

Supporting Information

for

Synthesis and Reactivity of

Ruthenium Phosphite Indenylidene Complexes

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1. General Information

All reactions were performed under an inert atmosphere of argon or nitrogen using standard Schlenk line and glovebox techniques. Solvents were dispensed from a solvent purification system. All other reagents were used without further purification. ^1H , ^{13}C -{ ^1H } and ^{31}P -{ ^1H } 1D and 2D Nuclear Magnetic Resonance (NMR) spectra were recorded on a Bruker AVANCE 400 Ultrashield spectrometer using the residual solvent peak as reference (CHCl_3 : $\delta_{\text{H}} = 7.26$ ppm, $\delta_{\text{C}} = 77.16$ ppm; CH_2Cl_2 , $\delta_{\text{H}} = 5.32$ ppm, $\delta_{\text{C}} = 53.80$ ppm.) at 298K. Variable temperature NMR spectra were carried out in CD_3NO_2 . Gas chromatography (GC) analyses were performed on an Agilent 7890A apparatus equipped with a flame ionization detector and a (5%-Phenyl)-methylpolysiloxane column (30 m, 320 μm , film: 0.25 μm). Flash chromatography was conducted using 40-63 μm silica. Analytical TLCs were performed on Merck pre-coated silica 60-F₂₅₄ plates. Elemental analyses were performed by the University of St Andrews Analytical Service. Calorimetric studies were performed on a CALVET C80 solution calorimeter.

2. Procedures for catalysis

Substrates **2**,¹ **4**,² **6**,³ **9**,² **13**,¹ **15**,⁴ **17**,² **19**,⁵ **21**, **23**,⁶ **25**,⁶ **27**,² **29**,² **31**,⁷ **33**,⁸ **35**,⁹ **37**,¹⁰ **39**,¹¹ **41**,² **43**,² **45**,¹² **47**,¹³ **55**,¹⁴ **57**,¹⁵ **63**,¹ **65**,¹⁶ and **67**¹⁷ were synthesized according to literature procedures. Substrate **11**, **59**, **61** were obtained commercially.

NMR spectra of the RCM products **3**,¹ **5**,¹⁸ **8**,¹⁹ **10**,² **12**,² **14**,¹ **16**,²⁰ **18**,²¹ **20**,⁵ **24**,⁶ **26**,² **28**,²² **30**,² **32**,² **34**,²³ **36**,¹⁷ **38**,¹⁰ **40**,² **42**,¹⁸ **44**,¹⁸ **48**,¹⁸ **50**,²⁴ **54**,¹⁹ **56**,²⁵ **58**,²⁶ **60**,²⁷ **62**,²⁸ **64**,¹ **66**,¹⁶ and **68**¹⁷ were compared to previously reported analyses.

– Procedure for Tables 3 – 6

A flame-dried schlenk was charged with a solution of the substrate (0.25 mmol) in 2.5 mL of solvent (0.1M, CH_2Cl_2 for room temperature experiments and toluene for 80°C) and **Caz-1** (1 to 2 mol%) was added. The reaction mixture was stirred at the appropriate temperature for the appropriate amount of time. The solvent was removed *in vacuo*. The conversion was determined by ^1H NMR (CDCl_3). Flash chromatography (pentane/diethylether - 9:1 to 8:2 v:v) on silica gel afforded the title compounds.

– Procedure for Figure 4 – Comparison of catalysts

A reaction tube (Radleys carousel 12 reaction station) was charged with a solution of di(methallyl)tosylamine **9** (0.5 mmol) in toluene (0.5 mL) and the ruthenium pre-catalyst (0.5 mol%) was added. The reaction mixture was stirred at 80°C and aliquots were taken every 5 to 20 minutes. Each aliquot was then added to a solution of 40 μL of ethylvinyl ether and

toluene. All samples were then subjected to GC analysis to determine the conversion of **9** to **10**.

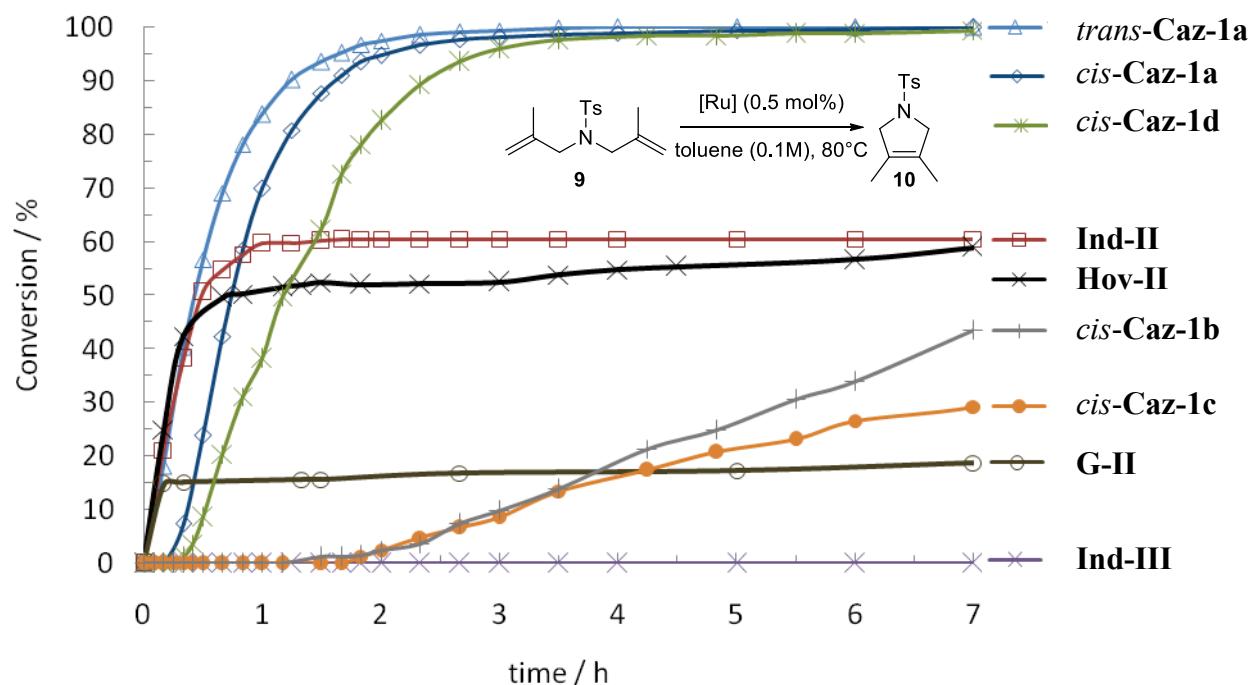


Figure S1. Comparative catalytic studies at low catalyst loading. Reaction conditions: **9** (0.5 mmol), pre-catalyst (0.5 mol%), toluene (0.1 M, 5 mL).

The same reaction conditions were used for the plot of Figure S2, with variable amounts of toluene to have concentrations of 0.05M, 0.1M and 1M. Albeit small variations were observed, the rate of those reactions seemed similar, indicating that concentration has no influence on this RCM.

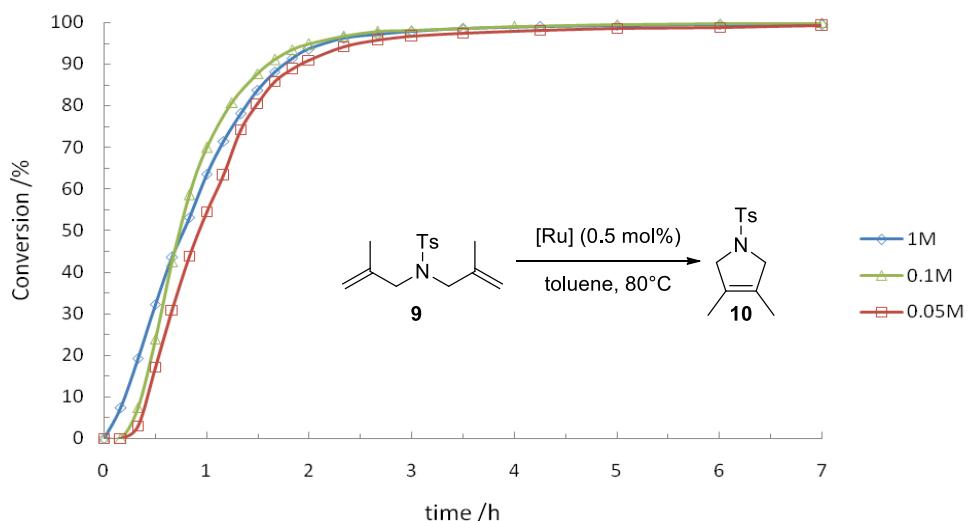
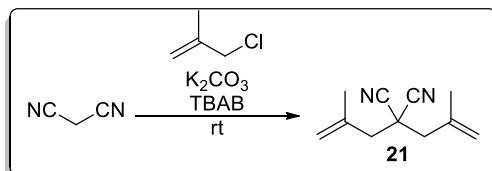


Figure S2. Comparative catalytic studies at low catalyst loading and variable concentration. Reaction conditions: **9** (0.5 mmol), pre-catalyst (0.5 mol%), toluene.

– Procedure for table 7 - Catalytic RCM at low catalyst loading

In the glovebox, a vial was charged with a stirring bar, substrate (0.25 mmol), pre-catalyst *cis*-**Caz-1** (from a stock solution of 2.2 mg in 2 mL of toluene), and 0.5 mL of toluene. The mixture was stirred outside the glovebox at the indicated temperature. After 20h, the reaction was stopped and solvent was evaporated. Flash chromatography (pentane/diethylether - 9:1 to 8:2 v:v) on silica gel afforded the title compounds.

3. Procedure for the synthesis of 2,2-bis(2-methylallyl)malononitrile **21**



In a flame dried flask under argon were added malononitrile (20 mmol, 1.32 g), 3-chloro-2-methylprop-1-ene (50 mmol, 4.9 mL) and tetrabutylammonium bromide (2 mmol, 645 mg). The neat mixture was stirred at room temperature for 30 min and potassium carbonate (50 mmol, 6.9 g) was added. The resulting mixture was stirred for an additional 56h. Water (50 mL) and dichloromethane (50 mL) were added. The aqueous phase was extracted with dichloromethane and the combined organic layers were washed with brine, dried over MgSO_4 and concentrated in vacuum. Purification by flash chromatography (Hexane/Et₂O 8:2) afforded the pure product as a white solid (2.89 g, 83% yield).

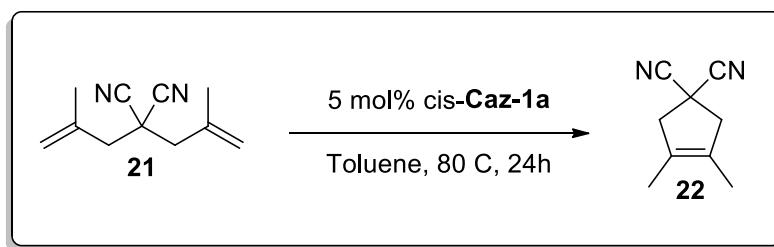
¹H NMR (CDCl_3 , 400 MHz): δ (ppm) = 5.18 (t, 2H, $^2J_{\text{HH}} = 1.3$ Hz), 5.10 (s, 2H), 2.65 (s, 4H), 1.98 (s, 6H).

¹³C-{¹H} NMR (CDCl_3 100.6 MHz) δ (ppm) = 137.3 (C^{IV} alkene), 118.9 (CH_2 alkene), 115.8 (C^{IV} CN), 45.7 (CH_2), 36.0 (C^{IV}), 23.2 (CH_3).

CI-HRMS calculated for $\text{C}_{11}\text{H}_{15}\text{N}_2$ [$\text{M} + \text{H}$]⁺ 175.1235 found 175.1239.

Elemental Analysis calculated for $\text{C}_{11}\text{H}_{14}\text{N}_2$: C, 75.82; H 8.10; N 16.08. Found: C 75.68; H 7.93; N 15.95.

4. Procedure for the synthesis of 3,4-dimethylcyclopent-3-ene-1,1-dicarbonitrile 22



A flame-dried schlenk was charged with a solution of the substrate (0.75 mmol) in 7.5 mL of toluene and *cis*-Caz-1a (32.7 mg, 0.0375mmol, 5 mol%) was added. The reaction mixture was stirred at 80 C for 24h . The conversion was determined by ^1H NMR (CDCl_3). Flash chromatography (pentane/dichloromethane/methanol - 70:30:1 v:v) on silica gel afforded the title compound (61 mg, 55%)

^1H NMR (CDCl_3 , 400 MHz): δ (ppm) = 3.12 (m, 4H, $^2J_{\text{HH}} = 0.8$ Hz), 1.69 (m, 6H, $^2J_{\text{HH}} = 0.8$ Hz)

^{13}C -{ ^1H } NMR (CDCl_3 100.6 MHz) δ (ppm) = 128.4 (C^{III} alkene), 117.4 (C^{VI} CN), 49.8 (CH_2), 30.4 (C^{I}), 13.3 (CH_3).

CI-HRMS calculated for $\text{C}_9\text{H}_{11}\text{N}_2$ $[\text{M} + \text{H}]^+$ 147.0922 found 147.0920

5. Synthesis and characterization of *cis*-Caz-1a²⁹

Dichloro-{*N,N'*-bis[2,4,6-(trimethyl)phenyl]imidazolin-2-ylidene}(3-phenylinden-1-

ylidene) (triisopropylphosphite) ruthenium *cis*-Caz-1a. According to the general procedure, 1 equiv of triisopropylphosphite was used and the reaction was stirred for 15h at 40°C. The product was obtained as a brown solid (194 g, 85%). **^1H NMR** (CD_2Cl_2 , 400 MHz): δ (ppm) = 8.87 (d, 1H, $^3J_{\text{HH}} = 7.2$ Hz, indenylidene H⁷). 7.73-7.69 (m, 2H, indenylidene H⁹), 7.46-7.50 (m, 1H, indenylidene H¹¹), 7.38-7.42 (m, 2H, indenylidene H¹⁰), 7.30-7.36 (m, 2H, indenylidene H⁵ and H⁶), 7.14 (d, $^3J_{\text{HH}} = 7.2$ Hz, 1H, indenylidene H⁴), 7.00 (s, 2H, mesityl CH), 6.48 (s, mesityl CH), 6.45 (s, 1H, indenylidene H²), 6.13 (s, 1H, mesityl CH), 4.82 (m, 1H, CH-CH₃), 4.30 (m, 1H, CH-CH₃), 3.76-3.91 (m, 3H, carbene H^{4'}H^{5'}), 3.58-3.67 (m, 1H, carbene H^{4'}), 3.23 (m, 1H, CH-CH₃), 2.73 (s, 3H, mesityl CH₃), 2.64 (s, 3H, mesityl CH₃),

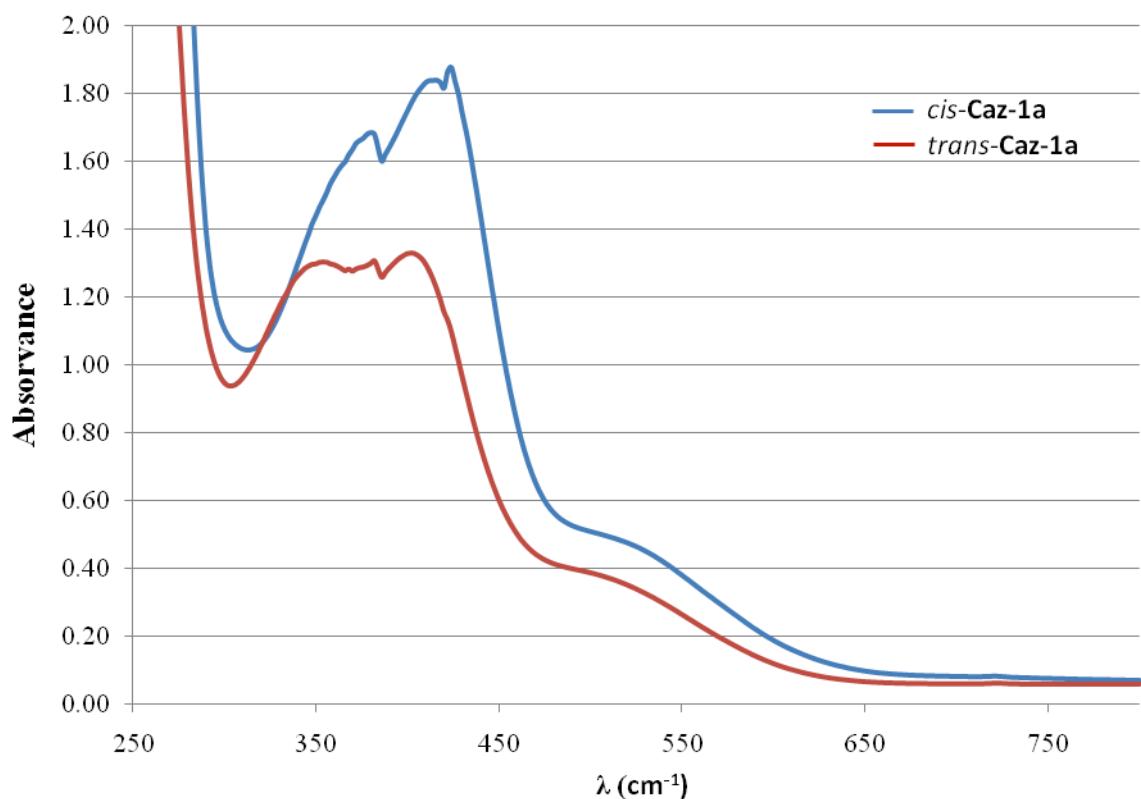
2.56 (s, 3H, mesityl CH₃), 2.33 (s, 3H, mesityl CH₃), 1.85 (s, 3H, mesityl CH₃), 1.58 (s, 3H, mesityl CH₃), 1.48 (d, ³J_{HH} = 6.2 Hz, 3H, CH-CH₃), 1.43 (d, ³J_{HH} = 6.1 Hz, 3H, CH-CH₃), 1.06 (d, ³J_{HH} = 6.0 Hz, 3H, CH-CH₃), 0.92 (d, ³J_{HH} = 5.8 Hz, 3H, CH-CH₃), 0.75 (d, ³J_{HH} = 6.0 Hz, 3H, CH-CH₃), 0.58 (d, ³J_{HH} = 5.9 Hz, 3H, CH-CH₃), ¹³C-{¹H} NMR (CDCl₃ 100.6 MHz) δ (ppm) = 292.1 (d, ²J_{CP} = 24.7 Hz, indenylidene C¹), 208.95 (d, ²J_{CP} = 13.4 Hz, carbene C²), 141.2 (d, ³J_{CP} = 2.6 Hz, indenylidene C^{7a}), 142.5 (s, C^{IV}), 140.4 (d, ³J_{CP} = 15.9 Hz, indenylidene C²), 139.2 (s, C^{IV}), 138.6 (s, C^{IV}), 138.5 (s, C^{IV}), 138.25 (s, C^{IV}), 138.1 (s, C^{IV}), 137.0 (s, C^{IV}), 136.9 (s, C^{IV}), 136.8 (s, C^{IV}), 135.9 (s, C^{IV}), 135.0 (s, C^{IV}), 130.5 (s, mesityl CH and indenylidene C⁷H), 130.31 (s, mesityl CH), 130.26 (s, mesityl CH), 129.8 (s, indenylidene C⁶H), 129.9 (s, indenylidene C⁵H), 128.7 (s, indenylidene C¹¹H), 129.2 (s, indenylidene C¹⁰H), 127.6 (s, indenylidene C⁹H), 117.4 (s, indenylidene C⁴H), 72.9 (d, ²J_{CP} = 3.6 Hz, CH-CH₃), 70.7 (d, ²J_{CP} = 9.3 Hz, CH-CH₃), 69.55 (d, ²J_{CP} = 11.7 Hz, CH-CH₃), 52.6 (s, carbene C^{5'}H₂), 52.0 (s, carbene C^{4'}H₂), 24.74 (s, CH-CH₃), 24.72 (s, CH-CH₃), 24.4 (s, CH-CH₃), 24.3 (s, CH-CH₃), 24.05 (s, CH-CH₃), 24.0 (s, CH-CH₃), 21.5 (s, mesityl CH₃), 21.4 (s, mesityl CH₃), 21.1 (s, mesityl CH₃), 20.6 (s, mesityl CH₃), 19.5 (s, mesityl CH₃), 19.1 (s, mesityl CH₃). ³¹P-{¹H} NMR (CD₂Cl₂, 162 MHz) δ (ppm) = 122.0. Ele. anal. Calcd. for C₄₅H₅₇Cl₂N₂O₃PRu: C, 61.64; H, 6.55; N, 3.19. Found: C, 61.21; H, 6.24; N, 3.15.

6. Crystallographic data for complexes *cis*-Caz-1a-d

Table S1

	<i>Cis</i> -P(O <i>i</i> Pr) ₃ ²⁹	<i>Cis</i> -P(OPh) ₃	<i>cis</i> -P(OEt) ₃	<i>cis</i> -P(OMe) ₃
Formula	C ₄₅ H ₅₇ Cl ₂ N ₂ O ₃ PRu	C ₅₄ H ₅₁ Cl ₂ N ₂ O ₃ PRu	C ₄₂ H ₅₁ Cl ₂ N ₂ O ₃ PRu	C ₃₉ H ₄₅ Cl ₂ N ₂ O ₃ PRu·CH ₄ O
<i>M</i> / g.mol ⁻¹	876.87	978.91	834.79	824.75
Crystal system	Monoclinic	Triclinic	Triclinic	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> -1	<i>P</i> -1	<i>P</i> 2 ₁ / <i>n</i>
<i>a</i> / Å	19.132 (2)	9.127 (2)	9.318 (2)	9.0518 (19)
<i>b</i> / Å	9.5576 (11)	11.772 (3)	18.306 (3)	25.921 (5)
<i>c</i> / Å	24.397 (3)	21.891 (6)	24.300 (4)	16.471 (3)
β / °	104.451 (3)	86.571 (9)	89.514 (16)	94.024 (5)
<i>V</i> / Å ³	4320.0 (9)	76.206 (8)	3989.9 (14)	3855.0 (13)
<i>Z</i>	4	2	4	4
ρ_{calcd} / g.cm ⁻³	1.348	1.441	1.390	1.421
μ (Mo K α)/ mm ⁻¹	0.564	0.549	0.607	0.629
<i>T</i> / K	125 (2)	93 (2)	93 (2)	93 (2)
Number of reflections	5696	8198	14091	5706
Number of unique reflections	7916	7277	10415	6942
<i>R</i> _{int}	0.132	0.056	0.084	0.054
<i>R</i> 1, w <i>R</i> 2 (<i>I</i> > 2 σ (<i>I</i>))	0.0897, 0.1676	0.0638, 0.1718	0.0778, 0.1971	0.0481, 0.1252
<i>R</i> 1, w <i>R</i> 2 (all data)	0.1341, 0.1900	0.0722, 0.1849	0.1000, 0.2130	0.0617, 0.1348
GOF	1.197	1.080	1.073	1.053

7. UV-Visible spectra of *cis*-Caz-1a and *trans*-Caz-1a.

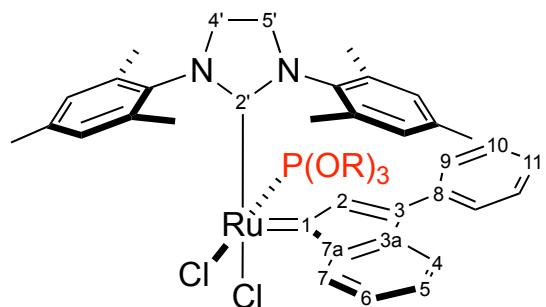


Concentration of the complexes 1.14×10^{-4} [M] in CH_2Cl_2 .

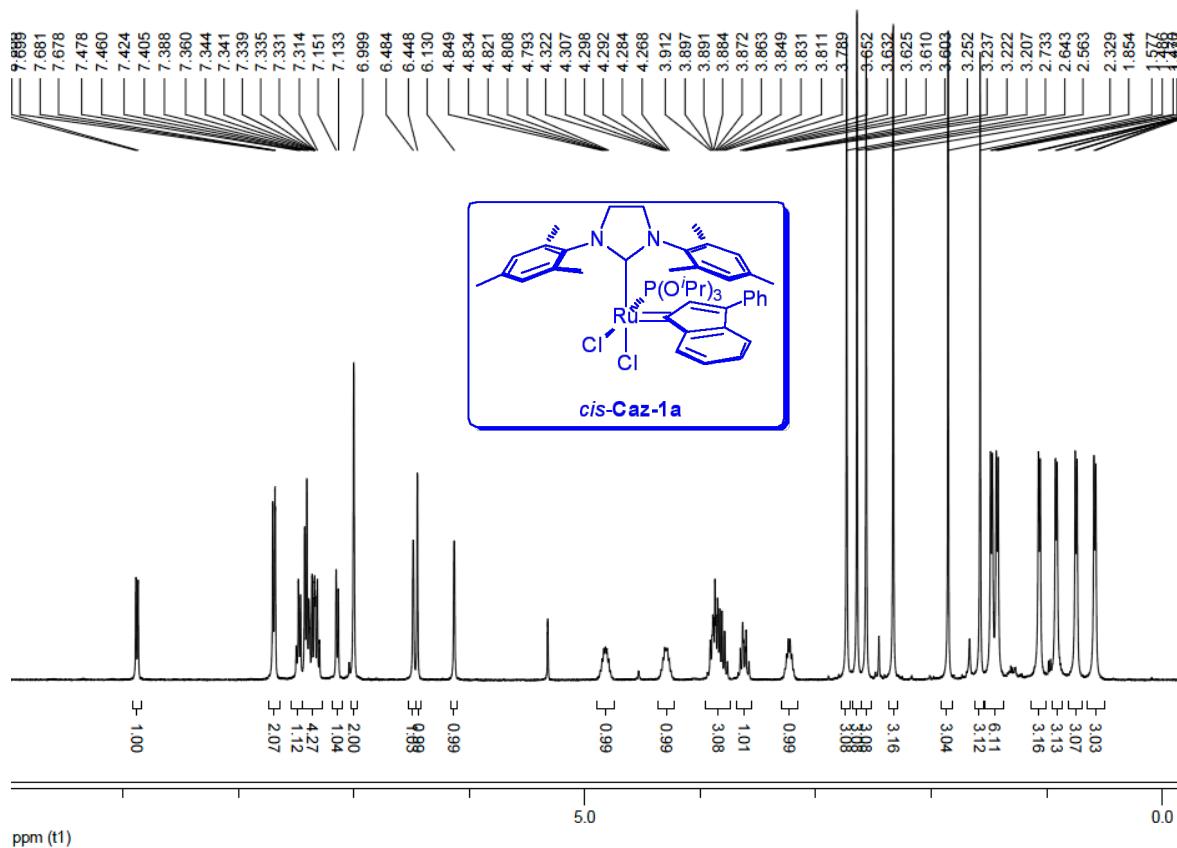
$\text{UV}_{\text{max}} \text{ } c\text{i}s\text{-Caz-1a} : 424, 414 \text{ and } 380 \text{ cm}^{-1}$

$\text{UV}_{\text{max}} \text{ } t\text{r}a\text{n}s\text{-Caz-1a} : 402, 382, 356 \text{ cm}^{-1}$

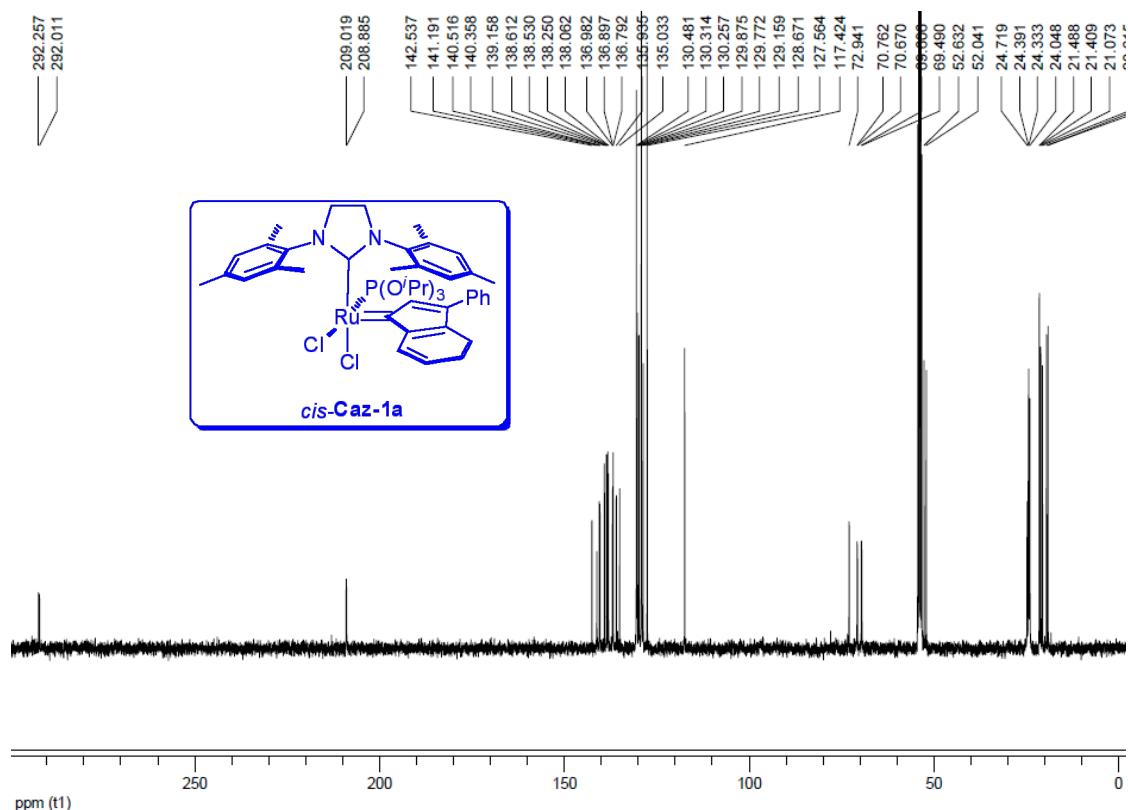
8. NMR Spectra of complexes *cis*-Caz-1a-d



