.



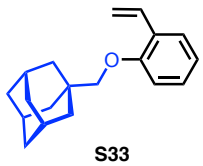
S30

(2-vinylphenoxy)cycloheptane (S30): The title compound was prepared on a 2.0-mmol scale from 2-(cycloheptyloxy)benzaldehyde **(S11)** according to the general Wittig procedure and was obtained as a colorless oil (85% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.51–7.47 (m, 1H), 7.23–7.17 (m, 1H), 7.09 (dd, J = 17.8, 11.1 Hz, 1H), 6.94–6.88 (m, 1H), 6.85 (d, J = 8.3 Hz, 1H), 5.75 (dt, J = 17.8, 1.3 Hz, 1H), 5.25 (dt, J = 11.1, 1.2 Hz, 1H), 4.46 (tt, J = 8.0, 4.2 Hz, 1H), 2.08–1.99 (m, 2H), 1.90–1.81 (m, 2H), 1.81–1.70 (m, 2H), 1.70–1.55 (m, 4H), 1.53–1.43 (m, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 155.18, 132.15, 128.76, 127.93, 126.63, 120.47, 114.14, 113.97, 78.60, 33.91, 28.57, 23.12; **HRMS** (FAB+) *m/z* Calcd for $C_{15}H_{20}O$ $[M]^+$ 216.1514, found 216.1508.



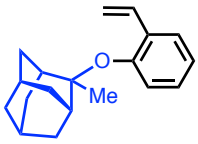
S31

(2-vinylphenoxy)cyclooctane (S31): The title compound was prepared on a 3.0-mmol scale from 2-(cyclooctyloxy)benzaldehyde **(S12)** according to the general Wittig procedure and was obtained as a colorless oil (646 mg, 93% yield). 7.51 (dd, J = 7.5, 1.2 Hz, 1H), 7.25–7.19 (m, 1H), 7.10 (dd, J_1 = 17.8 Hz, J_2 = 11.2 Hz, 1H), 6.93 (t, J = 7.5 Hz, 1H), 6.86 (d, J = 8.3 Hz, 1H), 5.76 (ddd, J_1 = 17.8 Hz, J_2 = 1.4 Hz, J_3 = 0.9 Hz, 1H), 5.30–5.20 (m, 1H), 4.46 (tt, J_1 = 8.0 Hz, J_2 = 3.8 Hz, 1H), 2.01–1.88 (m, 4H), 1.87–1.78 (m, 2H), 1.73–1.65 (m, 1H), 1.65–1.51 (m, 7H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 155.11, 132.16, 128.74, 127.96, 126.67, 120.44, 114.13, 113.94, 78.55, 31.69, 27.30, 25.74, 23.19; **HRMS** (FAB+) *m/z* Calcd for $C_{16}H_{22}O_2$ $[M]^+$ 230.1671, found 230.1671.



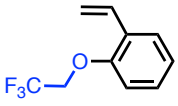
S33

(3*r*,5*r*,7*r*)-1-((2-vinylphenoxy)methyl)adamantane (S33): The title compound was prepared on a 3.0-mmol scale from 2-(((3*r*,5*r*,7*r*)-adamantan-1-yl)methoxy)benzaldehyde **(S14)** according to the general Wittig procedure and was obtained as a colorless oil (93% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.49 (dd, J = 7.6, 1.7 Hz, 1H), 7.21 (ddd, J = 8.3, 7.5, 1.7 Hz, 1H), 7.12 (dd, J = 17.8, 11.2 Hz, 1H), 6.93–6.87 (m, 1H), 6.87–6.82 (m, 1H), 5.77 (dd, J = 17.8, 1.6 Hz, 1H), 5.27 (dd, J = 11.2, 1.5 Hz, 1H), 3.53 (s, 2H), 2.04 (s, 3H), 1.81–1.66 (m, 12H); **^{13}C NMR** (125 MHz, $CDCL_3$) δ 156.67, 131.79, 128.93, 126.91, 126.37, 120.35, 114.12, 111.92, 78.69, 39.83, 37.30, 34.12, 28.37; **HRMS** (FAB+) *m/z* Calcd for $C_{19}H_{24}O$ $[M]^+$ 268.1827, found 268.1833.



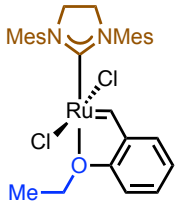
S34

(1*s*,2*s*,5*r*)-2-methyl-2-(2-vinylphenoxy)adamantane (S34): The title compound was prepared on a 3.0-mmol scale from 2-(((1*S*,2*S*,5*R*)-2-methyladamantan-2-yl)oxy)benzaldehyde **(S15)** according to the general Wittig procedure and was obtained as a colorless oil (57% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.57–7.51 (m, 1H), 7.21–7.11 (m, 2H), 6.98 (d, *J* = 7.7 Hz, 2H), 5.70 (dd, *J* = 17.8, 1.2 Hz, 1H), 5.22 (dd, *J* = 11.1, 1.2 Hz, 1H), 2.46 (d, *J* = 11.7 Hz, 2H), 2.19 (s, 2H), 1.95–1.80 (m, 6H), 1.76 (s, 2H), 1.61 (d, *J* = 12.2 Hz, 2H), 1.32 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 154.01, 133.02, 131.55, 128.28, 126.11, 121.81, 120.95, 113.53, 84.97, 38.60, 38.53, 35.31, 33.21, 27.63, 27.24, 22.27; **HRMS** (FAB+) *m/z* Calcd for $C_{19}H_{23}O$ $[(M+H)-H_2]^+$ 267.1749, found 267.1743.



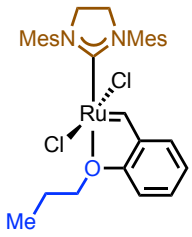
S36

1-(2,2,2-trifluoroethoxy)-2-vinylbenzene (S36): The title compound was prepared on a 3.0-mmol scale from 2-(2,2,2-trifluoroethoxy)benzaldehyde (**S17**) according to the general Wittig procedure and was obtained as a colorless oil (98% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.55–7.48 (m, 1H), 7.28–7.19 (m, 1H), 7.03 (td, *J* = 11.9, 11.2, 7.0 Hz, 2H), 6.82 (d, *J* = 8.2 Hz, 1H), 5.78 (dt, *J* = 17.8, 1.2 Hz, 1H), 5.32 (dt, *J* = 11.2, 1.1 Hz, 1H), 4.35 (q, *J* = 8.1 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 154.64, 130.88, 129.00, 127.83, 127.09, 123.51 (q, J_{CF} = 278.0 Hz), 122.86, 115.63, 112.97, 66.59 (q, J_{CF} = 35.6 Hz); **HRMS** (EI+) *m/z* Calcd for $C_{10}H_9F_3O$ $[M]^+$ 202.0606, found 202.0644.



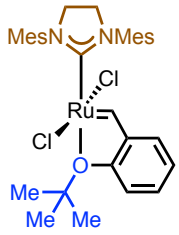
16

ethoxy catalyst (16): The title compound was prepared on a 0.2 mmol scale using the general chelation procedure and obtained as a green microcrystalline solid (62 mg, 51% yield, Method A). **^{1}H NMR** (500 MHz, CD_2Cl_2) δ 16.52 (s, 1H), 7.56 (ddd, J_1 = 8.8 Hz, J_2 = 7.1 Hz, J_3 = 2.0 Hz, 1H), 7.08 (bs, 4H), 7.00–6.92 (m, 2H), 6.88 (d, *J* = 8.3 Hz, 1H), 4.17 (q, *J* = 6.9 Hz, 2H), 4.16 (s, 4H), 2.44 (bs, 12H), 2.42 (bs, 6H), 1.13 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (125 MHz, CD_2Cl_2) δ 294.71, 211.58, 154.32, 145.56, 139.63, 139.54, 136.70 (bs), 130.06, 129.96, 123.68, 122.31, 112.82, 67.18, 52.25, 21.45, 19.75 (bs), 13.96; **HRMS** (FAB+) *m/z* Calcd for $C_{30}H_{36}Cl_2N_2ORu$ $[M]^+$ 612.1248, found 612.1256.



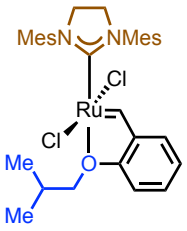
17

***n*-propoxy catalyst (17):** The title compound was prepared on a 0.2 mmol scale using the general chelation procedure and obtained as a green microcrystalline solid (98 mg, 78% yield, Method A). **^{1}H NMR** (500 MHz, CD_2Cl_2) δ 16.52 (s, 1H), 7.57 (ddd, J_1 = 8.7 Hz, J_2 = 7.0 Hz, J_3 = 2.2 Hz, 1H), 7.09 (s, 4H), 7.00–6.92 (m, 2H), 6.90 (d, *J* = 8.3 Hz, 1H), 4.16 (s, 4H), 4.02 (t, J = , 2H), 2.44 (s, 12H), 2.43 (s, 6H), 1.57 (h, *J* = 7.6 Hz, 2H), 0.79 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR** (125 MHz, CD_2Cl_2) δ 295.23, 211.53, 154.38, 145.67, 139.67, 139.50, 136.64 (bs), 130.08, 129.96, 123.74, 122.34, 113.10, 72.90, 52.20, 22.05, 21.48, 19.75 (bs), 9.97; **HRMS** (FAB+) *m/z* Calcd for $C_{31}H_{38}Cl_2N_2ORu$ $[M]^+$ 626.1405, found 626.1429.



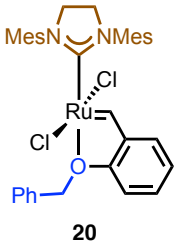
18

***tert*-butoxy catalyst (18):** The title compound was prepared on a 0.2 mmol scale using the general chelation procedure and obtained as a green microcrystalline solid (117 mg, 91% yield, Method A). **^{1}H NMR** (500 MHz, CD_2Cl_2) δ 16.50 (s, 1H), 7.50 (t, *J* = 7.5 Hz, 1H), 7.18–6.98 (m, 5H), 6.97–6.86 (m, 2H), 4.15 (s, 4H), 2.42 (bs, 18H), 1.52 (s, 9H); **^{13}C NMR** (125 MHz, CD_2Cl_2) δ 298.91, 211.77, 152.20, 146.99, 139.72 (bs), 139.47, 129.92, 129.54, 123.80, 122.57, 116.89, 88.30, 52.16 (bs), 28.88, 21.44, 19.64 (bs); **HRMS** (FAB+) *m/z* Calcd for $C_{32}H_{40}Cl_2N_2ORu$ $[M]^+$ 640.1562, found 640.1545.



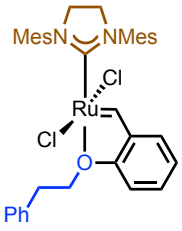
19

***iso*-butoxy catalyst (19):** The title compound was prepared on a 0.2 mmol scale using the general chelation procedure and obtained as a green microcrystalline solid (80 mg, 63% yield, Method A). **^{1}H NMR** (500 MHz, CD_2Cl_2) δ 16.57 (s, 1H), 7.56 (ddd, *J* = 8.8, 6.0, 3.1 Hz, 1H), 7.08 (s, 4H), 6.98–6.91 (m, 3H), 4.16 (s, 4H), 3.93 (d, *J* = 6.3 Hz, 2H), 2.44 (d, *J* = 10.4 Hz, 18H), 1.83 (dh, *J* = 13.1, 6.5 Hz, 1H), 0.83 (d, *J* = 6.7 Hz, 6H); **^{13}C NMR** (125 MHz, CD_2Cl_2) δ 296.13 (Ru,=CAr), 296.02 (Ru=CAr), 210.81, 154.71, 145.96, 139.52, 139.36, 136.50 (bs), 130.01, 129.83, 123.96, 122.40, 114.31, 78.60, 52.07 (bs), 28.42, 21.44, 19.84, 19.69 (bs); **HRMS** (FAB+) *m/z* Calcd for $C_{32}H_{40}Cl_2N_2ORu$ $[M]^+$ 640.1562, found 640.1586.



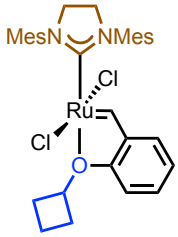
20

benzyloxy catalyst (20): The title compound was prepared on a 0.2 mmol scale according to the general chelation procedure and was obtained as a green microcrystalline solid (78 mg, 58% yield, Method A). **^{1}H** NMR (500 MHz, CD_2Cl_2) δ 16.55 (d, *J* = 1.0 Hz, 1H), 7.43–7.38 (m, 3H), 7.30–7.24 (m, 3H), 7.10–7.04 (m, 4H), 6.97–6.90 (m, 2H), 6.74 (d, *J* = 8.4 Hz, 1H), 5.26 (s, 2H), 4.11 (s, 4H), 2.44 (s, 12H), 2.42 (s, 6H); **^{13}C NMR** (125 MHz, CD_2Cl_2) δ 290.80, 209.83, 153.79, 144.75, 139.23, 139.00, 136.90, 135.44, 129.95, 129.88, 128.89, 128.58, 128.23, 123.89, 122.28, 114.16, 75.23, 52.38, 21.49, 19.55. Analytical data were in agreement with previously reported data.[12a]



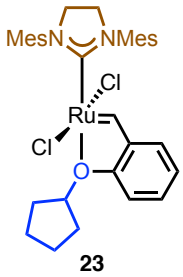
21

phenethoxy catalyst (21): The title compound was prepared on a 0.2 mmol scale according to the general chelation procedure and obtained as green microcrystalline solid (117 mg, 85% yield, Method A). **^{1}H NMR** (400 MHz, CD_2Cl_2) δ 16.45 (s, 1H), 7.54 (ddd, *J* = 8.5, 7.3, 1.8 Hz, 1H), 7.35–7.28 (m, 2H), 7.27–7.22 (m, 1H), 7.18–7.11 (m, 2H), 7.03 (d, *J* = 8.3 Hz, 4H), 7.02–6.94 (m, 2H), 6.85 (d, *J* = 8.3 Hz, 1H), 4.26–4.20 (m, 2H), 4.18 (s, 4H), 2.90–2.79 (m, 2H), 2.47 (s, 12H), 2.20 (s, 6H); **^{13}C NMR** (125 MHz, CD_2Cl_2) δ 294.77 (bs), 211.04, 153.97, 145.46, 139.61, 137.04, 136.27, 130.07, 129.88, 129.82, 128.95, 127.09, 123.88, 122.37, 113.03, 71.52, 52.07 (bs), 35.10, 21.20, 19.73 (bs); **HRMS** (FAB+) *m/z* Calcd for $C_{36}H_{40}Cl_2N_2ORu$ $[M]^+$ 688.1561, found 688.1586.



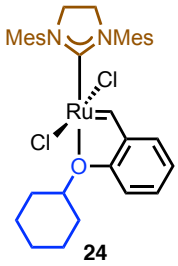
22

cyclobutoxy catalyst (22): The title compound was prepared on a 0.2 mmol scale using the general chelation procedure and obtained as a green microcrystalline solid (123 mg, 96% yield, Method A). **^{1}H NMR** (500 MHz, CD_2Cl_2) δ 16.48 (s, 1H), 7.52 (ddd, J = 8.3, 7.3, 1.8 Hz, 1H), 7.07 (s, 4H), 6.99–6.89 (m, 2H), 6.74 (d, J = 8.2 Hz, 1H), 4.76 (p, J = 7.4 Hz, 1H), 4.16 (s, 4H), 2.44 (s, 12H), 2.40 (s, 6H), 2.21–2.05 (m, 4H), 1.68 (qt, J = 9.9, 2.4 Hz, 1H), 1.55–1.50 (m, 1H); **^{13}C NMR** (125 MHz, CD_2Cl_2) δ 294.60 (Ru=CAr), 294.31 (Ru=CAr), 211.55, 153.08, 145.25, 139.56, 139.43, 136.56 (bs), 129.94, 129.78, 123.50, 122.17, 113.21, 76.34, 52.08, 31.19, 21.37, 19.67 (bs), 13.54; **HRMS** (FAB+) *m/z* Calcd for $C_{32}H_{38}Cl_2N_2ORu$ $[M]^+$ 638.1405, found 638.1386.



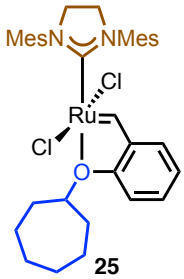
23

cyclopentyloxy catalyst (23): The title compound was prepared on a 0.2 mmol scale using the general chelation procedure and obtained as a green microcrystalline solid (124 mg, 95% yield, Method A). **^{1}H NMR** (500 MHz, CD_2Cl_2) δ 16.52 (s, 1H), 7.55 (ddd, J_1 = 8.4 Hz, J_2 = 7.3 Hz, J_3 = 1.8 Hz, 1H), 7.08 (bs, 4H), 6.97 (dd, J_1 = 7.6 Hz, J_2 = 1.7 Hz, 1H), 6.92 (td, J_1 = 7.4 Hz, J_2 = 0.7 Hz, 1H), 6.87 (d, J = 8.3 Hz, 1H), 4.91 (tt, J_1 = 7.4 Hz, J_2 = 4.8 Hz, 1H), 4.15 (s, 4H), 2.45 (bs, 12H), 2.43 (bs, 6H), 1.96–1.87 (m, 2H), 1.79–1.70 (m, 2H), 1.69–1.60 (m, 2H), 1.41–1.33 (m, 2H); **^{13}C NMR** (125 MHz, CD_2Cl_2) δ 296.27 (Ru=CAr), 296.13 (Ru=CAr), 211.73, 153.92, 145.83, 139.72 (bs), 139.50, 136.52 (bs), 130.03, 129.97, 123.08, 122.52, 113.82, 84.92, 52.19 (bs), 33.55, 24.81, 21.49, 19.82 (bs); **HRMS** (FAB+) *m/z* Calcd for $C_{33}H_{40}Cl_2N_2ORu$ $[M]^+$ 652.1562, found 652.1544.



24

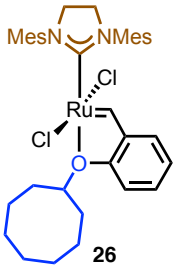
cyclohexyloxy catalyst (24): The title compound was prepared on a 0.2 mmol scale using the general chelation procedure and obtained as a green microcrystalline solid (126 mg, 94% yield, Method A). **^{1}H NMR** (500 MHz, CD_2Cl_2) δ 16.51 (s, 1H), 7.57–7.52 (m, 1H), 7.08 (s, 4H), 6.97 (dd, J_1 = 7.5 Hz, J_2 = 1.4 Hz, 1H), 6.90 (t, J = 7.4 Hz, 1H), 6.84 (d, J = 8.3 Hz, 1H), 4.50 (tt, J_1 = 10.9 Hz, J_2 = 3.9 Hz, 1H), 4.16 (s, 4H), 2.44 (bs, 12H), 2.42 (bs, 6H), 2.07 (d, J = 11.0 Hz, 2H), 1.67 (d, J = 13.1 Hz, 2H), 1.57 (d, J = 12.7 Hz, 1H), 1.42–1.30 (m, 2H), 1.25–1.14 (m, 2H), 1.07–0.99 (m, 1H); **^{13}C NMR** (125 MHz, CD_2Cl_2) δ 296.81 (Ru=CAr), 296.70 (Ru=CAr), 211.49, 152.43, 145.65, 139.61 (bs), 139.31, 129.85, 129.74 (bs), 122.78, 122.74, 113.28, 81.62, 51.96(bs), 31.76, 25.69, 25.38, 21.42, 19.55 (bs); **HRMS** (FAB+) *m/z* Calcd for $C_{34}H_{42}Cl_2N_2ORu$ $[M]^+$ 666.1718, found 666.1697.



25

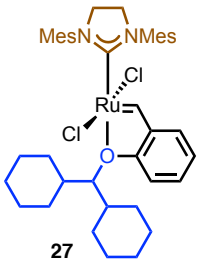
cycloheptyloxy catalyst (25): The title compound was prepared on a 0.2 mmol scale using the general chelation procedure and obtained as a green microcrystalline solid (134 mg, 98% yield, Method A). **^{1}H NMR** (500 MHz, CD_2Cl_2) δ 16.50 (s, 1H), 7.58–7.51 (m, 1H), 7.08 (s, 4H), 6.97 (dd, J = 7.5, 1.5 Hz, 1H), 6.94–6.88 (m, 1H), 6.76 (d, J = 8.3 Hz, 1H), 4.64 (tt, J = 8.9, 4.0 Hz, 1H), 4.15 (s, 4H), 2.45 (s, 12H), 2.42 (s, 6H), 2.09–1.99 (m, 2H), 1.67–1.56 (m, 4H), 1.56–1.45 (m, 4H), 1.30–1.24 (m, 2H); **^{13}C NMR** (125 MHz, CD_2Cl_2) δ 296.69 (Ru=CAr), 296.56 (Ru=CAr), 211.74, 152.72, 146.06, 139.75 (bs), 139.42, 136.71

(bs), 129.92, 129.90, 122.85, 122.78, 113.71, 84.17, 52.17 (bs), 33.67, 28.35, 23.72, 21.49, 19.84 (bs); **HRMS** (FAB+) *m/z* Calcd for $C_{35}H_{44}Cl_2N_2ORu$ $[M]^+$ 680.1875, found 680.1893.



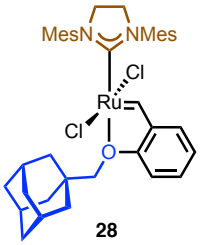
26

cyclooctyloxy catalyst (26): The title compound was prepared on a 0.2 mmol scale using the general chelation procedure and obtained as a green microcrystalline solid (107 mg, 77% yield, Method A) **^{1}H NMR** (500 MHz, CD_2Cl_2) δ 16.51 (s, 1H), 7.58–7.53 (m, 1H), 7.09 (s, 4H), 6.97 (dd, *J* = 7.6, 1.6 Hz, 1H), 6.91 (t, *J* = 7.3 Hz, 1H), 6.77 (d, *J* = 8.3 Hz, 1H), 4.74 (tt, *J* = 9.5, 2.9 Hz, 1H), 4.14 (s, 4H), 2.43 (s, 18H), 1.95–1.89 (m, 2H), 1.71–1.62 (m, 4H), 1.59–1.51 (m, 2H), 1.49–1.43 (m, 2H), 1.43–1.31 (m, 4H); **^{13}C NMR** (125 MHz, CD_2Cl_2) δ 296.44, 211.21, 152.45, 145.91, 139.52 (bs), 139.31, 129.87, 129.82, 122.77, 113.63, 84.03, 52.04 (bs), 32.89, 26.84, 26.55, 24.33, 21.45, 19.66 (bs); **HRMS** (FAB+) *m/z* Calcd for $C_{36}H_{46}Cl_2N_2ORu$ $[M]^+$ 694.2031, found 694.2036.



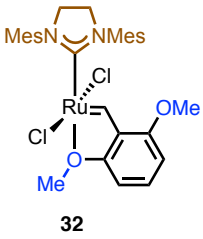
27

dicyclohexylmethoxy catalyst (27): The title compound was prepared on a 0.2 mmol scale using the general chelation procedure and obtained as a green microcrystalline solid (12 mg, 8% yield, Method A; 72 mg, 47%, Method C). **^{1}H NMR** (500 MHz, CD_2Cl_2) δ 16.72 (s, 1H), 7.46 (ddd, *J* = 8.9, 5.5, 3.6 Hz, 1H), 7.09 (d, *J* = 30.4 Hz, 4H), 6.98 (d, *J* = 8.6 Hz, 1H), 6.87–6.79 (m, 2H), 4.49 (t, *J* = 6.5 Hz, 1H), 4.08 (s, 4H), 2.70–2.28 (m, 18H), 1.86 (tdt, *J* = 11.0, 6.5, 3.3 Hz, 2H), 1.63 (d, *J* = 12.7 Hz, 2H), 1.53–1.33 (m, 8H), 1.22 (d, *J* = 12.2 Hz, 2H), 1.15 (ddq, *J* = 16.3, 7.6, 4.4, 3.9 Hz, 2H), 1.08–0.91 (m, 4H), 0.82 (qd, *J* = 11.8, 3.0 Hz, 2H); **^{13}C NMR** (125 MHz, CD_2Cl_2) δ 296.65 (Ru=CAr), 296.55 (Ru=CAr), 208.83, 156.38, 145.87, 139.65, 139.65, 139.18, 138.50, 135.44 (bs), 130.03, 122.32, 122.26, 114.32, 93.74, 52.68 (bs), 52.04 (bs), 39.68, 29.83, 29.12, 26.92, 26.56, 26.35, 21.45, 20.64, 18.62; **HRMS** (FAB+) *m/z* Calcd for $C_{41}H_{54}Cl_2N_2ORu$ $[M]^+$ 762.2657, found 762.2658.



28

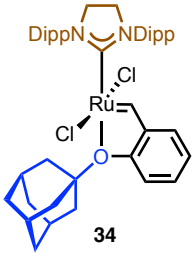
1-adamantanylmethoxy catalyst (28): The title compound was prepared on a 0.2 mmol scale using the general chelation procedure and obtained as a green microcrystalline solid (79 mg, 54% yield, Method B). **^{1}H NMR** (500 MHz, CD_2Cl_2) δ 16.59 (s, 1H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.07 (s, 4H), 6.98 (d, *J* = 8.3 Hz, 1H), 6.91 (dt, *J* = 16.0, 7.3 Hz, 2H), 4.12 (s, 4H), 3.97 (s, 2H), 2.45 (s, 12H), 2.40 (s, 6H), 1.92 (s, 3H), 1.71–1.59 (m, 6H), 1.54 (s, 6H); **^{13}C NMR** (125 MHz, CD_2Cl_2) δ 295.64 (Ru=CAr), 295.52 (Ru=CAr), 210.22, 155.90, 145.92, 139.38 (bs), 139.23, 135.49 (bs), 130.13, 129.92, 123.85, 122.21, 115.57, 82.91, 52.24 (bs), 39.31, 37.28, 34.68, 28.79, 21.40, 19.47 (bs); **HRMS** (FAB+) *m/z* Calcd for $C_{39}H_{48}Cl_2N_2ORu$ $[M]^+$ 732.2187, found 732.2184.



32

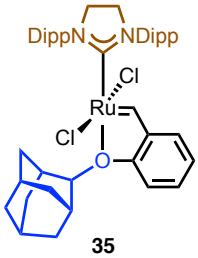
2,6-dimethoxy catalyst (32): The title compound was prepared on a 0.2 mmol scale according to the general chelation procedure and was obtained as a green microcrystalline solid (53 mg, 42%, Method A; 69 mg, 55% yield; Method B). **^{1}H NMR** (*trans* isomer, 400 MHz, CD_2Cl_2) δ 17.25 (s, 1H), 7.56 (t, *J* = 8.3 Hz, 1H), 7.08 (s, 4H), 6.51 (d, *J* = 8.3 Hz, 1H), 6.44 (d, *J* = 8.3 Hz, 1H), 4.09 (s, 4H), 3.81 (s, 3H), 3.74 (s, 3H), 2.44 (s, 12H), 2.42 (s, 6H); **^{13}C NMR** (*trans* isomer, 101 MHz, CD_2Cl_2) δ 286.20 (Ru=CAr), 285.83 (Ru=CAr), 211.18, 155.06,

147.43, 138.90, 138.82, 136.89 (bs), 134.93, 131.73, 129.90, 106.70, 104.74, 59.25, 56.19, 52.35, 21.54, 19.50. Analytical data were in agreement with previously reported data.[12b]



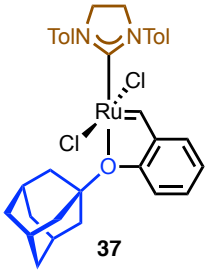
34

1-adamantyloxy/dipp catalyst (34): The title compound was prepared on a 0.2 mmol scale using the general chelation procedure and obtained as a green microcrystalline solid (103 mg, 64% yield, Method B). **^{1}H NMR** (500 MHz, CD_2Cl_2) δ 16.43 (s, 1H), 7.53 (t, *J* = 7.4 Hz, 2H), 7.43 (ddd, *J* = 8.8, 7.0, 2.1 Hz, 1H), 7.38 (d, *J* = 7.7 Hz, 4H), 7.26 (d, *J* = 8.4 Hz, 1H), 6.90–6.78 (m, 2H), 4.21 (s, 4H), 3.60 (s, 4H), 2.29 (s, 6H), 2.12 (s, 3H), 1.60 (s, 6H), 1.25 (d, *J* = 6.9 Hz, 24H); **^{13}C NMR** (125 MHz, CD_2Cl_2) δ 294.89 (Ru=CAr), 294.77 (Ru=CAr), 214.67, 152.51, 150.16, 146.33, 137.32 (bs), 130.17, 129.21, 124.78, 123.75, 122.40, 117.67, 89.17, 55.19 (bs), 41.49, 36.53, 32.46, 29.49, 27.19, 23.58; **HRMS** (FAB+) *m/z* Calcd for $C_{44}H_{59}Cl_2N_2ORu$ $[M+H]^+$ 803.3049, found 803.3036.



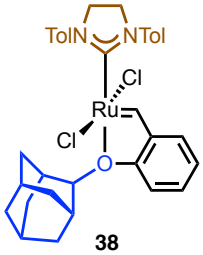
35

2-adamantyloxy/dipp catalyst (35): The title compound was prepared on a 0.2 mmol scale using the general chelation procedure and obtained as a green microcrystalline solid (67 mg, 42% yield, Method B). **^{1}H NMR** (500 MHz, CD_2Cl_2) δ 16.62 (s, 1H), 7.60–7.46 (m, 3H), 7.39 (d, *J* = 7.7 Hz, 4H), 6.90–6.83 (m, 1H), 6.80 (dd, *J* = 7.6, 1.8 Hz, 2H), 4.64 (s, 1H), 4.18 (s, 4H), 3.59 (s, 4H), 2.50 (s, 2H), 2.32 (d, *J* = 12.7 Hz, 2H), 1.82–1.55 (m, 9H), 1.35–1.01 (m, 25H); **^{13}C NMR** (125 MHz, CD_2Cl_2) δ 293.24 (Ru=CAr), 293.12 (Ru=CAr), 212.23, 154.33, 149.93, 144.36, 137.57 (bs), 130.39, 130.31, 125.07, 123.73, 122.96, 114.59, 88.55, 55.35 (bs), 38.29, 37.70, 31.67, 31.39, 29.46, 28.05, 27.55, 27.03, 23.79; **HRMS** (FAB+) *m/z* Calcd for $C_{44}H_{59}Cl_2N_2ORu$ $[M+H]^+$ 803.3049, found 803.3085.



37

1-adamantyloxy/*o*-tol catalyst (37): The title compound was prepared on a 0.2 mmol scale using the general chelation procedure and obtained as a green microcrystalline solid (53 mg, 40% yield, Method B). **^{1}H NMR** (500 MHz, CD_2Cl_2) δ 16.39 (s, 1H), 8.50 (s, 1H), 7.56–7.42 (m, 4H), 7.38 (s, 3H), 7.30 (d, *J* = 8.5 Hz, 2H), 6.86 (d, *J* = 5.3 Hz, 2H), 4.45–3.99 (m, 4H), 2.52 (s, 6H), 2.41–2.13 (m, 9H), 1.63 (s, 6H); **^{13}C NMR** (125 MHz, CD_2Cl_2) δ 297.91, 211.54, 152.62, 145.99, 142.64, 140.83, 139.24, 138.17, 131.92, 130.70, 129.48, 128.15, 127.62, 123.53, 122.44, 117.71, 88.71, 54.79 (bs), 52.71 (bs), 41.79, 36.55, 32.45, 19.78, 18.32; **HRMS** (FAB+) *m/z* Calcd for $C_{34}H_{38}Cl_2N_2ORu$ $[M]^+$ 662.1405, found 662.1437.



38

2-adamantyloxy/*o*-tol catalyst (40): The title compound was prepared on a 0.2 mmol scale using the general chelation procedure and obtained as a green microcrystalline solid (44 mg, 33% yield, Method B). **^{1}H NMR** (400 MHz, CD_2Cl_2) δ 16.57 (s, 1H), 8.27 (s, 1H), 7.63–7.17 (m, 8H), 6.98–6.74 (m, 3H), 4.69 (s, 1H), 4.20 (d, *J* = 143.8 Hz, 4H), 2.56 (s, 7H), 2.43–2.21 (m, 3H), 1.88–1.58 (m, 9H), 1.22–0.99 (m, 1H); **^{13}C NMR** (101 MHz, CD_2Cl2) δ 296.26, 209.09, 154.52, 143.98, 142.55, 140.59, 138.81, 137.57, 131.85, 131.05, 130.62, 130.26, 129.40, 128.05, 122.86, 114.44, 88.11, 52.95 (bs), 37.98, 37.60, 37.40, 31.66, 27.88, 27.34, 19.67, 18.36; **HRMS** (FAB+) *m/z* Calcd for $C_{34}H_{38}Cl_2N_2ORu$ $[M]^+$ 662.1405, found 662.1392.

Analysis of Collective Data

A positive correlation between the initiation rates and the benzylidenes ^{1}H NMR peaks (Figure **S6**) and a negative correlation between NHC ^{13}C NMR and the initiation rates are revealed in the data (Figure **S7**).

A weak positive correlation between the initiation rate and Ru–O bond length was found in the crystal structures (Figure **S8**). However, if the fast-initiating catalyst **27** is omitted, little or no correlation between the initiation rate and the Ru–O bond length would be obtained. As claimed in our earlier work, it seems that the Ru–O bond length would only be indicative of the fast initiation rate when it is exceptionally long, such as that of catalysts **15** (2.347 A) and **27** (2.394 A, entry 12, Table 3, main text). On the other hand, no correlation between the Ru=C bond length and the initiation rate was observed (Figure **S9**).

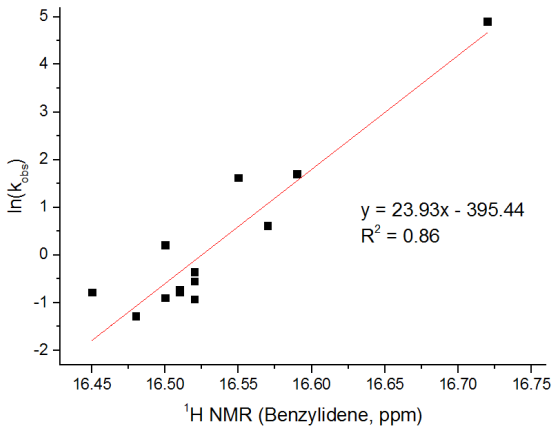


Figure S6: ln(k_{init}) vs. Benzylidene ^{1}H NMR Shift

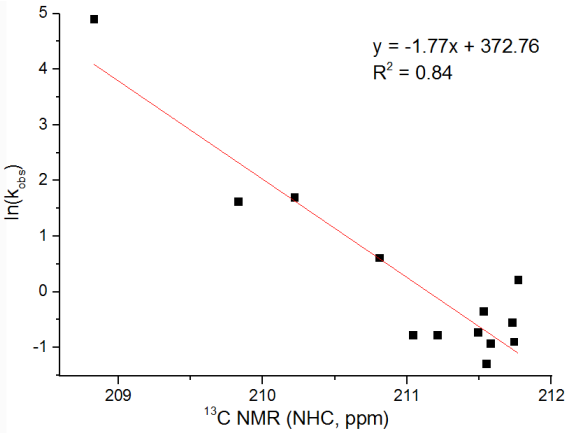


Figure S7: ln(k_{init}) vs. NHC ^{13}C NMR Shift

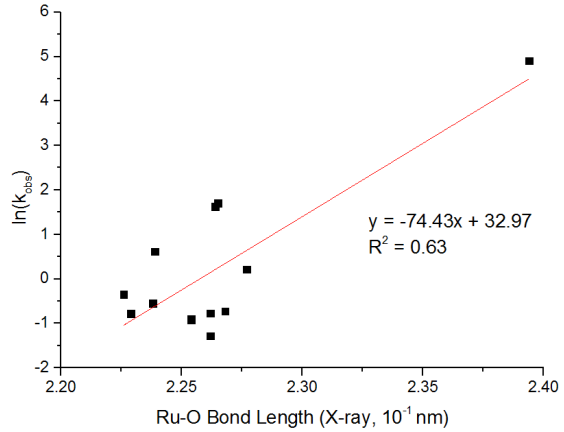


Figure S8: ln(k_{init}) vs. Ru–O Bond Length (X-ray)

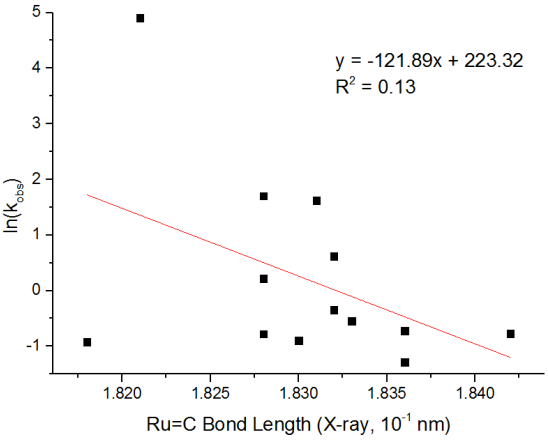


Figure S9: ln(k_{init}) vs. Ru=C Bond Length (X-ray)

X-RAY CRYSTALLOGRAPHY METHODS AND RESULTS

Table S2: Detailed summary of relevant Ru–O and Ru=C bond lengths from X-ray structures.

				Exp.(X-ray, Å)		
catalyst	**Ar =**	**R^1 =**	**R^2 =**	**Ru–O**	**Ru=C**	**CCDC**
16	Mes	Et	H	2.254(2)	1.818(3)	1825291
17	Mes	*n*-Pr	H	2.226(1)	1.832(1)	1825292
18	Mes	*t*-Butyl	H	2.274(1) 2.280(1)	1.828(1) 1.827(1)	1825279
19	Mes	*i*-Butyl	H	2.2388(9)	1.832(1)	1825280
20	Mes	Bn	H	2.2635(7)	1.831(1)	1825284
21	Mes	PhEt	H	2.229(3)	1.828(2)	1825287
22	Mes	*c*-Butyl	H	2.280(1) 2.244(2)	1.835(5) 1.836(2)	1825286
23	Mes	*c*-Pentyl	H	2.2383(9)	1.833(1)	1825275
24	Mes	*c*-Hexyl	H	2.268(2)	1.836(2)	1825289
25	Mes	*c*-Heptyl	H	2.254(1)	1.830(2)	1825278
26	Mes	*c*-Octyl	H	2.260(2) 2.263(2)	1.835(3) 1.848(3)	1825277
27	Mes	$CHCy_2$	H	2.394(2)	1.821(2)	1825288
28	Mes	CH_2-1-Ada	H	2.265(1)	1.828(3)	1825282
32	Mes	Methyl	OMe	2.218(1)	1.839(2)	1825290
33	Dipp	*i*-Propyl	H	2.2358(6) 2.2490(7)	1.832(1) 1.831(1)	1825276
34	Dipp	1-Ada	H	2.2486(9)	1.828(1)	1825281
35	Dipp	2-Ada	H	2.3233(8)	1.8294(8)	1825283
36	*o*-Tol	*i*-Propyl	H	2.298(1)	1.833(1)	635259
37	*o*-Tol	1-Ada	H	2.268(2)	1.827(2)	1825285
38	*o*-Tol	2-Ada	H	2.338(3)	1.828(4)	1825293

X-Ray Structure Determination

Low-temperature diffraction data (ϕ-and ω-scans) were collected on a Bruker AXS D8 VENTURE KAPPA diffractometer coupled to a PHOTON 100 CMOS detector with Cu K_α radiation (λ = 1.54178 Å) from an IμS micro-source for the structure of **16**. The structure was solved by direct methods using SHELXS[13] and refined against F^2 on all data by full-matrix least squares with SHELXL-2014[14] using established refinement techniques.[15] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the U value of the atoms they are linked to (1.5 times for methyl groups). Graphical representation of structures with 50% probability thermal ellipsoids was generated using Mercury visualization software.

16 crystallizes in the monoclinic space group $C2/c$ with one molecule in the asymmetric unit along with half a molecule of dichloromethane. The dichloromethane molecule is located near a crystallographic two-fold rotation axis. The dichloromethane did not strictly conform to the two-fold rotation. Therefore, it was disordered about the rotation axis and refined with the help of a similarity distance restraint on the carbon-chlorine distance.

Table S3. Crystal data and structure refinement for **16**.

Identification code	P16018	
Empirical formula	C30.50 H37 Cl3 N2 O Ru	
Formula weight	655.04	
Temperature	200(2) K	
Wavelength	1.54178 ≈	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 46.7355(14) ≈	α = 90∞.
	b = 8.5018(2) ≈	β = 98.7514(16)∞.
	c = 15.8550(4) ≈	γ = 90∞.
Volume	6226.4(3) ≈^{3}	
Z	8	
Density (calculated)	1.398 Mg/m^3	
Absorption coefficient	6.634 mm^{-1}	
F(000)	2696	
Crystal size	0.150 x 0.100 x 0.050 mm^3	
Theta range for data collection	1.913 to 74.818∞.	
Index ranges	-58<=h<=58, -10<=k<=10, -19<=l<=19	
Reflections collected	60726	
Independent reflections	6386 [R(int) = 0.0841]	

Completeness to theta = 67.679∞	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7538 and 0.6293
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6386 / 1 / 359
Goodness-of-fit on F^2	1.033
Final R indices [I>2sigma(I)]	R1 = 0.0372, wR2 = 0.0729
R indices (all data)	R1 = 0.0513, wR2 = 0.0778
Extinction coefficient	n/a
Largest diff. peak and hole	0.394 and -0.691 e.≈$^{-3}$

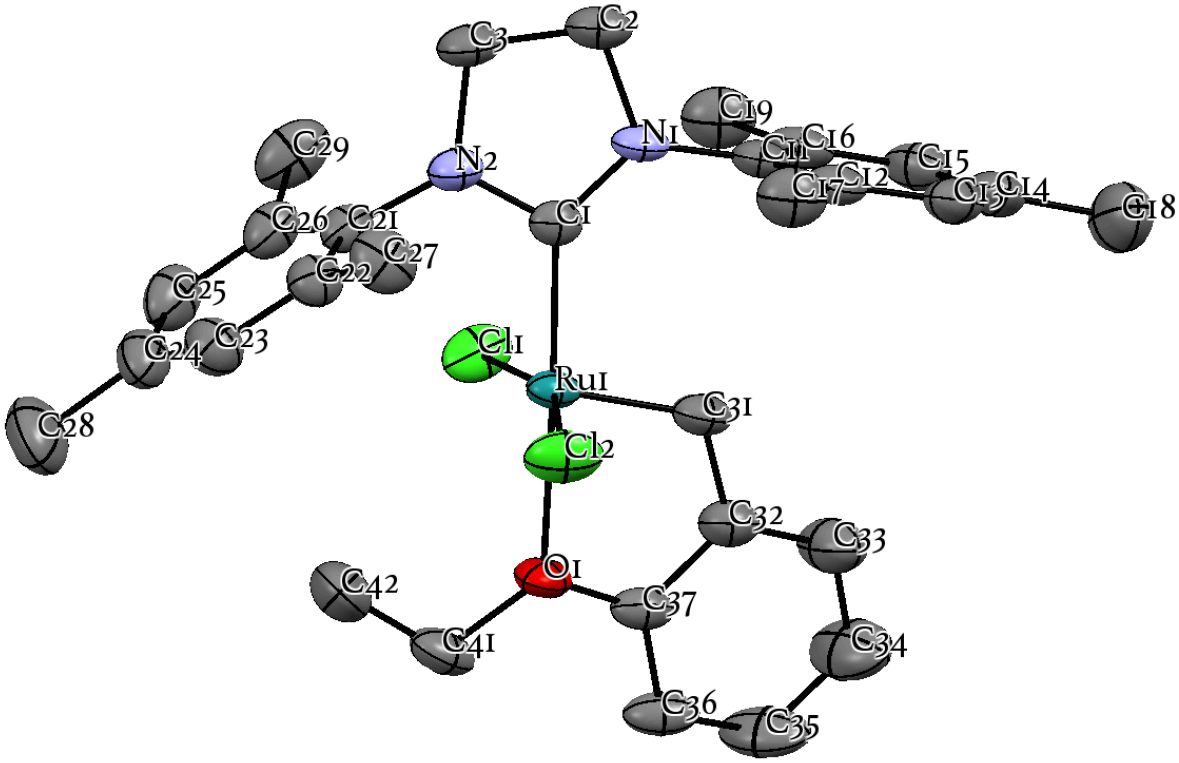


Figure S10: X-ray crystal structure of **16** with 50% probability ellipsoids. For clarity, hydrogen atoms and dichloromethane are omitted.

Low-temperature diffraction data (ϕ-and ω-scans) were collected on a Bruker Kappa diffractometer coupled to a Apex II CCD detector with graphite monochromated Mo K_α radiation (λ = 0.71073 Å) for the structure of compound **17**. The structure was solved by direct methods using SHELXS[13] and refined against F^2 on all data by full-matrix least squares with SHELXL-2013[14] using established refinement techniques.[15] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl groups). Graphical representation of structures with 50% probability thermal ellipsoids was generated using Mercury visualization software.

17 crystallizes in the monoclinic space group $P2_1/n$ with one molecule in the asymmetric unit.

Table S4. Crystal data and structure refinement for **17**.

Identification code	A14109	
Empirical formula	C31 H38 Cl2 N2 O Ru	
Formula weight	626.60	
Temperature	100(2) K	
Wavelength	0.71073 ≈	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 12.8981(10) ≈	α = 90∞.
	b = 11.0700(9) ≈	β = 99.745(4)∞.
	c = 20.9391(18) ≈	γ = 90∞.
Volume	2946.6(4) ≈3	
Z	4	
Density (calculated)	1.412 Mg/m3	
Absorption coefficient	0.740 mm-1	
F(000)	1296	
Crystal size	0.300 x 0.300 x 0.200 mm3	
Theta range for data collection	1.974 to 30.565∞.	
Index ranges	-18<=h<=18, -15<=k<=15, -29<=l<=29	
Reflections collected	55877	
Independent reflections	9002 [R(int) = 0.0385]	
Completeness to theta = 25.242∞	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6542	
Refinement method	Full-matrix least-squares on F2	

Data / restraints / parameters	9002 / 0 / 341
Goodness-of-fit on F^2	1.040
Final R indices [I>2sigma(I)]	R1 = 0.0246, wR2 = 0.0594
R indices (all data)	R1 = 0.0289, wR2 = 0.0617
Extinction coefficient	n/a
Largest diff. peak and hole	0.765 and -0.389 e.$\approx^{-3}$

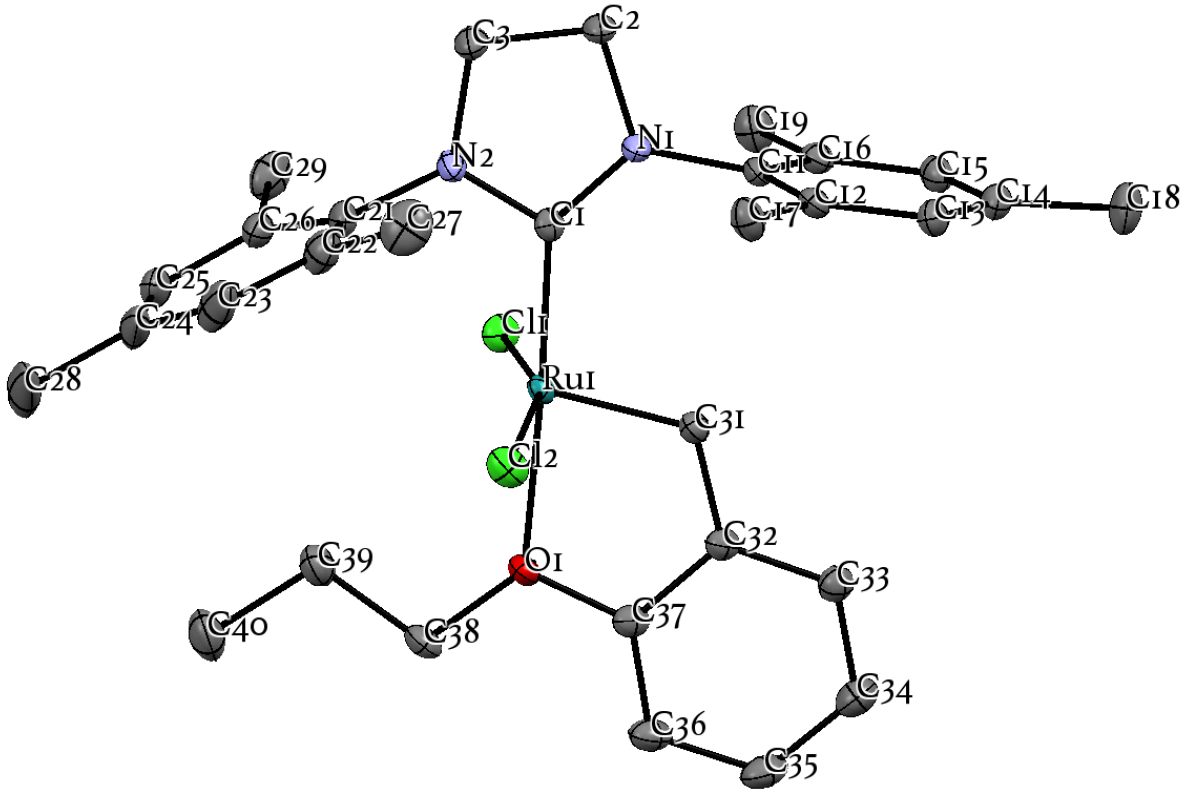


Figure S11: X-ray crystal structure of **17** with 50% probability ellipsoids. For clarity, hydrogen atoms are omitted.

Low-temperature diffraction data (ϕ-and ω-scans) were collected on a Bruker AXS KAPPA APEX II diffractometer coupled to a APEX II CCD detector with graphite monochromated Mo K_α radiation (λ = 0.71073 Å) for the structure of compound **18**. The structure was solved by direct methods using SHELXS[13] and refined against F^2 on all data by full-matrix least squares with SHELXL-2014[14] using established refinement techniques.[15] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the U value of the atoms they are linked to (1.5 times for methyl groups). Graphical representation of structures with 50% probability thermal ellipsoids was generated using Mercury visualization software.

18 crystallizes in the monoclinic space group $P2_1/n$ with two molecules in the asymmetric unit along with two molecules of dichloromethane.

Table S5. Crystal data and structure refinement for **18**.

Identification code	A15026	
Empirical formula	C33 H42 Cl4 N2 O Ru	
Formula weight	725.55	
Temperature	100(2) K	
Wavelength	0.71073 ≈	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 20.3523(12) ≈	α = 90∞.
	b = 14.3896(9) ≈	β = 98.786(3)∞.
	c = 23.6323(15) ≈	γ = 90∞.
Volume	6839.8(7) ≈^{3}	
Z	8	
Density (calculated)	1.409 Mg/m^3	
Absorption coefficient	0.799 mm^{-1}	
F(000)	2992	
Crystal size	0.500 x 0.400 x 0.300 mm^3	
Theta range for data collection	1.740 to 36.390∞.	
Index ranges	-33<=h<=33, -24<=k<=24, -39<=l<=39	
Reflections collected	204312	
Independent reflections	33268 [R(int) = 0.0519]	
Completeness to theta = 25.242∞	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7471 and 0.6939	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	33268 / 0 / 757
Goodness-of-fit on F^2	1.035
Final R indices [I>2sigma(I)]	R1 = 0.0357, wR2 = 0.0716
R indices (all data)	R1 = 0.0587, wR2 = 0.0803
Extinction coefficient	n/a
Largest diff. peak and hole	0.964 and -0.592 e.$\approx^{-3}$

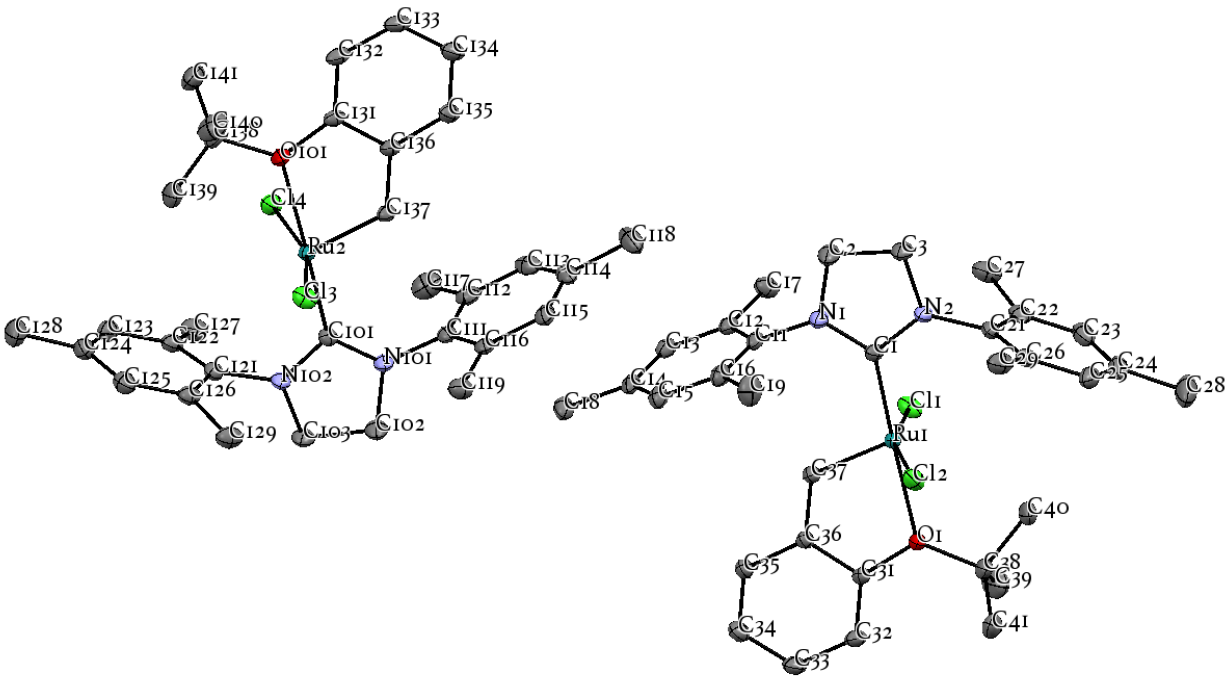


Figure S12: X-ray crystal structure of **18** with 50% probability ellipsoids. Two crystallographically inequivalent molecules are present in the unit cell; for clarity, hydrogen atoms and dichloromethane are omitted.

Low-temperature diffraction data (ϕ-and ω-scans) were collected on a Bruker Kappa diffractometer coupled to a Apex II CCD detector with graphite monochromated Mo K_α radiation (λ = 0.71073 Å) for the structure of compound **19**. The structure was solved by direct methods using SHELXS[13] and refined against F^2 on all data by full-matrix least squares with SHELXL-2013[14] using established refinement techniques.[15] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl groups). Graphical representation of structures with 50% probability thermal ellipsoids was generated using Mercury visualization software.

19 crystallizes in the orthorhombic space group *Pbcn* with one molecule in the asymmetric unit along with two and a half molecules of benzene. The half molecule of benzene is located about a two-fold rotation axis.

Table S6. Crystal data and structure refinement for **19**.

Identification code	A14175	
Empirical formula	C47 H55 Cl2 N2 O Ru	
Formula weight	835.90	
Temperature	100(2) K	
Wavelength	0.71073 ≈	
Crystal system	Orthorhombic	
Space group	P b c n	
Unit cell dimensions	a = 14.0951(7) ≈	α = 90∞.
	b = 23.0099(13) ≈	β = 90∞.
	c = 26.1818(15) ≈	γ = 90∞.
Volume	8491.5(8) ≈^{3}	
Z	8	
Density (calculated)	1.308 Mg/m^3	
Absorption coefficient	0.532 mm^{-1}	
F(000)	3496	
Crystal size	0.500 x 0.300 x 0.100 mm^3	
Theta range for data collection	1.556 to 36.382∞.	
Index ranges	-23<=h<=23, -32<=k<=38, -35<=l<=43	
Reflections collected	195657	
Independent reflections	20674 [R(int) = 0.0607]	
Completeness to theta = 25.242∞	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7471 and 0.6541	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	20674 / 0 / 486
Goodness-of-fit on F^2	1.067
Final R indices [I>2sigma(I)]	R1 = 0.0332, wR2 = 0.0770
R indices (all data)	R1 = 0.0579, wR2 = 0.0917
Extinction coefficient	n/a
Largest diff. peak and hole	0.814 and -0.719 e.$\approx^{-3}$

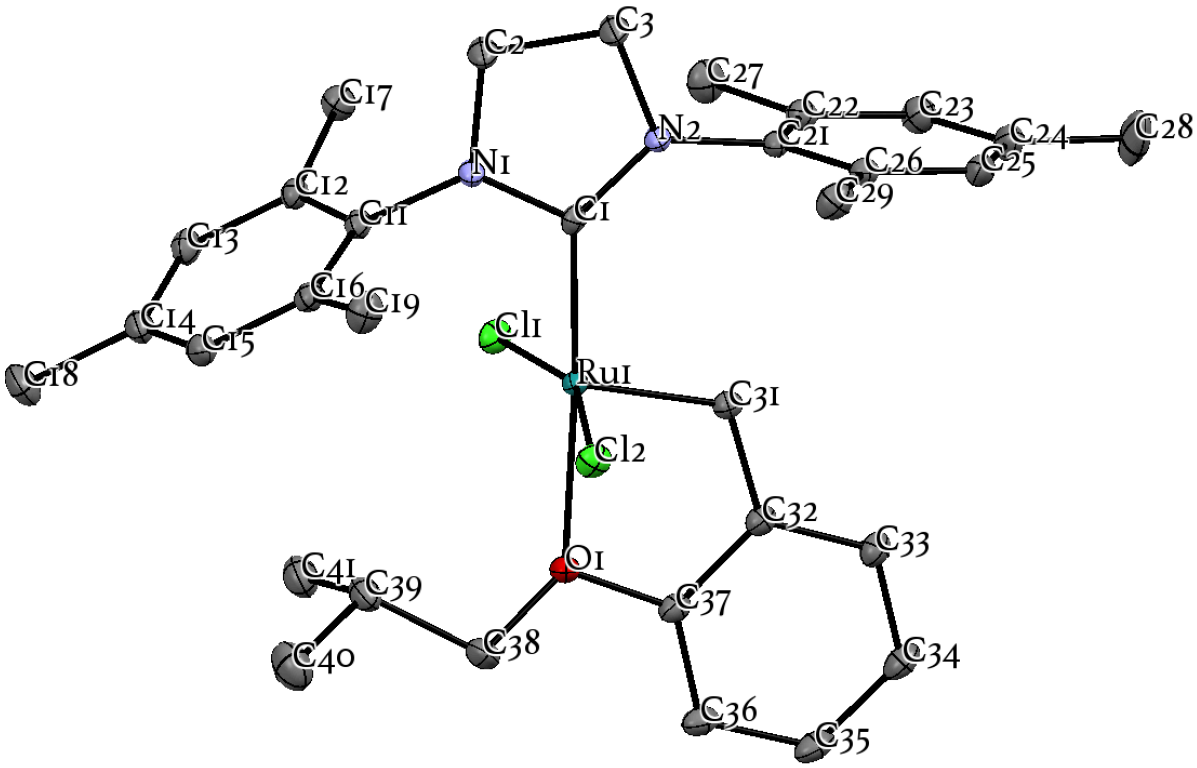


Figure S13: X-ray crystal structure of **19** with 50% probability ellipsoids. For clarity, hydrogen atoms and benzene are omitted.

Crystals were mounted on polyimide MiTeGen loops with STP Oil Treatment and placed under a nitrogen stream. Low temperature (100K) X-ray data were obtained with a Bruker AXS KAPPA APEX II diffractometer running at 50kV and 30mA (Mo K_α = 0.71073 Å; APEX II CCD detector equipped with a graphite monochromator. All diffractometer manipulations, including data collection, integration, and scaling were carried out using the Bruker APEX2 software.[16] Absorption corrections were applied using SADABS.[17] Space groups were determined on the basis of systematic absences and intensity statistics and the structures were solved by intrinsic phasing using XT and refined by full-matrix least squares on F^2 using XL.[14] All non-hydrogen atoms were refined using anisotropic displacement parameters. Hydrogen atoms were placed in idealized positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed at 1.2 times (1.5 times for methyl groups) the U_{eq} value of the bonded atom. Graphical representation of structures with 50% probability thermal ellipsoids was generated using Mercury visualization software.

Compound **20** crystallizes in the monoclinic space group $P2_1/c$ with one molecule and one half a molecule of benzene (on a center) in the asymmetric unit. The benzyl group is disordered over two positions with an 88:12 ratio.

Table S7. Crystal data and structure refinement for **20**.

Identification code	a14036	
Empirical formula	C38 H41 Cl2 N2 O Ru	
Formula weight	713.70	
Temperature	100 K	
Wavelength	0.71073 ≈	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 22.2405(10) ≈	α = 90∞
	b = 11.1477(5) ≈	β = 91.974(2)∞
	c = 13.6169(7) ≈	γ = 90∞
Volume	3374.0(3) ≈^{3}	
Z	4	
Density (calculated)	1.405 Mg/m^3	
Absorption coefficient	0.656 mm^{-1}	
F(000)	1476	
Crystal size	0.27 x 0.26 x 0.05 mm^3	
Theta range for data collection	1.832 to 43.981∞.	
Index ranges	-37<=h<=43, -21<=k<=21, -26<=l<=26	
Reflections collected	193890	
Independent reflections	26134 [R(int) = 0.0638]	

Completeness to theta = 25.000∞	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.8855
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	26134 / 15 / 432
Goodness-of-fit on F^2	1.006
Final R indices [I>2sigma(I)]	R1 = 0.0390, wR2 = 0.0742
R indices (all data)	R1 = 0.0726, wR2 = 0.0842
Extinction coefficient	n/a
Largest diff. peak and hole	1.149 and -0.966 e.≈$^{-3}$

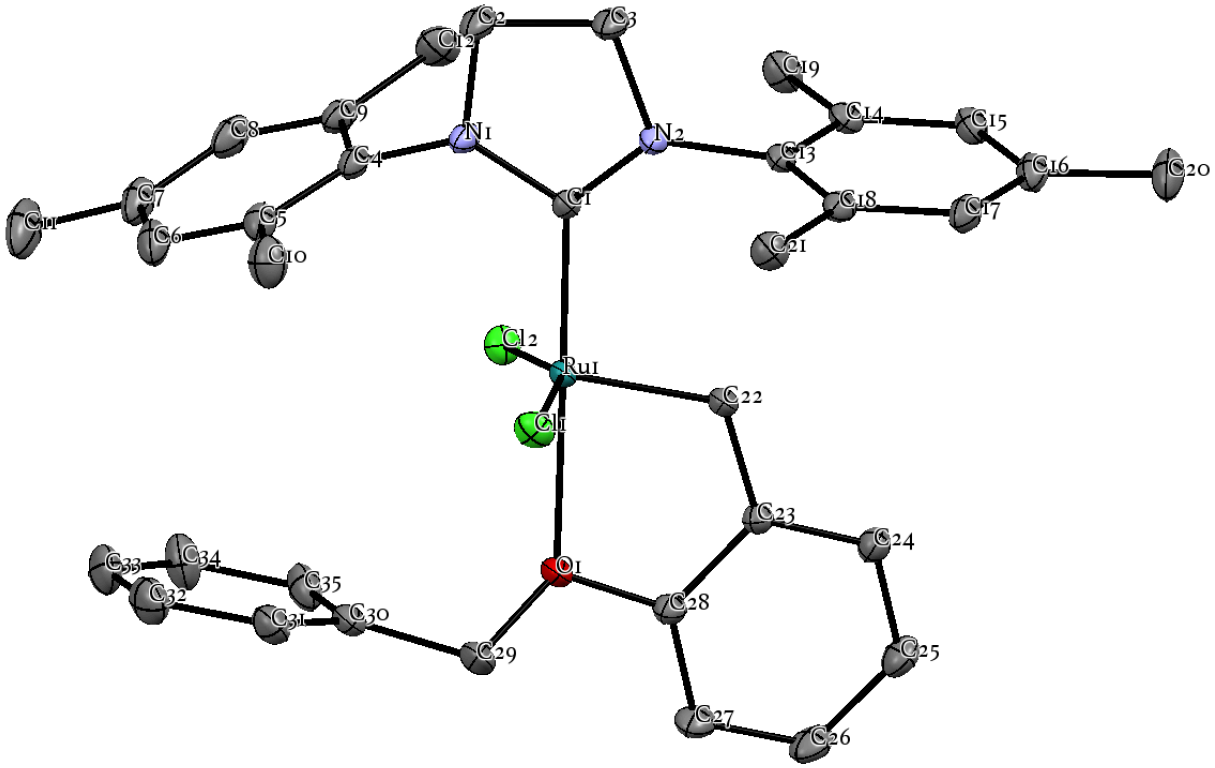


Figure S14: X-ray crystal structure of **20** with 50% probability ellipsoids. For clarity, hydrogen atoms and benzene are omitted.

Crystals were mounted on polyimide MiTeGen loops with STP Oil Treatment and placed under a nitrogen stream. Low temperature (100K) X-ray data were obtained with a Bruker AXS KAPPA APEX II diffractometer running at 50kV and 30mA (Mo K_α = 0.71073 Å; APEX II CCD detector equipped with a graphite monochromator. All diffractometer manipulations, including data collection, integration, and scaling were carried out using the Bruker APEX2 software.[16] Absorption corrections were applied using SADABS.[17] Space groups were determined on the basis of systematic absences and intensity statistics and the structures were solved by intrinsic phasing using XT and refined by full-matrix least squares on F^2 using XL.[14] All non-hydrogen atoms were refined using anisotropic displacement parameters. Hydrogen atoms were placed in idealized positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed at 1.2 times (1.5 times for methyl groups) the U_{eq} value of the bonded atom. Graphical representation of structures with 50% probability thermal ellipsoids was generated using Mercury visualization software.

Compound **21** crystallizes in the monoclinic space group $P2_1/n$ with one molecule in the asymmetric unit. The ruthenium, both chlorines, and the benzyl CH_2 carbon were disordered over two positions with a 78:22 ratio.

Table S8. Crystal data and structure refinement for **21.**

Identification code	a14170	
Empirical formula	C36 H40 Cl2 N2 O Ru	
Formula weight	688.67	
Temperature	100.15 K	
Wavelength	0.71073 ≈	
Crystal system	Monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 15.3743(5) ≈	α = 90∞
	b = 13.6512(4) ≈	β = 106.7820(18)∞
	c = 16.2548(5) ≈	γ = 90∞
Volume	3266.22(18) ≈^{3}	
Z	4	
Density (calculated)	1.400 Mg/m^3	
Absorption coefficient	0.674 mm^{-1}	
F(000)	1424	
Crystal size	0.47 x 0.36 x 0.04 mm^3	
Theta range for data collection	1.606 to 37.478∞.	
Index ranges	-26<=h<=26, -23<=k<=23, -27<=l<=26	
Reflections collected	162917	
Independent reflections	16536 [R(int) = 0.0530]	

Completeness to theta = 25.000∞	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.8180
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	16536 / 0 / 577
Goodness-of-fit on F^2	1.425
Final R indices [I>2sigma(I)]	R1 = 0.0322, wR2 = 0.0731
R indices (all data)	R1 = 0.0542, wR2 = 0.0799
Extinction coefficient	n/a
Largest diff. peak and hole	0.858 and -0.881 e.≈$^{-3}$

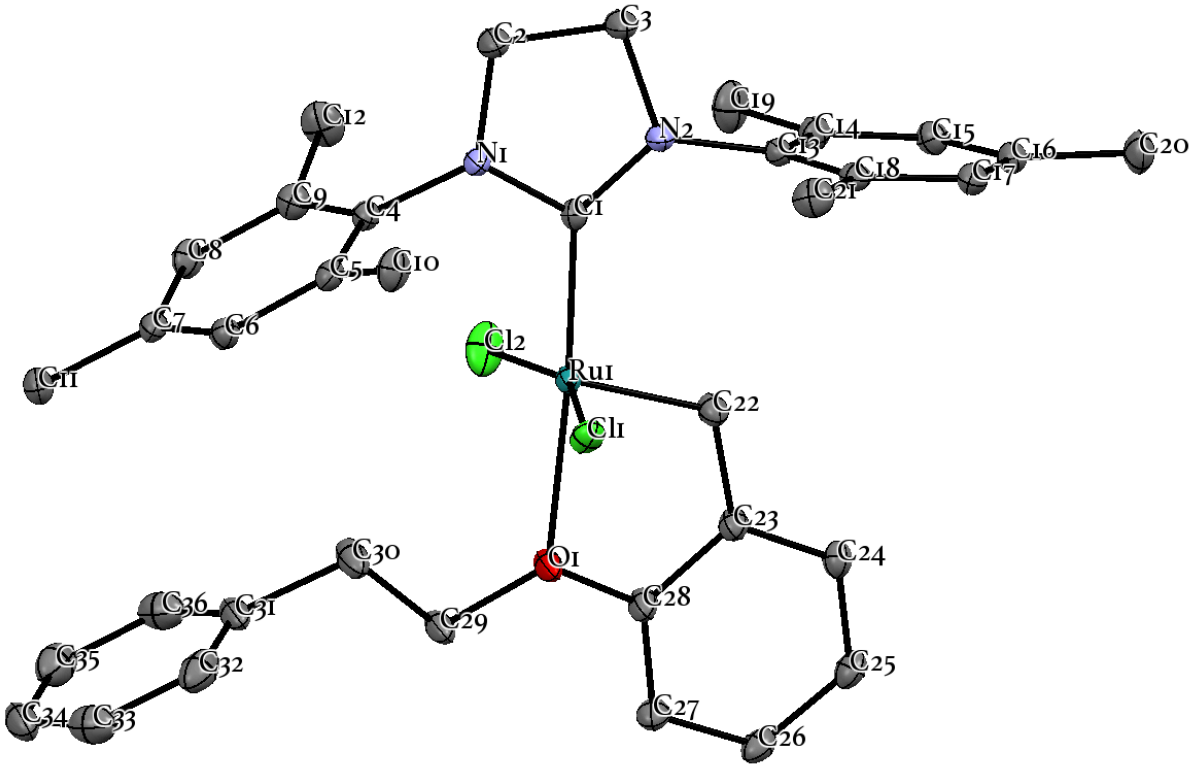


Figure S15: X-ray crystal structure of **21** with 50% probability ellipsoids. For clarity, hydrogen atoms are omitted.