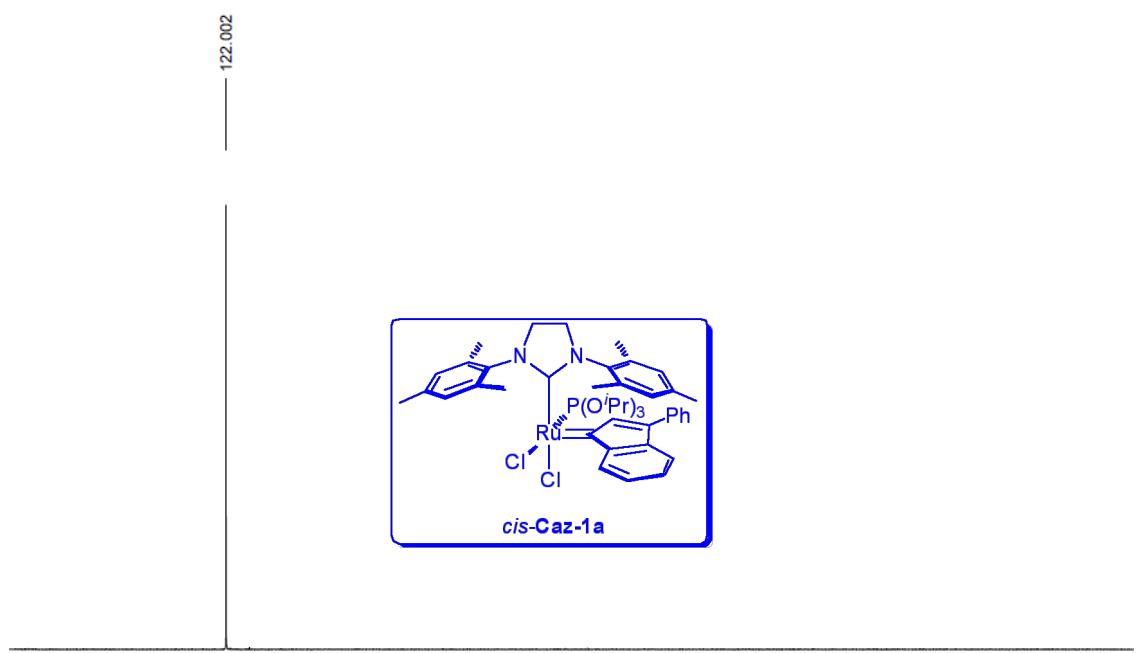
^1H NMR (CD_2Cl_2) of *cis*-Caz-1a



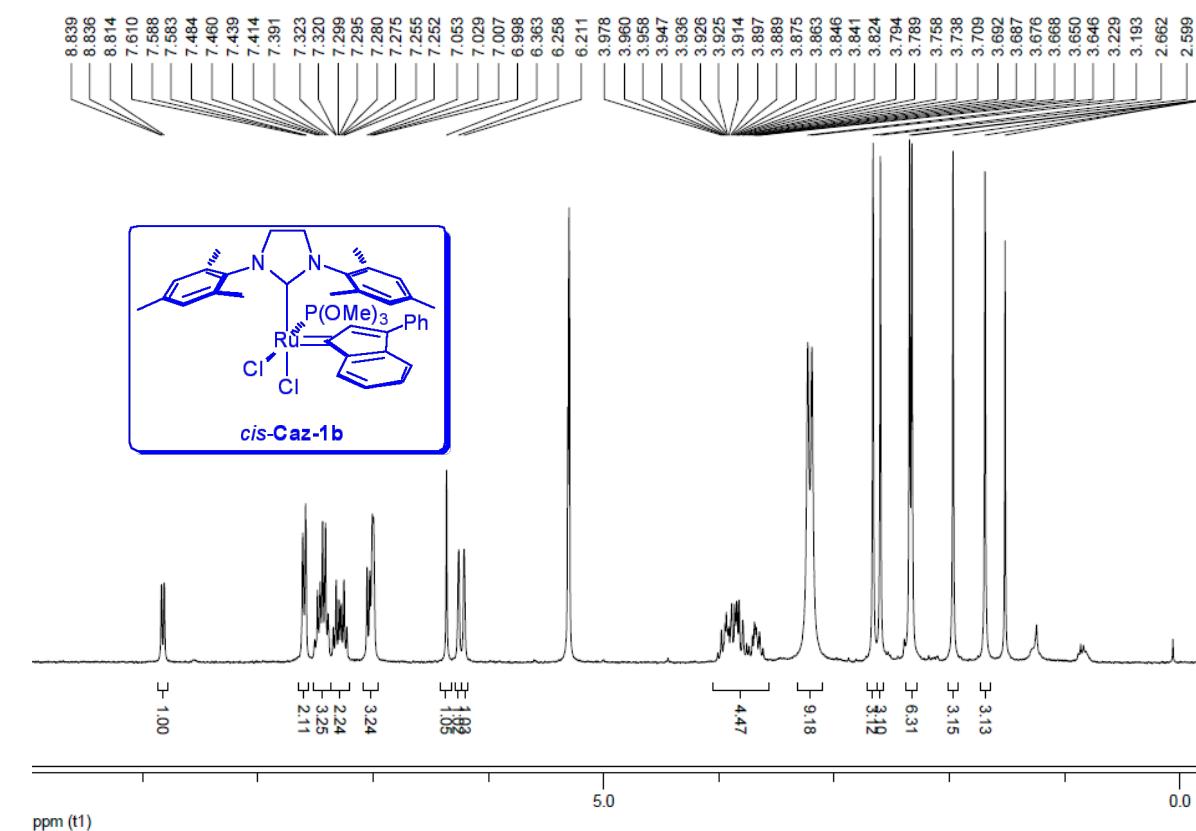
$^{13}\text{C}-\{^1\text{H}\}$ NMR (CD_2Cl_2) of *cis*-Caz-1a



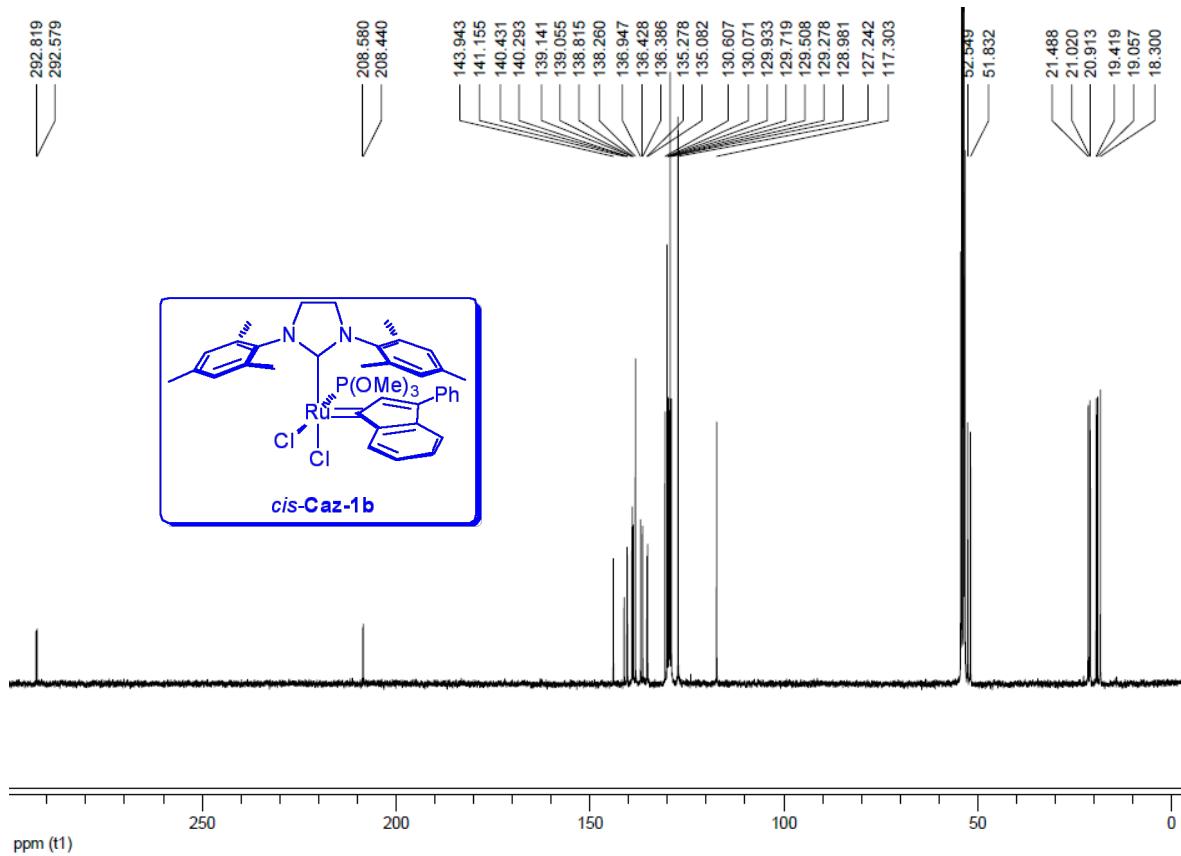
$^{31}\text{P}-\{\text{H}\}$ NMR (CD_2Cl_2) of *cis*-Caz-1a



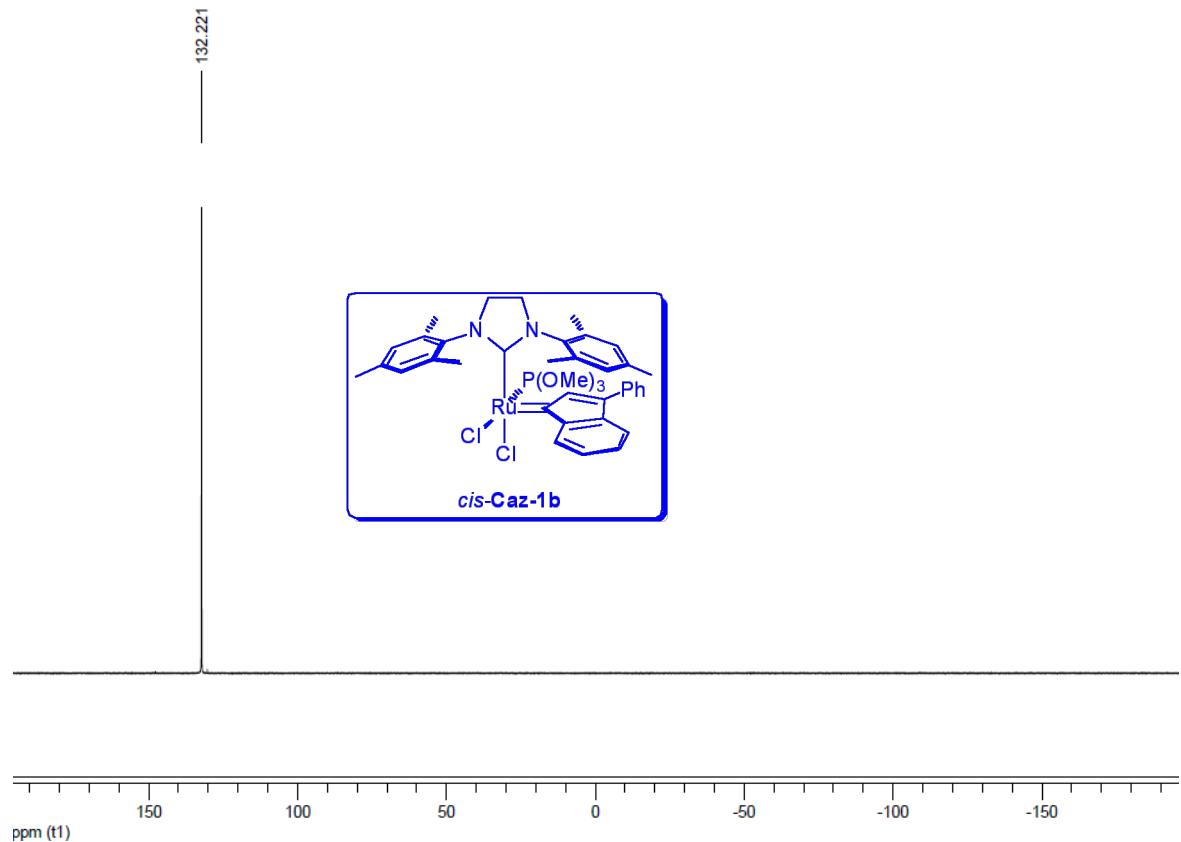
^1H NMR (CD_2Cl_2) of *cis*-Caz-1b



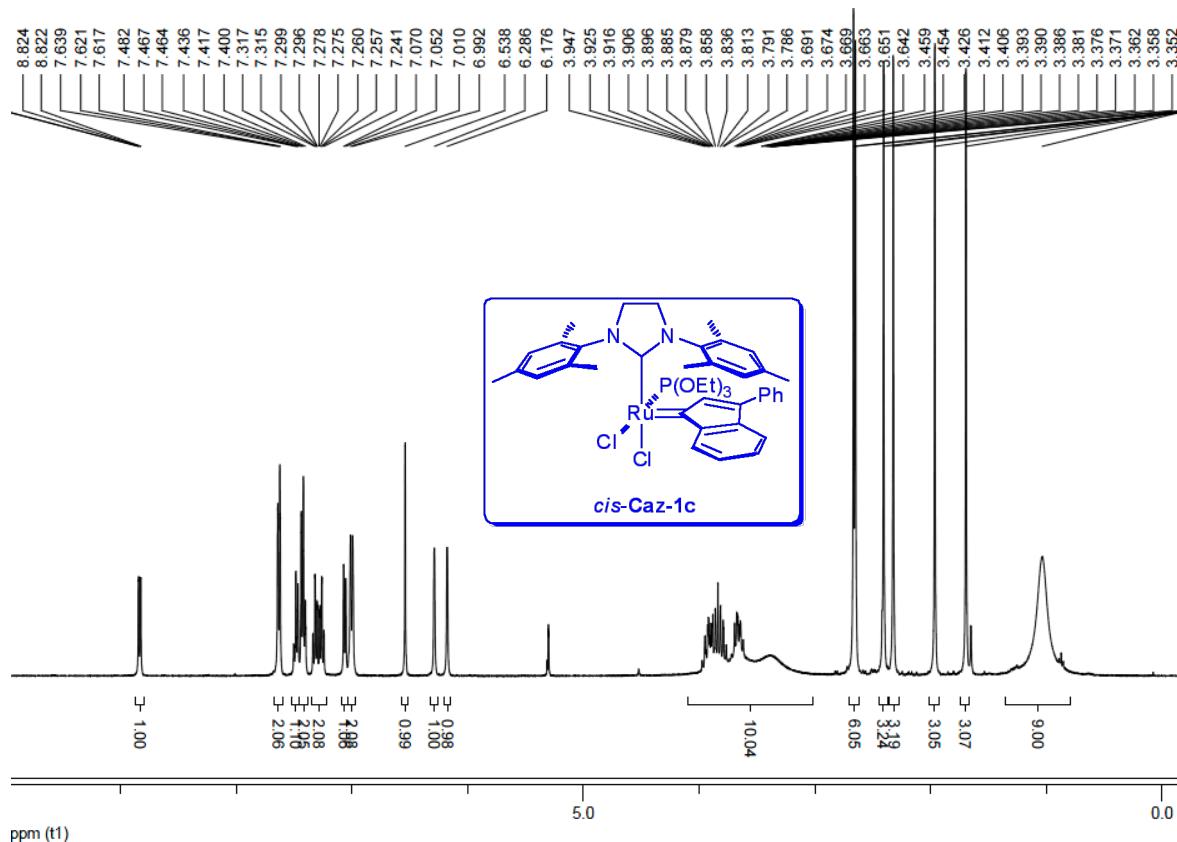
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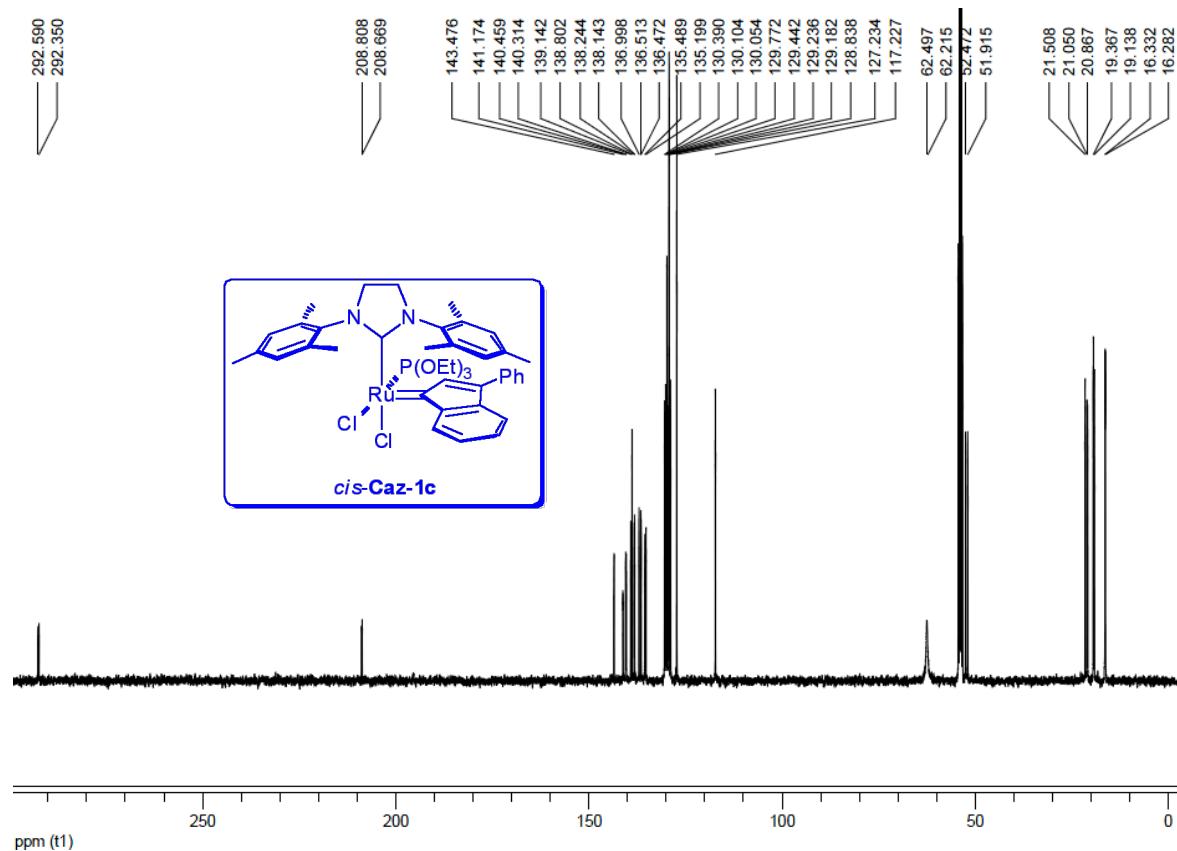
${}^31\text{P}-\{{}^1\text{H}\}$ NMR (CD_2Cl_2) of *cis*-Caz-1b



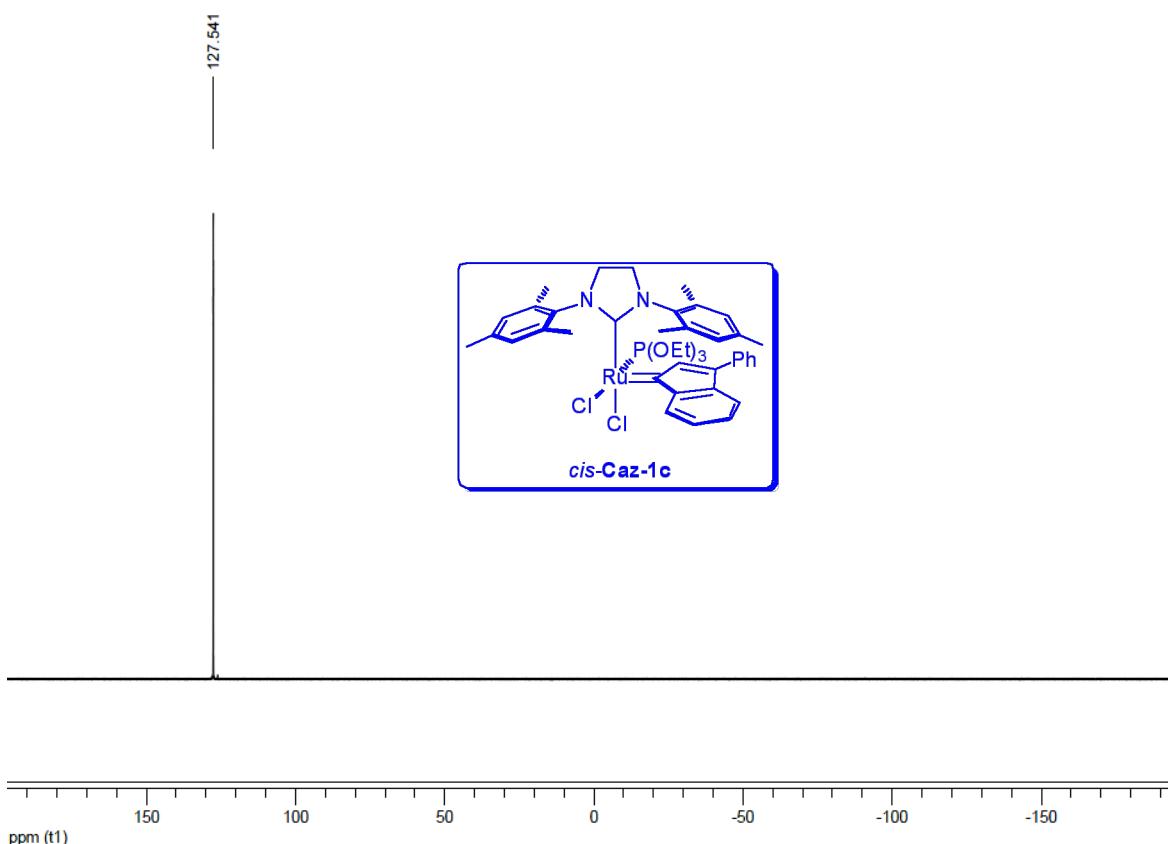
^1H NMR (CD_2Cl_2) of *cis*-Caz-1c



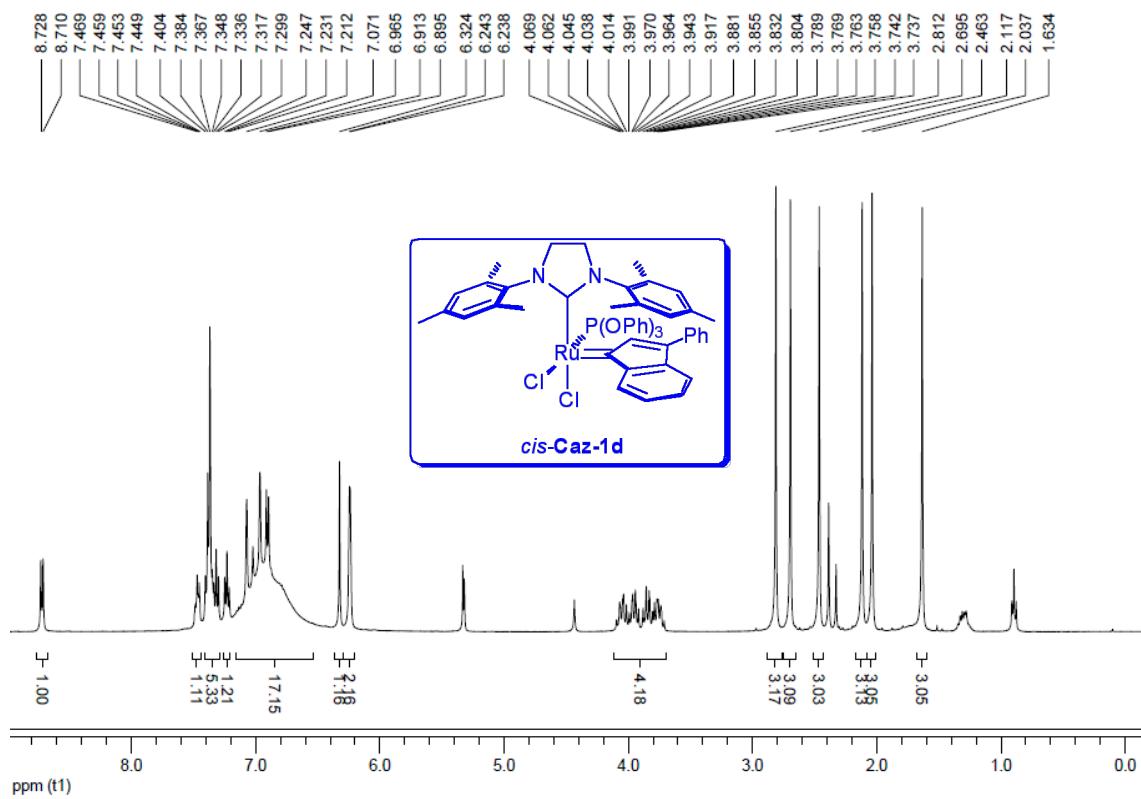
^{13}C -{ ^1H } NMR (CD_2Cl_2) of *cis*-Caz-1c



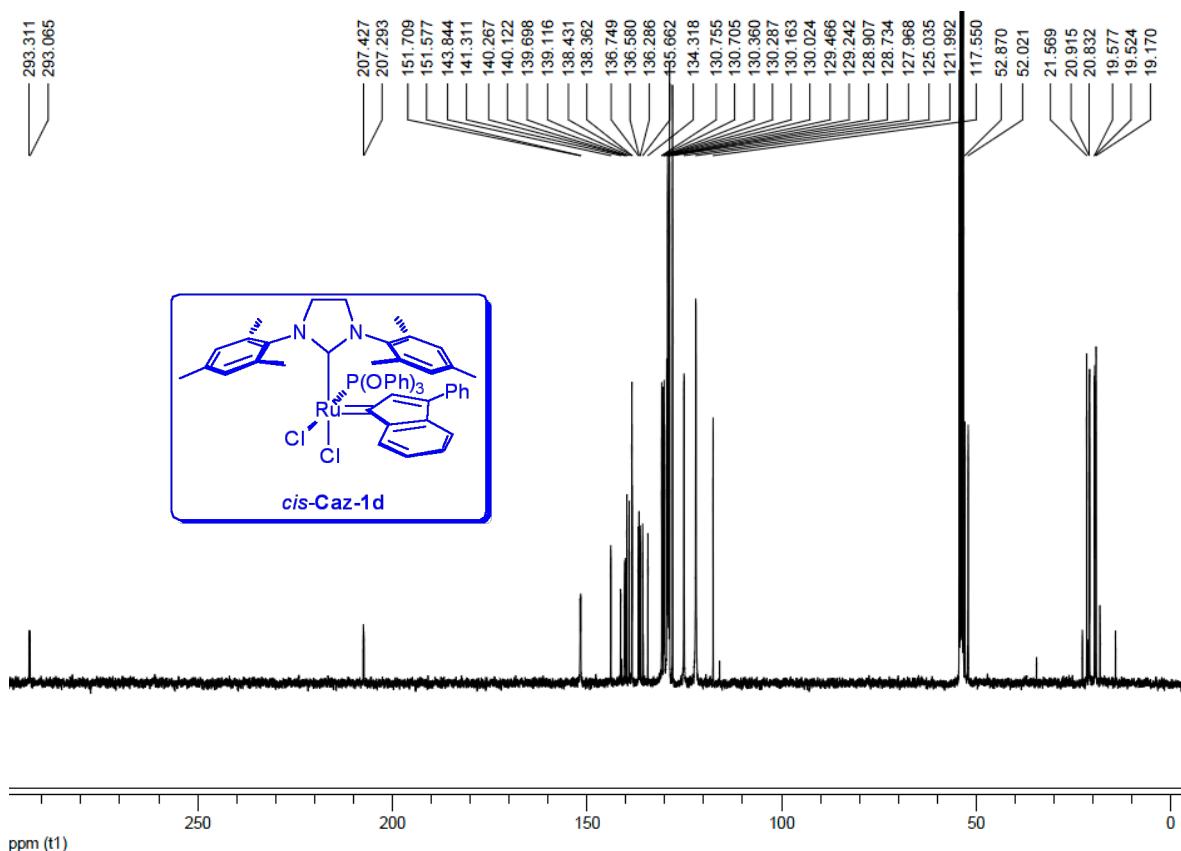
${}^{-31}\text{P}-\{{}^1\text{H}\}$ NMR (CD_2Cl_2) of *cis*-Caz-1c



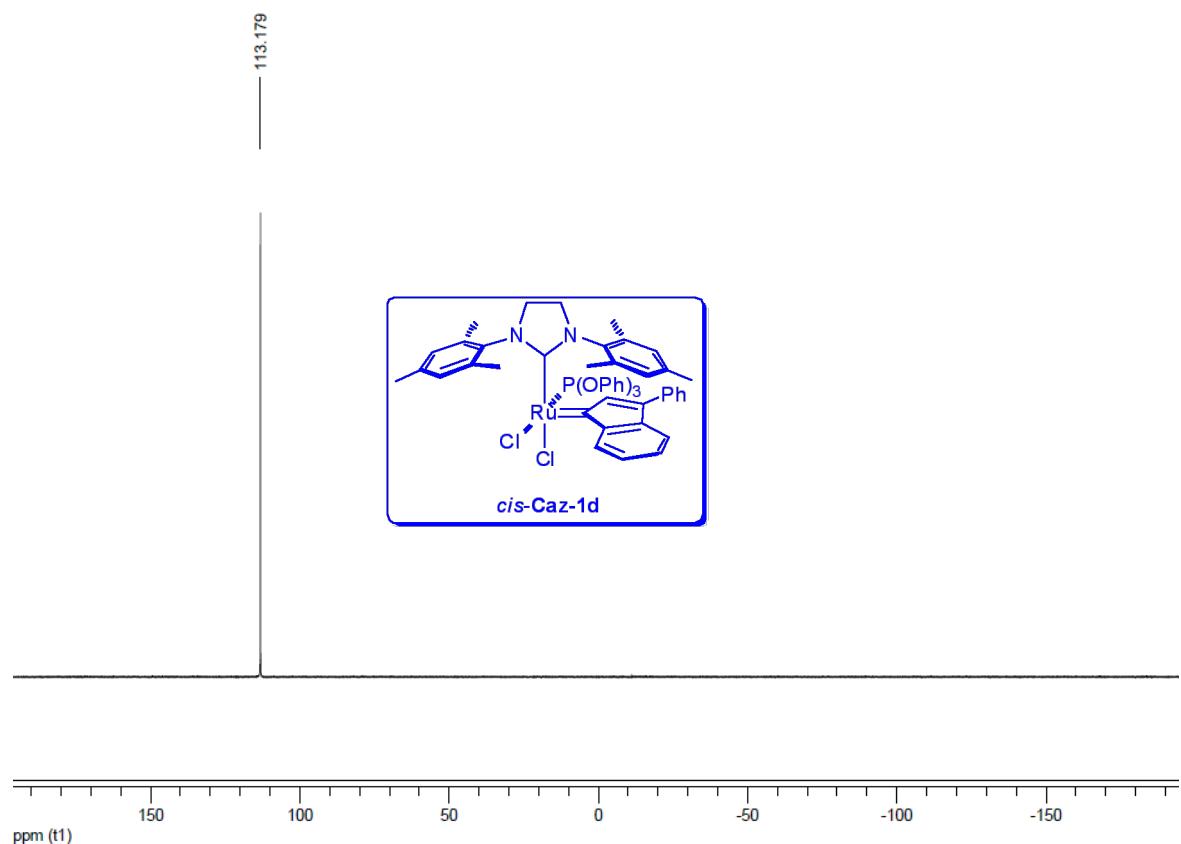
${}^1\text{H}$ NMR (CD_2Cl_2) of *cis*-Caz-1d



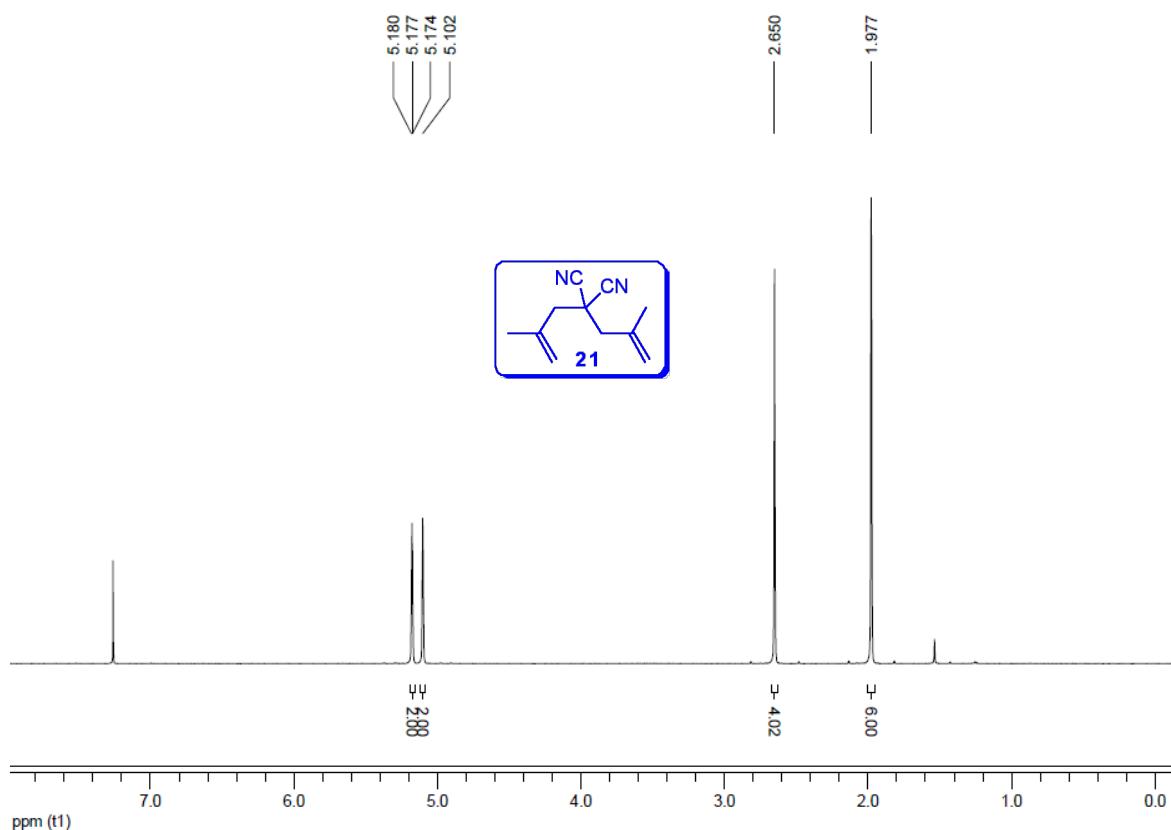
$^{13}\text{C}-\{\text{H}\}$ NMR (CD_2Cl_2) of *cis*-Caz-1d



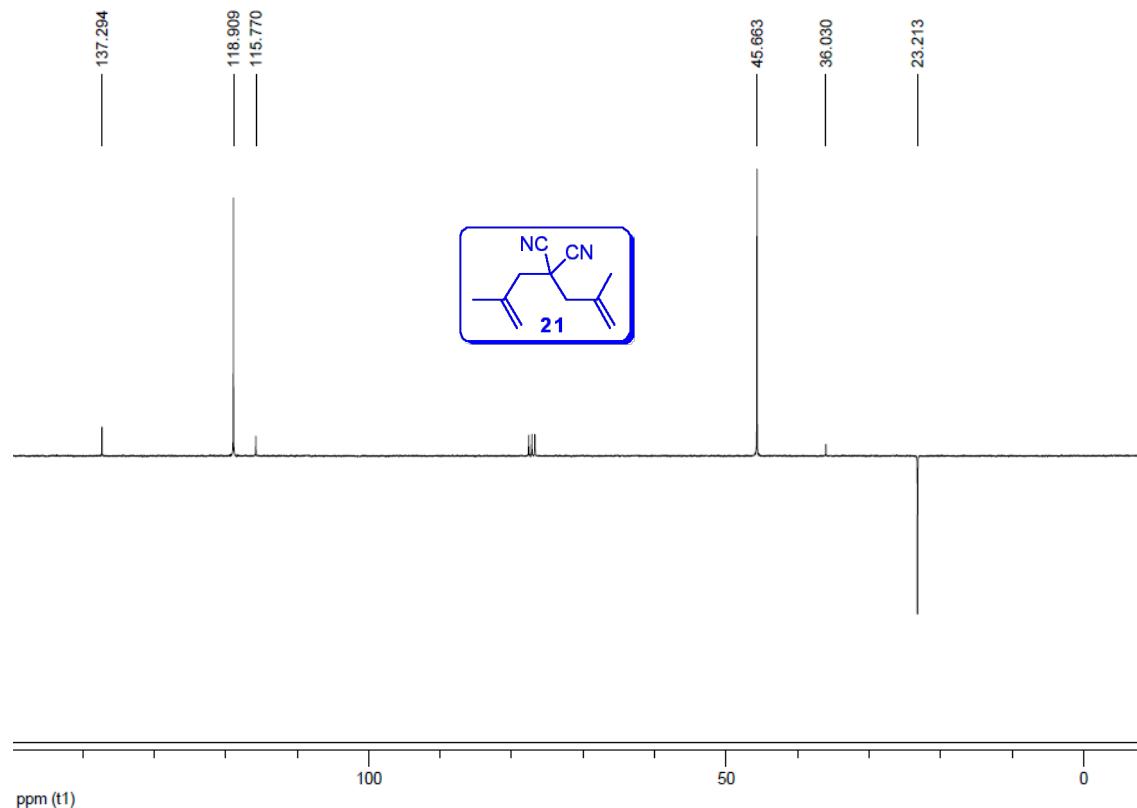
$^{31}\text{P}-\{\text{H}\}$ NMR (CD_2Cl_2) of *cis*-Caz-1d



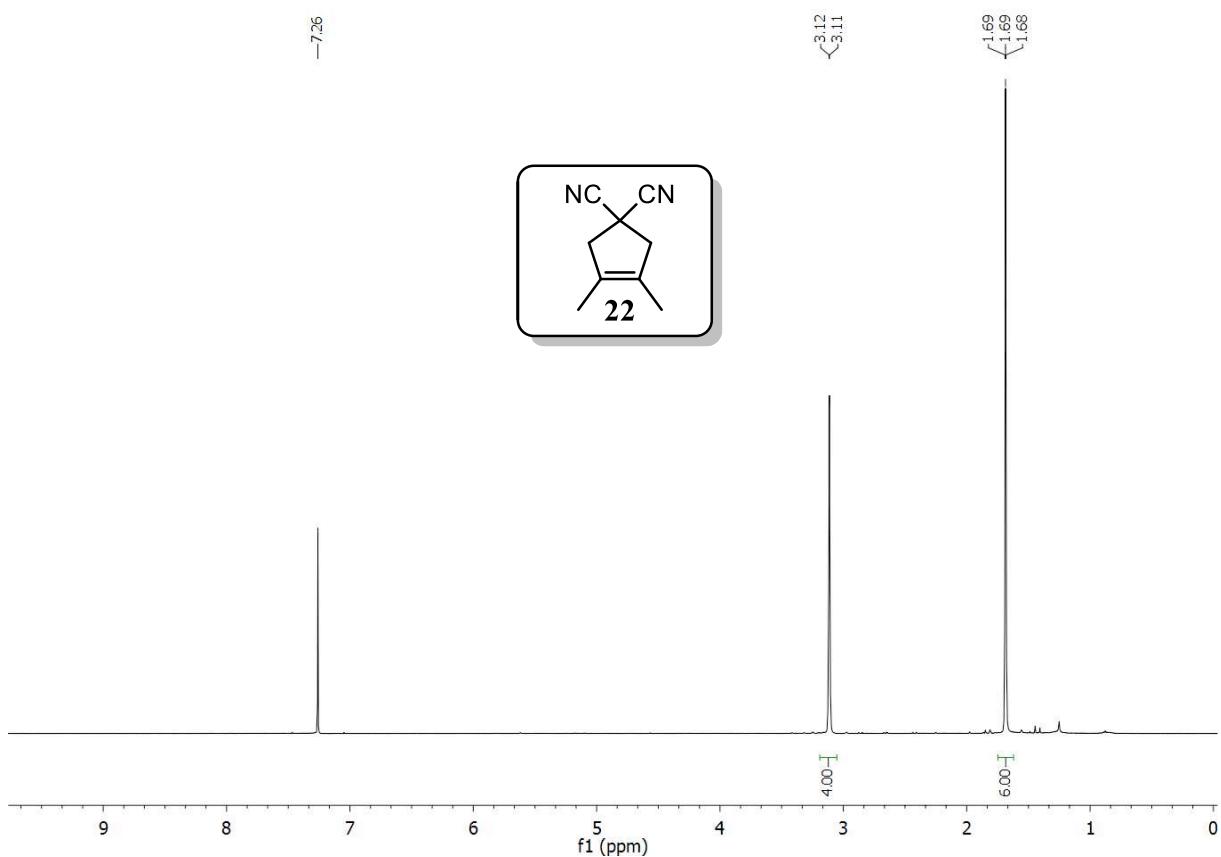
^1H NMR (CDCl_3) of 2,2-bis(2-methylallyl)malononitrile **21**



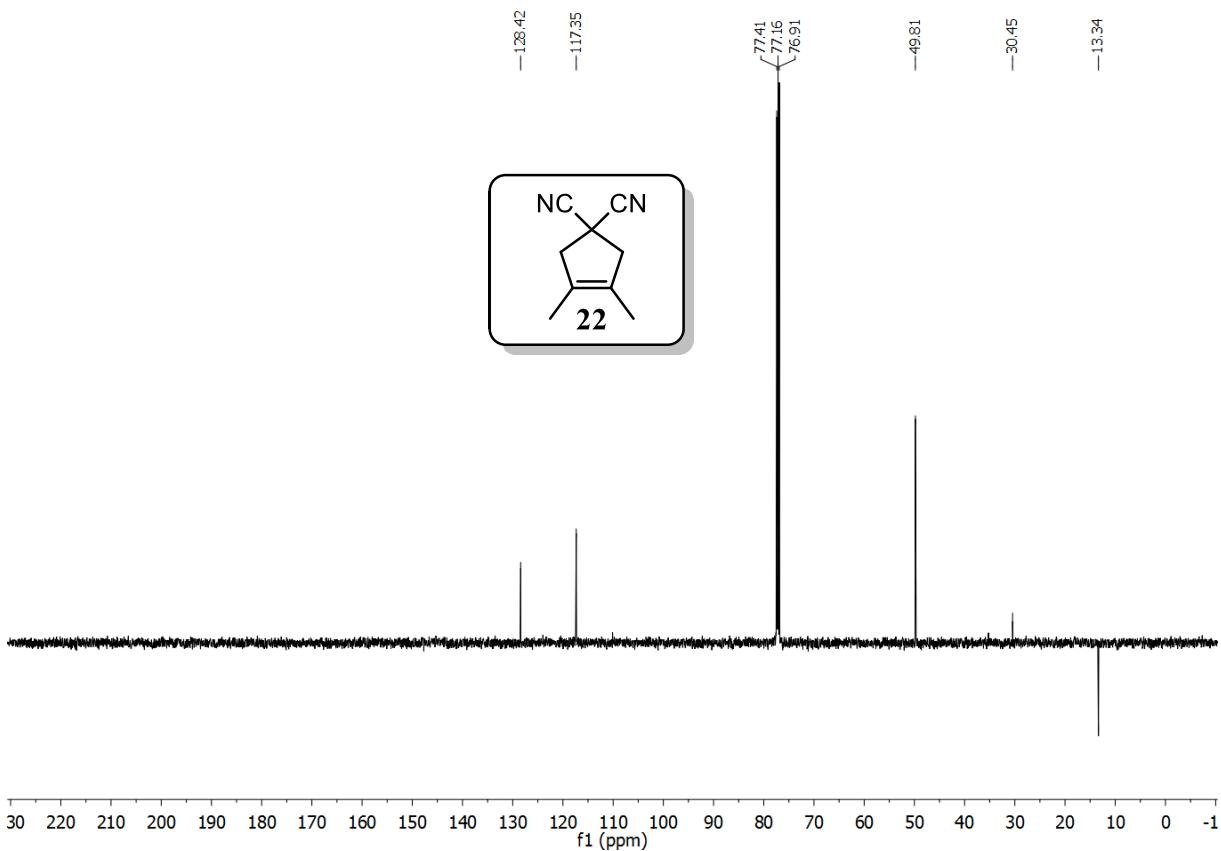
$^{13}\text{C}-\{^1\text{H}\}$ NMR (CDCl_3) of 2,2-bis(2-methylallyl)malononitrile **21**



^1H NMR (CDCl_3) of 3,4-dimethylcyclopent-3-ene-1,1-dicarbonitrile 22

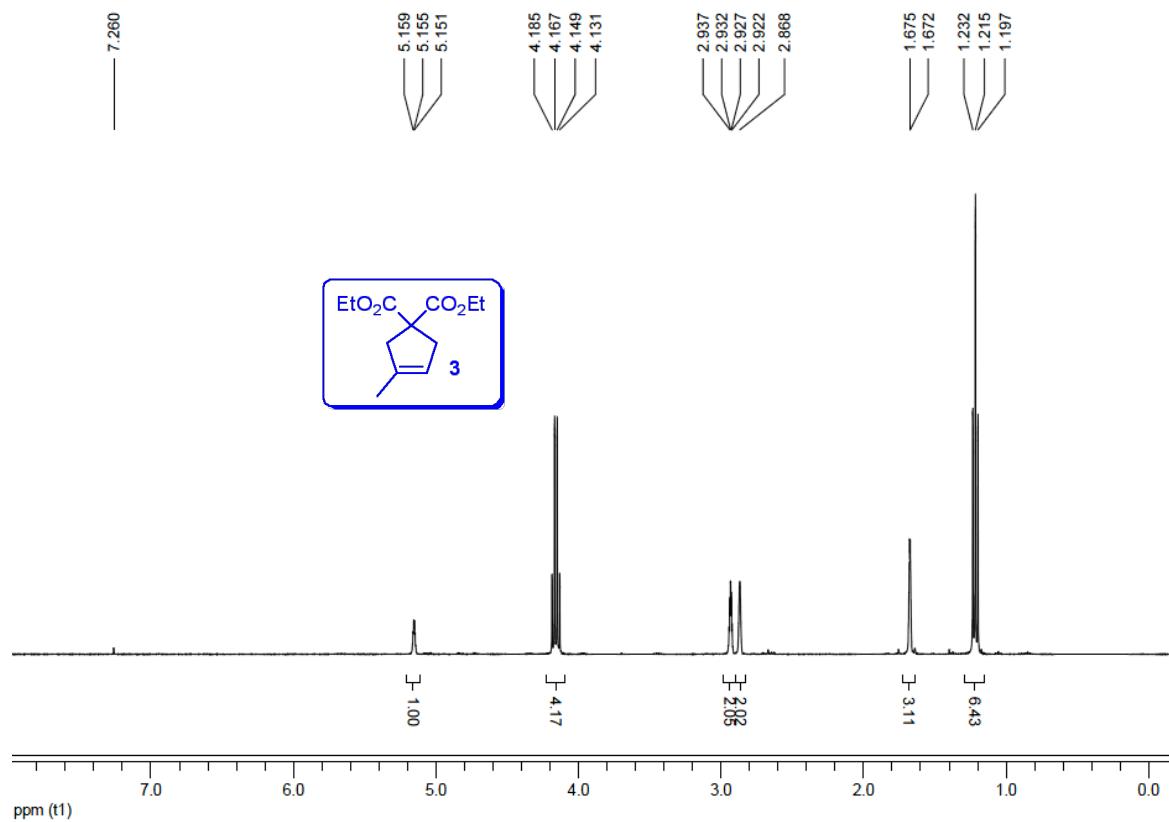


$^{13}\text{C}-\{^1\text{H}\}$ NMR (CDCl_3) of 3,4-dimethylcyclopent-3-ene-1,1-dicarbonitrile 22