Low-temperature diffraction data (ϕ-and ω-scans) were collected on a Bruker Kappa diffractometer coupled to a Apex II CCD detector with graphite monochromated Mo K_α radiation (λ = 0.71073 Å) for the structure of **22**. The structure was solved by direct methods using SHELXS[13] and refined against F^2 on all data by full-matrix least squares with SHELXL-2013[14] using established refinement techniques.[15] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl groups). All disordered atoms were refined with the help of similarity restraints on the 1,2- and 1,3- distances and displacement parameters as well as rigid bond restraints for anisotropic displacement parameters. Graphical representation of structures with 50% probability thermal ellipsoids was generated using Mercury visualization software.

22 crystallizes in the triclinic space group *P*-1 with two molecules in the asymmetric unit along with 3.572 molecules of benzene and 0.428 molecules of pentane at four unique positions. The second molecule (Ru2) is partially disordered. The ellipsoids for many atoms in the second molecule were elongated and the highest residual electron density maxima were located near the Ru and Cl atoms at positions consistent with a second component. Half of the second molecule was modeled as a two-part disorder. One of the four solvent positions was modeled as a mixture of 0.572(3) molecules of benzene and 0.428(3) molecules of pentane.

Table S9. Crystal data and structure refinement for **22**.

Identification code	A13168	
Empirical formula	C43.78 H51.30 Cl2 N2 O Ru	
Formula weight	793.53	
Temperature	100(2) K	
Wavelength	0.71073 ≈	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 13.917(2) ≈	α = 80.167(2)∞.
	b = 14.408(2) ≈	β = 73.341(2)∞.
	c = 21.533(3) ≈	γ = 75.237(2)∞.
Volume	3977.5(10) ≈^{3}	
Z	4	
Density (calculated)	1.325 Mg/m^3	
Absorption coefficient	0.563 mm^{-1}	
F(000)	1656	
Crystal size	0.250 x 0.250 x 0.200 mm^3	
Theta range for data collection	1.470 to 30.560∞.	
Index ranges	-19<=h<=19, -20<=k<=20, -30<=l<=30	

Reflections collected	115691
Independent reflections	24211 [R(int) = 0.0373]
Completeness to theta = 25.242∞	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7461 and 0.7017
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	24211 / 833 / 1085
Goodness-of-fit on F^2	1.018
Final R indices [I>2sigma(I)]	R1 = 0.0317, wR2 = 0.0751
R indices (all data)	R1 = 0.0428, wR2 = 0.0816
Extinction coefficient	n/a
Largest diff. peak and hole	1.159 and -0.429 e.≈$^{-3}$

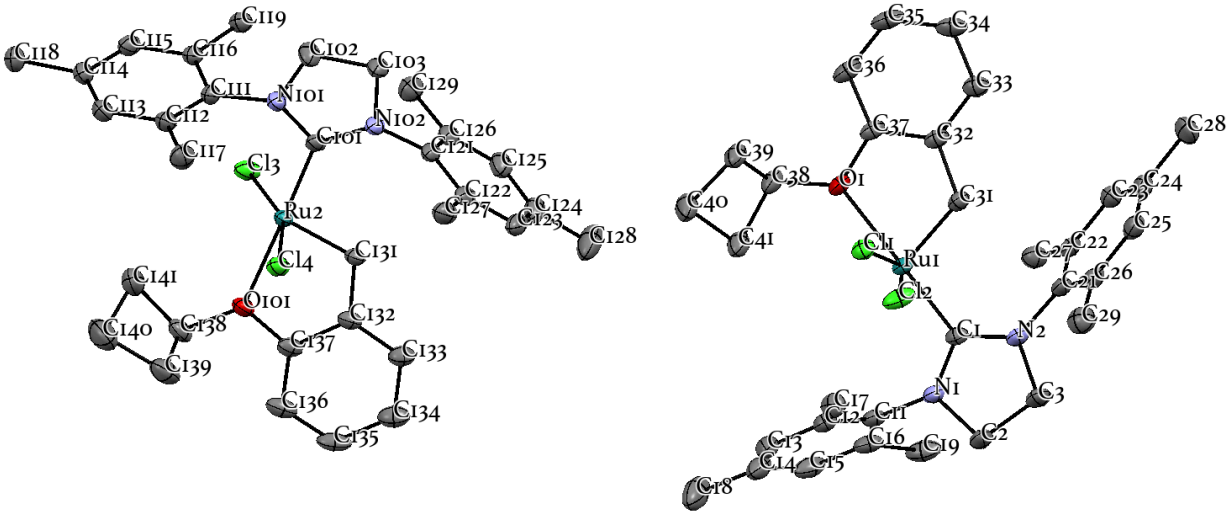


Figure S16. X-ray crystal structure of **22** with 50% probability ellipsoids. Two crystallographically equivalent molecules are present in the unit cell; for clarity, hydrogen atoms and benzene are omitted.

Low-temperature diffraction data (ϕ-and ω-scans) were collected on a Bruker AXS KAPPA APEX II diffractometer coupled to an APEX II CCD detector with graphite monochromated Mo K_α radiation (λ = 0.71073 Å) for the structure of **23**. The structure was solved by direct methods using SHELXS[13] and refined against F^2 on all data by full-matrix least squares with SHELXL-2014[14] using established refinement techniques.[15] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl groups). All disordered atoms were refined with the help of similarity restraints on the 1,2- and 1,3-distances and displacement parameters as well as rigid bond restraints for anisotropic displacement parameters. Graphical representation of structures with 50% probability thermal ellipsoids was generated using Mercury visualization software.

23 crystallizes in the monoclinic space group *C*2/*c* with one molecule in the asymmetric unit along with half a molecule of pentane. One atom in the cyclopentyl group was disordered over two positions. The pentane molecule is located near a crystallographic inversion center and disordered appropriately.

Table S10. Crystal data and structure refinement for **23**.

Identification code	A13195	
Empirical formula	C35.50 H46 Cl2 N2 O Ru	
Formula weight	688.71	
Temperature	100(2) K	
Wavelength	0.71073 ≈	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 29.3054(10) ≈	α = 90∞.
	b = 15.4122(5) ≈	β = 125.1577(15)∞.
	c = 17.7368(6) ≈	γ = 90∞.
Volume	6549.6(4) ≈^{3}	
Z	8	
Density (calculated)	1.397 Mg/m^3	
Absorption coefficient	0.672 mm^{-1}	
F(000)	2872	
Crystal size	0.600 x 0.400 x 0.300 mm^3	
Theta range for data collection	1.571 to 36.412∞.	
Index ranges	-48<=h<=48, -25<=k<=25, -29<=l<=29	
Reflections collected	250815	
Independent reflections	15972 [R(int) = 0.0362]	

Completeness to theta = 25.242∞	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7471 and 0.6539
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	15972 / 9 / 413
Goodness-of-fit on F^2	1.118
Final R indices [I>2sigma(I)]	R1 = 0.0347, wR2 = 0.0730
R indices (all data)	R1 = 0.0471, wR2 = 0.0850
Extinction coefficient	n/a
Largest diff. peak and hole	1.717 and -0.735 e.≈$^{-3}$

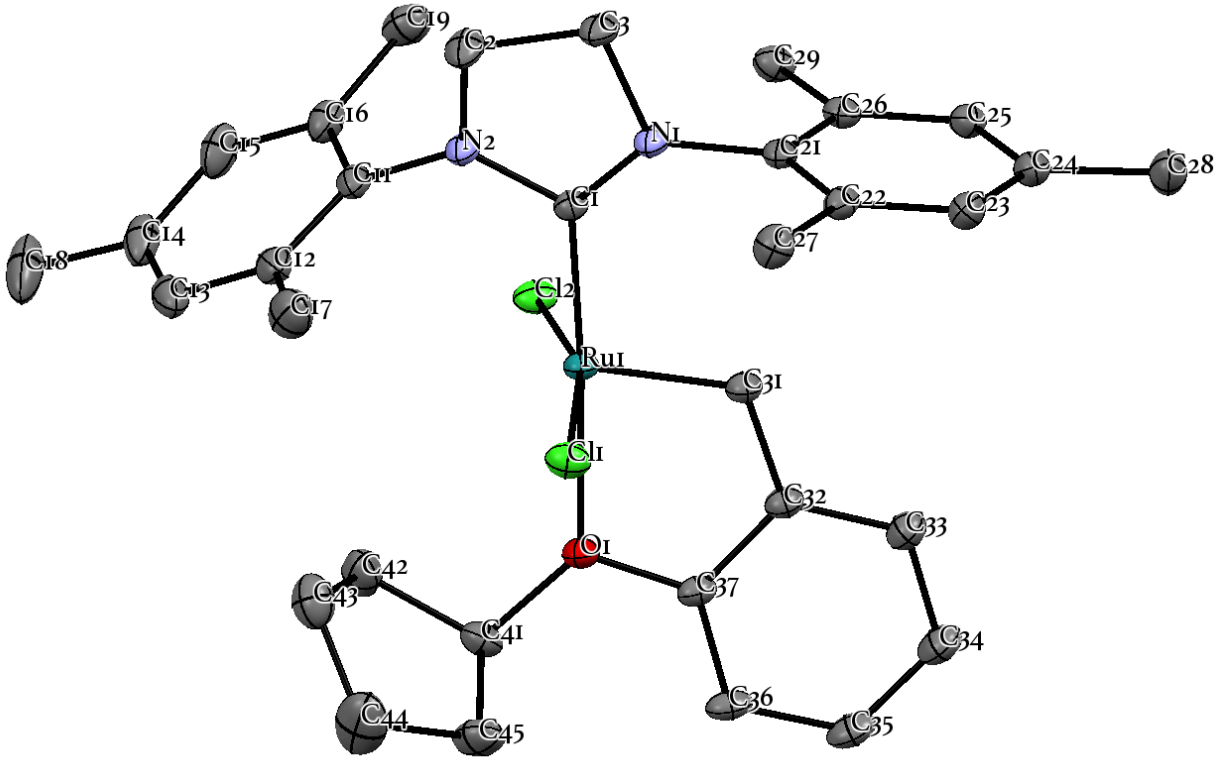


Figure S17. X-ray crystal structure of **23** with 50% probability ellipsoids. For clarity, hydrogen atoms and pentane are omitted.

Low-temperature diffraction data (ϕ-and ω-scans) were collected on a Bruker three-circle diffractometer coupled to a Bruker Smart 1000 CCD detector with graphite monochromated Mo K_α radiation (λ = 0.71073 Å) for the structure of **24**. The structure was solved by direct methods using SHELXS[13] and refined against F^2 on all data by full-matrix least squares with SHELXL-2013[14] using established refinement techniques.[15] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the U value of the atoms they are linked to (1.5 times for methyl groups). Graphical representation of structures with 50% probability thermal ellipsoids was generated using Mercury visualization software.

24 crystallizes in the monoclinic space group $P2_1/n$ with one molecule in the asymmetric unit along with one molecule of dichloromethane.

Table S11. Crystal data and structure refinement for **24**.

Identification code	S13028	
Empirical formula	C35 H44 Cl4 N2 O Ru	
Formula weight	751.59	
Temperature	100(2) K	
Wavelength	0.71073 ≈	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 13.5741(7) ≈	α = 90∞.
	b = 10.3883(5) ≈	β = 91.995(3)∞.
	c = 24.5146(13) ≈	γ = 90∞.
Volume	3454.8(3) ≈^{3}	
Z	4	
Density (calculated)	1.445 Mg/m^3	
Absorption coefficient	0.794 mm^{-1}	
F(000)	1552	
Crystal size	0.400 x 0.300 x 0.070 mm^3	
Theta range for data collection	1.662 to 30.596∞.	
Index ranges	-19<=h<=19, -14<=k<=14, -34<=l<=35	
Reflections collected	73040	
Independent reflections	10584 [R(int) = 0.0418]	
Completeness to theta = 25.242∞	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6303	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10584 / 0 / 394
Goodness-of-fit on F^2	1.152
Final R indices [I>2sigma(I)]	R1 = 0.0399, wR2 = 0.0909
R indices (all data)	R1 = 0.0497, wR2 = 0.0969
Extinction coefficient	n/a
Largest diff. peak and hole	1.827 and -0.803 e.$\approx^{-3}$

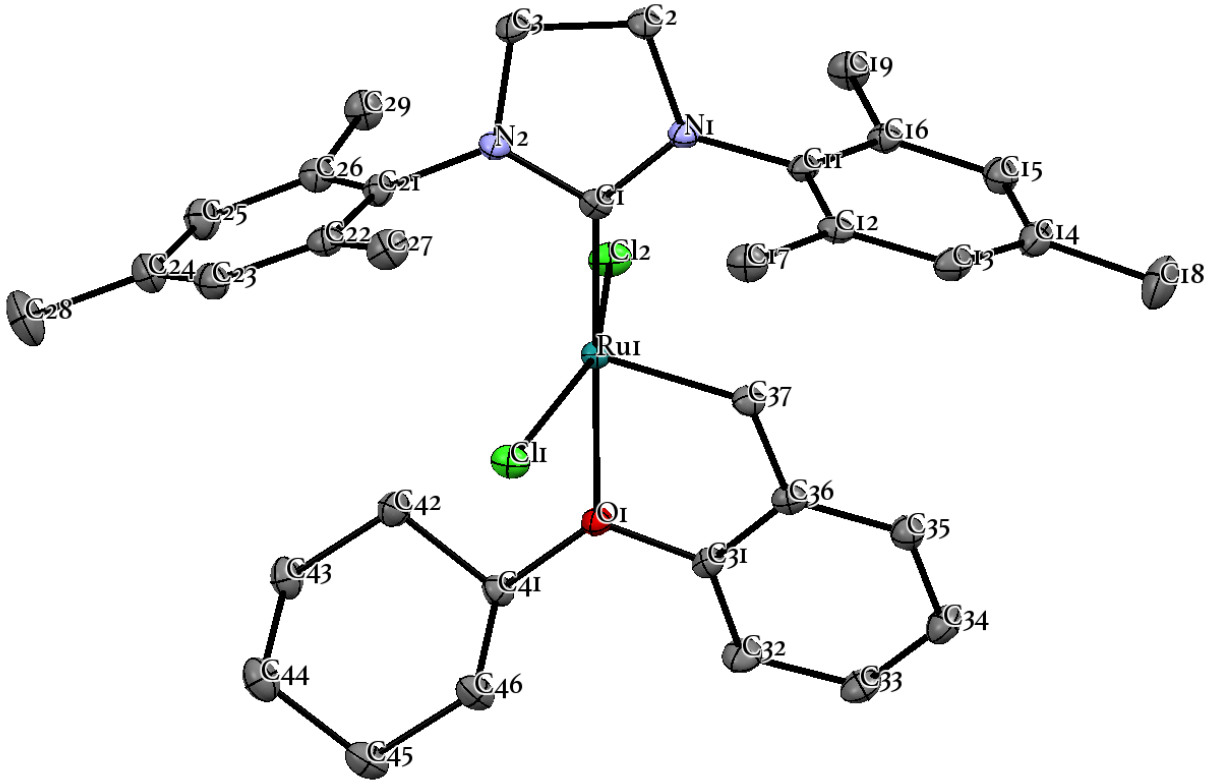


Figure S18. X-ray crystal structure of **24** with 50% probability ellipsoids. For clarity, hydrogen atoms and dichloromethane are omitted.

Low-temperature diffraction data (ϕ-and ω-scans) were collected on a Bruker AXS KAPPA APEX II diffractometer coupled to an APEX II CCD detector with graphite monochromated Mo K_α radiation (λ = 0.71073 Å) for the structure of **25**. The structure was solved by direct methods using SHELXS[13] and refined against F^2 on all data by full-matrix least squares with SHELXL-2014[14] using established refinement techniques.[15] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the U value of the atoms they are linked to (1.5 times for methyl groups). All disordered atoms were refined with the help of similarity restraints on the 1,2- and 1,3-distances and displacement parameters as well as rigid bond restraints for anisotropic displacement parameters. Graphical representation of structures with 50% probability thermal ellipsoids was generated using Mercury visualization software.

25 crystallizes in the monoclinic space group $P2_1/n$ with one molecule in the asymmetric unit along with one molecule of benzene. The N-heterocyclic carbene was modeled as a two component disorder.

Table S12. Crystal data and structure refinement for **25**.

Identification code	A13157	
Empirical formula	C41 H50 Cl2 N2 O Ru	
Formula weight	758.80	
Temperature	100(2) K	
Wavelength	0.71073 ≈	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 13.3139(5) ≈	α = 90∞.
	b = 10.3981(3) ≈	β = 91.215(2)∞.
	c = 27.1206(10) ≈	γ = 90∞.
Volume	3753.7(2) ≈^{3}	
Z	4	
Density (calculated)	1.343 Mg/m^3	
Absorption coefficient	0.594 mm^{-1}	
F(000)	1584	
Crystal size	0.200 x 0.180 x 0.170 mm^3	
Theta range for data collection	1.502 to 36.379∞.	
Index ranges	-22<=h<=22, -17<=k<=17, -45<=l<=45	
Reflections collected	210943	
Independent reflections	18268 [R(int) = 0.0641]	
Completeness to theta = 25.242∞	100.0 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7471 and 0.6904
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	18268 / 1485 / 644
Goodness-of-fit on F^2	1.113
Final R indices [I>2sigma(I)]	R1 = 0.0388, wR2 = 0.0779
R indices (all data)	R1 = 0.0571, wR2 = 0.0839
Extinction coefficient	n/a
Largest diff. peak and hole	0.917 and -1.416 e.$\approx^{-3}$

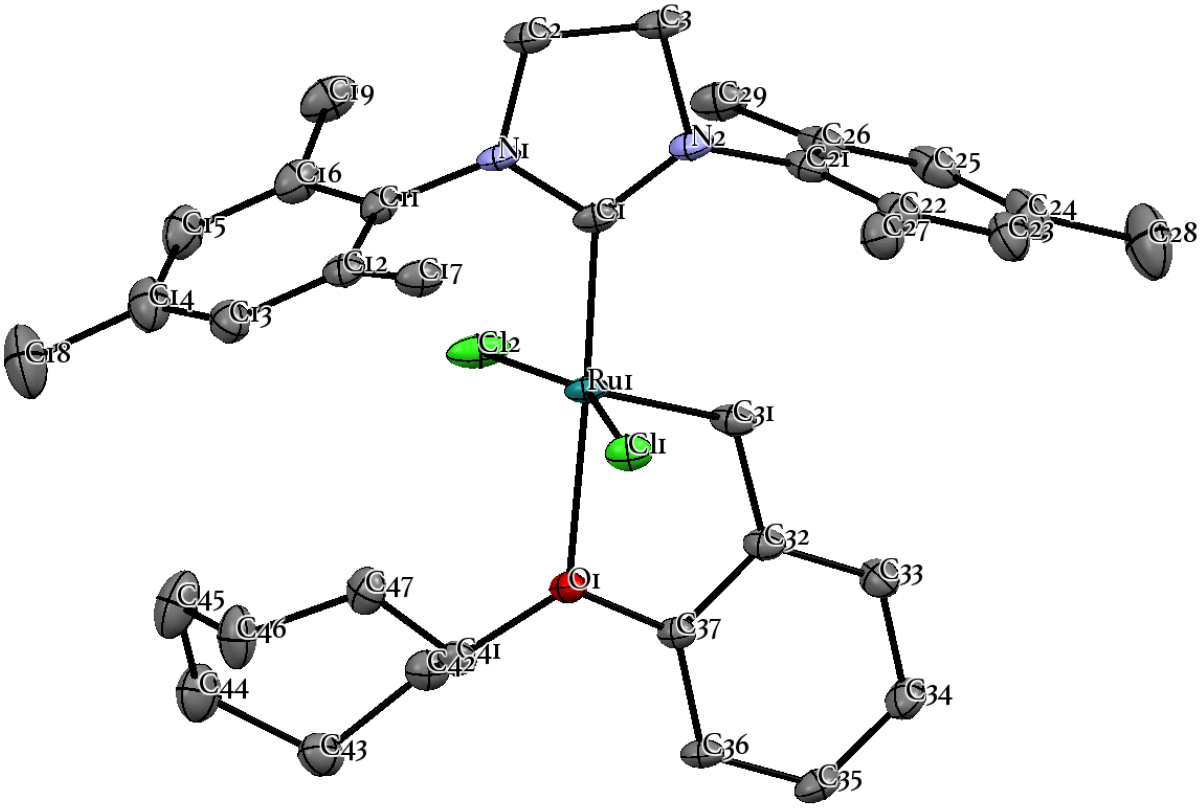


Figure S19. X-ray crystal structure of **25** with 50% probability ellipsoids. For clarity, hydrogen atoms and benzene are omitted.

Low-temperature diffraction data (ϕ-and ω-scans) were collected on a Bruker three-circle diffractometer coupled to a Bruker Smart 1000 CCD detector with graphite monochromated Mo K_α radiation (λ = 0.71073 Å) for the structure of **26**. The structure was solved by direct methods using SHELXS[13] and refined against F^2 on all data by full-matrix least squares with SHELXL-2014[14] using established refinement techniques.[15] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the U value of the atoms they are linked to (1.5 times for methyl groups). All disordered atoms were refined with the help of similarity restraints on the 1,2- and 1,3-distances and displacement parameters as well as enhanced rigid bond restraints for anisotropic displacement parameters. Graphical representation of structures with 50% probability thermal ellipsoids was generated using Mercury visualization software.

26 crystallizes in the monoclinic space group $P2_1/c$ with two molecules in the asymmetric unit along with two molecules of benzene. The highest electron density maxima are located near the Ru atoms. A portion of the cyclooctane group is disordered over two positions in both molecules and in one molecule one of the aryl groups is disordered over two positions. Both molecules of benzene were modeled as two component disorders. In addition to the above restraints, all disordered benzene molecules were restrained to be flat.

Table S13. Crystal data and structure refinement for **26**.

Identification code	S13032	
Empirical formula	C42 H52 Cl2 N2 O Ru	
Formula weight	772.82	
Temperature	100(2) K	
Wavelength	0.71073 ≈	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 26.6283(11) ≈	α = 90∞.
	b = 10.7110(5) ≈	β = 116.1997(19)∞.
	c = 29.9319(13) ≈	γ = 90∞.
Volume	7660.0(6) ≈^{3}	
Z	8	
Density (calculated)	1.340 Mg/m^3	
Absorption coefficient	0.583 mm^{-1}	
F(000)	3232	
Crystal size	0.400 x 0.340 x 0.220 mm^3	
Theta range for data collection	0.852 to 30.640∞.	
Index ranges	-37<=h<=38, -15<=k<=15, -42<=l<=42	
Reflections collected	220720	

Independent reflections	23406 [R(int) = 0.0988]
Completeness to theta = 25.242∞	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7461 and 0.6750
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	23406 / 2164 / 1122
Goodness-of-fit on F^2	1.070
Final R indices [I>2sigma(I)]	R1 = 0.0694, wR2 = 0.1719
R indices (all data)	R1 = 0.1129, wR2 = 0.1998
Extinction coefficient	n/a
Largest diff. peak and hole	5.620 and -2.377 e.≈$^{-3}$

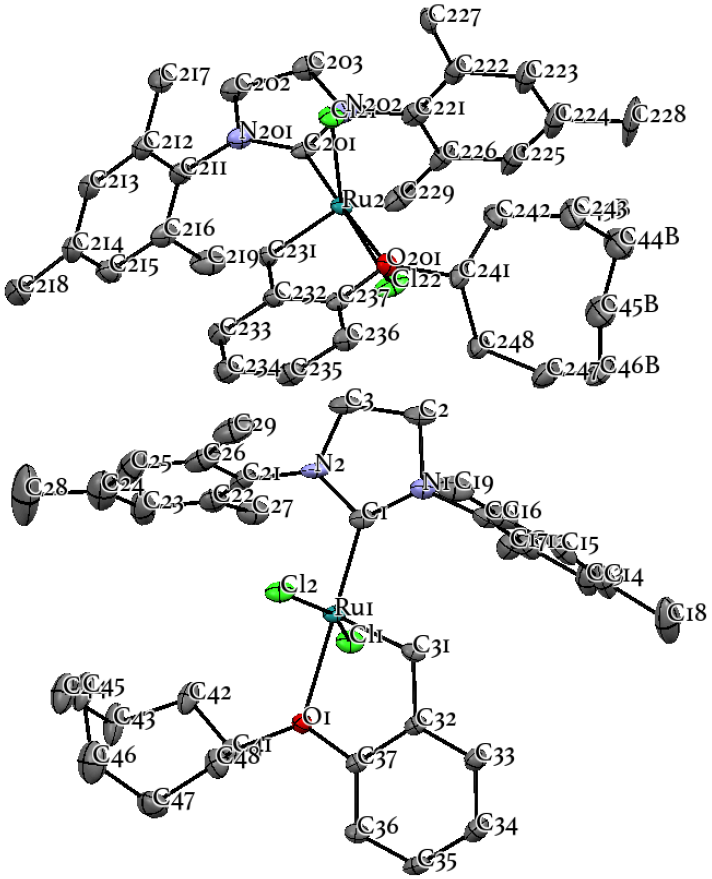


Figure S20. X-ray crystal structure of **26** with 50% probability ellipsoids. Two crystallographically inequivalent molecules are present in the unit cell; for clarity, hydrogen atoms and benzene are omitted.

Low-temperature diffraction data (ϕ-and ω-scans) were collected on Bruker Kappa diffractometer coupled to a Apex II CCD detector with graphite monochromated Mo K_α radiation (λ = 0.71073 Å) for the structure of **27**. The structure was solved by direct methods using SHELXS[13] and refined against F^2 on all data by full-matrix least squares with SHELXL-2013[14] using established refinement techniques.[15] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl groups). Graphical representation of structures with 50% probability thermal ellipsoids was generated using Mercury visualization software.

27 crystallizes in the orthorhombic space group *Pbca* with one molecule in the asymmetric unit along with one molecule of diethyl ether. The coordinates for the hydrogen atom bound to C31 was located in the difference Fourier synthesis and refined semi-freely with the help of a restraint on the C-H distance (0.95(4) Å).

Table S14. Crystal data and structure refinement for **27**.

Identification code	A14206	
Empirical formula	C45 H64 Cl2 N2 O2 Ru	
Formula weight	836.95	
Temperature	100(2) K	
Wavelength	0.71073 ≈	
Crystal system	Orthorhombic	
Space group	P b c a	
Unit cell dimensions	a = 13.9235(5) ≈	α = 90∞.
	b = 14.9583(6) ≈	β = 90∞.
	c = 40.1267(16) ≈	γ = 90∞.
Volume	8357.3(6) ≈^{3}	
Z	8	
Density (calculated)	1.330 Mg/m^3	
Absorption coefficient	0.542 mm^{-1}	
F(000)	3536	
Crystal size	0.150 x 0.100 x 0.050 mm^3	
Theta range for data collection	2.030 to 30.575∞.	
Index ranges	-19<=h<=17, -21<=k<=21, -57<=l<=44	
Reflections collected	76875	
Independent reflections	12759 [R(int) = 0.0895]	
Completeness to theta = 25.242∞	100.0 %	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	0.7461 and 0.6447
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12759 / 1 / 480
Goodness-of-fit on F^2	1.016
Final R indices [I>2sigma(I)]	R1 = 0.0467, wR2 = 0.0791
R indices (all data)	R1 = 0.0860, wR2 = 0.0889
Extinction coefficient	n/a
Largest diff. peak and hole	0.575 and -0.773 e.$\approx^{-3}$

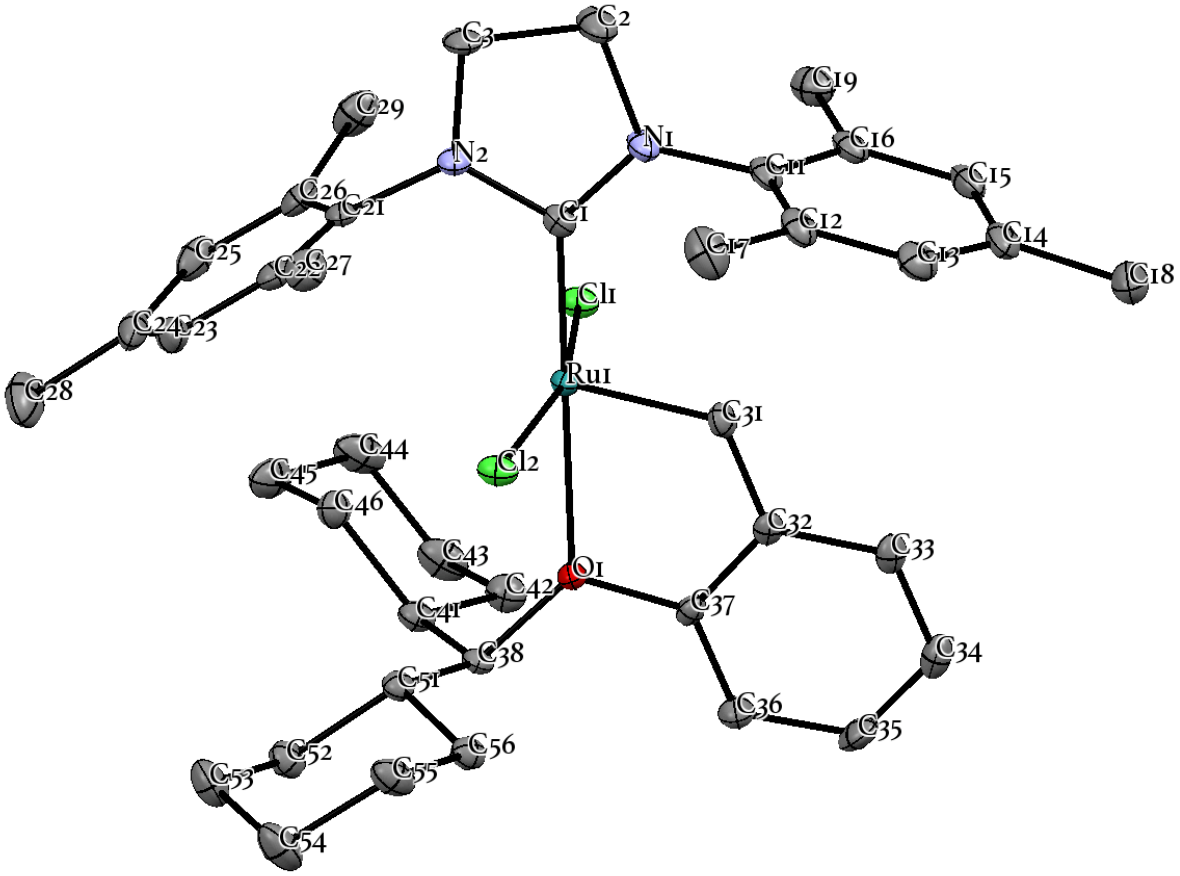


Figure S21. X-ray crystal structure of **27** with 50% probability ellipsoids. For clarity, hydrogen atoms and diethyl ether are omitted.

Low-temperature diffraction data (ϕ-and ω-scans) were collected on a Bruker AXS KAPPA APEX II diffractometer coupled to a APEX II CCD detector with graphite monochromated Mo K_α radiation (λ = 0.71073 Å) for the structure of **28**. The structure was solved by direct methods using SHELXS[13] and refined against F^2 on all data by full-matrix least squares with SHELXL-2014[14] using established refinement techniques.[15] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl groups). All disordered atoms were refined with the help of similarity restraints on the 1,2- and 1,3-distances and displacement parameters as well as rigid bond restraints for anisotropic displacement parameters. Graphical representation of structures with 50% probability thermal ellipsoids was generated using Mercury visualization software.

28 crystallizes in the monoclinic space group $P2_1/c$ with one molecule in the asymmetric unit along with 2.5 molecules of benzene. One of the benzene molecules is located on a crystallographic inversion center. Approximately half of the ruthenium complex was disordered over two positions including the ruthenium and chloride atoms. The occupancy of the two components refine to, 0.8128(12):0.1872(12).

Table S15. Crystal data and structure refinement for **28**.

Identification code	A15013	
Empirical formula	C54 H63 Cl2 N2 O Ru	
Formula weight	928.03	
Temperature	100(2) K	
Wavelength	0.71073 ≈	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 19.4578(8) ≈	α = 90∞.
	b = 14.5971(6) ≈	β = 114.788(2)∞.
	c = 18.2439(8) ≈	γ = 90∞.
Volume	4704.4(4) ≈^{3}	
Z	4	
Density (calculated)	1.310 Mg/m^3	
Absorption coefficient	0.487 mm^{-1}	
F(000)	1948	
Crystal size	0.500 x 0.300 x 0.200 mm^3	
Theta range for data collection	1.810 to 36.406∞.	
Index ranges	-32<=h<=30, -24<=k<=24, -30<=l<=30	
Reflections collected	147151	
Independent reflections	22890 [R(int) = 0.0560]	

Completeness to theta = 25.242∞	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7471 and 0.6546
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	22890 / 814 / 746
Goodness-of-fit on F^2	1.080
Final R indices [I>2sigma(I)]	R1 = 0.0449, wR2 = 0.0929
R indices (all data)	R1 = 0.0811, wR2 = 0.1104
Extinction coefficient	n/a
Largest diff. peak and hole	1.348 and -0.884 e.≈$^{-3}$

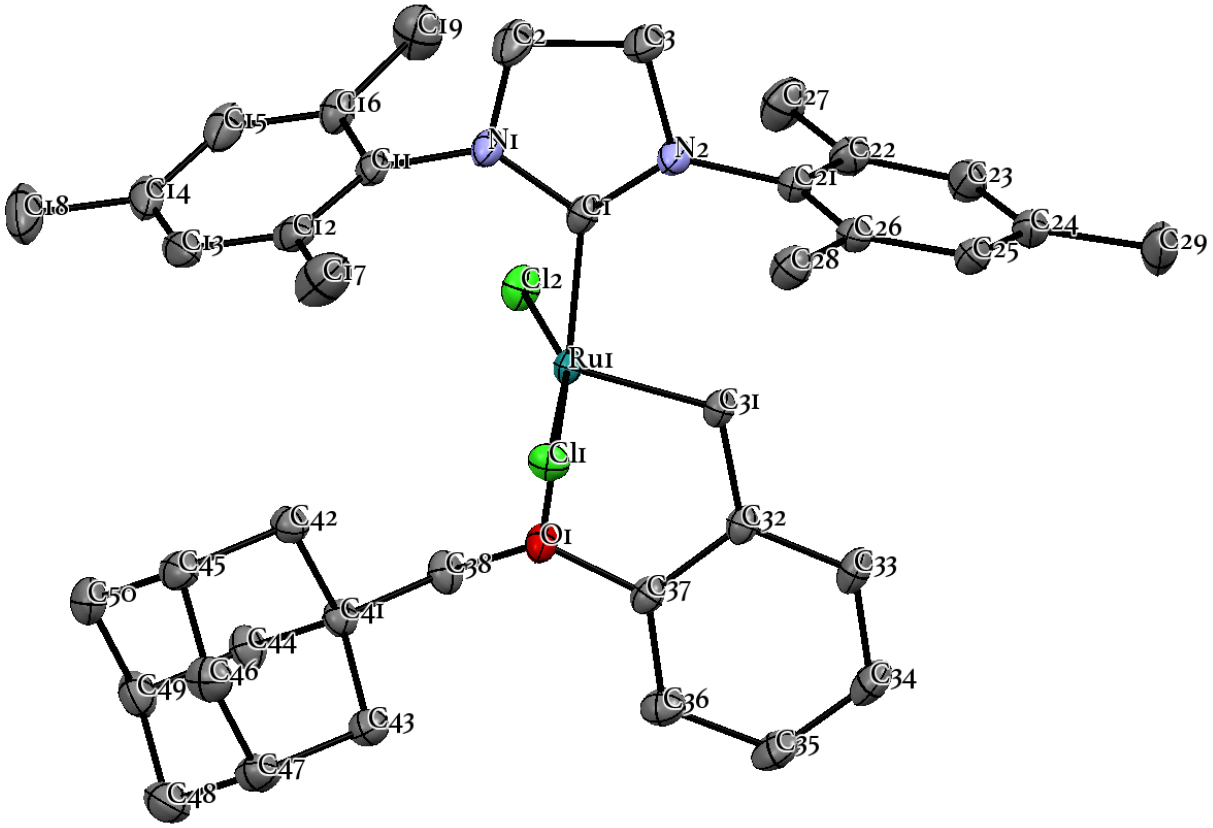


Figure S22. X-ray crystal structure of **28** with 50% probability ellipsoids. For clarity, hydrogen atoms and benzene are omitted.

Low-temperature diffraction data (ϕ-and ω-scans) were collected on a Bruker Kappa diffractometer coupled to a Apex II CCD detector with graphite monochromated Mo K_α radiation (λ = 0.71073 Å) for the structure of **32**. The structure was solved by direct methods using SHELXS[13] and refined against F^2 on all data by full-matrix least squares with SHELXL-2013[14] using established refinement techniques.[15] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl groups). Graphical representation of structures with 50% probability thermal ellipsoids was generated using Mercury visualization software.

32 crystallizes in the monoclinic space group $P2_1/n$ with one molecule in the asymmetric unit.

Table *S16*. Crystal data and structure refinement for **32**.

Identification code	A14127	
Empirical formula	C30 H36 Cl2 N2 O2 Ru	
Formula weight	628.58	
Temperature	100(2) K	
Wavelength	0.71073 ≈	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 12.9199(9) ≈	α = 90∞.
	b = 10.5216(8) ≈	β = 101.442(2)∞.
	c = 21.8706(17) ≈	γ = 90∞.
Volume	2914.0(4) ≈^{3}	
Z	4	
Density (calculated)	1.433 Mg/m^3	
Absorption coefficient	0.751 mm^{-1}	
F(000)	1296	
Crystal size	0.150 x 0.100 x 0.050 mm^3	
Theta range for data collection	1.698 to 30.505∞.	
Index ranges	-18<=h<=18, -15<=k<=15, -31<=l<=31	
Reflections collected	66594	
Independent reflections	8888 [R(int) = 0.0732]	
Completeness to theta = 25.242∞	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7465 and 0.6984	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8888 / 0 / 342
Goodness-of-fit on F^2	1.003
Final R indices [I>2sigma(I)]	R1 = 0.0337, wR2 = 0.0695
R indices (all data)	R1 = 0.0564, wR2 = 0.0769
Extinction coefficient	n/a
Largest diff. peak and hole	0.786 and -0.566 e.$\approx^{-3}$

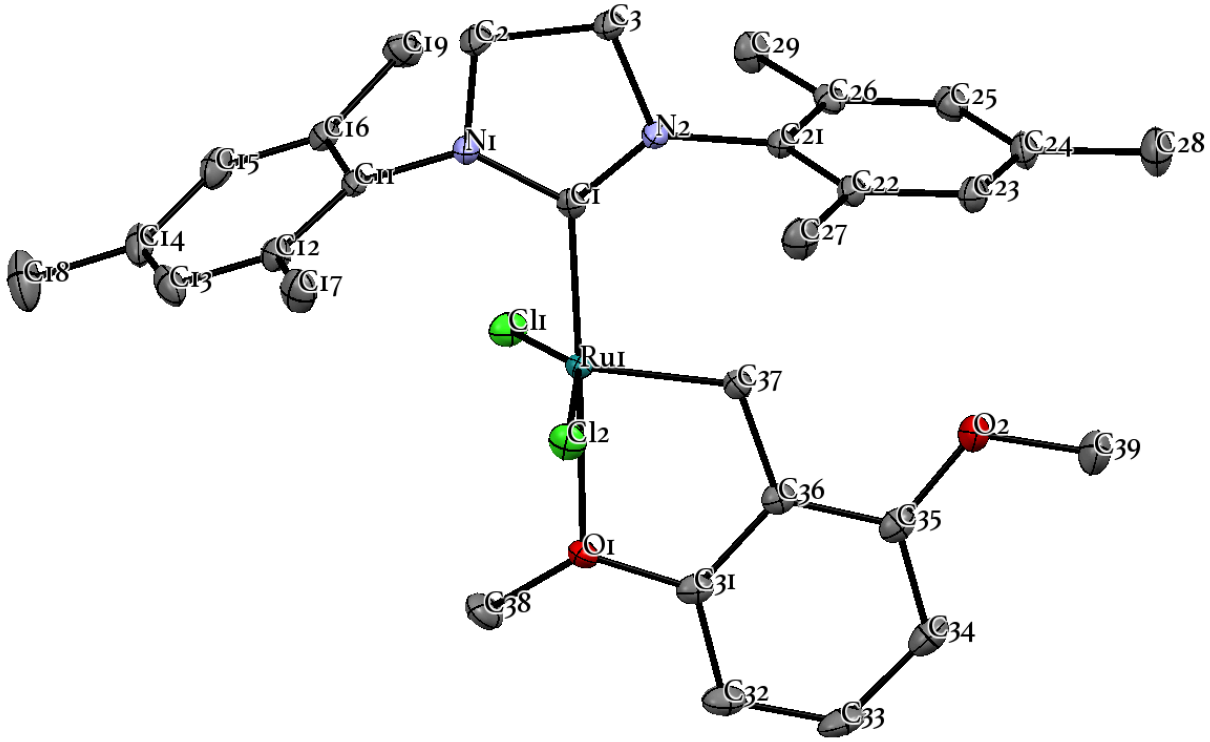


Figure *S23*. X-ray crystal structure of **32** with 50% probability ellipsoids. For clarity, hydrogen atoms are omitted.

Crystals were mounted on polyimide MiTeGen loops with STP Oil Treatment and placed under a nitrogen stream. Low temperature (100K) X-ray data were obtained with a Bruker AXS KAPPA APEX II diffractometer running at 50kV and 30mA (Mo K_α = 0.71073 Å; APEX II CCD detector equipped with a graphite monochromator. All diffractometer manipulations, including data collection, integration, and scaling were carried out using the Bruker APEX2 software.[16] Absorption corrections were applied using SADABS.[17] Space groups were determined on the basis of systematic absences and intensity statistics and the structures were solved by intrinsic phasing using XT and refined by full-matrix least squares on F^2 using XL.[14] All non-hydrogen atoms were refined using anisotropic displacement parameters. Hydrogen atoms were placed in idealized positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed at 1.2 times (1.5 times for methyl groups) the U_{eq} value of the bonded atom. Graphical representation of structures with 50% probability thermal ellipsoids was generated using Mercury visualization software.

Compound **33** crystallizes in the triclinic space group *P*-1 with two molecules and one half a molecule of dichloromethane (on a center) in the asymmetric unit.

Table *S17*. Crystal data and structure refinement for **33**.

Identification code	a14249	
Empirical formula	C37.25 H50.50 Cl2.50 N2 O Ru	
Formula weight	731.99	
Temperature	100 K	
Wavelength	0.71073 ≈	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.5483(5) ≈	α = 71.003(3)∞
	b = 19.8913(11) ≈	β = 83.298(3)∞
	c = 22.4058(13) ≈	γ = 80.481(3)∞
Volume	3544.6(4) ≈^{3}	
Z	4	
Density (calculated)	1.372 Mg/m^3	
Absorption coefficient	0.662 mm^{-1}	
F(000)	1530	
Crystal size	0.48 x 0.25 x 0.10 mm^3	
Theta range for data collection	1.668 to 43.728∞.	
Index ranges	-16<=h<=16, -38<=k<=38, -43<=l<=43	
Reflections collected	367490	
Independent reflections	53947 [R(int) = 0.0494]	
Completeness to theta = 25.000∞	100.0 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.9065
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	53947 / 0 / 1201
Goodness-of-fit on F^2	1.256
Final R indices [I>2sigma(I)]	R1 = 0.0354, wR2 = 0.0755
R indices (all data)	R1 = 0.0537, wR2 = 0.0801
Extinction coefficient	n/a
Largest diff. peak and hole	2.973 and -3.316 e.$\approx^{-3}$

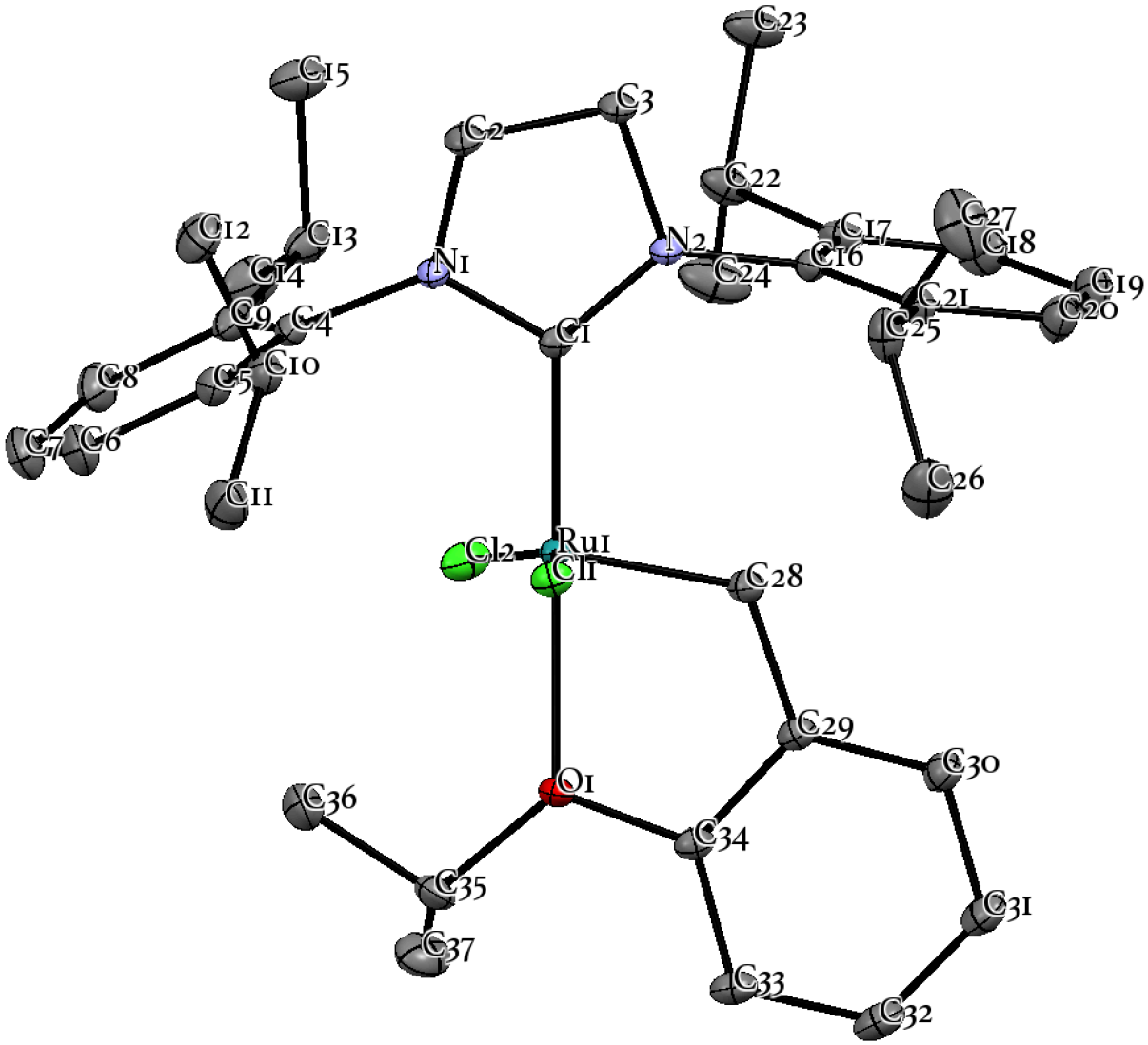


Figure *S24*. X-ray crystal structure of **33** with 50% probability ellipsoids. For clarity, hydrogen atoms and dichloromethane are omitted.

Low-temperature diffraction data (ϕ-and ω-scans) were collected on a Bruker AXS KAPPA APEX II diffractometer coupled to a APEX II CCD detector with graphite monochromated Mo K_α radiation (λ = 0.71073 Å) for the structure of **34**. The structure was solved by direct methods using SHELXS[13] and refined against F^2 on all data by full-matrix least squares with SHELXL-2014[14] using established refinement techniques.[15] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl groups). All disordered atoms were refined with the help of similarity restraints on the 1,2- and 1,3-distances and displacement parameters as well as rigid bond restraints for anisotropic displacement parameters. Graphical representation of structures with 50% probability thermal ellipsoids was generated using Mercury visualization software.

34 crystallizes in the monoclinic space group $P2_1/c$ with one molecule in the asymmetric unit along with two half molecules of hexane. The two half occupied molecules of pentane are located near crystallographic inversion centers and were disordered accordingly. They were refined with the help of similarity restraints on the 1,2- and 1,3-distances.

Table *S18*. Crystal data and structure refinement for **34**.

Identification code	A14410	
Empirical formula	C49 H70 Cl2 N2 O Ru	
Formula weight	875.04	
Temperature	100(2) K	
Wavelength	0.71073 ≈	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 11.5662(6) ≈	α = 90∞.
	b = 24.6231(13) ≈	β = 100.300(3)∞.
	c = 16.3227(8) ≈	γ = 90∞.
Volume	4573.7(4) ≈^{3}	
Z	4	
Density (calculated)	1.271 Mg/m^3	
Absorption coefficient	0.496 mm^{-1}	
F(000)	1856	
Crystal size	0.300 x 0.250 x 0.200 mm^3	
Theta range for data collection	1.514 to 36.318∞.	
Index ranges	-19<=h<=19, -41<=k<=41, -27<=l<=27	
Reflections collected	168417	
Independent reflections	22176 [R(int) = 0.0659]	

Completeness to theta = 25.242∞	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7475 and 0.6870
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	22176 / 43 / 553
Goodness-of-fit on F^2	1.021
Final R indices [I>2sigma(I)]	R1 = 0.0348, wR2 = 0.0768
R indices (all data)	R1 = 0.0514, wR2 = 0.0838
Extinction coefficient	n/a
Largest diff. peak and hole	1.012 and -0.755 e.≈$^{-3}$

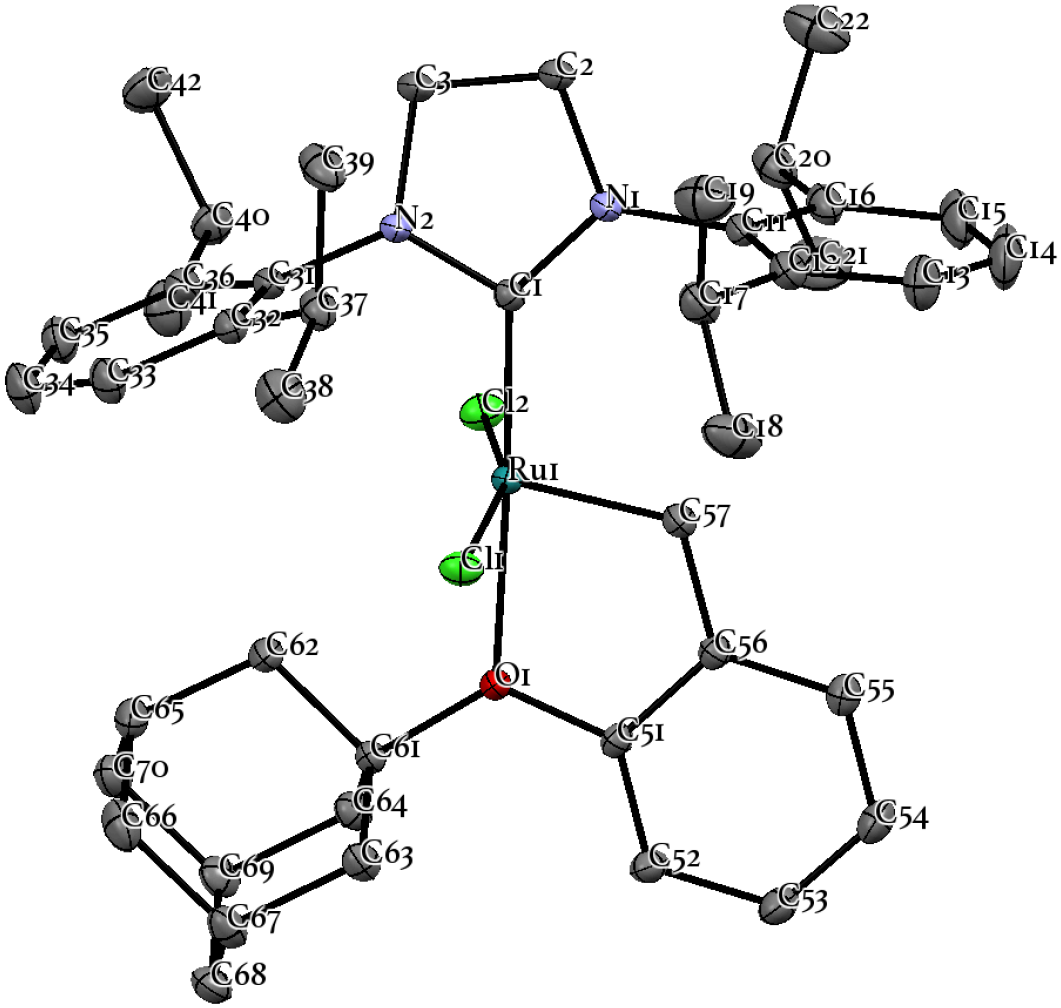


Figure *S25*: X-ray crystal structure of **34** with 50% probability ellipsoids. For clarity, hydrogen atoms and pentane are omitted.

Low-temperature diffraction data (ϕ-and ω-scans) were collected on a Bruker Kappa diffractometer coupled to a Apex II CCD detector with graphite monochromated Mo K_α radiation (λ = 0.71073 Å) for the structure of **35**. The structure was solved by direct methods using SHELXS[13] and refined against F^2 on all data by full-matrix least squares with SHELXL-2014[14] using established refinement techniques.[15] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl groups). Graphical representation of structures with 50% probability thermal ellipsoids was generated using Mercury visualization software.

35 crystallizes in the triclinic space group $P\bar{1}$ with one molecule in the asymmetric unit along with two molecules of ethyl acetate. The carbonyl group in one of the ethyl acetate molecules was disordered over two positions and refined with the help of similarity restraints on the 1,2- and 1,3- distances and displacement parameters as well as rigid bond restraints for anisotropic displacement parameters.

Table *S19*. Crystal data and structure refinement for **35**.

Identification code	A14271	
Empirical formula	C52 H74 Cl2 N2 O5 Ru	
Formula weight	979.10	
Temperature	100(2) K	
Wavelength	0.71073 ≈	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.2187(5) ≈	α = 88.374(3)°.
	b = 12.4464(5) ≈	β = 80.557(2)°.
	c = 17.9271(8) ≈	γ = 66.697(2)°.
Volume	2467.99(18) ≈^{3}	
Z	2	
Density (calculated)	1.318 Mg/m^3	
Absorption coefficient	0.473 mm^{-1}	
F(000)	1036	
Crystal size	0.400 x 0.300 x 0.050 mm^3	
Theta range for data collection	1.783 to 36.412°.	
Index ranges	-20<=h<=20, -20<=k<=20, -29<=l<=29	
Reflections collected	144904	
Independent reflections	24067 [R(int) = 0.0433]	
Completeness to theta = 25.242°	100.0 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7471 and 0.6665
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	24067 / 52 / 581
Goodness-of-fit on F^2	1.037
Final R indices [I>2sigma(I)]	R1 = 0.0293, wR2 = 0.0697
R indices (all data)	R1 = 0.0390, wR2 = 0.0741
Extinction coefficient	n/a
Largest diff. peak and hole	0.829 and -0.714 e.$\approx^{-3}$

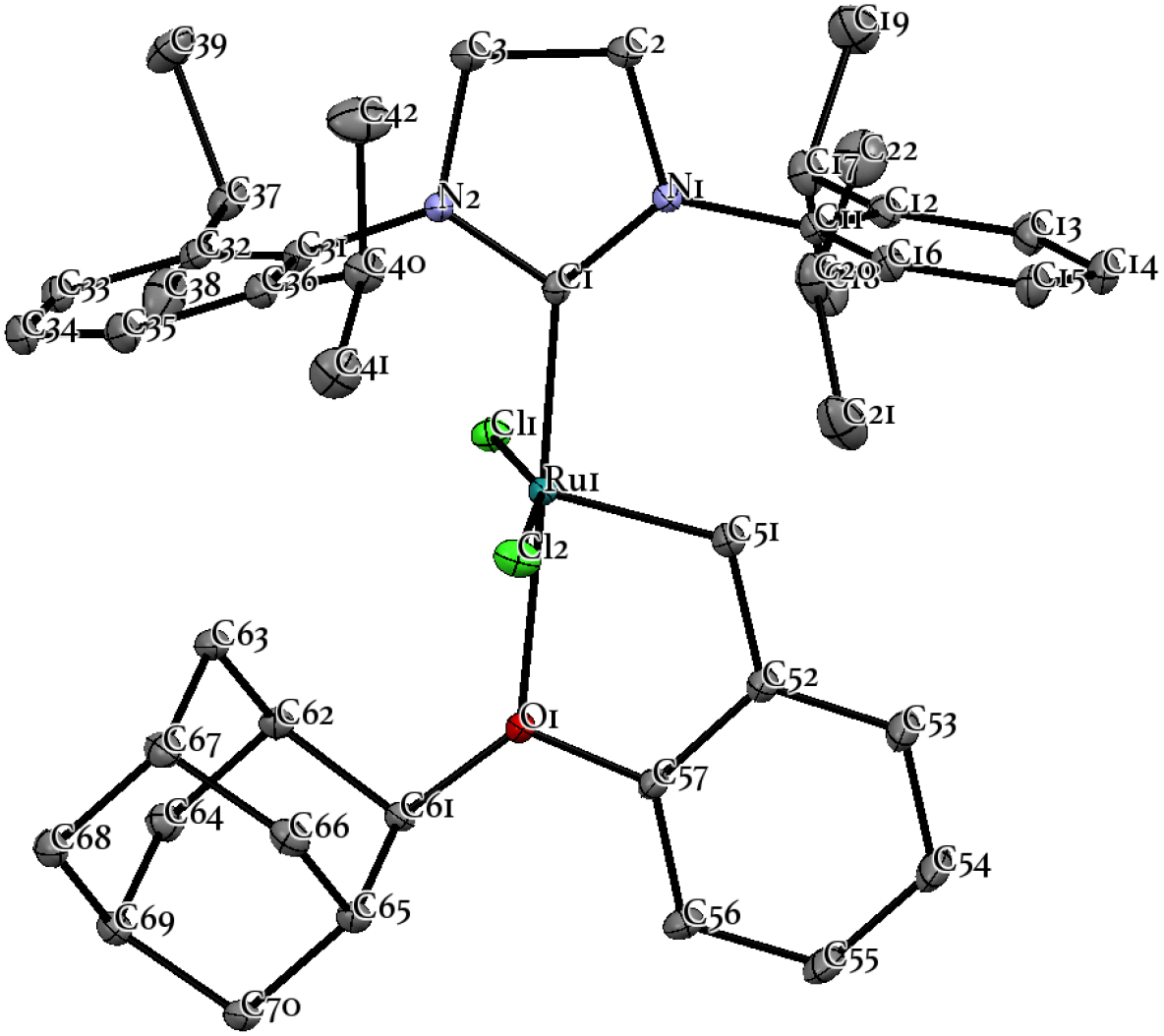


Figure *S26*: X-ray crystal structure of **35** with 50% probability ellipsoids. For clarity, hydrogen atoms and ethyl acetate are omitted.

Crystals were mounted on polyimide MiTeGen loops with STP Oil Treatment and placed under a nitrogen stream. Low temperature (100K) X-ray data were obtained with a Bruker AXS KAPPA APEX II diffractometer running at 50kV and 30mA (Mo K_α = 0.71073 Å; APEX II CCD detector equipped with a graphite monochromator. All diffractometer manipulations, including data collection, integration, and scaling were carried out using the Bruker APEX2 software.[16] Absorption corrections were applied using SADABS.[17] Space groups were determined on the basis of systematic absences and intensity statistics and the structures were solved by intrinsic phasing using XT and refined by full-matrix least squares on F^2 using XL.[14] All non-hydrogen atoms were refined using anisotropic displacement parameters. Hydrogen atoms were placed in idealized positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed at 1.2 times (1.5 times for methyl groups) the U_{eq} value of the bonded atom. Graphical representation of structures with 50% probability thermal ellipsoids was generated using Mercury visualization software.

Compound **37** crystallizes in the orthorhombic space group $P2_12_12_1$ with one molecule and two thirds of a pentane (on a 2_1) in the asymmetric unit. It is twinned by inversion with a 53:47 ratio.

Table *S20*. Crystal data and structure refinement for **37**.

Identification code	a14250	
Empirical formula	C37.33 H46 Cl2 N2 O Ru	
Formula weight	710.71	
Temperature	100 K	
Wavelength	0.71073 ≈	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 7.5671(5) ≈	α = 90∞
	b = 15.1815(11) ≈	β = 90∞
	c = 29.2865(19) ≈	γ = 90∞
Volume	3364.4(4) ≈^{3}	
Z	4	
Density (calculated)	1.403 Mg/m^3	
Absorption coefficient	0.657 mm^{-1}	
F(000)	1480	
Crystal size	0.49 x 0.05 x 0.04 mm^3	
Theta range for data collection	1.511 to 36.970∞.	
Index ranges	-12<=h<=12, -25<=k<=25, -48<=l<=49	
Reflections collected	186950	
Independent reflections	16795 [R(int) = 0.0768]	
Completeness to theta = 25.000∞	100.0 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.9273
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	16795 / 0 / 400
Goodness-of-fit on F^2	1.277
Final R indices [I>2sigma(I)]	R1 = 0.0398, wR2 = 0.0750
R indices (all data)	R1 = 0.0557, wR2 = 0.0783
Absolute structure parameter	0.47(2)
Extinction coefficient	n/a
Largest diff. peak and hole	0.936 and -0.848 e.$\approx^{-3}$

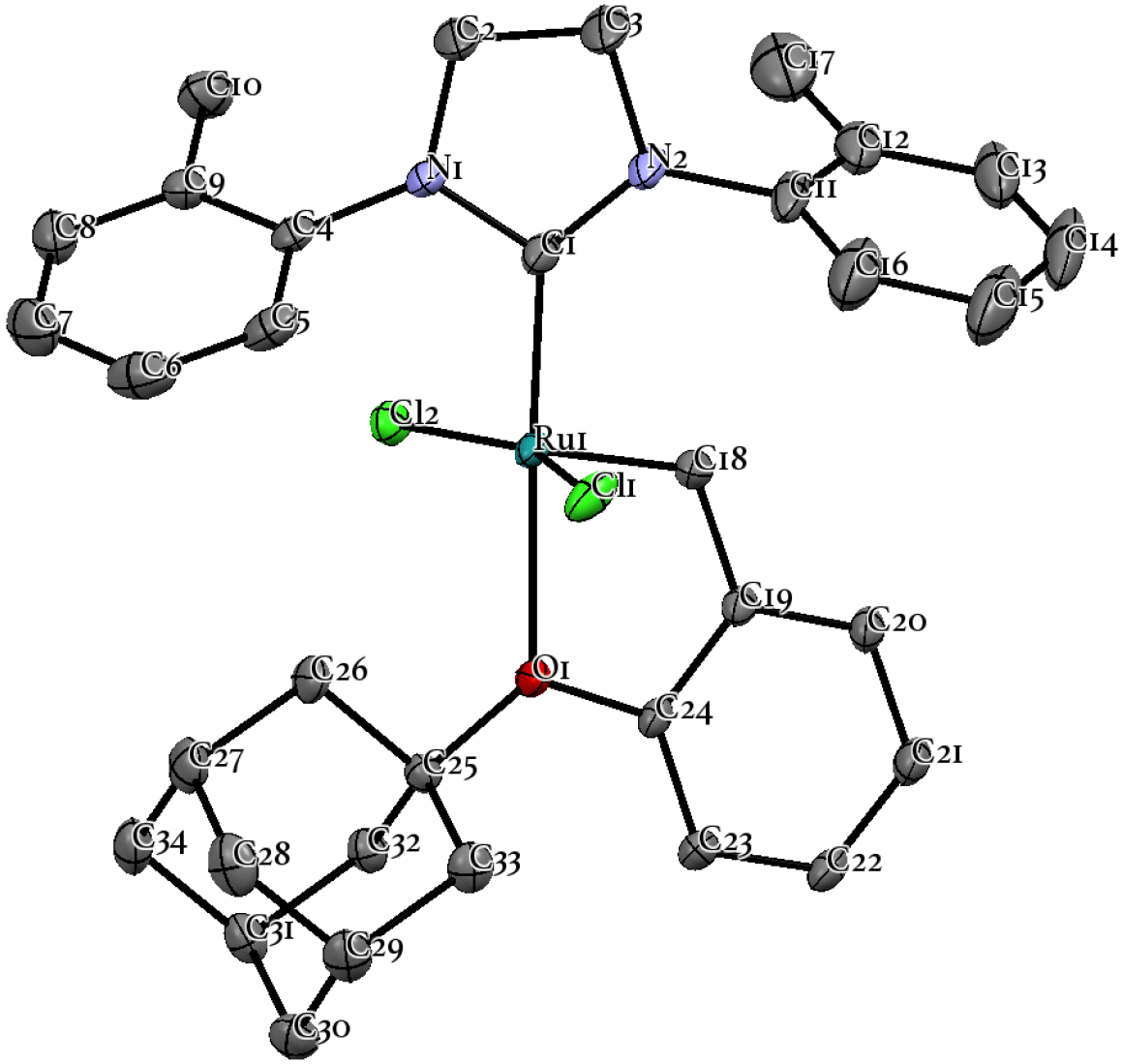


Figure *S27*: X-ray crystal structure of **37** with 50% probability ellipsoids. For clarity, hydrogen atoms and pentane are omitted.

Low-temperature diffraction data (ϕ-and ω-scans) were collected on a Bruker AXS D8 VENTURE KAPPA diffractometer coupled to a PHOTON 100 CMOS detector with Cu K_α radiation (λ = 1.54178 Å) from an IμS micro-source for the structure of **38**. The structure was solved by direct methods using SHELXS[13] and refined against F^2 on all data by full-matrix least squares with SHELXL-2014[14] using established refinement techniques.[15] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl groups). All disordered atoms were refined with the help of similarity restraints on the 1,2- and 1,3-distances and displacement parameters as well as rigid bond restraints for anisotropic displacement parameters. Graphical representation of structures with 50% probability thermal ellipsoids was generated using Mercury visualization software.

38 crystallizes in the orthorhombic space group *Pbca* with one molecule in the asymmetric unit. One of the aryl groups was disordered over two positions. The occupancy of the two components refined to 0.853(6):0.147(6).

Table *S21*. Crystal data and structure refinement for **38**.