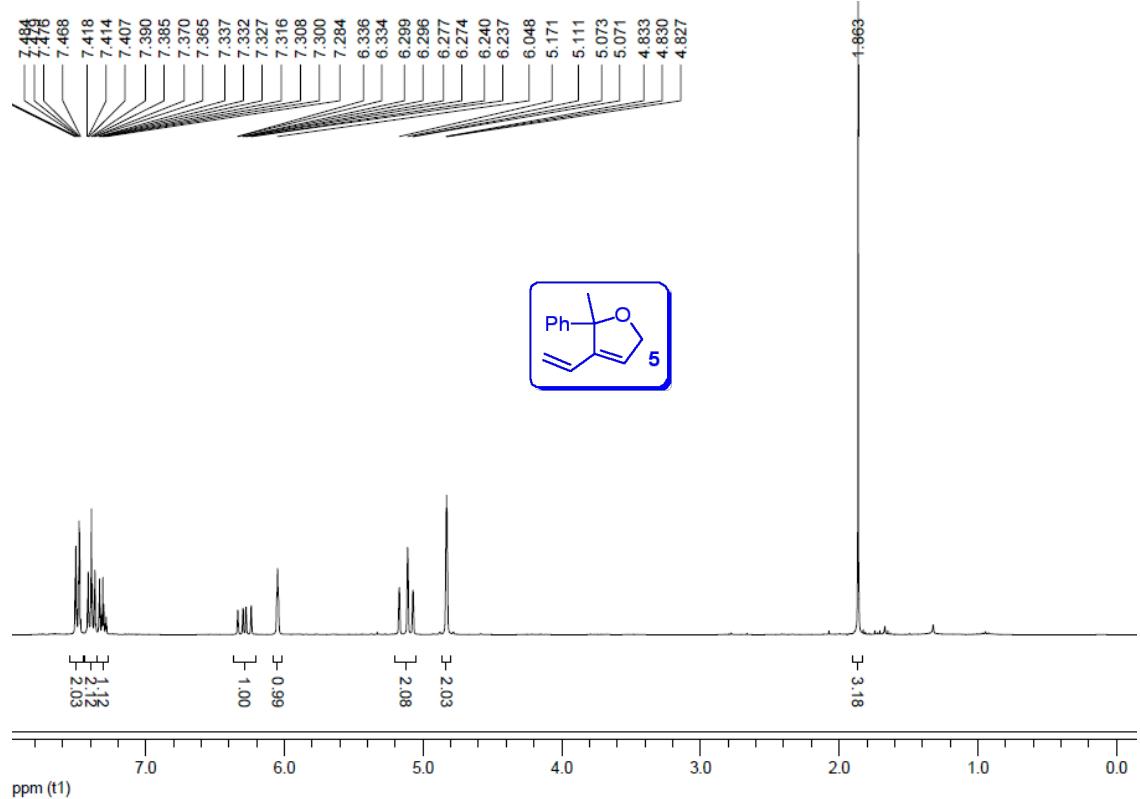


9. NMR Spectra of metathesis products

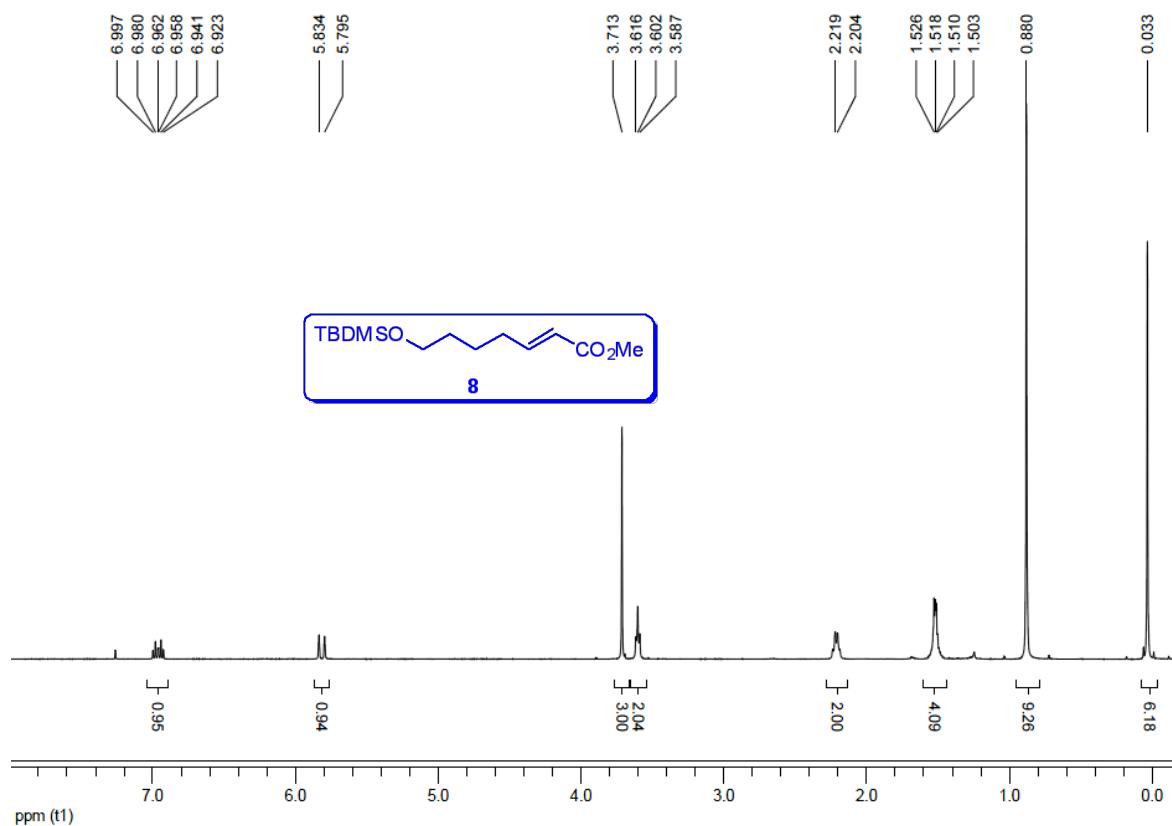
^1H NMR (CDCl_3) of 3



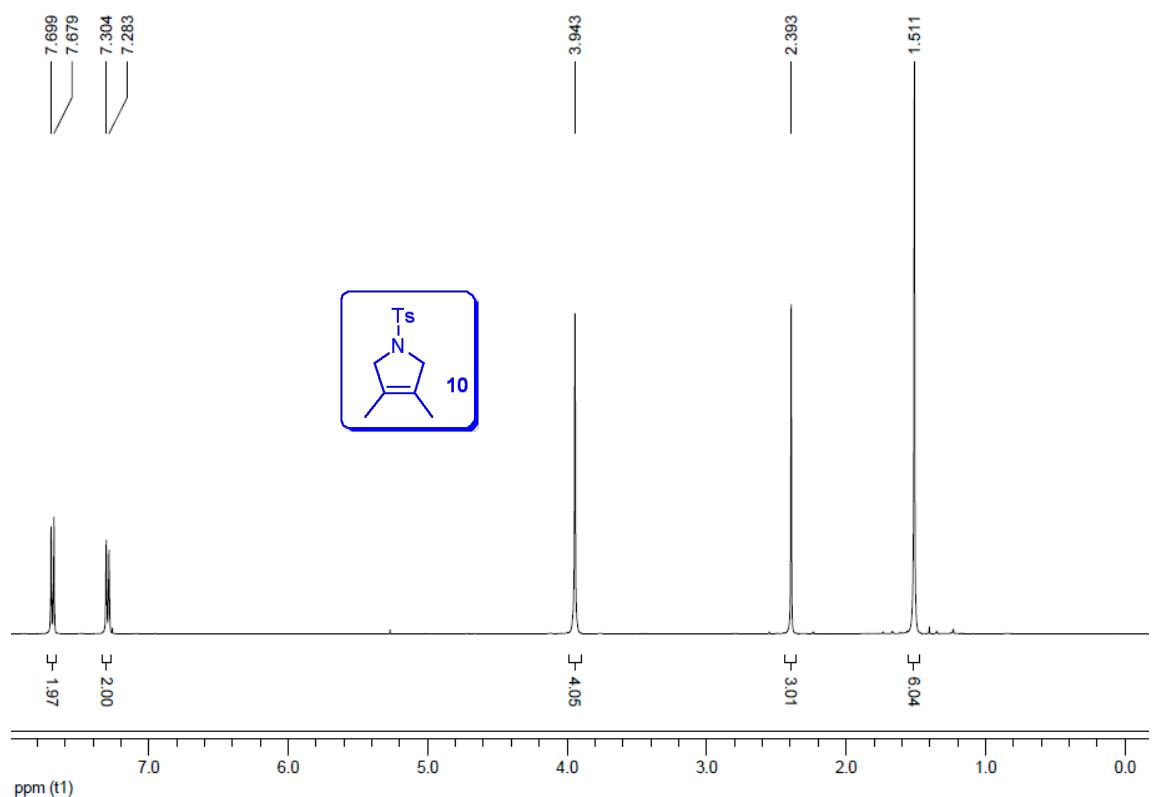
^1H NMR (CDCl_3) of 5



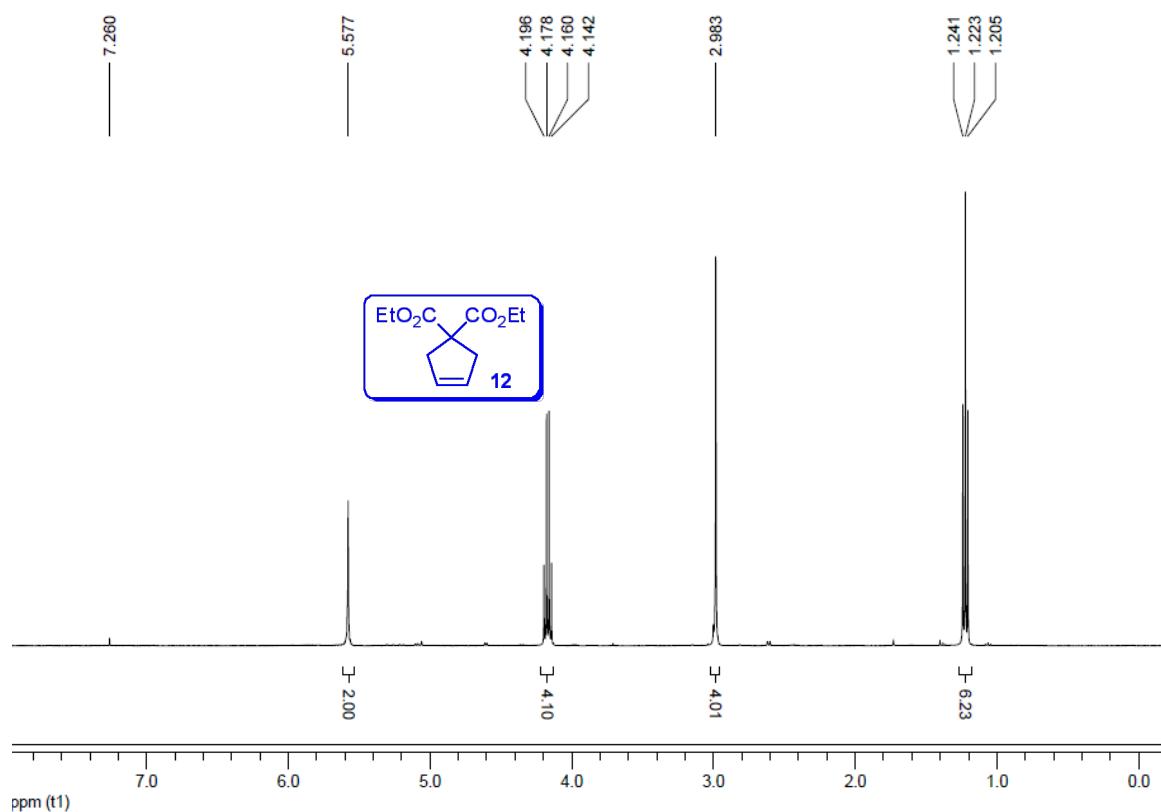
^1H NMR (CDCl_3) of **8**



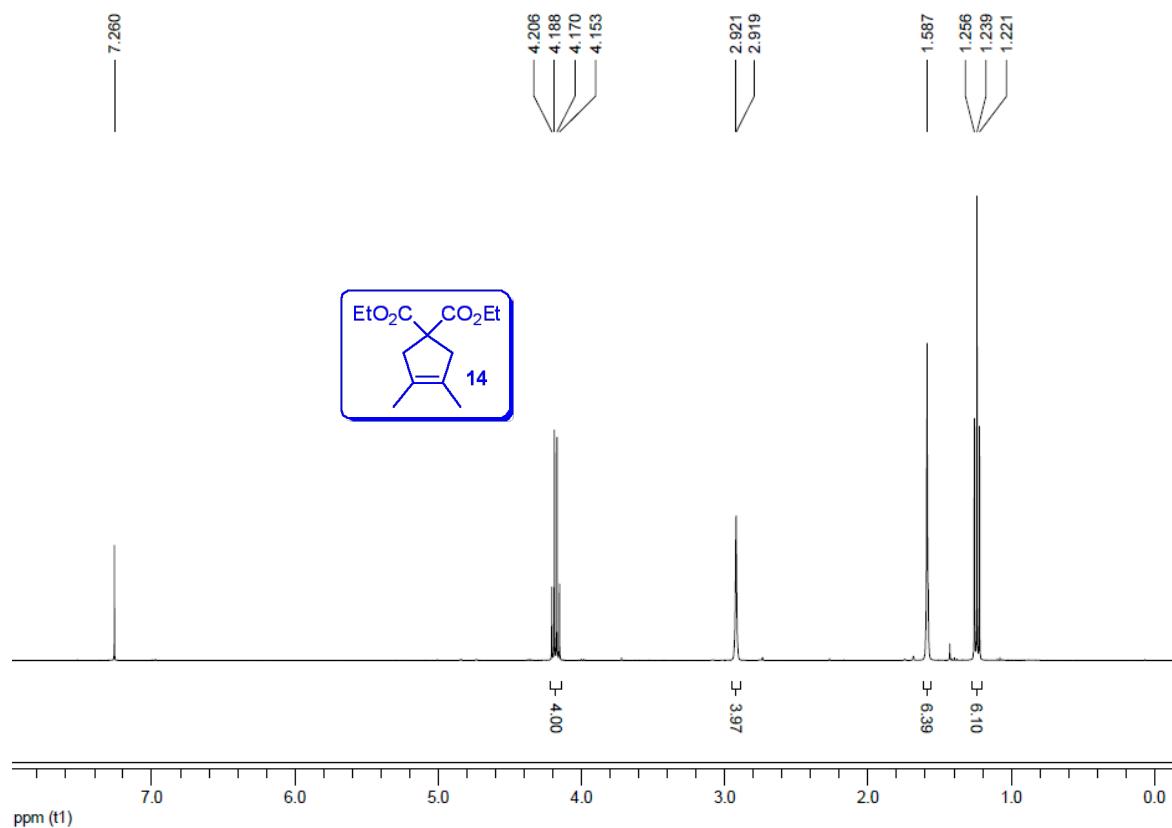
^1H NMR (CDCl_3) of **10**



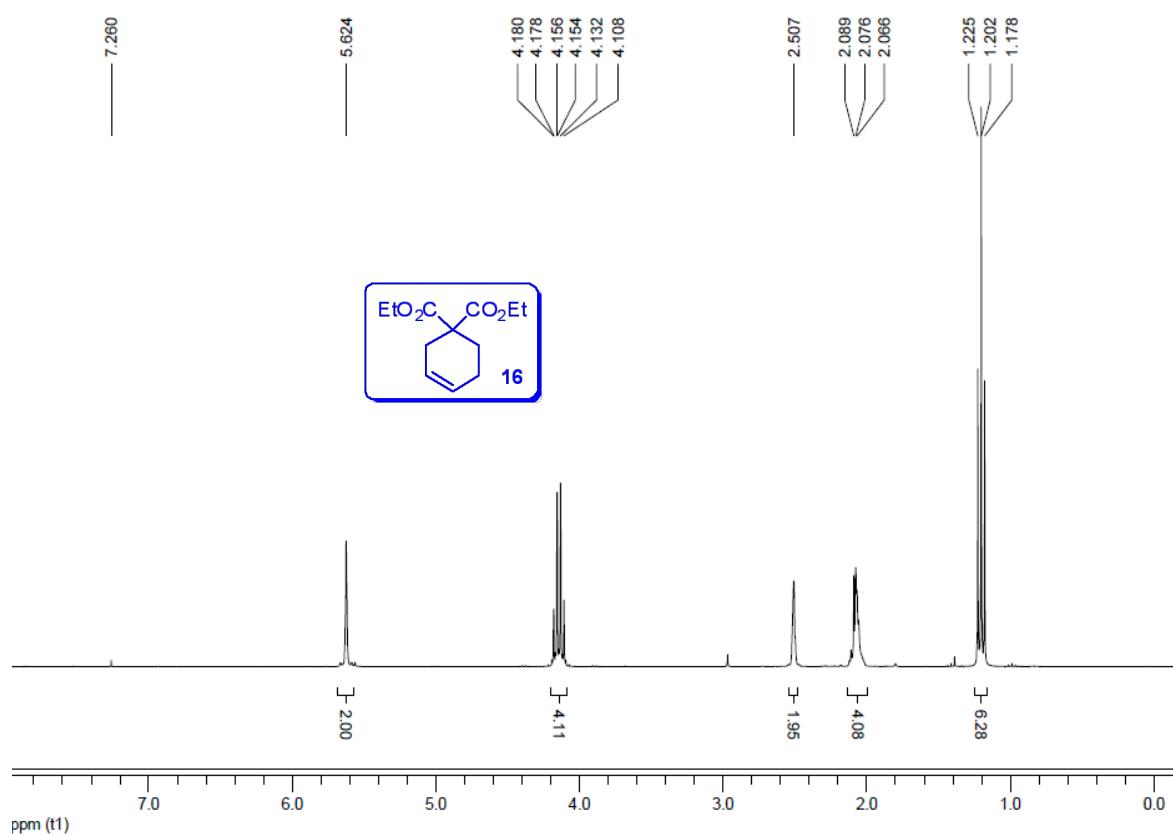
^1H NMR (CDCl_3) of 12



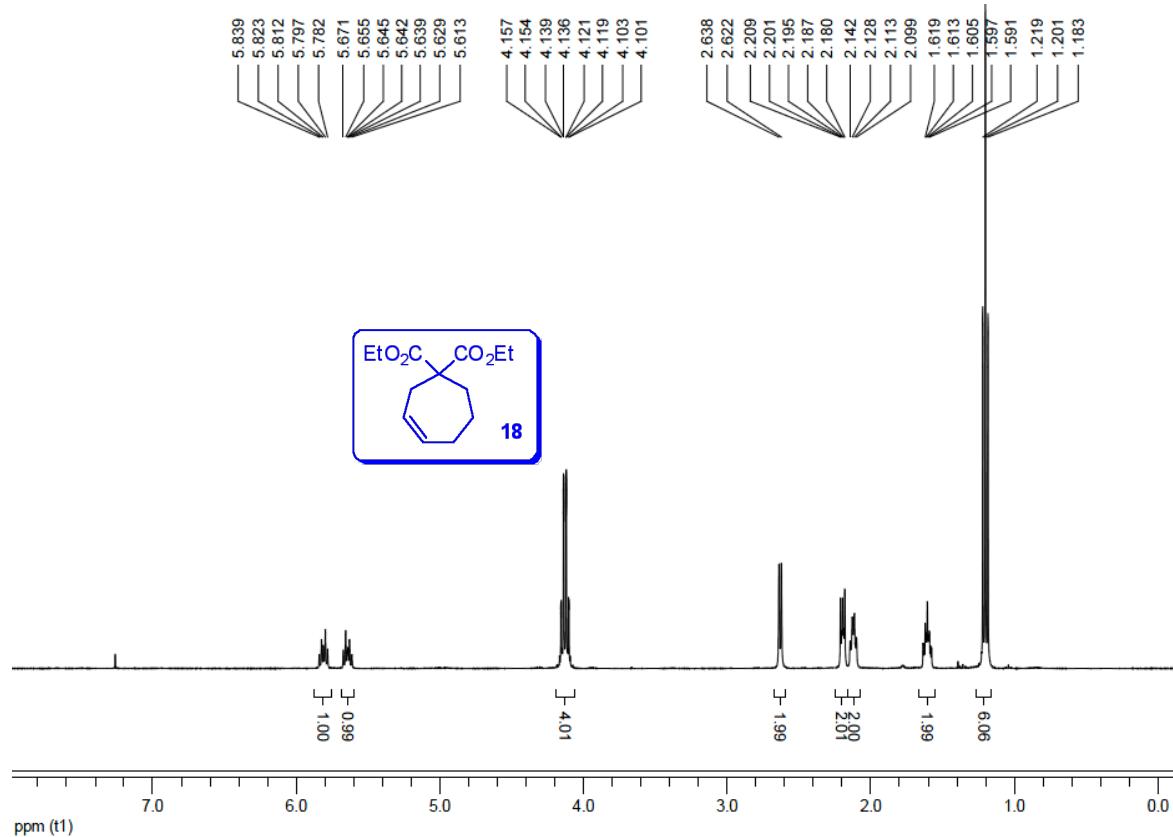
^1H NMR (CDCl_3) of 14



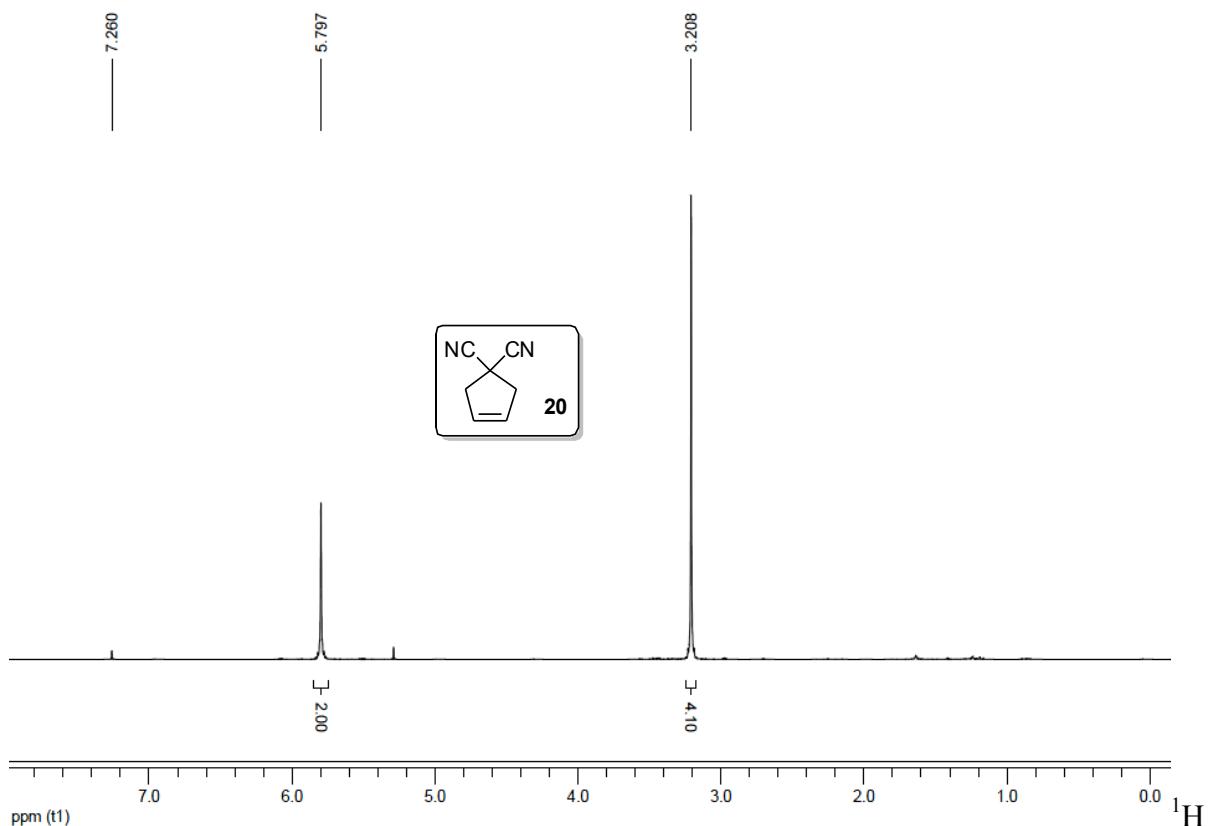
^1H NMR (CDCl_3) of 16



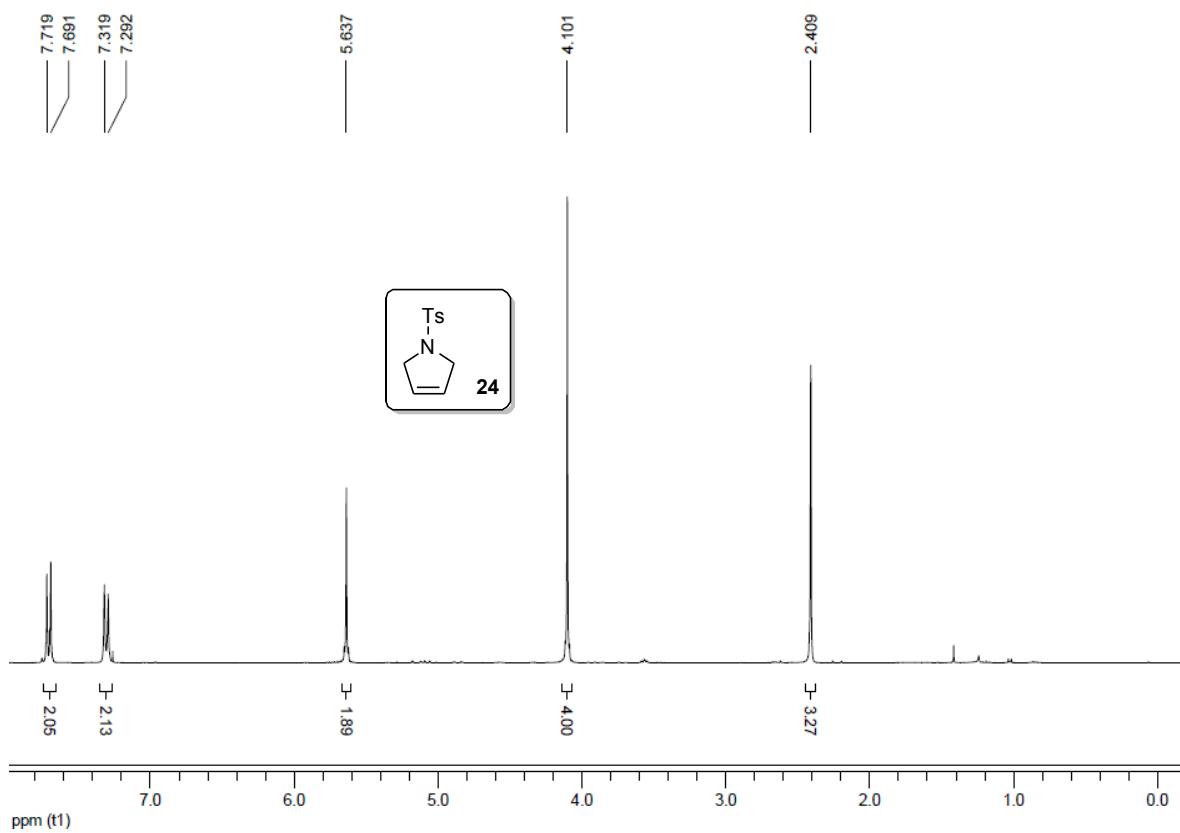
^1H NMR (CDCl_3) of 18



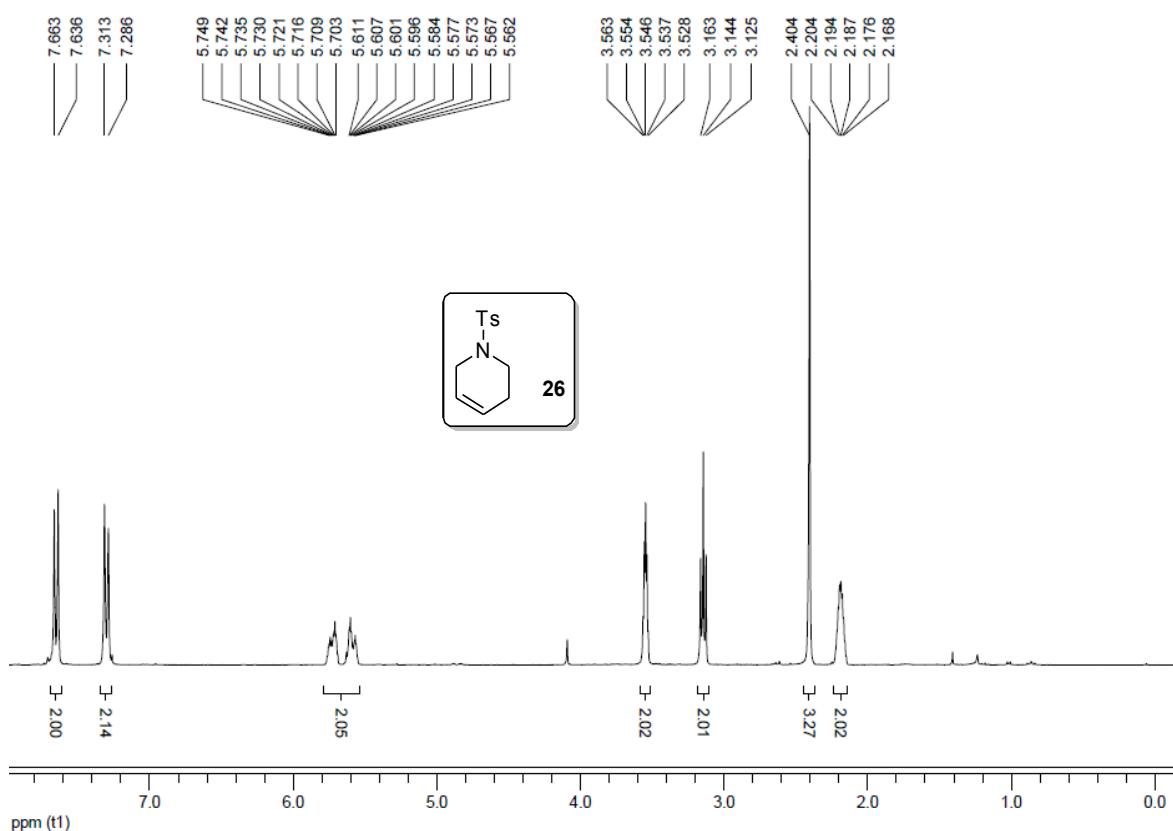
^1H NMR (CDCl_3) of **20**



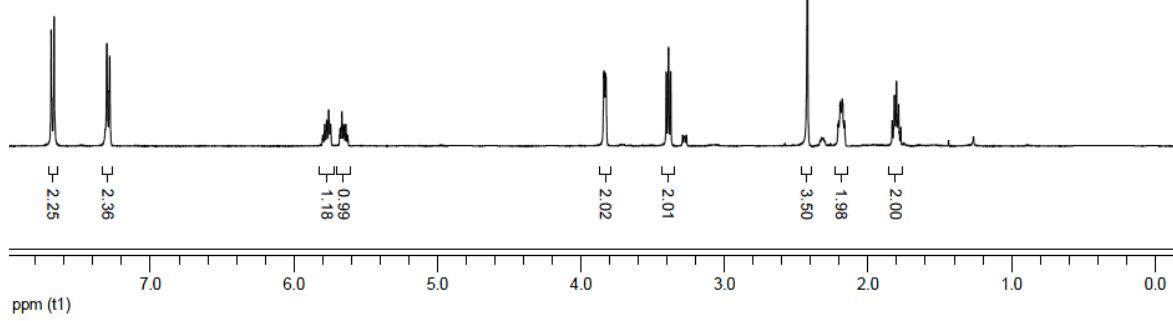
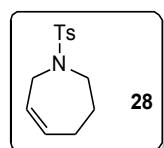
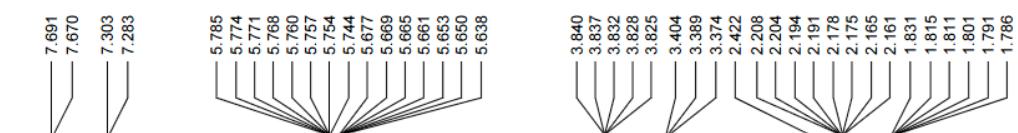
NMR (CDCl_3) of **24**



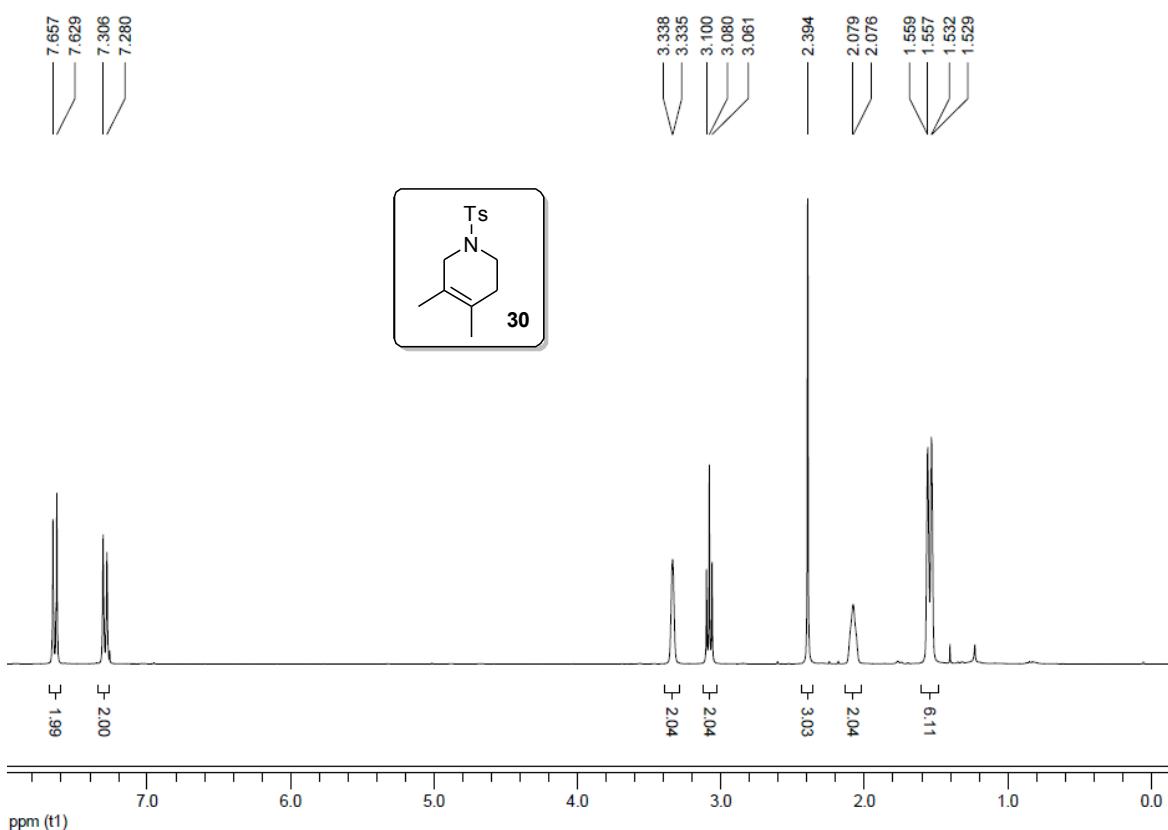
^1H NMR (CDCl_3) of 26



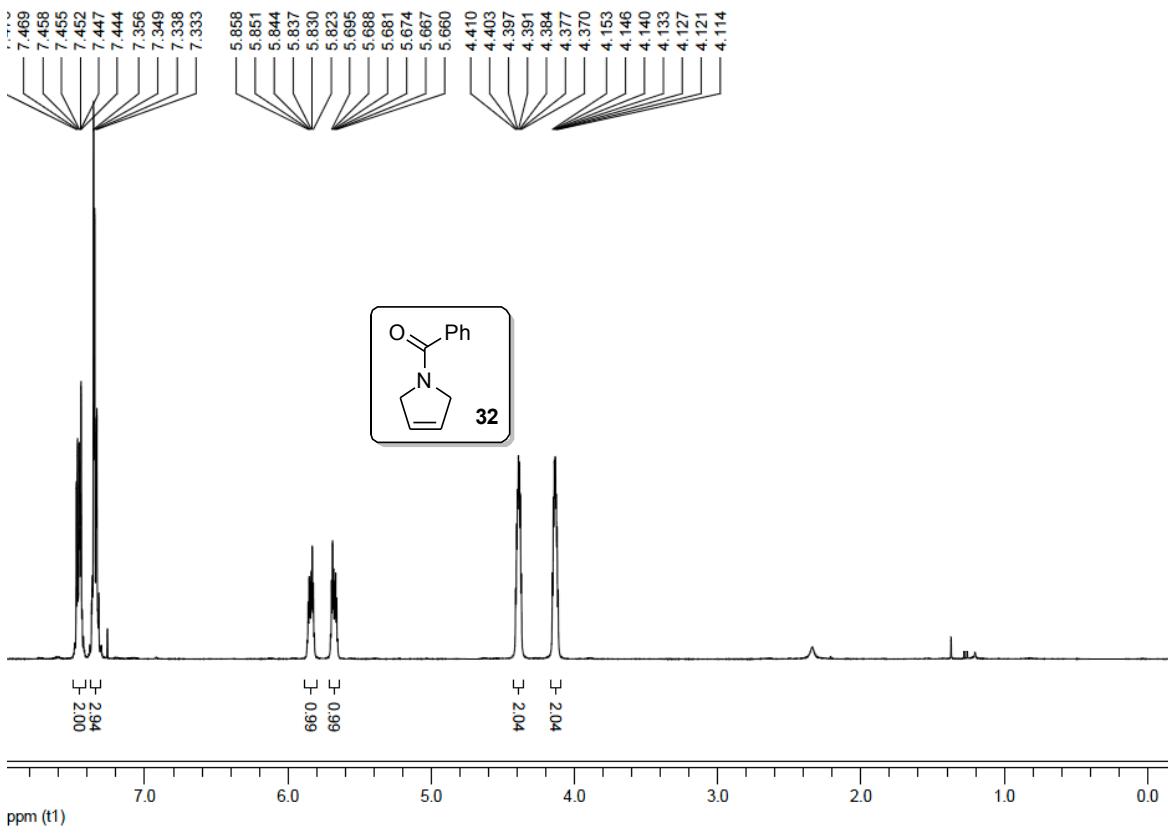
^1H NMR (CDCl_3) of 28



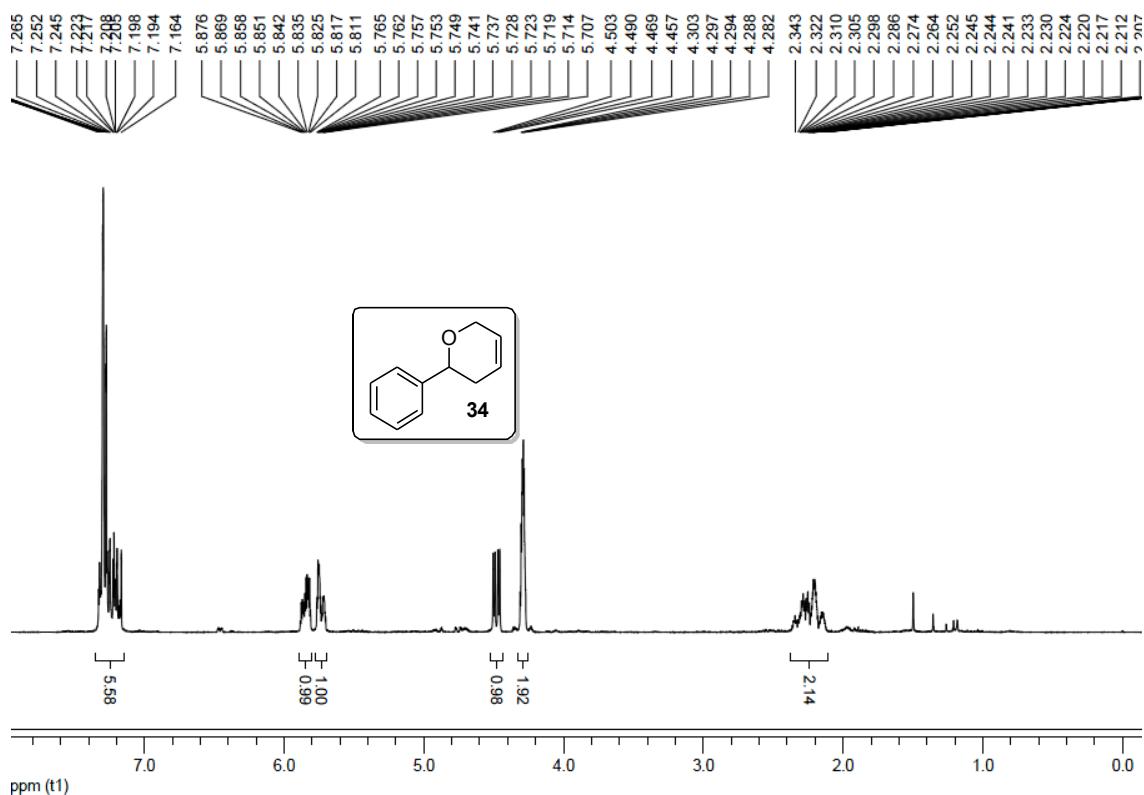
^1H NMR (CDCl_3) of 30



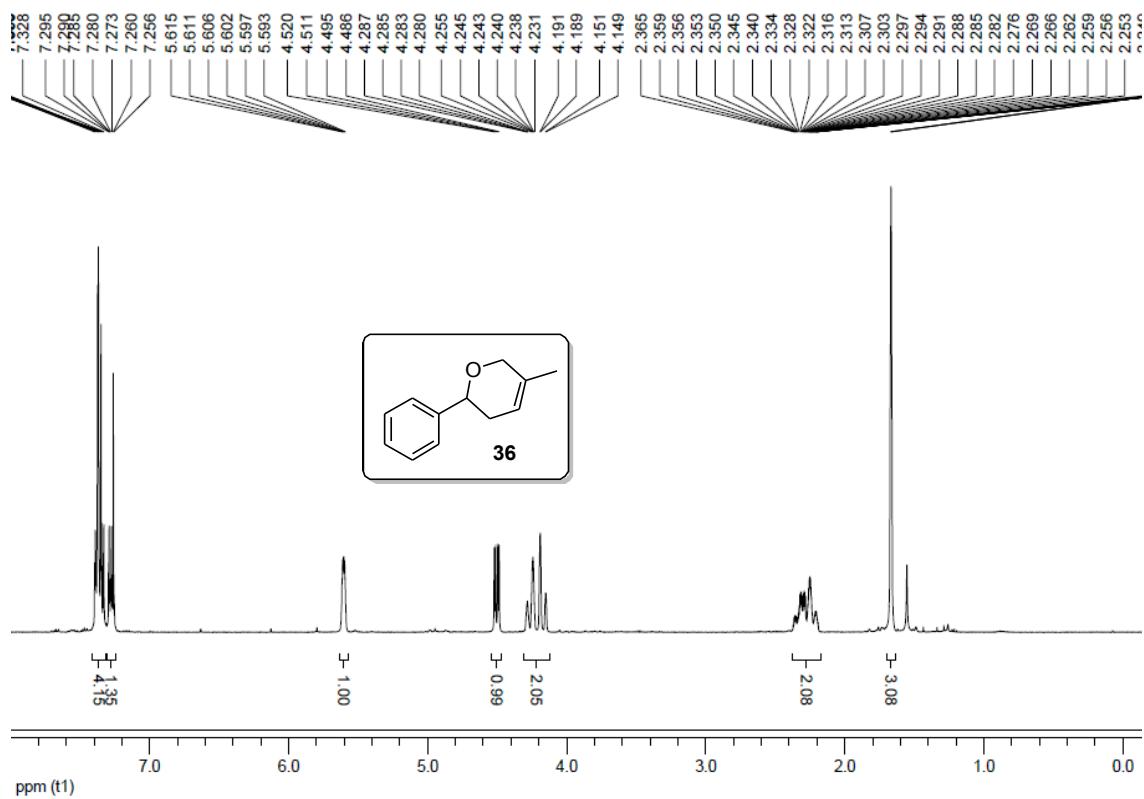
^1H NMR (CDCl_3) of 32



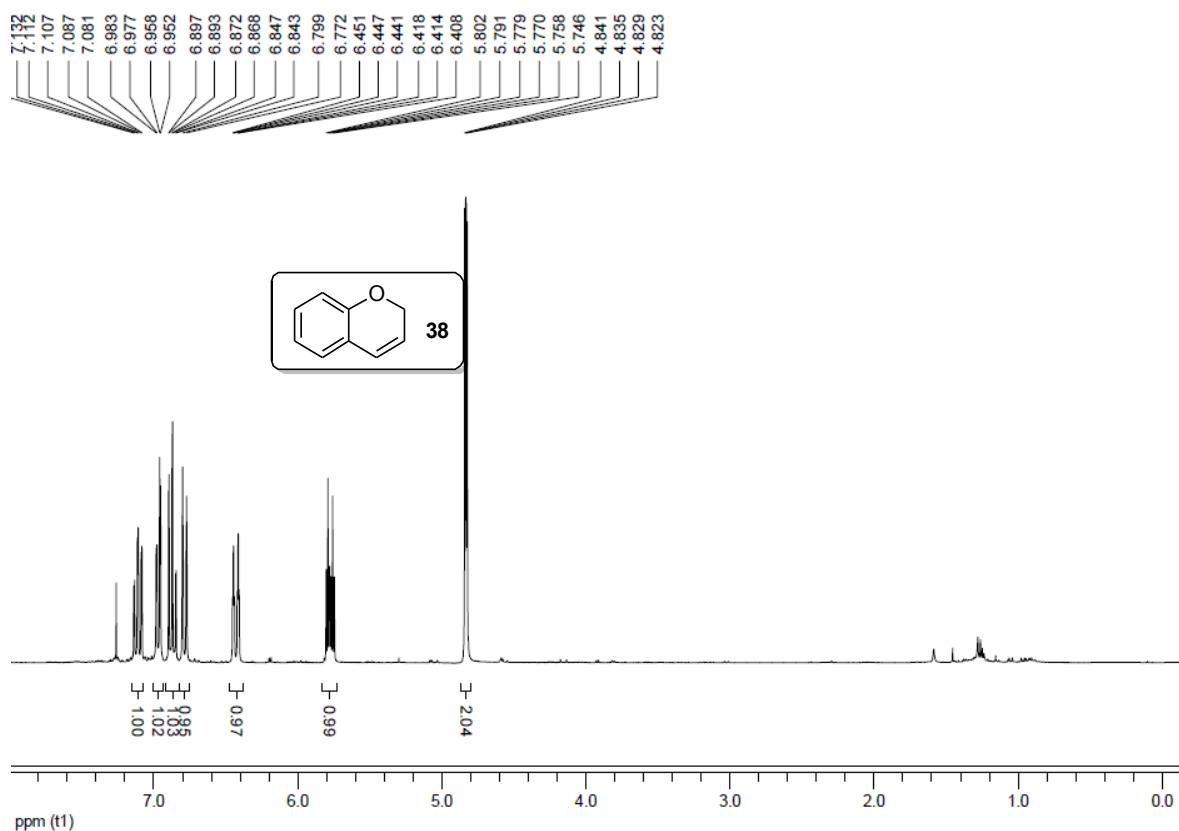
^1H NMR (CDCl_3) of 34



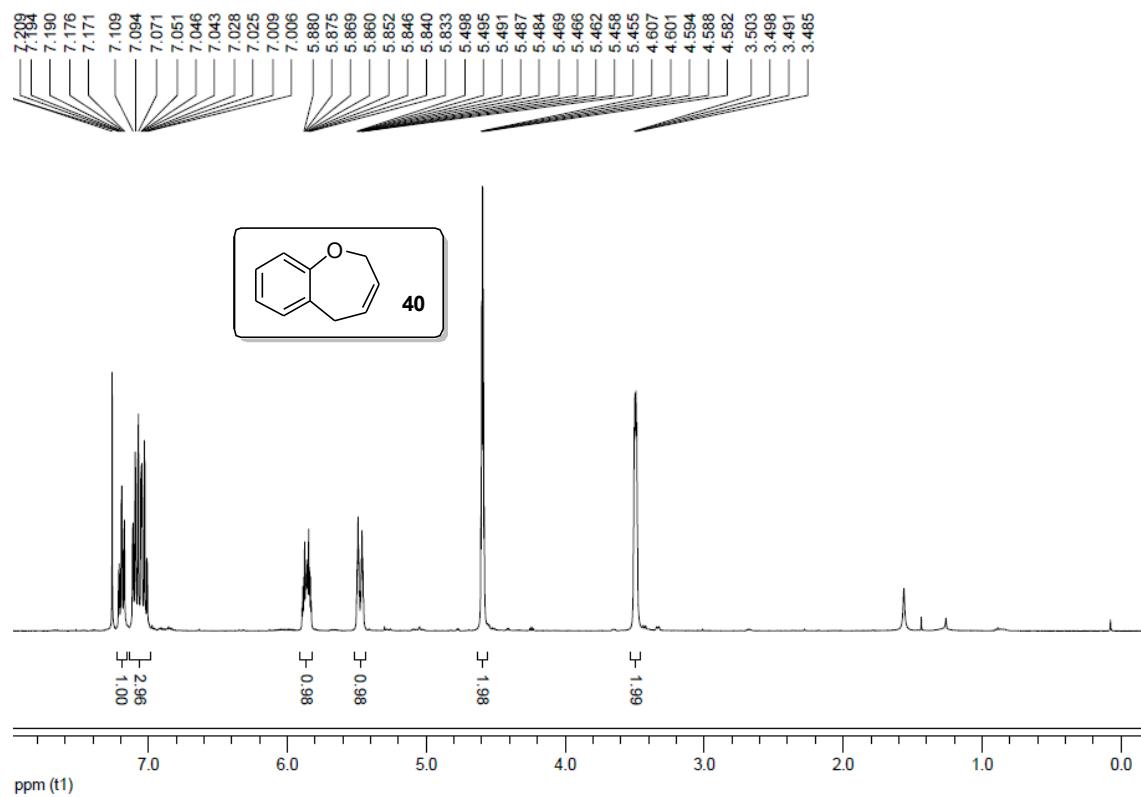
^1H NMR (CDCl_3) of 36



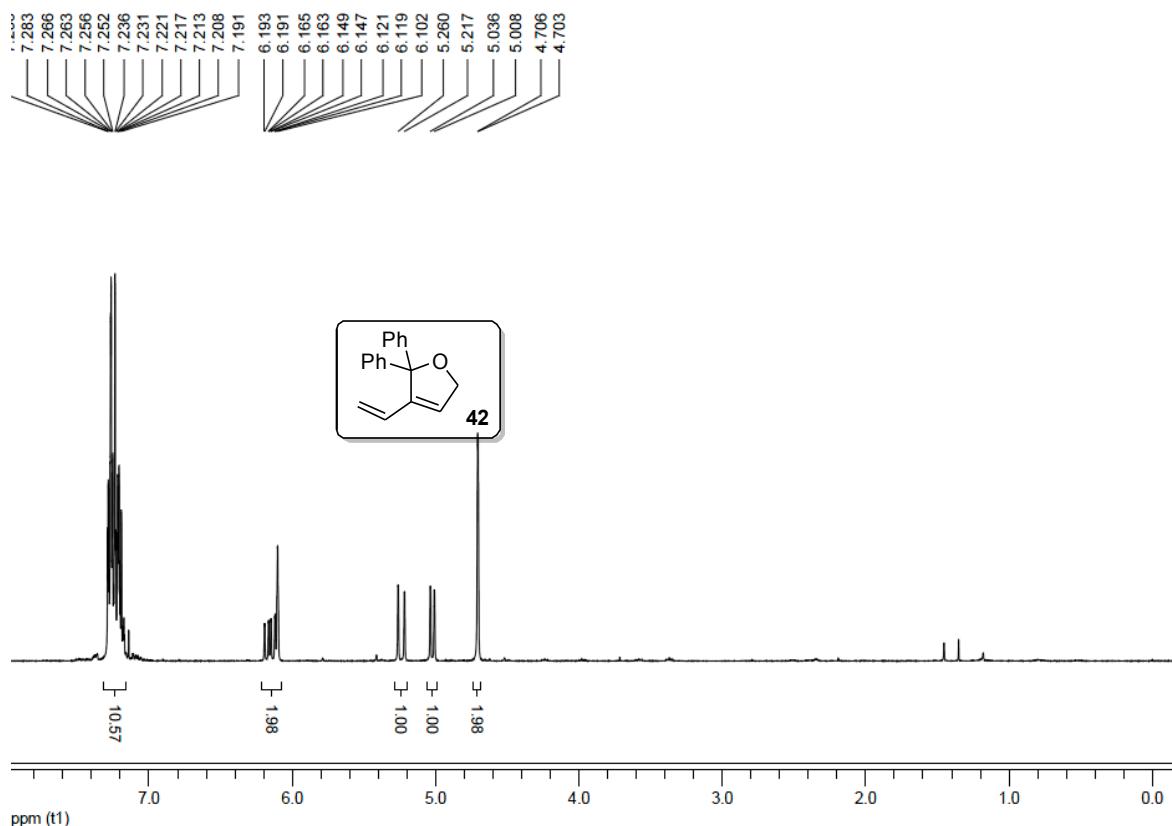
^1H NMR (CDCl_3) of 38



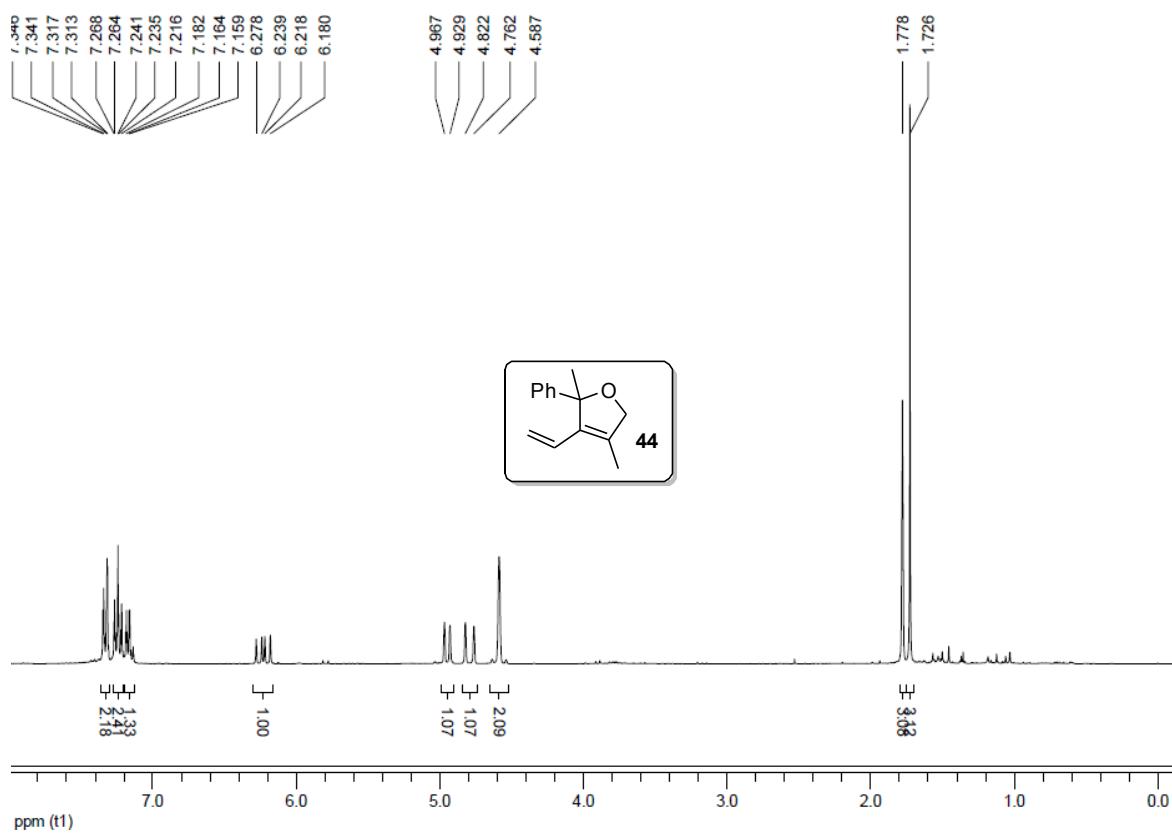
^1H NMR (CDCl_3) of 40



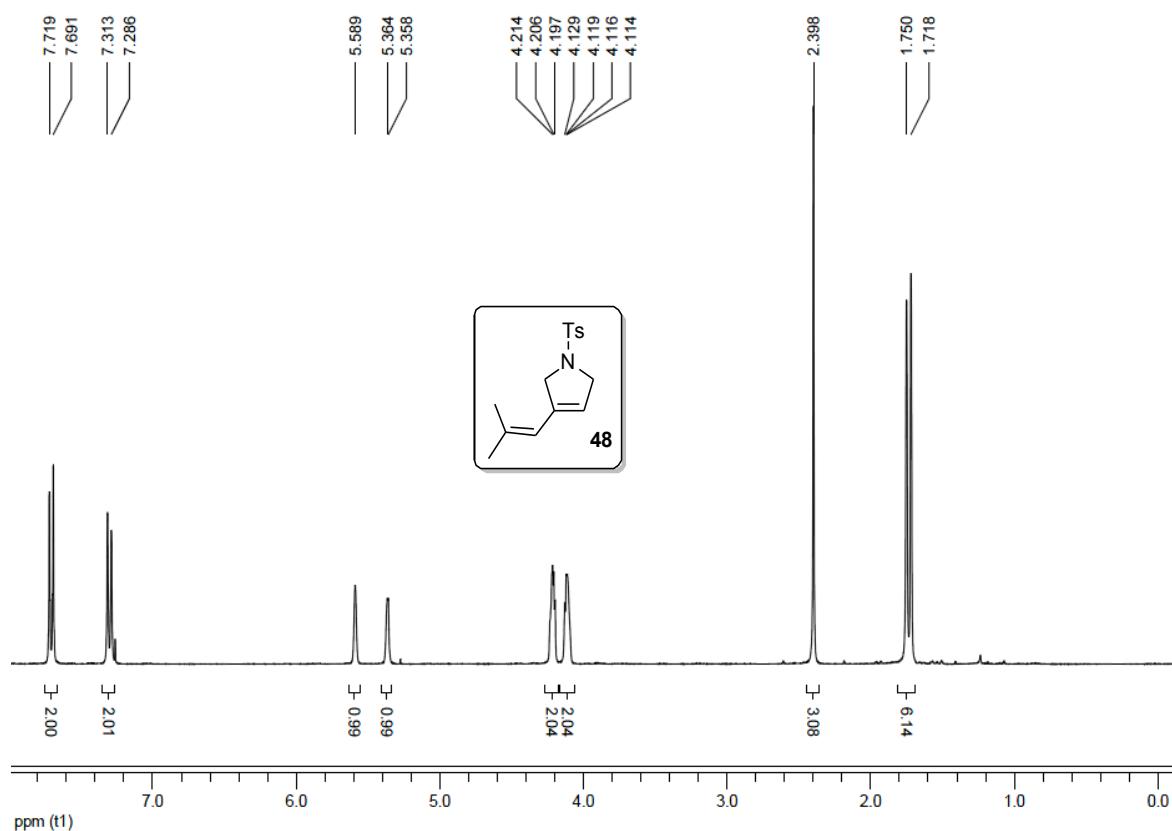
¹H NMR (CDCl_3) of 42



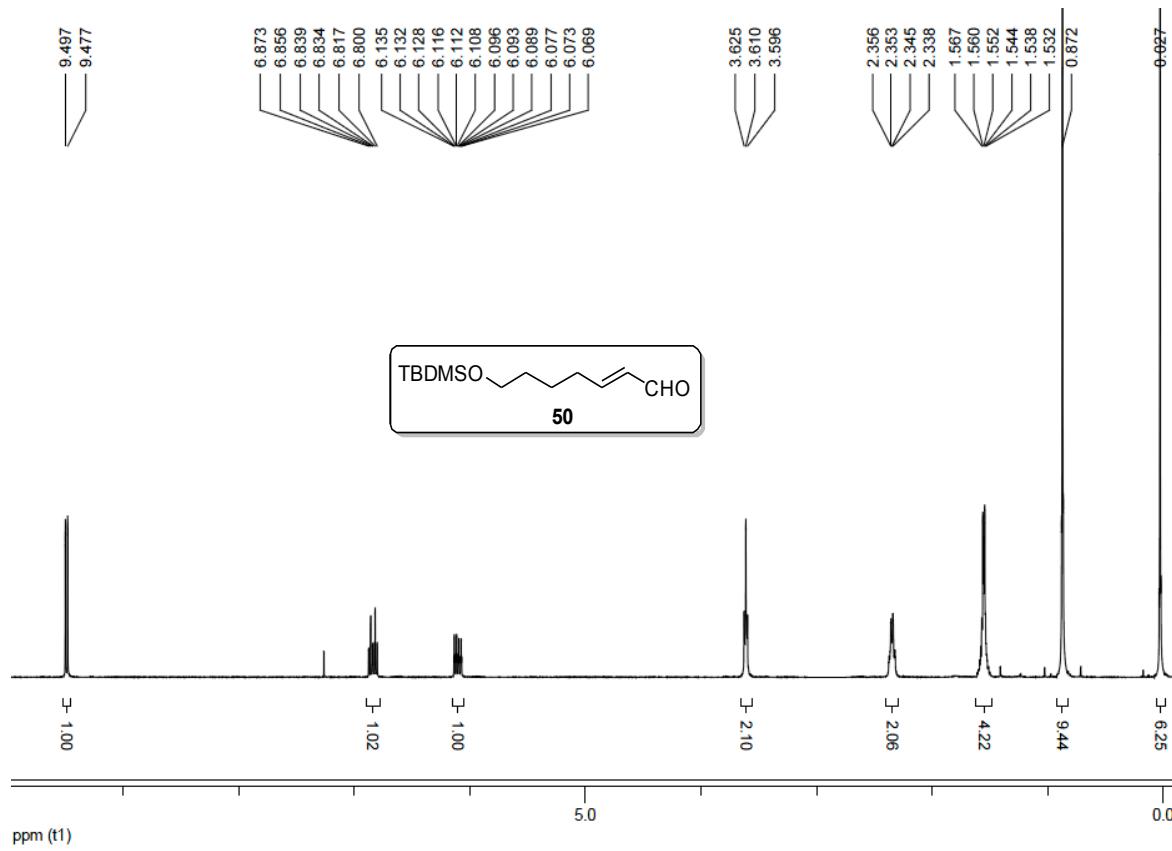
¹H NMR (CDCl_3) of 44



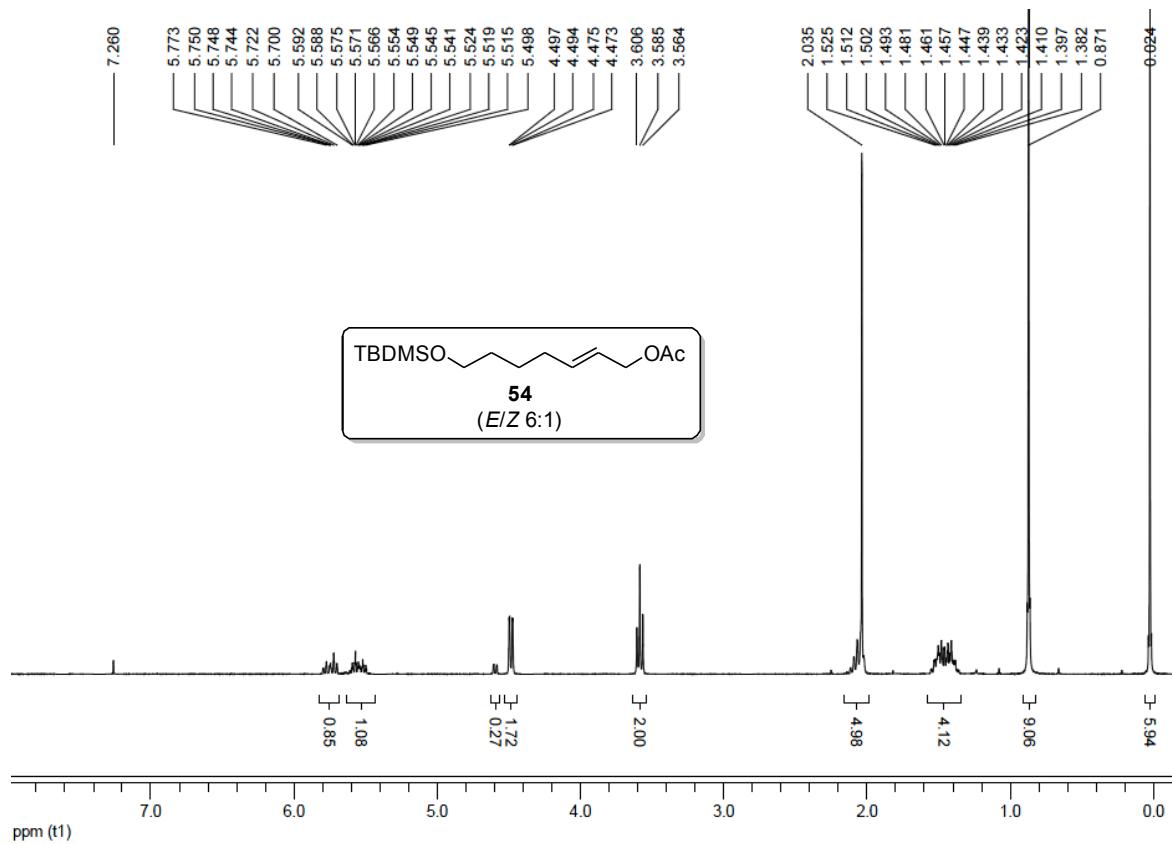
^1H NMR (CDCl_3) of 48



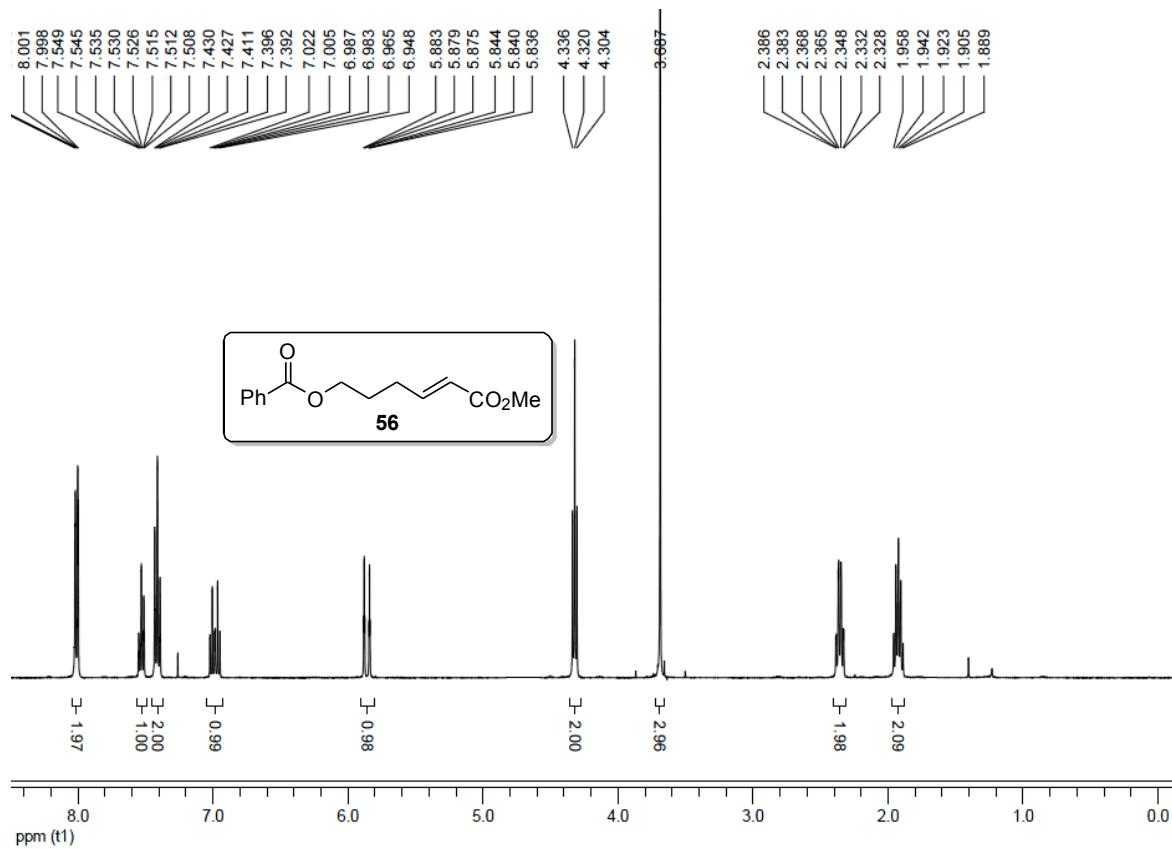
^1H NMR (CDCl_3) of 50



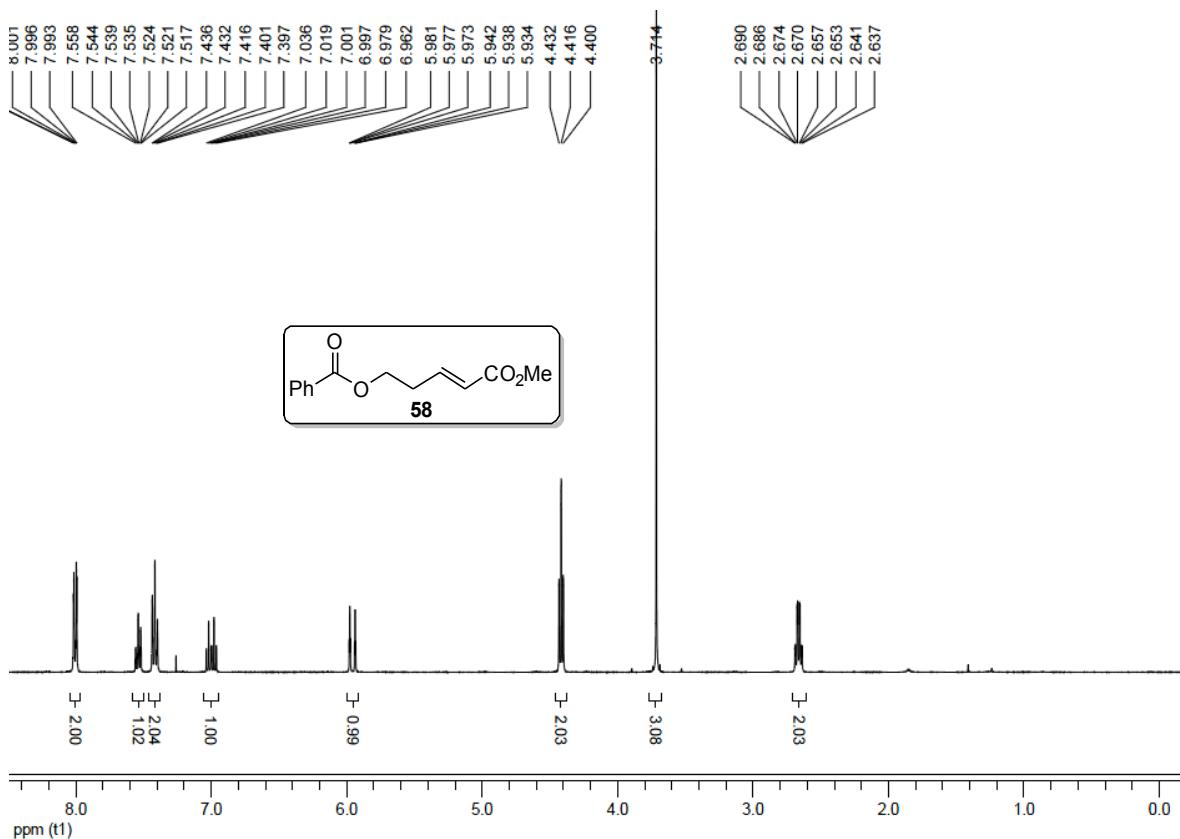
^1H NMR (CDCl_3) of **54** (*E/Z* 6:1)



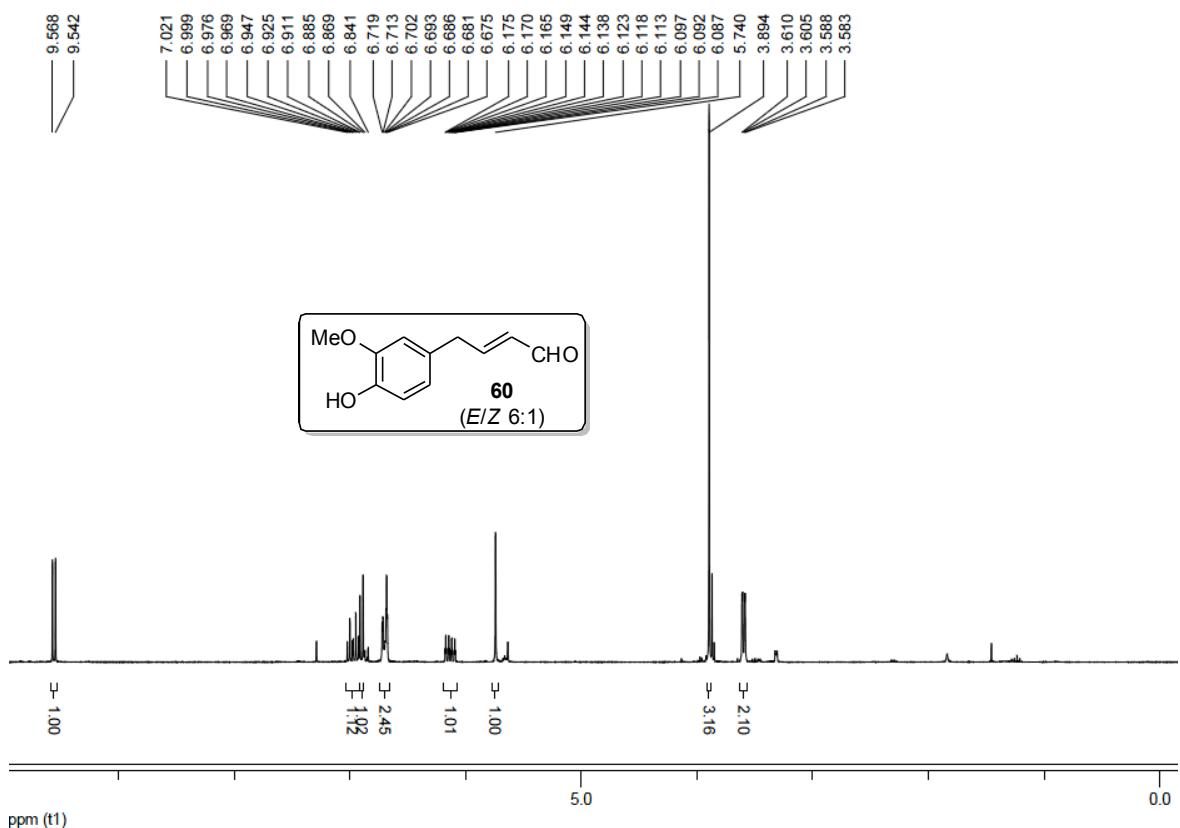
^1H NMR (CDCl_3) of **56** (*E/Z* > 20:1)



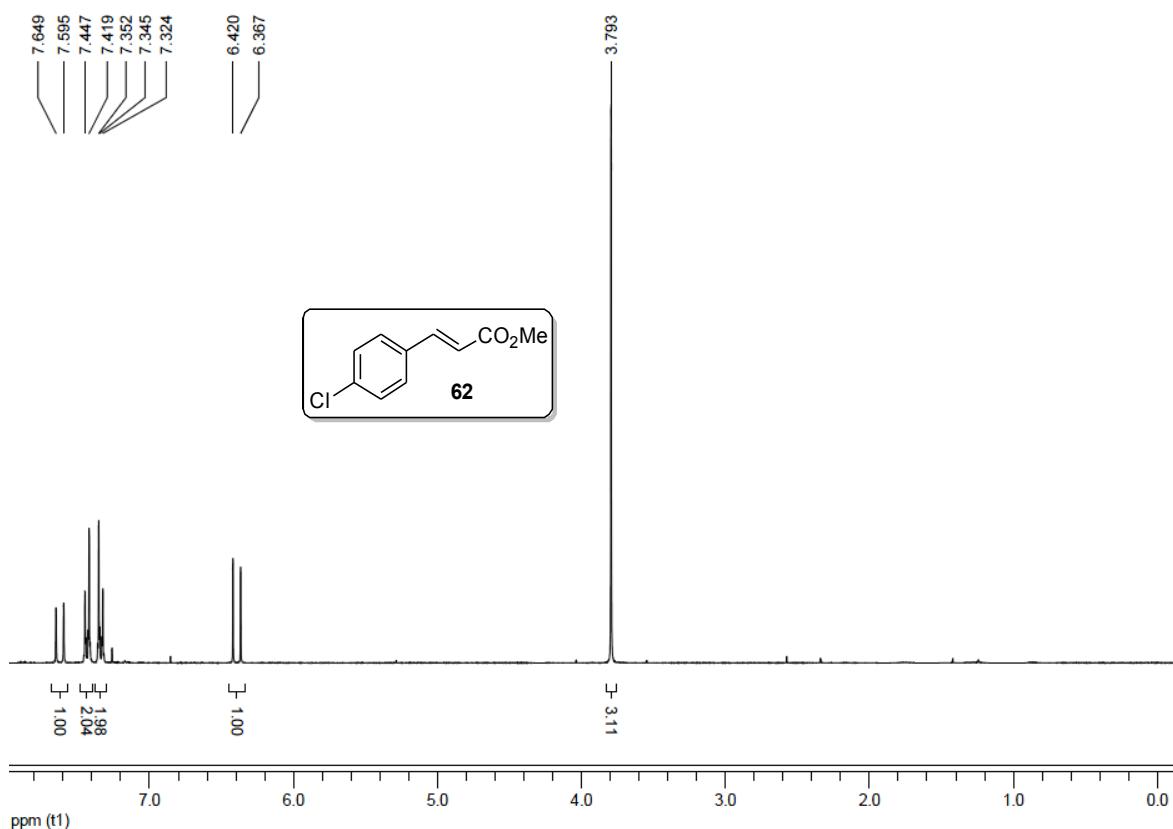
^1H NMR (CDCl_3) of **58** (*E/Z* > 20:1)



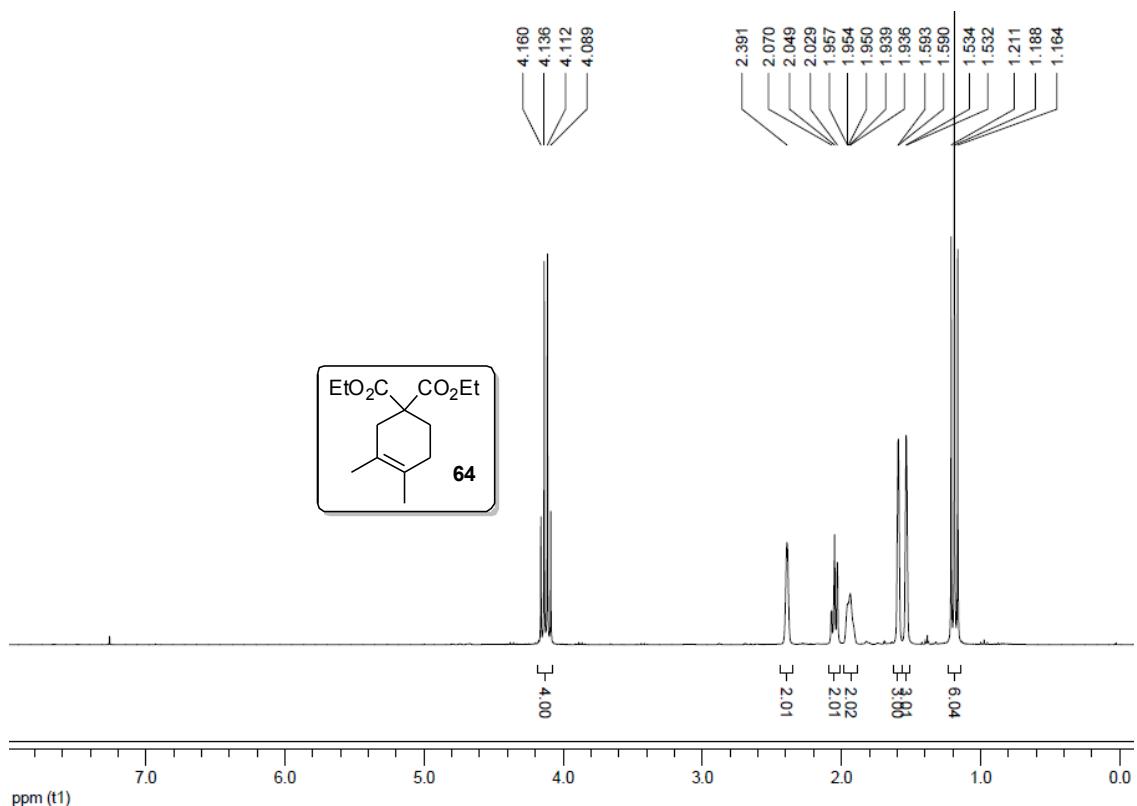
^1H NMR (CDCl_3) of **60** (*E/Z* 6:1)



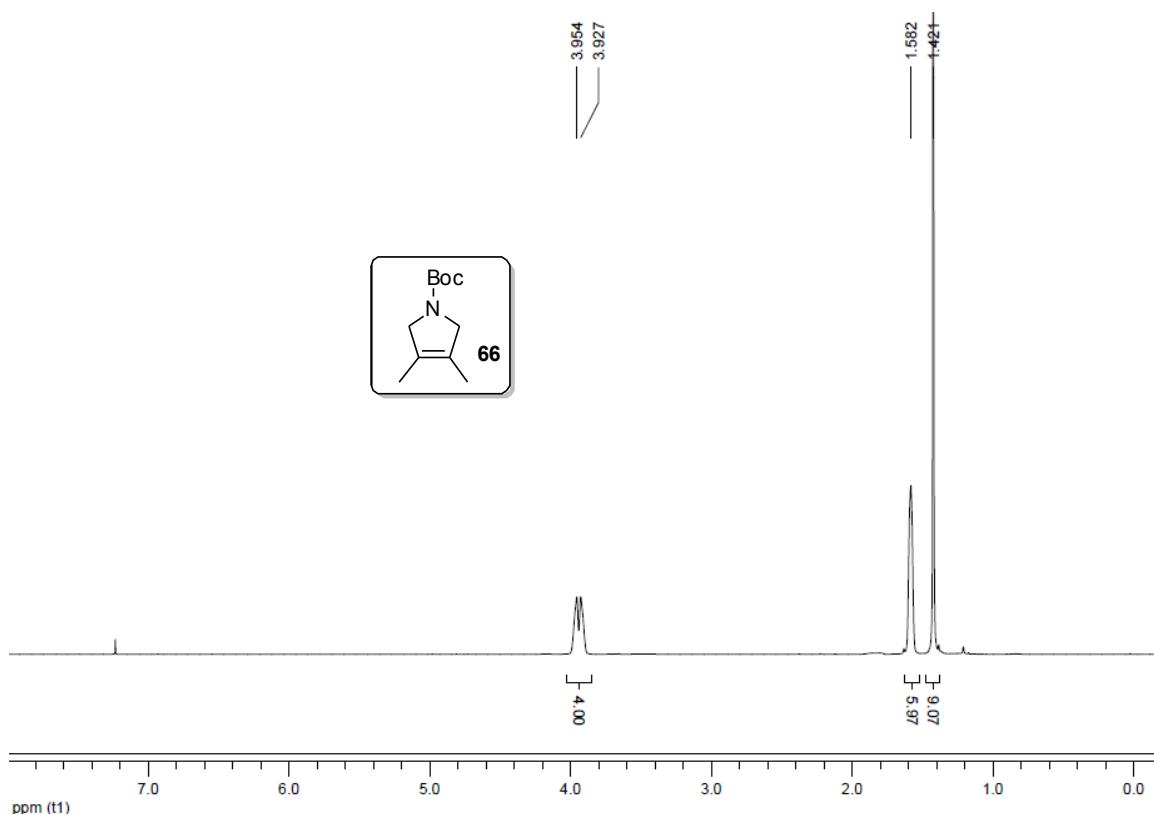
^1H NMR (CDCl_3) of 62 ($E/Z > 20:1$)



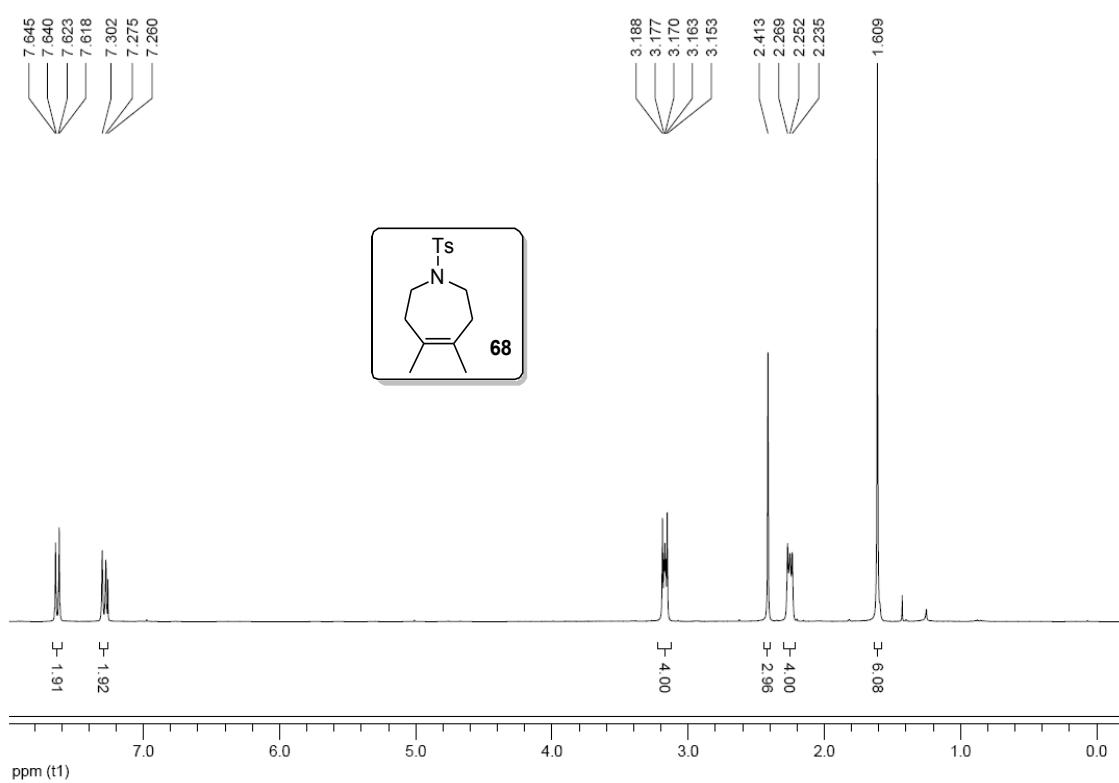
^1H NMR (CDCl_3) of 64



^1H NMR (CDCl_3) of 66



^1H NMR (CDCl_3) of 68



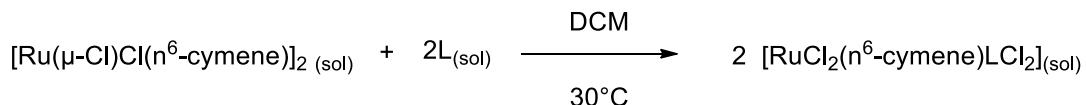
10. Calorimetric studies

Procedure for calorimetric experiments.

Two solutions containing separately the complex and the ligand were prepared: stock solution **A** containing 30 mg (0.048 mmol) of $[\text{Ru}(\mu\text{-Cl})\text{Cl}(\eta^6\text{-cymene})]_2$ in CH_2Cl_2 (0.75 mL) and stock solution **B** containing the ligand **L** (0.293 mmol, 6 eq) in CH_2Cl_2 (2 mL). The first container of the cell was charged with stock solution **B** (0.75 mL) and the second container with stock solution **A** (0.3 mL). The cell was placed in the calorimeter and the temperature stabilised to 30°C. The solutions were then mixed and thermogram recorded. The reported enthalpy of reaction was based on an average of at least 3 measurements.

Equation leading to BDE.

The reaction done in the vessel is described by this equation:



Considering it in term of energy and bond dissociation, we obtain the following equation:

$$2 D(\text{Ru} - \text{Cl}) = 2 D(\text{Ru} - \text{L}) + \Delta H_{rxn}$$

This equation could be modified to isolate and calculate the BDE of the inserted ligand directly from the enthalpy of reaction:

$$2 D(\text{Ru} - \text{L}) = D(\text{Ru} - \text{Cl}) - \Delta H_{rxn}$$

$$D(\text{Ru} - \text{L}) = \frac{D(\text{Ru} - \text{Cl}) - \Delta H_{rxn}}{2}$$