Identification code	P15121	
Empirical formula	C34 H38 Cl2 N2 O Ru	
Formula weight	662.63	
Temperature	100(2) K	
Wavelength	1.54178 ≈	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 18.6198(8) ≈	α = 90∞.
	b = 12.7525(5) ≈	β = 90∞.
	c = 25.1609(10) ≈	γ = 90∞.
Volume	5974.4(4) ≈^{3}	
Z	8	
Density (calculated)	1.473 Mg/m^3	
Absorption coefficient	6.121 mm^{-1}	
F(000)	2736	
Crystal size	0.250 x 0.050 x 0.050 mm^3	
Theta range for data collection	3.513 to 74.598∞.	
Index ranges	-22<=h<=20, -13<=k<=15, -31<=l<=30	
Reflections collected	36700	
Independent reflections	6038 [R(int) = 0.1186]	
Completeness to theta = 67.679∞	99.9 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7538 and 0.6175
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6038 / 412 / 428
Goodness-of-fit on F^2	1.013
Final R indices [I>2sigma(I)]	R1 = 0.0469, wR2 = 0.0838
R indices (all data)	R1 = 0.0761, wR2 = 0.0932
Extinction coefficient	n/a
Largest diff. peak and hole	0.589 and -0.806 e.$\approx^{-3}$

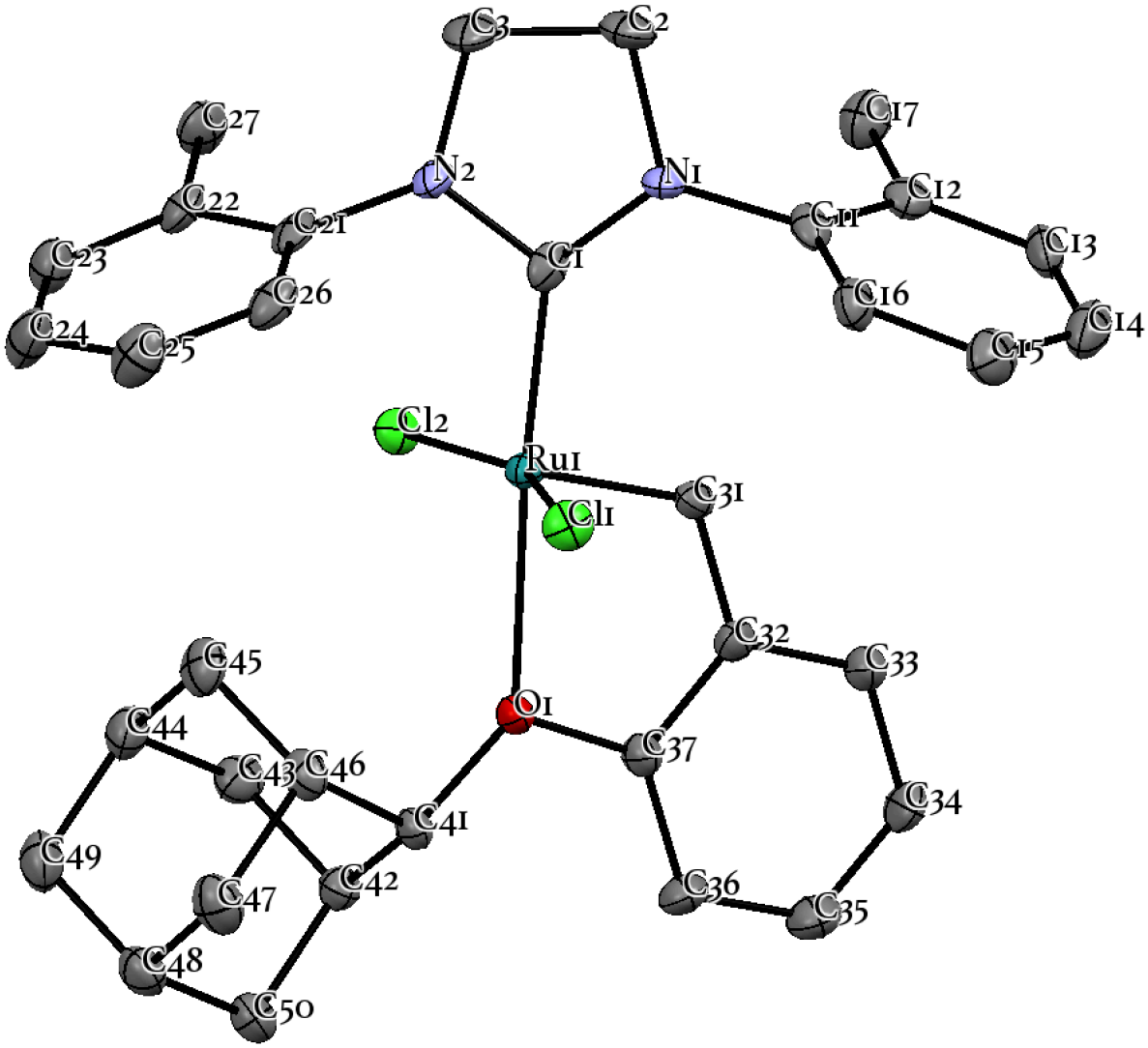
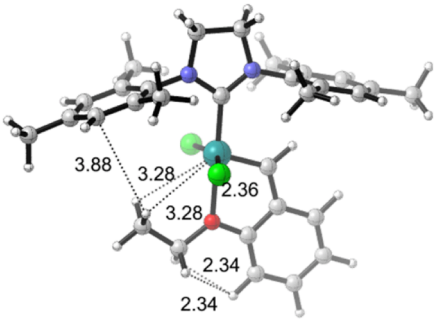


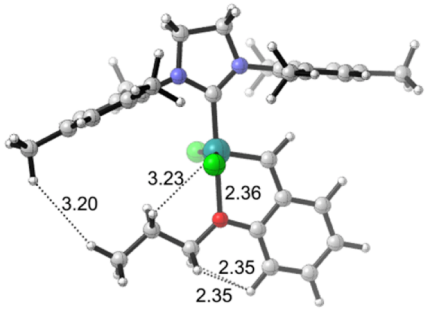
Figure *S28*: X-ray crystal structure of **38** with 50% probability ellipsoids. For clarity, hydrogen atoms are omitted.

COMPUTATIONAL METHODS AND RESULTS

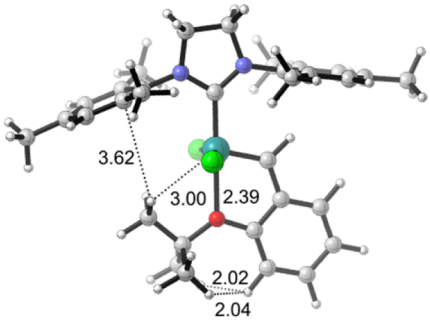
*3D Structures of the Optimized Geometries of Catalysts **16–38**:*



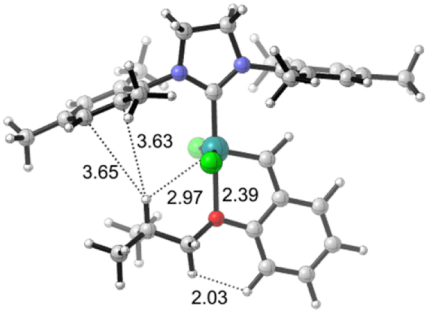
16
Ar = Mes, R^1 = Et, R^2 = H



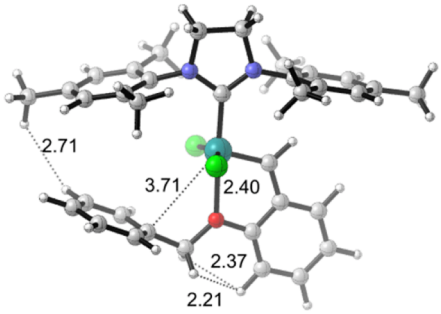
17
Ar = Mes, R^1 = *n*-Pr, R^2 = H



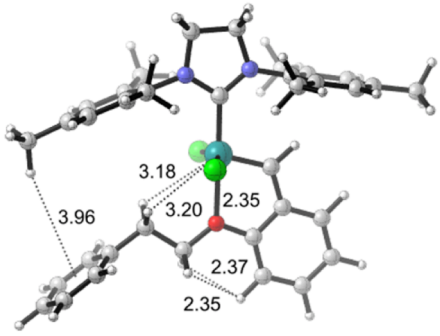
18
Ar = Mes, R^1 = *t*-Bu, R^2 = H



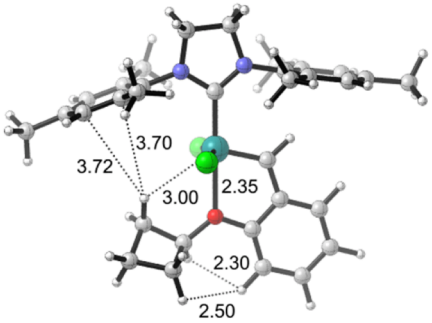
19
Ar = Mes, R^1 = *i*-Bu, R^2 = H



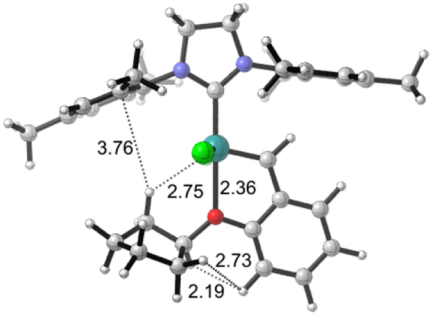
20
Ar = Mes, R^1 = Bn, R^2 = H



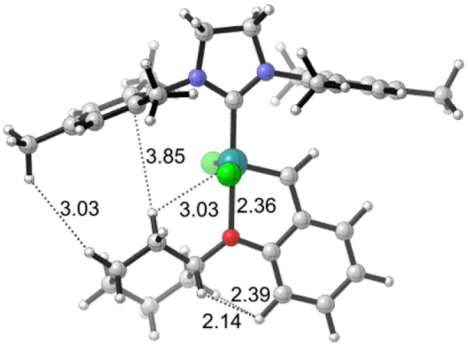
21
Ar = Mes, R^1 = PhEt, R^2 = H



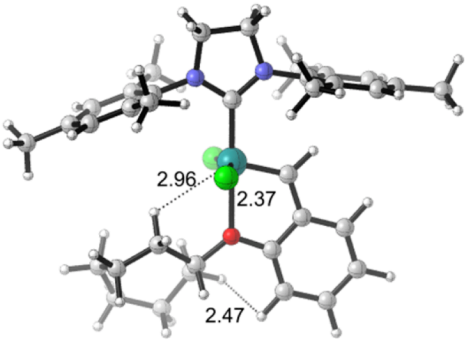
22
Ar = Mes, R^1 = *c*-Bu, R^2 = H



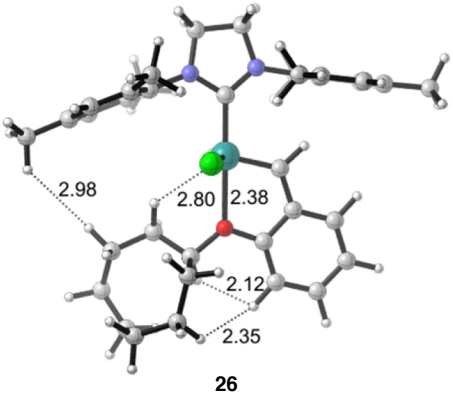
23
Ar = Mes, R^1 = *c*-Pentyl, R^2 = H



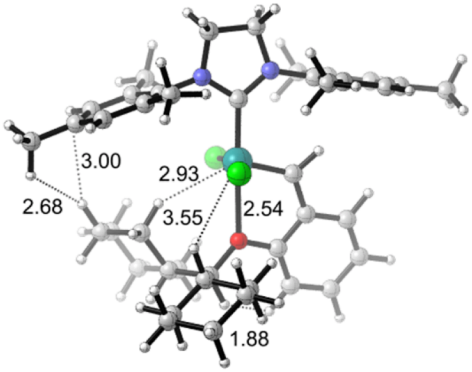
24
Ar = Mes, R^1 = *c*-Hexyl, R^2 = H



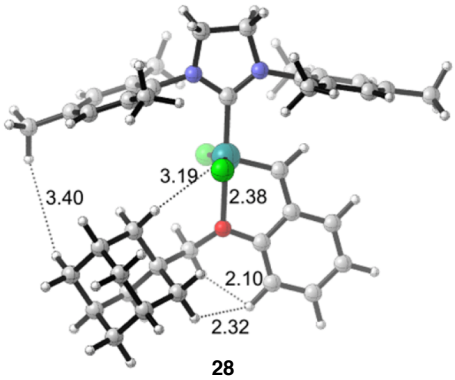
25
Ar = Mes, R^1 = *c*-Heptyl, R^2 = H



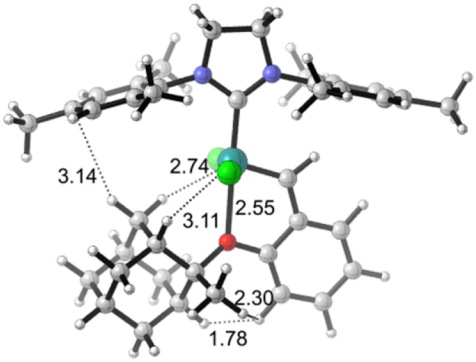
26
Ar = Mes, R^1 = *c*-Octyl, R^2 = H



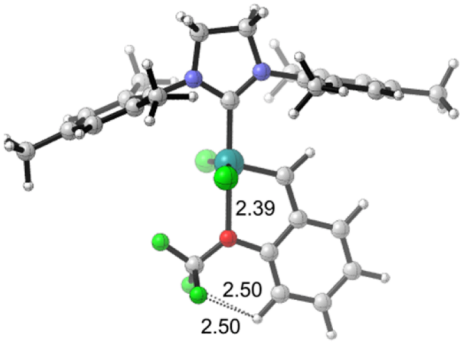
27
Ar = Mes, R^1 = $CHCy_2$, R^2 = H



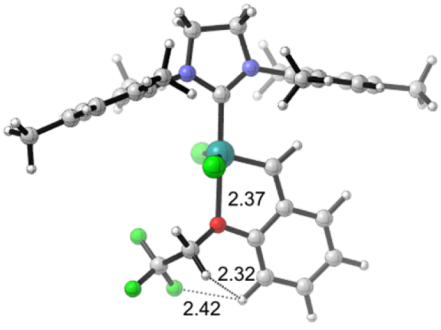
28
Ar = Mes, R^1 = CH_2-1-Ada, R^2 = H



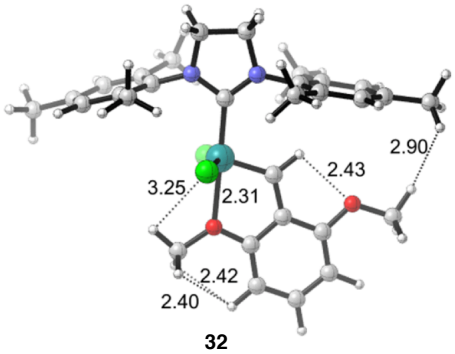
29
Ar = Mes, R^1 = 2–Me-2-Ada, R^2 = H



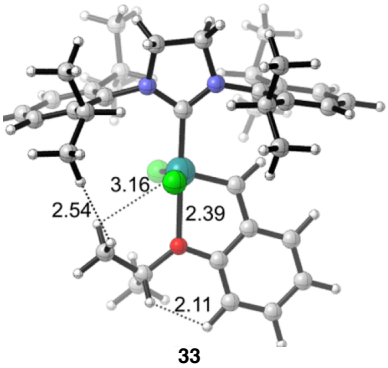
30
Ar = Mes, R^1 = CF_3, R^2 = H



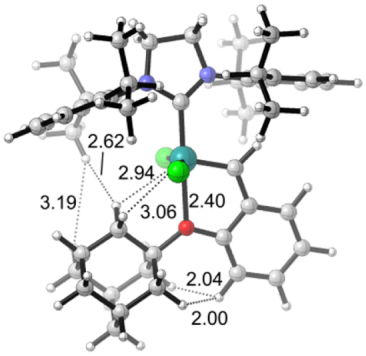
31
Ar = Mes, R^1 = CH_2CF_3, R^2 = H



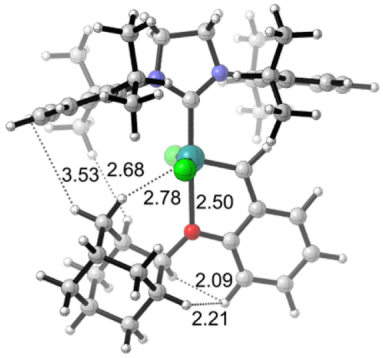
32
Ar = Mes, R^1 = Me, R^2 = OMe



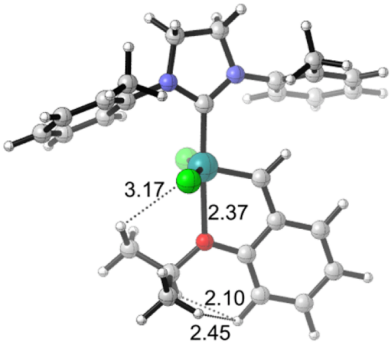
33
Ar = DIPP, R^1 = *i*-Pr, R^2 = H



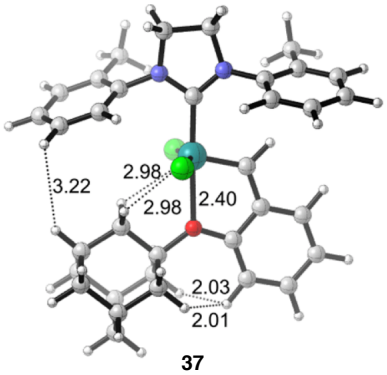
34
Ar = DIPP, R^1 = 1-Ada, R^2 = H



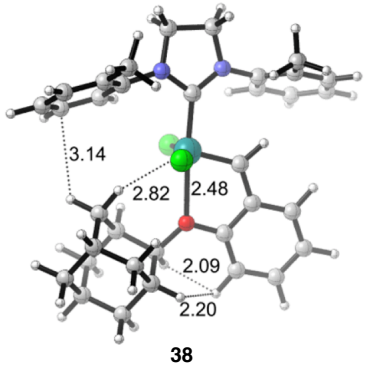
35
Ar = DIPP, R^1 = 2-Ada, R^2 = H



36
Ar = *o*-Tol, R^1 = *i*-Pr, R^2 = H



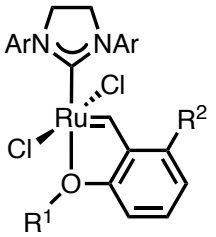
37
Ar = *o*-Tol, R^1 = 1-Ada, R^2 = H



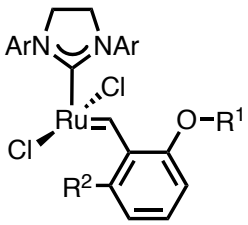
38
Ar = *o*-Tol, R^1 = 2-Ada, R^2 = H

Figure S29: Optimized geometries of catalysts 16–38. Geometries were optimized using B3LYP/LANL2DZ-6-31G(d) in gas phase. All distances are shown in Å.

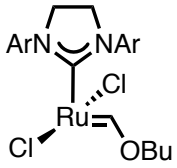
The Cartesian Coordinates (Å) and M06 single point energies, enthalpies at 298K, and Gibbs free energies at 298K for the optimized structures



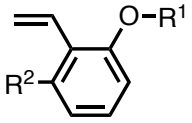
A



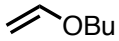
B



C



D



BVE

catalyst	Ar =	R^1 =	R^2 =
16	Mes	Et	H
17	Mes	*n*-Pr	H
18	Mes	*t*-Bu	H
19	Mes	*i*-Bu	H
20	Mes	Bn	H
21	Mes	PhEt	H
22	Mes	*c*-Butyl	H
23	Mes	*c*-Pentyl	H
24	Mes	*c*-Hexyl	H
25	Mes	*c*-Heptyl	H
26	Mes	*c*-Octyl	H
27	Mes	$CHCy_2$	H
28	Mes	CH_2-1-Ada	H
29	Mes	2-Me-2-Ada	H
30	Mes	CF_3	H
31	Mes	CH_2CF_3	H
32	Mes	Me	OMe
33	Dipp	*i*-Pr	H
34	Dipp	1-Ada	H
35	Dipp	2-Ada	H
36	*o*-Tol	*i*-Pr	H
37	*o*-Tol	1-Ada	H
38	*o*-Tol	2-Ada	H

A is the 16-electron ground-state chelated precatalyst,
B is the 14-electron non-chelated complex by dissociation of Ru–O bond,
C is the 14-electron Fischer carbene complex formed from the reaction of **A** and butyl vinyl ether,
D is the olefin product from the reaction of **A** and butyl vinyl ether.

For Cartesian coordinates listed below, the geometry optimizations were performed with B3LYP/LANL2DZ--6-31G(d). Single point energies listed below were calculated with M06/SDD--6-311+G(d,p) and the SMD solvation model in toluene.

16-A

M06 SCF energy: -2364.334009 a.u.
Enthalpy at 298K: -2363.696874 a.u.
Gibbs free energy at 298K: -2363.811949 a.u.
Cartesian Coordinates

Ru	0.181716	0.613800	0.000196
C	0.300006	-1.389750	0.000052
N	-0.646776	-2.363871	-0.000264
C	-0.087692	-3.730155	0.000403
C	1.427155	-3.481761	-0.001171
N	1.513790	-2.011754	0.000153
H	1.922026	-3.890437	-0.889052
H	1.924247	-3.892226	0.884610
H	-0.429419	-4.278896	-0.883986
H	-0.427760	-4.277322	0.886439
C	2.808966	-1.384612	0.000059
C	3.461555	-1.142311	1.227589
C	4.716741	-0.525735	1.198721
C	5.350243	-0.186501	0.000027
C	4.716609	-0.525612	-1.198736
C	3.461466	-1.142086	-1.227573
H	5.215093	-0.317254	2.143236
H	5.214917	-0.317087	-2.143281
C	2.901237	-1.614132	-2.548256
H	3.251972	-2.634577	-2.762289
H	1.812165	-1.607493	-2.565085
H	3.242551	-0.973044	-3.365770
C	2.901497	-1.614624	2.548238
H	3.243554	-0.974170	3.365941
H	3.251639	-2.635407	2.761648
H	1.812439	-1.607307	2.565426
C	6.683995	0.523255	-0.000220
H	7.278207	0.261747	-0.882486
H	7.270441	0.276901	0.891483
H	6.550350	1.613240	-0.010314
C	-2.074094	-2.230333	-0.000110
C	-2.759227	-2.196323	1.228623
C	-4.155744	-2.115281	1.201259
H	-4.695822	-2.076766	2.144978
C	-4.155830	-2.115328	-1.201346
C	-2.759317	-2.196396	-1.228784
H	-4.695969	-2.076844	-2.145030
C	-4.872140	-2.077801	-0.000021

C	-2.016260	-2.199513	-2.543899
H	-2.719126	-2.169860	-3.381963
H	-1.399544	-3.099439	-2.663150
H	-1.346180	-1.335852	-2.628708
H	-1.399068	-3.098853	2.663011
C	-2.016134	-2.199181	2.543722
H	-2.718996	-2.169771	3.381797
H	-1.346363	-1.335272	2.628517
C	-6.382822	-2.027600	0.000043
H	-6.767414	-1.512207	0.886579
H	-6.812077	-3.038588	0.000670
H	-6.767518	-1.513242	-0.887046
Cl	0.583894	0.821862	2.367530
Cl	0.583817	0.822092	-2.367116
C	-1.641224	0.902545	0.000319
H	-2.389954	0.112504	0.000521
C	-2.163768	2.249887	0.000150
C	-1.260461	3.341088	0.000060
C	-1.718640	4.657277	-0.000148
C	-3.097729	4.891991	-0.000282
C	-4.012813	3.835227	-0.000196
C	-3.544626	2.524742	0.000036
H	-4.238907	1.688276	0.000102
H	-5.079771	4.036667	-0.000335
H	-3.455372	5.918113	-0.000443
H	-1.028793	5.492519	-0.000193
O	0.049420	2.968778	0.000272
C	1.080378	3.979812	-0.000335
H	0.945329	4.602283	0.892101
H	0.945093	4.601417	-0.893332
C	2.438953	3.306229	-0.000123
H	3.215728	4.080093	-0.000423
H	2.564779	2.685707	0.891726
H	2.564750	2.685077	-0.891539

16-B

M06 SCF energy: -2364.31128584 a.u.
Enthalpy at 298K: -2363.674508 a.u.
Gibbs free energy at 298K: -2363.791196 a.u.
Cartesian Coordinates

Ru	-0.508855	0.821893	-0.345544
C	-0.991575	-1.073947	-0.083738
N	-0.242685	-2.207717	-0.144765
C	-1.045785	-3.430875	0.056650
C	-2.482020	-2.908140	-0.037218
N	-2.294392	-1.450712	0.066496
H	-2.955521	-3.159893	-0.993975

H	-3.124984	-3.270135	0.770099
H	-0.821435	-3.872126	1.035896
H	-0.807774	-4.171197	-0.712067
Cl	-0.938731	1.747743	1.808267
Cl	-0.830679	0.737068	-2.717447
C	-3.442119	-0.601175	0.259760
C	-3.823876	-0.285355	1.581556
C	-4.950445	0.516656	1.770516
C	-5.711109	0.991089	0.696283
C	-5.349678	0.595251	-0.592684
C	-4.236273	-0.218202	-0.838857
C	-3.982248	-0.721027	-2.240138
H	-2.920079	-0.759953	-2.485770
H	-4.407192	-1.726914	-2.370269
H	-4.465732	-0.070228	-2.974849
H	-5.956182	0.913673	-1.437848
C	-6.891172	1.904761	0.928844
H	-6.564940	2.948993	1.022083
H	-7.422104	1.648580	1.852471
H	-7.605642	1.858152	0.100272
H	-5.241260	0.777104	2.785778
C	-3.068951	-0.820195	2.774527
H	-2.067128	-0.386083	2.831952
H	-3.596559	-0.572160	3.700465
H	-2.965326	-1.912076	2.733466
C	1.184102	-2.357932	-0.189296
C	1.910384	-2.370246	1.015760
C	3.285094	-2.625449	0.954809
C	3.941602	-2.859853	-0.257071
C	3.185464	-2.842120	-1.433721
C	1.807791	-2.601558	-1.427337
C	1.023924	-2.603908	-2.717607
H	0.510398	-1.649828	-2.877091
H	1.687319	-2.784799	-3.568676
H	0.257038	-3.389637	-2.725293
C	1.245396	-2.082016	2.342203
H	0.791572	-1.083972	2.355740
H	0.448757	-2.800459	2.571157
H	1.975116	-2.131425	3.155775
H	3.854226	-2.643508	1.881779
H	3.678223	-3.025541	-2.386227
C	5.431853	-3.107230	-0.301055
H	5.975155	-2.201252	-0.600623
H	5.687119	-3.888950	-1.025234
H	5.816885	-3.413256	0.677218
C	1.333725	0.821153	-0.222493
H	1.886721	0.009065	0.244158

C	2.105002	2.008670	-0.552880
C	1.695027	2.922177	-1.548692
C	2.437070	4.061535	-1.843160
C	3.613435	4.314410	-1.137584
C	4.054818	3.436437	-0.144573
C	3.313195	2.289592	0.155268
H	4.970903	3.656966	0.390055
H	4.202962	5.200682	-1.357525
H	2.105119	4.739958	-2.622999
H	0.803307	2.692963	-2.123503
O	3.660428	1.401002	1.122326
C	4.816941	1.656598	1.921375
H	4.717077	2.636095	2.408174
C	4.916725	0.546832	2.952927
H	5.008670	-0.426610	2.461738
H	4.025831	0.532103	3.588377
H	5.795917	0.703448	3.587259
H	5.711472	1.682536	1.283055

16-D

M06 SCF energy: -463.264771505 a.u.
Enthalpy at 298K: -463.0579075 a.u.
Gibbs free energy at 298K: -463.1060065 a.u.
Cartesian Coordinates

C	1.414013	-1.733390	-0.138000
H	0.645186	-2.374027	-0.560819
C	1.074755	-0.301578	-0.085015
C	-0.277753	0.106838	-0.211938
C	-0.614442	1.465079	-0.166410
C	0.381682	2.429152	-0.000155
C	1.717777	2.049073	0.117475
C	2.048227	0.696416	0.068777
H	3.091045	0.399021	0.131048
H	2.496044	2.797278	0.236181
H	0.103745	3.479299	0.032576
H	-1.646817	1.782560	-0.253740
O	-1.185086	-0.902665	-0.381679
C	-2.577807	-0.613606	-0.513275
H	-2.728735	0.233462	-1.194660
C	2.550913	-2.296517	0.292908
H	3.348325	-1.729016	0.766182
H	2.715780	-3.365263	0.192924
C	-3.258472	-0.385056	0.833258
H	-2.856132	0.492817	1.347484
H	-4.334992	-0.236080	0.688741
H	-3.113929	-1.255411	1.481237

H	-2.992195	-1.501784	-0.999473

17-A

M06 SCF energy: -2403.624817 a.u.
Enthalpy at 298K: -2402.957811 a.u.
Gibbs free energy at 298K: -2403.076692 a.u.
Cartesian Coordinates

Ru	-0.143477	0.501295	0.003675
C	-0.050035	-1.503107	0.050154
N	0.997917	-2.365340	0.128119
C	0.587159	-3.783653	0.149305
C	-0.932962	-3.689592	0.313452
N	-1.188388	-2.257385	0.082994
C	-2.549776	-1.791592	0.016951
C	-3.190707	-1.752243	-1.242040
C	-4.512562	-1.304922	-1.297405
C	-5.218917	-0.930598	-0.148566
C	-4.585986	-1.071257	1.087216
C	-3.264717	-1.523638	1.201307
C	-2.705797	-1.805745	2.575690
C	-2.506704	-2.231539	-2.499533
C	-6.630597	-0.400955	-0.246373
C	2.401720	-2.083722	0.053500
C	3.027608	-2.017447	-1.205803
C	4.408369	-1.794458	-1.242455
C	4.508954	-1.718236	1.156781
C	3.130471	-1.940180	1.248372
C	5.167049	-1.647109	-0.075758
C	2.445159	-1.979595	2.593576
C	2.236366	-2.127644	-2.488041
C	6.663311	-1.444939	-0.145886
Cl	-0.653152	0.676801	-2.346702
Cl	-0.448607	0.676927	2.390296
C	1.637179	0.981231	-0.082504
C	2.015211	2.375879	-0.091769
C	1.004302	3.367301	-0.043435
C	1.323148	4.724088	-0.046728
C	2.669374	5.100449	-0.098572
C	3.688418	4.144502	-0.147526
C	3.359069	2.792552	-0.144575
O	-0.258682	2.861438	0.003114
C	-1.389965	3.754519	0.061913
C	-2.669477	2.934825	0.110114
C	-3.905980	3.839933	0.169082
H	-1.264100	-3.974119	1.319698
H	-1.480395	-4.300207	-0.410688

H	1.075659	-4.308927	0.975482
H	0.881399	-4.275365	-0.786089
H	-5.006406	-1.257946	-2.265555
H	-5.136011	-0.841841	1.997755
H	-3.024997	-2.803637	2.910375
H	-1.618434	-1.755373	2.605230
H	-3.080343	-1.081648	3.304785
H	-3.205823	-2.213262	-3.341200
H	-2.146916	-3.262966	-2.391928
H	-1.652369	-1.599329	-2.754863
H	-7.184416	-0.880991	-1.060765
H	-6.633481	0.678876	-0.447085
H	-7.185599	-0.560784	0.684062
H	4.901457	-1.729993	-2.210206
H	5.080643	-1.595377	2.074211
H	3.174637	-1.859733	3.400289
H	1.923490	-2.931118	2.757657
H	1.696418	-1.183622	2.684718
H	1.701467	-3.082775	-2.560465
H	2.899989	-2.056631	-3.355073
H	1.486515	-1.331582	-2.566936
H	6.953352	-0.903499	-1.052717
H	7.192043	-2.407557	-0.160064
H	7.033893	-0.884490	0.718924
H	2.463533	0.274644	-0.133719
H	4.135471	2.032622	-0.181142
H	4.727790	4.456070	-0.187421
H	2.918913	6.158081	-0.100799
H	0.550130	5.482297	-0.010254
H	-1.365628	4.397960	-0.826532
H	-1.287566	4.380053	0.957560
H	-2.709281	2.293094	-0.777143
H	-2.633575	2.280749	0.988409
H	-3.973589	4.488899	-0.712740
H	-4.818845	3.236692	0.207066
H	-3.895500	4.481328	1.059028

17-B

M06 SCF energy: -2403.602044 a.u.
Enthalpy at 298K: -2402.935304 a.u.
Gibbs free energy at 298K: -2403.057426 a.u.
Cartesian Coordinates

Ru	-0.560261	0.668271	0.559765
C	-1.133857	-1.111446	-0.066400
N	-0.456237	-2.284111	-0.195005
C	-1.320014	-3.394499	-0.645135
C	-2.726457	-2.799558	-0.521515

N	-2.447147	-1.365861	-0.333947
C	-3.528213	-0.416152	-0.395803
C	-3.825374	0.179135	-1.641172
C	-4.885010	1.085272	-1.703726
C	-5.662206	1.396248	-0.582302
C	-5.390363	0.729443	0.613526
C	-4.346448	-0.197360	0.729776
C	-4.197217	-0.985844	2.009483
C	-3.054395	-0.168360	-2.891911
C	-6.766418	2.423243	-0.669332
C	0.956171	-2.531202	-0.132052
C	1.735338	-2.363051	-1.292154
C	3.094863	-2.686804	-1.226096
C	2.877428	-3.325521	1.077955
C	1.512564	-3.020658	1.064120
C	3.684206	-3.170418	-0.054049
C	0.674095	-3.197431	2.307122
C	1.146775	-1.797370	-2.564230
C	5.149161	-3.539689	-0.014411
Cl	-0.766422	1.989723	-1.418989
Cl	-1.029128	0.204868	2.860698
C	1.281446	0.544465	0.532275
C	2.120219	1.594471	1.084274
C	3.380429	1.874388	0.472769
C	4.187743	2.901816	0.970875
C	3.766845	3.647933	2.074105
C	2.543581	3.386039	2.693026
C	1.731187	2.372169	2.196572
O	3.703923	1.089487	-0.588742
C	4.852083	1.379869	-1.394343
C	4.614278	2.527643	-2.377087
C	3.450870	2.269019	-3.340469
H	-3.271960	-3.193181	0.344692
H	-3.339477	-2.957317	-1.413613
H	-1.169229	-4.272414	-0.010776
H	-1.069191	-3.672914	-1.676300
H	-5.109542	1.560353	-2.656110
H	-6.014030	0.920008	1.484344
H	-4.747007	-1.935698	1.938426
H	-3.156349	-1.204855	2.250202
H	-4.618094	-0.432143	2.853995
H	-3.531724	0.280083	-3.768511
H	-3.012284	-1.252799	-3.055088
H	-2.028605	0.206945	-2.838910
H	-7.276292	2.383562	-1.638418
H	-6.365780	3.439167	-0.555855
H	-7.515026	2.277030	0.116340

H	3.707667	-2.553708	-2.115213
H	3.320375	-3.693486	2.001045
H	1.286443	-3.572275	3.132762
H	-0.141503	-3.915123	2.148997
H	0.215929	-2.252510	2.618997
H	1.893645	-1.791795	-3.363689
H	0.798345	-0.767597	-2.421053
H	0.287720	-2.379197	-2.918874
H	5.711247	-3.036920	-0.808200
H	5.290066	-4.620662	-0.147911
H	5.603347	-3.271049	0.945606
H	1.801461	-0.224096	-0.033496
H	0.795896	2.130405	2.692149
H	2.228854	3.962353	3.557524
H	4.408987	4.440753	2.448997
H	5.139288	3.133037	0.507133
H	5.030623	0.447053	-1.938439
H	5.727183	1.564101	-0.758243
H	4.436773	3.456260	-1.821388
H	5.548282	2.673517	-2.937939
H	2.506224	2.149183	-2.800837
H	3.334241	3.103538	-4.040105
H	3.621788	1.359560	-3.930517

17-D

M06 SCF energy: -502.558441 a.u.
Enthalpy at 298K: -502.321627 a.u.
Gibbs free energy at 298K: -502.373458 a.u.
Cartesian Coordinates

C	0.852508	1.999273	-0.017416
C	1.254148	0.583692	0.026546
C	0.269408	-0.431641	-0.080990
C	0.632496	-1.783043	-0.043608
C	1.973655	-2.142843	0.103293
C	2.956569	-1.161225	0.220147
C	2.588477	0.182412	0.185918
O	-1.019728	-0.003222	-0.229803
C	-2.068085	-0.964295	-0.334180
C	-3.388673	-0.212386	-0.452148
C	-3.743008	0.605846	0.793481
C	1.656078	3.050115	-0.230993
H	-0.208480	2.181591	0.128090
H	3.351197	0.946779	0.302713
H	3.999289	-1.437464	0.347109
H	2.241757	-3.195638	0.131955
H	-0.120072	-2.557735	-0.131465
H	-1.902504	-1.597505	-1.217559

H	-2.070195	-1.613043	0.554541
H	-4.174139	-0.953337	-0.652260
H	-3.338949	0.440454	-1.332577
H	-4.695873	1.129541	0.659895
H	-3.836222	-0.038764	1.676341
H	-2.971732	1.352828	1.004318
H	2.721183	2.950912	-0.424432
H	1.261121	4.061724	-0.228537

18-A

M06 SCF energy: -2442.92180573 a.u.
Enthalpy at 298K: -2442.226313 a.u.
Gibbs free energy at 298K: -2442.346264 a.u.
Cartesian Coordinates

Ru	0.162154	0.388595	0.000832
C	0.104937	-1.617168	0.039277
N	-0.926147	-2.500392	0.106546
C	-0.488213	-3.910648	0.111728
C	1.029918	-3.789575	0.277552
N	1.257542	-2.349977	0.064790
H	1.589028	-4.380616	-0.453842
H	1.366201	-4.080183	1.280383
H	-0.772681	-4.397392	-0.829245
H	-0.966683	-4.454704	0.931608
C	2.608998	-1.854761	0.016436
C	3.307008	-1.585977	1.210694
C	4.619719	-1.105283	1.114800
C	5.261712	-0.937564	-0.112853
C	4.573973	-1.312193	-1.273027
C	3.261048	-1.787091	-1.235886
H	5.156156	-0.875120	2.033207
H	5.076339	-1.244743	-2.235617
C	2.599257	-2.266386	-2.505234
H	2.266427	-3.308494	-2.414293
H	1.729769	-1.654157	-2.758639
H	3.303934	-2.218177	-3.341097
C	2.740534	-1.894361	2.576313
H	3.091314	-1.169422	3.316274
H	3.078241	-2.888322	2.904454
H	1.652113	-1.868201	2.594982
C	6.664211	-0.381109	-0.190980
H	7.244575	-0.864965	-0.984526
H	7.202306	-0.513285	0.753539
H	6.649859	0.694477	-0.411840
C	-2.335497	-2.244628	0.041879
C	-3.059822	-2.124206	1.242128

C	-4.442435	-1.925247	1.160514
H	-5.010597	-1.820032	2.082322
C	-4.354966	-1.980756	-1.239628
C	-2.970309	-2.180291	-1.213075
H	-4.854977	-1.917783	-2.203927
C	-5.109005	-1.854991	-0.067480
C	-2.186132	-2.268410	-2.501223
H	-2.857351	-2.206320	-3.363104
H	-1.633188	-3.212488	-2.582203
H	-1.452619	-1.457417	-2.581443
H	-1.818816	-3.102385	2.732060
C	-2.366839	-2.163287	2.583349
H	-3.095244	-2.073951	3.395008
H	-1.639529	-1.348503	2.681885
C	-6.608825	-1.677238	-0.127220
H	-6.983407	-1.129443	0.743961
H	-7.121780	-2.648294	-0.145577
H	-6.913159	-1.133871	-1.028199
Cl	0.446588	0.554961	2.399348
Cl	0.613510	0.559203	-2.370433
C	-1.622385	0.835566	-0.070940
H	-2.438802	0.116695	-0.113718
C	-2.023554	2.221532	-0.080914
C	-1.040570	3.248379	-0.040471
C	-1.442433	4.587371	-0.047052
C	-2.803146	4.902944	-0.093255
C	-3.782921	3.907989	-0.134339
C	-3.386594	2.576806	-0.128347
H	-4.123698	1.778415	-0.158536
H	-4.835363	4.172245	-0.170181
H	-3.093359	5.950301	-0.097239
H	-0.723540	5.391838	-0.017233
O	0.238396	2.774048	0.000217
C	1.470985	3.605566	0.066820
C	1.594451	4.446966	-1.209702
H	0.839156	5.230729	-1.294934
H	2.577284	4.930919	-1.222119
H	1.518094	3.795500	-2.085418
C	1.478822	4.411268	1.371906
H	2.455389	4.894967	1.484719
H	0.716674	5.192141	1.410444
H	1.325964	3.735170	2.218495
C	2.609893	2.581330	0.102439
H	2.532049	1.941758	0.985909
H	2.604405	1.960702	-0.797917
H	3.565207	3.116350	0.147085

18-B

M06 SCF energy: -2442.89999205 a.u.
Enthalpy at 298K: -2442.205094 a.u.
Gibbs free energy at 298K: -2442.330948 a.u.
Cartesian Coordinates

Ru	-0.623802	-0.657232	0.562741
C	-1.268947	1.114553	-0.028801
N	-0.635681	2.313913	-0.117220
C	-1.548848	3.420173	-0.469095
C	-2.929390	2.751786	-0.431831
N	-2.593038	1.326685	-0.272084
H	-3.505944	2.906690	-1.349115
H	-3.536215	3.092038	0.414947
H	-1.297387	3.818243	-1.459119
H	-1.450387	4.233554	0.256054
C	-3.633371	0.336438	-0.380633
C	-4.470515	0.065389	0.719627
C	-5.475953	-0.896516	0.559505
C	-5.693856	-1.549026	-0.655170
C	-4.901475	-1.187731	-1.750399
C	-3.877845	-0.244709	-1.644011
H	-6.113124	-1.127455	1.410547
H	-5.085354	-1.650877	-2.717290
C	-3.089094	0.151635	-2.868922
H	-3.031649	1.241160	-2.982811
H	-2.068132	-0.237825	-2.820175
H	-3.560196	-0.252597	-3.770109
C	-4.381318	0.831128	2.018477
H	-4.787368	0.238353	2.843584
H	-4.977008	1.753772	1.959282
H	-3.356264	1.096279	2.279910
C	-6.757402	-2.613225	-0.789008
H	-7.244981	-2.572648	-1.769435
H	-7.529300	-2.509584	-0.019296
H	-6.322802	-3.616114	-0.685009
C	0.771455	2.597106	-0.088639
C	1.366843	3.030037	1.109079
C	2.727265	3.359209	1.084717
H	3.200648	3.686123	2.007941
C	2.856409	2.871412	-1.261877
C	1.502411	2.526206	-1.290661
H	3.430924	2.815669	-2.184037
C	3.490120	3.280554	-0.083372
C	0.859779	2.064698	-2.578884
H	1.591066	2.058912	-3.392271
H	0.033585	2.718047	-2.886261

H	0.449716	1.052481	-2.486707
H	-0.244502	3.859585	2.301855
C	0.577116	3.136842	2.391033
H	1.220545	3.471150	3.210429
H	0.132237	2.176243	2.671248
C	4.965956	3.603147	-0.072474
H	5.225950	4.266278	0.759033
H	5.278720	4.086807	-1.004537
H	5.565093	2.689510	0.036577
Cl	-1.153297	-0.189236	2.849515
Cl	-0.771961	-1.995859	-1.414907
C	1.213513	-0.469277	0.529481
H	1.700846	0.256984	-0.117879
C	2.107050	-1.417720	1.180747
C	3.379920	-1.698380	0.599055
C	4.264779	-2.565059	1.247986
C	3.898753	-3.188842	2.441402
C	2.648104	-2.944169	3.012956
C	1.768262	-2.065232	2.391611
H	0.817010	-1.829913	2.857093
H	2.368185	-3.420022	3.948116
H	4.600747	-3.860630	2.928719
H	5.245956	-2.739794	0.822659
O	3.707124	-1.056933	-0.560562
C	3.988758	-1.785588	-1.811777
C	3.149283	-3.061433	-1.918333
H	2.080841	-2.839761	-1.826336
H	3.320162	-3.524921	-2.896470
H	3.420377	-3.792642	-1.150543
C	3.580910	-0.782320	-2.894347
H	3.811839	-1.178561	-3.889152
H	2.507045	-0.582275	-2.840962
H	4.120148	0.161388	-2.760611
C	5.492890	-2.079273	-1.904838
H	6.071202	-1.170200	-1.708929
H	5.805460	-2.851303	-1.195722
H	5.743631	-2.436898	-2.910162

18-D

M06 SCF energy: -541.85257294 a.u.
Enthalpy at 298K: -541.5875749 a.u.
Gibbs free energy at 298K: -541.6425279 a.u.
Cartesian Coordinates

C	-1.442074	1.923281	-0.011670
H	-0.452169	2.349292	-0.145985
C	-1.485076	0.451916	0.013178

C	-0.287742	-0.286646	0.200948
C	-0.327928	-1.687195	0.232888
C	-1.534693	-2.364870	0.060746
C	-2.718677	-1.653763	-0.137205
C	-2.681989	-0.262772	-0.157259
H	-3.598973	0.291930	-0.333594
H	-3.659680	-2.177312	-0.279716
H	-1.543205	-3.451396	0.085408
H	0.576827	-2.253634	0.410361
O	0.841312	0.458475	0.414300
C	2.182155	0.108963	-0.044615
C	-2.482725	2.754955	0.132637
H	-3.496561	2.408329	0.316511
H	-2.345908	3.831159	0.081823
C	2.893602	1.469104	-0.051554
H	3.944688	1.353380	-0.336979
H	2.412799	2.149679	-0.761506
H	2.850990	1.923981	0.943296
C	2.871014	-0.819083	0.969430
H	2.463557	-1.833246	0.960885
H	3.940782	-0.892042	0.742639
H	2.761137	-0.413914	1.980442
C	2.164796	-0.481256	-1.459671
H	1.663825	-1.451308	-1.503296
H	1.653919	0.197990	-2.150379
H	3.193504	-0.616491	-1.811430

19-A

M06 SCF energy: -2442.91821782 a.u.
Enthalpy at 298K: -2442.221847 a.u.
Gibbs free energy at 298K: -2442.343853 a.u.
Cartesian Coordinates

Ru	-0.107912	0.419337	0.051629
C	0.109468	-1.572152	-0.081302
N	1.209340	-2.361845	-0.199399
C	0.887608	-3.800500	-0.286655
C	-0.635578	-3.793577	-0.449243
N	-0.979654	-2.393179	-0.148691
H	-1.143059	-4.472372	0.242506
H	-0.948981	-4.047695	-1.469118
H	1.212531	-4.314799	0.626074
H	1.406991	-4.255898	-1.135031
C	-2.366731	-2.015538	-0.059044
C	-3.100779	-1.737206	-1.229329
C	-4.446980	-1.372290	-1.093375
C	-5.083511	-1.330816	0.147967

C	-4.351467	-1.714671	1.277454
C	-3.004613	-2.075488	1.200902
H	-5.012998	-1.134085	-1.991596
H	-4.844015	-1.744044	2.246967
C	-2.289045	-2.572180	2.433823
H	-1.882419	-3.580451	2.281379
H	-1.463295	-1.911860	2.710553
H	-2.981878	-2.621628	3.279400
C	-2.528184	-1.921862	-2.614858
H	-2.998237	-1.234309	-3.323903
H	-2.728691	-2.943652	-2.969066
H	-1.454840	-1.739175	-2.654701
C	-6.526054	-0.899124	0.272686
H	-7.063124	-1.503062	1.012786
H	-7.054549	-0.982089	-0.682688
H	-6.598117	0.147194	0.598162
C	2.593060	-1.995756	-0.109909
C	3.310932	-1.755582	-1.296177
C	4.672132	-1.450275	-1.191986
H	5.234610	-1.252215	-2.102023
C	4.578676	-1.637329	1.201297
C	3.214655	-1.946238	1.152082
H	5.067572	-1.585532	2.171855
C	5.325350	-1.390741	0.044006
C	2.434375	-2.164912	2.427111
H	3.098718	-2.118930	3.295328
H	1.938443	-3.143319	2.443206
H	1.652860	-1.406221	2.555436
H	2.185325	-2.765930	-2.854843
C	2.630946	-1.785217	-2.644307
H	3.349431	-1.572110	-3.441618
H	1.823419	-1.046071	-2.701928
C	6.805920	-1.097156	0.123664
H	7.127236	-0.431773	-0.684863
H	7.396689	-2.019179	0.038658
H	7.072013	-0.628415	1.076946
Cl	-0.414520	0.687334	-2.332933
Cl	-0.562902	0.424324	2.418591
C	1.635680	1.004499	0.160353
H	2.502816	0.348824	0.217853
C	1.928671	2.419058	0.182606
C	0.868070	3.353945	0.103086
C	1.129281	4.722622	0.050240
C	2.453702	5.166464	0.105063
C	3.517416	4.264717	0.207466
C	3.251504	2.900797	0.244958
H	4.061731	2.179016	0.309689

H	4.540039	4.627231	0.250019
H	2.650447	6.234580	0.069773
H	0.327204	5.446862	-0.021030
O	-0.382243	2.793737	0.116172
C	-1.480488	3.489316	-0.532478
H	-1.300426	3.441398	-1.610766
H	-1.481132	4.532961	-0.202193
C	-2.807388	2.838731	-0.153047
H	-2.723038	1.766097	-0.371647
C	-3.911877	3.418449	-1.051441
H	-3.706101	3.237600	-2.112731
H	-4.018560	4.501646	-0.904319
H	-4.876582	2.958258	-0.811981
C	-3.130201	3.020286	1.335627
H	-2.353697	2.578608	1.966117
H	-4.080587	2.533291	1.582820
H	-3.226580	4.085858	1.586451

19-B

M06 SCF energy: -2442.89514184 a.u.
Enthalpy at 298K: -2442.199255 a.u.
Gibbs free energy at 298K: -2442.325653 a.u.
Cartesian Coordinates

Ru	0.700584	0.684704	-0.589512
C	1.210290	-1.124306	0.017436
N	0.498550	-2.276809	0.115846
C	1.343745	-3.442046	0.447337
C	2.688333	-2.796286	0.800973
N	2.502112	-1.405994	0.351119
H	3.532471	-3.257708	0.280895
H	2.895449	-2.818153	1.877929
H	1.413643	-4.110193	-0.419130
H	0.906201	-4.005061	1.276917
C	3.582162	-0.464095	0.503775
C	3.771317	0.180664	1.743110
C	4.832165	1.084096	1.861726
C	5.717219	1.331747	0.809946
C	5.552700	0.607947	-0.375290
C	4.509363	-0.306127	-0.548912
H	4.968492	1.603900	2.807624
H	6.262093	0.747733	-1.187934
C	4.443007	-1.137827	-1.807392
H	4.586173	-2.204142	-1.584883
H	3.485930	-1.028576	-2.322403
H	5.236145	-0.840917	-2.500135

C	2.931217	-0.131517	2.959331
H	2.859494	0.741986	3.612390
H	3.392313	-0.942993	3.541265
H	1.913609	-0.425762	2.701924
C	6.822397	2.351924	0.948817
H	7.686669	2.095594	0.326675
H	7.161667	2.438349	1.986640
H	6.478344	3.346316	0.635071
C	-0.906926	-2.495323	-0.072823
C	-1.752090	-2.406249	1.050694
C	-3.111373	-2.679696	0.879357
H	-3.773446	-2.609407	1.739754
C	-2.768787	-3.130706	-1.453851
C	-1.397284	-2.872982	-1.334617
H	-3.162132	-3.413076	-2.427829
C	-3.641343	-3.034584	-0.366986
C	-0.492000	-2.988828	-2.537546
H	-1.069443	-3.262910	-3.425500
H	0.276488	-3.759804	-2.396095
H	0.027738	-2.047370	-2.745133
H	-0.410815	-2.653683	2.746633
C	-1.216171	-1.992905	2.402265
H	-2.009036	-2.020261	3.155664
H	-0.807092	-0.975574	2.377491
C	-5.122274	-3.284475	-0.529803
H	-5.679194	-2.338666	-0.543492
H	-5.521810	-3.882653	0.297186
H	-5.340338	-3.809558	-1.465112
Cl	0.714110	1.893178	1.475250
Cl	1.394890	0.315282	-2.847844
C	-1.135735	0.581712	-0.731500
H	-1.719794	-0.167642	-0.199484
C	-1.917063	1.632849	-1.369273
C	-3.201939	1.953562	-0.850149
C	-3.985304	2.939303	-1.447908
C	-3.514593	3.626778	-2.567714
C	-2.252116	3.333567	-3.091064
C	-1.463186	2.352199	-2.499317
H	-0.502278	2.091689	-2.931234
H	-1.888000	3.860611	-3.968117
H	-4.134973	4.389276	-3.031270
H	-4.963250	3.151396	-1.025954
O	-3.690767	1.284745	0.244299
C	-3.358438	1.883047	1.517073
H	-3.703230	2.928426	1.521731
H	-2.267692	1.882892	1.644690
C	-4.044609	1.090079	2.626621

H	-3.707211	0.048533	2.528569
C	-5.572346	1.117875	2.483119
H	-5.881918	0.740753	1.503864
H	-5.954553	2.142026	2.588973
H	-6.050115	0.504395	3.256197
C	-3.592203	1.622268	3.994561
H	-3.894560	2.668695	4.130229
H	-2.503136	1.571526	4.107006
H	-4.044933	1.040874	4.805904

19-D

M06 SCF energy: -541.8520645 a.u.
Enthalpy at 298K: -541.5857535 a.u.
Gibbs free energy at 298K: -541.6404235 a.u.
Cartesian Coordinates

C	-1.460768	1.938154	-0.314633
H	-0.480561	2.190286	-0.710288
C	-1.709559	0.499072	-0.128407
C	-0.616566	-0.402018	-0.062371
C	-0.833815	-1.774262	0.105717
C	-2.136180	-2.267239	0.212673
C	-3.225167	-1.399711	0.144989
C	-3.002327	-0.034891	-0.030076
H	-3.850116	0.638963	-0.114255
H	-4.239514	-1.781805	0.214371
H	-2.291344	-3.335091	0.341901
H	0.002196	-2.461727	0.157832
O	0.625537	0.158482	-0.163978
C	1.776889	-0.680814	-0.134834
C	-2.312699	2.932861	-0.031927
H	-3.292647	2.761914	0.406607
H	-2.045170	3.967771	-0.223832
H	1.730594	-1.403675	-0.962483
H	1.804278	-1.246287	0.809309
C	3.020859	0.199657	-0.260701
H	2.910454	0.777092	-1.189388
C	4.271091	-0.683651	-0.383275
H	4.208606	-1.359618	-1.244626
H	5.168602	-0.067608	-0.506182
H	4.412784	-1.296716	0.516343
C	3.136523	1.182604	0.912203
H	2.239017	1.801846	0.997948
H	3.268157	0.644011	1.860122
H	4.000689	1.844211	0.782294

20-A

M06 SCF energy: -2555.965558 a.u.
Enthalpy at 298K: -2555.272655 a.u.
Gibbs free energy at 298K: -2555.395938 a.u.
Cartesian Coordinates

Ru	-0.088935	0.414282	-0.000837
Cl	0.098719	0.632924	2.392536
Cl	0.586075	0.444389	-2.313022
O	0.161429	2.803447	-0.098697
N	0.677604	-2.437588	0.202457
N	-1.501151	-2.299339	0.375504
C	-0.372028	-1.567244	0.154866
C	0.285810	-3.800733	0.603984
H	0.642256	-4.005828	1.621127
H	0.730459	-4.541182	-0.066913
C	-1.239382	-3.745712	0.515227
H	-1.633234	-4.285290	-0.355443
H	-1.735303	-4.137753	1.407769
C	2.070626	-2.207440	-0.082370
C	2.973197	-1.916638	0.955922
C	4.336334	-1.819794	0.638846
H	5.037421	-1.590268	1.438781
C	4.816225	-2.025727	-0.652497
C	3.895825	-2.363786	-1.652722
H	4.253369	-2.560766	-2.661226
C	2.530262	-2.473564	-1.393856
C	2.556365	-1.745429	2.397378
H	1.507898	-1.991826	2.565615
H	2.679069	-0.705257	2.715737
H	3.178560	-2.373494	3.046979
C	6.287327	-1.894521	-0.970831
H	6.509850	-0.916606	-1.418784
H	6.613153	-2.656700	-1.687759
H	6.903314	-1.989949	-0.070455
C	1.589729	-2.900363	-2.494733
H	1.004420	-3.785648	-2.214590
H	2.152262	-3.150554	-3.399479
H	0.889858	-2.096365	-2.740261
C	-2.877740	-1.907334	0.274211
C	-3.494155	-1.880342	-0.991887
C	-4.853719	-1.555815	-1.057343
H	-5.336265	-1.520659	-2.031884
C	-5.603509	-1.272996	0.089457
C	-4.957848	-1.315514	1.329810
H	-5.523020	-1.090895	2.231978
C	-3.601393	-1.636416	1.450480
C	-2.709501	-2.126787	-2.259393

H	-1.967891	-1.336918	-2.431142
H	-3.378434	-2.157113	-3.124809
H	-2.161707	-3.075957	-2.229469
C	-7.078980	-0.958778	-0.004882
H	-7.338961	-0.540202	-0.982847
H	-7.386529	-0.242630	0.764810
H	-7.686028	-1.863540	0.133789
C	-2.936609	-1.656968	2.805899
H	-2.541336	-2.651697	3.049839
H	-3.652923	-1.387951	3.588225
H	-2.095082	-0.956475	2.850305
C	-1.822121	0.999352	-0.228289
H	-2.686701	0.341250	-0.268908
C	-2.118677	2.402993	-0.389911
C	-3.429482	2.865794	-0.614695
H	-4.235624	2.137247	-0.646395
C	-3.689541	4.219991	-0.799416
H	-4.703568	4.566049	-0.975347
C	-2.630945	5.131054	-0.762239
H	-2.821517	6.190451	-0.911177
C	-1.316782	4.707706	-0.536273
H	-0.518174	5.438490	-0.516778
C	-1.066189	3.348852	-0.343701
C	1.307301	3.695806	-0.102256
H	1.108763	4.486237	0.629421
H	1.373372	4.143088	-1.100055
C	2.580535	2.978939	0.247125
C	2.998879	2.898955	1.581670
H	2.359390	3.290491	2.367788
C	4.224775	2.317054	1.903400
H	4.542843	2.265270	2.941135
C	5.043391	1.811763	0.890499
H	6.004922	1.369682	1.138492
C	4.626059	1.874406	-0.440693
H	5.255478	1.473997	-1.230387
C	3.398598	2.453859	-0.761498
H	3.064885	2.489733	-1.794482

20-B

M06 SCF energy: -2555.946125 a.u.
Enthalpy at 298K: -2555.253664 a.u.
Gibbs free energy at 298K: -2555.381817 a.u.
Cartesian Coordinates

Ru	1.097129	-0.914089	0.052942
C	1.416076	0.960417	0.591350
N	0.630950	1.864860	1.228530

C	1.349050	3.114753	1.550621
C	2.659245	2.963916	0.769441
N	2.628190	1.546193	0.371046
H	3.544741	3.173436	1.376061
H	2.693392	3.603497	-0.121328
H	1.510928	3.183405	2.632987
H	0.760487	3.982166	1.238588
C	3.747115	0.980734	-0.339001
C	3.841055	1.139302	-1.736199
C	4.941174	0.574520	-2.391550
C	5.952127	-0.096337	-1.700893
C	5.872606	-0.153758	-0.305074
C	4.795364	0.388887	0.399641
H	5.007375	0.671532	-3.473119
H	6.676062	-0.626714	0.255284
C	4.810224	0.395226	1.909262
H	4.897313	1.419358	2.297931
H	3.906270	-0.051373	2.328495
H	5.669434	-0.169121	2.283656
C	2.858942	1.968027	-2.530325
H	2.727220	1.555621	-3.533923
H	3.236601	2.995075	-2.640538
H	1.872863	2.008604	-2.067822
C	7.102403	-0.741495	-2.437351
H	8.024600	-0.712200	-1.846785
H	7.294380	-0.247410	-3.395669
H	6.887312	-1.796735	-2.651566
C	-0.736017	1.743078	1.647558
C	-1.745886	2.177421	0.768250
C	-3.073755	2.098999	1.197270
H	-3.863952	2.405309	0.516333
C	-2.378253	1.207401	3.317582
C	-1.032990	1.262398	2.934924
H	-2.623473	0.825074	4.306141
C	-3.409610	1.618094	2.467701
C	0.050936	0.790188	3.875082
H	-0.385441	0.428404	4.810911
H	0.750420	1.596654	4.130759
H	0.640147	-0.023049	3.437283
H	-0.773563	3.567973	-0.590232
C	-1.415605	2.677893	-0.618841
H	-2.328463	2.942302	-1.159013
H	-0.886310	1.917369	-1.205051
C	-4.853122	1.562931	2.910491
H	-5.513925	1.315378	2.072949
H	-5.183083	2.531177	3.310707
H	-5.003393	0.815902	3.696639

Cl	0.755679	-0.615257	-2.298782
Cl	2.167561	-1.876364	1.961288
C	-0.680485	-1.181895	0.463316
H	-1.378347	-0.358736	0.603925
C	-1.289890	-2.504027	0.395420
C	-2.641697	-2.622381	-0.027668
C	-3.264756	-3.866737	-0.091234
C	-2.562260	-5.020197	0.262529
C	-1.230473	-4.930102	0.676339
C	-0.601889	-3.690256	0.740428
H	0.416914	-3.614128	1.106643
H	-0.685497	-5.825001	0.962192
H	-3.056822	-5.986797	0.217180
H	-4.300828	-3.914545	-0.413486
O	-3.357032	-1.497826	-0.368024
C	-3.262235	-1.128213	-1.758156
H	-3.532216	-2.002297	-2.370815
H	-2.226304	-0.860802	-2.005152
C	-4.200447	0.020819	-2.036107
C	-5.965020	2.118867	-2.649535
C	-5.423326	0.138613	-1.363385
C	-3.870381	0.963633	-3.017130
C	-4.749440	2.003930	-3.327036
C	-6.297678	1.184050	-1.665510
H	-5.677194	-0.586363	-0.596585
H	-2.919111	0.883733	-3.538266
H	-4.480511	2.727035	-4.092660
H	-7.243062	1.266293	-1.135014
H	-6.648069	2.930508	-2.885801

20-D

M06 SCF energy: -654.8998025 a.u.
Enthalpy at 298K: -654.6370615 a.u.
Gibbs free energy at 298K: -654.6944495 a.u.
Cartesian Coordinates

C	-1.874807	1.983648	-0.411118
H	-0.848756	2.035635	-0.765224
C	-2.388068	0.624006	-0.174165
C	-1.480102	-0.452077	-0.007318
C	-1.946484	-1.752909	0.210714
C	-3.320104	-2.000602	0.269353
C	-4.230596	-0.958617	0.103079
C	-3.758578	0.333722	-0.122197
H	-4.466865	1.141358	-0.283046
H	-5.299181	-1.150425	0.134583
H	-3.670470	-3.015403	0.437692

H	-1.251893	-2.575172	0.336403
O	-0.153687	-0.123122	-0.070499
C	-2.545866	3.127017	-0.217675
H	-3.559144	3.155900	0.175230
H	-2.088480	4.086410	-0.440738
C	0.822842	-1.144008	0.118817
H	0.656027	-1.626449	1.094211
H	0.721179	-1.917661	-0.655025
C	2.197175	-0.520509	0.064022
C	3.236034	-1.165748	-0.614508
C	2.461590	0.685792	0.725916
C	4.522766	-0.622740	-0.626516
H	3.038371	-2.097110	-1.140768
C	3.743565	1.234051	0.706296
H	1.655362	1.196988	1.243389
C	4.778951	0.579750	0.033207
H	5.319881	-1.134553	-1.159144
H	3.935766	2.173156	1.218545
H	5.777798	1.007655	0.020442

21-A

M06 SCF energy: -2595.262149 a.u.
Enthalpy at 298K: -2594.539134 a.u.
Gibbs free energy at 298K: -2594.66809 a.u.
Cartesian Coordinates

Ru	-0.288214	0.200186	0.012525
C	-1.255880	-1.558245	0.038106
N	-2.576393	-1.876781	0.043949
C	-2.826122	-3.329384	0.134592
C	-1.423567	-3.923827	-0.038254
N	-0.560996	-2.733479	0.053397
C	0.869842	-2.889193	-0.003766
C	1.589911	-3.036129	1.202330
C	2.980290	-3.161643	1.130634
C	3.662081	-3.182835	-0.090663
C	2.907525	-3.143950	-1.265398
C	1.513239	-3.022239	-1.251501
C	0.753802	-3.139468	-2.551993
C	0.894792	-3.122650	2.539615
C	5.170411	-3.249859	-0.137530
C	-3.711611	-1.000834	0.045999
C	-4.258462	-0.575217	1.270857
C	-5.396343	0.238516	1.234467
C	-5.423322	0.179452	-1.167077
C	-4.286193	-0.635277	-1.185592
C	-5.995731	0.623158	0.030167

C	-3.670537	-1.065290	-2.496162
C	-3.619684	-0.939317	2.590148
C	-7.246052	1.472473	0.023658
Cl	0.095964	0.252766	2.397284
Cl	0.197413	0.120456	-2.349140
C	-1.669454	1.422715	-0.057575
C	-1.378232	2.837876	-0.089980
C	-0.027379	3.265061	-0.069813
C	0.303817	4.617870	-0.104262
C	-0.726424	5.562701	-0.157492
C	-2.068603	5.171824	-0.176936
C	-2.387881	3.817749	-0.143732
O	0.870411	2.242089	-0.014956
C	2.285359	2.520947	-0.009997
C	3.047170	1.198143	0.054943
C	4.542884	1.440827	0.064828
C	5.270657	1.480694	-1.132989
C	5.226426	1.657611	1.269937
C	6.644201	1.730929	-1.128036
C	6.599482	1.908846	1.278853
C	7.312736	1.947077	0.078753
H	-1.291676	-4.411151	-1.011845
H	-1.166694	-4.646605	0.741885
H	-3.524471	-3.644825	-0.646660
H	-3.270483	-3.575433	1.106466
H	3.542882	-3.255584	2.056869
H	3.412430	-3.219844	-2.226305
H	0.571069	-4.199149	-2.783836
H	-0.201158	-2.615494	-2.529504
H	1.332138	-2.717628	-3.378308
H	1.624857	-3.297690	3.335793
H	0.178320	-3.954490	2.561653
H	0.352226	-2.203199	2.772766
H	5.521903	-3.776884	-1.031239
H	5.577992	-3.759362	0.742268
H	5.604669	-2.241606	-0.161339
H	-5.821940	0.582851	2.174710
H	-5.869766	0.476441	-2.113783
H	-4.273264	-0.712186	-3.338358
H	-3.598021	-2.157327	-2.575400
H	-2.655174	-0.666870	-2.610967
H	-4.180529	-0.500981	3.421113
H	-2.585754	-0.579635	2.648208
H	-3.594304	-2.025009	2.747641
H	-7.282965	2.139007	0.891909
H	-8.148745	0.847574	0.055560
H	-7.309495	2.086941	-0.880705

H	-2.725828	1.160670	-0.083517
H	-3.424934	3.492224	-0.159049
H	-2.854464	5.919900	-0.218261
H	-0.469477	6.618188	-0.184040
H	1.337135	4.943587	-0.090432
H	2.513899	3.147275	0.860142
H	2.534615	3.073397	-0.923493
H	2.736928	0.662547	0.958774
H	2.761684	0.588951	-0.809430
H	4.755352	1.307072	-2.075277
H	4.677372	1.619764	2.208486
H	7.192128	1.753322	-2.066591
H	7.112699	2.069447	2.223520
H	8.382409	2.139285	0.084411

21-B

M06 SCF energy: -2595.242606 a.u.
Enthalpy at 298K: -2594.520038 a.u.
Gibbs free energy at 298K: -2594.650002 a.u.
Cartesian Coordinates

Ru	-0.996924	-0.138114	-1.015866
C	-1.501428	-0.845391	0.755268
N	-0.857930	-1.682154	1.613102
C	-1.661405	-1.992879	2.813152
C	-3.043153	-1.443938	2.445397
N	-2.749810	-0.621568	1.259440
C	-3.762303	0.260672	0.738382
C	-4.764487	-0.235904	-0.117870
C	-5.733963	0.661400	-0.584077
C	-5.756145	2.001287	-0.193035
C	-4.796329	2.437055	0.727261
C	-3.800071	1.589174	1.213501
C	-2.818791	2.089182	2.246132
C	-4.877305	-1.699587	-0.472910
C	-6.787257	2.957612	-0.744484
C	0.502040	-2.143760	1.595938
C	0.784048	-3.421190	1.076328
C	2.101842	-3.883191	1.147916
C	2.804688	-1.864793	2.241011
C	1.502500	-1.354023	2.192837
C	3.125657	-3.122256	1.722160
C	1.204720	0.024350	2.735772
C	-0.293598	-4.277512	0.455497
C	4.543618	-3.643518	1.762101
Cl	-1.835508	-2.029120	-2.216084
Cl	-0.871742	2.217131	-0.636358

C	0.820607	-0.468327	-1.080417
C	1.597413	-0.261563	-2.288906
C	2.992348	0.032913	-2.189300
C	3.741103	0.280358	-3.344878
C	3.130241	0.222240	-4.599206
C	1.773083	-0.080857	-4.722926
C	1.021402	-0.316557	-3.577820
O	3.499708	0.053023	-0.928213
C	4.849324	0.451969	-0.683641
C	5.024319	1.979815	-0.663028
C	4.280564	2.654953	0.470648
C	2.919426	2.970031	0.353894
C	4.935243	2.948872	1.674920
C	2.230720	3.562476	1.413702
C	4.250385	3.542132	2.737356
C	2.894298	3.850558	2.608823
H	-3.487057	-0.832216	3.236007
H	-3.752916	-2.239196	2.186888
H	-1.231187	-1.498016	3.692658
H	-1.664152	-3.070746	2.997519
H	-6.500254	0.291113	-1.261707
H	-4.822423	3.466582	1.077406
H	-2.806339	1.450396	3.138501
H	-1.804094	2.122599	1.840567
H	-3.086477	3.100581	2.566614
H	-3.906879	-2.162559	-0.657336
H	-5.480754	-1.829770	-1.376207
H	-5.378963	-2.253111	0.333977
H	-6.379348	3.527894	-1.589395
H	-7.106324	3.683735	0.011493
H	-7.675005	2.427809	-1.105372
H	2.331553	-4.867749	0.745742
H	3.585261	-1.258791	2.695901
H	0.488596	-0.006033	3.566936
H	0.779626	0.676552	1.965166
H	2.117620	0.501249	3.102428
H	-1.094564	-4.505078	1.170900
H	0.123224	-5.230271	0.115248
H	-0.759135	-3.780237	-0.402193
H	5.027180	-3.551355	0.780575
H	4.573538	-4.704298	2.035909
H	5.154107	-3.090612	2.483498
H	1.394828	-0.696949	-0.186717
H	-0.024792	-0.594511	-3.665620
H	1.308374	-0.138917	-5.702220
H	3.729242	0.414196	-5.485574
H	4.795707	0.520805	-3.282177

H	5.524359	-0.014629	-1.411778
H	5.077221	0.034996	0.300972
H	6.100515	2.180737	-0.577804
H	4.701959	2.389298	-1.627723
H	2.384145	2.751649	-0.565893
H	5.994166	2.718766	1.779520
H	1.175358	3.790385	1.295165
H	4.778035	3.769811	3.660301
H	2.360336	4.317775	3.432374

21-D

M06 SCF energy: -694.194941 a.u.
Enthalpy at 298K: -693.902147 a.u.
Gibbs free energy at 298K: -693.963323 a.u.
Cartesian Coordinates