Unfortunately the BDE Ru-Cl for $[\text{Ru}(\mu\text{-Cl})\text{Cl}(\eta^6\text{-cymene})]_2$ is not described in the literature, therefore we were not able to calculate properly the absolute BDE. In order to compare different ligands we decided to deduce only the “relative” BDE. Starting from the previous equation, relative BDE were calculated using this general equation. That gives the value for R-L BDE ($\text{kcal}\cdot\text{mol}^{-1}$):

$$D(\text{Ru} - \text{L}) = \frac{| - \Delta H_{rxn} |}{2}$$

NMR analyses obtained for $[\text{RuCl}_2(\eta^6\text{-cymene})\{\text{P}(\text{O}-\text{C}_6\text{H}_5)_3\}]$,^{30,31} $[\text{RuCl}_2(\eta^6\text{-cymene})\{\text{P}(\text{OMe})_3\}]$,^{29,30} $[\text{RuCl}_2(\eta^6\text{-cymene})\{\text{P}(\text{OEt})_3\}]$ ^{30,32} and $[\text{RuCl}_2(\eta^6\text{-cymene})\{\text{P}(\text{O}^i\text{Pr})_3\}]$ ³³ were similar to literature data.

Table S2. Calorimetric studies carried out on $[\text{RuCl}_2(p\text{-cymene})]_2$.

Ligand (L)	Complex formed	$-\Delta H_{\text{rxn}}$ (kcal.mol ⁻¹)	Relative BDE (kcal.mol ⁻¹)	TEP ³⁴ (cm ⁻¹)	Cone angle ³³
P(OPh) ₃	$[\text{RuCl}_2(\eta^6\text{-cymene})\{\text{P}(\text{OPh})_3\}]$	34.1 ± 0.4	17.05	2085.3	128
P(OMe) ₃	$[\text{RuCl}_2(\eta^6\text{-cymene})]\{\text{P}(\text{OMe})_3\}]$	42.8 ± 0.6	21.40	2079.5	107
P(OEt) ₃	$[\text{RuCl}_2(\eta^6\text{-cymene})]\{\text{P}(\text{OEt})_3\}]$	42.9 ± 0.5	21.45	2077.0	110
P(O <i>i</i> Pr) ₃	$[\text{RuCl}_2(\eta^6\text{-cymene})]\{\text{P}(\text{O}^i\text{Pr})_3\}]$	43.2 ± 0.4	21.60	2075.9	130

11. DFT Calculations

DFT static calculations were performed at the GGA level with the Gaussian09 package,³⁵ using the BP86 functional of Becke and Perdew.³⁶ The electronic configuration of the molecular systems was described with the standard split-valence basis set with a polarization function of Ahlrichs and co-workers for H, C, N, O, P, and Cl (SVP keyword in Gaussian09),³⁷ For Ru we used the small-core, quasi-relativistic Stuttgart/Dresden effective core potential, with an associated (8s7p6d)/[6s5p3d] valence basis set contracted according to a (311111/22111/411) scheme (standard SDD keywords in gaussian09).³⁸ The geometry optimizations were performed without symmetry constraints, and the characterization of the located stationary points was performed by analytical frequency calculations. Solvent effects including contributions of non electrostatic terms have been estimated in single point calculations on the gas phase optimized structures with triple zeta valence plus polarization (TZVP keyword in Gaussian), based on the polarizable continuous solvation model PCM,

using toluene and nitromethane as the solvents,³⁹ employing the BP86 and M06 functionals.^{36,40}

Table S3. xyz coordinate data sets for DFT (SIMes)(Cl₂)(L)Ru=Indenylidene complexes optimized complexes.