C	3.243737	1.827957	-0.126091
C	3.194871	0.358109	-0.060279
C	1.941271	-0.302491	-0.004914
C	1.872292	-1.698857	0.054498
C	3.045503	-2.456256	0.058710
C	4.288553	-1.828123	-0.002802
C	4.349873	-0.437295	-0.066634
O	0.839011	0.506883	-0.005213
C	-0.457484	-0.080724	0.010296
C	-1.478305	1.059053	-0.031814
C	-2.899658	0.537435	-0.014189
C	-3.564509	0.307293	1.198320
C	-3.568153	0.236582	-1.208961
C	-4.860357	-0.210804	1.218127
C	-4.864133	-0.281397	-1.194373
C	-5.514114	-0.507689	0.020538
C	4.306648	2.601660	0.132724
H	2.308861	2.307652	-0.402164
H	5.317213	0.050769	-0.142651
H	5.202629	-2.414708	-0.012401
H	2.978589	-3.539986	0.103792
H	0.913319	-2.201540	0.101329
H	-0.592621	-0.681970	0.920346
H	-0.586360	-0.744652	-0.856172
H	-1.296746	1.715913	0.826739
H	-1.296046	1.652331	-0.935369
H	-3.063761	0.543243	2.135092
H	-3.070092	0.416702	-2.159448
H	-5.360746	-0.377663	2.168456
H	-5.367475	-0.503632	-2.131719
H	-6.524526	-0.907409	0.033798

H	5.264825	2.201363	0.454197
H	4.244637	3.681809	0.038940

22-A

M06 SCF energy: -2441.686094 a.u.
Enthalpy at 298K: -2441.012895 a.u.
Gibbs free energy at 298K: -2441.131741 a.u.
Cartesian Coordinates

Ru	-0.141464	0.406451	0.060794
C	0.022400	-1.590178	-0.074501
N	1.100461	-2.408458	-0.205550
C	0.742496	-3.839261	-0.276898
C	-0.781892	-3.796069	-0.417159
N	-1.087245	-2.385681	-0.121490
C	-2.464464	-1.976729	-0.018520
C	-3.208476	-1.698828	-1.182839
C	-4.545146	-1.305908	-1.034314
C	-5.164432	-1.235460	0.214614
C	-4.425363	-1.619254	1.339213
C	-3.086847	-2.008103	1.249865
C	-2.365243	-2.502403	2.480303
C	-2.657969	-1.911845	-2.573231
C	-6.595970	-0.772003	0.351402
C	2.494332	-2.078894	-0.138954
C	3.201150	-1.870356	-1.337698
C	4.572193	-1.604007	-1.256482
C	4.508061	-1.763847	1.139820
C	3.135290	-2.033486	1.113405
C	5.244819	-1.551467	-0.030674
C	2.366587	-2.215083	2.401114
C	2.499515	-1.889669	-2.675070
C	6.734295	-1.300737	0.025417
Cl	-0.523881	0.673000	-2.307403
Cl	-0.602259	0.471730	2.423343
C	1.623981	0.946255	0.117072
C	1.952509	2.351450	0.187116
C	0.904004	3.303072	0.210617
C	1.169293	4.669358	0.279249
C	2.500307	5.095417	0.329873
C	3.556729	4.179115	0.309086
C	3.280527	2.817422	0.236825
O	-0.338750	2.747420	0.158576
C	-1.513528	3.570054	0.251504
C	-1.970750	4.336117	-1.011376
C	-2.838079	2.793597	0.242986
C	-3.425351	3.928715	-0.644581

H	-1.295599	-4.457405	0.286928
H	-1.116649	-4.049608	-1.430330
H	1.068062	-4.354541	0.635152
H	1.238162	-4.313916	-1.128985
H	-5.118194	-1.068214	-1.928247
H	-4.905675	-1.626944	2.315273
H	-3.055016	-2.553040	3.328397
H	-1.955503	-3.509115	2.327349
H	-1.540264	-1.839248	2.753277
H	-3.125974	-1.225733	-3.285055
H	-2.880458	-2.934604	-2.911312
H	-1.582382	-1.747607	-2.629331
H	-7.126322	-1.331307	1.130265
H	-7.147661	-0.888615	-0.587285
H	-6.641947	0.289532	0.628727
H	5.126558	-1.430972	-2.176520
H	5.012234	-1.715496	2.102744
H	1.846228	-3.180189	2.436947
H	1.606400	-1.435019	2.528251
H	3.042973	-2.174113	3.260225
H	2.021441	-2.857952	-2.871108
H	3.211285	-1.703716	-3.485065
H	1.713281	-1.127315	-2.725995
H	7.066908	-0.670401	-0.806210
H	7.296134	-2.242491	-0.036400
H	7.024449	-0.811423	0.961244
H	2.475225	0.268150	0.106543
H	4.086441	2.088155	0.218754
H	4.583776	4.529396	0.347250
H	2.708988	6.160556	0.382640
H	0.365359	5.395456	0.283825
H	-1.412250	4.211451	1.133547
H	-1.622932	3.812843	-1.906733
H	-1.729787	5.401124	-1.087904
H	-2.732509	1.867052	-0.328493
H	-3.296670	2.573921	1.209760
H	-4.078308	3.627523	-1.467372
H	-3.933370	4.697249	-0.053090

22-B

M06 SCF energy: -2441.661447 a.u.
Enthalpy at 298K: -2440.988729 a.u.
Gibbs free energy at 298K: -2441.111547 a.u.
Cartesian Coordinates

Ru	-0.577090	0.548941	-0.702771
C	-1.191708	-1.125090	0.149155

N	-0.543566	-2.293655	0.394446
C	-1.434307	-3.336176	0.943586
C	-2.824774	-2.703807	0.805337
N	-2.507774	-1.309335	0.451319
C	-3.556178	-0.321054	0.439279
C	-4.406202	-0.200345	-0.677369
C	-5.417226	0.768285	-0.632064
C	-5.626979	1.572206	0.489642
C	-4.819267	1.362433	1.612996
C	-3.790192	0.419756	1.618085
C	-2.984570	0.186893	2.873486
C	-4.322304	-1.126482	-1.867423
C	-6.696261	2.639001	0.495602
C	0.865968	-2.564789	0.369167
C	1.428499	-3.186453	-0.758736
C	2.794493	-3.491402	-0.726856
C	2.993496	-2.606180	1.496222
C	1.634911	-2.279662	1.514541
C	3.594147	-3.204964	0.382780
C	1.027811	-1.600208	2.720426
C	0.599086	-3.511008	-1.977563
C	5.074030	-3.508457	0.375669
Cl	-1.095173	-0.238786	-2.899966
Cl	-0.746751	2.143676	1.071135
C	1.261230	0.395351	-0.657151
C	2.134618	1.278123	-1.417892
C	3.398216	1.646934	-0.876480
C	4.278810	2.441839	-1.608546
C	3.923113	2.899251	-2.878569
C	2.679075	2.566981	-3.421537
C	1.796790	1.768591	-2.700851
O	3.781461	1.205997	0.367233
C	3.264046	1.959166	1.476306
C	3.704642	1.432844	2.851594
C	3.909502	3.326297	1.813934
C	3.827125	2.913208	3.310349
H	-3.406647	-2.740297	1.731140
H	-3.417855	-3.168597	0.009048
H	-1.168847	-3.549135	1.986138
H	-1.328061	-4.262367	0.371451
H	-6.065105	0.882098	-1.498571
H	-4.994270	1.948835	2.512196
H	-3.011900	-0.865838	3.183296
H	-1.939099	0.472253	2.730296
H	-3.384695	0.784442	3.698029
H	-4.767831	-0.659099	-2.750664
H	-4.884427	-2.051420	-1.673016

H	-3.295186	-1.392190	-2.120528
H	-6.271807	3.619783	0.243771
H	-7.164287	2.733117	1.481833
H	-7.482254	2.425118	-0.236176
H	3.243118	-3.964832	-1.597389
H	3.598865	-2.380304	2.371368
H	1.768529	-1.503365	3.519523
H	0.176461	-2.158788	3.127400
H	0.662276	-0.596207	2.473801
H	0.144162	-2.610584	-2.404092
H	-0.218283	-4.204518	-1.740370
H	1.216985	-3.982834	-2.747457
H	5.323973	-4.270697	-0.369364
H	5.415881	-3.863668	1.354253
H	5.656457	-2.609393	0.135380
H	1.770907	-0.250146	0.057182
H	0.852973	1.465548	-3.142377
H	2.403254	2.916238	-4.412232
H	4.618298	3.516268	-3.441793
H	5.239599	2.690575	-1.169129
H	2.173826	2.040600	1.393184
H	4.687278	0.955823	2.772770
H	3.020020	0.771079	3.389772
H	4.948178	3.355546	1.467814
H	3.390858	4.233591	1.491870
H	4.675544	3.171540	3.950050
H	2.907638	3.271734	3.782706

22-D

M06 SCF energy: -540.618745 a.u.
Enthalpy at 298K: -540.37571 a.u.
Gibbs free energy at 298K: -540.427386 a.u.
Cartesian Coordinates

C	1.684868	1.910521	-0.051585
C	1.655717	0.438693	-0.048902
C	0.413126	-0.240414	-0.112049
C	0.364038	-1.638988	-0.115205
C	1.546078	-2.379903	-0.063921
C	2.780043	-1.732408	-0.010998
C	2.822112	-0.339627	-0.007391
O	-0.701853	0.552198	-0.154167
C	-1.972417	-0.030152	-0.391940
C	-2.748393	-0.664322	0.794256
C	-3.097508	1.011329	-0.537890
C	-4.020573	0.056242	0.268903
C	2.707565	2.686429	0.332195

H	0.769749	2.387821	-0.391166
H	3.783764	0.165198	0.006078
H	3.702242	-2.305494	0.018261
H	1.494542	-3.465450	-0.067426
H	-0.589700	-2.152795	-0.142365
H	-1.919340	-0.704940	-1.256407
H	-2.400503	-0.236936	1.740122
H	-2.767840	-1.755369	0.879263
H	-2.846763	1.908450	0.036817
H	-3.394940	1.303183	-1.549384
H	-4.682792	0.509066	1.011488
H	-4.617707	-0.588306	-0.383956
H	3.638660	2.284920	0.724129
H	2.637514	3.768666	0.275036

23-A

M06 SCF energy: -2481.0058 a.u.
Enthalpy at 298K: -2480.301674 a.u.
Gibbs free energy at 298K: -2480.423071 a.u.
Cartesian Coordinates

Ru	-0.099829	0.312647	0.081187
C	0.247213	-1.659517	-0.086330
N	1.394981	-2.379459	-0.185588
C	1.167789	-3.829000	-0.347641
C	-0.350091	-3.956585	-0.169699
N	-0.786813	-2.550447	-0.123488
C	-2.190084	-2.260185	0.018762
C	-2.977944	-2.102316	-1.143316
C	-4.338188	-1.821797	-0.986234
C	-4.937852	-1.734906	0.275014
C	-4.149108	-1.993261	1.397738
C	-2.782758	-2.281342	1.297842
C	-2.029823	-2.698928	2.538947
C	-2.407258	-2.303755	-2.526264
C	-6.400250	-1.381689	0.415168
C	2.751130	-1.914647	-0.199140
C	3.366810	-1.607872	-1.427250
C	4.706489	-1.205399	-1.407721
C	4.790238	-1.425856	0.983161
C	3.451958	-1.832950	1.018358
C	5.436213	-1.111608	-0.217255
C	2.772653	-2.123953	2.335768
C	2.601223	-1.658016	-2.728179
C	6.893045	-0.709016	-0.233311
Cl	-0.557984	0.619487	-2.272982
Cl	-0.470211	0.236052	2.461188

C	1.606882	1.011489	0.129007
C	1.803924	2.433661	0.281599
C	0.674431	3.287216	0.355062
C	0.828660	4.665434	0.506384
C	2.118459	5.198511	0.594021
C	3.249289	4.379240	0.526036
C	3.087651	3.006859	0.368023
O	-0.517018	2.633175	0.264194
C	-1.765200	3.379232	0.337351
C	-2.065806	4.167743	-0.968358
C	-2.930863	2.389745	0.522669
C	-3.301432	3.482966	-1.586722
C	-4.060244	2.943386	-0.363139
H	-0.623016	-4.466892	0.761563
H	-0.833548	-4.481474	-0.999405
H	1.735198	-4.387999	0.403211
H	1.505964	-4.155858	-1.337984
H	-4.947357	-1.683961	-1.876976
H	-4.606661	-1.984263	2.384878
H	-2.163981	-3.776834	2.712952
H	-0.963908	-2.482845	2.476082
H	-2.412003	-2.174325	3.418717
H	-1.558539	-1.643374	-2.716164
H	-3.169331	-2.102630	-3.285363
H	-2.072561	-3.340854	-2.666046
H	-6.829015	-1.800966	1.331589
H	-6.985468	-1.749318	-0.434832
H	-6.540602	-0.293277	0.458995
H	5.190115	-0.955014	-2.349687
H	5.338657	-1.350026	1.919679
H	3.489517	-2.061784	3.160128
H	2.330422	-3.127899	2.355836
H	1.961527	-1.412191	2.532921
H	2.193638	-2.657154	-2.926515
H	3.253720	-1.396982	-3.566877
H	1.755318	-0.960430	-2.722588
H	7.101704	0.010549	-1.032423
H	7.541878	-1.578717	-0.403570
H	7.196094	-0.259092	0.717933
H	2.517058	0.418631	0.062340
H	3.951666	2.349641	0.311990
H	4.242940	4.811675	0.593689
H	2.234352	6.272484	0.712722
H	-0.029081	5.325305	0.547290
H	-1.673438	4.042286	1.202912
H	-1.201745	4.174116	-1.638120
H	-2.295863	5.210673	-0.714408

H	-3.198912	2.252944	1.573291
H	-2.620567	1.412678	0.136689
H	-3.896162	4.164968	-2.203742
H	-2.978953	2.647357	-2.218245
H	-4.589877	3.759451	0.148291
H	-4.801352	2.177432	-0.614610

23-B

M06 SCF energy: -2480.982711 a.u.
Enthalpy at 298K: -2480.278795 a.u.
Gibbs free energy at 298K: -2480.403005 a.u.
Cartesian Coordinates

Ru	0.722117	0.510407	-0.766972
C	1.343042	-1.104360	0.183718
N	0.720528	-2.286459	0.439689
C	1.604703	-3.263138	1.107752
C	2.981477	-2.598139	1.006641
N	2.642554	-1.230338	0.577689
C	3.664376	-0.214607	0.580761
C	3.821770	0.571895	1.742083
C	4.830957	1.536228	1.755445
C	5.690195	1.725404	0.667591
C	5.554219	0.879277	-0.434398
C	4.567431	-0.112867	-0.495719
C	4.561467	-1.080284	-1.655452
C	2.953805	0.371493	2.961076
C	6.736556	2.814518	0.689339
C	-0.669897	-2.626963	0.330913
C	-1.529735	-2.339057	1.408337
C	-2.860283	-2.761297	1.322878
C	-2.462949	-3.722413	-0.840376
C	-1.119982	-3.330215	-0.800897
C	-3.346727	-3.453755	0.208636
C	-0.195770	-3.653111	-1.950091
C	-1.053030	-1.558260	2.611793
C	-4.782030	-3.923390	0.153963
Cl	0.769087	2.174371	0.947756
Cl	1.362673	-0.348873	-2.910532
C	-1.111257	0.310459	-0.794618
C	-1.945256	1.193194	-1.596285
C	-3.197973	1.638895	-1.073457
C	-4.004732	2.497351	-1.827925
C	-3.588073	2.916947	-3.093431
C	-2.367708	2.495267	-3.621965
C	-1.555923	1.647419	-2.874761
O	-3.514952	1.182717	0.165234

C	-4.634630	1.734102	0.891389
C	-4.779769	0.881378	2.165263
C	-4.306286	3.141587	1.413036
C	-3.964452	1.608943	3.275717
C	-3.368489	2.869290	2.601651
H	3.623756	-3.079266	0.259450
H	3.519670	-2.578109	1.958813
H	1.557344	-4.228290	0.595620
H	1.284136	-3.413581	2.146017
H	4.947966	2.156653	2.641190
H	6.243093	0.977781	-1.270632
H	5.096975	-2.003146	-1.389283
H	3.552568	-1.345896	-1.974218
H	5.076117	-0.647722	-2.518637
H	3.337205	0.958881	3.800930
H	2.927505	-0.679627	3.274799
H	1.926625	0.693028	2.766885
H	7.151215	2.953344	1.694016
H	6.306578	3.776481	0.380693
H	7.563335	2.591895	0.006656
H	-3.532900	-2.542319	2.149639
H	-2.824324	-4.255408	-1.717132
H	0.645140	-4.281684	-1.629347
H	0.230744	-2.745812	-2.391079
H	-0.733291	-4.197500	-2.732348
H	-0.220363	-2.054218	3.125668
H	-1.863122	-1.441368	3.337899
H	-0.704803	-0.557668	2.329565
H	-5.444279	-3.254650	0.713968
H	-4.888065	-4.926143	0.589485
H	-5.146494	-3.976807	-0.877230
H	-1.636667	-0.334582	-0.093360
H	-0.620267	1.284005	-3.287482
H	-2.052881	2.819168	-4.609218
H	-4.229868	3.582495	-3.665011
H	-4.950498	2.850952	-1.435423
H	-5.527613	1.688086	0.257225
H	-4.427718	-0.134714	1.966503
H	-5.839294	0.813167	2.435905
H	-5.239408	3.611748	1.753851
H	-3.867346	3.788984	0.648412
H	-4.625066	1.890628	4.103770
H	-3.182884	0.969185	3.697099
H	-3.299321	3.721394	3.285423
H	-2.358785	2.664352	2.229724

23-D

M06 SCF energy: -579.937903 a.u.
Enthalpy at 298K: -579.663821 a.u.
Gibbs free energy at 298K: -579.718563 a.u.
Cartesian Coordinates

C	1.539808	2.013304	0.136847
C	1.779036	0.561737	0.078895
C	0.692486	-0.338102	0.234759
C	0.906830	-1.721391	0.183481
C	2.194208	-2.224518	-0.014751
C	3.275727	-1.357168	-0.160290
C	3.058315	0.018168	-0.107442
O	-0.529420	0.240241	0.437235
C	-1.704225	-0.572878	0.613100
C	-2.812712	0.366777	1.144570
C	-2.231413	-1.076633	-0.743246
C	-3.748794	0.674170	-0.058329
C	-3.005379	0.130914	-1.295505
C	2.358914	2.973676	-0.312890
H	0.593334	2.306670	0.582166
H	3.903061	0.695650	-0.192407
H	4.279645	-1.745900	-0.304151
H	2.343659	-3.300412	-0.050782
H	0.078970	-2.412191	0.288356
H	-1.473245	-1.378406	1.319338
H	-2.343921	1.267643	1.550403
H	-3.357904	-0.111238	1.965095
H	-2.916752	-1.917827	-0.567779
H	-1.431483	-1.429767	-1.400457
H	-4.702368	0.145627	0.062932
H	-3.983698	1.739923	-0.142512
H	-3.677898	-0.130318	-2.119226
H	-2.294269	0.876532	-1.670066
H	3.303252	2.761224	-0.807785
H	2.098168	4.022533	-0.206204

24-A

M06 SCF energy: -2520.308059 a.u.
Enthalpy at 298K: -2519.573368 a.u.
Gibbs free energy at 298K: -2519.6948 a.u.
Cartesian Coordinates

Ru	-0.021145	0.200425	-0.083162
C	0.677729	-1.676798	0.044735
N	1.937704	-2.182544	0.099467
C	1.972136	-3.653437	0.221641
C	0.507474	-4.042879	-0.004373

N	-0.178751	-2.740820	0.052662
H	0.120622	-4.717347	0.765307
H	0.344883	-4.511056	-0.982995
H	2.336544	-3.940313	1.215621
H	2.649298	-4.081808	-0.523455
C	-1.616433	-2.700622	-0.020606
C	-2.262314	-2.754519	-1.271970
C	-3.662307	-2.705226	-1.295449
C	-4.423672	-2.655826	-0.127024
C	-3.752356	-2.709406	1.100180
C	-2.358691	-2.752031	1.181153
H	-4.165641	-2.723139	-2.260095
H	-4.328770	-2.732352	2.022514
C	-1.687919	-2.923330	2.522633
H	-1.147344	-3.878303	2.574083
H	-0.978963	-2.117967	2.726151
H	-2.433995	-2.927110	3.323088
C	-1.519328	-2.971196	-2.569064
H	-1.994694	-2.422979	-3.386983
H	-1.536790	-4.038864	-2.832622
H	-0.484030	-2.636848	-2.521949
C	-5.930664	-2.559832	-0.182057
H	-6.398648	-3.104068	0.645696
H	-6.324666	-2.962619	-1.121107
H	-6.262606	-1.515240	-0.110353
C	3.185266	-1.478510	0.161514
C	3.885512	-1.232432	-1.034150
C	5.124097	-0.587364	-0.951429
H	5.669014	-0.382092	-1.870508
C	4.951622	-0.462833	1.441437
C	3.708336	-1.104563	1.413590
H	5.360987	-0.159120	2.402619
C	5.676083	-0.198476	0.274163
C	2.940059	-1.338313	2.693275
H	3.512632	-0.980425	3.554294
H	2.730833	-2.402820	2.857462
H	1.975235	-0.817566	2.685216
H	3.112654	-2.691591	-2.444781
C	3.306017	-1.613421	-2.375787
H	3.997944	-1.350628	-3.181745
H	2.353375	-1.103038	-2.560948
C	7.033285	0.463944	0.337063
H	7.223734	1.074353	-0.552251
H	7.836030	-0.283475	0.394810
H	7.125318	1.107585	1.218247
Cl	-0.259520	0.105389	-2.483200
Cl	-0.620092	0.347677	2.254172

C	1.522596	1.209866	-0.037567
H	2.523918	0.800468	0.085089
C	1.455951	2.644790	-0.190021
C	0.190964	3.272195	-0.318309
C	0.094133	4.652977	-0.493907
C	1.264731	5.415909	-0.538226
C	2.524401	4.823220	-0.406527
C	2.613622	3.446380	-0.233358
H	3.581401	2.961432	-0.133314
H	3.422207	5.432884	-0.440222
H	1.184038	6.490915	-0.675456
H	-0.867634	5.140670	-0.594366
O	-0.858007	2.404302	-0.266848
C	-2.238004	2.876232	-0.255649
C	-4.608890	2.109548	-0.605323
C	-4.086982	3.884380	1.128173
C	-5.012961	2.719440	0.746177
C	-2.607500	3.460166	1.111457
C	-3.128630	1.689658	-0.617489
H	-4.789918	2.842424	-1.405891
H	-4.239905	4.715919	0.423312
H	-4.955301	1.944541	1.523668
H	-2.419621	2.687713	1.866701
H	-2.967543	0.895067	0.123061
H	-2.321977	3.637657	-1.042342
H	-5.233717	1.238307	-0.836637
H	-4.345298	4.269973	2.121845
H	-6.056094	3.059074	0.714138
H	-1.963379	4.311819	1.357551
H	-2.833151	1.292132	-1.593417

24-B

M06 SCF energy: -2520.28653 a.u.
Enthalpy at 298K: -2519.552438 a.u.
Gibbs free energy at 298K: -2519.678504 a.u.
Cartesian Coordinates

Ru	0.739309	-0.234259	0.888849
C	1.404251	1.070133	-0.439642
N	0.814293	2.146213	-1.022834
C	1.769481	2.968825	-1.793006
C	3.013658	2.076691	-1.849003
N	2.705561	1.040133	-0.848569
H	3.931821	2.607505	-1.582546
H	3.157182	1.616049	-2.834365
H	1.954832	3.913837	-1.268637
H	1.362453	3.201708	-2.781094

C	3.673942	0.002760	-0.594931
C	3.733236	-1.115472	-1.451091
C	4.694821	-2.096475	-1.189751
C	5.606799	-1.980384	-0.138187
C	5.573837	-0.818032	0.638551
C	4.633317	0.193616	0.422661
H	4.730063	-2.973677	-1.832227
H	6.307661	-0.685263	1.430416
C	4.707488	1.470691	1.224479
H	4.903388	2.335901	0.576759
H	3.780685	1.666409	1.769133
H	5.523976	1.415605	1.950798
C	2.861555	-1.248762	-2.677828
H	2.665739	-2.301196	-2.898382
H	3.367251	-0.815682	-3.553286
H	1.894808	-0.758641	-2.560536
C	6.601828	-3.079314	0.151655
H	7.516985	-2.683610	0.605033
H	6.878416	-3.621624	-0.758853
H	6.181587	-3.812851	0.852331
C	-0.553575	2.577063	-0.964947
C	-1.432663	2.131084	-1.971128
C	-2.748824	2.600334	-1.956658
H	-3.436740	2.259739	-2.727399
C	-2.295481	3.931030	-0.010745
C	-0.964354	3.496908	0.015574
H	-2.627908	4.634000	0.749876
C	-3.203361	3.491581	-0.977674
C	-0.017038	4.008850	1.073515
H	-0.537796	4.685256	1.757807
H	0.818650	4.568354	0.633267
H	0.413900	3.191871	1.661324
H	-0.117751	1.531142	-3.596383
C	-0.977082	1.152578	-3.029360
H	-1.781041	0.954545	-3.744359
H	-0.672778	0.195381	-2.589150
C	-4.643572	3.946932	-0.958085
H	-5.285274	3.192936	-0.483806
H	-5.028033	4.107950	-1.971470
H	-4.762055	4.879244	-0.396610
Cl	0.607222	-2.238022	-0.406381
Cl	1.545182	1.028539	2.753637
C	-1.078572	0.094505	0.932610
H	-1.598440	0.568009	0.099497
C	-1.945172	-0.436441	1.976809
C	-3.282731	-0.817023	1.664098
C	-4.150582	-1.234659	2.674090

C	-3.714473	-1.308517	3.997021
C	-2.397346	-0.971654	4.320748
C	-1.526425	-0.543807	3.324634
H	-0.521362	-0.227309	3.582600
H	-2.054441	-1.024994	5.349879
H	-4.402389	-1.635379	4.772445
H	-5.165638	-1.503289	2.399102
O	-3.764085	-0.748587	0.384191
C	-3.320620	-1.770949	-0.554733
C	-3.425857	-4.199406	-1.231479
C	-3.474148	-2.383239	-2.999482
C	-3.943140	-3.797054	-2.621075
C	-3.858554	-1.355772	-1.921525
C	-3.819093	-3.164529	-0.162226
H	-2.330976	-4.287036	-1.260266
H	-2.381946	-2.386847	-3.123755
H	-5.043001	-3.826288	-2.622178
H	-4.952538	-1.274389	-1.852612
H	-4.913239	-3.128834	-0.057646
H	-2.222377	-1.775096	-0.572743
H	-3.812632	-5.186721	-0.950082
H	-3.899782	-2.084142	-3.965779
H	-3.608988	-4.521006	-3.375050
H	-3.479833	-0.358922	-2.173120
H	-3.408486	-3.452319	0.812320

24-D

M06 SCF energy: -619.2398792 a.u.
Enthalpy at 298K: -618.9353942 a.u.
Gibbs free energy at 298K: -618.9911872 a.u.
Cartesian Coordinates

C	-2.306831	1.911083	0.113611
H	-1.393565	2.409849	-0.198438
C	-2.294465	0.444873	-0.019812
C	-1.058985	-0.239059	-0.160719
C	-1.034266	-1.633567	-0.288047
C	-2.226604	-2.359801	-0.285309
C	-3.450988	-1.705169	-0.159249
C	-3.471480	-0.317762	-0.033103
H	-4.424815	0.198046	0.037711
H	-4.380744	-2.266531	-0.168181
H	-2.189285	-3.441270	-0.386508
H	-0.093741	-2.162749	-0.383566
O	0.054996	0.552964	-0.165786
C	-3.313291	2.657102	0.588963
H	-4.240727	2.229011	0.961121

H	-3.232697	3.739325	0.631137
C	1.370264	-0.005701	-0.298963
C	2.263883	1.114461	-0.836686
C	1.889643	-0.533196	1.045083
H	1.345716	-0.818562	-1.038942
C	3.724786	0.650477	-0.955693
H	2.195258	1.969493	-0.150259
H	1.878926	1.451564	-1.806254
C	3.349913	-1.003032	0.930614
H	1.815322	0.283386	1.776161
H	1.249434	-1.343903	1.410731
C	4.256635	0.108692	0.380388
H	4.348952	1.480411	-1.308736
H	3.795457	-0.137697	-1.719912
H	3.708115	-1.340441	1.910927
H	3.402579	-1.877290	0.264553
H	5.281814	-0.262710	0.257986
H	4.304750	0.929957	1.110305

25-A

M06 SCF energy: -2559.591055 a.u.
Enthalpy at 298K: -2558.826029 a.u.
Gibbs free energy at 298K: -2558.952011 a.u.
Cartesian Coordinates

Ru	-0.078684	-0.146207	-0.131137
C	-0.953491	1.653189	0.036447
N	-2.257463	2.031862	0.099521
C	-2.436205	3.492114	0.225487
C	-1.020259	4.024452	-0.014810
N	-0.207167	2.797381	0.043769
C	1.227967	2.906661	-0.004620
C	1.886860	3.041355	-1.243106
C	3.284461	3.143828	-1.239892
C	4.025145	3.168380	-0.057331
C	3.329438	3.138305	1.156944
C	1.938449	3.027017	1.211422
C	1.228973	3.106266	2.541549
C	1.144862	3.188691	-2.550427
C	5.534178	3.239517	-0.081896
C	-3.430784	1.212161	0.189761
C	-4.138074	0.906427	-0.987525
C	-5.310324	0.150814	-0.874621
C	-5.061612	0.036361	1.512005
C	-3.883702	0.789172	1.453876
C	-5.790673	-0.290209	0.363096
C	-3.105934	1.089984	2.713717

C	-3.632745	1.342853	-2.342128
C	-7.079728	-1.073515	0.460306
Cl	0.042446	-0.002920	-2.538178
Cl	0.620538	-0.262636	2.178928
C	-1.518215	-1.295828	-0.043604
C	-1.324188	-2.719078	-0.192477
C	-0.012117	-3.230627	-0.359369
C	0.202488	-4.601179	-0.513829
C	-0.895039	-5.467070	-0.507408
C	-2.198466	-4.987962	-0.344550
C	-2.405521	-3.622079	-0.187347
O	0.954592	-2.270620	-0.364446
C	2.377383	-2.619509	-0.381345
C	2.810730	-3.107222	1.007569
C	3.099773	-1.384617	-0.916116
C	4.198715	-3.777654	0.985420
C	4.633454	-1.503382	-0.985243
C	5.413020	-2.836666	1.127465
C	5.324947	-1.483193	0.390818
H	-0.696019	4.738758	0.747680
H	-0.912932	4.500013	-0.997389
H	-2.816992	3.740091	1.223929
H	-3.159932	3.852306	-0.511688
H	3.800302	3.225537	-2.194482
H	3.882739	3.216218	2.090369
H	0.565601	3.980615	2.585559
H	0.630246	2.212765	2.730954
H	1.954888	3.205120	3.354299
H	1.738671	2.795361	-3.380528
H	0.959487	4.253127	-2.756649
H	0.193686	2.657784	-2.556810
H	5.977957	2.244351	0.054800
H	5.919296	3.876372	0.722443
H	5.902433	3.634080	-1.034636
H	-5.859732	-0.099941	-1.779594
H	-5.415647	-0.305295	2.482447
H	-3.623526	0.685575	3.588808
H	-2.984360	2.168702	2.873002
H	-2.100392	0.654116	2.681116
H	-4.316091	1.014590	-3.131172
H	-2.639900	0.927719	-2.551783
H	-3.546903	2.434830	-2.412590
H	-7.263816	-1.657677	-0.447583
H	-7.940092	-0.404375	0.596046
H	-7.068015	-1.762048	1.311998
H	-2.549665	-0.980790	0.104084
H	-3.409199	-3.224361	-0.060361

H	-3.038212	-5.676202	-0.340187
H	-0.721227	-6.532836	-0.629524
H	1.200227	-5.004072	-0.635816
H	2.493111	-3.432330	-1.109881
H	2.768420	-2.270095	1.712804
H	2.069803	-3.835140	1.356707
H	2.849186	-0.529759	-0.273707
H	2.692431	-1.162609	-1.907802
H	4.292760	-4.355686	0.054284
H	4.248730	-4.518802	1.792390
H	4.988862	-0.644742	-1.567875
H	4.929801	-2.395497	-1.556386
H	5.585714	-2.632268	2.192312
H	6.300980	-3.381610	0.779292
H	6.345657	-1.094290	0.279729
H	4.796136	-0.756308	1.021791

25-B

M06 SCF energy: -2559.567838 a.u.
Enthalpy at 298K: -2558.803228 a.u.
Gibbs free energy at 298K: -2558.93216 a.u.
Cartesian Coordinates

Ru	-1.245355	0.728272	-0.546289
C	-1.699803	-1.098388	0.048925
N	-0.983710	-2.253981	0.042809
C	-1.780395	-3.425289	0.461600
C	-3.095104	-2.794807	0.935094
N	-2.948405	-1.391516	0.514132
C	-4.021551	-0.466910	0.780263
C	-5.024093	-0.281108	-0.195945
C	-6.064600	0.607644	0.090003
C	-6.152506	1.279682	1.313305
C	-5.189359	1.005527	2.286734
C	-4.127457	0.125670	2.054489
C	-3.192834	-0.217552	3.190697
C	-5.034061	-1.057464	-1.490819
C	-7.259797	2.273551	1.573874
C	0.375953	-2.494472	-0.349142
C	0.666260	-2.869521	-1.673246
C	1.989112	-3.205151	-1.984951
C	2.678026	-2.819033	0.282004
C	1.373978	-2.468161	0.644028
C	3.006579	-3.189469	-1.027297
C	1.055543	-2.052017	2.061684
C	-0.401425	-2.912848	-2.739417
C	4.427072	-3.547605	-1.398037

Cl	-2.095191	0.447326	-2.769269
Cl	-1.159079	1.865043	1.547642
C	0.579626	0.653476	-0.811967
C	1.277190	1.791813	-1.391924
C	2.574878	2.148002	-0.909467
C	3.231943	3.265380	-1.437771
C	2.621807	4.034443	-2.431578
C	1.357565	3.702807	-2.917892
C	0.696276	2.594753	-2.397565
O	3.074953	1.361644	0.078025
C	4.256306	1.754707	0.813999
C	5.537062	1.329143	0.067182
C	4.051339	1.154368	2.210290
C	6.047350	-0.101764	0.317754
C	5.299214	1.127106	3.112532
C	6.910801	-0.242443	1.584854
C	6.171046	-0.127230	2.926332
H	-3.220445	-2.850268	2.022977
H	-3.975943	-3.244661	0.467467
H	-1.260328	-3.974826	1.252280
H	-1.920610	-4.104557	-0.387167
H	-6.833182	0.768374	-0.662825
H	-5.263034	1.485625	3.260095
H	-3.580387	-1.077096	3.757274
H	-2.185812	-0.453957	2.846467
H	-3.108288	0.621950	3.885654
H	-5.902603	-0.777164	-2.094469
H	-5.099551	-2.138114	-1.305480
H	-4.135733	-0.874460	-2.085327
H	-7.488071	2.349847	2.642289
H	-8.179776	1.998242	1.046663
H	-6.974895	3.276254	1.228840
H	2.225276	-3.494568	-3.006610
H	3.454292	-2.809954	1.044533
H	1.956601	-2.077810	2.681917
H	0.315448	-2.714096	2.528788
H	0.646640	-1.035558	2.099473
H	-1.192502	-3.633822	-2.496070
H	0.029123	-3.211692	-3.699855
H	-0.881798	-1.937158	-2.867738
H	4.461278	-4.163347	-2.302626
H	4.924773	-4.099213	-0.592594
H	5.025215	-2.647521	-1.591262
H	1.205000	-0.134338	-0.397385
H	-0.272158	2.304807	-2.792885
H	0.894118	4.295021	-3.700916
H	3.151259	4.896841	-2.828384

H	4.217342	3.544670	-1.085656
H	4.248545	2.848012	0.901846
H	5.352638	1.469656	-1.003608
H	6.338243	2.035143	0.328226
H	3.671106	0.132824	2.086106
H	3.243921	1.718729	2.690229
H	6.662244	-0.396686	-0.542512
H	5.203220	-0.804186	0.341091
H	4.966960	1.156503	4.157573
H	5.902012	2.035311	2.966124
H	7.425821	-1.212425	1.559794
H	7.703011	0.520228	1.543544
H	6.913951	-0.169870	3.734321
H	5.528824	-1.010633	3.059644

25-D

M06 SCF energy: -658.522892 a.u.
Enthalpy at 298K: -658.188209 a.u.
Gibbs free energy at 298K: -658.247084 a.u.
Cartesian Coordinates

C	2.201501	2.030865	0.077882
C	2.442944	0.578547	0.057054
C	1.357294	-0.318850	0.235408
C	1.576178	-1.702501	0.216916
C	2.864887	-2.207218	0.031297
C	3.944753	-1.341616	-0.134295
C	3.723730	0.034033	-0.114681
O	0.136472	0.265468	0.421698
C	-1.058266	-0.523829	0.595330
C	-1.568984	-1.040292	-0.762684
C	-2.009962	0.398620	1.373276
C	-2.385817	-0.047991	-1.610681
C	-3.503964	0.027084	1.325496
C	-3.883176	-0.016882	-1.256770
C	-4.244749	0.598916	0.103327
C	3.013880	2.978384	-0.409672
H	1.260212	2.335386	0.526588
H	4.566559	0.711865	-0.214906
H	4.949675	-1.731454	-0.267739
H	3.016332	-3.283396	0.021244
H	0.751626	-2.394560	0.339043
H	-0.816609	-1.386766	1.229192
H	-0.695065	-1.379587	-1.329920
H	-2.176741	-1.938830	-0.584606
H	-1.882839	1.415638	0.981706
H	-1.659842	0.431215	2.411824

H	-2.294010	-0.341859	-2.664019
H	-1.947181	0.956700	-1.540404
H	-3.982886	0.427024	2.228079
H	-3.635344	-1.063517	1.377138
H	-4.423744	0.535441	-2.037313
H	-4.265007	-1.048291	-1.297268
H	-5.326456	0.483926	0.256479
H	-4.057462	1.682300	0.068876
H	3.951317	2.751518	-0.911322
H	2.754197	4.029881	-0.329490

26-A

M06 SCF energy: -2598.878177 a.u.
Enthalpy at 298K: -2598.209621 a.u.
Gibbs free energy at 298K: -2598.209621 a.u.
Cartesian Coordinates

Ru	-0.178921	0.043420	-0.072983
C	-1.432151	-1.522385	-0.005283
N	-2.788844	-1.608516	-0.029639
C	-3.285810	-2.996910	0.043384
C	-2.009218	-3.818455	-0.155913
N	-0.953870	-2.802298	-0.001163
C	0.422981	-3.223204	0.040079
C	1.000155	-3.522104	1.295154
C	2.334146	-3.933287	1.329182
C	3.093693	-4.088015	0.163649
C	2.464178	-3.876110	-1.063837
C	1.125822	-3.470668	-1.156034
C	0.467984	-3.420531	-2.514521
C	0.196889	-3.470175	2.572242
C	4.549677	-4.485252	0.236174
C	-3.758736	-0.554346	0.037358
C	-4.166242	-0.067016	1.293642
C	-5.155008	0.922522	1.325865
C	-5.310567	0.913005	-1.071460
C	-4.327050	-0.078196	-1.158519
C	-5.741638	1.422629	0.158070
C	-3.868832	-0.590173	-2.503374
C	-3.524477	-0.548766	2.573684
C	-6.834404	2.464802	0.224790
Cl	0.446062	-0.050667	2.257174
Cl	0.013423	-0.067183	-2.477304
C	-1.334190	1.478553	0.007762
C	-0.825361	2.826750	-0.082279
C	0.573462	3.041355	-0.181351
C	1.088598	4.335617	-0.267073

C	0.208434	5.421916	-0.265916
C	-1.174067	5.236632	-0.173390
C	-1.681627	3.945363	-0.080158
O	1.309485	1.895223	-0.188224
C	2.777118	1.936954	-0.140679
C	3.218688	0.544451	-0.603351
C	3.252791	2.346097	1.268417
C	4.692623	0.176542	-0.375114
C	4.466433	3.296865	1.309098
C	5.764807	0.997687	-1.107854
C	5.830534	2.801015	0.789212
C	5.899526	2.487167	-0.724516
H	-1.953189	-4.269870	-1.154166
H	-1.891279	-4.613510	0.586059
H	-4.036452	-3.174955	-0.732133
H	-3.754845	-3.177432	1.018675
H	2.788506	-4.148101	2.293956
H	3.018334	-4.047520	-1.984499
H	0.074125	-4.413624	-2.776179
H	-0.343590	-2.695546	-2.562071
H	1.192003	-3.144217	-3.286480
H	0.821500	-3.752496	3.425178
H	-0.648619	-4.170375	2.538346
H	-0.195212	-2.468063	2.759068
H	4.885019	-4.954375	-0.694758
H	4.734307	-5.186815	1.057375
H	5.188984	-3.609426	0.410585
H	-5.470932	1.313993	2.290601
H	-5.748957	1.296372	-1.990447
H	-4.415043	-0.092143	-3.310217
H	-4.038631	-1.669712	-2.607414
H	-2.797038	-0.416693	-2.654491
H	-3.614879	-1.635168	2.695795
H	-3.999064	-0.079514	3.440757
H	-2.454190	-0.311055	2.600379
H	-6.728758	3.101486	1.109595
H	-7.825896	1.995327	0.279175
H	-6.829685	3.108925	-0.661040
H	-2.414546	1.393931	0.111416
H	-2.752692	3.774780	-0.006431
H	-1.842587	6.092204	-0.171798
H	0.616882	6.426601	-0.334990
H	2.154922	4.511821	-0.330732
H	3.075466	2.685987	-0.880257
H	2.947321	0.424204	-1.658076
H	2.616567	-0.181021	-0.041915
H	3.438886	1.447278	1.866751

H	2.422316	2.855895	1.767730
H	4.905600	0.179550	0.701000
H	4.802733	-0.870096	-0.687672
H	4.210353	4.215713	0.758934
H	4.596840	3.606960	2.354505
H	6.730249	0.509434	-0.912983
H	5.604547	0.924040	-2.192634
H	6.156764	1.928231	1.371392
H	6.556998	3.591865	1.016599
H	6.862076	2.837068	-1.119193
H	5.144204	3.084974	-1.251282

26-B

M06 SCF energy: -2598.855242 a.u.
Enthalpy at 298K: -2598.060686 a.u.
Gibbs free energy at 298K: -2598.19019 a.u.
Cartesian Coordinates

Ru	-0.962038	-0.038927	-0.972857
C	-1.762681	-0.847402	0.644622
N	-1.370132	-1.903117	1.405732
C	-2.358324	-2.255896	2.445625
C	-3.561260	-1.375848	2.085691
N	-3.001690	-0.469474	1.067828
C	-3.767531	0.672866	0.639305
C	-4.780144	0.527247	-0.328365
C	-5.508598	1.666990	-0.693713
C	-5.290151	2.911096	-0.100287
C	-4.335050	2.998267	0.919107
C	-3.571331	1.898722	1.312092
C	-2.587700	2.031293	2.449664
C	-5.163437	-0.812084	-0.911825
C	-6.062283	4.132342	-0.540687
C	-0.095500	-2.562502	1.447028
C	0.082796	-3.767847	0.746048
C	1.319395	-4.415346	0.855915
C	2.130316	-2.724083	2.353413
C	0.916728	-2.035179	2.272988
C	2.356277	-3.909376	1.643835
C	0.722161	-0.743184	3.033563
C	-1.016477	-4.361386	-0.101506
C	3.694192	-4.607193	1.713118
Cl	-2.085699	-1.588503	-2.406639
Cl	-0.443555	2.192231	-0.290875
C	0.771140	-0.679047	-0.951426
C	1.650947	-0.622022	-2.111904
C	3.048815	-0.401766	-1.936701

C	3.913135	-0.468021	-3.031400
C	3.419532	-0.719625	-4.311289
C	2.047690	-0.897115	-4.510598
C	1.177889	-0.846563	-3.426832
O	3.589736	-0.161079	-0.704294
C	3.333663	1.139092	-0.077315
C	3.968885	2.255198	-0.919218
C	3.835340	0.958935	1.360067
C	3.630394	3.692144	-0.452772
C	3.485291	2.110947	2.331565
C	4.736675	4.413861	0.345105
C	4.620810	3.115069	2.627017
C	5.458445	3.610505	1.438315
H	-3.944991	-0.804077	2.935901
H	-4.389643	-1.953442	1.659278
H	-1.955321	-2.034067	3.441047
H	-2.584142	-3.325207	2.403084
H	-6.278658	1.567978	-1.455782
H	-4.178843	3.949345	1.423365
H	-1.558239	1.966167	2.085900
H	-2.708003	2.999632	2.944825
H	-2.730595	1.250214	3.206926
H	-5.627693	-0.685541	-1.894508
H	-5.901706	-1.311899	-0.267993
H	-4.307250	-1.475874	-1.037271
H	-5.470687	4.738334	-1.239349
H	-6.315928	4.775541	0.309497
H	-6.991887	3.858386	-1.050151
H	1.471694	-5.342310	0.307639
H	2.920458	-2.322210	2.984054
H	0.556865	0.103492	2.357260
H	-0.140576	-0.785089	3.709326
H	1.603430	-0.519369	3.641759
H	-1.896515	-4.621230	0.501743
H	-0.671413	-5.278339	-0.588546
H	-1.351181	-3.664170	-0.876359
H	3.610822	-5.663364	1.437160
H	4.125470	-4.550611	2.718780
H	4.413182	-4.143119	1.025366
H	1.252637	-0.994916	-0.025494
H	0.120873	-1.042408	-3.571264
H	1.658144	-1.092796	-5.505341
H	4.106018	-0.767257	-5.152616
H	4.972516	-0.309093	-2.856163
H	2.247427	1.300827	-0.056981
H	3.599621	2.126176	-1.942400
H	5.055240	2.099630	-0.966727

H	4.917409	0.772792	1.342029
H	3.379571	0.029156	1.717880
H	3.415278	4.304845	-1.336725
H	2.692690	3.678539	0.113020
H	2.596581	2.636492	1.966136
H	3.183576	1.676694	3.293502
H	5.504418	4.753419	-0.364908
H	4.311268	5.327243	0.785028
H	5.315491	2.643905	3.337340
H	4.192019	3.978400	3.155592
H	5.969605	2.754379	0.978386
H	6.262521	4.242473	1.840189

26-D

M06 SCF energy: -697.809634 a.u.
Enthalpy at 298K: -697.444777 a.u.
Gibbs free energy at 298K: -697.505681 a.u.
Cartesian Coordinates

C	3.059297	1.748968	-0.359609
C	2.849873	0.324946	-0.049478
C	1.529477	-0.185386	0.061111
C	1.318262	-1.539773	0.349299
C	2.405746	-2.395253	0.538184
C	3.709273	-1.913491	0.429969
C	3.915671	-0.567893	0.132046
O	0.530083	0.727430	-0.116043
C	-0.860119	0.351781	-0.011380
C	-1.327640	-0.376927	-1.291863
C	-1.563046	1.691293	0.269612
C	-2.337289	-1.524260	-1.085292
C	-3.084632	1.754883	0.074883
C	-3.745922	-1.202248	-0.548076
C	-3.958221	0.894789	1.000617
C	-3.804278	-0.636413	0.891029
C	4.183189	2.449667	-0.156378
H	2.198680	2.260245	-0.781713
H	4.929823	-0.195731	0.018316
H	4.556917	-2.579730	0.561483
H	2.223833	-3.443603	0.759789
H	0.313271	-1.936482	0.427583
H	-0.964088	-0.312389	0.854233
H	-0.438995	-0.811174	-1.763737
H	-1.719400	0.354227	-2.010811
H	-1.104731	2.422777	-0.408641
H	-1.300287	2.010081	1.286616
H	-2.453766	-2.033199	-2.051653

H	-1.881893	-2.267975	-0.413609
H	-3.381997	2.802508	0.215542
H	-3.328032	1.525211	-0.970096
H	-4.265188	-0.525696	-1.241039
H	-4.312884	-2.141547	-0.578732
H	-5.005459	1.148300	0.783375
H	-3.787402	1.193700	2.044581
H	-4.655351	-1.085797	1.418527
H	-2.917688	-0.969503	1.445742
H	5.071001	2.021379	0.302106
H	4.245132	3.496864	-0.437561

27-A

M06 SCF energy: -2794.151889 a.u.
Enthalpy at 298K: -2793.229557 a.u.
Gibbs free energy at 298K: -2793.365952 a.u.
Cartesian Coordinates

Cl	-0.170280	-0.456579	-2.445929
Cl	0.103433	0.079561	2.302559
Ru	-0.360147	-0.084032	-0.061385
C	-1.556271	-1.666971	0.216005
N	-2.906604	-1.779214	0.321664
C	-3.914335	-0.761606	0.237458
C	-4.370638	-0.162754	1.427303
C	-3.755221	-0.502809	2.764163
H	-4.256527	0.044985	3.567858
H	-2.688146	-0.251775	2.791145
H	-3.839249	-1.573251	2.991229
C	-5.389629	0.791112	1.336639
H	-5.741509	1.268691	2.248662
C	-5.963770	1.146511	0.110924
C	-7.089527	2.153087	0.046587
H	-6.989068	2.918140	0.823986
H	-8.063347	1.667109	0.194267
H	-7.122536	2.656982	-0.925082
C	-5.489601	0.523676	-1.048525
H	-5.920937	0.790887	-2.010911
C	-4.471846	-0.436713	-1.013138
C	-3.970208	-1.064474	-2.291749
H	-2.906727	-0.854301	-2.454012
H	-4.528878	-0.681263	-3.150962
H	-4.086211	-2.155621	-2.284844
C	-3.366762	-3.175688	0.458534
H	-3.910441	-3.481742	-0.443148
H	-4.045861	-3.269652	1.311283
C	-2.056449	-3.945509	0.646887

H	-1.926442	-4.308443	1.673503
H	-1.959764	-4.798613	-0.030992
N	-1.039215	-2.924422	0.340751
C	0.348293	-3.313669	0.354676
C	1.043806	-3.391496	1.578218
C	0.378370	-3.170672	2.916250
H	0.079103	-4.137598	3.346612
H	-0.497587	-2.527172	2.850000
H	1.069349	-2.698895	3.620300
C	2.385583	-3.792704	1.552289
H	2.932636	-3.832008	2.492028
C	3.027651	-4.163707	0.370241
C	4.485761	-4.558960	0.364321
H	4.816461	-4.889606	1.354434
H	5.121401	-3.712576	0.072052
H	4.679212	-5.368731	-0.348103
C	2.277461	-4.172581	-0.811552
H	2.740319	-4.518354	-1.733352
C	0.939267	-3.771929	-0.845104
C	0.148125	-3.908695	-2.123495
H	0.787387	-4.288436	-2.926313
H	-0.270836	-2.952763	-2.446071
H	-0.681039	-4.618802	-2.001792
C	-1.569424	1.299588	-0.182159
H	-2.628031	1.199107	0.050763
C	-1.174380	2.612267	-0.631671
C	-2.161062	3.579132	-0.921847
H	-3.201569	3.313472	-0.753105
C	-1.823139	4.826696	-1.427636
H	-2.591900	5.559262	-1.653610
C	-0.475061	5.119370	-1.653370
H	-0.190836	6.084401	-2.064548
C	0.528856	4.193385	-1.363626
H	1.556710	4.460883	-1.569434
C	0.193113	2.941798	-0.836577
O	1.079498	1.961776	-0.491410
C	2.515941	2.259862	-0.293880
H	2.664942	3.304543	-0.576022
C	3.360667	1.411536	-1.262425
H	4.389358	1.778347	-1.121843
C	2.992414	1.685807	-2.735816
H	1.956712	1.374603	-2.912411
H	3.047953	2.765339	-2.937945
C	3.921235	0.930987	-3.700179
H	3.609138	1.115600	-4.736117
H	4.945721	1.323602	-3.606663
C	3.927488	-0.576431	-3.406564

H	2.927790	-0.985422	-3.605693
H	4.625980	-1.091703	-4.079387
C	4.298396	-0.851282	-1.941855
H	5.339842	-0.539458	-1.765633
H	4.251885	-1.927667	-1.733899
C	3.369778	-0.101764	-0.971501
H	2.353515	-0.498383	-1.078294
H	3.681711	-0.293781	0.062225
C	2.836536	2.141719	1.209118
H	2.565803	1.133429	1.542118
C	4.340967	2.361533	1.488789
H	4.947873	1.617456	0.960713
H	4.645423	3.347116	1.101112
C	4.659077	2.289927	2.992031
H	4.460834	1.268588	3.348321
H	5.729558	2.474896	3.151127
C	3.815004	3.278871	3.806381
H	4.099197	4.307130	3.534729
H	4.029494	3.168468	4.877436
C	2.319468	3.071756	3.533003
H	2.006889	2.089320	3.911776
H	1.725069	3.819602	4.073824
C	1.999626	3.143937	2.032903
H	2.199246	4.164809	1.668101
H	0.935203	2.944351	1.882871

27-B

M06 SCF energy: -2794.132326 a.u.
Enthalpy at 298K: -2793.210384 a.u.
Gibbs free energy at 298K: -2793.350208 a.u.
Cartesian Coordinates

Ru	-1.629325	0.089769	1.014028
C	-2.226374	1.104106	-0.572406
N	-1.647651	2.138390	-1.240149
C	-2.515687	2.686538	-2.302543
C	-3.857672	1.998935	-2.031279
N	-3.487448	0.947904	-1.067669
H	-4.591621	2.679052	-1.583141
H	-4.302708	1.555812	-2.926965
H	-2.106556	2.438882	-3.289827
H	-2.570077	3.775702	-2.221620
Cl	-1.579656	-2.174949	0.260691
Cl	-2.446615	1.776647	2.508227
C	-4.441181	-0.085588	-0.752686
C	-4.418206	-1.270435	-1.518515
C	-5.366744	-2.255991	-1.241239

C	-6.335655	-2.092483	-0.245442
C	-6.371179	-0.880484	0.446519
C	-5.452084	0.147253	0.199967
C	-5.621181	1.476455	0.897245
H	-4.673013	1.891109	1.245193
H	-6.090646	2.210476	0.226736
H	-6.277273	1.370434	1.766462
H	-7.144129	-0.716271	1.194190
C	-7.314378	-3.198891	0.070354
H	-6.872397	-3.925948	0.764302
H	-7.604601	-3.748519	-0.831999
H	-8.223766	-2.809510	0.539930
H	-5.345420	-3.177976	-1.817976
C	-3.415144	-1.479274	-2.627209
H	-2.409708	-1.621008	-2.220002
H	-3.670353	-2.370058	-3.209321
H	-3.384004	-0.627661	-3.318005
C	-0.292163	2.610998	-1.192942
C	0.677500	1.978258	-1.993329
C	1.969484	2.514144	-2.017853
C	2.308812	3.655662	-1.284752
C	1.315211	4.266297	-0.513445
C	0.008564	3.770437	-0.454270
C	-1.038629	4.477721	0.370651
H	-1.488182	3.806732	1.109273
H	-0.599284	5.329468	0.898604
H	-1.853826	4.864622	-0.255275
C	0.345307	0.747560	-2.805271
H	-0.047577	-0.059201	-2.176653
H	-0.412426	0.954449	-3.571485
H	1.235431	0.372269	-3.317897
H	2.725141	2.030729	-2.633290
H	1.558489	5.160776	0.056051
C	3.713107	4.212588	-1.313537
H	4.291374	3.875648	-0.443313
H	3.709716	5.308076	-1.294043
H	4.253740	3.891240	-2.210026
C	0.201264	0.344605	1.037914
H	0.761535	0.628362	0.148319
C	0.988728	-0.041910	2.199222
C	0.483050	0.092178	3.512506
C	1.232397	-0.271149	4.625096
C	2.519396	-0.777937	4.442401
C	3.055552	-0.928110	3.162891
C	2.304410	-0.580884	2.033696
H	4.063332	-1.310331	3.060378
H	3.125087	-1.054750	5.301552

H	0.823791	-0.144388	5.622852
H	-0.498615	0.535894	3.642267
O	2.735734	-0.710699	0.752532
C	3.872665	-1.531167	0.371907
H	4.317636	-1.973637	1.269206
C	4.917798	-0.598937	-0.277043
C	5.412088	0.462961	0.728336
C	6.120234	-1.371862	-0.859417
H	4.418334	-0.068407	-1.101106
C	6.458744	1.405400	0.115067
H	5.859598	-0.047271	1.595749
H	4.562490	1.040713	1.107390
C	7.175733	-0.431183	-1.465370
H	6.585531	-1.969898	-0.060189
H	5.789707	-2.081295	-1.626202
C	7.649682	0.626994	-0.460340
H	5.989783	1.993138	-0.687745
H	6.799948	2.125449	0.869979
H	6.744021	0.072895	-2.342890
H	8.026479	-1.018944	-1.833032
H	8.362825	1.311989	-0.936575
H	8.190546	0.132752	0.360478
C	3.354735	-2.699980	-0.492839
C	2.400116	-3.611459	0.306850
C	2.693573	-2.264773	-1.814408
H	4.241615	-3.303497	-0.740307
C	1.954195	-4.828194	-0.519047
H	1.511229	-3.040429	0.602415
H	2.890359	-3.943335	1.232945
C	2.232896	-3.476403	-2.642300
H	1.828165	-1.632224	-1.582121
H	3.385232	-1.654188	-2.410051
C	1.299166	-4.392524	-1.837885
H	1.255806	-5.437806	0.067301
H	2.825755	-5.465575	-0.734987
H	1.733987	-3.132440	-3.557944
H	3.115543	-4.049479	-2.966007
H	1.024060	-5.271378	-2.435731
H	0.367842	-3.855237	-1.611756

27-D

M06 SCF energy: -893.0857918 a.u.
Enthalpy at 298K: -892.5941338 a.u.
Gibbs free energy at 298K: -892.6672298 a.u.
Cartesian Coordinates

C	-2.780555	-0.277946	1.762985

H	-1.850567	0.002038	2.250131
C	-2.636099	-1.151233	0.585580
C	-1.403514	-1.195812	-0.114981
C	-1.255137	-2.037137	-1.224605
C	-2.323770	-2.821569	-1.660284
C	-3.543800	-2.790036	-0.984827
C	-3.682237	-1.969148	0.131743
H	-4.618160	-1.967816	0.683281
H	-4.372060	-3.411813	-1.312039
H	-2.189725	-3.470032	-2.522130
H	-0.306349	-2.097883	-1.744489
O	-0.402933	-0.410124	0.388920
C	0.689698	0.085947	-0.420222
H	0.618451	-0.342224	-1.427337
C	-3.932448	0.194157	2.258940
H	-4.896595	-0.009143	1.799463
H	-3.944064	0.817140	3.148512
C	2.003765	-0.400118	0.228544
C	2.066843	-1.941223	0.277346
C	3.258901	0.155153	-0.477075
H	2.008407	-0.038792	1.267335
C	3.358513	-2.447073	0.936712
H	2.014501	-2.334784	-0.750120
H	1.193125	-2.331219	0.809407
C	4.558727	-0.358858	0.165710
H	3.236697	-0.140735	-1.537768
H	3.260456	1.251038	-0.460429
C	4.603700	-1.891468	0.231820
H	3.374434	-3.544432	0.933354
H	3.370755	-2.138839	1.992727
H	5.423356	0.026005	-0.390113
H	4.638361	0.048229	1.184632
H	5.515788	-2.222950	0.744512
H	4.653378	-2.298155	-0.789413
C	0.528387	1.616396	-0.561974
C	-0.778824	1.978948	-1.296972
C	0.617513	2.382190	0.773458
H	1.358913	1.953021	-1.201091
C	-0.915880	3.495076	-1.506765
H	-1.633752	1.618336	-0.710711
H	-0.820001	1.459835	-2.264411
C	0.471992	3.899679	0.571641
H	-0.177336	2.022473	1.440086
H	1.569235	2.172206	1.277354
C	-0.821232	4.255008	-0.175158
H	-1.867030	3.718321	-2.006835
H	-0.119146	3.844588	-2.180770

H	0.503215	4.408950	1.543556
H	1.333926	4.272582	-0.002224
H	-0.876521	5.337617	-0.347786
H	-1.685477	3.991838	0.452258

28-A

M06 SCF energy: -2714.370608 a.u.
Enthalpy at 298K: -2713.531409 a.u.
Gibbs free energy at 298K: -2713.658436 a.u.
Cartesian Coordinates

C	-2.780555	-0.277946	1.762985
H	-1.850567	0.002038	2.250131
C	-2.636099	-1.151233	0.585580
C	-1.403514	-1.195812	-0.114981
C	-1.255137	-2.037137	-1.224605
C	-2.323770	-2.821569	-1.660284
C	-3.543800	-2.790036	-0.984827
C	-3.682237	-1.969148	0.131743
H	-4.618160	-1.967816	0.683281
H	-4.372060	-3.411813	-1.312039
H	-2.189725	-3.470032	-2.522130
H	-0.306349	-2.097883	-1.744489
O	-0.402933	-0.410124	0.388920
C	0.689698	0.085947	-0.420222
H	0.618451	-0.342224	-1.427337
C	-3.932448	0.194157	2.258940
H	-4.896595	-0.009143	1.799463
H	-3.944064	0.817140	3.148512
C	2.003765	-0.400118	0.228544
C	2.066843	-1.941223	0.277346
C	3.258901	0.155153	-0.477075
H	2.008407	-0.038792	1.267335
C	3.358513	-2.447073	0.936712
H	2.014501	-2.334784	-0.750120
H	1.193125	-2.331219	0.809407
C	4.558727	-0.358858	0.165710
H	3.236697	-0.140735	-1.537768
H	3.260456	1.251038	-0.460429
C	4.603700	-1.891468	0.231820
H	3.374434	-3.544432	0.933354
H	3.370755	-2.138839	1.992727
H	5.423356	0.026005	-0.390113
H	4.638361	0.048229	1.184632
H	5.515788	-2.222950	0.744512
H	4.653378	-2.298155	-0.789413
C	0.528387	1.616396	-0.561974

C	-0.778824	1.978948	-1.296972
C	0.617513	2.382190	0.773458
H	1.358913	1.953021	-1.201091
C	-0.915880	3.495076	-1.506765
H	-1.633752	1.618336	-0.710711
H	-0.820001	1.459835	-2.264411
C	0.471992	3.899679	0.571641
H	-0.177336	2.022473	1.440086
H	1.569235	2.172206	1.277354
C	-0.821232	4.255008	-0.175158
H	-1.867030	3.718321	-2.006835
H	-0.119146	3.844588	-2.180770
H	0.503215	4.408950	1.543556
H	1.333926	4.272582	-0.002224
H	-0.876521	5.337617	-0.347786
H	-1.685477	3.991838	0.452258

28-B

M06 SCF energy: -2714.349239 a.u.
Enthalpy at 298K: -2713.510296 a.u.
Gibbs free energy at 298K: -2713.64158 a.u.
Cartesian Coordinates

Ru	-1.442472	-0.079188	0.920310
C	-2.233768	0.717616	-0.702992
N	-1.886584	1.812418	-1.429806
C	-2.821440	2.080932	-2.541222
C	-3.968323	1.101248	-2.265071
N	-3.403349	0.237619	-1.214552
C	-4.114536	-0.946380	-0.806560
C	-5.170025	-0.855308	0.121844
C	-5.833695	-2.035450	0.481073
C	-5.511763	-3.270404	-0.083962
C	-4.522287	-3.306610	-1.073129
C	-3.820630	-2.163649	-1.459721
C	-2.808459	-2.241317	-2.577261
C	-5.670326	0.463836	0.661058
C	-6.213066	-4.534556	0.353991
C	-0.688819	2.599888	-1.361815
C	-0.698367	3.800307	-0.628422
C	0.458668	4.586244	-0.639861
C	1.568374	3.021252	-2.084066
C	0.437547	2.197929	-2.103822
C	1.601036	4.214943	-1.356311
C	0.452383	0.896601	-2.872230
C	-1.910543	4.228976	0.162806
C	2.846285	5.070715	-1.324533

Cl	-2.807659	1.210250	2.405796
Cl	-0.551317	-2.129055	0.062293
C	0.178436	0.791885	1.084305
C	0.997888	0.649354	2.275987
C	2.422836	0.673989	2.154891
C	3.221252	0.522970	3.293033
C	2.629828	0.350129	4.545747
C	1.241654	0.324120	4.688022
C	0.440161	0.468078	3.561427
O	2.892747	0.847323	0.892067
C	4.280288	0.739908	0.547062
C	4.631532	-0.610188	-0.095024
C	6.127792	-0.577591	-0.496100
C	4.405527	-1.797511	0.873024
C	3.782251	-0.842223	-1.369238
C	6.532058	-1.903040	-1.175082
C	4.805606	-3.124948	0.194117
C	4.183911	-2.166420	-2.049997
C	6.296652	-3.072796	-0.197205
C	5.675162	-2.112769	-2.440868
C	3.946620	-3.333825	-1.070143
H	-4.244898	0.507374	-3.141336
H	-4.869172	1.604496	-1.893954
H	-2.328664	1.892702	-3.502828
H	-3.139927	3.127376	-2.523136
H	-6.635308	-1.977159	1.214422
H	-4.290144	-4.251018	-1.560335
H	-3.015629	-1.505088	-3.364462
H	-1.795709	-2.063963	-2.205511
H	-2.828652	-3.233355	-3.038498
H	-6.104801	0.335343	1.656766
H	-6.461540	0.862584	0.009422
H	-4.879932	1.209224	0.747174
H	-6.348612	-5.229130	-0.482460
H	-7.197428	-4.320348	0.783308
H	-5.628723	-5.060697	1.120341
H	0.464615	5.514249	-0.072046
H	2.445458	2.718336	-2.652035
H	1.410620	0.763082	-3.382582
H	-0.335268	0.857462	-3.634707
H	0.300792	0.036930	-2.208960
H	-2.791403	4.357199	-0.479465
H	-1.725026	5.184966	0.661717
H	-2.173349	3.487346	0.925294
H	3.466492	4.833018	-0.449953
H	2.599595	6.136304	-1.264919
H	3.463452	4.914205	-2.215530

H	0.650174	1.298025	0.245715
H	-0.640260	0.492350	3.662188
H	0.789261	0.200808	5.667126
H	3.269784	0.235754	5.416918
H	4.301610	0.525680	3.219587
H	4.921482	0.943119	1.410907
H	4.445451	1.543569	-0.179869
H	6.751384	-0.408707	0.394409
H	6.313960	0.264560	-1.179183
H	3.352729	-1.838937	1.176332
H	4.999990	-1.653432	1.787032
H	3.929536	-0.002247	-2.065257
H	2.718773	-0.860265	-1.104389
H	7.594372	-1.857438	-1.449866
H	4.635852	-3.951435	0.896293
H	3.570502	-2.310210	-2.949203
H	6.920092	-2.946713	0.699374
H	6.598819	-4.019755	-0.665451
H	5.850715	-1.295936	-3.155487
H	5.969547	-3.044723	-2.942940
H	4.208259	-4.287668	-1.549112
H	2.883854	-3.388337	-0.800552

28-D

M06 SCF energy: -813.305276 a.u.
Enthalpy at 298K: -812.896408 a.u.
Gibbs free energy at 298K: -812.958089 a.u.
Cartesian Coordinates

C	2.789498	2.001830	-0.124638
C	3.297120	0.621314	-0.065033
C	2.385823	-0.463918	-0.002922
C	2.852292	-1.782608	0.049539
C	4.224849	-2.039704	0.040815
C	5.137566	-0.988271	-0.027159
C	4.667105	0.322328	-0.084588
O	1.060119	-0.133315	0.011088
C	0.081676	-1.170784	0.034013
C	-1.317713	-0.552326	0.015723
C	-1.540651	0.289909	-1.264399
C	-2.361387	-1.697139	0.038314
C	-1.546604	0.346942	1.255392
C	-2.969028	0.871542	-1.281181
C	-3.793118	-1.121516	0.021390
C	-2.975364	0.927946	1.238844
C	-3.993040	-0.281402	-1.257458
C	-3.173164	1.766760	-0.041055

C	-3.999583	-0.225232	1.260246
C	3.480185	3.115818	0.153529
H	1.747086	2.098637	-0.415402
H	5.376127	1.141080	-0.166993
H	6.205490	-1.185326	-0.047295
H	4.573148	-3.068377	0.080925
H	2.155601	-2.610772	0.101673
H	0.212355	-1.780061	0.941131
H	0.217676	-1.826238	-0.839617
H	-1.380556	-0.339828	-2.152017
H	-0.800459	1.097465	-1.310225
H	-2.217631	-2.315224	0.936494
H	-2.212669	-2.355579	-0.829881
H	-0.805011	1.154349	1.268281
H	-1.391665	-0.242732	2.170954
H	-3.106364	1.467459	-2.193199
H	-4.514843	-1.948864	0.038164
H	-3.117791	1.563890	2.122578
H	-3.870662	-0.913617	-2.148098
H	-5.015813	0.118985	-1.288347
H	-2.461075	2.603358	-0.058157
H	-4.181126	2.204225	-0.053729
H	-5.022365	0.176304	1.267878
H	-3.882189	-0.817035	2.178849
H	4.513556	3.100642	0.490735
H	3.019457	4.094841	0.060357

29-A

M06 SCF energy: -2714.362453 a.u.
Enthalpy at 298K: -2713.523599 a.u.
Gibbs free energy at 298K: -2713.649557 a.u.
Cartesian Coordinates

Ru	-0.294307	0.009213	-0.034178
C	-1.490826	1.611328	-0.059687
N	-2.841753	1.741912	-0.147228
C	-3.290104	3.148922	-0.131887
C	-1.977919	3.919698	-0.295610
N	-0.966925	2.872791	-0.065919
C	0.419114	3.254855	0.031557
C	1.179334	3.468383	-1.136721
C	2.516911	3.858918	-0.991988
C	3.093637	4.088338	0.258715
C	2.281838	3.963087	1.391303
C	0.944691	3.567657	1.305638
C	0.090363	3.539210	2.549561
C	0.582137	3.397541	-2.522024

C	4.549382	4.471742	0.387140
C	-3.857141	0.729543	-0.088987
C	-4.404549	0.247005	-1.293024
C	-5.427661	-0.703671	-1.217352
C	-5.359146	-0.655415	1.182985
C	-4.332748	0.296261	1.163093
C	-5.920423	-1.166188	0.007878
C	-3.732557	0.796635	2.455804
C	-3.887794	0.711094	-2.633854
C	-7.051983	-2.167025	0.058175
Cl	-0.099217	0.048561	-2.458099
Cl	0.095571	0.075531	2.362645
C	-1.499412	-1.370984	0.063992
C	-1.065301	-2.735340	0.225617
C	0.311136	-3.099032	0.184273
C	0.648929	-4.446860	0.363796
C	-0.340306	-5.407381	0.581817
C	-1.692642	-5.062549	0.627074
C	-2.040812	-3.732477	0.446992
O	1.192180	-2.067796	-0.015120
C	2.547392	-2.250590	-0.662874
C	3.555060	-2.940903	0.304803
C	3.079965	-0.810359	-0.911157
C	3.673544	-2.153778	1.628414
C	4.951925	-3.012127	-0.363640
C	3.232819	-0.020297	0.407849
C	4.478244	-0.872676	-1.577388
C	4.216709	-0.738116	1.349152
C	5.477531	-1.594628	-0.651689
C	5.602419	-0.827069	0.679859
C	2.293128	-2.990176	-1.981547
H	-1.863379	4.730837	0.429205
H	-1.862164	4.340020	-1.302103
H	-3.794366	3.371646	0.816591
H	-3.999299	3.331639	-0.944291
H	3.113713	4.006978	-1.889762
H	2.695463	4.190909	2.371213
H	-0.806486	4.161491	2.435193
H	-0.232632	2.521913	2.786046
H	0.653173	3.925984	3.404629
H	1.346172	3.135264	-3.259897
H	0.177868	4.379549	-2.808096
H	-0.210755	2.654274	-2.600311
H	4.713731	5.147010	1.233981
H	4.916448	4.965159	-0.519051
H	5.176705	3.585735	0.553627
H	-5.848678	-1.092520	-2.142163

H	-5.727101	-1.005619	2.145076
H	-4.257731	0.365371	3.313397
H	-3.799859	1.888137	2.543899
H	-2.671553	0.532334	2.538079
H	-2.820282	0.492257	-2.750538
H	-4.011254	1.794021	-2.764559
H	-4.431165	0.218090	-3.445678
H	-6.991507	-2.883285	-0.768492
H	-8.026516	-1.666377	-0.018645
H	-7.048753	-2.729966	0.997351
H	-2.579297	-1.237829	0.032634
H	-3.083172	-3.425371	0.474988
H	-2.452996	-5.818267	0.798628
H	-0.037384	-6.442133	0.719103
H	1.676206	-4.772581	0.337638
H	3.248129	-3.965287	0.523666
H	2.382104	-0.299479	-1.580330
H	4.348921	-2.696533	2.304247
H	2.698845	-2.087472	2.123801
H	4.917847	-3.607832	-1.283977
H	5.633625	-3.535752	0.320485
H	2.274702	0.099537	0.918197
H	3.594220	0.988816	0.169298
H	4.438738	-1.363015	-2.557003
H	4.812739	0.156566	-1.763367
H	4.291434	-0.183961	2.293415
H	6.458930	-1.656613	-1.140981
H	5.998290	0.182017	0.497253
H	6.317389	-1.336453	1.341891
H	1.911508	-4.001506	-1.821101
H	1.558463	-2.429961	-2.567990
H	3.206453	-3.078669	-2.572013

29-B

M06 SCF energy: -2714.347983 a.u.
Enthalpy at 298K: -2713.509401 a.u.
Gibbs free energy at 298K: -2713.638328 a.u.
Cartesian Coordinates

Ru	1.359307	-0.077438	-0.965475
C	2.148973	0.829934	0.600603
N	1.762385	1.943476	1.282334
C	2.726658	2.332486	2.331363
C	3.929087	1.429416	2.037950
N	3.372369	0.461539	1.077132
C	4.136605	-0.708989	0.729897
C	5.157936	-0.629586	-0.236689

C	5.884840	-1.792718	-0.521333
C	5.654320	-2.995896	0.147907
C	4.688608	-3.014571	1.160282
C	3.926263	-1.888828	1.475246
C	2.925877	-1.945804	2.604340
C	5.545798	0.668202	-0.904871
C	6.424210	-4.245918	-0.207834
C	0.510186	2.645656	1.244901
C	0.394148	3.809117	0.462956
C	-0.817417	4.509030	0.500925
C	-1.729210	2.949383	2.080482
C	-0.541305	2.211159	2.075062
C	-1.888758	4.098798	1.299265
C	-0.415273	0.966421	2.923432
C	1.532669	4.302662	-0.396290
C	-3.172542	4.895066	1.343285
Cl	2.480624	1.379355	-2.501977
Cl	0.839686	-2.267321	-0.165148
C	-0.378201	0.548677	-0.971236
C	-1.257709	0.379582	-2.118284
C	-2.647042	0.092973	-1.911169
C	-3.496977	-0.001399	-3.020506
C	-2.992487	0.147746	-4.314209
C	-1.638642	0.397623	-4.534080
C	-0.785101	0.509285	-3.442152
O	-2.998085	-0.083810	-0.613861
C	-4.310536	-0.476770	-0.094207
C	-4.025522	-0.689306	1.422692
C	-4.785052	-1.843284	-0.669772
C	-2.932896	-1.764714	1.622966
C	-5.305081	-1.152831	2.157365
C	-3.690184	-2.916487	-0.471001
C	-6.069645	-2.304457	0.062396
C	-3.406474	-3.107063	1.032672
C	-5.789329	-2.492094	1.566095
C	-4.693461	-3.562139	1.750133
C	-5.274937	0.696134	-0.324201
H	4.305635	0.913036	2.925847
H	4.761375	1.977488	1.580545
H	2.297820	2.153361	3.324974
H	2.962343	3.397442	2.251379
H	6.662448	-1.745823	-1.280771
H	4.521864	-3.931724	1.720916
H	3.057006	-1.115197	3.309114
H	1.902510	-1.905491	2.219695
H	3.038058	-2.878986	3.164637
H	6.060900	0.474467	-1.850605

H	6.241319	1.235220	-0.269176
H	4.684329	1.300692	-1.124151
H	6.634345	-4.854184	0.678993
H	7.377084	-4.007575	-0.691902
H	5.851257	-4.873895	-0.902716
H	-0.922023	5.401965	-0.111549
H	-2.549156	2.616724	2.713584
H	-1.352322	0.765507	3.450621
H	0.372068	1.063029	3.681661
H	-0.173990	0.085048	2.319443
H	2.422426	4.531850	0.204722
H	1.246583	5.218617	-0.921988
H	1.830419	3.556027	-1.139511
H	-3.357875	5.407796	0.393679
H	-3.136333	5.663775	2.127006
H	-4.034991	4.254696	1.557515
H	-0.853970	0.912007	-0.062119
H	0.261994	0.749998	-3.592074
H	-1.253840	0.517844	-5.542111
H	-3.676919	0.064908	-5.154723
H	-4.551184	-0.198845	-2.894137
H	-3.682776	0.269179	1.834217
H	-5.012054	-1.751541	-1.735679
H	-2.736136	-1.874895	2.698680
H	-1.994701	-1.461924	1.150449
H	-6.099174	-0.398088	2.098795
H	-5.073725	-1.274444	3.224193
H	-2.769411	-2.636498	-0.993109
H	-4.035403	-3.860426	-0.914385
H	-6.890107	-1.591781	-0.090092
H	-6.399252	-3.254377	-0.379551
H	-2.618637	-3.859252	1.161261
H	-6.709390	-2.808326	2.075462
H	-5.036803	-4.524581	1.345301
H	-4.496291	-3.717701	2.820117
H	-4.843232	1.605718	0.107463
H	-5.454494	0.883721	-1.385468
H	-6.245350	0.524534	0.145875

29-D

M06 SCF energy: -813.301727 a.u.
Enthalpy at 298K: -812.893654 a.u.
Gibbs free energy at 298K: -812.954759 a.u.
Cartesian Coordinates

C	2.659784	1.894974	-0.432065
C	2.847944	0.447663	-0.236493

C	1.731753	-0.421634	-0.284679
C	1.905986	-1.803597	-0.138330
C	3.175019	-2.336380	0.083832
C	4.285878	-1.491383	0.140336
C	4.117489	-0.120820	-0.032152
O	0.497839	0.115125	-0.569180
C	-0.567123	0.210843	0.441482
C	-1.369232	-1.120026	0.509224
C	-1.511938	1.304362	-0.126378
C	-1.839896	-1.522490	-0.906535
C	-2.615075	-0.952503	1.413971
C	-1.983448	0.908332	-1.544429
C	-2.757695	1.472963	0.774701
C	-2.758385	-0.424249	-1.483196
C	-3.536915	0.143832	0.844275
C	-3.993404	-0.258525	-0.573190
C	0.056562	0.607529	1.782931
C	3.511419	2.864396	-0.070877
H	1.724936	2.172394	-0.911698
H	4.987740	0.529372	-0.028296
H	5.280000	-1.901224	0.295646
H	3.295990	-3.410730	0.194340
H	1.045210	-2.457696	-0.218444
H	-0.727317	-1.903125	0.931405
H	-0.953858	2.248609	-0.171541
H	-2.381469	-2.477054	-0.851990
H	-0.977615	-1.673070	-1.564347
H	-2.325423	-0.712552	2.444438
H	-3.152206	-1.909886	1.458567
H	-1.123349	0.819175	-2.214532
H	-2.629754	1.701826	-1.944660
H	-2.478510	1.806101	1.781855
H	-3.395740	2.261569	0.353304
H	-3.079581	-0.709241	-2.493812
H	-4.412308	0.263620	1.496346
H	-4.666321	0.507392	-0.983592
H	-4.564040	-1.197070	-0.532322
H	0.724979	-0.177796	2.150568
H	0.641029	1.526769	1.672427
H	-0.703845	0.779427	2.547360
H	4.446629	2.665345	0.446548
H	3.289757	3.907120	-0.278695

30-A

M06 SCF energy: -2622.775283 a.u.
Enthalpy at 298K: -2622.190296 a.u.

Gibbs free energy at 298K: -2622.31132 a.u.
Cartesian Coordinates

Ru	-0.179590	0.358056	0.000330
C	-0.126909	-1.642274	-0.002061
N	0.897468	-2.532117	-0.004433
C	0.449482	-3.939773	-0.003811
C	-1.081254	-3.813585	-0.012247
N	-1.286211	-2.355637	-0.003717
H	-1.548593	-4.266697	0.868701
H	-1.537423	-4.254407	-0.905365
H	0.828451	-4.455679	0.885076
H	0.838136	-4.459751	-0.885958
C	-2.626992	-1.829126	-0.001460
C	-3.295298	-1.629328	-1.228112
C	-4.590602	-1.103365	-1.195902
C	-5.245092	-0.813646	0.004196
C	-4.588963	-1.112720	1.201394
C	-3.293835	-1.638669	1.227760
H	-5.102484	-0.925265	-2.139317
H	-5.099606	-0.941895	2.146830
C	-2.704117	-2.075013	2.548014
H	-3.026042	-3.100620	2.781780
H	-1.615515	-2.041756	2.551359
H	-3.050156	-1.429375	3.359716
C	-2.708171	-2.055774	-2.552749
H	-3.048400	-1.398551	-3.357584
H	-3.038246	-3.076142	-2.797715
H	-1.619344	-2.031102	-2.555349
C	-6.623938	-0.196888	0.007965
H	-7.200669	-0.507448	0.885938
H	-7.190158	-0.473075	-0.888026
H	-6.562892	0.899232	0.029885
C	2.307883	-2.276255	-0.001950
C	2.988422	-2.177473	-1.229897
C	4.371717	-1.968716	-1.200251
H	4.906891	-1.879681	-2.143288
C	4.368540	-1.971529	1.202534
C	2.985164	-2.180296	1.228067
H	4.901221	-1.884557	2.147181
C	5.080237	-1.866931	0.002185
C	2.243908	-2.248532	2.542476
H	2.941330	-2.163281	3.381163
H	1.703232	-3.196271	2.658663
H	1.504819	-1.443092	2.629447
H	1.707691	-3.189864	-2.663892
C	2.250603	-2.243578	-2.546312
H	2.950521	-2.160066	-3.383099

H	1.513756	-1.436255	-2.635067
C	6.579670	-1.676713	0.004407
H	6.916236	-1.128193	-0.881771
H	7.100720	-2.643519	0.004797
H	6.913703	-1.128877	0.891972
Cl	-0.591473	0.535707	-2.357670
Cl	-0.605860	0.532295	2.355855
C	1.607985	0.808463	0.006283
H	2.424506	0.088885	0.010667
C	2.025982	2.199374	0.006146
C	1.070139	3.235181	0.003115
C	1.419890	4.577344	0.002372
C	2.780397	4.904492	0.004673
C	3.761273	3.909629	0.007784
C	3.385150	2.569847	0.008599
H	4.134946	1.783377	0.010928
H	4.812408	4.181724	0.009573
H	3.067106	5.952052	0.004027
H	0.670393	5.357734	0.000093
O	-0.236633	2.747584	0.001335
C	-1.333211	3.573200	-0.003520
F	-2.410158	2.801318	-0.004784
F	-1.351630	4.362140	-1.088466
F	-1.357545	4.366704	1.078043

30-B

M06 SCF energy: -2622.767547 a.u.
Enthalpy at 298K: -2622.182489 a.u.
Gibbs free energy at 298K: -2622.300607 a.u.
Cartesian Coordinates

Ru	-0.694738	-0.771152	0.340193
C	-1.197193	1.123553	0.082927
N	-0.473190	2.268541	0.154739
C	-1.292186	3.475258	-0.081156
C	-2.721640	2.923438	-0.054615
N	-2.500577	1.468238	-0.118872
C	-3.624723	0.582781	-0.286834
C	-4.400173	0.203020	0.825378
C	-5.484709	-0.657190	0.608021
C	-5.836744	-1.100560	-0.667227
C	-5.099745	-0.626130	-1.759211
C	-4.003328	0.221620	-1.599248
C	-3.283701	0.764230	-2.810578
C	-4.170225	0.758980	2.210944
C	-6.983028	-2.063014	-0.869929
C	0.949037	2.434254	0.248124

C	1.527228	2.661430	1.508140
C	2.910731	2.871520	1.567714
C	3.092865	2.660497	-0.818093
C	1.719255	2.435531	-0.931998
C	3.709336	2.870911	0.421631
C	1.104880	2.135028	-2.279693
C	0.696566	2.649988	2.769595
C	5.204680	3.066986	0.503108
Cl	-1.193321	-0.823081	2.671158
Cl	-0.945014	-1.615423	-1.863987
C	1.147548	-0.722775	0.422084
C	1.915511	-1.923070	0.730442
C	3.286820	-2.023543	0.400622
C	4.034888	-3.163561	0.665664
C	3.421824	-4.259847	1.273652
C	2.070056	-4.198651	1.622593
C	1.333706	-3.049344	1.360063
O	3.947865	-0.908804	-0.141118
C	4.141210	-0.869415	-1.484317
F	4.785480	-1.956460	-1.949021
F	4.891564	0.206699	-1.748984
F	2.988216	-0.766218	-2.166507
H	-3.326586	3.257294	-0.902429
H	-3.253010	3.181250	0.869596
H	-1.030051	3.923029	-1.047421
H	-1.104439	4.217856	0.699363
H	-6.075032	-0.974227	1.465202
H	-5.387488	-0.922635	-2.765369
H	-3.280560	1.862003	-2.819187
H	-2.246271	0.422186	-2.844622
H	-3.777790	0.429080	-3.727361
H	-4.422570	0.017204	2.974099
H	-4.816771	1.632891	2.376601
H	-3.134797	1.053244	2.380456
H	-7.546614	-1.830821	-1.780533
H	-7.678186	-2.044420	-0.024200
H	-6.615929	-3.092831	-0.970788
H	3.373409	3.031270	2.539042
H	3.701108	2.644654	-1.718783
H	1.855293	2.224175	-3.070352
H	0.282932	2.818371	-2.524683
H	0.700316	1.116553	-2.315094
H	0.186946	1.689409	2.906067
H	-0.077755	3.428034	2.755265
H	1.326763	2.830369	3.645562
H	5.729040	2.202984	0.077899
H	5.538550	3.190982	1.537854

H	5.524815	3.951024	-0.062441
H	1.727356	0.160426	0.170238
H	0.298159	-2.992771	1.682413
H	1.593753	-5.042492	2.112490
H	4.003497	-5.152816	1.482962
H	5.085732	-3.180793	0.399386

30-D

M06 SCF energy: -721.720958 a.u.
Enthalpy at 298K: -721.720958 a.u.
Gibbs free energy at 298K: -721.616508 a.u.
Cartesian Coordinates

C	0.897645	1.971679	-0.335029
C	1.243237	0.547176	-0.199038
C	0.279380	-0.449950	-0.427869
C	0.562393	-1.808813	-0.323895
C	1.848204	-2.212497	0.030433
C	2.834546	-1.249782	0.262894
C	2.535072	0.103489	0.141201
O	-1.006087	-0.061956	-0.852887
C	-1.997801	-0.051148	0.073274
F	-3.099952	0.406336	-0.521946
F	-1.711608	0.741301	1.122259
F	-2.259107	-1.280072	0.564919
C	1.611611	3.003890	0.131066
H	-0.032397	2.174869	-0.858255
H	3.318140	0.839406	0.295564
H	3.843273	-1.555856	0.525294
H	2.079313	-3.270322	0.113405
H	-0.222463	-2.529490	-0.523674
H	2.532943	2.879377	0.693977
H	1.280177	4.025317	-0.028529

31-A

M06 SCF energy: -2662.064624 a.u.
Enthalpy at 298K: -2661.448867 a.u.
Gibbs free energy at 298K: -2661.569169 a.u.
Cartesian Coordinates

Ru	0.121856	0.226961	0.044913
C	-0.400677	-1.705139	-0.099786
N	-1.609313	-2.311354	-0.235146
C	-1.511417	-3.782617	-0.325221
C	-0.006412	-4.006201	-0.499897
N	0.548549	-2.681637	-0.171100
C	1.976306	-2.524133	-0.056978

C	2.574624	-2.720841	1.208491
C	3.958110	-2.572387	1.315909
C	4.760122	-2.264911	0.210058
C	4.147100	-2.165456	-1.039020
C	2.763697	-2.316641	-1.206234
C	2.200121	-2.354392	-2.606930
C	1.766508	-3.138323	2.413727
C	6.247828	-2.055117	0.367942
C	-2.920383	-1.739593	-0.128230
C	-3.509092	-1.593330	1.142571
C	-4.811407	-1.086294	1.210596
C	-4.913023	-0.897785	-1.181952
C	-3.613448	-1.401736	-1.305151
C	-5.531092	-0.736510	0.062590
C	-2.971189	-1.542813	-2.664578
C	-2.747913	-1.913992	2.407841
C	-6.950206	-0.226027	0.163152
Cl	0.781468	0.161837	2.369147
Cl	0.354521	0.449002	-2.328215
C	-1.504405	1.073326	0.230520
C	-1.573551	2.520299	0.245477
C	-0.381118	3.275577	0.216198
C	-0.393061	4.665367	0.215314
C	-1.625955	5.324933	0.260163
C	-2.825770	4.608129	0.296268
C	-2.797420	3.216926	0.284607
O	0.763943	2.506833	0.170148
C	1.958832	2.962675	0.801644
C	2.983100	3.413866	-0.225931
F	2.542771	4.460961	-0.958746
F	4.099381	3.810640	0.425807
F	3.317161	2.430756	-1.071352
H	0.260468	-4.279299	-1.528375
H	0.395037	-4.770254	0.171795
H	-2.100908	-4.152810	-1.168812
H	-1.903018	-4.242198	0.590920
H	4.422785	-2.706645	2.290262
H	4.757949	-1.980180	-1.920200
H	2.362109	-3.349546	-3.045879
H	1.136370	-2.123766	-2.640159
H	2.703927	-1.626621	-3.249389
H	2.416307	-3.246504	3.287362
H	1.273880	-4.106160	2.249333
H	0.998346	-2.400765	2.656042
H	6.782983	-2.253068	-0.566665
H	6.664896	-2.705369	1.144923
H	6.469932	-1.019721	0.658446

H	-5.272865	-0.960384	2.187839
H	-5.454423	-0.623439	-2.084877
H	-3.664329	-1.228569	-3.450744
H	-2.684187	-2.581386	-2.873546
H	-2.062226	-0.935287	-2.743465
H	-3.389854	-1.786537	3.284584
H	-1.875775	-1.260055	2.527146
H	-2.377311	-2.946075	2.416883
H	-7.119554	0.307156	1.104700
H	-7.671789	-1.053127	0.124361
H	-7.191874	0.452996	-0.661451
H	-2.460082	0.559550	0.320741
H	-3.720415	2.643402	0.307445
H	-3.774483	5.135384	0.327555
H	-1.642100	6.411145	0.254992
H	0.529344	5.228434	0.142904
H	2.357392	2.117980	1.366648
H	1.747139	3.785078	1.488854

31-B

M06 SCF energy: -2662.048288 a.u.
Enthalpy at 298K: -2661.432725 a.u.
Gibbs free energy at 298K: -2661.554552 a.u.
Cartesian Coordinates

Ru	-0.924131	0.756103	-0.532756
C	-1.373507	-1.101564	-0.033446
N	-0.649508	-2.249366	-0.099301
C	-1.416965	-3.430467	0.346003
C	-2.847808	-2.890399	0.425387
N	-2.639213	-1.433893	0.350425
C	-3.749436	-0.548146	0.591450
C	-4.664813	-0.260535	-0.439694
C	-5.735470	0.594698	-0.148128
C	-5.939793	1.121595	1.127906
C	-5.060765	0.741199	2.148331
C	-3.969407	-0.095376	1.910497
C	-3.078262	-0.516969	3.054038
C	-4.590281	-0.907195	-1.802900
C	-7.078704	2.074453	1.404667
C	0.752913	-2.426275	-0.350270
C	1.176396	-2.779641	-1.642556
C	2.543040	-3.008579	-1.846536
C	3.011974	-2.570377	0.467553
C	1.660396	-2.327875	0.723429
C	3.474187	-2.907489	-0.810471
C	1.209613	-1.928693	2.110346

C	0.201583	-2.900900	-2.789343
C	4.945708	-3.153176	-1.050356
Cl	-1.553494	0.488684	-2.822456
Cl	-1.092786	1.896616	1.548118
C	0.917100	0.736468	-0.639196
C	1.631521	1.914914	-1.112146
C	2.907363	2.244885	-0.571648
C	3.565063	3.412862	-0.958611
C	2.981348	4.259727	-1.905772
C	1.745758	3.948141	-2.470338
C	1.081548	2.791361	-2.072013
O	3.418187	1.363027	0.343973
C	4.575347	1.734528	1.054363
C	4.942469	0.591313	1.984725
F	3.922701	0.229472	2.779585
F	5.342305	-0.501668	1.300724
F	5.970895	0.980829	2.767189
H	-3.357050	-3.156957	1.355844
H	-3.468783	-3.224818	-0.414642
H	-1.043248	-3.777691	1.317204
H	-1.305848	-4.247012	-0.372905
H	-6.435251	0.839626	-0.944330
H	-5.227785	1.106459	3.159200
H	-2.959756	-1.606785	3.098847
H	-2.083208	-0.072881	2.959963
H	-3.503975	-0.190080	4.007572
H	-5.070702	-0.275094	-2.555628
H	-5.124595	-1.868391	-1.797761
H	-3.566174	-1.082069	-2.133100
H	-7.504281	1.913070	2.401387
H	-7.882072	1.965603	0.668610
H	-6.735544	3.116613	1.364145
H	2.884418	-3.269348	-2.845885
H	3.723677	-2.472222	1.282031
H	2.073900	-1.758899	2.757597
H	0.590506	-2.704345	2.579836
H	0.619252	-1.006059	2.095135
H	0.720756	-3.207314	-3.702488
H	-0.308615	-1.951726	-2.985819
H	-0.575717	-3.648633	-2.585080
H	5.170093	-3.233929	-2.118569
H	5.278870	-4.081936	-0.569174
H	5.550904	-2.340017	-0.634152
H	1.524606	-0.061210	-0.219101
H	0.135092	2.522894	-2.531624
H	1.302313	4.598372	-3.218011
H	3.507063	5.163696	-2.200756

H	4.526656	3.677881	-0.534383
H	4.403279	2.633308	1.659640
H	5.433495	1.907219	0.392664

31-D

M06 SCF energy: -761.004052 a.u.
Enthalpy at 298K: -760.818447 a.u.
Gibbs free energy at 298K: -760.873156 a.u.
Cartesian Coordinates

C	1.533171	1.967629	0.117174
C	1.873492	0.536169	0.058864
C	0.842899	-0.431700	-0.011297
C	1.134886	-1.797053	-0.060774
C	2.465095	-2.223289	-0.041109
C	3.498356	-1.291085	0.034051
C	3.195238	0.068353	0.088499
O	-0.437399	0.066248	-0.037056
C	-1.515430	-0.836531	-0.034269
C	-2.791896	-0.013520	0.002983
F	-2.857124	0.756368	1.102813
F	-2.904015	0.785468	-1.071350
F	-3.852079	-0.851597	0.014405
C	2.360868	2.988110	-0.143295
H	0.504291	2.188487	0.387161
H	4.000655	0.791391	0.176289
H	4.533370	-1.618782	0.061954
H	2.683847	-3.286780	-0.078786
H	0.341058	-2.533270	-0.119414
H	-1.502447	-1.490410	0.847283
H	-1.534751	-1.457950	-0.938936
H	3.391257	2.846997	-0.459586
H	2.020793	4.015689	-0.057285

32-A

M06 SCF energy: -2439.525611 a.u.
Enthalpy at 298K: -2438.882958 a.u.
Gibbs free energy at 298K: -2439.002416 a.u.
Cartesian Coordinates

Ru	-0.40471000	0.69195800	0.05066900
C	-0.78315800	-1.27917200	-0.01129400
N	0.03091400	-2.36657300	-0.05612400
C	-0.70237400	-3.64849700	-0.05650100
C	-2.16127000	-3.20395000	-0.20453100
N	-2.06758000	-1.74422700	-0.03721100
H	-2.81879400	-3.63711800	0.55545900

H	-2.57547500	-3.44427800	-1.19113800
H	-0.51800200	-4.18796300	0.88033000
H	-0.36167600	-4.28093900	-0.88219700
C	-3.27909600	-0.96593000	-0.04432400
C	-3.87264500	-0.60071900	-1.26938800
C	-5.05629000	0.14651200	-1.23351300
C	-5.67919000	0.49384300	-0.03341500
C	-5.11540400	0.03041800	1.16037500
C	-3.93285800	-0.71355600	1.18227400
H	-5.50670800	0.45019800	-2.17639900
H	-5.61585900	0.24071000	2.10315600
C	-3.42827700	-1.28586300	2.48475000
H	-3.44214900	-2.38421300	2.46486500
H	-2.40785700	-0.96171300	2.70029300
H	-4.06716300	-0.96595500	3.31351800
C	-3.34363000	-1.06897000	-2.60447000
H	-3.50956000	-0.31115700	-3.37494000
H	-3.87365500	-1.98062500	-2.91749500
H	-2.27378800	-1.27280500	-2.58303400
C	-6.93341200	1.33645800	-0.02237400
H	-7.58394000	1.07679200	0.81997000
H	-7.50738700	1.21439600	-0.94715400
H	-6.69140400	2.40352300	0.07212700
C	1.46240800	-2.43762500	-0.01028900
C	2.17588700	-2.50654500	-1.22047100
C	3.56238500	-2.68577900	-1.15977000
H	4.12448500	-2.73686800	-2.08997300
C	3.49836100	-2.71117300	1.24135500
C	2.11118300	-2.53344200	1.23547400
H	4.01141500	-2.78201700	2.19832800
C	4.23927800	-2.80160700	0.05804300
C	1.34726400	-2.41456500	2.53295300
H	2.02397400	-2.51514900	3.38694600
H	0.57785700	-3.19110100	2.62908200
H	0.83782000	-1.44696000	2.61146300
H	0.73089500	-3.14950600	-2.71095600
C	1.47533600	-2.35886000	-2.55048800
H	2.19530000	-2.41320600	-3.37273600
H	0.94608300	-1.40120300	-2.61984000
C	5.73071700	-3.04682800	0.09825900
H	6.21784900	-2.71610700	-0.82547700
H	5.95449500	-4.11555300	0.21727100
H	6.20198000	-2.52617200	0.93966000
Cl	-0.79690100	1.03515400	-2.30117400
Cl	-0.75397300	0.91770600	2.42853200
C	1.44684100	0.76070000	0.01848700
H	2.09009300	-0.11431900	-0.00103600

C	2.11689800	2.03862900	0.00743200
C	3.53006000	2.18278100	-0.05311500
C	4.11244700	3.45533300	-0.06771200
C	3.29474600	4.58593500	-0.02321000
C	1.90308500	4.49151300	0.03601300
C	1.33820700	3.21908200	0.05020500
H	1.29219300	5.38512400	0.06747500
H	3.75640200	5.56945400	-0.03578600
H	5.18764600	3.57627000	-0.11399700
O	4.23677400	1.02678000	-0.09743300
C	5.65242600	1.09251000	-0.17788000
H	5.99355500	0.05712500	-0.21251100
H	6.08170900	1.58939400	0.70147900
H	5.97773700	1.61513700	-1.08636500
O	0.00246800	2.96809200	0.10742100
C	-0.93943700	4.04000300	0.15972600
H	-0.76332600	4.65528200	1.04777000
H	-0.87599800	4.64465100	-0.75055800
H	-1.91688100	3.56491900	0.22570400

32-D

M06 SCF energy: -538.460335 a.u.
Enthalpy at 298K: -538.247684 a.u.
Gibbs free energy at 298K: -538.298289 a.u.
Cartesian Coordinates

C	-0.027314	1.971601	0.000027
C	0.021382	0.502982	0.000038
C	1.295234	-0.126685	0.000195
C	1.433634	-1.518779	0.000117
C	0.291890	-2.315414	-0.000098
C	-0.977683	-1.745634	-0.000207
C	-1.109992	-0.350957	-0.000096
O	2.371475	0.717384	0.000499
C	3.676107	0.166246	-0.000291
O	-2.327908	0.264411	-0.000153
C	-3.501196	-0.531048	0.000242
C	-1.079893	2.806473	-0.000196
H	0.958729	2.425359	0.000134
H	-1.851678	-2.384674	-0.000414
H	0.393124	-3.397291	-0.000197
H	2.412638	-1.981177	0.000284
H	3.859432	-0.443453	0.894338
H	4.358625	1.018420	-0.000528
H	3.858440	-0.443206	-0.895283
H	-4.336379	0.172071	0.000589
H	-3.561370	-1.164007	-0.894705

H	-3.560678	-1.164097	0.895167
H	-2.108600	2.475664	-0.000293
H	-0.903849	3.879311	-0.000251

33-A

M06 SCF energy: -2639.37114 a.u.
Enthalpy at 298K: -2638.524401 a.u.
Gibbs free energy at 298K: -2638.652743 a.u.
Cartesian Coordinates

Ru	-0.204729	0.879459	-0.002058
Cl	-0.282378	1.128271	2.390671
Cl	0.551659	1.294999	-2.241245
O	-1.153710	3.067709	-0.108655
N	1.894545	-1.170229	0.381673
N	-0.065400	-2.162457	0.413077
C	0.550315	-0.961194	0.209879
C	2.171857	-2.498985	0.963111
H	2.317875	-2.409080	2.046014
H	3.071159	-2.937443	0.528506
C	0.896237	-3.261589	0.629934
H	0.989700	-3.866512	-0.282375
H	0.558553	-3.910442	1.441351
C	2.994556	-0.267368	0.116708
C	3.583424	0.459924	1.179593
C	4.676683	1.287705	0.885803
H	5.135624	1.860804	1.685338
C	5.193137	1.374574	-0.400422
H	6.039518	2.025084	-0.606062
C	4.640770	0.606231	-1.420927
H	5.069816	0.660224	-2.415632
C	3.548887	-0.237525	-1.191465
C	3.154113	0.308906	2.637023
H	2.160913	-0.145959	2.656751
C	3.035310	1.652009	3.379901
H	4.009286	2.140457	3.504928
H	2.621566	1.483579	4.380327
H	2.362874	2.334681	2.855824
C	4.141604	-0.613078	3.388295
H	4.254445	-1.587998	2.901075
H	3.798806	-0.783416	4.416128
H	5.138126	-0.157648	3.438287
C	3.061491	-1.143189	-2.322850
H	2.006592	-1.363113	-2.142330
C	3.154246	-0.502992	-3.719820
H	2.675793	0.477870	-3.739182
H	2.644445	-1.144449	-4.448223

H	4.193478	-0.401240	-4.055984
C	3.847422	-2.474501	-2.331762
H	4.913061	-2.291826	-2.516178
H	3.477158	-3.130179	-3.129441
H	3.768221	-3.020977	-1.386821
C	-1.438269	-2.532133	0.192060
C	-1.851169	-2.894088	-1.111979
C	-3.178451	-3.305319	-1.289924
H	-3.521128	-3.578781	-2.283901
C	-4.062873	-3.373691	-0.217194
H	-5.088124	-3.697787	-0.376945
C	-3.629239	-3.036607	1.061815
H	-4.322817	-3.102993	1.894889
C	-2.314331	-2.614678	1.298413
C	-0.918375	-2.861247	-2.320062
H	0.054111	-2.486331	-1.989682
C	-0.702809	-4.277419	-2.893693
H	-0.330302	-4.972647	-2.132045
H	0.024494	-4.248736	-3.713536
H	-1.635481	-4.693969	-3.292177
C	-1.415711	-1.896973	-3.414668
H	-2.402026	-2.191321	-3.793167
H	-0.719833	-1.901847	-4.261531
H	-1.472598	-0.869994	-3.042766
C	-1.877097	-2.286541	2.722687
H	-0.895154	-1.809010	2.671879
C	-2.820227	-1.282653	3.410959
H	-2.890306	-0.354265	2.838034
H	-2.430190	-1.028810	4.402802
H	-3.828677	-1.692636	3.546024
C	-1.748245	-3.573290	3.565612
H	-2.717402	-4.075100	3.676385
H	-1.378466	-3.334789	4.569816
H	-1.056770	-4.294138	3.112830
C	-1.984190	0.529182	-0.336421
H	-2.389426	-0.469006	-0.490884
C	-2.944186	1.606342	-0.409297
C	-4.321155	1.364776	-0.585848
H	-4.657368	0.334985	-0.676660
C	-5.231375	2.414760	-0.635120
H	-6.290723	2.218532	-0.769642
C	-4.767896	3.727907	-0.509825
H	-5.470398	4.556147	-0.547148
C	-3.408404	4.005223	-0.339044
H	-3.080179	5.033322	-0.249838
C	-2.499712	2.947219	-0.287642
C	-0.501682	4.377401	-0.145170

H	-1.103565	5.044748	0.482738
C	0.867889	4.200805	0.493305
H	0.773606	3.775531	1.495818
H	1.360098	5.177308	0.564680
H	1.496125	3.542840	-0.116125
C	-0.429793	4.887416	-1.581815
H	0.143551	4.183961	-2.192089
H	0.064520	5.865619	-1.598310
H	-1.423122	5.000196	-2.026318

33-B

M06 SCF energy: -2639.349362 a.u.
Enthalpy at 298K: -2638.502898 a.u.
Gibbs free energy at 298K: -2638.634188 a.u.
Cartesian Coordinates

Ru	-0.246329	-1.175765	-0.256757
Cl	-0.639379	-2.373474	1.776222
Cl	-0.501683	-0.933936	-2.602624
O	4.106110	-0.318681	-1.100832
N	-2.413442	0.662219	0.384592
N	-0.551285	1.418265	1.292259
C	-1.063663	0.454937	0.475222
C	-2.880021	1.692129	1.331281
H	-3.375436	1.216714	2.186047
H	-3.592717	2.364506	0.849364
C	-1.577528	2.384399	1.733221
H	-1.434531	3.345563	1.223411
H	-1.498681	2.554127	2.809968
C	-3.357044	0.040615	-0.519883
C	-4.112676	-1.079760	-0.100352
C	-5.019386	-1.636753	-1.013338
H	-5.599114	-2.505922	-0.719296
C	-5.203223	-1.090166	-2.277470
H	-5.907475	-1.543756	-2.970064
C	-4.506169	0.056868	-2.643664
H	-4.683344	0.499445	-3.619016
C	-3.585126	0.654548	-1.778017
C	-4.065205	-1.633772	1.321132
H	-3.153771	-1.270986	1.802479
C	-4.013435	-3.171377	1.374536
H	-4.943416	-3.626166	1.012625
H	-3.868910	-3.498637	2.409914
H	-3.179623	-3.561540	0.785654
C	-5.278984	-1.120177	2.128245
H	-5.334067	-0.025400	2.140295
H	-5.221749	-1.469240	3.166373

H	-6.218906	-1.489586	1.700407
C	-2.953770	1.985963	-2.180214
H	-2.124906	2.185049	-1.495308
C	-2.375308	1.998341	-3.606651
H	-1.651212	1.192693	-3.742695
H	-1.874522	2.956697	-3.792769
H	-3.160669	1.894420	-4.364552
C	-3.983577	3.128505	-2.025727
H	-4.819030	2.992412	-2.722574
H	-3.518674	4.097428	-2.245162
H	-4.407424	3.175866	-1.016041
C	0.822467	1.772118	1.540874
C	1.472942	2.648478	0.639290
C	2.771356	3.068164	0.952630
H	3.290446	3.739337	0.274336
C	3.403694	2.647296	2.119045
H	4.409997	2.989754	2.346832
C	2.741801	1.796050	2.998096
H	3.238776	1.479306	3.910182
C	1.440964	1.345071	2.737240
C	0.815041	3.166217	-0.637873
H	-0.173434	2.707643	-0.721054
C	0.617799	4.695643	-0.586003
H	0.045865	5.004007	0.297011
H	0.081003	5.041015	-1.477424
H	1.579821	5.220676	-0.553778
C	1.594998	2.764762	-1.905105
H	2.589626	3.226546	-1.923592
H	1.056513	3.101475	-2.798470
H	1.715969	1.680070	-1.976116
C	0.738810	0.455325	3.757734
H	-0.179713	0.077555	3.301835
C	1.581933	-0.775059	4.139706
H	1.839774	-1.363567	3.255294
H	1.008681	-1.422255	4.812436
H	2.507111	-0.493590	4.657479
C	0.359167	1.262273	5.017688
H	1.251560	1.639022	5.532475
H	-0.192058	0.629543	5.723224
H	-0.269825	2.127992	4.777510
C	1.571292	-0.855606	-0.139093
H	1.984559	0.144218	-0.024060
C	2.525994	-1.925105	-0.379567
C	2.199164	-3.279683	-0.138140
H	1.233247	-3.507617	0.301829
C	3.099874	-4.307677	-0.388710
H	2.823660	-5.337097	-0.182769

C	4.362846	-3.998055	-0.894300
H	5.079488	-4.789448	-1.098045
C	4.728982	-2.674489	-1.143577
H	5.714966	-2.470391	-1.542095
C	3.829259	-1.631779	-0.889803
C	5.371074	0.089681	-1.664890
H	6.168469	-0.509943	-1.207870
C	5.361973	-0.099361	-3.181829
H	5.178265	-1.141330	-3.459309
H	6.325126	0.204588	-3.607559
H	4.574492	0.515167	-3.630910
C	5.562689	1.545006	-1.255831
H	4.774697	2.170434	-1.687128
H	6.531671	1.910835	-1.612592
H	5.526156	1.646661	-0.167329

34-A

M06 SCF energy: -2910.820282 a.u.
Enthalpy at 298K: -2909.83086 a.u.
Gibbs free energy at 298K: -2909.966944 a.u.
Cartesian Coordinates

Cl	0.410876	0.306509	-2.400259
Cl	0.478280	-0.419861	2.282351
Ru	0.090694	-0.304564	-0.095999
C	-1.587133	0.741175	0.199326
C	-3.790219	1.469805	0.651999
H	-4.473753	1.246789	1.474616
H	-4.384714	1.661659	-0.251376
N	-2.871504	0.337544	0.422516
C	-3.470650	-0.958545	0.244426
C	-3.958973	-1.322527	-1.032512
C	-3.815387	-0.431667	-2.264076
H	-3.242537	0.455194	-1.979388
C	-3.026035	-1.124919	-3.391603
H	-2.018356	-1.392804	-3.062074
H	-2.922394	-0.447381	-4.246739
H	-3.536289	-2.029979	-3.742561
C	-5.193935	0.040362	-2.771494
H	-5.800969	-0.803703	-3.119885
H	-5.073233	0.732139	-3.613403
H	-5.763165	0.553473	-1.987358
C	-4.602270	-2.560461	-1.160766
H	-4.977749	-2.865172	-2.133605
C	-4.771169	-3.403552	-0.066027
H	-5.276050	-4.358601	-0.187277
C	-4.300634	-3.017239	1.185704

H	-4.444601	-3.676353	2.036665
C	-3.646896	-1.792188	1.372441
C	-3.174692	-1.401951	2.769620
H	-2.548006	-0.511429	2.677852
C	-2.299252	-2.490725	3.417630
H	-2.861127	-3.415478	3.597859
H	-1.923456	-2.136863	4.384002
H	-1.432181	-2.720079	2.792501
C	-4.375263	-1.059970	3.677244
H	-4.993709	-0.258743	3.254941
H	-4.026692	-0.734130	4.664329
H	-5.023876	-1.932615	3.822125
C	-2.821136	2.601688	0.966909
H	-3.107996	3.556838	0.525241
H	-2.700324	2.740719	2.047288
N	-1.563082	2.101393	0.377963
C	-0.471645	3.021473	0.137750
C	-0.330958	3.586431	-1.158886
C	-1.326172	3.334997	-2.292416
H	-1.771796	2.349479	-2.138078
C	-0.688808	3.329319	-3.693986
H	-0.378894	4.334141	-4.006612
H	-1.424895	2.979355	-4.426967
H	0.173294	2.661356	-3.736206
C	-2.452699	4.393931	-2.263612
H	-2.995008	4.412125	-1.312967
H	-3.180331	4.197476	-3.060520
H	-2.042303	5.398159	-2.424353
C	0.717133	4.489422	-1.370673
H	0.857719	4.917445	-2.357334
C	1.576971	4.859247	-0.341405
H	2.385042	5.561003	-0.532480
C	1.378989	4.355096	0.937704
H	2.024855	4.684655	1.745242
C	0.349191	3.443932	1.213654
C	0.099149	3.049595	2.668396
H	-0.523089	2.151175	2.679419
C	1.385278	2.706357	3.442300
H	1.963161	1.933763	2.930404
H	1.124378	2.320011	4.433892
H	2.020852	3.587371	3.591918
C	-0.649433	4.186919	3.402096
H	-0.028672	5.089640	3.455324
H	-0.889982	3.884744	4.428679
H	-1.583522	4.464718	2.901793
O	2.097883	-1.607993	-0.298909
C	1.742373	-2.922158	-0.409712

C	2.598934	-4.026222	-0.465030
H	3.670150	-3.911513	-0.405600
C	2.067874	-5.312029	-0.598064
H	2.753042	-6.154653	-0.639223
C	0.690245	-5.528846	-0.679201
H	0.295437	-6.534731	-0.784272
C	-0.163879	-4.435524	-0.617925
H	-1.241440	-4.570233	-0.668225
C	0.336529	-3.125194	-0.476145
C	-0.563563	-2.002120	-0.377152
H	-1.619112	-2.242024	-0.493053
C	3.484395	-1.090478	-0.210908
C	3.326141	0.439051	-0.127619
H	2.723440	0.691413	0.752248
H	2.794121	0.793837	-1.016124
C	4.292516	-1.422919	-1.480190
H	3.753586	-1.036130	-2.353035
H	4.405725	-2.500940	-1.623446
C	4.185251	-1.581245	1.069626
H	4.291317	-2.670081	1.082458
H	3.570155	-1.306880	1.934243
C	4.713762	1.109944	-0.025949
H	4.570034	2.195990	0.033844
C	5.546026	0.757720	-1.274133
H	5.056734	1.144360	-2.177872
H	6.536625	1.229607	-1.215975
C	5.692751	-0.773565	-1.365235
H	6.276282	-1.039606	-2.255993
C	6.404288	-1.300642	-0.100060
H	7.412467	-0.870196	-0.031271
H	6.528130	-2.391293	-0.161200
C	5.585361	-0.927933	1.154860
H	6.093194	-1.302131	2.052987
C	5.438290	0.604200	1.237030
H	4.871835	0.881206	2.135995
H	6.427578	1.074827	1.321305

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M06 SCF energy: -2910.802022 a.u.
Enthalpy at 298K: -2909.812978 a.u.
Gibbs free energy at 298K: -2909.950363 a.u.
Cartesian Coordinates

Cl	0.204806	1.837697	-1.768899
Cl	2.061937	-2.385631	-1.502643
Ru	0.867343	-0.349447	-1.111495
C	1.847321	-0.128877	0.584567

C	2.741714	-0.417720	2.747961
H	2.991698	-1.342511	3.273915
H	2.473394	0.340406	3.493936
N	1.614246	-0.647278	1.822187
C	0.365615	-1.093277	2.384675
C	-0.488510	-0.134417	2.979035
C	-0.142858	1.351928	3.051175
H	0.817795	1.502250	2.553186
C	-1.160385	2.238577	2.310770
H	-1.226323	1.968517	1.252364
H	-0.855936	3.290508	2.369000
H	-2.159466	2.159408	2.754439
C	0.017619	1.814024	4.514706
H	-0.929749	1.744835	5.061615
H	0.346037	2.859516	4.550420
H	0.753734	1.206406	5.053719
C	-1.679494	-0.587286	3.559770
H	-2.357450	0.130296	4.013246
C	-2.004693	-1.940674	3.573443
H	-2.936118	-2.271459	4.025060
C	-1.129964	-2.870565	3.020570
H	-1.383664	-3.925847	3.053089
C	0.073430	-2.474760	2.422058
C	1.032012	-3.531943	1.884292
H	1.797441	-3.024312	1.292297
C	0.343692	-4.540310	0.947002
H	-0.403204	-5.147180	1.473411
H	1.090248	-5.223937	0.528158
H	-0.146482	-4.033438	0.111539
C	1.730635	-4.268681	3.047624
H	2.259711	-3.575936	3.713227
H	2.461161	-4.988171	2.659374
H	1.007103	-4.821749	3.659120
C	3.851400	0.049797	1.805713
H	4.415357	0.902988	2.187397
H	4.556610	-0.756772	1.578523
N	3.100592	0.419835	0.589611
C	3.724216	1.246044	-0.422950
C	3.424075	2.634790	-0.443578
C	2.487479	3.295795	0.567706
H	1.733864	2.558814	0.854299
C	1.728635	4.514266	0.011778
H	2.391067	5.374319	-0.145002
H	0.964578	4.827235	0.733074
H	1.229084	4.273997	-0.928880
C	3.264440	3.720600	1.834313
H	3.766113	2.880579	2.325117

H	2.585374	4.177462	2.564763
H	4.033281	4.461205	1.583205
C	4.075077	3.431167	-1.390618
H	3.848570	4.490502	-1.439266
C	5.009690	2.895395	-2.271631
H	5.499871	3.535809	-3.000359
C	5.326346	1.545374	-2.205216
H	6.075650	1.139227	-2.877184
C	4.704648	0.692925	-1.281513
C	5.176871	-0.757059	-1.201389
H	4.451013	-1.323001	-0.612529
C	5.250989	-1.441067	-2.579388
H	4.296958	-1.370421	-3.107085
H	5.482694	-2.504334	-2.450785
H	6.036039	-1.007902	-3.210561
C	6.552643	-0.836223	-0.502026
H	7.319823	-0.316882	-1.088947
H	6.865761	-1.881593	-0.392355
H	6.540069	-0.378645	0.493862
O	-3.616622	-1.078070	-0.187707
C	-3.094086	-1.743071	-1.263278
C	-3.914942	-2.542281	-2.066329
H	-4.964937	-2.631020	-1.813933
C	-3.391743	-3.229818	-3.160628
H	-4.048815	-3.841493	-3.773416
C	-2.029319	-3.143741	-3.457008
H	-1.614575	-3.683248	-4.303301
C	-1.193562	-2.397571	-2.636132
H	-0.125543	-2.400067	-2.823068
C	-1.688494	-1.688484	-1.512449
C	-0.798293	-0.982286	-0.599641
H	-1.222793	-0.751340	0.377379
C	-4.414311	0.138833	-0.377581
C	-5.789802	-0.145326	-1.013761
H	-6.310881	-0.916732	-0.431047
H	-5.665066	-0.524751	-2.034033
C	-3.667319	1.181904	-1.223698
H	-3.512445	0.799314	-2.240426
H	-2.672333	1.372894	-0.805219
C	-4.624027	0.669123	1.048132
H	-3.646376	0.831156	1.513437
H	-5.142601	-0.095216	1.641488
C	-6.619597	1.159544	-1.055638
H	-7.595988	0.944278	-1.509165
C	-5.870185	2.208466	-1.903166
H	-5.747301	1.845039	-2.932605
H	-6.456971	3.135556	-1.959615

C	-4.491560	2.489120	-1.270372
H	-3.947725	3.227519	-1.872081
C	-4.687260	3.026481	0.162654
H	-5.254022	3.967509	0.138500
H	-3.713116	3.252173	0.616163
C	-5.439804	1.978248	1.009087
H	-5.571333	2.351687	2.033262
C	-6.817820	1.697875	0.375431
H	-7.371800	0.967614	0.981554
H	-7.418783	2.617121	0.351932

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M06 SCF energy: -2910.819091 a.u.
Enthalpy at 298K: -2909.829432 a.u.
Gibbs free energy at 298K: -2909.966916 a.u.
Cartesian Coordinates

Cl	-0.284399	0.460697	2.426647
Cl	-0.579047	-0.161156	-2.273035
Ru	-0.101502	0.354254	0.027429
C	1.495081	-0.829927	0.168056
N	2.824657	-0.543701	0.279011
C	3.520767	0.699871	0.077604
C	3.871104	1.477490	1.205406
C	3.489527	1.082125	2.628679
H	2.763491	0.267494	2.568200
C	2.803694	2.228209	3.394598
H	3.480741	3.075825	3.557316
H	2.476537	1.872161	4.377619
H	1.917354	2.582132	2.861402
C	4.723500	0.575155	3.405421
H	5.210434	-0.267719	2.900221
H	4.432606	0.244761	4.409568
H	5.474551	1.366777	3.517768
C	4.615640	2.644531	0.990304
H	4.892291	3.261433	1.840210
C	5.009035	3.026548	-0.289227
H	5.587505	3.935699	-0.432431
C	4.668196	2.237753	-1.384434
H	4.984948	2.538553	-2.379034
C	3.926437	1.059395	-1.229382
C	3.600036	0.221995	-2.463668
H	2.952882	-0.603596	-2.154879
C	2.818327	1.023194	-3.522814
H	1.868047	1.387737	-3.123242
H	2.587902	0.381345	-4.380583
H	3.398722	1.876990	-3.892384

C	4.881255	-0.382823	-3.075694
H	5.551649	0.400290	-3.449390
H	4.628638	-1.034836	-3.920093
H	5.443481	-0.974997	-2.344072
C	3.654096	-1.759744	0.398781
H	4.438842	-1.615584	1.144706
H	4.127409	-1.988711	-0.565437
C	2.621341	-2.801071	0.805201
H	2.778563	-3.777192	0.344886
H	2.585015	-2.930270	1.893338
N	1.366139	-2.186400	0.328288
C	0.193253	-3.016693	0.152911
C	-0.572092	-3.406807	1.280007
C	-0.201181	-3.042759	2.716197
H	0.483416	-2.191694	2.689234
C	-1.409068	-2.607911	3.566396
H	-1.956219	-1.793120	3.087430
H	-1.061309	-2.245039	4.540010
H	-2.099536	-3.438906	3.754558
C	0.508463	-4.234240	3.399728
H	-0.171402	-5.089600	3.495719
H	0.838591	-3.954100	4.407433
H	1.384346	-4.576894	2.837899
C	-1.671501	-4.251367	1.069361
H	-2.275028	-4.554721	1.918948
C	-1.992956	-4.719625	-0.198115
H	-2.853254	-5.369306	-0.338168
C	-1.192432	-4.379377	-1.284130
H	-1.431523	-4.778715	-2.263838
C	-0.078291	-3.545321	-1.138484
C	0.840514	-3.327249	-2.341084
H	1.356395	-2.374580	-2.201553
C	0.096892	-3.245217	-3.686701
H	0.793881	-2.920560	-4.467891
H	-0.722085	-2.525050	-3.645427
H	-0.299039	-4.220386	-3.995819
C	1.897684	-4.452739	-2.427050
H	2.518002	-4.525010	-1.528113
H	2.564868	-4.281740	-3.280651
H	1.414063	-5.426673	-2.569780
C	0.671082	1.996637	-0.275018
H	1.735830	2.141379	-0.447113
C	-0.117445	3.203918	-0.306946
C	0.509394	4.457495	-0.468382
H	1.588849	4.477432	-0.595417
C	-0.221670	5.638172	-0.449088
H	0.273700	6.596657	-0.570032

C	-1.605482	5.573293	-0.266593
H	-2.193702	6.486846	-0.245563
C	-2.262039	4.349355	-0.115382
H	-3.336093	4.344468	0.012043
C	-1.527260	3.159182	-0.142224
O	-2.057541	1.906510	-0.013693
C	-3.477237	1.780578	0.332240
H	-3.676086	2.574166	1.061708
C	-3.749739	0.431915	1.016511
H	-3.055390	0.319342	1.855085
C	-3.610522	-0.749842	0.036564
H	-2.585177	-0.831670	-0.339581
H	-3.826744	-1.684997	0.570108
C	-5.208585	0.483933	1.534583
H	-5.431924	-0.449037	2.068561
H	-5.329359	1.300608	2.260358
C	-4.394983	1.940580	-0.898396
H	-4.159968	2.874492	-1.421726
C	-4.228163	0.753604	-1.869253
H	-3.202021	0.712454	-2.249067
H	-4.892232	0.904137	-2.731781
C	-4.577511	-0.564953	-1.149941
H	-4.462636	-1.403030	-1.848783
C	-6.029372	-0.510334	-0.631095
H	-6.728283	-0.391975	-1.471220
H	-6.289243	-1.453157	-0.129524
C	-6.184392	0.669255	0.352121
H	-7.215351	0.708553	0.728383
C	-5.850773	1.987320	-0.377064
H	-5.992021	2.842184	0.300388
H	-6.534212	2.137180	-1.223331

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M06 SCF energy: -2910.796876 a.u.
Enthalpy at 298K: -2909.807387 a.u.
Gibbs free energy at 298K: -2909.945481 a.u.
Cartesian Coordinates

N	2.972515	-0.754376	0.521341
C	3.970345	-0.308278	1.510484
C	3.221452	0.793358	2.262297
N	2.068317	1.066353	1.379070
C	1.934788	0.125556	0.397934
H	4.861884	0.070459	0.996597
H	4.270350	-1.138767	2.153888
H	3.817054	1.699817	2.393298
H	2.873109	0.466468	3.249122

Ru	0.756006	0.091540	-1.183740
Cl	2.198367	1.612569	-2.329471
Cl	-0.276381	-2.046899	-1.193389
C	3.139927	-2.043794	-0.111443
C	3.916313	-2.162433	-1.285957
C	4.075447	-3.440902	-1.838668
C	3.515235	-4.563359	-1.240719
C	2.804139	-4.432699	-0.051901
H	2.393672	-5.318121	0.424723
H	4.658415	-3.555732	-2.747255
H	4.249175	-0.061100	-1.499448
C	4.653914	-0.985881	-1.918135
C	2.610348	-3.182835	0.543890
C	1.915158	-3.114942	1.901841
H	1.748956	-2.061232	2.144043
C	1.153231	2.099589	1.802350
C	0.154450	1.777234	2.753903
C	-0.682065	2.803759	3.208880
C	-0.527838	4.111523	2.760349
C	0.487871	4.417291	1.861239
C	1.355841	3.431392	1.372456
H	0.618246	5.444482	1.535086
H	-1.460422	2.574152	3.930940
C	-0.018135	0.377478	3.338966
C	2.506209	3.844172	0.460460
H	2.927418	2.940292	0.014710
H	0.637246	-0.304389	2.790366
C	-0.685104	1.082253	-0.616575
H	-0.959529	1.114684	0.438661
C	-1.641277	1.684576	-1.544190
C	-3.042675	1.527683	-1.326333
C	-3.952577	2.236073	-2.118979
C	-3.493379	3.051044	-3.156454
C	-2.129792	3.165988	-3.424351
C	-1.216739	2.483314	-2.624719
H	-0.150896	2.584356	-2.799044
H	-1.777682	3.789561	-4.240477
H	-4.217404	3.588450	-3.763490
H	-5.017989	2.149000	-1.944576
O	-3.391555	0.661542	-0.339432
C	-4.767664	0.264220	-0.151516
H	-5.375595	1.174945	-0.048067
C	-4.824909	-0.531856	1.165072
C	-5.314177	-0.610084	-1.303972
H	-4.403515	0.089488	1.965145
C	-4.025695	-1.847758	1.036518
C	-6.303996	-0.855406	1.470851

H	-5.250759	-0.063285	-2.250630
C	-4.513677	-1.923913	-1.416785
C	-6.795010	-0.926698	-0.990824
H	-4.066523	-2.387661	1.992798
H	-2.972118	-1.638771	0.824724
C	-4.617445	-2.711304	-0.095052
H	-6.884078	0.071063	1.588031
H	-6.368806	-1.393850	2.425826
C	-6.895271	-1.713397	0.332658
H	-3.462528	-1.718143	-1.647999
H	-4.916787	-2.518515	-2.247980
H	-7.381155	0.001476	-0.924725
H	-7.222439	-1.512561	-1.815402
H	-4.046052	-3.644073	-0.179276
C	-6.096206	-3.028020	0.210038
H	-7.948522	-1.936085	0.549284
H	-6.522298	-3.653005	-0.587257
H	-6.175958	-3.603105	1.143354
C	4.461513	-0.903247	-3.443501
H	4.931368	0.009219	-3.826456
H	4.920199	-1.754126	-3.961367
H	3.401721	-0.865400	-3.709225
C	6.158220	-1.052118	-1.573777
H	6.622051	-1.948047	-2.004020
H	6.680853	-0.176309	-1.976666
H	6.330152	-1.082770	-0.491389
C	2.821819	-3.708665	3.002709
H	2.995275	-4.777775	2.833046
H	3.803154	-3.220878	3.037646
H	2.352210	-3.598624	3.987826
C	0.538126	-3.803518	1.916556
H	-0.116352	-3.383053	1.149409
H	0.624267	-4.882233	1.740722
H	0.066034	-3.671277	2.898296
C	0.400033	0.344965	4.825082
H	-0.263037	0.971510	5.433220
H	0.344168	-0.677889	5.216247
H	1.422261	0.710988	4.973923
C	-1.452093	-0.160074	3.182599
H	-1.775657	-0.145234	2.138930
H	-1.506641	-1.195598	3.537649
H	-2.169338	0.427356	3.767961
C	3.614499	4.549459	1.272989
H	3.248306	5.486062	1.711103
H	3.983842	3.927005	2.096609
H	4.465317	4.792169	0.625370
C	2.049987	4.743932	-0.702579

H	1.711284	5.726908	-0.352929
H	2.885269	4.908389	-1.391922
H	1.239853	4.276578	-1.267616
H	-1.189154	4.894115	3.122968
H	3.647900	-5.543789	-1.690705

36-A

M06 SCF energy: -2246.449104 a.u.
Enthalpy at 298K: -2245.900502 a.u.
Gibbs free energy at 298K: -2246.001359 a.u.
Cartesian Coordinates

Ru	-0.067865	-0.427482	-0.122822
Cl	0.109553	-0.379172	-2.537613
Cl	-1.005962	-0.988660	2.021489
O	0.902974	-2.592758	-0.170599
N	-2.144174	1.632818	-0.057571
N	-0.195378	2.641658	-0.077149
C	-0.799972	1.419401	-0.075603
C	-2.505674	3.060011	-0.000775
H	-2.907020	3.317462	0.985451
H	-3.262394	3.292755	-0.755357
C	-1.161298	3.743349	-0.268744
H	-1.079049	4.125041	-1.294753
H	-0.959492	4.567209	0.420725
C	-3.159947	0.626569	-0.184322
C	-4.074757	0.391219	0.862636
C	-5.077665	-0.559813	0.641944
H	-5.785904	-0.762971	1.441543
C	-5.174593	-1.265425	-0.558565
H	-5.963252	-2.001451	-0.690416
C	-4.255863	-1.026520	-1.578687
H	-4.316991	-1.566972	-2.518966
C	-3.255988	-0.069992	-1.394743
H	-2.536708	0.135130	-2.180721
C	-3.974743	1.093175	2.194599
H	-4.564581	0.563624	2.948718
H	-4.355384	2.122655	2.151217
H	-2.936419	1.119321	2.539103
C	1.190204	2.939219	-0.295967
C	1.927574	3.571285	0.725058
C	3.264884	3.893868	0.457325
H	3.853718	4.374063	1.235375
C	3.853295	3.602582	-0.774201
H	4.894098	3.861257	-0.949961
C	3.106008	2.975345	-1.772004
H	3.556487	2.734867	-2.730599

C	1.770678	2.650735	-1.535402
H	1.182009	2.133731	-2.286257
C	1.321982	3.869198	2.076608
H	0.675510	4.756980	2.049845
H	2.104619	4.064579	2.815981
H	0.711180	3.034401	2.435430
C	1.663982	-0.092231	0.408831
H	2.026985	0.885885	0.727088
C	2.634674	-1.161326	0.454199
C	3.984595	-0.933117	0.785092
H	4.295898	0.082712	1.014949
C	4.902376	-1.977550	0.809776
H	5.941226	-1.790811	1.064350
C	4.473036	-3.272569	0.504926
H	5.181169	-4.096630	0.523179
C	3.139931	-3.537037	0.177079
H	2.836489	-4.551788	-0.048537
C	2.224850	-2.483985	0.148779
C	0.271091	-3.901903	-0.338594
H	0.948864	-4.499643	-0.958927
C	-1.022630	-3.670706	-1.105160
H	-1.734599	-3.096541	-0.503425
H	-1.476804	-4.640180	-1.340043
H	-0.830737	-3.130690	-2.036067
C	0.051818	-4.551380	1.025058
H	0.993124	-4.704014	1.561755
H	-0.428136	-5.528128	0.894228
H	-0.592940	-3.913193	1.636377

36-B

M06 SCF energy: -2246.426483 a.u.
Enthalpy at 298K: -2245.878588 a.u.
Gibbs free energy at 298K: -2245.983056 a.u.
Cartesian Coordinates

Ru	-0.462031	-0.708851	-0.620337
Cl	-0.732796	-0.262763	-2.962850
Cl	-0.838520	-1.960035	1.379991
O	3.649078	-0.621007	1.313088
N	-2.642463	0.981705	0.240496
N	-0.829865	2.223096	0.091148
C	-1.315501	0.957863	-0.054231
C	-3.115063	2.314408	0.652215
H	-3.338545	2.329023	1.724614
H	-4.022828	2.583213	0.104762
C	-1.917024	3.203615	0.300707
H	-2.072704	3.773621	-0.624116

H	-1.661810	3.905136	1.098366
C	-3.551927	-0.121329	0.102270
C	-4.175196	-0.683007	1.234469
C	-5.087729	-1.721656	1.018798
H	-5.571039	-2.176315	1.879988
C	-5.367463	-2.202972	-0.261236
H	-6.073521	-3.019012	-0.388563
C	-4.732813	-1.642842	-1.367868
H	-4.936089	-2.009823	-2.369559
C	-3.833567	-0.591195	-1.185762
H	-3.336831	-0.136371	-2.036475
C	-3.856801	-0.228438	2.637604
H	-4.192236	-0.973668	3.364699
H	-4.354429	0.717569	2.890867
H	-2.778203	-0.097104	2.767799
C	0.450211	2.735388	-0.308016
C	1.287076	3.322612	0.661050
C	2.502236	3.869132	0.226904
H	3.167609	4.315015	0.962193
C	2.877344	3.839243	-1.115887
H	3.829445	4.265062	-1.420433
C	2.033011	3.255512	-2.061242
H	2.317232	3.221107	-3.108930
C	0.814876	2.710555	-1.658687
H	0.155496	2.234110	-2.376566
C	0.913997	3.362604	2.124592
H	0.263621	4.217380	2.357500
H	1.807519	3.463676	2.748228
H	0.382063	2.456219	2.431027
C	1.299325	-0.287561	-0.274502
H	1.576081	0.528200	0.396292
C	2.401736	-1.130771	-0.710398
C	2.380369	-1.809562	-1.951070
H	1.516116	-1.684062	-2.596578
C	3.468681	-2.563726	-2.376796
H	3.436844	-3.061171	-3.341694
C	4.607304	-2.659450	-1.571202
H	5.463290	-3.241462	-1.902587
C	4.650153	-2.013158	-0.335136
H	5.522622	-2.081110	0.307027
C	3.561193	-1.259981	0.105854
C	2.888609	-1.179484	2.428575
H	1.861501	-1.365636	2.090325
C	2.891156	-0.102346	3.503783
H	3.915946	0.118579	3.823573
H	2.319000	-0.438314	4.375009
H	2.440838	0.821630	3.128182

C	3.512818	-2.488903	2.903274
H	3.527123	-3.235152	2.102644
H	2.928404	-2.900725	3.733561
H	4.540849	-2.325444	3.247697

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M06 SCF energy: -2517.898431 a.u.
Enthalpy at 298K: -2517.207239 a.u.
Gibbs free energy at 298K: -2517.315455 a.u.
Cartesian Coordinates

Ru	0.403953	0.012448	-0.004437
Cl	0.231603	-0.156022	2.412787
Cl	-0.057685	0.804640	-2.236549
O	-1.566387	-1.342230	-0.179013
N	2.049549	2.431273	0.095782
N	3.375991	0.699852	0.325024
C	2.078568	1.067450	0.140088
C	3.332956	3.036741	0.492054
H	3.264551	3.408047	1.523374
H	3.593258	3.874575	-0.159116
C	4.296247	1.855358	0.356994
H	4.986878	1.765420	1.199800
H	4.881202	1.906323	-0.568679
C	0.868648	3.249142	0.106555
C	0.031700	3.223517	1.227175
H	0.256703	2.542377	2.041815
C	-1.089799	4.054050	1.283398
H	-1.737918	4.025957	2.154818
C	-1.356768	4.921832	0.226212
H	-2.222347	5.578223	0.260392
C	-0.509517	4.948633	-0.883678
H	-0.729525	5.619204	-1.710709
C	0.613540	4.118957	-0.973114
C	1.486682	4.136597	-2.202564
H	1.046103	4.771499	-2.977181
H	1.591020	3.124535	-2.605826
H	2.492295	4.526087	-1.994903
C	3.903484	-0.610619	0.560628
C	4.725190	-1.225244	-0.405265
C	5.263613	-2.482071	-0.095813
H	5.894986	-2.975524	-0.831099
C	4.994502	-3.113447	1.118936
H	5.423366	-4.090094	1.326892
C	4.167784	-2.493429	2.057144
H	3.940181	-2.981220	3.000485
C	3.629249	-1.237783	1.780769

H	2.961438	-0.748071	2.481815
C	4.995762	-0.590235	-1.749633
H	4.109930	-0.073620	-2.134024
H	5.290581	-1.348800	-2.481308
H	5.811961	0.143329	-1.701889
C	1.094691	-1.627427	-0.467583
H	2.152686	-1.816508	-0.654824
C	0.223211	-2.762759	-0.652620
C	0.748320	-4.027850	-0.983997
H	1.825797	-4.123826	-1.091479
C	-0.080963	-5.127445	-1.163435
H	0.333979	-6.098197	-1.416852
C	-1.459782	-4.962405	-1.012785
H	-2.126124	-5.809845	-1.150460
C	-2.015443	-3.722454	-0.685873
H	-3.086695	-3.646099	-0.581304
C	-1.183210	-2.613993	-0.501317
C	-2.960788	-0.878931	0.012077
C	-2.827091	0.619592	0.336468
H	-2.318551	1.122451	-0.493292
H	-2.210752	0.736738	1.234123
C	-4.223881	1.238457	0.564465
H	-4.098035	2.304210	0.792877
C	-4.914306	0.524248	1.742839
H	-4.334231	0.665088	2.664467
H	-5.909927	0.954829	1.917931
C	-5.036457	-0.978023	1.420616
H	-5.520615	-1.499899	2.256036
C	-5.872706	-1.163193	0.135564
H	-5.980150	-2.232479	-0.096125
H	-6.886206	-0.768276	0.288621
C	-5.194579	-0.428587	-1.041386
H	-5.790650	-0.562064	-1.953237
C	-3.786089	-1.024672	-1.280093
H	-3.881803	-2.070079	-1.587259
H	-3.268945	-0.495743	-2.089186
C	-3.626289	-1.580262	1.210943
H	-3.000898	-1.430146	2.098794
H	-3.713050	-2.659452	1.056363
C	-5.073160	1.071727	-0.710811
H	-6.070996	1.507351	-0.563020
H	-4.607601	1.606585	-1.548952

37-B

M06 SCF energy: -2517.879853 a.u.
Enthalpy at 298K: -2517.189505 a.u.