L=/	L=P(OMe) ₃ in cis	L=P(OMe) ₃ in trans
<p>Ru 1.053578 0.892545 -0.230047 Cl 1.515637 1.688459 1.893612 Cl 1.602025 1.237545 -2.470795 N 0.706643 -2.102000 -0.752613 N 2.758075 -1.424595 -0.245192 C -1.067381 3.280483 -1.618861 C -1.968166 4.314469 -1.966420 C -0.808114 1.060643 -0.202937 C -3.726731 3.283758 -0.606772 C 3.844938 -0.680153 0.340770 C -3.002992 1.053677 0.599709 C 1.552641 -3.280922 -1.041350 C -2.745937 -2.272860 -2.210040 C -4.209124 0.672962 1.352242 C 5.898139 0.592462 0.117356 C -1.502222 2.256910 -0.766418 C -2.847951 2.245564 -0.273812 C -2.796875 -3.106829 0.055141 C -5.507808 0.824949 0.798604 C 4.793613 -0.248511 -1.999440 C -1.363464 -2.007011 -2.119039 C 6.019438 0.696293 1.515823 C -0.613683 -1.470789 -3.313330 C -4.100941 0.113132 0.2652400 C 2.943391 -2.855708 -0.542958 C 3.971943 -0.652383 1.756820 C 4.835368 -0.101622 -0.497243 C 5.055973 0.048308 2.314944 C 1.445809 -1.010795 -0.357569 C -6.647925 0.428906 1.515882 C -0.715857 -2.272251 -0.886208 C -0.723900 -3.171629 1.507530 C -1.421934 -2.849244 0.204262 C -1.795515 0.369545 0.608655 C -4.971994 -3.052379 -1.254805 C 2.979438 -1.359712 2.649412 C -3.483837 -2.813035 -1.140247 C 5.242042 -0.274628 3.369190 C -3.276506 4.319841 -1.460116 C 6.521995 -0.119133 2.804934 C 7.142518 1.488215 2.146261 C 3.260897 -3.403802 0.372822 H 3.734671 -2.999064 -1.308256 H 1.161051 -4.179835 -0.521175 H 1.538530 -3.495434 -2.132962 H 3.826877 0.099777 -2.418490 H 5.607898 0.333716 -2.473410 H 4.924758 -1.309137 2.308423 H 1.983027 -0.875309 2.589659 H 2.853427 -2.427099 2.368734 H 3.307366 -1.325694 3.706529 H 7.490390 1.024385 3.092027 H 8.012194 1.582733 1.465263 H 6.805856 2.518725 2.395505 H -1.279972 -1.395119 4.194645 H -0.180506 -0.468537 -3.114932 H 0.239126 -2.126396 -3.592481 H -1.456509 -3.451576 2.289578 H -0.016986 -4.024256 1.402720 H -0.128103 -2.313946 1.883977 H -5.538867 -2.247399 -0.737819 H -5.305301 -3.068630 2.311729 H -5.269568 -4.011423 -0.782486 H -3.350493 -3.540633 0.904728 H -3.258680 -2.055348 -3.161993 H 6.662301 1.059144 -0.526712 H 5.150178 0.086596 3.413117 H -0.041735 3.273160 -2.018027 H -1.633191 5.124504 -2.633239 H -3.964515 5.138181 -1.726231 H -4.751079 3.312362 -0.204921 H -5.617574 1.225003 -0.220596 H -7.645025 0.546919 1.061838 H -7.418383 -0.420719 3.369776 H -5.133447 -0.693165 4.382683 H -3.103811 0.014641 3.109405 H -1.597411 -0.538350 1.184735 </p> <p>Ru 0.894219 -0.245852 0.918547 Cl 1.693749 -1.853234 2.506296 Cl 1.169486 1.381612 2.699859 P 1.107535 -1.870240 -0.628786 O 2.621958 -2.327113 -1.100590 O 0.523539 -1.553448 -2.156738 O 0.502037 -3.384680 -0.345576 N 0.319922 2.399265 -0.657137 N 2.451820 1.832069 -0.539649 C -1.531307 -0.306311 3.460351 C -2.554663 -0.460952 4.425991 C -0.995325 -0.421384 0.871047 C -4.190408 -0.924759 2.667082 C 3.683822 1.073841 -0.549489 C -3.204336 -0.905740 0.225452 C 1.023149 3.600917 -1.164172 C -3.288478 3.154914 0.029818 C 4.368649 -1.221789 -0.616021 C 5.834086 0.471967 0.406631 C -1.850650 -0.426839 2.102087 C -3.192096 -0.736479 1.703108 C -3.091449 2.150474 -2.156148 C -5.678868 -0.785874 -0.284226 C 4.378650 0.044701 1.730425 C -1.898554 0.3038119 0.247224 C 0.633897 -2.534326 -3.204848 C 6.175831 -0.272592 -0.737265 C -1.280905 3.614039 1.497176 C -4.206849 -1.978783 -1.807537 C 2.505828 3.232628 -1.010219 C 4.032038 0.393461 -1.749804 C 4.616290 1.176093 0.521392 C 5.266905 -0.278497 -1.812677 C 1.173365 1.401466 -0.279311 C -6.774917 -0.974671 -1.104781 C -1.117671 2.421641 -0.762951 C -0.865193 3.398543 -3.092617 C -1.704574 1.995042 -1.987152 C -1.903335 -0.745204 -0.226087 C 3.500896 -3.083652 -0.252491 C 5.395198 2.871616 -1.370566 C 3.128162 0.418791 -2.959441 C -3.905922 2.724461 -1.158100 C -5.302126 -2.290491 -2.624325 C -3.864843 -0.769877 4.036461 C -0.510065 -3.270793 0.613817 C -6.594266 -1.853409 -2.276310 C 7.477430 -1.039297 -0.809488 C 3.074710 2.298209 -1.961780 C 3.027365 3.866657 -0.261629 C 0.729457 3.801845 -2.217788 C 0.735200 4.487221 -0.561869 C 3.463130 1.748334 2.284841 C 5.243653 1.998122 2.420376 C 4.239213 3.109716 1.443962 C 2.130777 -0.010267 -2.741012 C 2.966075 1.455119 -3.328385 C 3.574299 -1.601019 -3.791612 C 7.836590 -1.141349 -1.853816 C 8.275227 -0.549699 -0.214837 C 7.356810 -2.068149 -0.403303 C -2.042138 3.733430 2.293122 C -0.458717 2.980397 1.886627 C -0.859702 4.626361 1.300644 C -1.492561 1.152102 -3.971887 C -0.073456 2.098415 -3.437576 C -0.348817 0.473126 -2.762027 C -5.902446 1.883802 -1.314909 C -5.855459 3.531420 -0.608184 C -5.622449 3.292056 -2.372746 C -3.550041 1.818007 -3.102644 C -3.902468 3.622849 0.817621 C 6.550755 0.534405 1.242644 C 5.527917 -0.814031 -2.741002 C 3.057462 -4.073950 -0.018824 C 4.440142 -3.218835 -0.822808 C 3.708740 -2.545469 0.694859 </p> <p>Ru -0.787960 0.362251 0.085006 Cl -0.620883 0.905096 -2.270763 Cl -1.597208 -0.041029 2.326902 P -0.997438 2.641538 0.498221 O -2.538371 3.202078 0.332792 O -0.228822 3.640014 -0.545968 O -0.674085 3.304862 1.985025 N -0.499038 -2.556821 -1.038569 N -2.580534 -1.8355840 -1.042630 C 1.585759 -0.871872 2.619440 C 2.606783 -1.217834 3.538795 C 1.077422 0.446984 0.377035 C 4.283837 -0.121211 2.135886 C -3.793543 -1.115967 -0.737616 C 3.321972 1.024687 -0.028686 C -1.225179 -3.627890 -1.763436 C 2.468531 -3.790512 0.860476 C 4.521797 1.560562 -0.690252 C -5.661335 -0.726206 0.768963 C 1.918780 -0.159798 1.461610 C 3.281541 0.208573 1.215824 C 3.232005 -2.818692 -1.216458 C 5.761139 0.868126 -0.669283 C -3.920335 -2.421516 1.462050 C 1.135829 -3.465186 0.551521 C -0.448700 5.059960 -0.525302 C -6.233238 0.192956 -0.134582 C 0.016332 -3.811314 1.505605 C 4.456532 2.786019 -1.405636 C -2.658415 -3.074480 -1.850382 C -4.383043 -0.260470 -1.706723 C 4.459902 -1.402705 0.488187 C -5.586244 0.395226 -1.366809 C -1.310062 -1.542207 -0.638947 C 6.885840 1.381451 -1.334175 C 0.872511 -2.797089 -0.673130 C 1.624601 -1.841478 -2.919143 C 1.911379 -2.486340 -1.585266 C 2.021393 1.188410 -0.469475 C -3.554376 2.929872 1.314488 C 4.980011 -3.790036 0.380846 C -3.812205 -0.096998 -3.094736 C 3.534072 -3.466059 -0.003805 C 5.582375 3.298557 -2.064170 C 3.937927 -0.848128 3.301198 C 0.435607 2.857612 2.781533 C 6.804332 2.600197 -2.030272 C -7.509611 0.926265 0.213539 C -2.959034 -2.831832 -2.891986 C -3.421590 -3.762738 -1.429286 C -0.765779 -3.796132 -2.759490 C -1.160609 -4.583047 -1.197339 C -3.016205 -2.025094 1.971989 C -4.675231 -2.661745 2.236260 C -3.633747 -3.367884 0.957243 C -2.703827 -0.081324 -3.090413 C -4.154692 -0.924452 -3.756885 C -4.161808 0.848282 -3.554910 C -7.967410 1.399830 -0.677829 C -8.260454 0.245571 0.666440 C -7.319265 1.731517 0.956708 C 0.409943 -4.304870 2.415373 C -0.543752 -2.905055 1.818704 C -0.725061 -4.501340 1.046813 C 2.562612 -1.513517 -3.408384 C 1.125315 -2.554057 -3.613463 C 0.951587 -0.963116 -2.815314 C 5.320468 -3.094030 1.170027 C 5.049025 -4.817104 0.792746 C 5.648980 -3.704840 -0.483245 C 4.049725 -2.568187 -1.912893 C 2.680733 -4.303948 1.813136 C -6.173869 -0.939441 1.722280 C -6.037374 1.076190 -2.108005 C -3.343920 3.482743 2.253358 C -4.509747 3.280878 0.879355 C -3.624172 1.844846 1.538665 </p>		

	H -0.009792 -2.185650 -4.036165 H 1.683051 -2.618825 -3.555222 H 0.288120 -3.527667 -2.854761 H -1.521932 -3.618556 0.170541 H -0.341626 -4.787769 0.886017 H -0.426479 -3.105364 1.528167 H -0.495987 -0.093449 3.763334 H -2.309086 -0.352853 5.494301 H -4.648446 -0.910247 4.798342 H -5.211710 -1.217670 2.380790 H -5.831046 -0.166675 0.611635 H -7.780455 -0.742538 -0.827152 H -7.456312 -2.103388 -2.914883 H -5.149973 -2.889472 -3.536531 H -3.204082 -2.347023 -2.074080 H -1.585832 -0.802642 -1.272762	H 0.380147 5.517476 -1.099681 H -1.415201 5.312065 -1.007392 H -0.440348 5.453565 0.512799 H 1.399395 2.969450 2.240242 H 0.453649 3.502557 3.681826 H 0.296551 1.800339 3.086474 H 0.536798 -1.126528 2.818777 H 2.346120 -1.773730 4.453620 H 4.721520 -1.109610 4.030599 H 5.324155 0.203108 1.980658 H 5.828834 -0.103587 -0.158401 H 7.834112 0.820618 -1.313399 H 7.689351 3.004899 -2.546540 H 5.508929 4.255090 -2.606030 H 3.507795 3.344432 -1.421420 H 1.710321 1.716694 -1.378375
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L=P(OEt) ₃ in <i>cis</i>				L=P(OEt) ₃ in <i>trans</i>			
Ru	-0.814374	-0.163305	0.995220	Ru	-0.718017	0.105077	-0.014045
Cl	-1.006993	-2.071578	2.492818	Cl	-1.559394	-0.165751	2.237344
Cl	-1.639293	1.110620	2.852262	Cl	-0.527248	0.491412	-2.402607
P	-1.143998	1.694413	-0.247720	P	-1.030267	2.406714	0.194797
O	-2.691722	2.121458	-0.621980	O	-2.568440	2.864698	-0.168389
O	-0.556318	1.712673	-1.806630	O	-0.195290	3.351701	-0.846761
O	-0.640955	3.166856	0.322633	O	-0.894741	3.188864	1.652406
N	-0.137372	-2.525672	-0.938297	N	-0.299907	-2.868922	-0.914534
N	-2.291244	-2.076660	-0.744754	N	-2.406008	-2.232722	-1.028444
C	-2.278311	-3.443118	-1.309545	C	-2.408130	-3.525471	-1.752701
C	1.062140	0.110370	0.953031	C	1.137807	0.268385	0.303665
C	6.550789	2.237520	-1.989447	C	6.836717	2.444237	-2.149650
C	3.237374	0.792073	0.372733	C	3.370877	0.887233	-0.105186
C	3.258666	0.385016	1.802505	C	3.331543	0.169751	1.198322
C	1.649142	-0.397576	3.483058	C	1.645274	-0.848530	2.656323
C	5.242618	2.695146	-2.235813	C	5.592021	3.093654	-2.254036
C	-3.556265	-1.382635	-0.676728	C	-3.663394	-1.567165	-0.787624
C	-4.236147	-2.686443	1.433752	C	-3.739728	-2.722457	1.495164
C	-4.495808	-1.667644	0.351449	C	-4.334031	-1.818066	0.443639
C	4.265074	0.460787	2.773192	C	4.325863	-0.054671	2.157838
C	5.701957	0.830557	-0.187633	C	5.827217	0.773674	-0.689671
C	-1.031505	-1.622477	-0.434602	C	-1.159624	-1.859922	-0.612719
C	0.412562	3.405879	1.286454	C	0.207008	2.944929	2.559045
C	-5.750845	-1.023189	0.299896	C	-5.590731	-1.220279	0.653445
C	6.117489	-0.160818	-0.749374	C	-6.211318	-0.415937	-0.324151
C	5.188847	0.040159	-1.790099	C	-5.549365	-0.243627	-1.553670
C	-7.464567	0.527000	-0.760148	C	-7.552166	0.230775	-0.055272
C	1.297131	-2.462019	-1.063154	C	1.076278	-3.020040	-0.520097
C	-0.794859	-3.658428	-1.631452	C	-0.967271	-4.025364	-1.559479
C	-3.637921	2.634565	0.353115	C	-3.692806	2.532446	0.693591
C	-4.114822	4.012957	-0.080886	C	-4.256753	3.795065	1.329234
C	2.118869	-3.198758	-0.172845	C	1.357196	-3.580719	0.753716
C	3.508244	-3.221605	-0.420589	C	2.700305	3.821284	1.093820
C	4.088702	-2.577543	-1.528120	C	3.758329	-3.518995	0.212277
C	4.375838	1.282305	-0.419493	C	4.565223	1.417429	-0.781324
C	6.773082	1.301867	-0.963645	C	6.946547	1.280352	-1.368734
C	3.235920	-1.883511	-2.410928	C	3.439169	-2.981909	-1.048918
C	1.846257	-1.818254	-2.206520	C	2.108649	-2.737028	-1.448655
C	1.939438	-0.046111	2.159020	C	1.975942	-0.221391	1.449916
C	1.543220	-3.983767	0.979311	C	0.245552	-3.906577	1.724305
C	5.577966	-2.635296	-1.781120	C	5.193077	-3.752986	0.628041
C	0.966729	-1.087563	3.194042	C	1.804759	-2.213387	-2.830890
C	3.969977	0.074611	4.103247	C	3.981124	-0.699505	3.370738
C	2.681143	-0.352025	4.451034	C	2.657450	-1.090450	3.615613
C	-0.769138	2.867038	-2.661892	C	-0.495177	4.760213	-1.008394
C	0.126103	2.479613	-3.884997	C	0.695461	5.432398	-1.672458
C	0.177403	4.768741	1.918626	C	-0.291994	3.060722	3.990151
C	4.172244	2.225233	-1.462552	C	4.471595	2.586880	-1.581874
C	1.936335	0.652977	-0.084978	C	2.075750	0.970156	-0.581950
C	-3.918083	-0.563436	-1.783281	C	-4.290015	-0.822761	-1.822922
C	-2.985432	-0.374116	-2.955322	C	-3.690740	-0.698056	-3.202927
H	-4.450044	-3.713721	1.061232	H	-3.376963	-3.678464	1.062328
H	-3.187385	-2.664588	1.793147	H	-2.873753	-2.226398	1.985418
H	-4.902053	-2.513708	2.302194	H	-4.488259	-2.962040	2.275737
H	-2.665038	-1.347088	-3.386060	H	-3.900967	-1.610155	-3.806146
H	-3.481228	0.201953	-3.761028	H	-4.136211	0.157037	-3.748736
H	-2.063965	0.168472	-2.662976	H	-2.592211	-0.547358	-3.167603
H	0.174289	-1.744602	-3.612835	H	1.326739	-2.994857	-3.463458
H	0.446236	-0.225584	-2.726517	H	1.105698	-1.349854	-2.798931
H	1.565509	-0.707029	-4.044812	H	2.733201	-1.899787	-3.347092
H	2.343449	-4.313392	1.670529	H	0.655345	-4.262788	2.689467
H	0.794212	-3.396479	1.550920	H	-0.392505	-3.020564	1.925051
H	1.025432	-4.901884	0.619863	H	-0.425550	-4.704104	1.336166
H	-8.238519	-0.080706	-0.248829	H	-8.251600	-0.473710	0.441260
H	-7.419025	1.504959	-0.231526	H	-7.446258	1.106702	0.621873
H	-7.811838	0.732304	-1.793225	H	-8.029702	0.589769	-0.988798
H	-5.464928	0.678363	-2.646285	H	-6.033279	0.347629	-2.349249
H	-6.474153	-1.229982	1.106608	H	-6.108619	-1.406835	1.609432
H	6.087261	-3.320608	-1.074516	H	5.330933	-4.762302	1.069882
H	5.800077	-2.980507	2.813179	H	5.890866	-3.654539	-0.227441
H	6.039228	-1.630014	-1.672243	H	5.501280	-3.017576	1.403120
H	3.664278	-1.380901	-3.294398	H	4.250841	-2.751392	-1.759088
H	4.153428	-3.784851	0.274434	H	2.926793	-4.247075	2.085529
H	-0.109812	1.841933	-4.476647	H	0.913971	4.965684	-2.654347
H	-0.020123	3.632885	4.541171	H	0.477971	6.507833	-1.840124
H	1.197168	2.707696	-3.599718	H	1.602760	5.357157	-1.038838
H	-0.542865	3.788455	-2.084423	H	-0.710125	5.210312	-0.014476
H	-3.269563	4.730116	-0.102480	H	-3.506070	4.268770	1.992616
H	-4.575761	3.981697	-1.090020	H	-4.559713	4.530770	0.555667
H	-4.875359	4.393455	0.633220	H	-5.152224	3.546114	1.937180
H	0.992021	4.993078	2.638117	H	0.552763	2.919609	4.696071
H	0.159162	5.572848	1.154121	H	-0.739465	4.058212	4.179905
H	-0.784528	-4.782902	2.469680	H	-1.052230	2.280393	4.193150
H	0.393406	2.609423	0.2058910	H	0.628621	1.934373	2.373051
H	-3.168771	2.662653	1.357985	H	-3.376369	1.796818	1.463828
H	0.629560	-0.704385	3.757134	H	0.599807	-1.119589	2.860150
H	2.458981	-0.641433	5.490344	H	2.396208	-1.580370	4.567214
H	4.759565	0.126700	4.870076	H	4.758932	-0.878373	4.130687
H	5.267270	0.842254	2.525733	H	5.358652	0.289042	1.994148
H	5.885775	0.073890	0.588887	H	5.918929	-0.156727	-0.110057
H	7.791993	0.931279	-0.767056	H	7.913378	0.757405	-1.291569
H	7.393164	2.611298	-2.592853	H	7.717453	2.844346	-2.676731
H	5.057933	3.433828	-3.032245	H	5.496142	4.007403	-2.862192
H	3.156256	2.608813	-1.644484	H	3.503978	3.107093	-1.653513
H	1.602841	0.866163	-1.106073	H	1.766147	1.420256	-1.531990
H	-0.403505	-4.620502	1.243404	H	-0.901197	-4.919298	-0.900853
H	-0.572606	-3.620109	-2.721839	H	-0.463515	-4.275076	-2.516013
H	-2.655554	-4.167280	0.554865	H	-3.171763	4.207081	-1.322611
H	-2.936346	-3.501438	-2.201056	H	-2.661805	-3.362473	-2.822188
H	-4.473990	1.905077	0.390708	H	-4.441152	2.034730	0.041794
H	-1.842065	2.903357	-2.947916	H	-1.410201	4.855449	-1.630864
H	1.392821	3.370372	0.762491	H	1.002179	3.694575	2.347250

L=P(O'Pr) ₃ in <i>cis</i>				L=P(O'Pr) ₃ in <i>trans</i>			
Ru	-0.768813	-0.275422	0.996898	Ru	-0.706709	-0.036665	-0.037614
Cl	-0.927110	-2.155990	2.532893	Cl	-1.589385	-0.187238	2.204951
Cl	-1.675722	1.016247	2.801740	Cl	-0.578324	0.269854	-2.432781
P	-1.061625	1.603122	-0.253819	P	-0.939081	2.304900	0.131298
O	-2.617349	2.087459	0.551561	O	-2.482187	2.842134	-0.109387
O	-0.528442	1.583444	-1.829474	O	-0.156764	3.151897	-1.029374
O	-0.447322	3.050121	0.273839	O	-0.627858	3.126996	1.538748
N	-0.017177	-2.658258	-0.884472	N	-0.144505	-3.002449	-0.894989
N	-2.185474	-2.322066	-0.641595	N	-2.285893	-2.496434	-0.965383
C	-2.111600	-3.706230	-1.157031	C	-2.236035	-3.823047	-1.623846
C	1.109839	-0.011587	0.989695	C	1.148518	0.098862	0.280443
C	6.740168	1.797450	-1.922658	C	6.898657	2.116500	-2.185791
C	3.316313	0.577433	0.416987	C	3.390319	0.683046	-0.124401
C	3.298631	0.241457	1.866912	C	3.334263	-0.016478	1.188688
C	1.634639	-0.415334	3.550500	C	1.619848	-0.990528	2.647182
C	5.443365	2.213654	-2.278569	C	5.668998	2.790033	-2.313193
C	-3.492278	-1.709062	-0.587829	C	-3.594060	-1.955543	-0.686671
C	-4.106887	-3.028248	1.535979	C	-3.468656	-3.035762	1.629681
C	-4.426720	-2.058864	0.424814	C	-4.202293	-2.260291	0.563035
C	4.283627	0.344442	2.858027	C	4.315642	-0.235679	2.163234
C	5.804298	0.560419	-0.040832	C	5.845065	0.504180	-0.692003
C	-0.945081	-1.784368	-0.389636	C	-1.058140	2.044430	-0.568321
C	0.441732	3.348628	1.395495	C	0.386964	2.748671	2.517755
C	-5.734546	-1.535426	0.328773	C	-5.529685	-1.842801	0.780075
C	-6.155366	-0.736404	-0.748987	C	-6.275041	-1.170094	-0.207831
C	-5.221746	-0.463066	-1.768136	C	-5.657712	-0.928543	-1.449890
C	-7.561058	-0.182755	-0.807431	C	-7.690782	-0.712173	0.061690
C	1.408692	-2.540236	-1.050887	C	1.241220	-3.112934	-0.522594
C	-0.627840	-3.856786	-1.506835	C	-0.735979	-4.151029	-1.621929
C	-3.384152	2.942108	0.363132	C	-3.502187	2.844244	0.944319
C	-3.534044	4.319325	-0.284424	C	-3.651321	4.268584	1.478610
C	2.282097	-3.206206	-0.154617	C	2.258854	-2.796575	-1.457030
C	3.661037	-3.211951	-0.456381	C	1.549576	-3.706631	0.731255
C	4.181876	-2.619939	-1.620760	C	2.899392	-3.933837	1.051035
C	4.489397	0.982830	-0.373453	C	3.941832	-3.596289	0.163450
C	6.912073	0.964082	-0.803596	C	4.597742	1.172473	-0.806909
C	3.280404	-1.981913	-2.497881	C	6.978869	0.969777	-1.376305
C	1.899107	-1.933410	-2.240761	C	3.597855	-3.035318	-1.080187
C	1.961867	-0.137536	2.217245	C	2.258854	-2.796575	-1.457030
C	1.773199	-3.940412	1.061017	C	1.973548	-0.391894	1.432771
C	5.659449	-2.665966	-1.934997	C	1.454651	-4.101957	1.694562
C	0.966149	-1.258576	3.219198	C	5.385478	-3.815549	0.555220
C	3.951232	0.032011	4.198516	C	1.940819	-2.257839	-2.830659
C	2.645792	-0.347285	4.538421	C	3.949871	-0.856534	3.382244
C	-0.605714	2.785808	-2.669953	C	2.618545	-1.227450	3.621001
C	0.810477	1.146846	-3.112293	C	-0.406544	4.567175	-1.303767
C	-4.715908	2.260134	0.648826	C	0.952673	5.250667	-1.435340
C	-1.554920	2.523550	-3.836376	C	-4.783896	2.293090	0.330121
C	-0.294661	4.274132	2.362489	C	-1.262901	4.677429	-2.564256
C	1.714597	3.982519	0.836466	C	-0.196191	3.043269	3.897172
C	4.337632	1.812941	-1.516902	C	1.684770	3.502843	2.230903
C	2.014666	0.468289	-0.053028	C	4.534078	2.324092	-1.635959
C	3.900968	-0.943411	-1.716099	C	2.096061	0.787146	-0.603818
C	2.957838	-0.697100	-2.867240	C	-4.330413	-1.319954	-1.723480
H	4.268454	-4.076710	1.196930	H	-2.997725	-3.956630	1.225526
H	-3.059426	-2.937174	1.886879	H	-2.660469	-2.412324	2.069408
H	-4.777760	-2.865102	2.402722	H	-4.157622	-3.334042	2.443954
H	-2.545967	-1.647974	3.268911	H	-3.755622	-2.058846	-3.686346
H	-3.477072	-0.179431	-3.697008	H	-4.366219	-0.383072	-3.675021
H	-2.092881	-0.074121	-2.563716	H	-2.710182	-0.738120	-3.066001
H	0.175352	-1.948460	-3.584349	H	1.623958	-3.075156	-3.517607
H	0.441946	0.392686	2.761869	H	1.122323	-1.507812	-2.806018
H	1.523411	-0.896201	-4.105598	H	2.835083	-1.786417	-3.283841
H	2.587831	-4.094865	1.795748	H	0.880537	-4.487304	2.641359
H	0.942446	-3.401300	1.561624	H	-0.209478	-3.247067	1.936487
H	1.392491	-4.950587	0.786341	H	-0.195772	4.900219	1.273866
H	8.286004	-0.850161	-0.298650	H	-8.198984	-1.364681	0.800535
H	-7.619495	0.806177	-0.300840	H	-7.702260	0.320121	0.476302
H	7.900662	-0.034136	1.852784	H	-8.300394	-0.696672	-0.864607
H	-5.533936	0.129263	2.644747	H	-6.230128	-0.427472	-2.248735
H	-6.456091	-1.792871	1.122484	H	-6.001289	-2.073164	1.750234
H	6.199675	-3.361210	-1.261779	H	5.537444	-4.814105	1.016026
H	5.840696	-2.990415	-2.981381	H	6.066011	-3.731300	-0.315595
H	6.120658	-1.660961	-1.823059	H	5.706294	-3.062578	1.308605
H	3.663241	-1.513821	-3.420356	H	4.396763	-2.777496	-1.795647
H	4.346108	-3.724241	0.239907	H	3.143528	-4.384395	2.027497
H	-2.570693	2.290077	-3.464573	H	-2.226999	4.153476	-2.420402
H	-1.618274	3.423582	-4.483401	H	-1.468659	5.742989	-2.799415
H	-1.199578	1.676590	-4.459636	H	-0.740084	4.220163	-3.429381
H	1.268052	2.319121	-3.693482	H	1.530422	4.807996	-2.273422
H	0.795215	4.051927	-3.754607	H	0.820648	6.333265	-1.641153
H	1.448891	3.361513	-2.233057	H	1.543757	5.143095	-0.504576
H	-1.011949	3.610973	-2.048500	H	-0.955721	4.999389	-0.438652
H	-4.556381	1.265584	1.108573	H	-4.636371	1.259649	-0.039453
H	-5.312469	2.877965	1.352097	H	-5.593219	2.279299	1.089342
H	-5.299003	2.127474	-0.285369	H	-5.114397	2.926698	-0.519621
H	-2.542543	4.786430	-0.447344	H	-2.692484	4.625693	1.900991
H	-0.458630	4.243536	-1.260405	H	-3.966926	4.959240	0.668192
H	-4.126109	4.989704	0.373239	H	-4.421079	4.300849	2.278054
H	0.372259	4.541767	3.208185	H	0.530074	2.759164	4.686396
H	-0.602256	5.212012	1.854156	H	-0.425940	4.123977	4.009082
H	-1.185412	3.767592	2.781871	H	-1.123902	2.458779	4.054610
H	2.240304	3.288190	0.152908	H	2.078172	3.246131	1.225870
H	1.479716	4.918913	0.287728	H	1.523054	4.600479	2.280715
H	2.411077	4.232590	1.663007	H	2.459670	3.230865	2.976196
H	0.681847	2.396446	1.915224	H	0.558551	1.655095	2.428096
H	-2.813003	3.031968	1.308405	H	-3.160191	2.169150	1.759172
H	0.601534	-0.679987	3.816526	H	0.567108	-1.239593	2.843934
H	2.394187	-0.579112	5.585437	H	2.342555	-1.696620	4.578880
H	4.725804	0.105236	4.978841	H	4.717270	-1.031464	4.153577
H	5.299176	0.693572	2.619491	H	5.353869	0.095019	2.006768
H	5.953665	-0.124776	0.805489	H	5.912202	-0.413384	-0.089115
H	7.919964	0.618447	-0.522836	H	7.933779	0.428409	-1.280253
H	7.610477	2.119745	-2.516032	H	7.790809	2.484820	-2.716790
H	5.294241	2.865593	3.154179	H	5.596541	3.691057	-2.943151
H	3.332967	2.161690	-1.797593	H	3.579300	2.864753	-1.726145
H	1.697157	0.653937	-1.085000	H	1.794156	1.229510	-1.560428
H	-0.1775508	-4.776723	-0.1084460	H	-0.495938	-5.101988	-1.100194
H	-0.433084	-3.858902	-2.603215	H	-0.307829	-4.210382	-2.645272

H -2.433942 -4.420270 -0.368394	H -2.845867 -4.554158 -1.049164
H -2.785736 -3.829697 -2.029754	H -2.661871 -3.761576 -2.646812