Gibbs free energy at 298K: -2517.300614 a.u.
Cartesian Coordinates

Ru	-1.373688	0.138765	1.001153
C	-2.186515	0.364229	-0.762516
N	-1.913919	1.223028	-1.782612
C	-2.825361	1.026419	-2.930783
C	-3.919274	0.133082	-2.337847
N	-3.265358	-0.385436	-1.123888
H	-4.213983	-0.680482	-3.005231
H	-4.819812	0.697281	-2.061107
H	-2.299820	0.537037	-3.758493
H	-3.201471	1.991583	-3.279836
C	-3.986349	-1.283115	-0.262903
C	-4.675431	-0.765681	0.838776
C	-5.413951	-1.616720	1.663407
C	-5.478267	-2.976136	1.365720
C	-4.797464	-3.481027	0.255660
C	-4.035787	-2.655315	-0.577533
H	-5.936634	-1.211981	2.525097
H	-4.840980	-4.545210	0.037860
C	-3.257962	-3.232517	-1.733705
H	-3.577024	-2.823448	-2.701005
H	-2.190515	-3.018389	-1.614644
H	-3.385924	-4.318135	-1.778990
C	-0.977748	2.309283	-1.815588
C	-1.193843	3.414405	-0.984667
C	-0.332796	4.508593	-1.039826
H	-0.499206	5.357303	-0.382908
C	0.941316	3.402684	-2.766480
C	0.098626	2.283712	-2.724232
H	1.783836	3.395843	-3.453804
C	0.734163	4.505597	-1.939272
C	0.374017	1.095245	-3.616104
H	1.432666	1.058098	-3.889775
H	-0.199067	1.142187	-4.552294
H	0.120096	0.151939	-3.121647
Cl	-2.610706	1.941906	1.988901
Cl	-0.761423	-2.159181	0.792822
C	0.287817	0.873252	0.665752
H	0.670494	0.955817	-0.351693
C	1.240729	1.220237	1.707960
C	2.638171	1.212593	1.424638
C	3.550332	1.616646	2.403878
C	3.106546	1.989207	3.673439
C	1.742238	1.979444	3.976988
C	0.823104	1.608153	3.002874
H	-0.240941	1.660791	3.212377

H	1.396546	2.284416	4.960288
H	3.830130	2.300161	4.422577
H	4.605456	1.654112	2.157512
O	3.054532	0.878406	0.164902
C	3.695001	-0.413184	-0.107974
C	5.207266	-0.352329	0.180372
C	3.061746	-1.571182	0.678921
C	3.474339	-0.632278	-1.612824
H	5.378866	-0.192592	1.251396
H	5.644648	0.499687	-0.356509
C	5.871683	-1.678636	-0.256606
H	1.980891	-1.613932	0.500463
H	3.204367	-1.417441	1.756294
C	3.724636	-2.899670	0.245047
H	3.896766	0.217927	-2.164631
H	2.396486	-0.651699	-1.814084
C	4.130603	-1.956703	-2.054844
H	6.948118	-1.626821	-0.046819
C	5.239518	-2.844457	0.532617
C	5.644800	-1.896653	-1.766586
H	3.267392	-3.720594	0.810811
C	3.497696	-3.121216	-1.264793
H	3.963299	-2.101346	-3.130326
H	5.415889	-2.711535	1.608882
H	5.712946	-3.793238	0.245132
H	6.107876	-1.081873	-2.340556
H	6.127877	-2.829312	-2.088380
H	3.944438	-4.075215	-1.576832
H	2.422151	-3.183508	-1.476329
H	-2.018722	3.391086	-0.280728
H	1.410196	5.354627	-1.991222
H	-4.618596	0.296893	1.052513
H	-6.053194	-3.648214	1.997072

38-A

M06 SCF energy: -2517.89657 a.u.
Enthalpy at 298K: -2517.204843 a.u.
Gibbs free energy at 298K: -2517.313609 a.u.
Cartesian Coordinates

Ru	0.357463	-0.020906	0.038628
Cl	-0.201037	-0.765507	-2.190798
Cl	0.314141	0.178199	2.452866
O	-1.533046	1.590749	-0.001467
N	1.834191	-2.543962	0.103133
N	3.286314	-0.901093	0.189233
C	1.956555	-1.186112	0.106920

C	3.101928	-3.225441	0.420394
H	3.253688	-4.095174	-0.223403
H	3.087773	-3.565353	1.464620
C	4.127194	-2.116549	0.177707
H	4.888870	-2.055896	0.959526
H	4.628719	-2.227200	-0.790612
C	0.611289	-3.288631	0.228042
C	0.214414	-4.154390	-0.811241
C	-0.930695	-4.931291	-0.602045
H	-1.259223	-5.599391	-1.394331
C	-1.659703	-4.861144	0.586961
C	-1.252290	-3.998465	1.602814
H	-1.809192	-3.934613	2.533264
C	-0.109256	-3.216653	1.425161
C	3.915717	0.370889	0.381871
C	3.742451	1.030386	1.603767
C	4.376188	2.250133	1.835196
H	4.226079	2.763987	2.780196
C	5.198130	2.801056	0.850744
C	5.368009	2.137007	-0.364430
H	5.996458	2.576951	-1.135329
C	4.732303	0.915780	-0.629419
C	1.158154	1.553826	-0.471892
H	2.198475	1.625754	-0.791445
C	0.423140	2.793925	-0.506590
C	1.082134	4.010066	-0.780101
H	2.146604	3.978587	-0.997792
C	0.403075	5.221359	-0.748158
H	0.923116	6.151817	-0.954459
C	-0.959578	5.224438	-0.439693
H	-1.506322	6.162979	-0.405015
C	-1.648428	4.037136	-0.178243
H	-2.705379	4.084453	0.045990
C	-0.967112	2.816282	-0.220501
C	-2.932955	1.537304	0.431826
H	-3.049703	2.351422	1.156751
C	-3.914475	1.720056	-0.745228
H	-3.668862	2.632073	-1.300802
C	-5.331574	1.847033	-0.137959
H	-5.388558	2.720206	0.528418
H	-6.058518	2.014779	-0.943631
C	-5.681880	0.560434	0.638102
H	-6.684261	0.657561	1.076140
C	-4.644817	0.346817	1.761706
H	-4.879900	-0.564644	2.326927
H	-4.680975	1.180613	2.477016
C	-3.224991	0.213900	1.156447

H	-2.485995	0.080284	1.953115
C	-3.207155	-0.989815	0.192004
H	-2.213607	-1.134256	-0.244698
H	-3.438113	-1.901997	0.757786
C	-4.234200	-0.776256	-0.936396
H	-4.203990	-1.630513	-1.624315
C	-5.647133	-0.639744	-0.331896
H	-5.921522	-1.561152	0.200816
H	-6.390691	-0.498487	-1.129138
C	-3.860412	0.509843	-1.700236
H	-2.858961	0.409042	-2.132932
H	-4.560750	0.679275	-2.529883
H	-2.544021	-5.479857	0.714821
H	5.700789	3.748947	1.023442
C	0.968459	-4.230917	-2.115185
H	1.980691	-4.636749	-1.986966
H	0.444664	-4.879789	-2.823557
H	1.058338	-3.235012	-2.560280
C	4.896285	0.248863	-1.975520
H	5.663287	-0.537030	-1.954927
H	3.960922	-0.211293	-2.311279
H	5.206098	0.977816	-2.730673
H	3.077344	0.596917	2.343409
H	0.223672	-2.538307	2.204002

38-B

M06 SCF energy: -2517.878764 a.u.
Enthalpy at 298K: -2517.187494 a.u.
Gibbs free energy at 298K: -2517.29871 a.u.
Cartesian Coordinates

Ru	-1.372729	0.263521	-0.985859
Cl	-0.659112	-2.017193	-1.026899
Cl	-2.701624	2.119884	-1.727762
O	3.114923	0.736317	-0.439461
N	-3.170867	-0.517798	1.138254
N	-1.825245	1.040966	1.917122
C	-2.118909	0.287711	0.822450
C	-3.792475	-0.144121	2.420342
H	-4.041073	-1.030171	3.009597
H	-4.716776	0.418283	2.233586
C	-2.700573	0.715264	3.065043
H	-3.086553	1.634576	3.513292
H	-2.142412	0.163334	3.828950
C	-3.903521	-1.340688	0.213808
C	-3.902998	-2.739750	0.378588
C	-4.682955	-3.492969	-0.505171

H	-4.690511	-4.575161	-0.402427
C	-5.428534	-2.892063	-1.521814
C	-5.413160	-1.507108	-1.671737
H	-5.987030	-1.027458	-2.459188
C	-4.657861	-0.728521	-0.792640
C	-0.905945	2.136029	2.031288
C	-1.146437	3.301813	1.294590
C	-0.299171	4.399903	1.428233
H	-0.485047	5.296220	0.843740
C	0.778259	4.340492	2.313172
C	1.008290	3.178610	3.048245
H	1.857319	3.129202	3.725716
C	0.180380	2.053983	2.924907
C	0.284799	1.003821	-0.664694
H	0.716931	1.036069	0.337263
C	1.177423	1.400977	-1.742873
C	0.692616	1.960405	-2.948293
H	-0.377384	2.108416	-3.059702
C	1.563318	2.384928	-3.946157
H	1.167946	2.828549	-4.855177
C	2.943680	2.259822	-3.764715
H	3.628980	2.597296	-4.537832
C	3.450678	1.698086	-2.592168
H	4.519718	1.591139	-2.438050
C	2.586072	1.261049	-1.587581
C	3.030552	-0.710293	-0.264952
H	2.046187	-1.040567	-0.620344
C	4.141128	-1.443390	-1.042531
H	4.043492	-1.213740	-2.111356
C	3.957629	-2.962777	-0.818384
H	2.977473	-3.285258	-1.193496
H	4.717992	-3.511559	-1.390623
C	4.083550	-3.284765	0.685159
H	3.956560	-4.364225	0.840839
C	2.985766	-2.519672	1.453374
H	3.045693	-2.745500	2.527201
H	1.991671	-2.835325	1.110397
C	3.165492	-1.000596	1.236314
H	2.380625	-0.450509	1.769554
C	4.555124	-0.561113	1.743541
H	4.678524	0.519696	1.607295
H	4.634385	-0.765040	2.820694
C	5.652929	-1.327266	0.975140
H	6.641890	-1.016520	1.337898
C	5.472571	-2.844659	1.194828
H	5.576030	-3.086458	2.262202
H	6.260560	-3.398347	0.665050

C	5.529813	-1.008044	-0.529494
H	5.675757	0.065757	-0.696849
H	6.311904	-1.533119	-1.095067
H	-6.016345	-3.509168	-2.195944
H	1.443424	5.192146	2.426005
C	-3.057151	-3.416428	1.428102
H	-3.312147	-3.094956	2.445848
H	-3.186660	-4.501934	1.384418
H	-1.998314	-3.191160	1.261045
C	0.481788	0.805970	3.722564
H	-0.086264	0.772472	4.662260
H	0.242610	-0.102096	3.159695
H	1.542312	0.767979	3.989330
H	-1.979749	3.323791	0.600356
H	-4.638763	0.352119	-0.889991

Mes-C

M06 SCF energy: -2211.97056191 a.u.
Enthalpy at 298K: -2211.359315 a.u.
Gibbs free energy at 298K: -2211.474863 a.u.
Cartesian Coordinates

Ru	0.386698	0.837894	-0.537314
C	0.772725	-0.938566	0.212287
N	-0.016366	-1.998142	0.537262
C	0.757970	-3.174563	0.979722
C	2.173192	-2.604559	1.141230
N	2.061492	-1.289441	0.489476
H	2.937214	-3.214243	0.649993
H	2.456226	-2.482132	2.193888
H	0.708655	-3.965650	0.221482
H	0.348297	-3.573261	1.912741
C	3.219113	-0.440485	0.371218
C	3.625184	0.346938	1.468243
C	4.757401	1.154368	1.316083
C	5.504881	1.170499	0.136166
C	5.121850	0.313677	-0.900828
C	3.996324	-0.509349	-0.805697
H	5.063725	1.781528	2.150563
H	5.718642	0.276046	-1.809492
C	3.666457	-1.466024	-1.925730
H	3.547156	-2.493121	-1.558192
H	2.738390	-1.182799	-2.431570
H	4.470687	-1.470581	-2.667714
C	2.940073	0.283488	2.812819
H	3.032948	1.237957	3.337673
H	3.409310	-0.486900	3.442207

H	1.875168	0.066154	2.730066
C	6.695532	2.087358	-0.016822
H	7.456958	1.651129	-0.672494
H	7.161241	2.306377	0.949917
H	6.396298	3.046609	-0.459456
C	-1.438547	-2.117971	0.413306
C	-2.240706	-1.792843	1.523770
C	-3.626242	-1.948375	1.405963
H	-4.256411	-1.692842	2.255303
C	-3.389153	-2.732733	-0.853226
C	-1.997681	-2.596399	-0.786596
H	-3.834094	-3.093211	-1.778268
C	-4.219258	-2.420680	0.229293
C	-1.138557	-2.915886	-1.986959
H	-1.753558	-3.294096	-2.809021
H	-0.386866	-3.681449	-1.758775
H	-0.599849	-2.029708	-2.343056
H	-0.887786	-1.923170	3.219200
C	-1.633431	-1.241138	2.792487
H	-2.405589	-1.079064	3.550565
H	-1.126653	-0.285321	2.610820
C	-5.715152	-2.618016	0.140220
H	-6.252359	-1.919866	0.790942
H	-5.997916	-3.633047	0.449664
H	-6.078383	-2.478983	-0.883541
Cl	0.425864	2.122720	1.496378
Cl	0.784197	0.348468	-2.853199
C	-1.452639	0.815632	-0.644396
H	-2.147633	0.102828	-0.188124
O	-2.049908	1.804076	-1.284607
C	-3.494085	1.936706	-1.210775
C	-3.879018	2.983110	-0.172856
H	-3.925023	0.954425	-0.979293
H	-3.806240	2.230311	-2.216611
C	-5.398245	3.194511	-0.100173
H	-3.492483	2.672597	0.806785
H	-3.377909	3.926851	-0.421932
C	-5.797091	4.251686	0.935122
H	-5.774659	3.490912	-1.089423
H	-5.889759	2.241339	0.141806
H	-6.884411	4.382305	0.969239
H	-5.461232	3.968336	1.939692
H	-5.349822	5.224371	0.698638

DIPP-C

M06 SCF energy: -2447.710947 a.u.

Enthalpy at 298K: -2446.919201 a.u.
Gibbs free energy at 298K: -2447.046392 a.u.
Cartesian Coordinates

Ru	-0.067378	0.696998	1.154423
C	-0.664391	-0.199671	-0.483295
N	0.012779	-0.849783	-1.475831
C	-0.886962	-1.334986	-2.540130
C	-2.148068	-0.514462	-2.285615
N	-1.974584	-0.113789	-0.876513
H	-3.069770	-1.082369	-2.420119
H	-2.190214	0.373652	-2.927269
H	-1.057398	-2.414330	-2.428656
H	-0.448191	-1.153729	-3.524221
C	-3.099235	0.373311	-0.106680
C	-3.537285	1.711860	-0.262613
C	-4.648617	2.128994	0.483545
C	-5.321688	1.256658	1.329278
C	-4.913957	-0.070240	1.424045
C	-3.813010	-0.547969	0.705753
H	-4.994591	3.153292	0.390237
H	-5.463567	-0.749378	2.066611
C	-3.489188	-2.041206	0.753406
H	-2.430602	-2.163972	0.509573
C	-2.927335	2.682580	-1.271562
H	-1.933405	2.316797	-1.543512
C	1.373991	-1.309611	-1.481161
C	2.352016	-0.540434	-2.153623
C	3.665173	-1.028665	-2.178332
H	4.435698	-0.455303	-2.685355
C	3.015715	-2.991779	-0.938143
C	1.685616	-2.554220	-0.884343
H	3.281825	-3.940784	-0.481051
C	3.999026	-2.236948	-1.572299
C	0.639845	-3.438259	-0.208406
H	-0.313081	-2.901747	-0.209681
C	2.021266	0.766021	-2.869691
H	1.001717	1.049716	-2.595533
Cl	0.375192	2.800007	0.091030
Cl	-0.877984	-0.720317	2.890821
C	1.690880	0.160094	1.263948
H	2.232979	-0.521479	0.601499
O	2.422490	0.631723	2.257488
C	3.835580	0.305628	2.333627
C	4.676804	1.487653	1.870289
H	4.023862	-0.590142	1.728592
H	4.019868	0.066971	3.384721
C	6.181195	1.225632	2.032644

H	4.442665	1.702515	0.819307
H	4.383573	2.374357	2.446118
C	7.038177	2.410910	1.575348
H	6.400769	0.999701	3.085590
H	6.461767	0.329088	1.461638
H	8.105876	2.199212	1.700254
H	6.863164	2.640999	0.517630
H	6.805322	3.312918	2.153504
C	-3.801603	2.739461	-2.545768
H	-4.791456	3.153108	-2.318312
H	-3.334669	3.383573	-3.300716
H	-3.957979	1.750593	-2.991115
C	-2.738814	4.105454	-0.714091
H	-2.188598	4.713541	-1.440729
H	-3.698641	4.603528	-0.531731
H	-2.161879	4.095692	0.212973
C	-4.323792	-2.806834	-0.299151
H	-5.394165	-2.724415	-0.075288
H	-4.174300	-2.429306	-1.316056
H	-4.061393	-3.871834	-0.293693
C	-3.712545	-2.683797	2.134541
H	-3.195090	-2.126783	2.917652
H	-4.777867	-2.750196	2.386813
H	-3.321094	-3.707877	2.127528
C	0.440807	-4.750431	-0.996231
H	0.174444	-4.560634	-2.042632
H	1.352593	-5.359418	-0.994100
H	-0.359070	-5.347641	-0.543375
C	0.979227	-3.733434	1.265549
H	0.204923	-4.372746	1.704575
H	1.936866	-4.258931	1.362888
H	1.015714	-2.815460	1.859048
C	2.073401	0.573987	-4.400694
H	3.087197	0.322467	-4.735335
H	1.408573	-0.230897	-4.736287
H	1.772452	1.496736	-4.910293
C	2.934015	1.928949	-2.439671
H	3.986050	1.738337	-2.684616
H	2.635104	2.845482	-2.960522
H	2.844111	2.121977	-1.367123
H	-6.177009	1.605011	1.902489
H	5.024295	-2.596757	-1.604326

Tol-C

M06 SCF energy: -2054.789469 a.u.
Enthalpy at 298K: -2054.295996 a.u.
Gibbs free energy at 298K: -2054.394433 a.u.

Cartesian Coordinates

Ru	0.449332	-1.039511	0.057320
C	0.972569	0.822720	-0.168005
N	0.266755	1.982043	-0.296034
C	1.151193	3.157750	-0.441644
C	2.510900	2.513208	-0.733950
N	2.296236	1.132375	-0.271229
H	3.331254	2.988885	-0.191211
H	2.755328	2.514904	-1.804730
H	1.169006	3.744688	0.484057
H	0.796865	3.798124	-1.253727
C	3.352058	0.162330	-0.370953
C	3.382989	-0.699412	-1.473207
C	4.412095	-1.635146	-1.599607
C	5.416767	-1.685277	-0.636028
C	5.382641	-0.813507	0.454813
C	4.354062	0.119826	0.618656
H	4.423771	-2.310433	-2.450006
H	6.161003	-0.870085	1.211657
C	4.298640	1.000220	1.841927
H	4.361536	2.068117	1.595399
H	3.360782	0.833588	2.382577
H	5.128124	0.770848	2.517294
C	-1.150349	2.138802	-0.419230
C	-1.787756	1.645230	-1.563797
C	-3.161582	1.817955	-1.728209
H	-3.650061	1.426850	-2.616025
C	-3.253810	2.988062	0.383450
C	-1.875892	2.818197	0.580357
H	-3.830696	3.506372	1.145836
C	-3.895416	2.498773	-0.754671
C	-1.218950	3.326169	1.842949
H	-1.957506	3.443249	2.641962
H	-0.749730	4.307969	1.694189
H	-0.441278	2.640522	2.195881
Cl	-0.042190	-1.438472	-2.267744
Cl	1.430993	-1.398549	2.214750
C	-1.264547	-0.784494	0.681251
H	-1.711630	0.162041	1.011922
O	-2.059069	-1.827679	0.833589
C	-3.411146	-1.652110	1.330111
C	-4.412421	-1.830355	0.196686
H	-3.493519	-0.660537	1.792591
H	-3.537815	-2.413175	2.105431
C	-5.864446	-1.754501	0.690176
H	-4.229770	-1.057864	-0.561487
H	-4.227760	-2.798360	-0.285730

C	-6.881658	-1.941755	-0.440569
H	-6.029271	-2.520833	1.460580
H	-6.035695	-0.785380	1.180079
H	-7.908710	-1.886124	-0.063130
H	-6.765021	-1.169362	-1.210277
H	-6.755841	-2.915979	-0.927599
H	6.225630	-2.405401	-0.725166
H	2.595790	-0.644105	-2.218773
H	-1.203964	1.097574	-2.296367
H	-4.965097	2.646106	-0.877332

BVE

M06 SCF energy: -310.917999723 a.u.
Enthalpy at 298K: -310.7367107 a.u.
Gibbs free energy at 298K: -310.7799437 a.u.
Cartesian Coordinates

C	2.311896	-0.679565	-0.156377
O	0.988378	-0.501057	-0.393845
C	0.421468	0.758835	-0.032864
C	-1.063263	0.731317	-0.371430
C	-1.863436	-0.301218	0.433422
C	-3.350611	-0.318431	0.066488
C	3.186426	0.178740	0.379768
H	2.608261	-1.675577	-0.475818
H	0.937105	1.559499	-0.582479
H	0.578396	0.933991	1.042127
H	-1.174082	0.534485	-1.446262
H	-1.467042	1.738010	-0.193128
H	-1.427627	-1.293879	0.270518
H	-1.751152	-0.086625	1.506002
H	-3.817962	0.657935	0.246682
H	-3.494248	-0.562791	-0.993283
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H	4.218740	-0.129829	0.498415

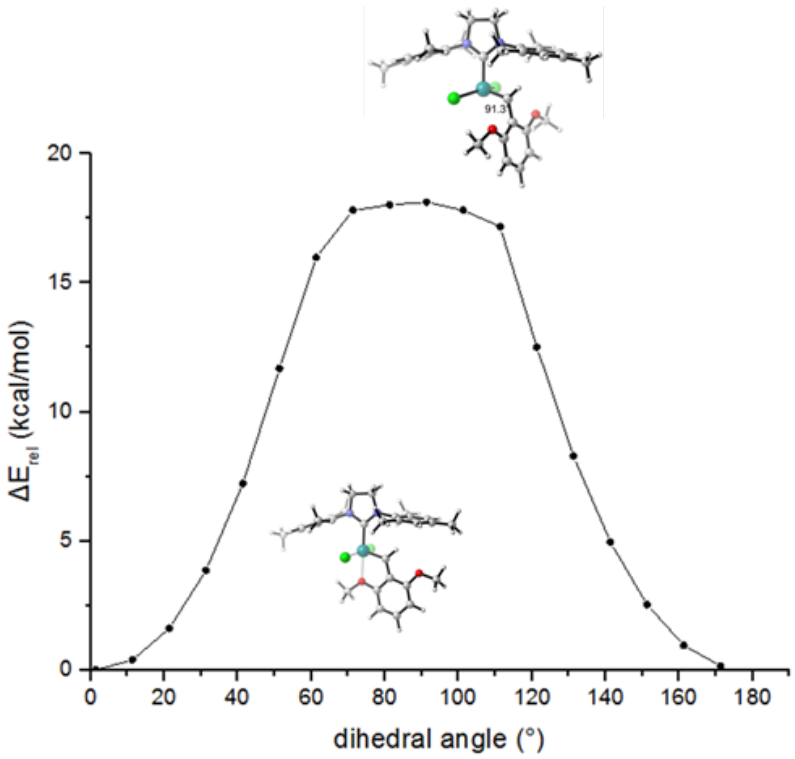

Figure S30: Energy scan of catalyst **32** around the $C_{benzylidene}$-C_{aryl} bond. No stable non-chelated 14 e^- complex intermediate was found.

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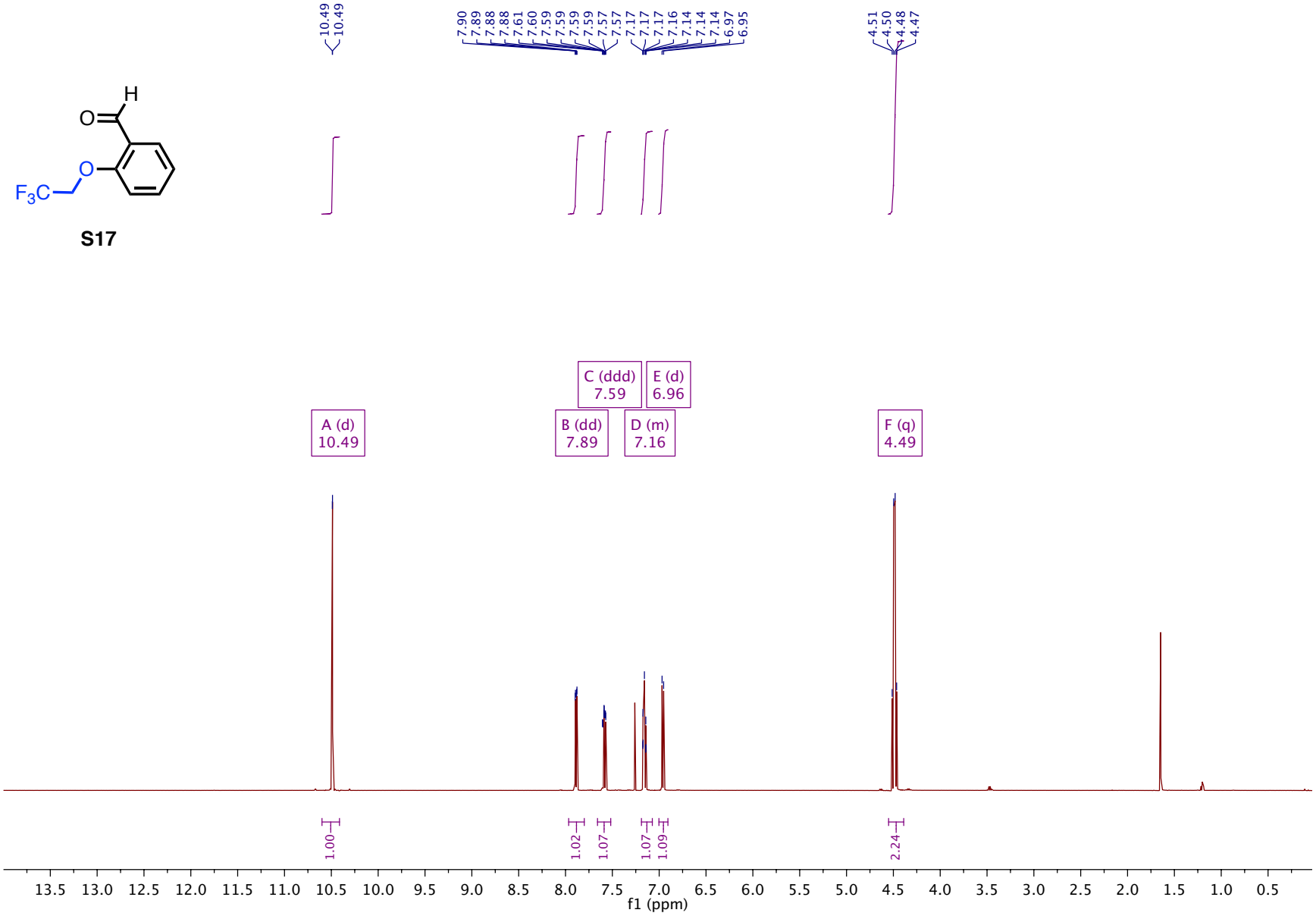
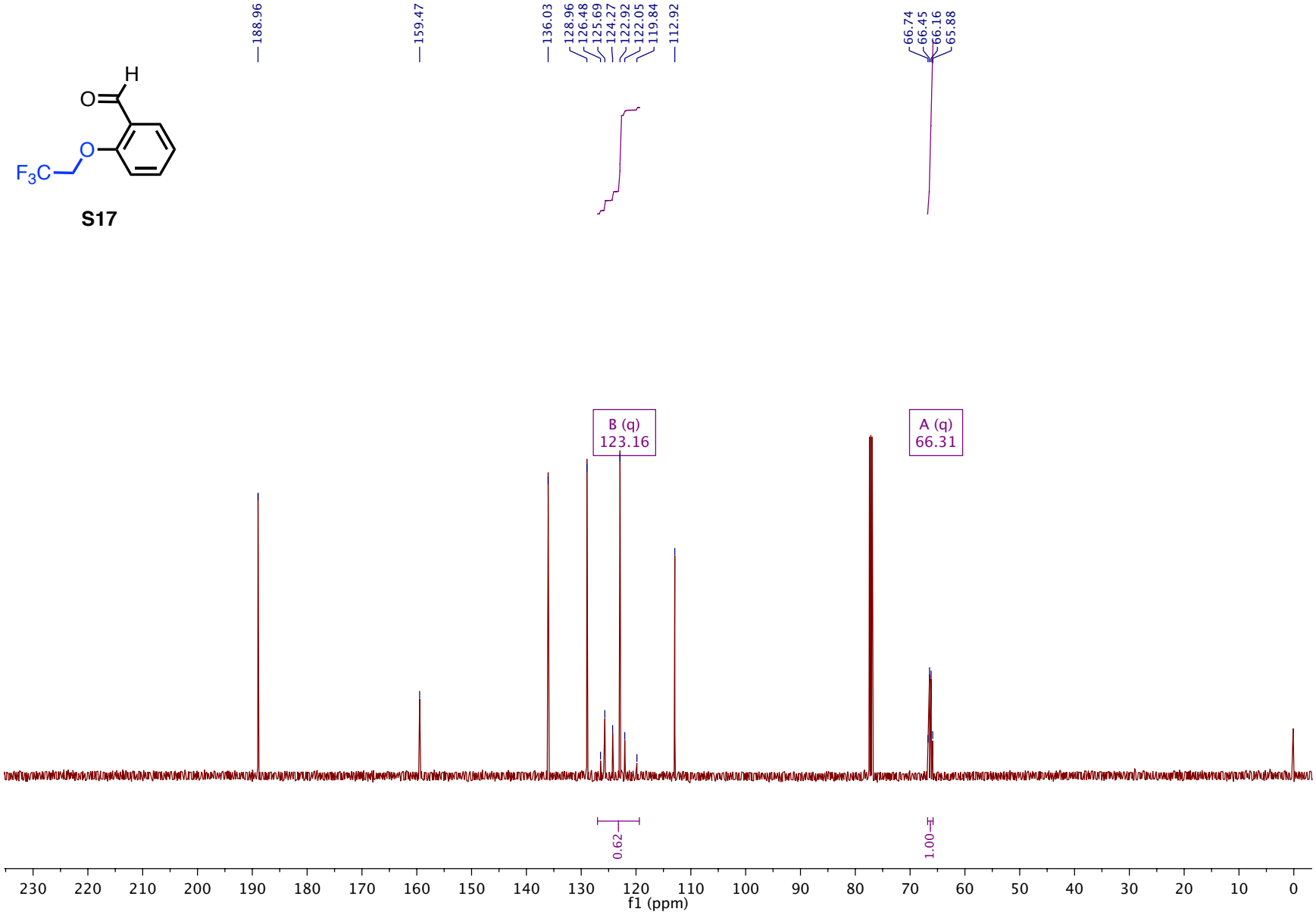
^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **S17.**

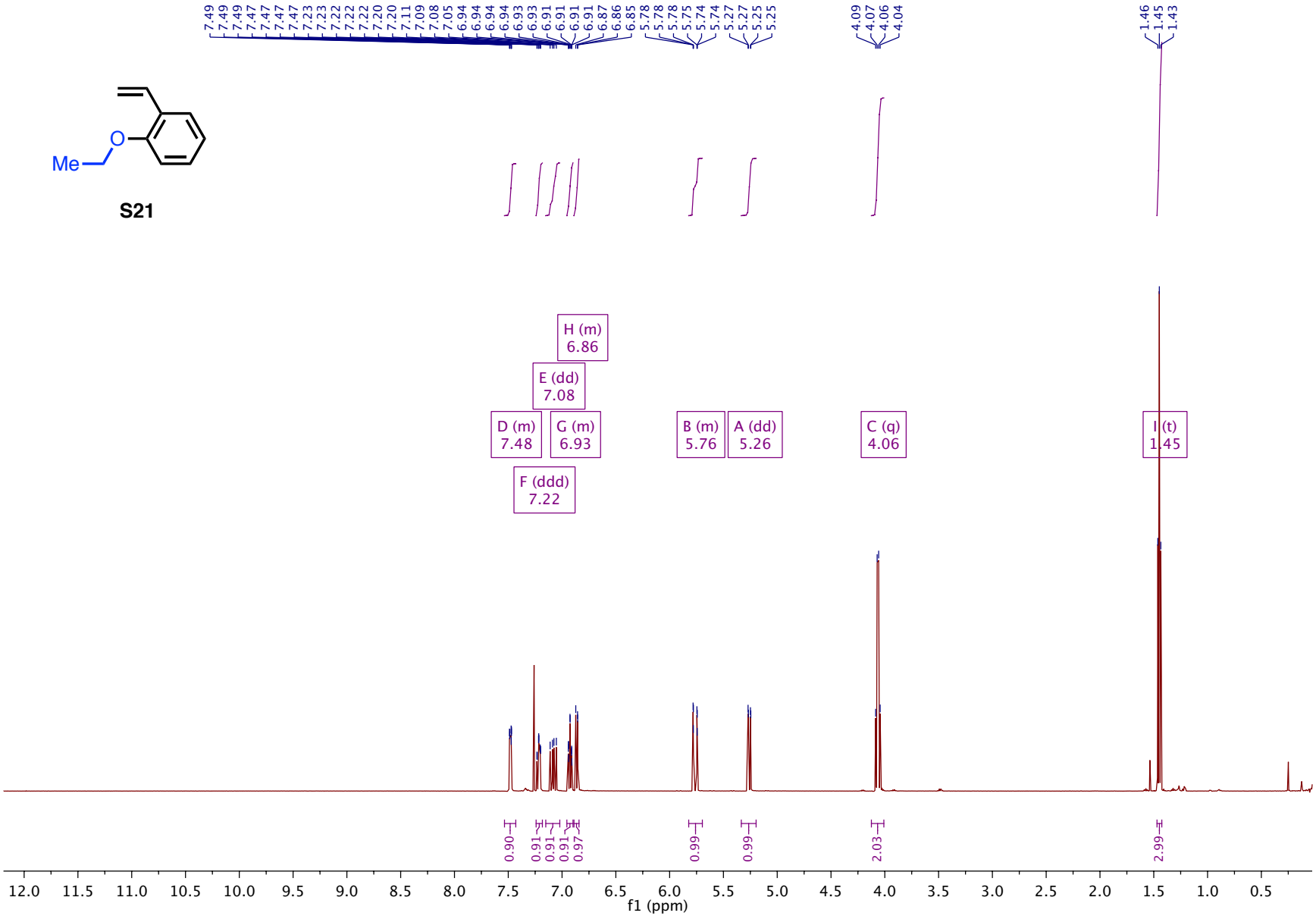


^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **S17.**

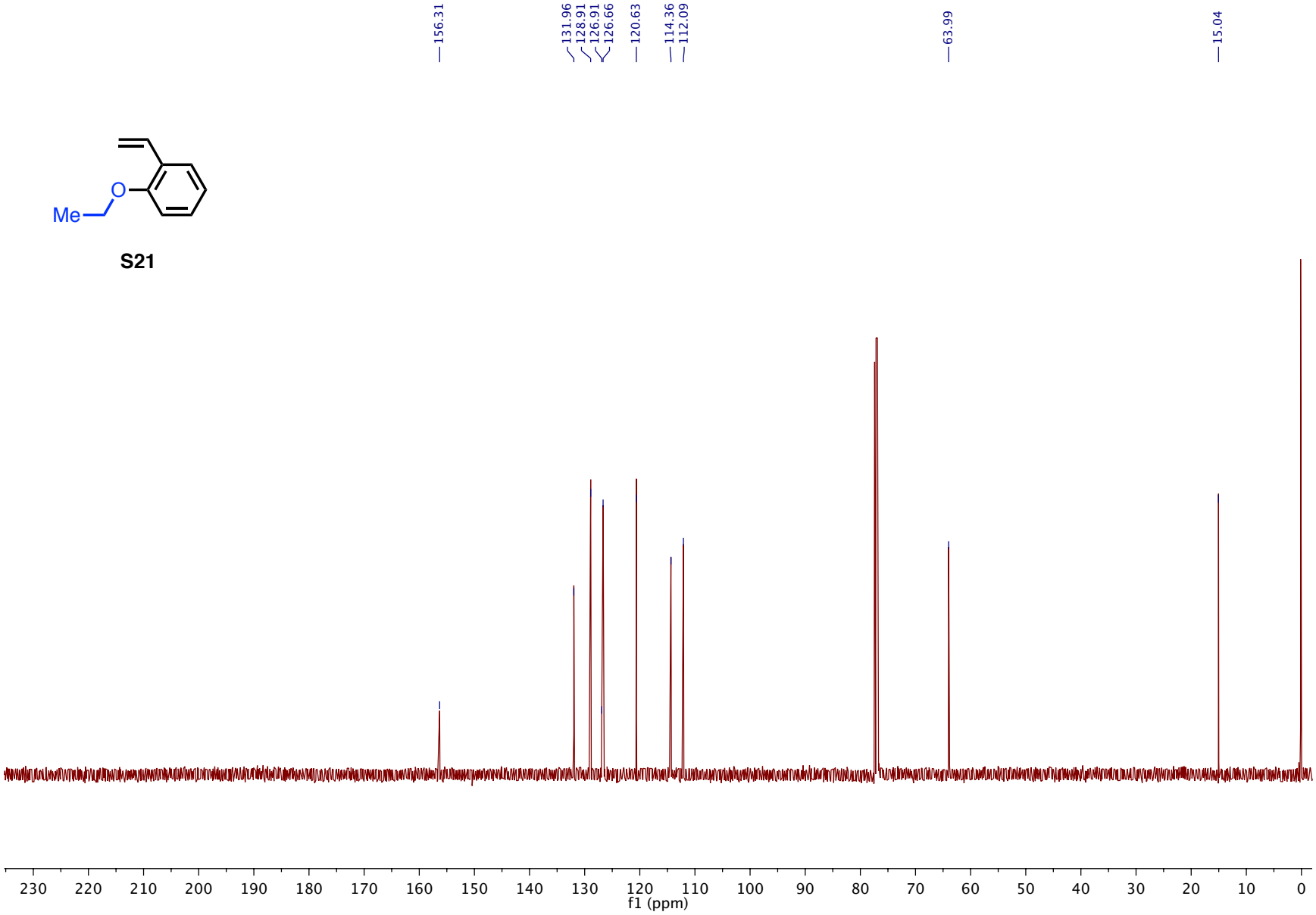


S17

^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **S21.**

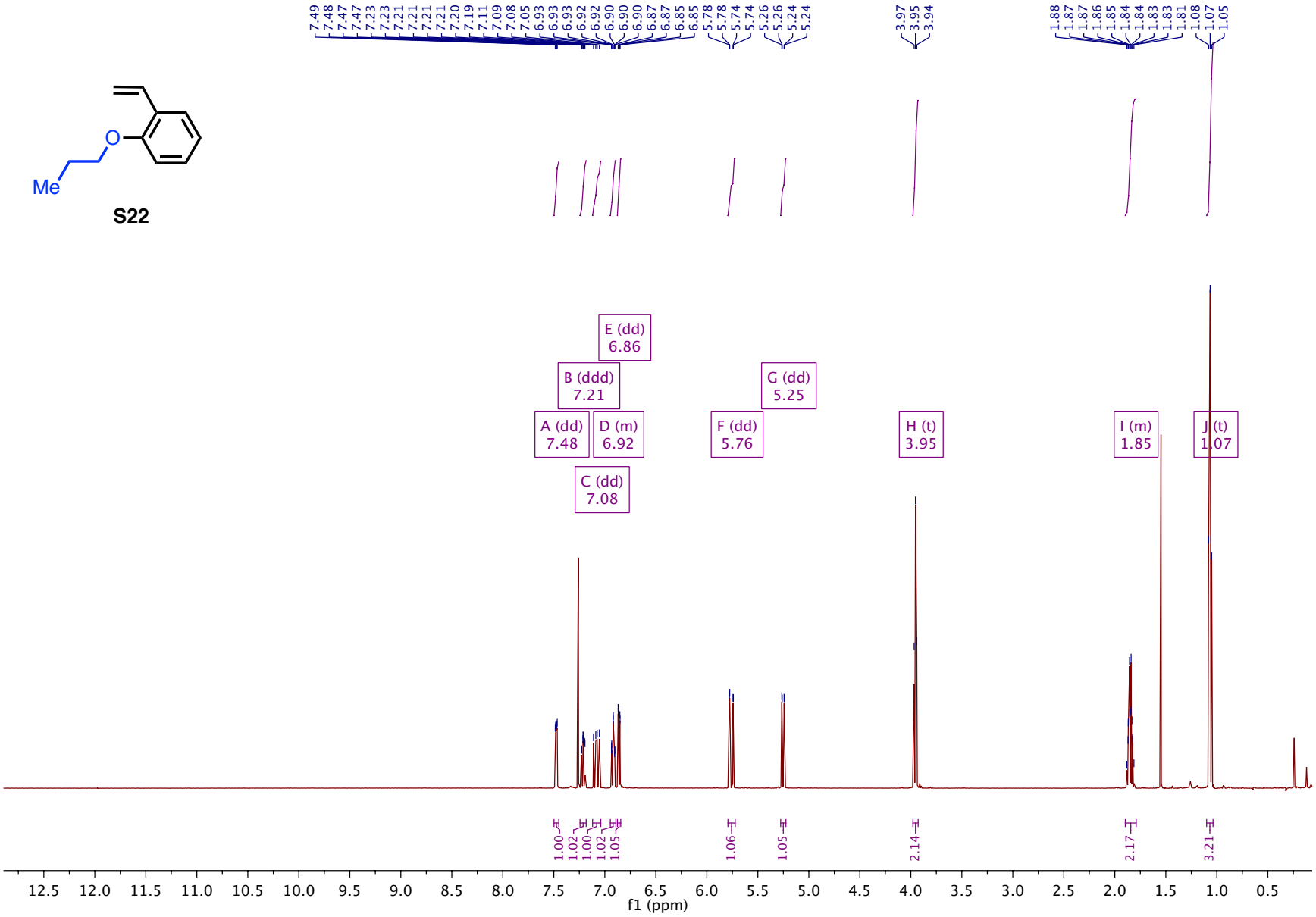


^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **S21.**

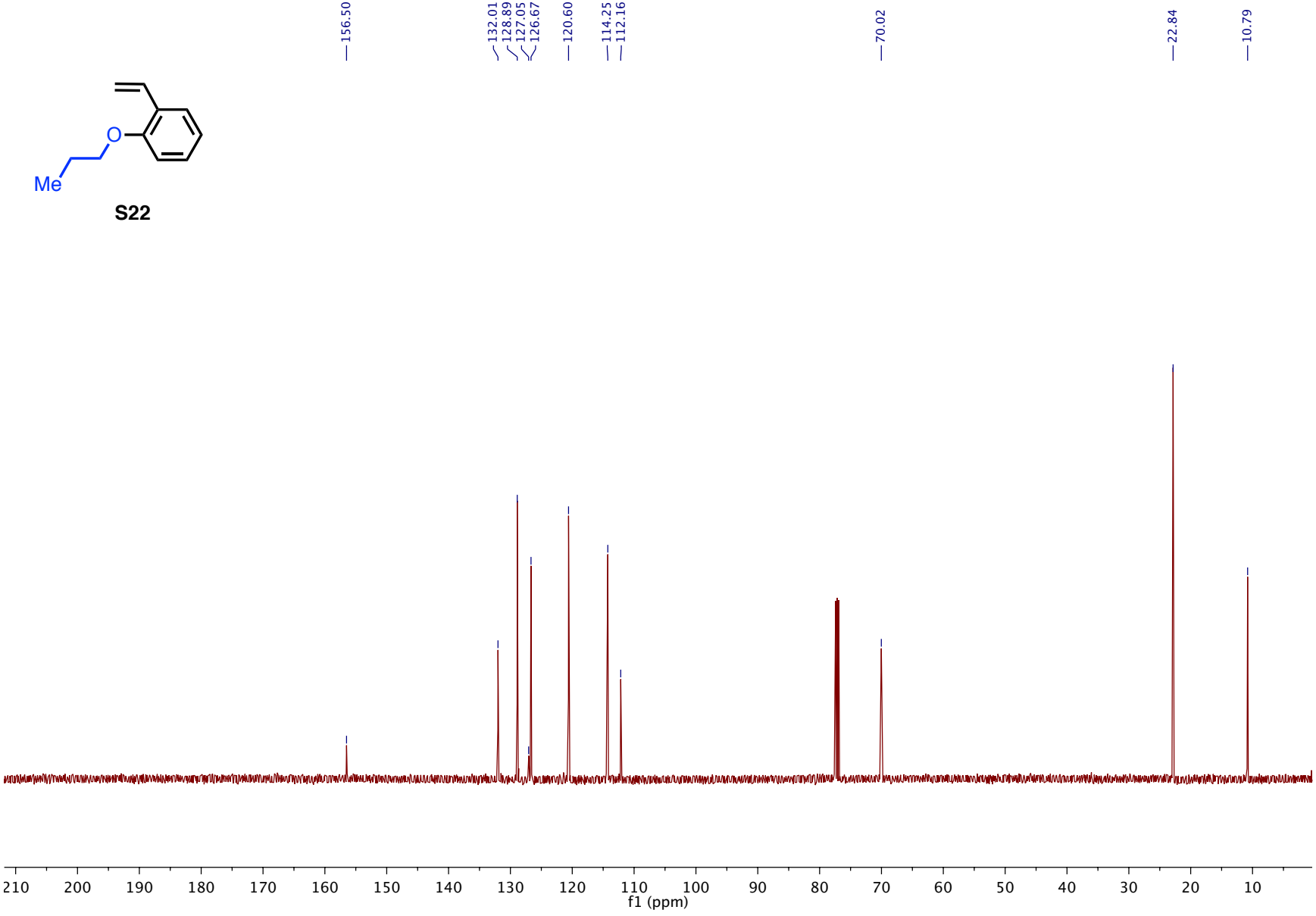


S21

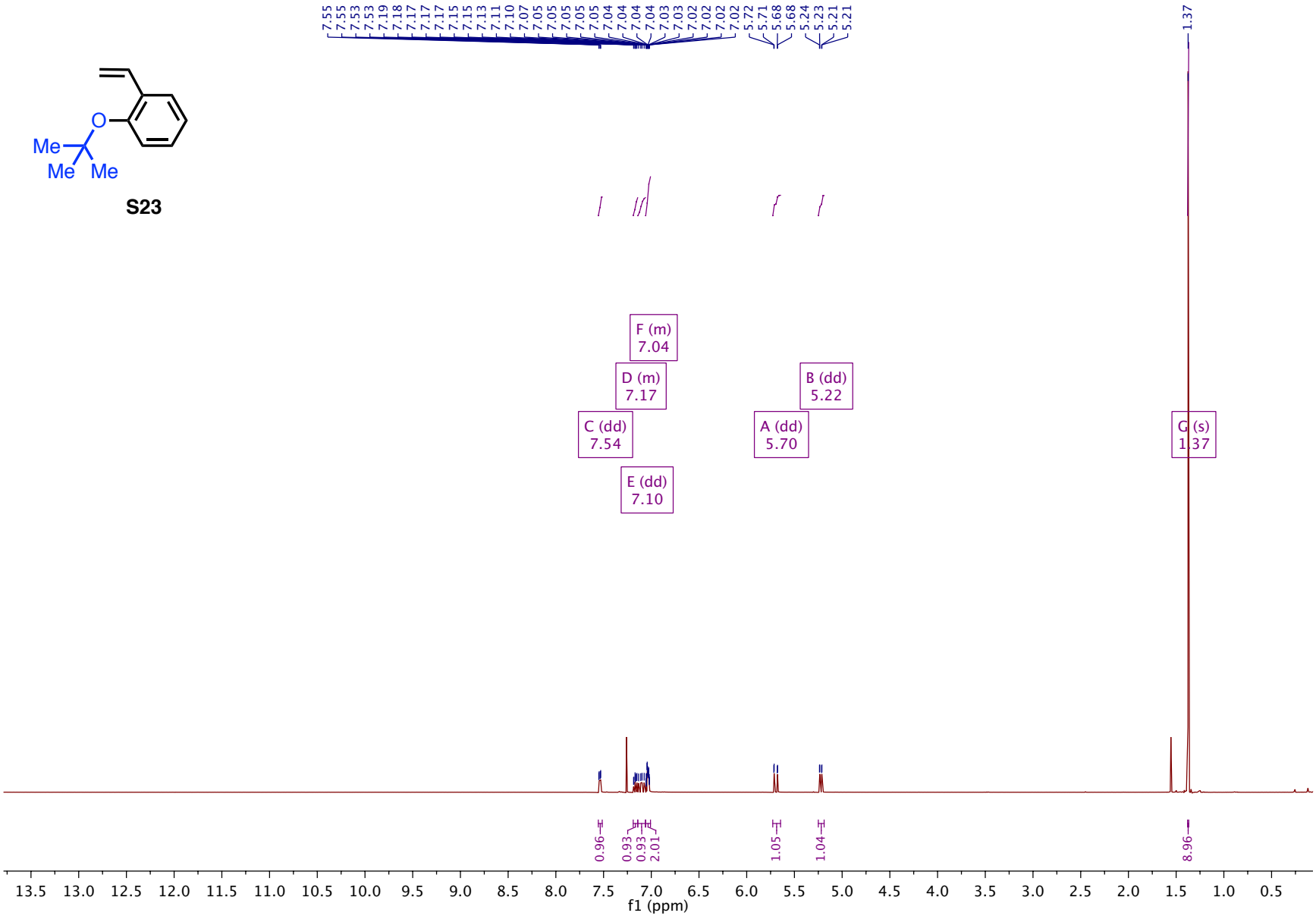
^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **S22.**



^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **S22.**



^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **S23.**



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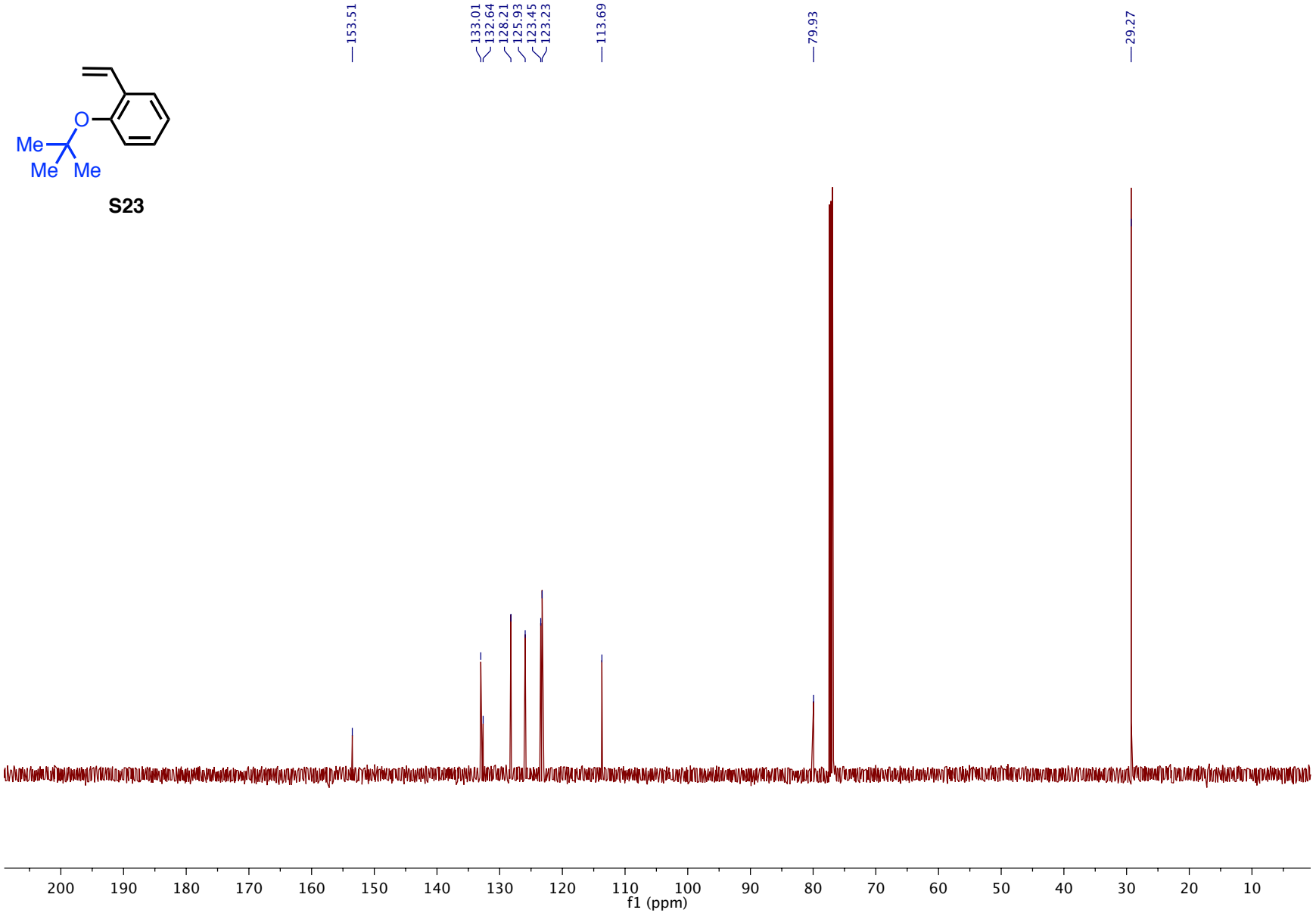
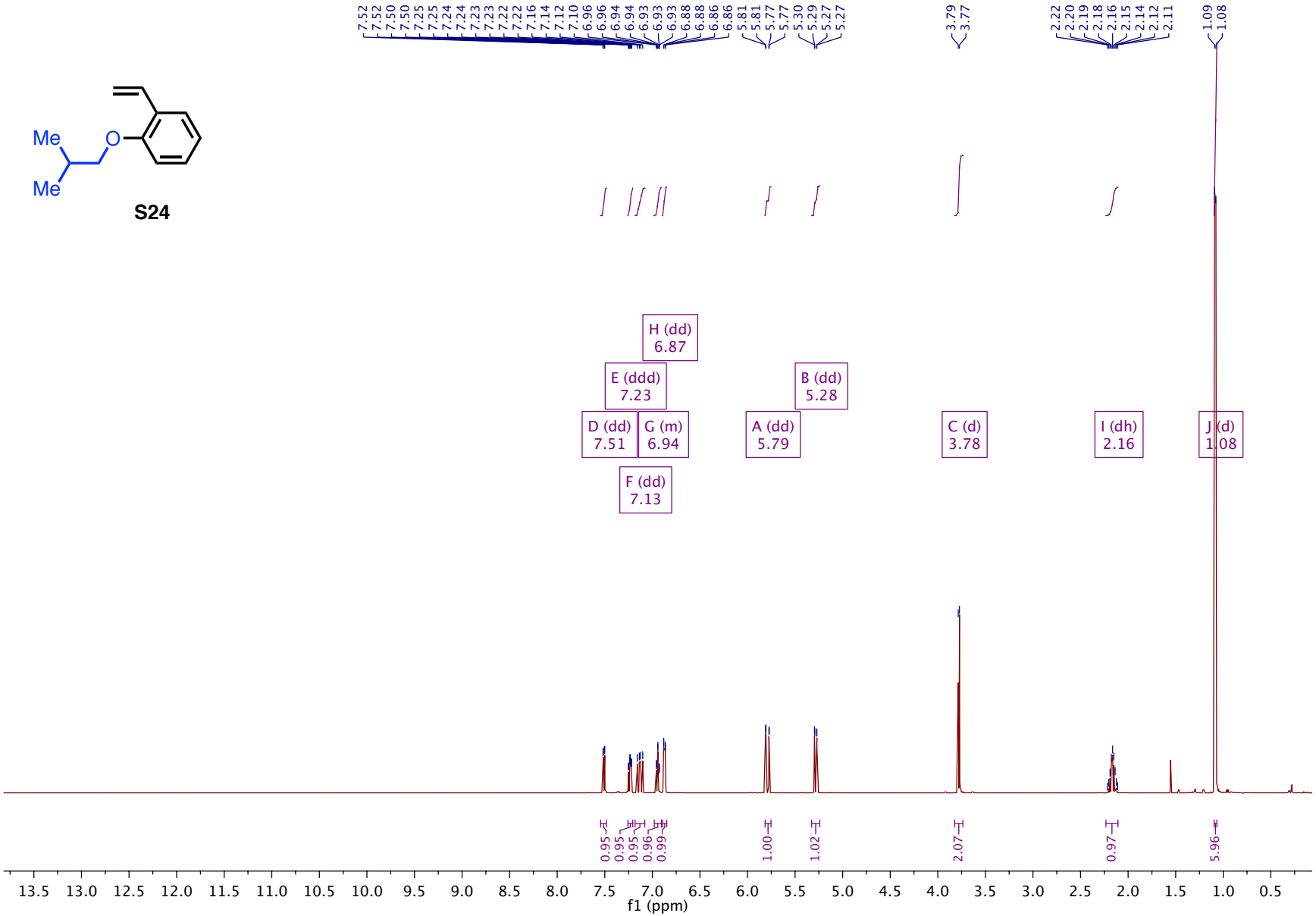
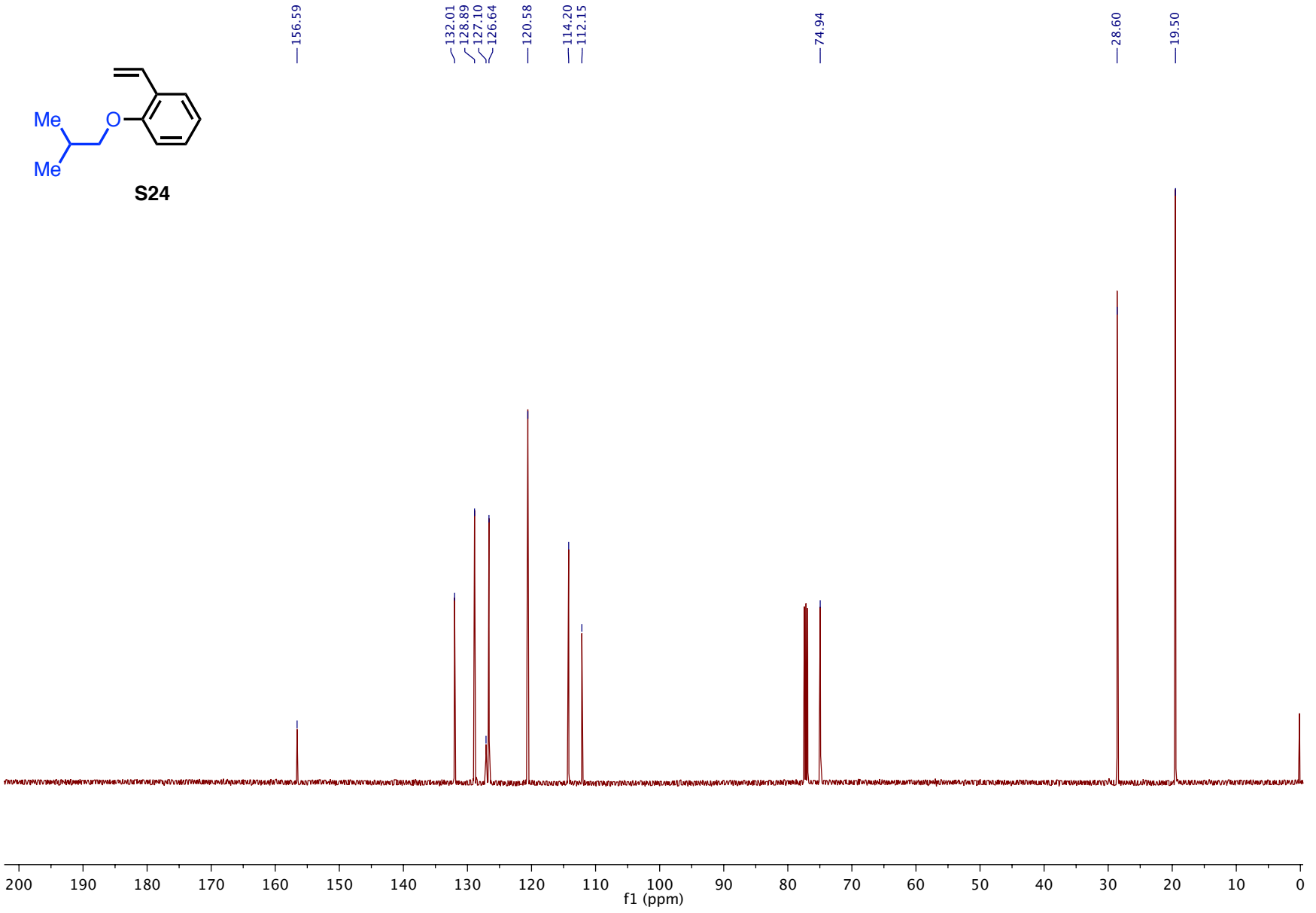


^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **S24.**



^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **S24.**



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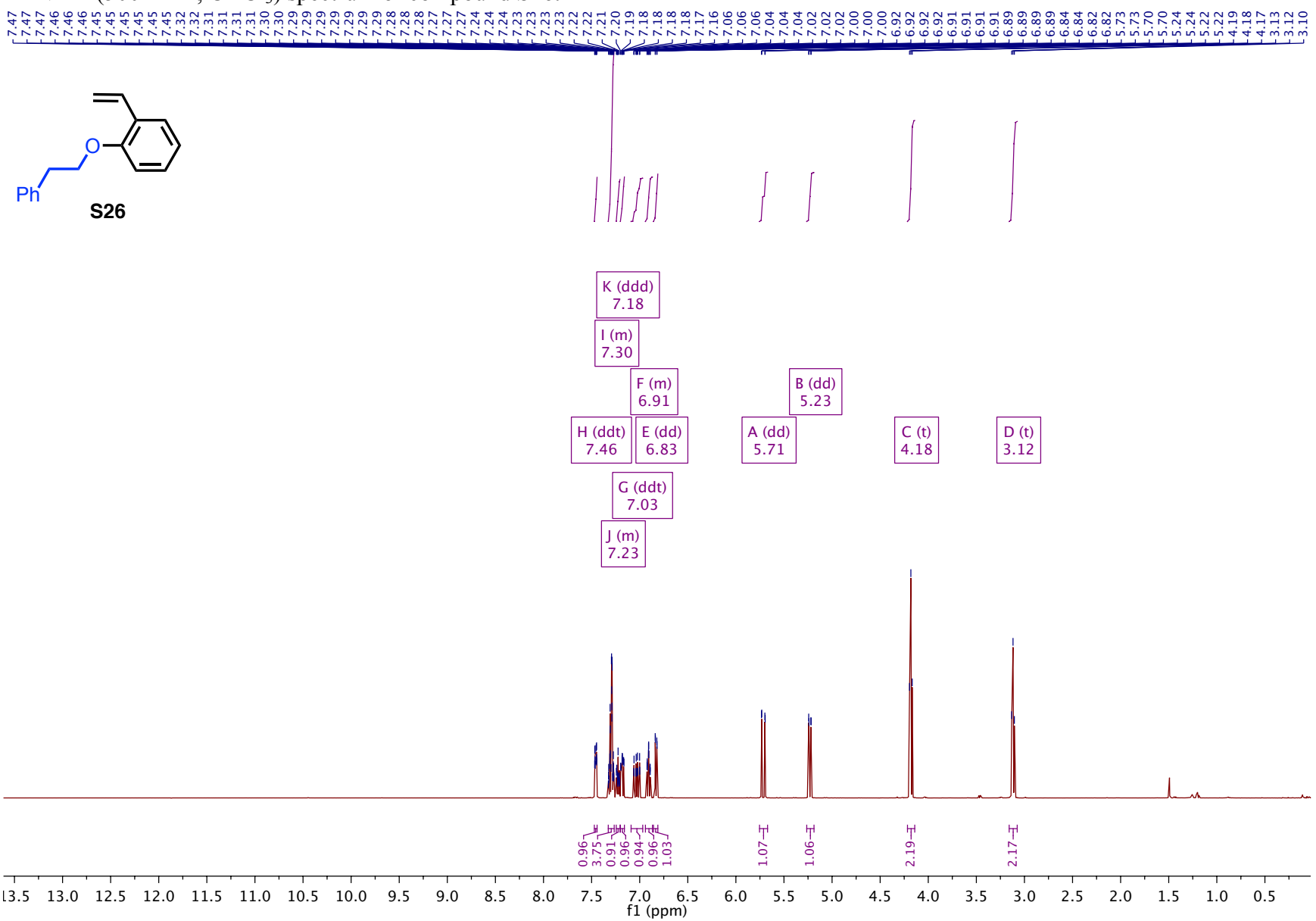

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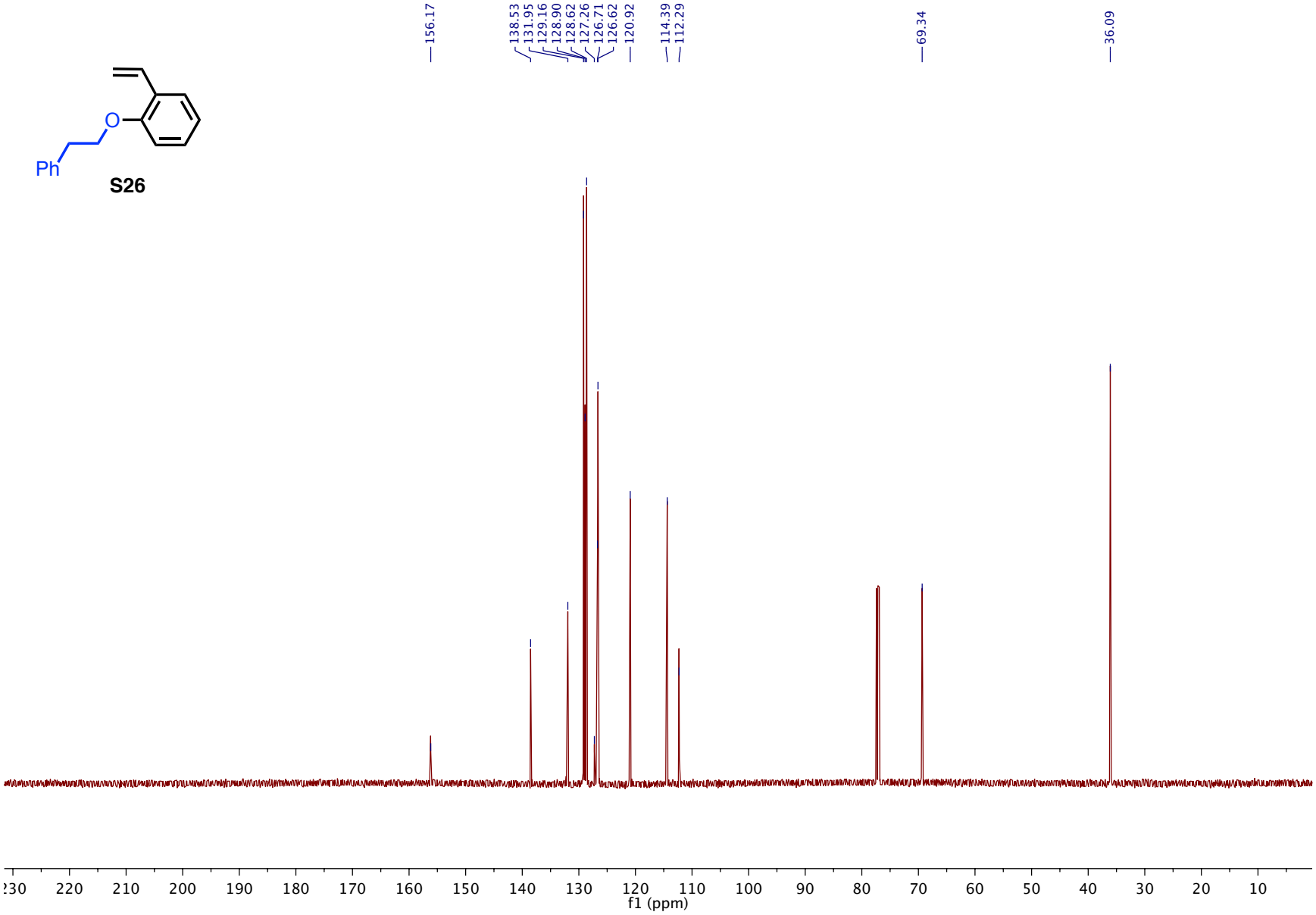

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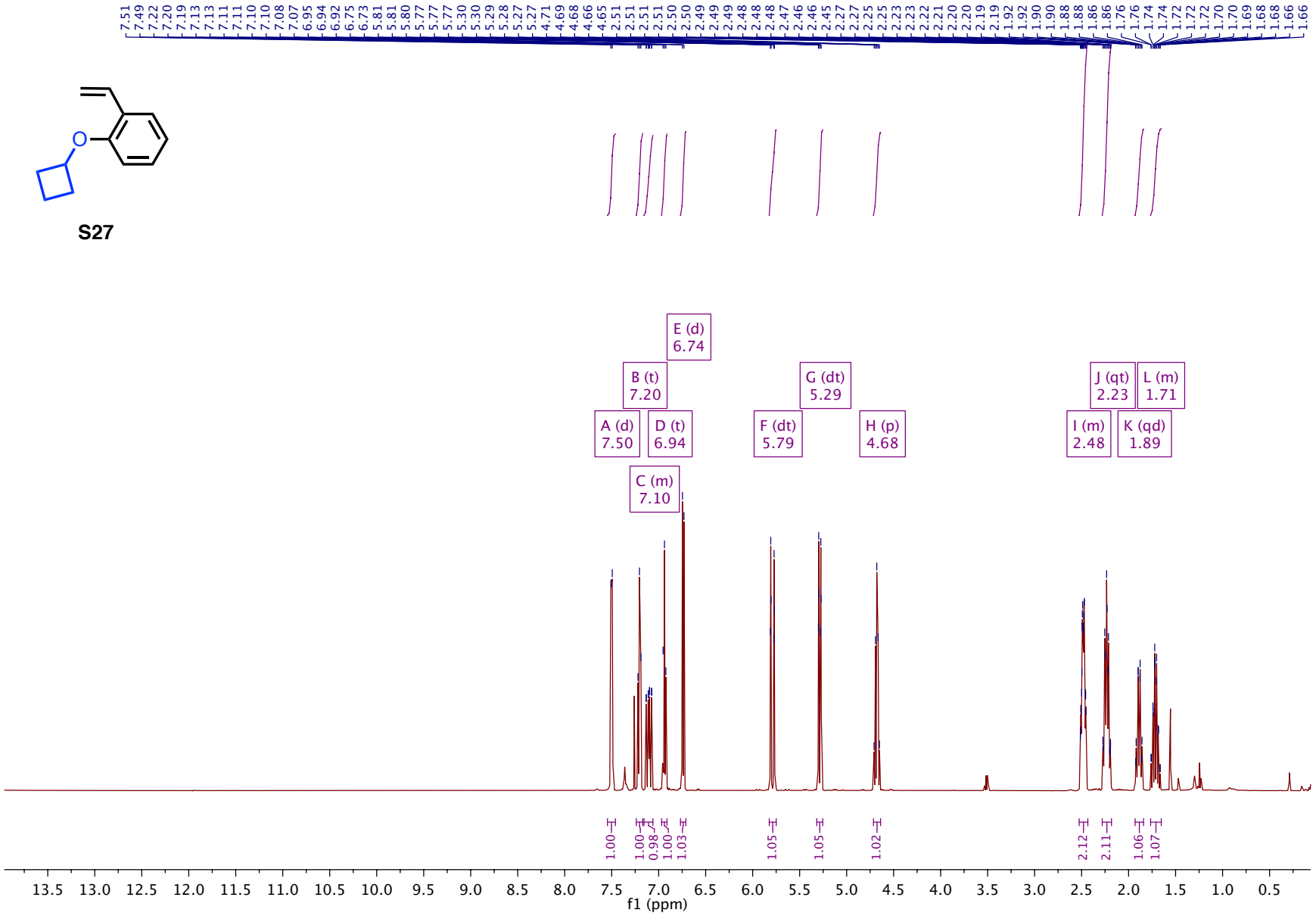

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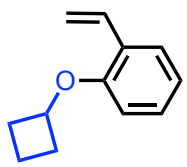

S27

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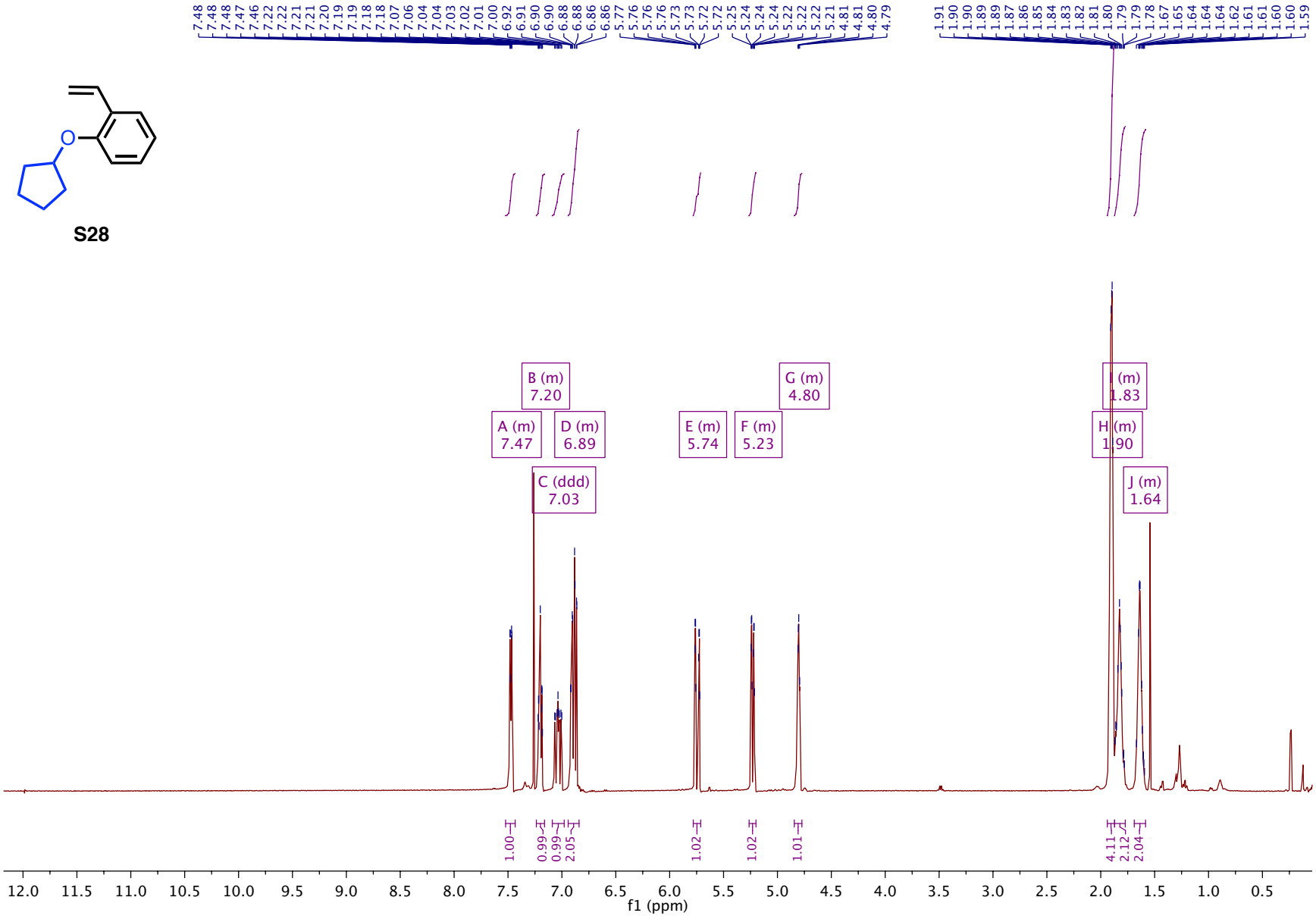

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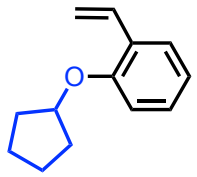
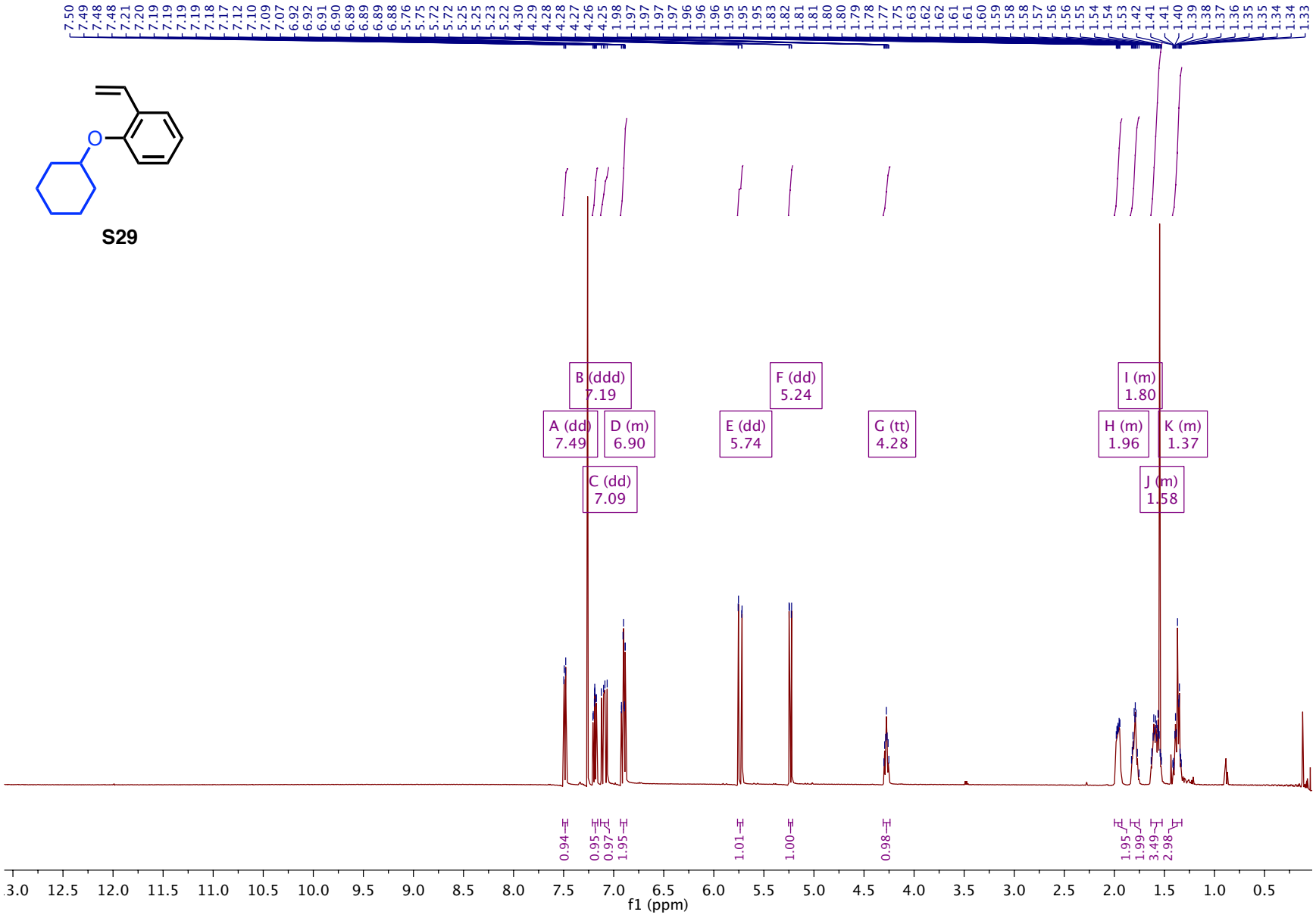


S28

^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **S29.**



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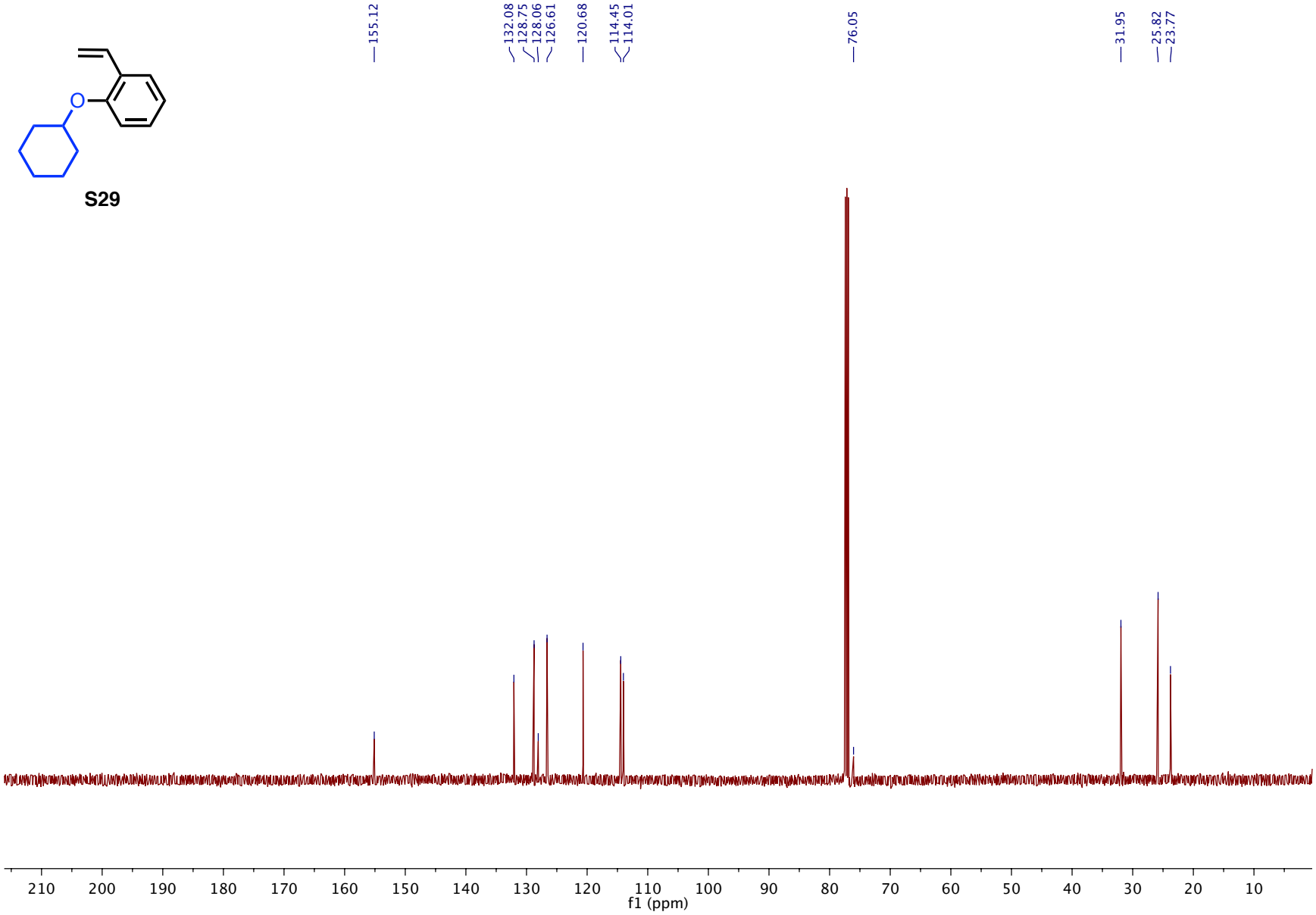
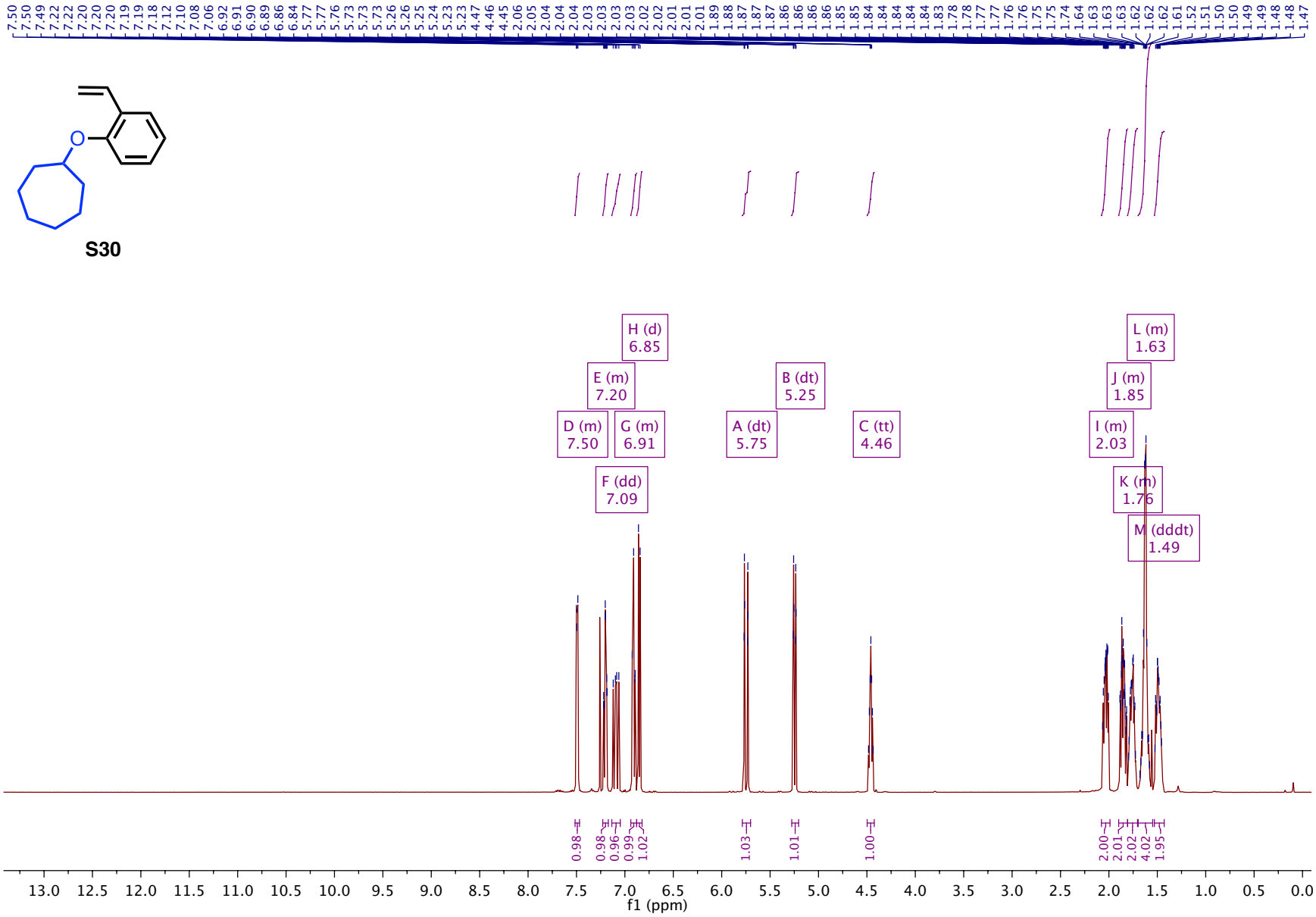
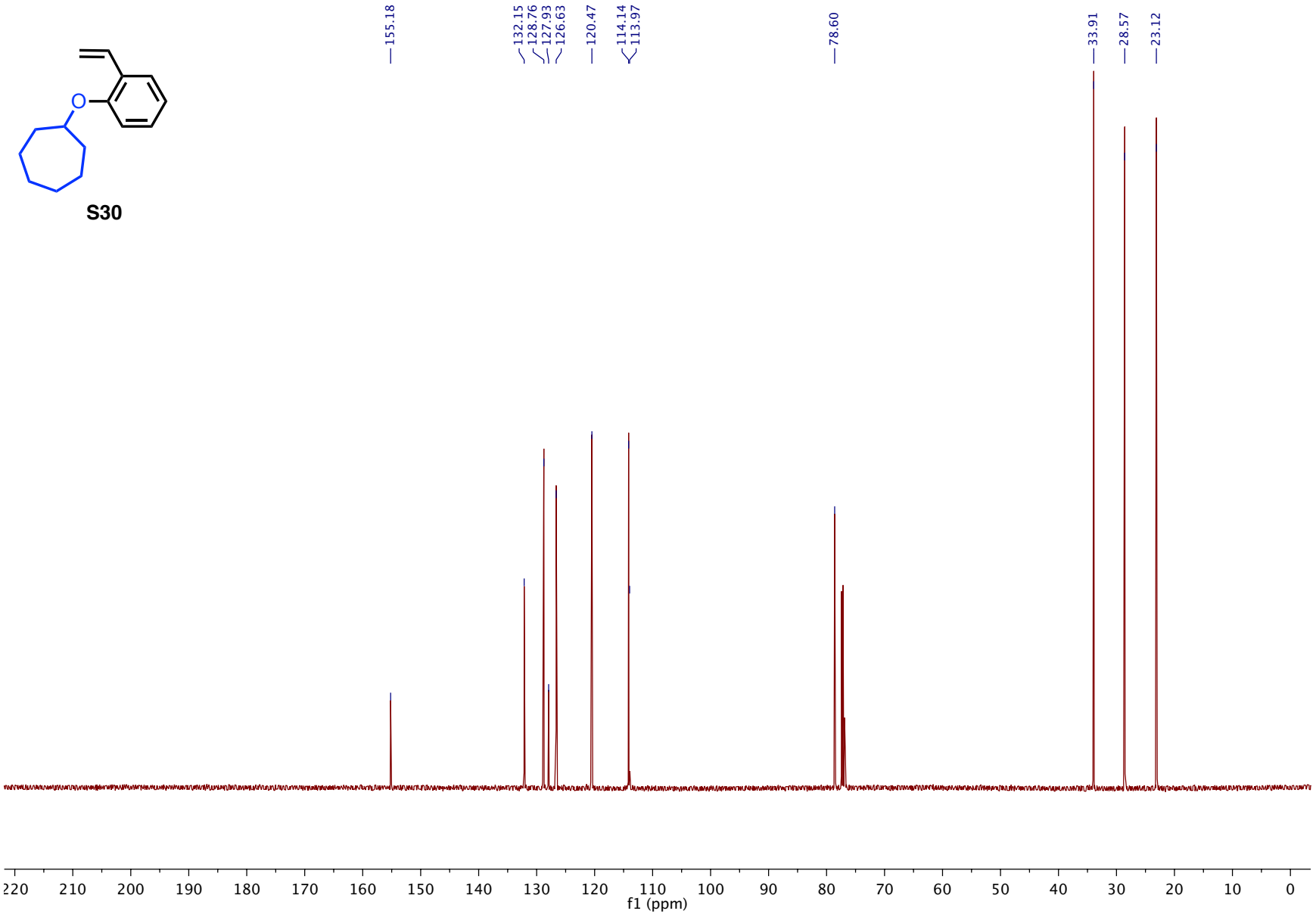


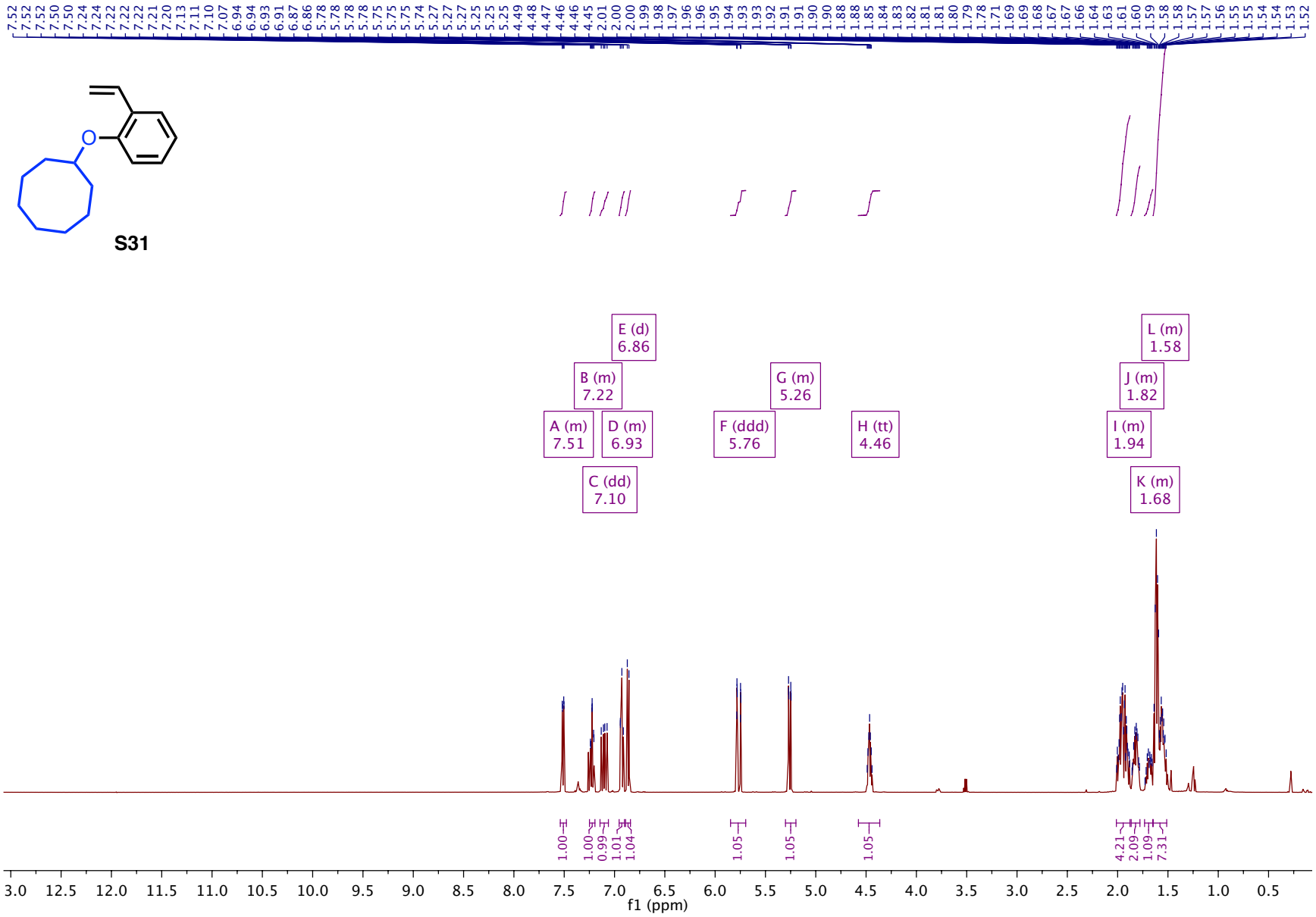
^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **S30.**



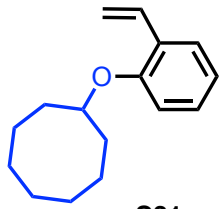
^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **S30.**



^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **S31.**

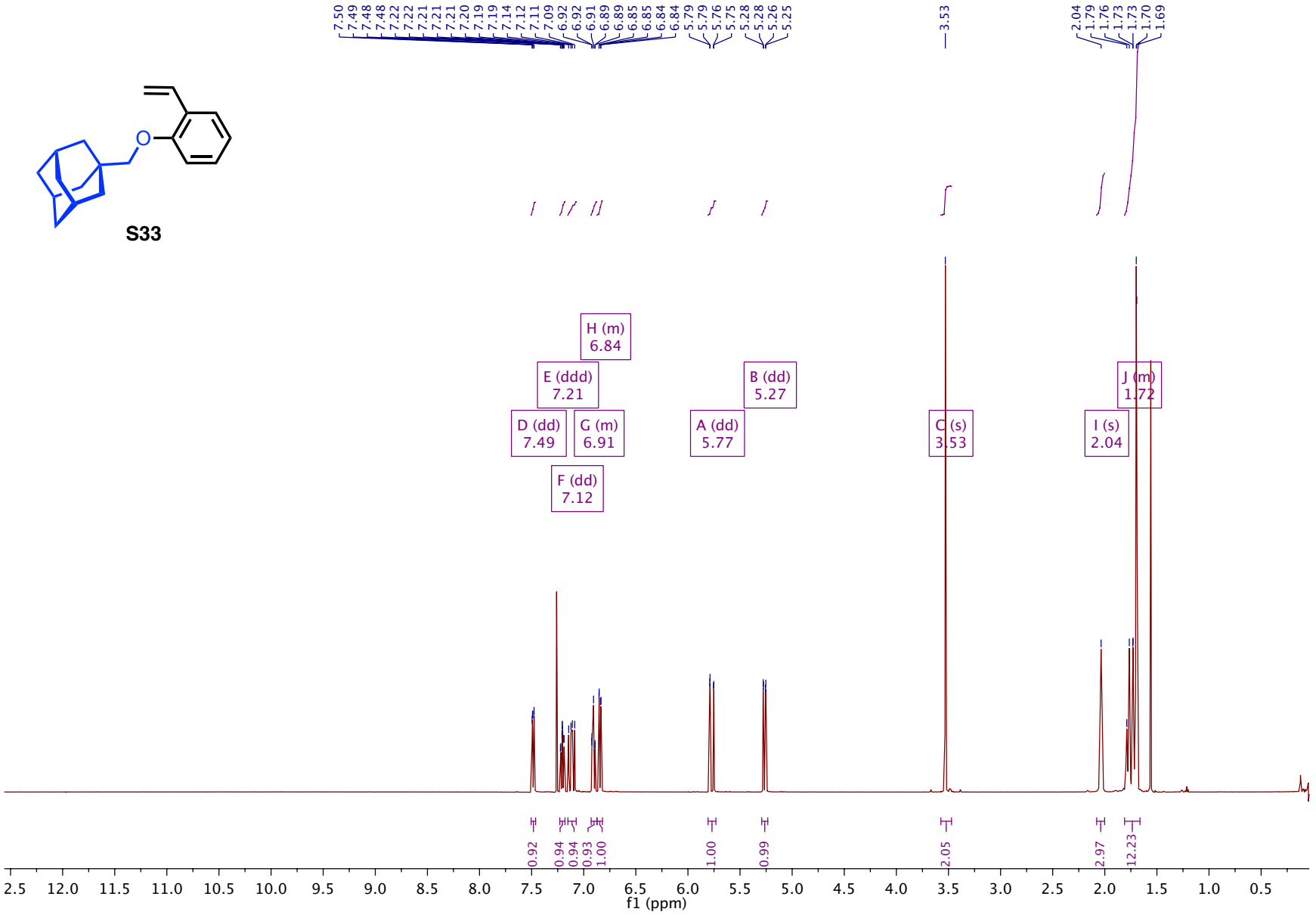


^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **S31.**

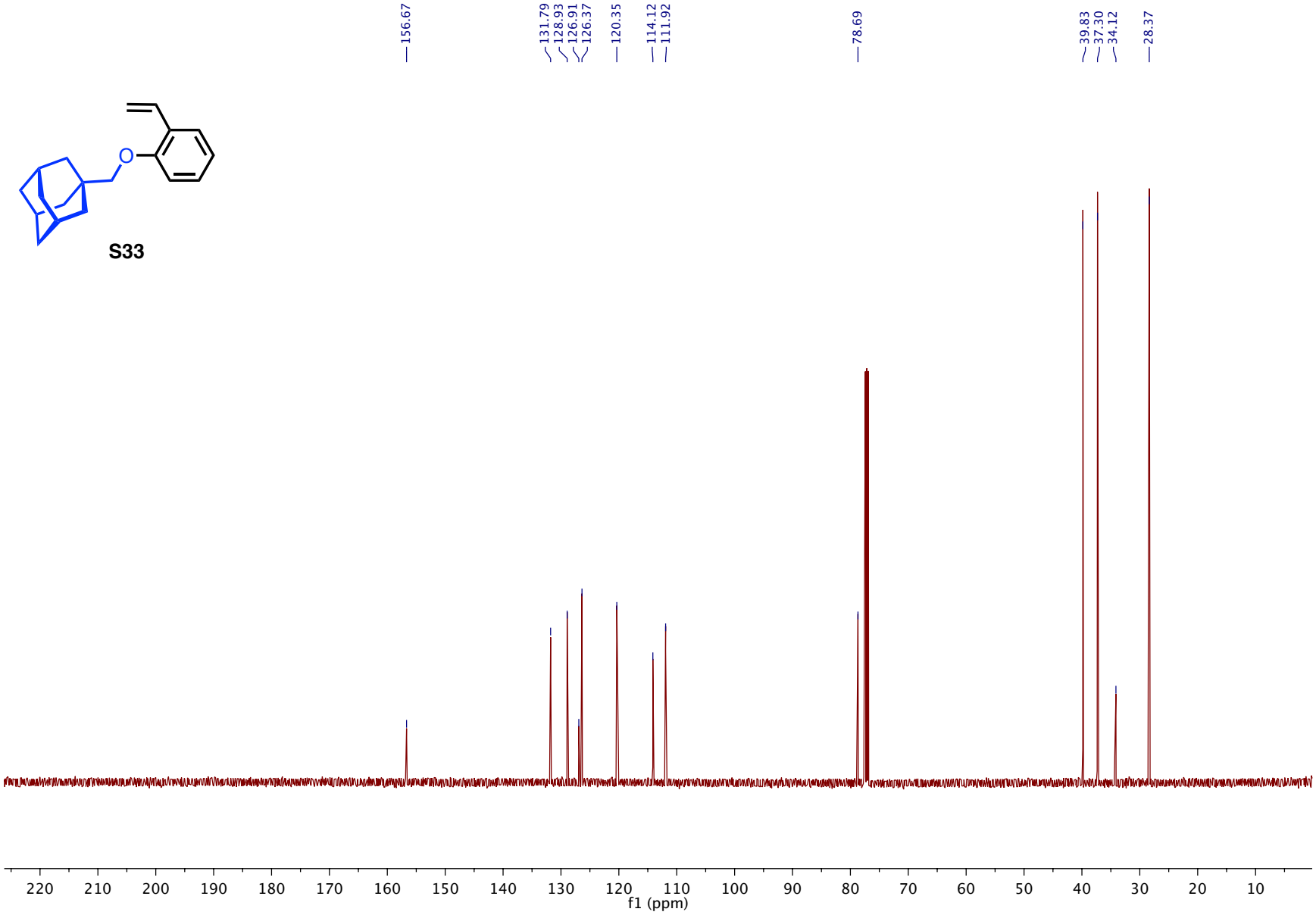


S31

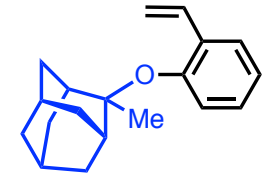
^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **S33.**



^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **S33.**

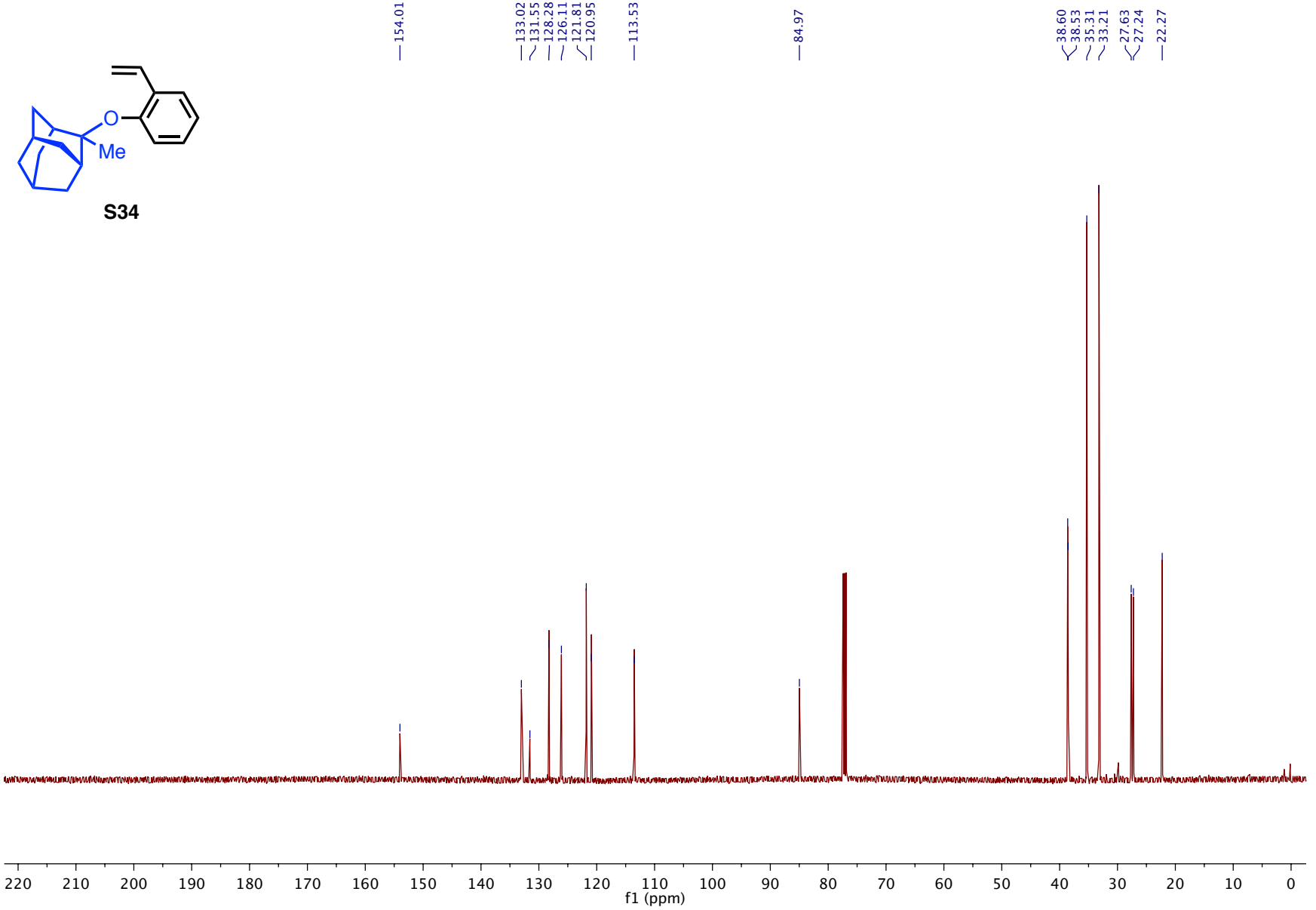


^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **S34.**

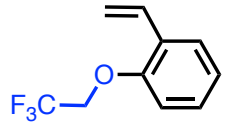


S34

^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **S34.**

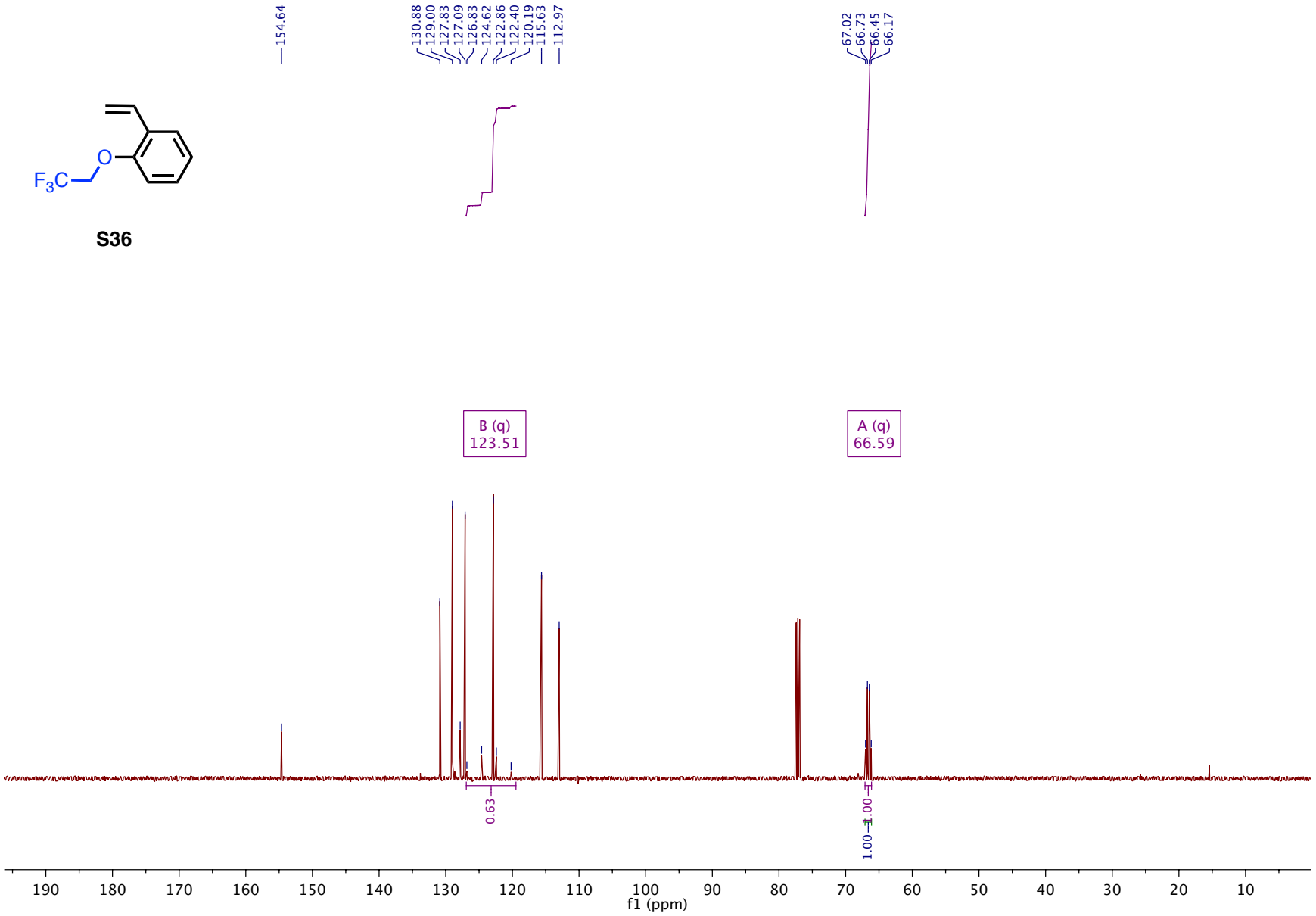


^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **S36.**

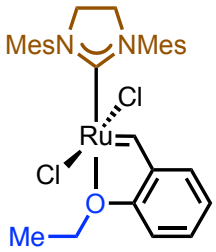


S36

^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **S36.**

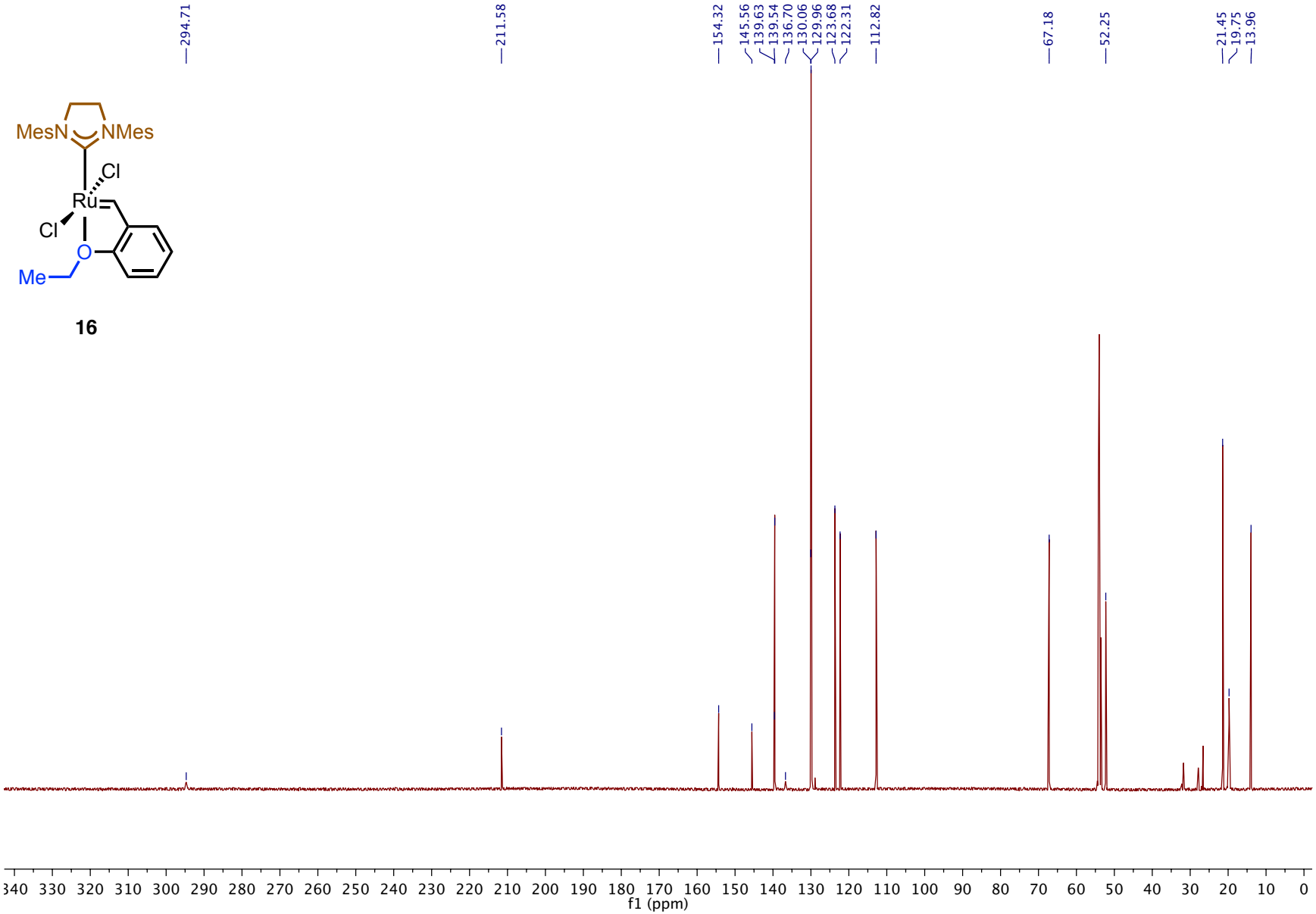


^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of catalyst **16.**



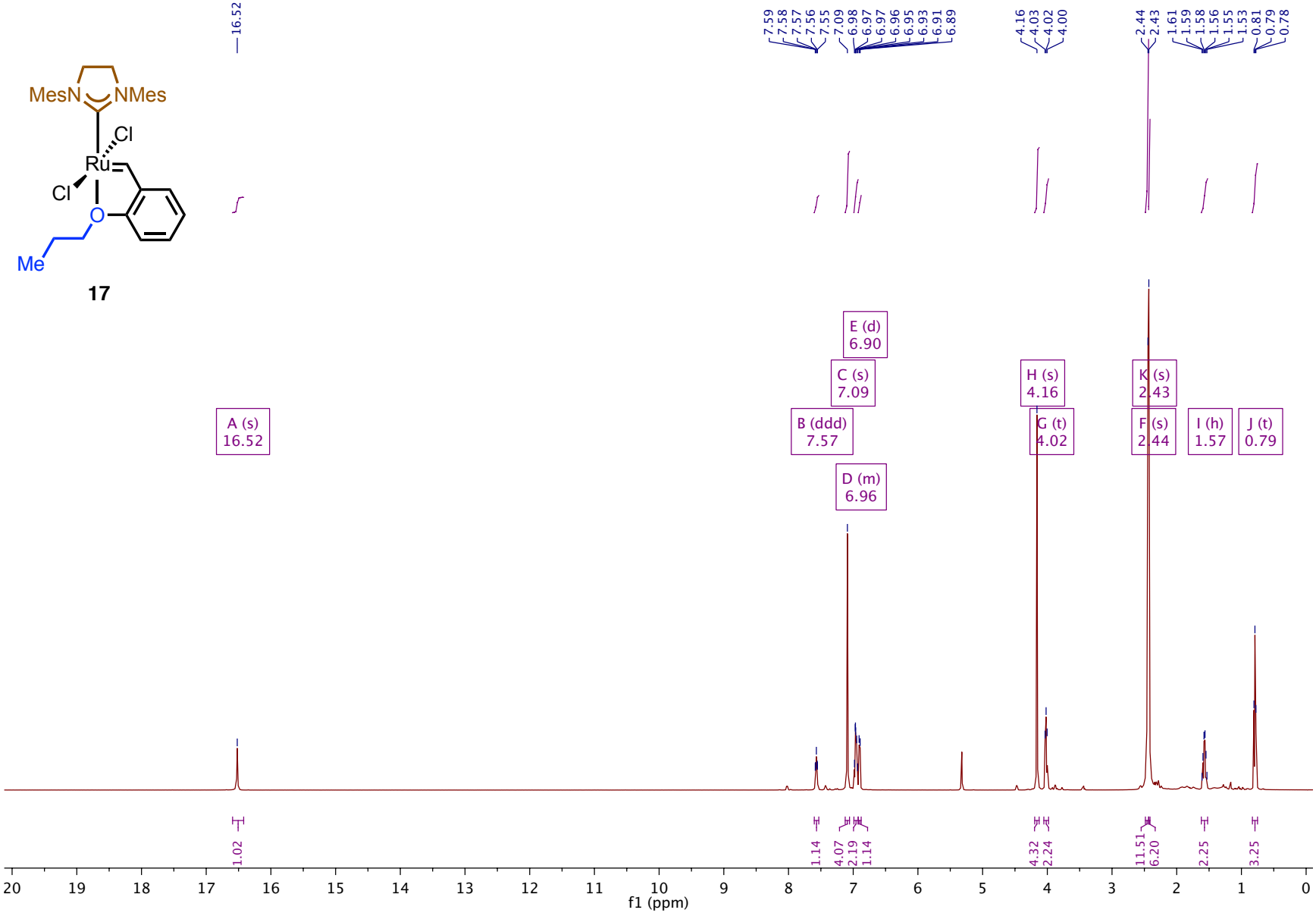
16

^{13}C NMR (125 MHz, CD_2Cl_2) spectrum of catalyst **16.**



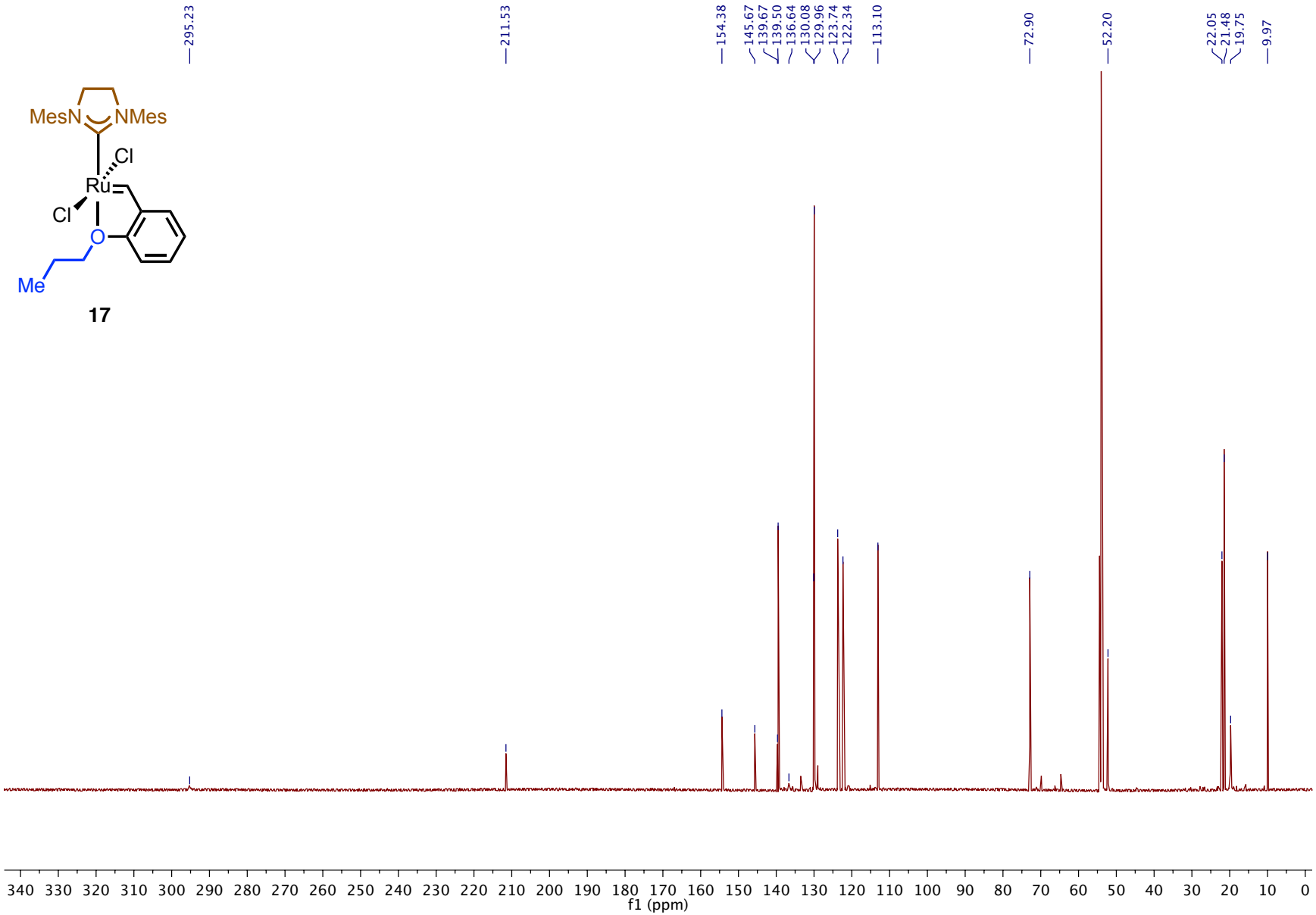
16

^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of catalyst **17.**

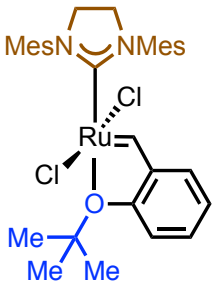


17

^{13}C NMR (125 MHz, CD_2Cl_2) spectrum of catalyst **17.**

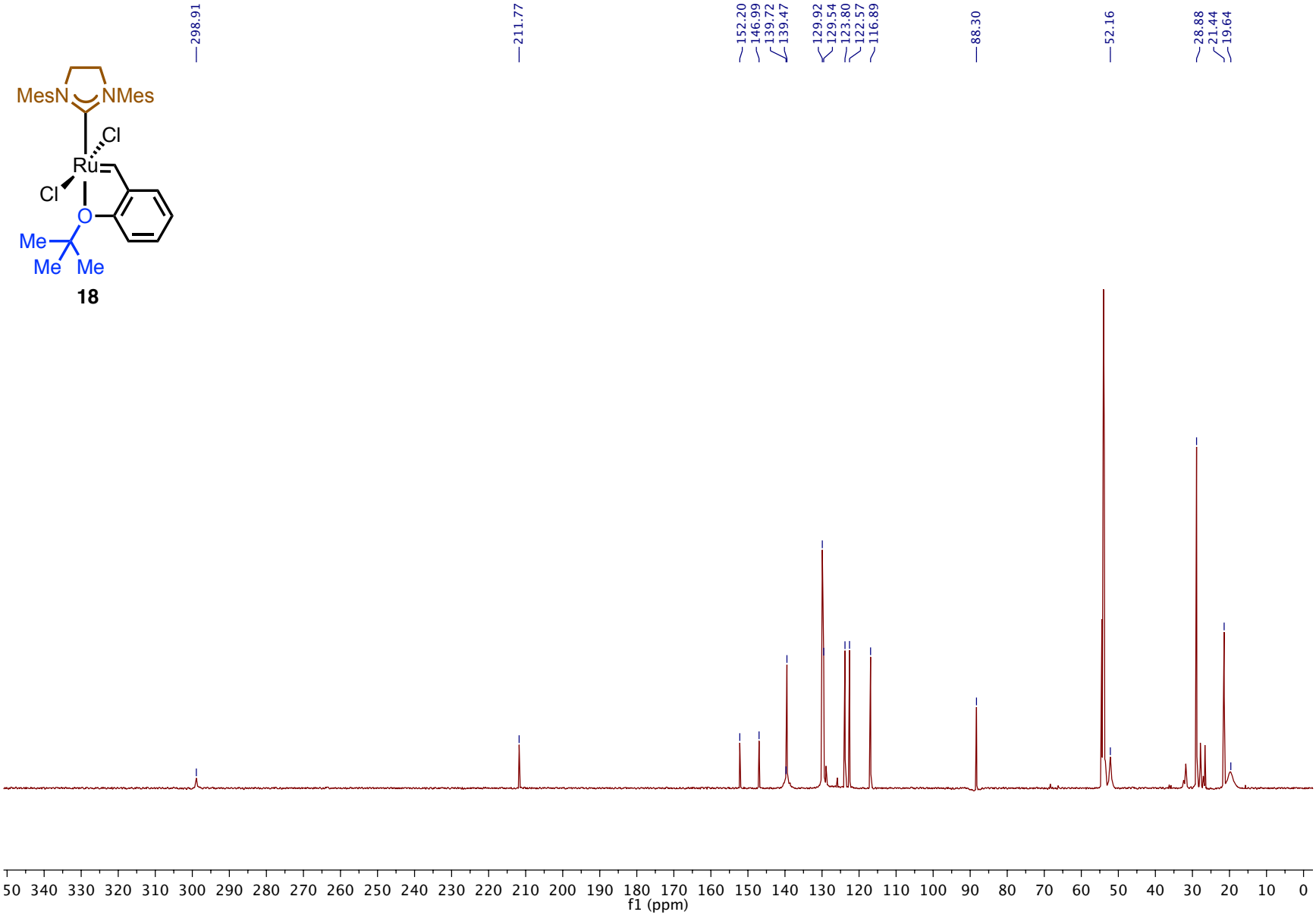


^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of catalyst **18.**

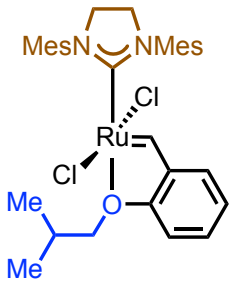


18

^{13}C NMR (125 MHz, CD_2Cl_2) spectrum of catalyst **18.**

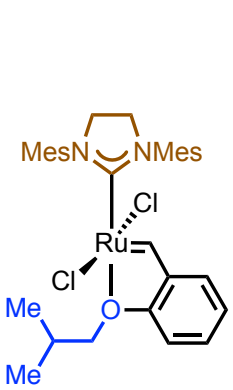


^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of catalyst **19.**



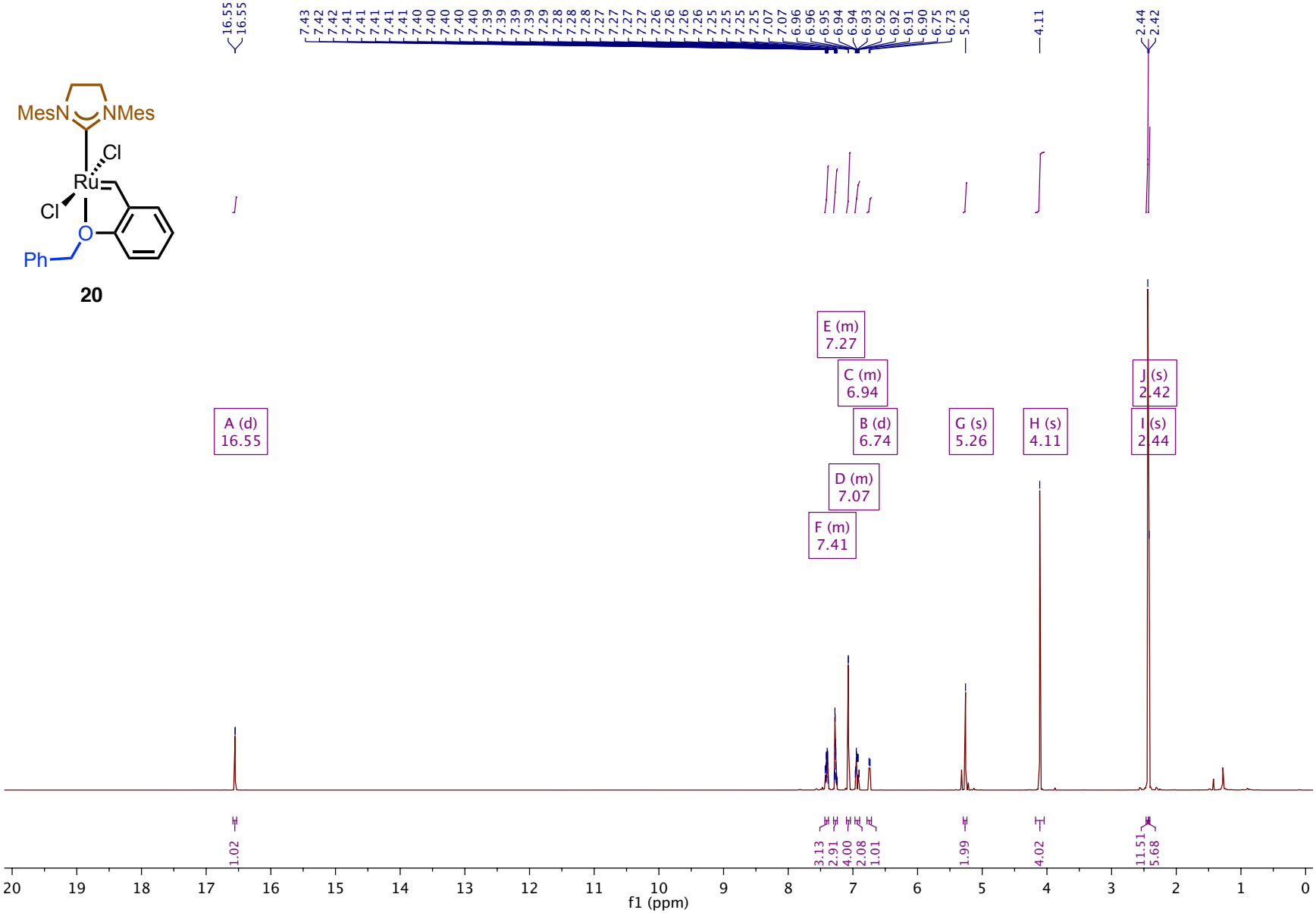
19

^{13}C NMR (125 MHz, CD_2Cl_2) spectrum of catalyst **19.**

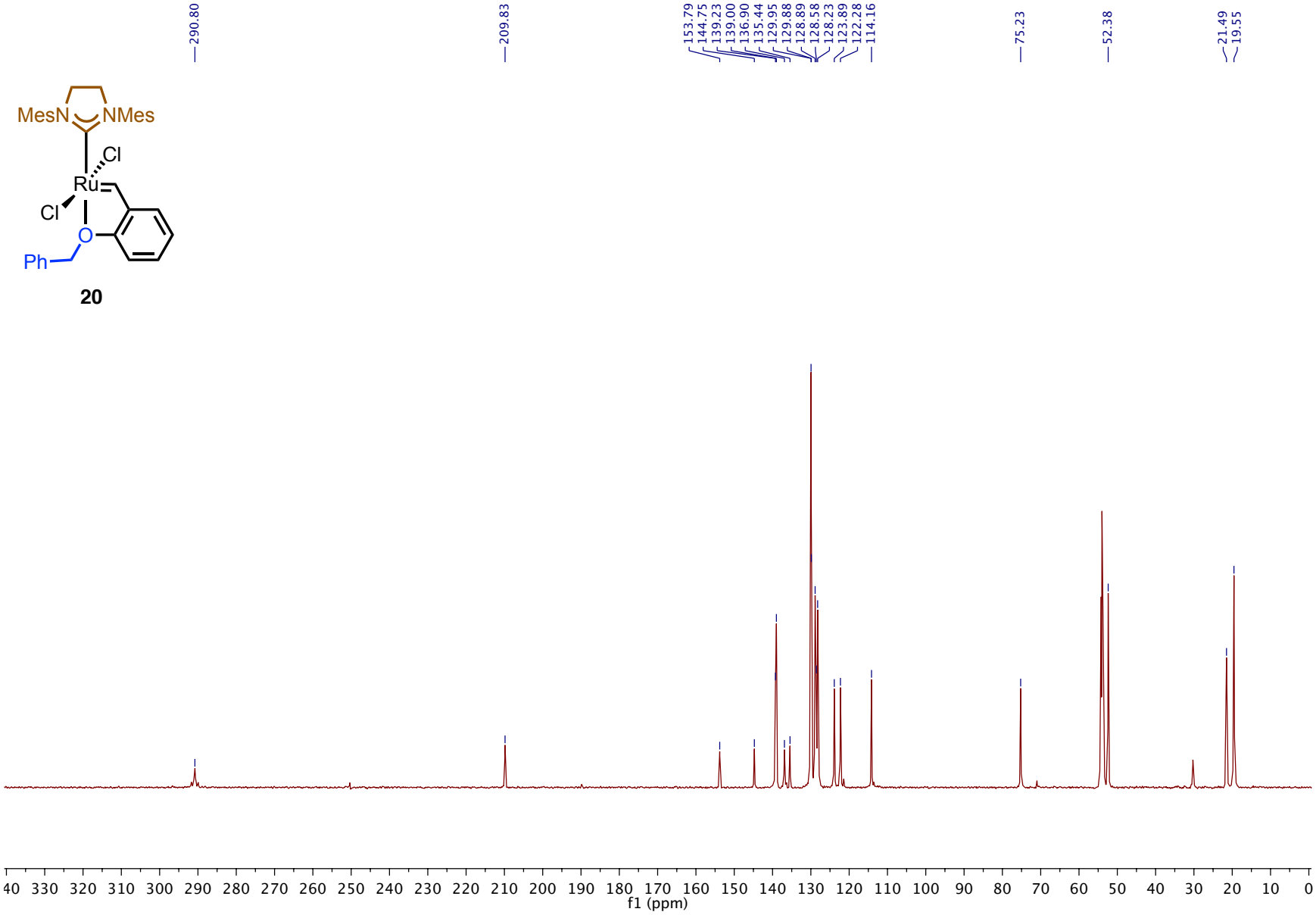


19

^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of catalyst **20.**

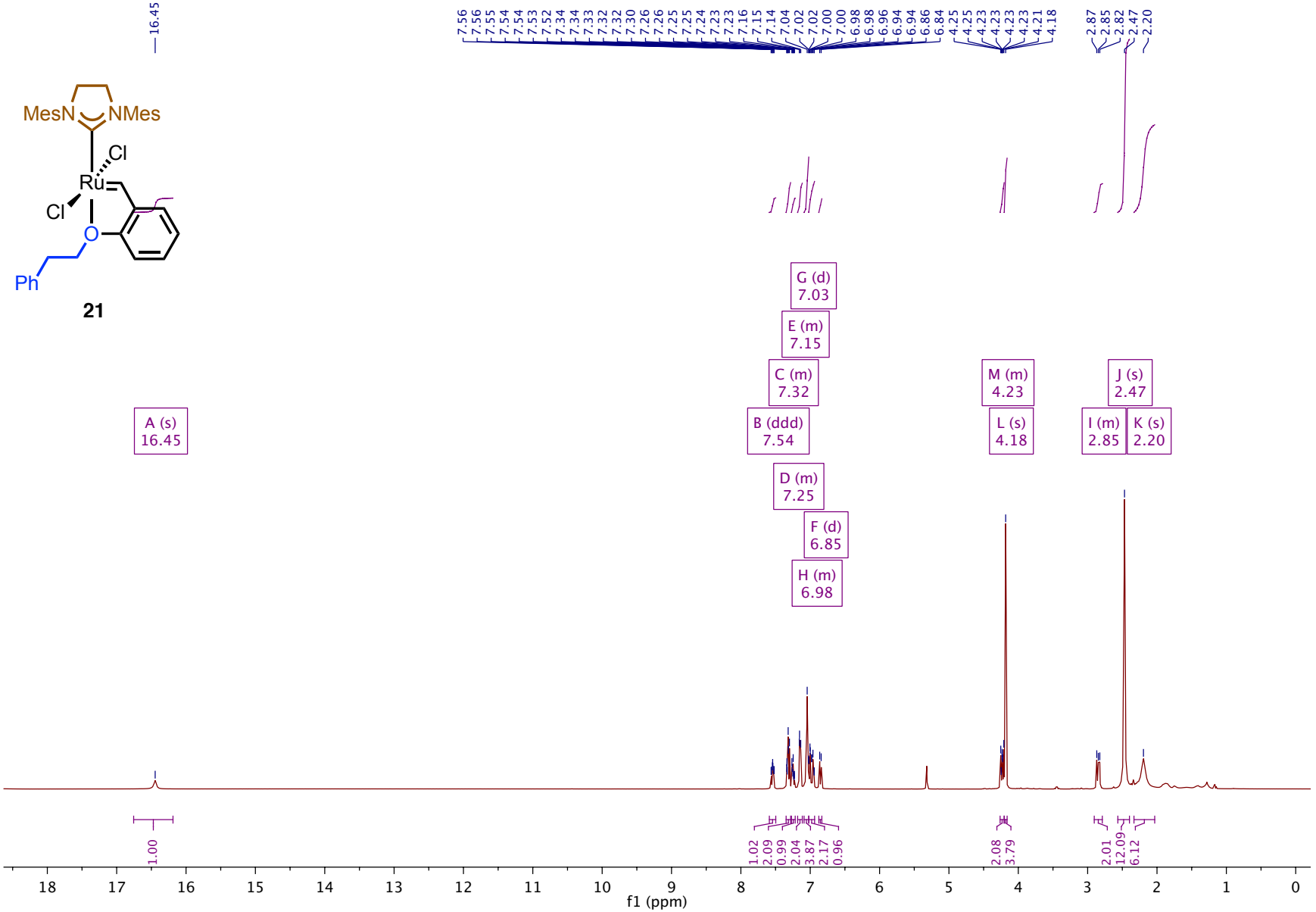


^{13}C NMR (125 MHz, CD_2Cl_2) spectrum of catalyst **20.**

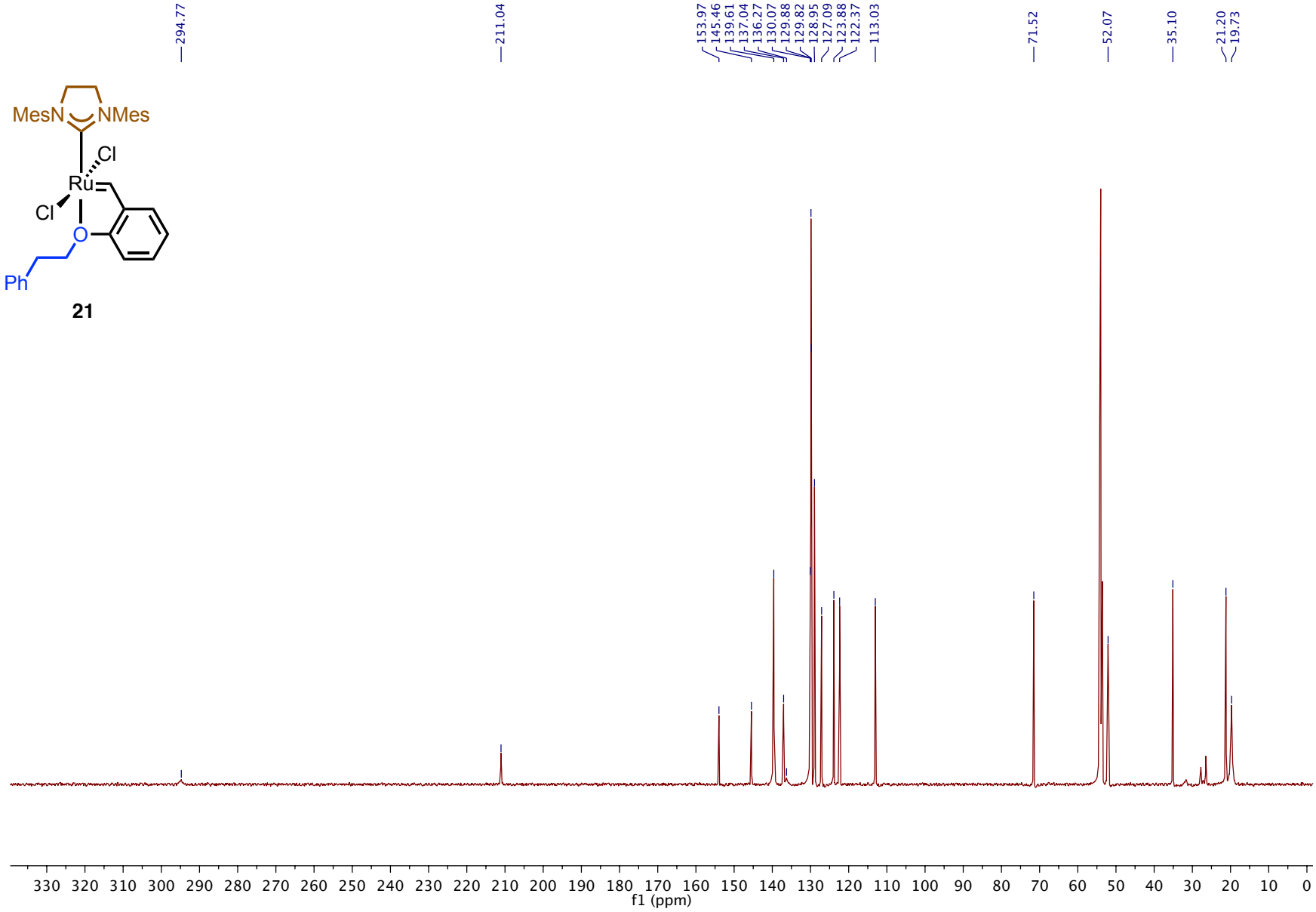


20

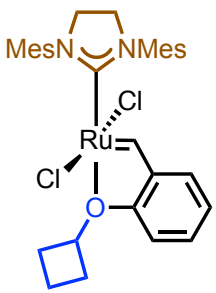
^{1}H NMR (400 MHz, CD_2Cl_2) spectrum of catalyst **21.**



^{13}C NMR (125 MHz, CD_2Cl_2) spectrum of catalyst **21.**

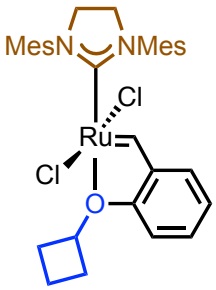


^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of catalyst **22.**



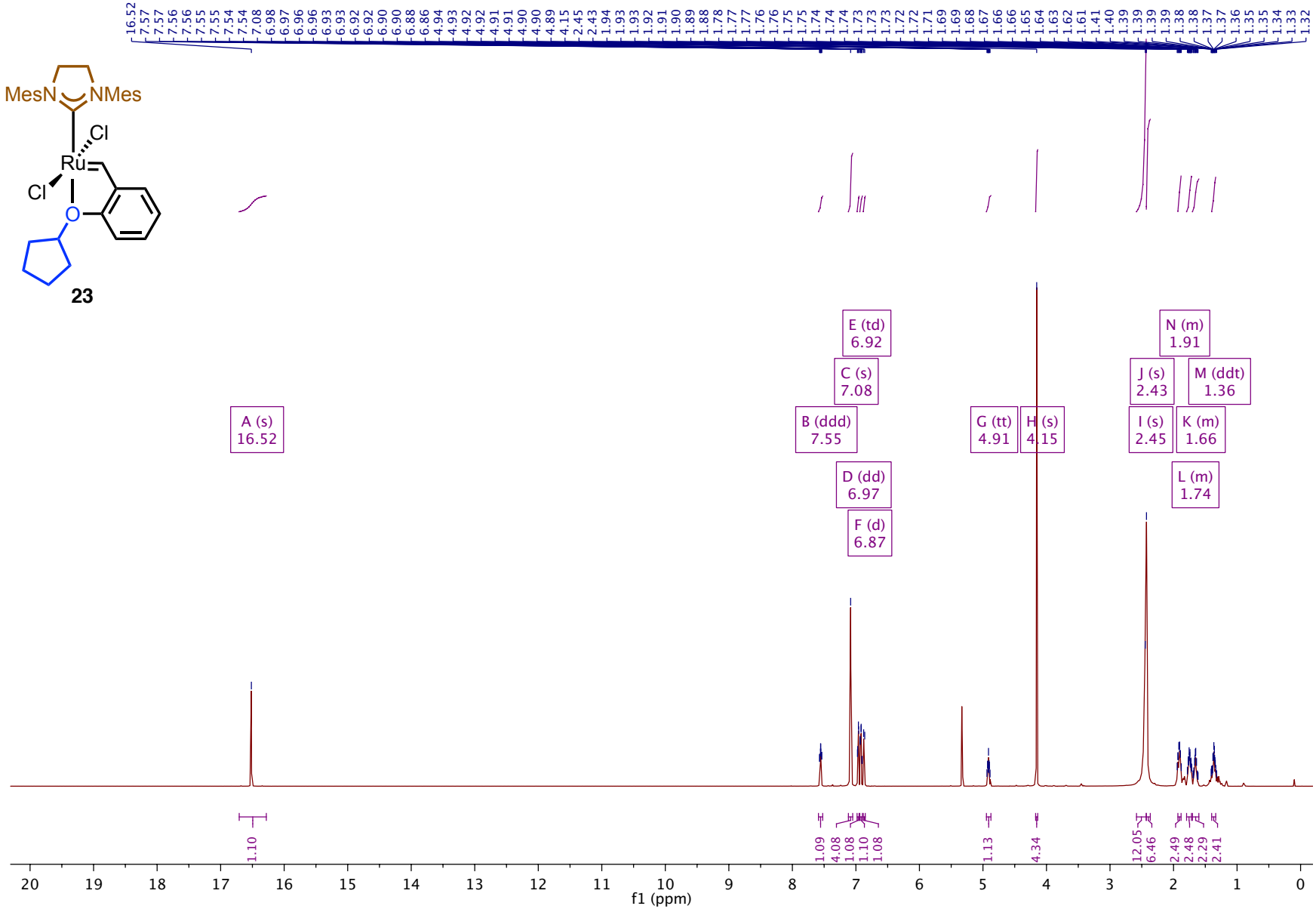
22

^{13}C NMR (125 MHz, CD_2Cl_2) spectrum of catalyst **22.**

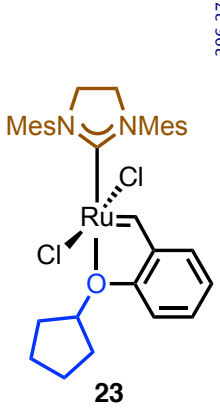


22

^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of catalyst **23.**

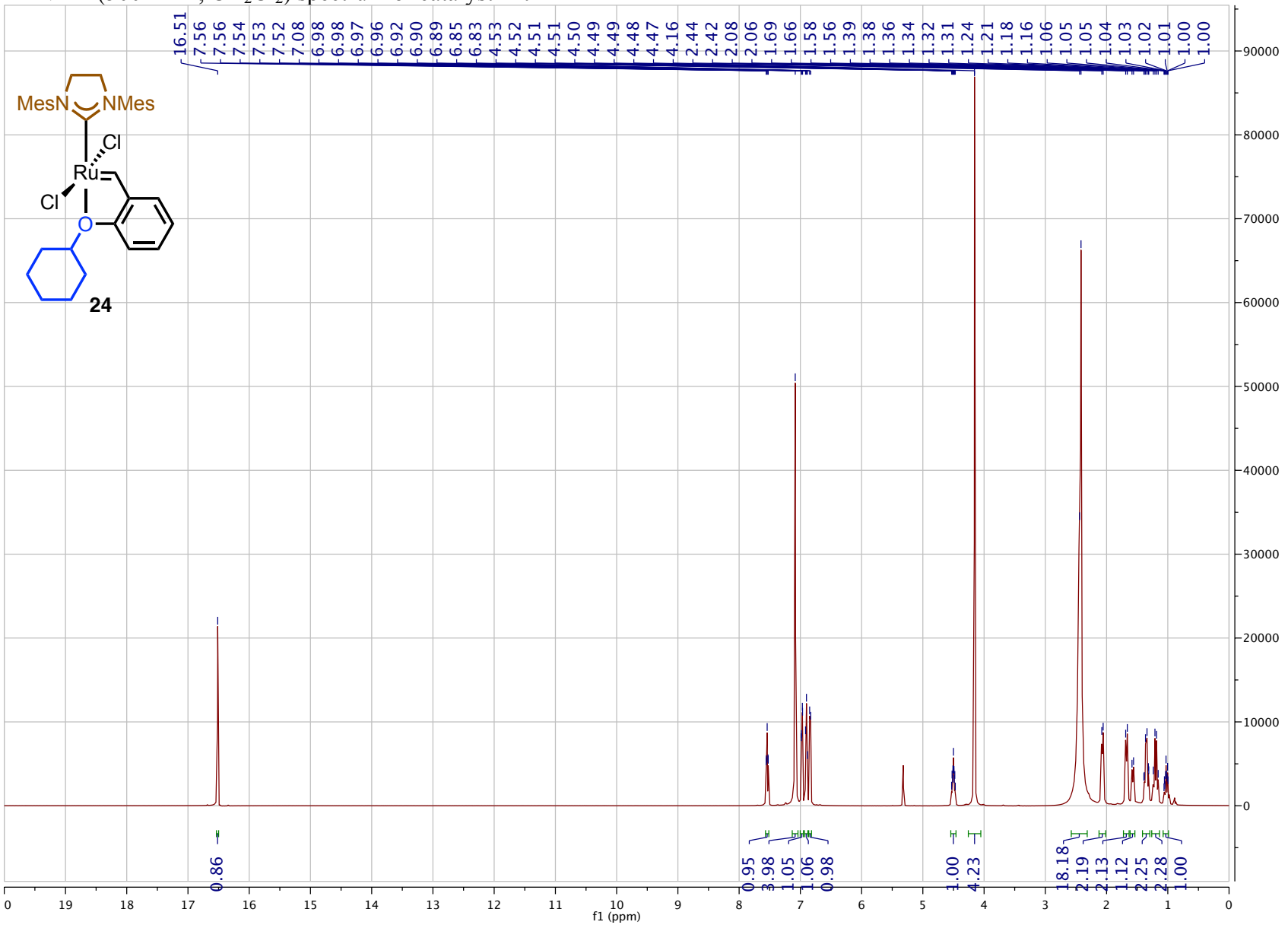


^{13}C NMR (125 MHz, CD_2Cl_2) spectrum of catalyst **23.**

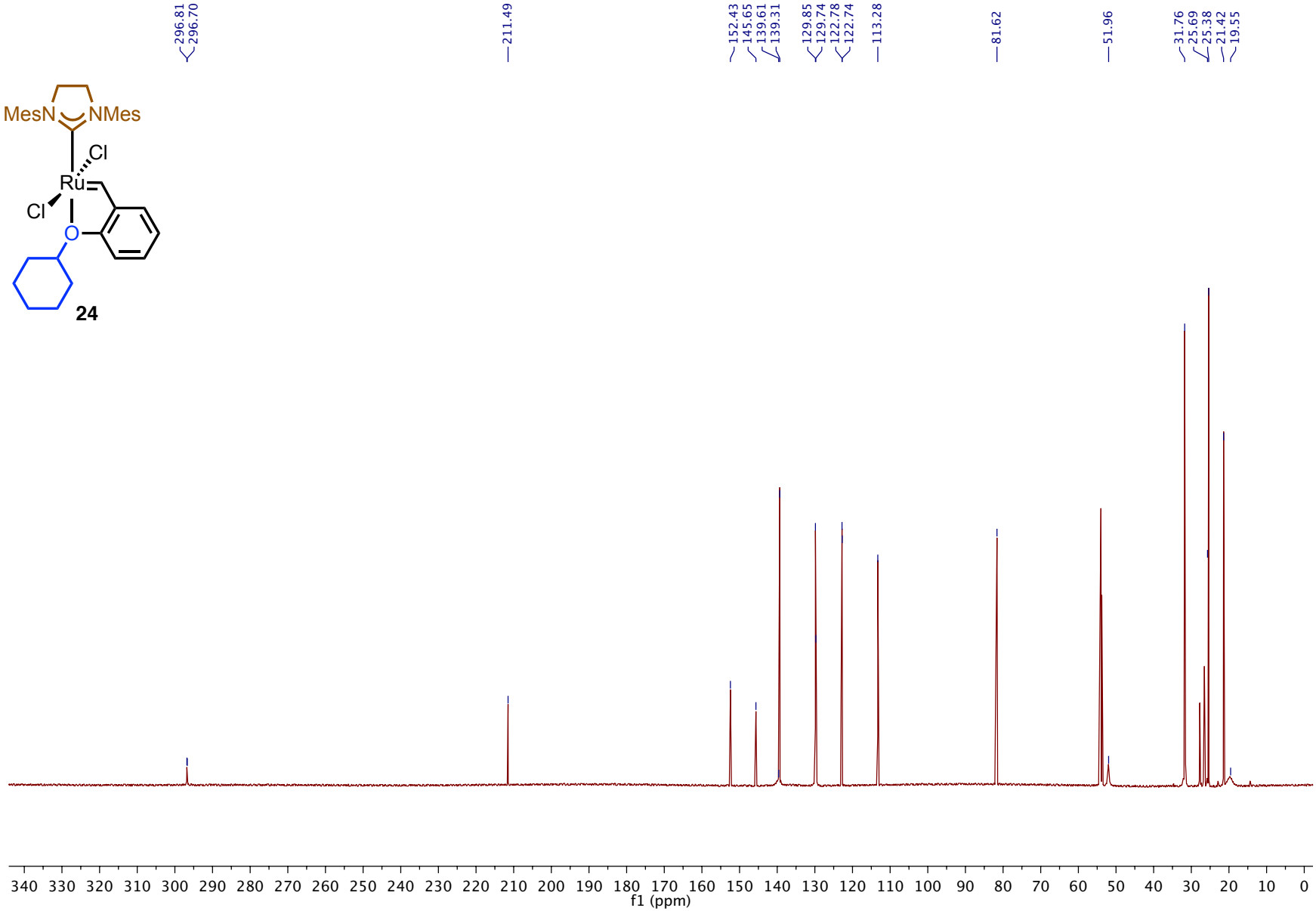


23

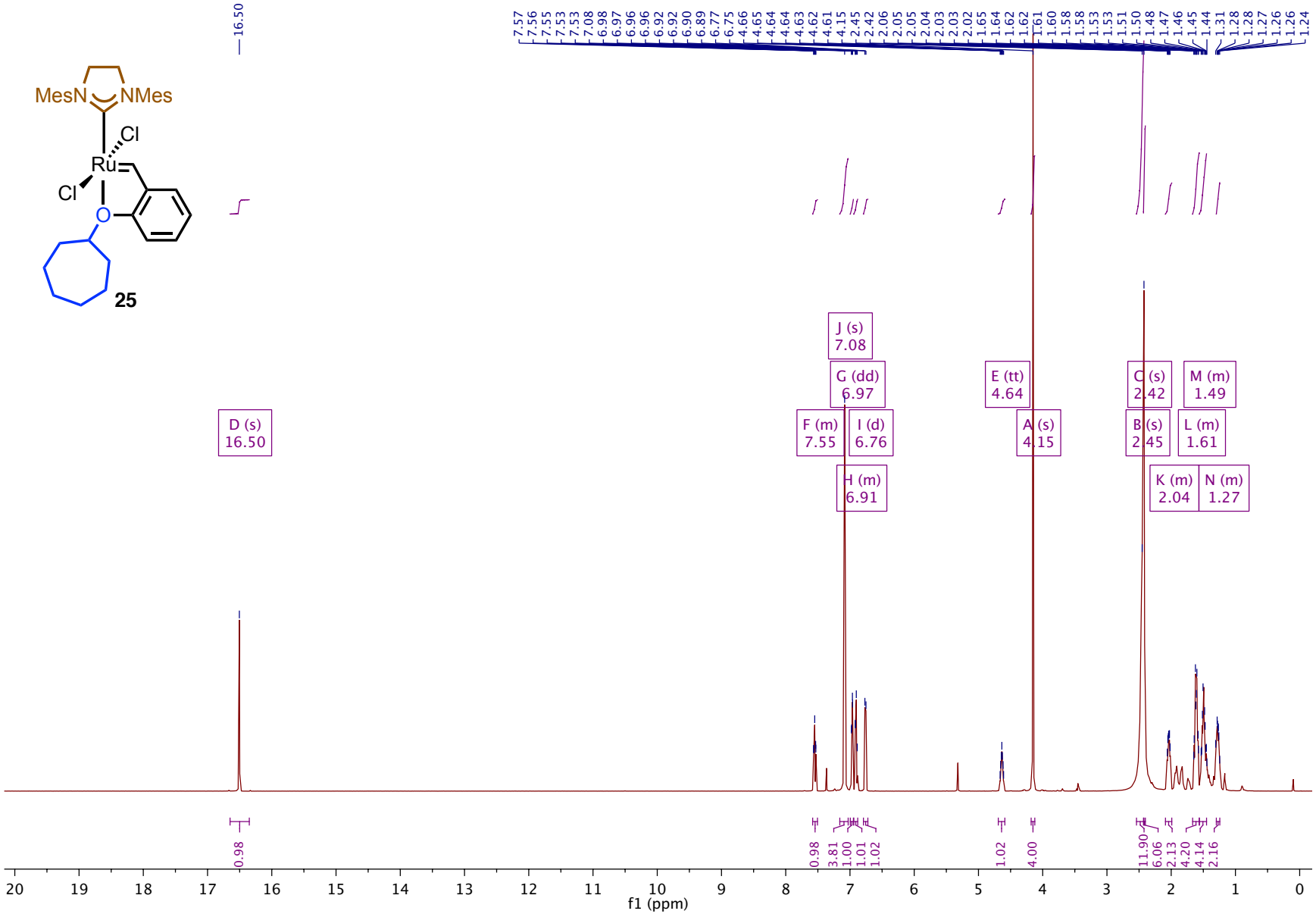
^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of catalyst **24.**



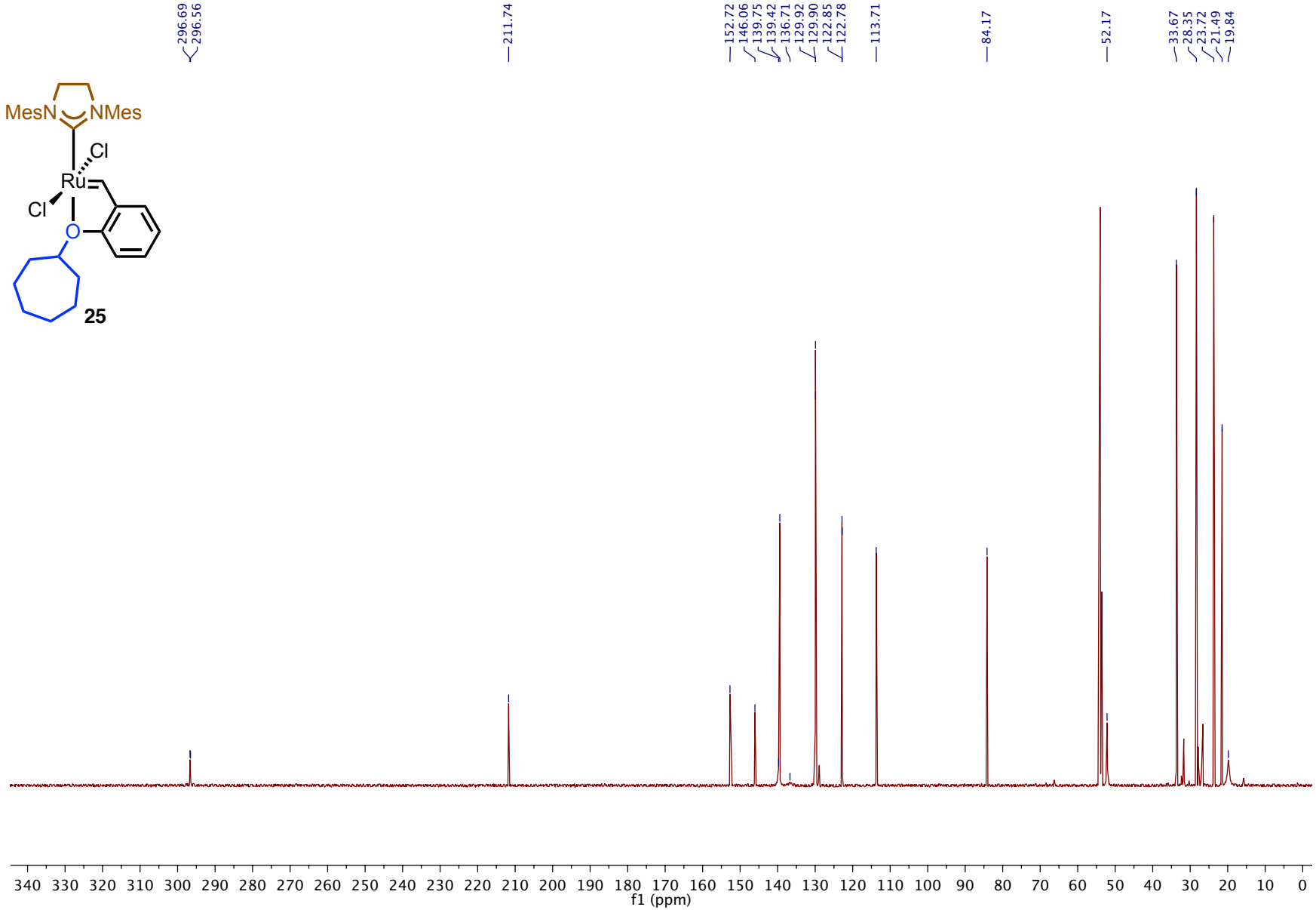
^{13}C NMR (125 MHz, CD_2Cl_2) spectrum of catalyst **24.**



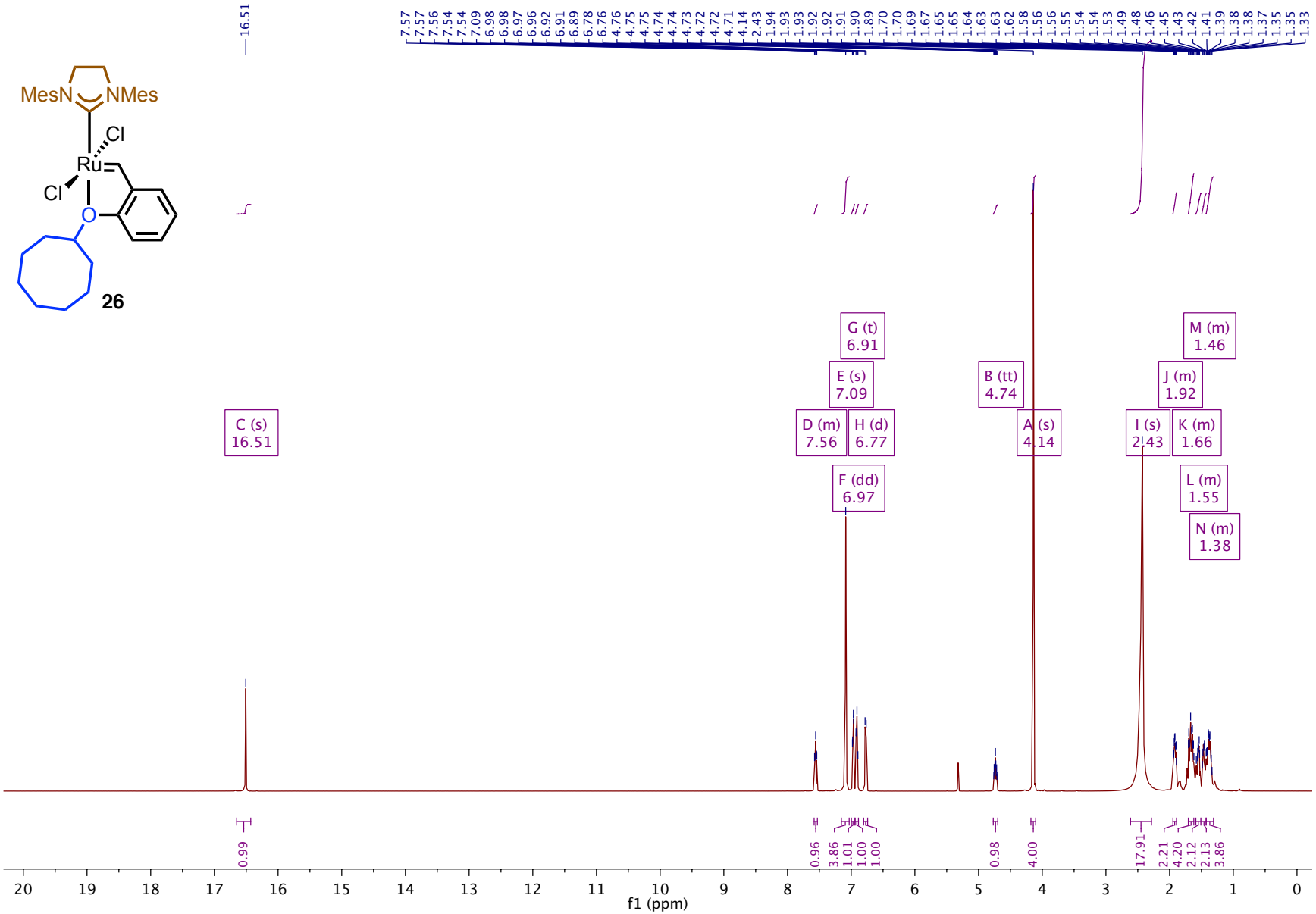
^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of catalyst **25.**



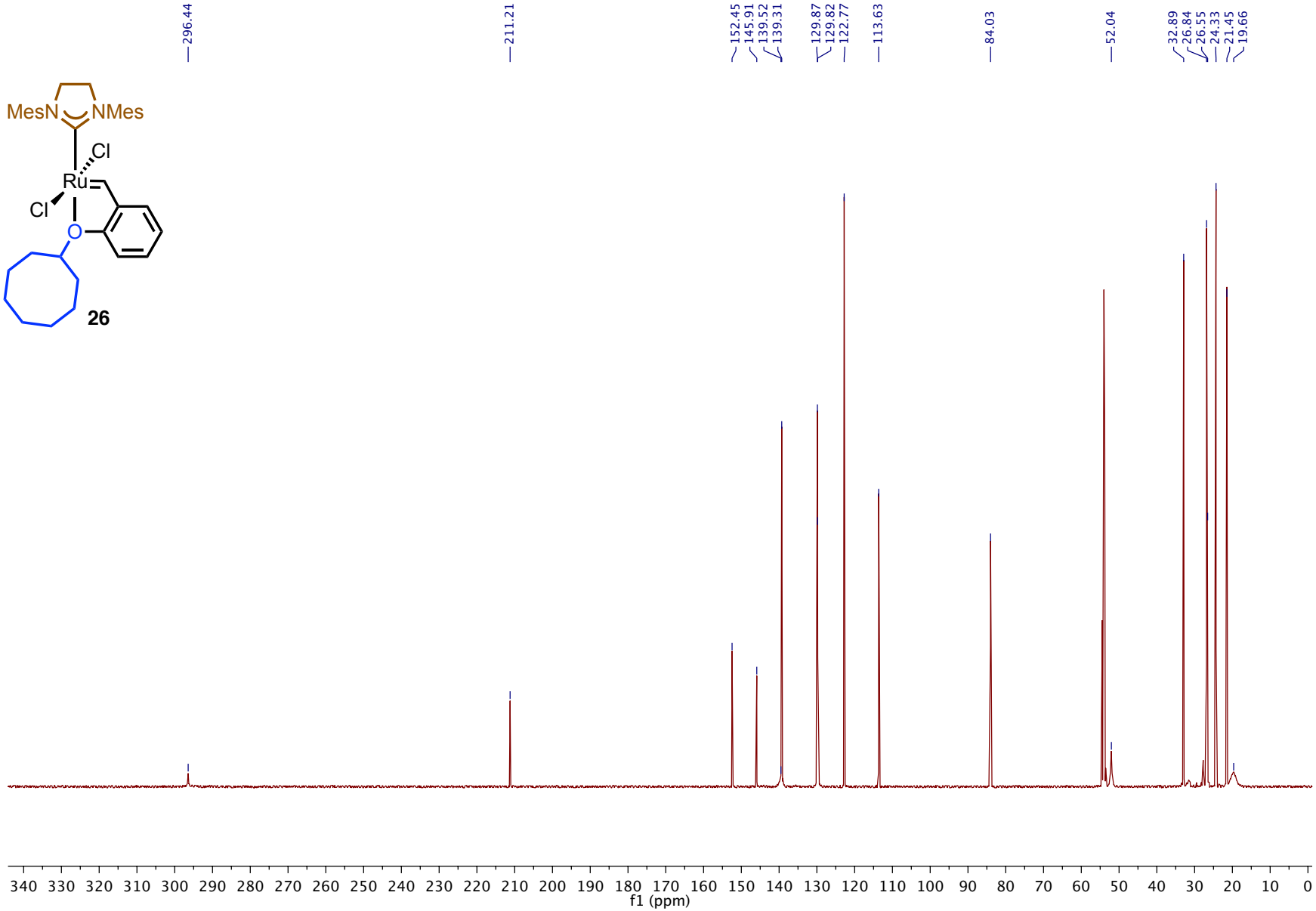
^{13}C NMR (125 MHz, CD_2Cl_2) spectrum of catalyst **25.**



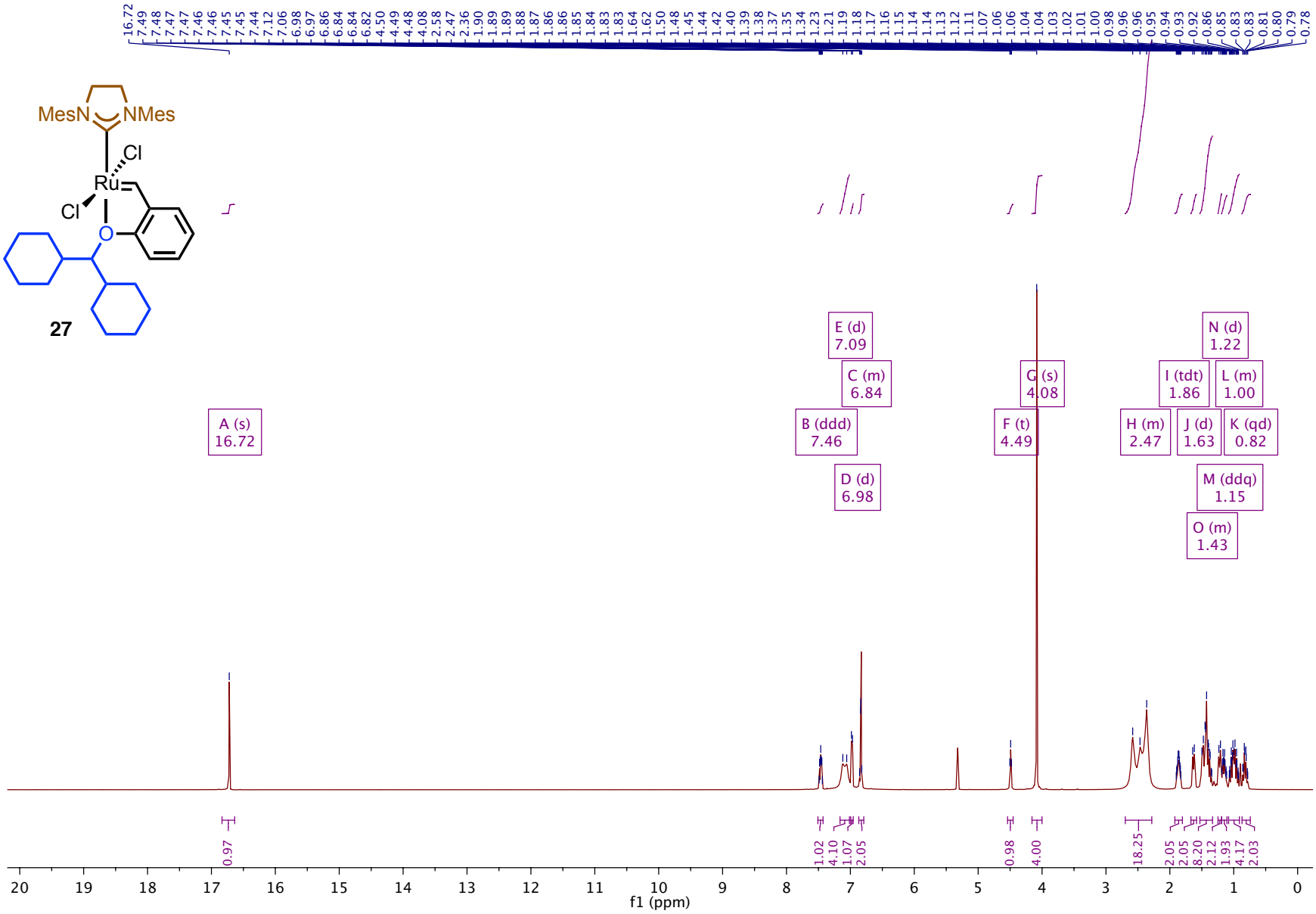
^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of catalyst **26.**



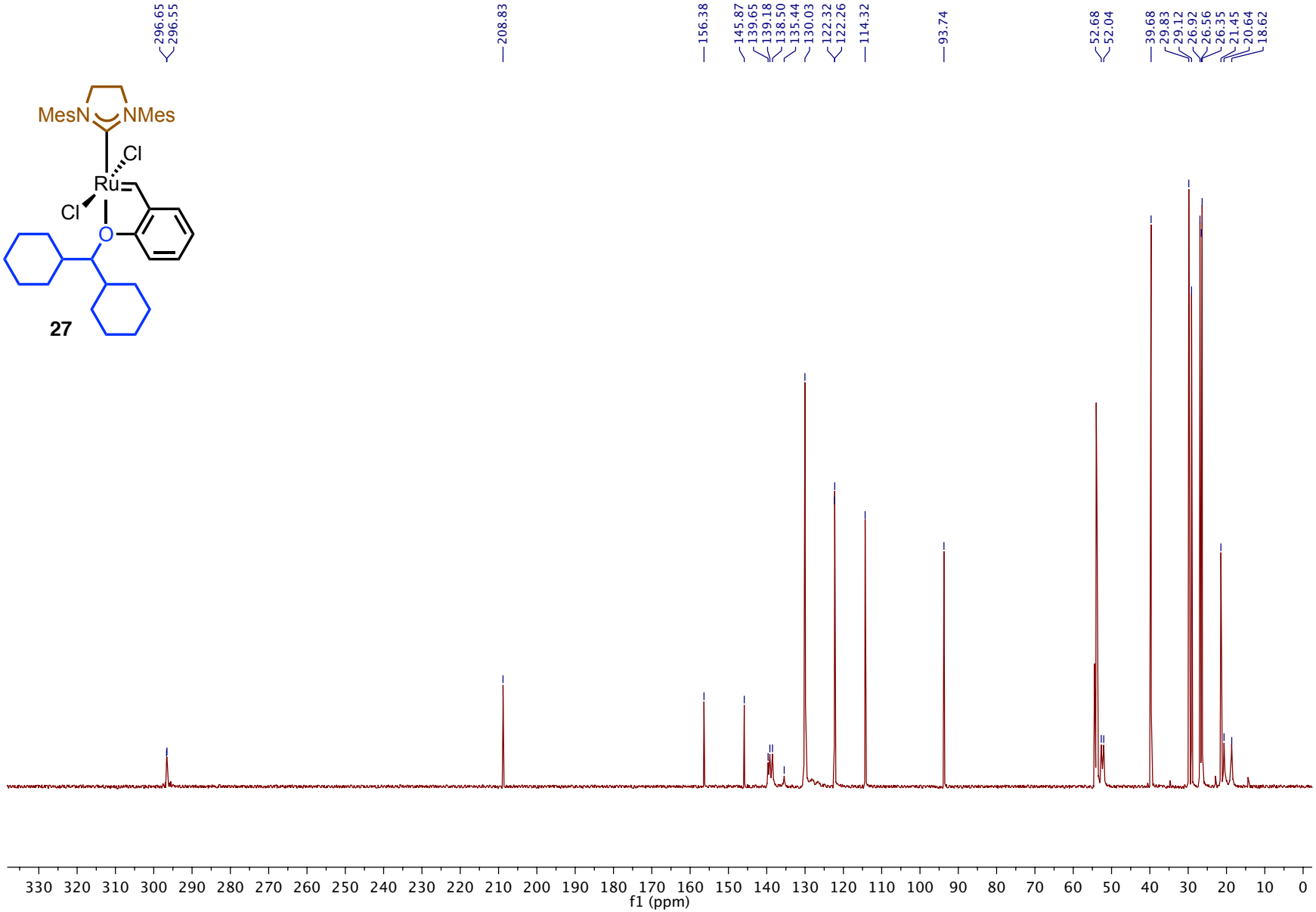
^{13}C NMR (125 MHz, CD_2Cl_2) spectrum of catalyst **26.**



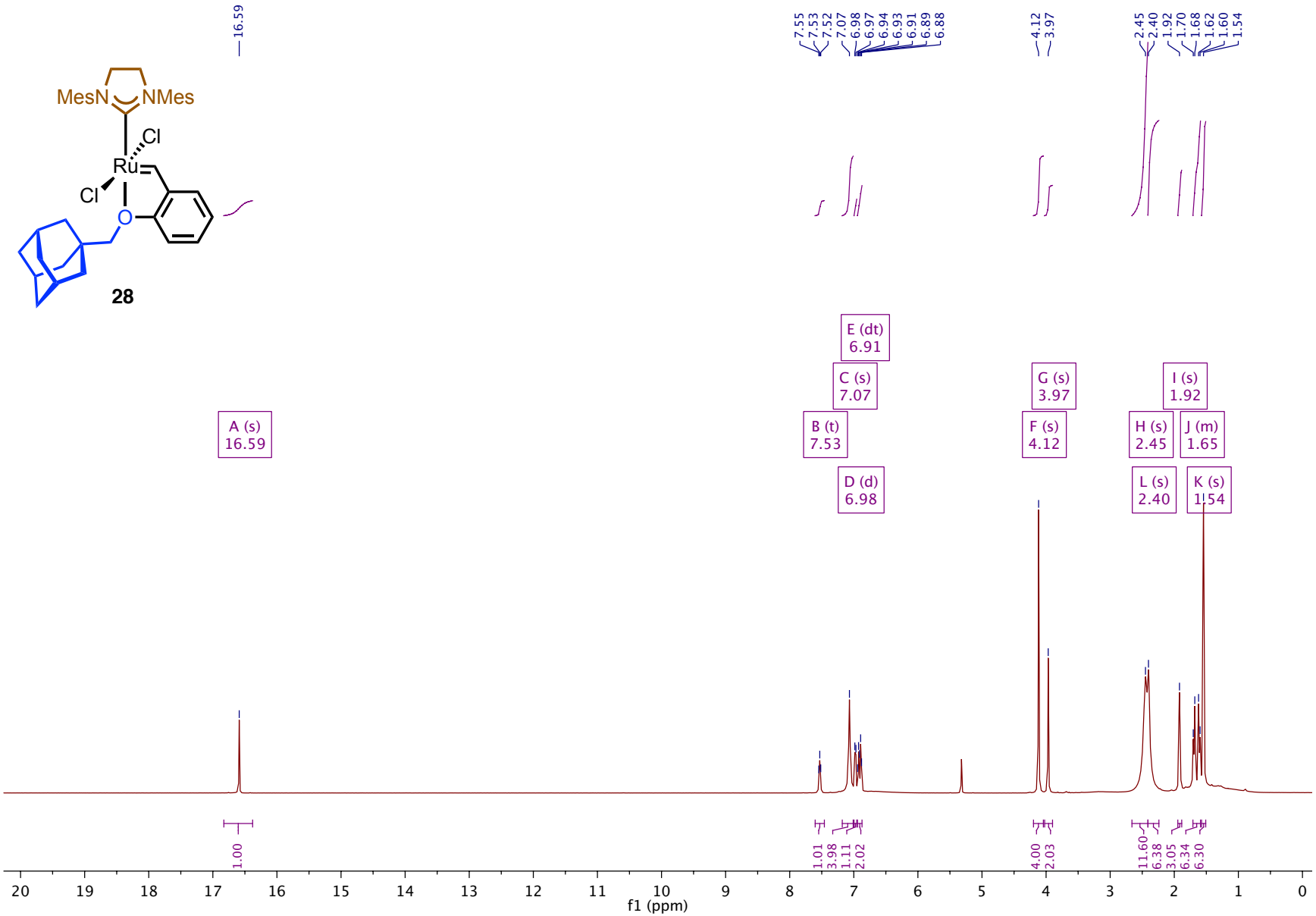
^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of catalyst **27.**



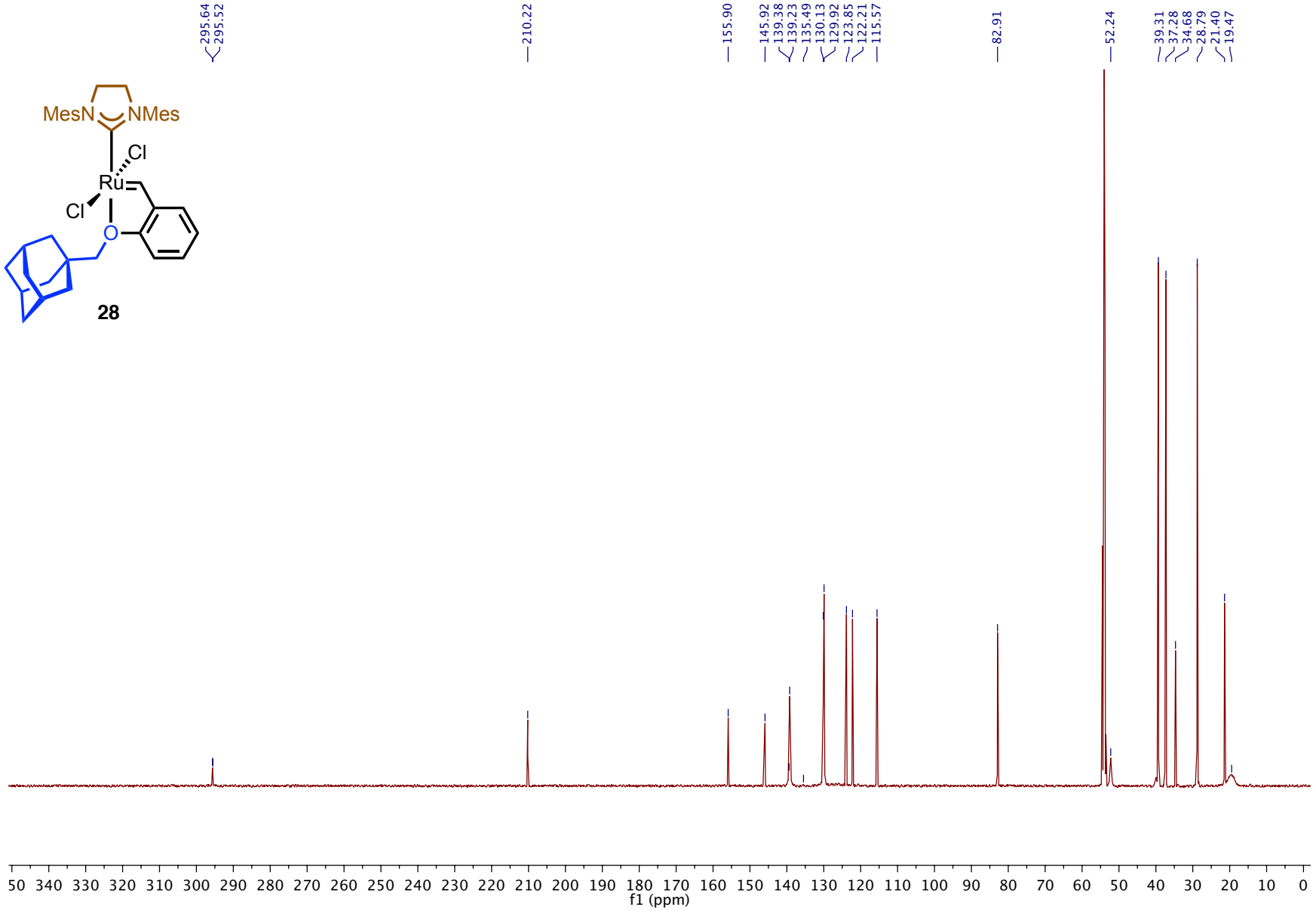
^{13}C NMR (125 MHz, CD_2Cl_2) spectrum of catalyst **27.**



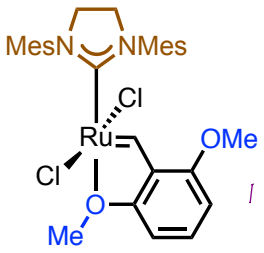
^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of catalyst **28.**



^{13}C NMR (125 MHz, CD_2Cl_2) spectrum of catalyst **28.**

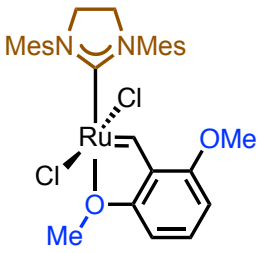


^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of catalyst **32.** (*trans* isomer)



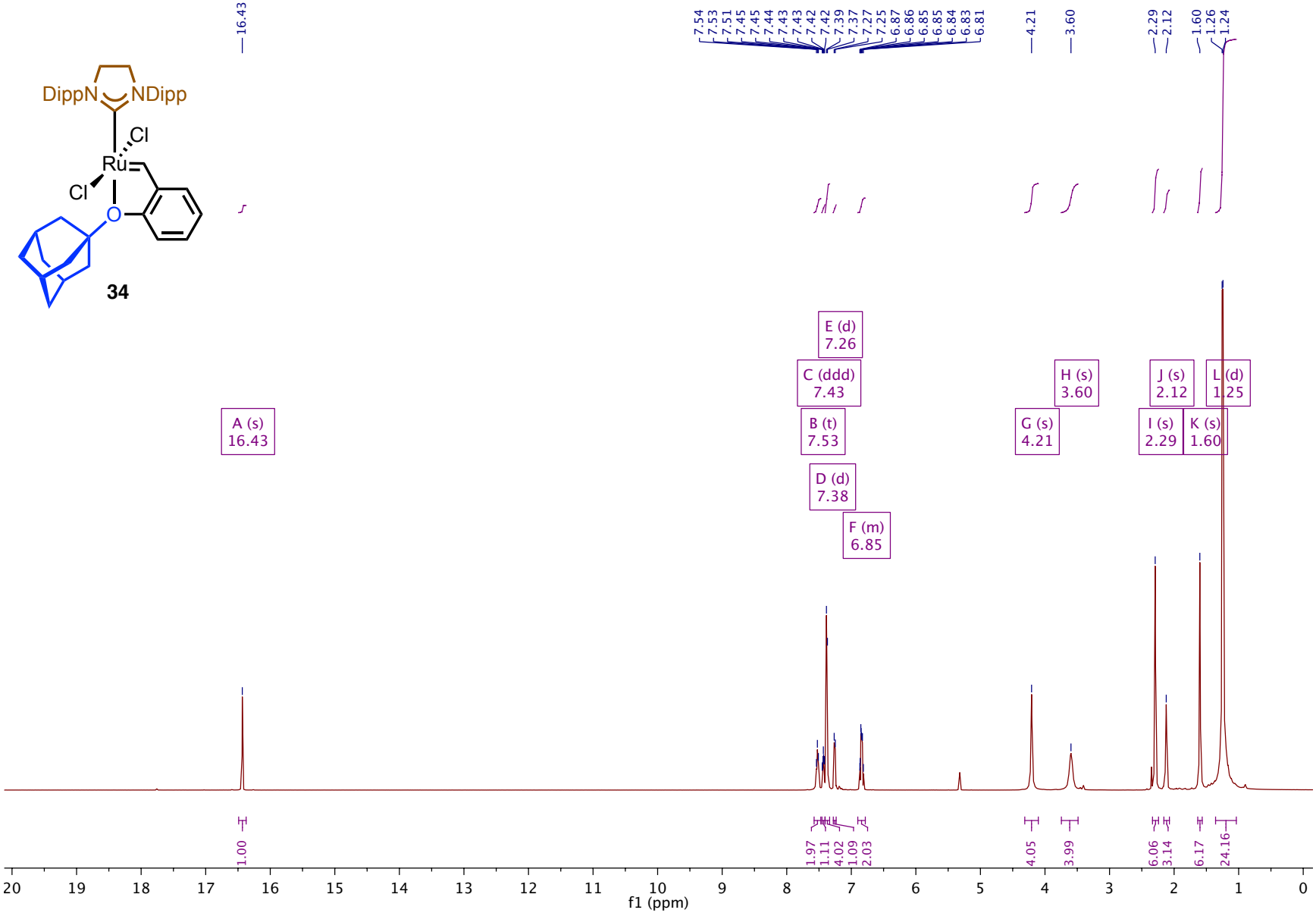
32

^{13}C NMR (125 MHz, CD_2Cl_2) spectrum of catalyst **32.** (*trans* isomer)

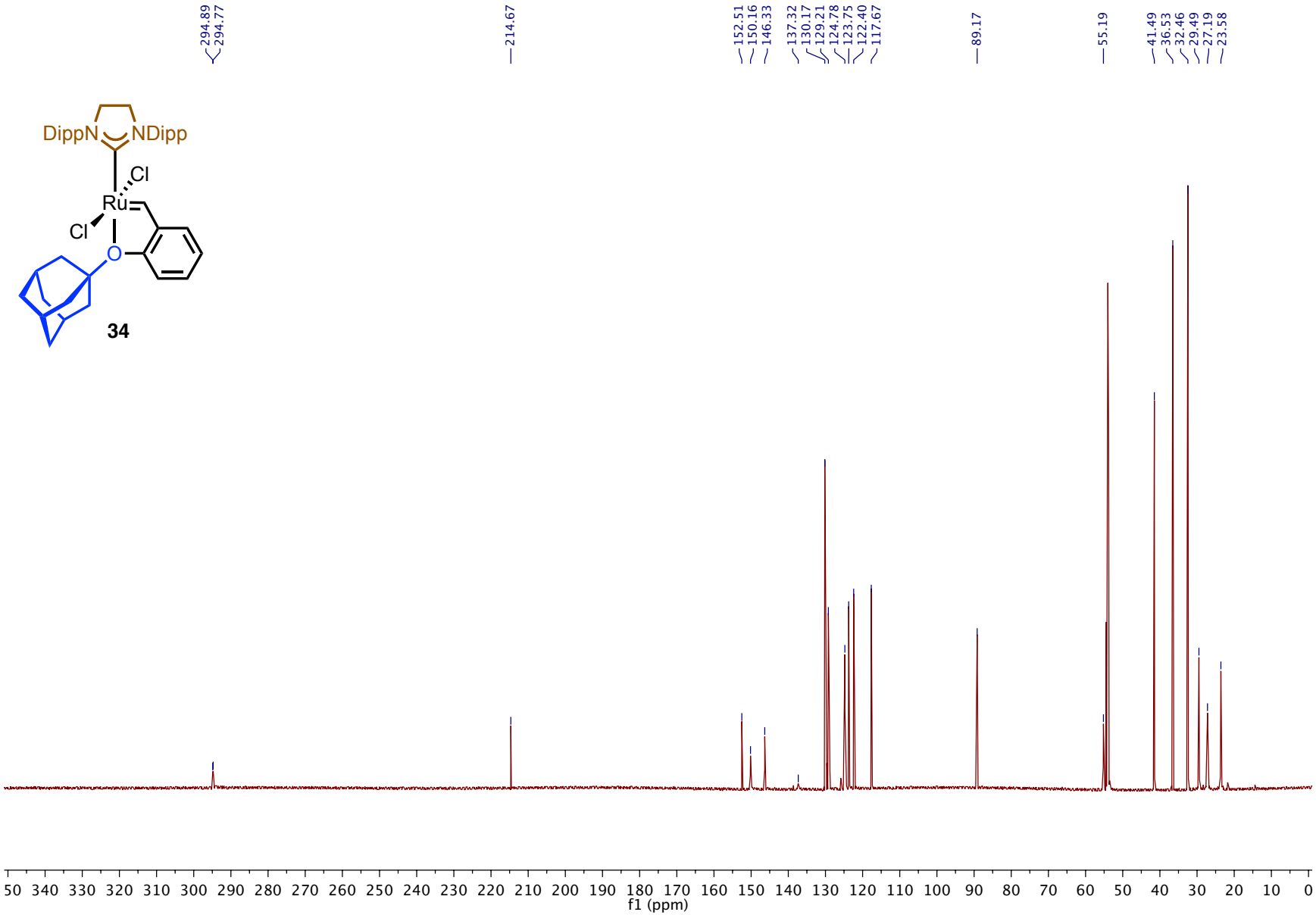


32

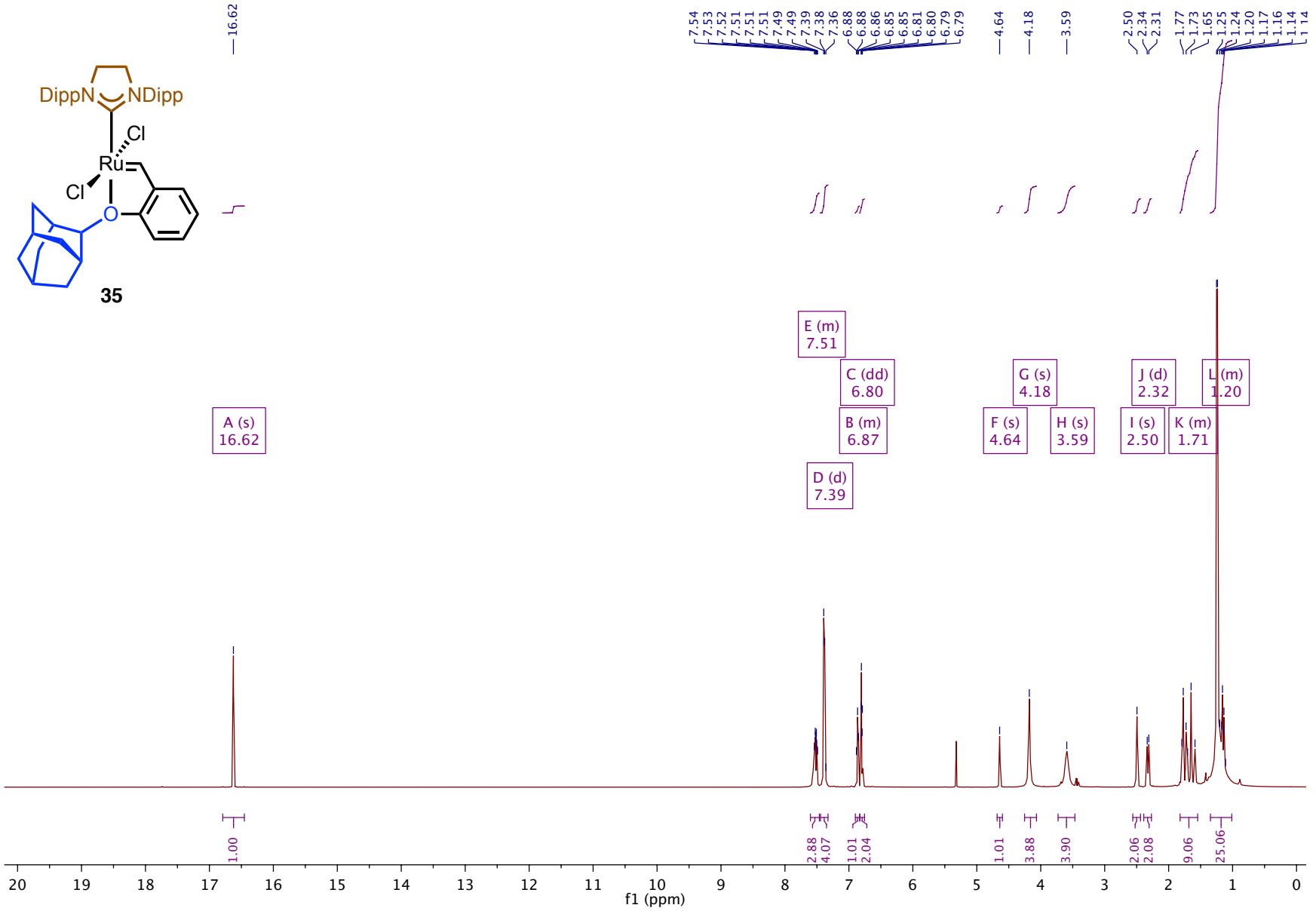
^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of catalyst **34.**



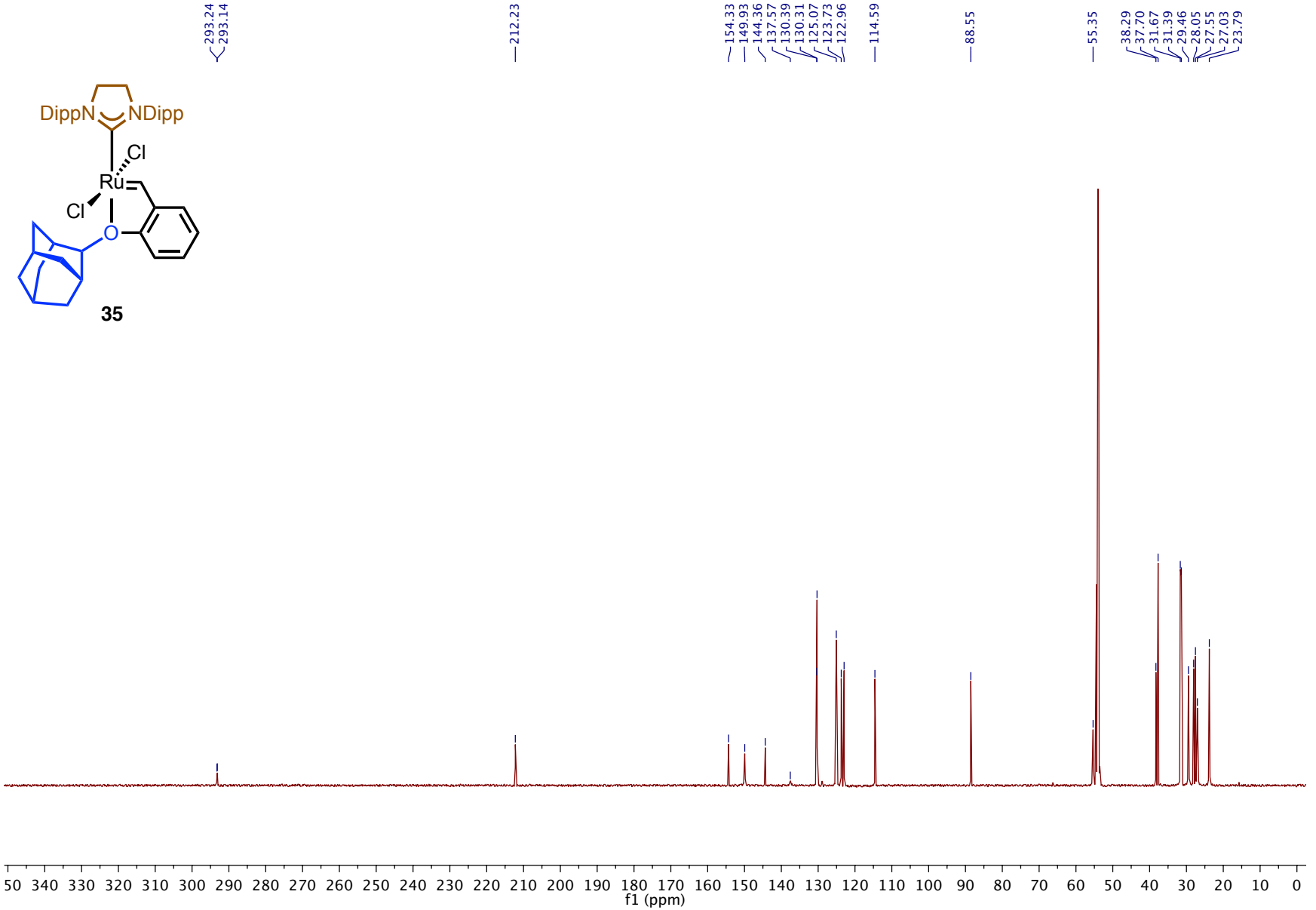
^{13}C NMR (125 MHz, CD_2Cl_2) spectrum of catalyst **34.**



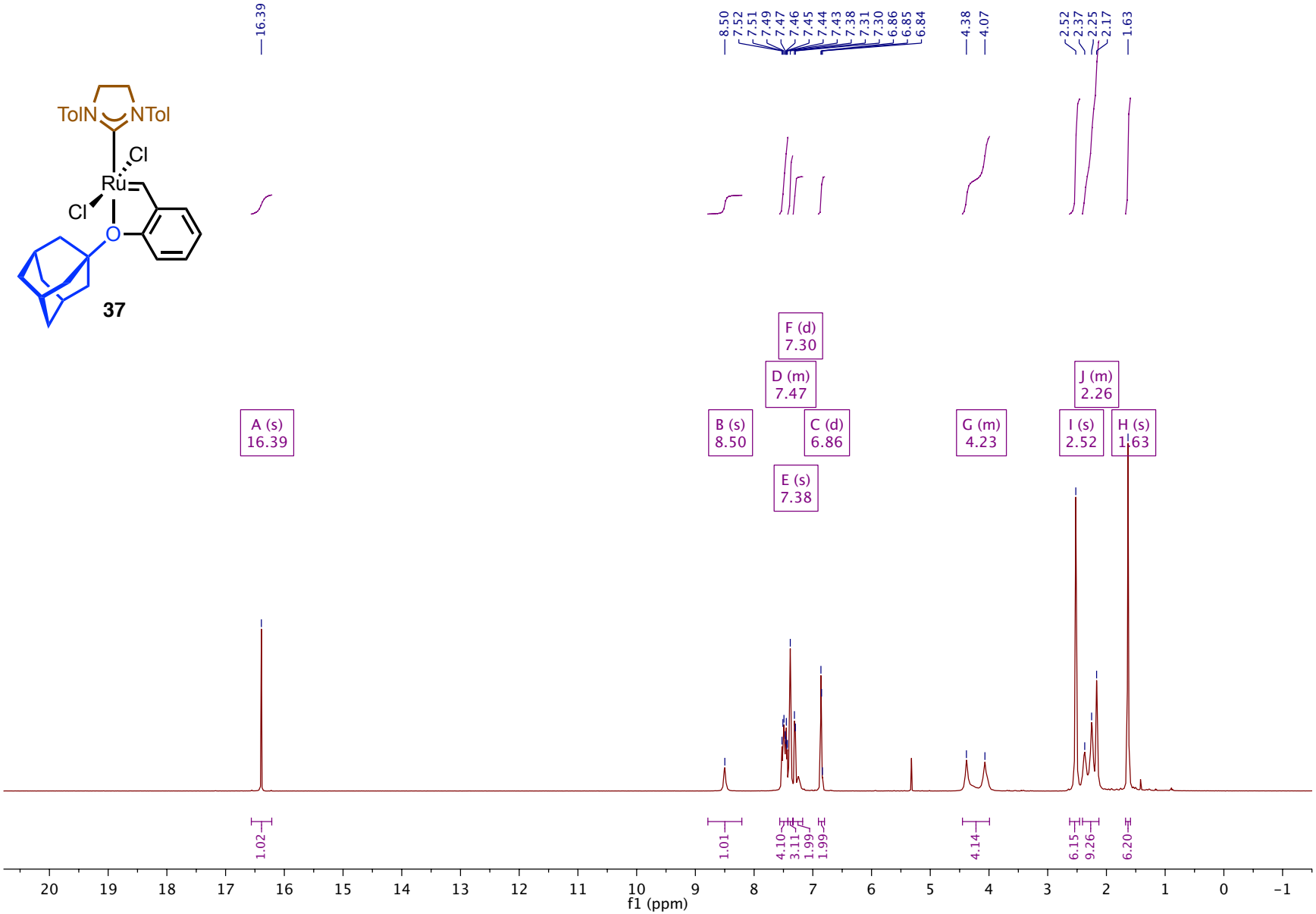
^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of catalyst **35.**



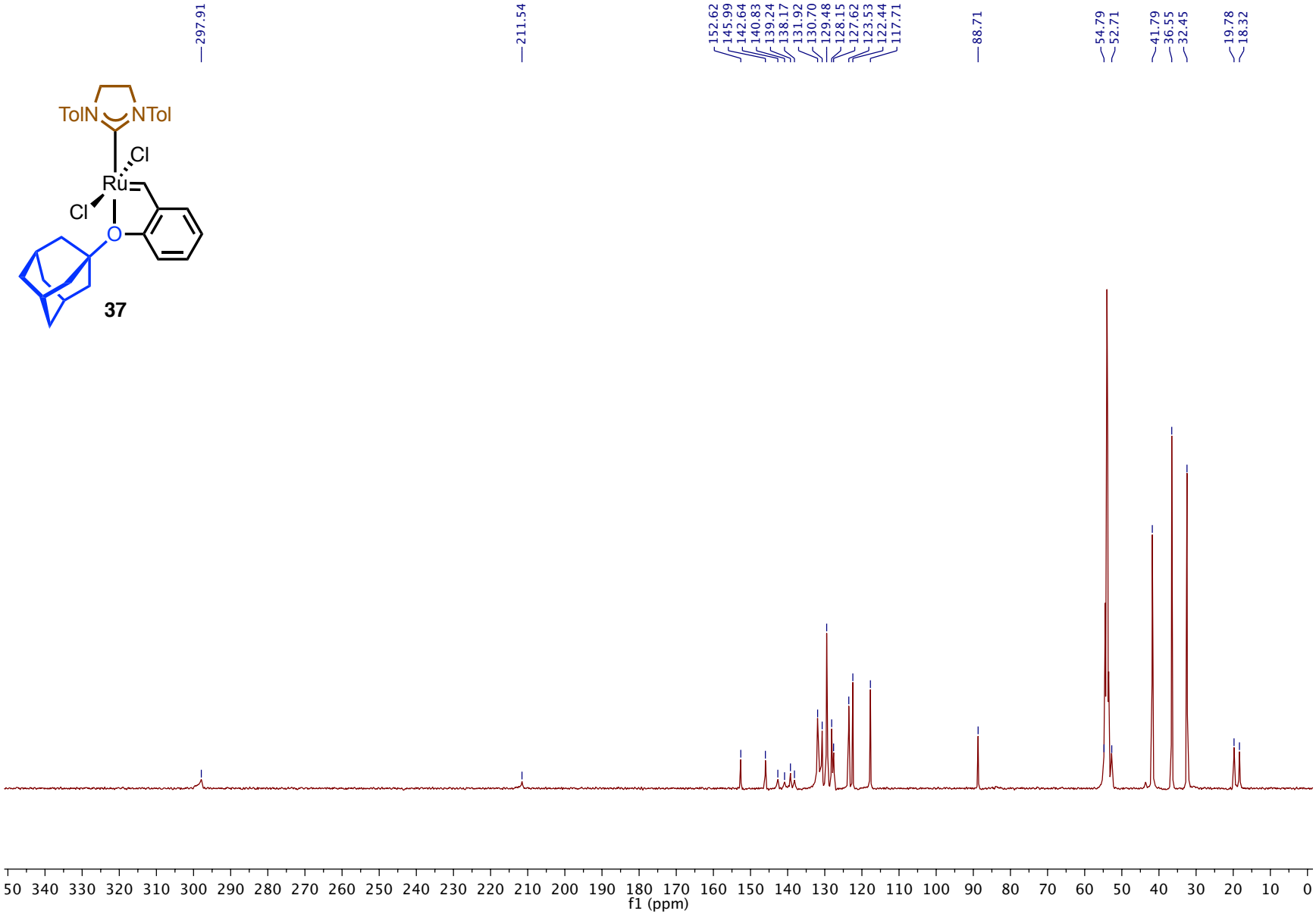
^{13}C NMR (125 MHz, CD_2Cl_2) spectrum of catalyst **35.**



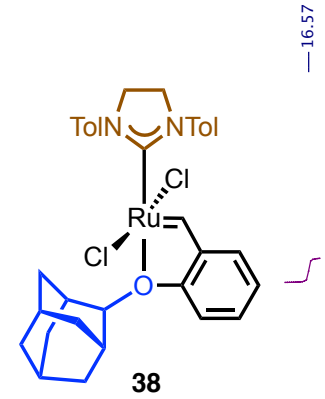
^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of catalyst **37.**



^{13}C NMR (125 MHz, CD_2Cl_2) spectrum of catalyst **37.**



^{1}H NMR (400 MHz, CD_2Cl_2) spectrum of catalyst **38.**



38

^{13}C NMR (101 MHz, CD_2Cl_2) spectrum of catalyst **38.**