L=P(OCy) ₃ in cis			L=P(OCy) ₃ in trans				
Ru	0.488992	-0.908837	-1.030466	Ru	-0.457269	-0.690484	-0.203617
Cl	0.428791	-2.830896	-2.521110	Cl	-1.394892	-0.944931	2.000539
Cl	1.436090	0.252392	-2.902603	Cl	-0.335868	-0.405378	-2.600959
P	1.028547	0.946498	0.176775	P	-1.067818	1.590817	-0.088113
O	2.639654	1.241400	0.419994	O	-2.661867	1.898454	-0.390901
O	0.538666	1.023056	1.765336	O	-0.374789	2.532459	-1.235764
O	0.599776	2.450513	-0.376362	N	-0.933977	2.463176	1.318246
N	-0.514867	-3.164455	0.882581	N	0.655428	-3.505713	-1.046731
N	1.679008	-3.069601	0.657272	N	-1.544731	-3.409032	-1.066522
C	1.446338	-4.436213	1.173771	C	-1.260001	-4.661542	-1.804307
C	-1.345558	-0.434036	-1.004037	C	1.335325	-0.243376	0.166182
C	6.672989	2.077887	1.955835	C	6.774054	2.637579	-2.140904
C	-3.457730	0.413744	-0.405265	C	3.468748	0.678363	-0.179577
C	-3.507863	0.450848	-1.847578	C	3.490807	-0.039197	1.125129
C	-1.960657	-0.834826	-3.542891	C	1.898834	-1.249858	2.546704
C	-5.330414	2.346920	2.283056	C	5.463912	3.133119	-2.281245
C	3.047963	-2.609711	0.626220	C	-2.925472	-3.122748	-0.761050
C	3.540834	-3.974649	-1.499757	C	-2.549133	-4.178299	1.538830
C	3.953444	-3.062910	-0.370197	C	3.440989	-3.552054	0.495258
C	-4.494396	0.234013	-2.824661	C	4.470996	-0.117790	2.122681
C	-5.920494	0.697817	0.091707	C	5.933127	0.860438	-0.700386
C	0.507344	-2.401357	0.387395	C	-0.414668	-2.735240	-0.692824
C	5.313573	-2.701870	-0.243023	C	4.817937	-3.402608	0.739219
C	5.804258	-1.963842	0.847568	C	-5.698327	-2.874679	-0.227727
C	4.887445	-1.578685	1.847107	C	-5.160531	-2.491216	-1.469103
C	7.265559	-1.589126	0.951882	C	-7.179283	-2.762951	0.059854
C	-1.917057	-2.881721	1.052756	C	2.042238	-3.371852	-0.682335
C	-0.042608	-4.411034	1.529847	C	0.267896	-4.775271	-1.706677
C	-2.865481	-3.463209	0.174829	C	2.457851	-3.888931	0.575164
C	-4.234327	-3.306836	0.482500	C	3.828914	-3.880791	0.884897
C	-4.676415	-2.640106	1.639058	C	4.791906	-3.382416	-0.016110
C	-4.559858	0.970821	0.394749	C	4.605909	1.348170	-0.828656
C	-6.960287	1.245427	0.859949	C	7.001563	1.496354	-1.351777
C	-3.703043	-2.090129	2.499294	C	4.347794	-2.899951	-1.260779
C	-2.327352	-2.199710	2.232789	C	2.984934	-2.389128	-1.628908
C	-2.229517	-0.490094	-2.212165	C	2.195794	-0.612517	1.336747
C	-2.448165	-4.276738	-1.025459	C	1.454852	-4.457919	1.551466
C	-6.147283	-2.515344	1.963906	C	6.256230	-3.358734	0.360282
C	-1.314467	-1.615166	3.189092	C	2.572747	-2.445439	-3.008544
C	-4.224538	-0.144713	-4.162401	C	4.168734	-0.785369	3.334380
C	-2.976761	-0.675937	4.515183	C	2.897287	-1.339603	3.545313
C	-4.291864	1.801680	1.516332	C	4.394357	2.496871	-1.636869
C	-2.169019	0.162971	0.044726	C	2.181909	0.598067	-0.685188
C	3.521017	-1.897023	1.765109	C	3.786405	-2.617781	-1.770653
C	2.588025	-1.541937	2.896116	C	3.291272	-2.275801	-3.155825
H	3.579251	-5.039635	-1.176238	H	-1.900604	-4.969974	1.108626
H	2.514545	-3.763342	-1.861155	H	-1.884920	-3.406509	1.984964
H	4.236985	-3.876353	2.356398	H	-3.150147	-4.630301	2.352093
H	2.068591	-2.440238	3.294070	H	-3.236392	-3.186528	-3.794555
H	3.143876	-1.077103	3.733359	H	-3.987675	-1.575846	-3.658843
H	1.802133	-0.831205	2.571355	H	-2.284627	-1.809171	-3.137656
H	-0.632377	-2.392597	3.596005	H	2.372801	-3.317606	-3.671762
H	-0.671568	-0.855692	2.696101	H	1.650166	-1.828163	-2.987806
H	-1.818793	-1.134940	4.050761	H	3.380976	-1.857473	-3.486566
H	-3.278477	-4.356172	-1.754469	H	1.935862	-4.699118	2.519125
H	-1.563994	-3.844619	-1.538355	H	0.624128	-3.750081	1.744150
H	-2.180047	-5.316332	-0.727891	H	0.994436	-5.395422	1.167764
H	7.7896579	-2.203970	0.279443	H	-7.629358	-3.763130	0.240666
H	7.425497	-0.524236	0.672729	H	-7.371137	-2.156613	0.970113
H	7.644603	-1.709739	1.988076	H	-7.726672	-2.295029	-0.782329
H	5.248705	-1.027273	2.731607	H	-5.832448	-2.093168	-2.248054
H	6.016026	-3.039684	-1.023538	H	5.218378	-3.731563	1.713106
H	-6.770642	-3.129189	1.283513	H	6.588091	-4.335534	0.771224
H	-6.359342	-2.835437	3.005993	H	6.900198	-3.115923	-0.508520
H	-6.485352	-1.460523	1.874152	H	6.449604	-2.598641	1.149100
H	-4.025498	-1.563722	3.413359	H	5.086127	-2.516753	-1.985043
H	-4.978176	-3.750315	-0.200649	H	4.153051	-4.273443	1.863032
H	-0.969247	-1.221548	3.818960	H	0.885238	-1.639967	2.720981
H	-2.773943	-0.959447	5.560061	H	2.668068	-1.840127	4.499678
H	-5.001521	-0.003928	4.931009	H	4.935064	-0.849678	4.123677
H	-5.461080	0.697825	2.578819	H	5.454356	0.359349	1.991661
H	-6.162674	0.016136	-0.735638	H	6.118930	-0.051283	-0.113978
H	-8.006342	1.014111	0.602121	H	8.021695	1.093435	-1.246259
H	-7.489455	2.513363	2.553419	H	7.614452	3.139851	-2.645948
H	-5.091414	2.996306	3.140429	H	5.276120	4.028262	-2.895551
H	-3.248084	2.034797	1.774476	H	3.374318	2.898971	-1.736295
H	-1.806919	0.328150	1.065415	H	1.834855	1.004064	-1.642784
H	-0.599776	-5.281539	1.128976	H	0.602395	-5.641483	-1.094465
H	-0.229371	-4.366377	2.626805	H	0.759771	-4.855986	-2.698187
H	1.679623	-5.183062	0.383788	H	-1.795953	-5.513288	-1.334260
H	2.104961	-4.638072	2.043496	H	-1.614908	-4.574848	-2.853370
C	3.483708	1.924269	-0.557970	C	-3.722229	1.738076	0.599947
C	3.977035	3.243982	0.047765	C	-4.092386	3.107332	1.187102
C	4.642401	1.008141	-0.952253	C	4.917584	1.083613	-0.097589
C	2.873554	2.139293	-1.461129	C	-3.356073	1.068199	1.410844
C	4.944579	3.963233	-0.912951	C	-5.295384	2.997121	2.142564
C	4.494394	3.019965	1.008713	C	-4.342885	3.788928	0.342060
C	3.104999	3.889202	0.285303	C	-3.208882	3.534040	1.702995
C	5.603873	1.725868	-1.917893	C	-6.125047	0.975999	0.852403
H	5.181521	0.705534	-0.027656	H	-5.184658	1.704322	-0.983090
H	4.236767	0.082497	-1.409183	H	-4.625834	0.083031	-0.478434
C	6.113412	3.052606	-1.327695	C	-6.504417	2.340119	1.455033
H	5.321669	4.896941	-0.442207	H	-5.563314	4.003615	2.530581
H	4.386578	4.279228	-1.824126	H	-5.004233	2.390942	3.031248
H	6.454498	1.057265	-2.171321	H	-6.989609	0.534702	0.311735
H	5.074144	1.927527	-2.876976	H	-5.879032	0.266469	1.675597
H	6.770145	3.576294	-2.055965	H	-7.345832	2.226888	2.172864
H	6.745601	2.839428	-0.434386	H	-6.872900	3.009980	0.643806
C	-0.341862	2.834298	-1.417650	C	0.139997	2.328409	2.289439
C	-1.477248	3.648189	-0.784202	C	1.190006	3.425069	2.065807
C	0.394681	3.652561	-2.485465	C	-0.477925	2.408709	3.689911
H	-0.750600	1.914300	-1.891004	H	0.612978	1.329268	2.165192
C	-2.461547	4.163841	-1.850808	C	2.272961	3.401202	3.161761
H	-1.025483	4.507493	-0.237608	H	0.668293	4.409446	2.068629
H	-2.010296	3.025627	-0.036869	H	1.649905	3.300504	1.062686
C	-0.585769	4.163775	-3.558650	C	0.609650	2.377842	4.780690
H	0.896972	4.512751	-1.986634	H	-1.058926	3.356579	3.762179
H	1.179034	3.017320	-2.944477	H	-1.192407	1.569137	3.814652
C	-1.738790	4.973470	-2.940370	C	1.656580	3.484801	4.568708

H	-3.254423	4.773793	-1.3666780		H	2.992455	4.232255	2.997517
H	-2.980097	3.295795	-2.317594		H	2.861149	2.459719	3.073608
H	-0.036840	4.772901	-4.308671		H	0.138958	2.469502	5.783346
H	-1.002373	3.292057	-4.112689		H	1.116290	1.385896	4.763974
H	-2.456819	5.290065	-3.727712		H	2.451362	3.420395	5.343282
H	-1.331527	5.909810	-2.492747		H	1.171230	4.479895	4.699990
C	0.790994	2.216555	2.574321		C	-0.799321	3.896846	-1.521240
C	-0.545667	2.759376	3.092332		C	0.455088	4.769344	-1.646774
C	1.748481	1.879254	3.721899		C	-1.632872	3.922034	-2.808591
H	1.262367	2.985566	1.924748		H	-1.418091	4.265076	-0.671286
C	-0.333333	3.976641	4.013900		C	0.092633	6.214042	-2.039618
H	-1.064185	1.947346	3.650718		H	1.110790	4.318978	-2.426024
H	-1.188206	3.026954	2.227860		H	1.021713	4.747483	-0.692792
C	1.964759	3.099735	4.637538		C	-1.997419	5.365495	-3.205121
H	1.315378	1.039906	4.311053		H	-1.035397	3.441643	-3.615089
H	2.709596	1.523644	3.298806		H	-2.540228	3.301562	-2.665401
C	0.630958	3.653368	5.168141		C	-0.747698	6.255341	-3.327868
H	-1.311420	4.329020	4.406286		H	1.018224	6.818319	-2.154692
H	0.081301	4.820421	3.415914		H	-0.483471	6.686713	-1.210716
H	2.638513	2.826969	5.478040		H	-2.569853	5.361679	-4.157605
H	2.491296	3.898184	4.065753		H	-2.679978	5.798532	-2.437383
H	0.805461	4.557504	5.790498		H	-1.036895	7.301536	-3.567901
H	0.160689	2.897932	5.839269		H	-0.126097	5.898530	-4.181362

L=P(OPh) ₃ in <i>cis</i>				L=P(OPh) ₃ in <i>trans</i>			
Ru	0.399661	-1.077422	-0.967969	Ru	-0.217803	-0.723532	-0.048371
Cl	1.300988	-0.477724	-3.105104	Cl	-0.428144	-0.447278	-2.453577
Cl	0.047499	-3.239524	-1.997538	Cl	-0.613148	-1.161880	2.295672
P	1.248932	0.848889	-0.182115	P	-1.304467	1.296739	0.148599
O	2.893480	0.896569	-0.019514	O	-2.918489	1.096712	-0.149338
O	0.806715	1.311021	1.379899	O	-0.907192	2.455764	-0.988657
O	1.090838	2.281362	-1.022578	O	-1.474745	2.166767	1.561421
N	-0.643867	-2.865836	1.387699	N	1.085923	-3.556669	-0.401919
N	1.550447	-2.846819	1.141918	N	-1.094778	-3.594035	-0.701833
C	-2.275661	-1.304886	-3.250410	C	2.575271	-0.403793	2.385129
C	-3.377578	-1.281440	-4.139670	C	3.681565	-0.124967	3.224297
C	-1.366229	-0.376630	-0.945645	C	1.477145	0.132552	0.030152
C	-4.625199	0.160239	-2.606488	C	4.704338	1.235792	1.470516
C	2.918361	-2.429140	0.934104	C	-2.486871	-3.236406	-0.850791
C	-3.316798	0.822432	-0.421111	C	3.270899	1.459827	-0.718911
C	-0.177292	-3.936374	2.301721	C	0.821127	-4.954669	-0.822586
C	-4.375312	-3.031721	1.043569	C	4.363665	-3.173121	1.335134
C	-4.275568	1.657075	0.316802	C	4.113950	2.291680	-1.591449
C	5.071075	-2.605210	-0.170004	C	-4.702599	-2.921824	0.089838
C	-2.369847	-0.624992	-2.030403	C	2.536836	0.132088	1.094798
C	-3.553130	-1.115063	-1.708105	C	3.619133	0.951385	0.634889
C	-3.806349	-1.326176	2.651988	C	4.603638	-2.404312	-0.944200
C	-5.673281	1.409451	0.271774	C	5.526856	2.155133	-1.619356
C	3.234567	-4.130988	-0.970721	C	-2.867987	-3.697215	1.644555
C	-3.012273	-3.309404	0.801082	C	2.998265	-3.443002	1.128613
C	5.647459	-1.688450	0.725447	C	-5.231082	-2.621567	-1.180323
C	-2.634443	-4.452483	-0.108436	C	2.140449	-3.990992	2.246309
C	-3.818611	2.730259	2.128165	C	3.518433	3.241006	-2.464365
C	1.310903	-4.056691	1.956944	C	-0.710275	-5.022229	-0.805347
C	3.487309	-1.548857	1.898371	C	-3.005527	-3.037945	-2.160063
C	3.724830	-3.020823	-0.072886	C	-3.347250	-3.256900	0.281726
C	4.840413	-1.193850	1.770587	C	-4.370516	-2.715031	-2.290664
C	0.386421	-2.245124	0.736657	C	-0.033681	-2.787834	-0.405940
C	-6.572319	2.202328	1.001708	C	6.309127	2.934916	-2.485652
C	-2.043272	-2.530832	1.484438	C	2.449825	-3.171410	-0.151612
C	-1.405634	-0.798945	3.238554	C	2.674271	-2.445320	-2.591784
C	-2.435460	-1.551948	2.438813	C	3.245214	-2.670984	-1.212285
C	-2.014520	0.553523	-0.028148	C	1.999716	1.009652	-1.025827
C	-6.264341	-1.815968	2.239763	C	6.635550	-2.325730	0.585370
C	2.674018	-1.029681	3.060697	C	-2.151216	-3.219046	-3.391668
C	-4.797300	-2.054294	1.961804	C	5.182778	-2.646312	0.316246
C	-4.718180	3.522052	1.854577	C	4.302979	4.023365	-3.322389
C	-4.535185	-0.558212	-3.824259	C	4.733702	0.682359	2.774908
C	-6.101033	3.264926	1.794017	C	5.702831	3.875231	-3.337157
C	7.079961	-1.233462	0.570407	C	-6.677699	-2.214312	-1.343129
H	1.972114	-0.463685	2.847653	H	-1.139306	-5.475455	-1.721575
H	1.536205	-4.963760	1.354266	H	-1.105887	-5.583619	0.069800
H	-0.358734	-3.639298	3.359285	H	1.250732	-5.129311	-1.834141
H	-0.741806	-4.871422	2.113020	H	1.300857	-5.669237	-0.123753
H	2.146725	-4.076901	-1.168339	H	-1.988725	-3.113639	1.987313
H	3.755540	-2.250319	-0.051522	H	-3.671873	-3.577896	2.397153
H	3.458522	-5.120482	-0.511461	H	-2.582044	-4.772249	1.640476
H	1.7722018	-0.484129	2.722124	H	-1.267749	-2.548120	-3.365001
H	2.325415	-1.855094	3.719790	H	-1.786635	-4.266174	-3.484133
H	3.273470	-0.338414	3.684060	H	-2.731606	-2.3991562	-4.307166
H	7.577357	-1.103508	1.553832	H	-7.041414	-2.393213	-2.375166
H	7.676816	-1.949926	-0.028894	H	-7.339741	-2.762128	-0.641333
H	7.120773	-0.250319	0.051522	H	-6.805702	-1.130676	-1.128860
H	-3.459711	-4.684534	-0.810336	H	2.715000	-4.051224	3.191265
H	-1.722272	-4.232015	-0.699436	H	1.246536	-3.354461	2.421037
H	-2.444917	-5.379185	0.480338	H	1.767842	-5.015190	2.023513
H	-1.891299	-0.147073	3.863427	H	3.436379	-2.006725	-3.264956
H	-0.838780	-1.459130	3.922617	H	2.334707	-3.398338	-3.054090
H	-0.659176	-0.295003	2.585055	H	1.793452	-1.767436	-2.576181
H	-6.501747	-0.732098	2.258195	H	6.727530	-1.360204	1.130052
H	-6.909123	-2.299273	1.478768	H	7.115705	-3.100840	1.217962
H	-6.554312	-2.227420	3.231614	H	7.218295	-2.236495	-0.353449
H	-4.108792	-0.559555	3.384857	H	5.231018	-2.004844	-1.758639
H	-5.131834	-3.622288	0.499954	H	4.797744	-3.371923	2.329183
H	5.692634	-3.039156	-0.971198	H	-5.369500	-2.913547	0.968025
H	5.278760	-0.506981	2.513968	H	-4.773329	-2.540158	-3.302426
H	-1.354507	-1.845651	-3.510262	H	1.732486	-1.008335	2.747006
H	-3.312047	-1.827040	-0.094303	H	3.704287	-0.540531	4.244182
H	-5.378815	-0.531078	-4.532635	H	5.583233	0.904605	3.440715
H	-5.518101	0.768223	-2.397359	H	5.513278	1.905497	1.140259
H	-6.052749	0.560261	-0.314470	H	6.009607	1.400124	-0.981332
H	-7.651844	1.987526	0.953879	H	7.403012	2.803209	-2.499363
H	-6.807936	3.891269	2.361077	H	6.318821	4.491189	-4.011495
H	-4.338824	4.355502	2.467297	H	3.818867	4.759892	-3.983375
H	-2.742655	2.958556	1.159099	H	2.425532	3.373016	-2.445963
H	-1.546105	0.927729	0.888904	H	1.462153	1.191361	-1.962912
C	3.896954	1.585924	-0.696455	C	-4.006920	1.205249	0.714495
C	4.920636	2.138937	0.096679	C	-5.085272	1.998405	0.285241
C	3.936525	1.682959	-2.098239	C	-4.061141	0.498547	1.929520
C	5.994724	2.799524	-0.524078	C	-6.236664	2.083277	1.086991
C	4.860283	2.044078	2.190474	C	-5.004787	2.539079	-0.669415
C	5.014738	2.352949	-2.701560	C	-5.217475	0.600939	2.721970
C	3.137598	2.122010	-2.699443	C	-3.204531	-0.117373	2.246615
C	6.045100	2.912664	-1.925051	C	-6.307311	1.388121	2.307429
C	6.795039	3.233171	0.097032	H	-7.082788	2.705309	0.753545
C	5.047026	2.430209	-3.800116	H	-5.263766	0.052541	3.676578
C	6.885428	3.434074	-2.409637	H	-7.209267	1.461068	2.935179
C	1.242695	2.382486	2.154725	C	-1.766387	3.440177	-1.459324
C	0.812875	2.371978	3.498588	C	-2.331097	3.249474	-2.732863
C	2.049463	3.437984	1.681966	C	-2.003878	4.614229	-0.723475
C	1.189238	3.409309	4.365433	C	-3.144717	4.257328	-3.276453
C	0.180615	1.543972	3.848815	H	-2.116449	2.313276	-3.270030
C	2.420106	4.468554	2.565919	C	-2.822775	5.612740	-1.280128
C	2.379105	3.470082	0.636183	H	-1.545492	4.740105	0.268308
C	1.997934	4.464034	3.905466	C	-3.393921	5.439226	-2.553526
C	0.845743	3.388691	5.412093	H	-3.587391	4.116646	-4.275567
C	3.051474	5.288354	2.187761	H	-3.011883	6.536332	-0.710143
C	2.294490	5.276941	4.586214	H	-4.032168	6.226652	-2.984302
C	-0.059176	2.880182	-1.537949	C	-0.474310	2.615764	2.411950
C	-0.557249	2.496454	2.795373	C	0.757859	3.102659	1.937546
C	-0.637415	3.945587	-0.821309	C	-0.774191	2.626633	3.787051
C	-1.661199	3.184012	-3.327448	C	1.697995	3.595921	2.860134
C	-0.073864	1.668393	-3.335945	H	0.979201	3.096530	0.859841
C	-1.734671	4.628545	-1.372682	C	0.170786	3.131139	4.692748

H	-0.211135	4.238872	0.149961	H	-1.746598	2.236970	4.121481
C	-2.253142	4.247673	-2.623246	C	1.410757	3.615343	4.235002
H	-2.058990	2.881282	-4.308851	H	2.666042	3.968611	2.490727
H	-2.186255	5.466328	-0.817998	H	-0.063276	3.139806	5.769317
H	-3.115796	4.783043	-3.049753	H	2.151815	4.005205	4.950066

L=PMe ₃ in <i>cis</i>				L=PMe ₃ in <i>trans</i>			
Ru	-0.948698	-0.949282	-0.356895	Ru	0.872418	-0.547379	-0.063004
Cl	-1.640359	-3.253761	-0.325396	Cl	0.647151	-0.243870	-2.481633
Cl	-1.180432	-1.117318	-2.776488	Cl	1.703004	-0.939649	2.177939
P	-1.266248	-1.131352	1.953488	P	1.219698	-2.856374	-0.557637
N	-0.431416	1.990480	-1.260497	N	0.552579	2.508254	0.489639
N	-2.547496	1.500503	-0.839460	N	2.652295	1.919936	0.179091
C	1.555767	-2.820950	-1.921580	C	-1.298856	-2.195118	2.488420
C	2.608458	-3.630738	-2.409978	C	-2.243975	-2.895197	3.275945
C	0.923990	-0.983708	-0.131026	C	-0.967812	-0.803856	0.241179
C	4.170724	-2.622365	0.818781	C	4.018173	-2.340145	1.689911
C	3.728164	1.063747	-0.133328	C	3.852046	1.178590	-0.123176
C	3.102738	-0.792614	0.745558	C	-3.250773	-0.863039	-0.347837
C	-1.177186	3.165368	-1.766519	C	1.292927	3.771447	0.721349
C	3.177905	2.115243	-2.285002	C	-2.886879	2.451743	1.953914
C	4.236873	-0.348231	1.570936	C	-4.494585	-0.671497	-1.112446
C	-5.801583	-0.195472	0.022800	C	5.858352	0.021006	0.609815
C	1.824368	-1.895943	-0.905196	C	1.713829	-1.561913	1.309449
C	3.142977	-1.790609	-0.355845	C	3.095089	-1.612156	0.927983
C	2.963914	2.998958	-0.051485	C	-3.031130	3.087331	-0.374719
C	5.554163	-0.260954	1.047480	C	-5.755109	-0.523167	-0.476182
C	-4.486061	-0.384189	-2.117900	C	4.391688	1.063851	2.381790
C	1.794119	1.841480	-2.349058	C	-1.487999	2.298688	1.857364
C	-1.009838	0.263400	3.154570	C	0.071479	-3.626080	-1.778337
C	-6.092448	0.359905	1.283223	C	6.247342	-0.213371	-0.722889
C	1.193332	1.307102	3.624592	C	-0.668108	1.897142	3.060336
C	4.039958	0.024020	2.927419	C	-4.456372	-0.604870	-2.530856
C	-2.635876	2.699085	-1.697929	C	2.752604	3.372357	0.446873
C	-4.037696	1.705781	1.100344	C	4.262874	1.043810	-1.480074
C	-4.652568	0.152787	-0.719173	C	4.685559	0.731239	0.938478
C	-5.205859	1.328727	1.792132	C	5.447782	0.328910	-1.748214
C	-1.251382	1.029169	-0.720257	C	1.365497	1.454744	0.206797
C	6.622653	0.177668	1.845947	C	6.924057	-0.316602	-1.226736
C	1.003360	2.130444	-1.207024	C	-0.880511	2.540937	0.600918
C	0.739596	3.136430	1.131291	C	-0.980541	3.169965	-1.869685
C	1.582511	2.739300	-0.058513	C	-1.641006	2.937894	-0.530504
C	1.792391	-0.356595	0.865239	C	-2.004366	-0.396438	-0.718061
C	-2.980512	-1.673225	2.390862	C	2.882178	-3.006873	-1.352545
C	5.269266	2.974711	-1.113046	C	5.170447	3.033019	0.988382
C	3.198518	2.843010	1.639911	C	3.495281	1.679765	-2.612691
C	3.785135	2.690483	-1.154885	C	-3.674563	2.852658	0.858349
C	5.107776	0.460865	3.723677	C	-5.625120	-0.401783	-3.277776
C	3.896189	-3.538055	-1.862996	C	-3.584524	-2.980157	2.874950
C	-0.238194	-2.463357	2.727649	C	1.290248	-4.080559	0.819685
C	6.407050	0.538266	3.187779	C	-6.866698	-0.258178	-2.630294
C	-7.315187	-0.069473	2.062113	C	7.490252	-1.012064	-1.047694
H	3.316649	3.454286	1.254974	H	3.186741	3.896394	-0.432450
H	-3.034114	2.421569	-2.699120	H	3.420427	3.560993	1.313258
H	-0.974093	4.054783	-1.127382	H	0.923665	4.566377	0.039472
H	-0.853824	3.411293	-2.797977	H	1.128547	4.122627	1.763061
H	-3.519044	-0.906661	-2.272145	H	3.310208	0.992486	2.606012
H	-5.309017	-1.080949	-2.369124	H	4.923670	0.370518	3.062468
H	-4.506890	0.441338	-2.862070	H	4.743581	2.091973	2.625760
H	-2.124965	2.732856	1.399341	H	2.528248	1.158341	2.789011
H	-3.526684	3.813897	1.204634	H	3.254983	2.742955	-2.400780
H	-3.307549	2.938933	2.738716	H	4.084621	1.646974	-3.550120
H	-7.671416	0.730865	2.741891	H	8.010762	-0.612161	-1.942100
H	-8.150571	-0.350310	1.389161	H	8.208082	-1.017048	-0.202807
H	-7.092993	-0.959595	2.691203	H	7.236654	-2.072396	-1.269222
H	1.982279	0.917999	-4.297775	H	-1.318741	1.708752	3.936364
H	0.457113	0.499074	3.431302	H	0.069074	0.981641	2.865364
H	0.659911	2.110770	-4.181283	H	0.053819	2.692704	3.347959
H	1.376208	3.403240	1.997655	H	-1.729588	3.445917	-2.637655
H	0.104083	4.022452	0.909378	H	-0.229745	3.989294	-1.830677
H	0.055995	2.321675	1.440747	H	-0.442363	2.259836	-2.215668
H	5.777185	2.318866	-0.373057	H	-5.716576	2.333942	0.319320
H	5.747125	2.807707	-2.098822	H	-5.516615	2.851750	0.2025510
H	5.473116	4.022267	0.805538	H	5.479347	4.061183	0.701887
H	3.411977	3.460980	0.844270	H	-3.631216	3.393367	-1.248242
H	3.797036	1.878903	-3.166612	H	-3.371387	2.260019	2.925949
H	-6.505945	-0.918110	-0.421901	H	6.496367	-0.346872	1.431080
H	-5.433983	1.818600	2.754061	H	5.764790	0.214577	-2.798728
H	-3.063990	-1.845973	3.484106	H	3.115829	-4.064984	-1.593316
H	-3.713827	-0.905052	2.078600	H	2.885185	-2.400008	-2.279482
H	3.183531	2.609578	1.835749	H	3.653345	2.604946	0.664774
H	0.046231	0.595283	3.145083	H	-0.936181	-3.698857	-1.322281
H	-1.654225	1.120320	2.886035	H	0.011616	-2.952935	-2.656362
H	-1.264962	-0.072310	4.181494	H	0.417550	-4.635036	-2.083306
H	-0.522100	-2.616009	3.789300	H	0.277823	-4.199371	1.253768
H	-0.404902	-3.391467	2.147121	H	1.653574	-5.062701	0.453241
H	0.833759	-2.192052	2.660228	H	1.959155	-3.686407	1.609892
H	0.536736	-2.906949	3.225350	H	-0.243444	-2.131807	2.791792
H	2.404986	-4.351542	3.217718	H	-1.915747	-3.385015	4.206746
H	4.701903	-4.190499	-2.236337	H	-4.308464	-3.546958	3.482409
H	5.174915	-2.593339	-0.369185	H	-5.067518	-2.432845	1.371645
H	5.731835	-0.510894	-0.008548	H	-5.812009	-0.535568	0.622222
H	7.634403	0.240902	1.414014	H	-7.889220	-0.196336	-0.708650
H	7.247762	0.874410	3.815137	H	-7.785616	-0.103676	-3.217908
H	4.928468	0.732699	4.776319	H	-5.568914	-0.363905	-4.377552
H	3.032843	-0.062251	3.364412	H	-3.492270	-0.739342	-3.045684
H	1.456807	0.410905	1.571451	H	-1.787339	0.188133	-1.617024

L=PEt ₃ in cis				L=PEt ₃ in trans			
Ru	0.850248	-0.079766	1.059938	Ru	-0.814341	0.292581	-0.039529
Cl	0.852042	1.695096	2.723751	Cl	-1.710940	0.444664	2.196533
Cl	1.677159	-1.428204	2.870619	Cl	-0.471912	0.088872	-2.465890
P	1.375714	-1.941626	-0.305590	P	-1.415732	2.585349	-0.538558
N	0.180384	2.491941	-0.586382	N	-0.149086	-2.758209	-0.025333
N	2.325795	1.956864	-0.490967	N	-2.306327	-2.338919	-0.192351
C	2.339469	3.401341	-0.798126	C	-2.215578	-3.791826	-0.460578
C	-0.990010	-0.428933	0.859290	C	0.991896	0.664543	0.334738
C	-6.225258	-2.226718	-2.711286	C	7.045325	0.648056	-2.255982
C	-3.097217	-1.093931	0.043849	C	3.298170	0.866035	-0.118555
C	3.214796	-0.918750	1.515841	C	3.042906	1.495675	1.203957
C	1.743499	-0.310533	3.388256	C	1.134408	1.924959	2.678835
C	-4.891965	-2.611424	-2.946459	C	5.829255	0.787587	-2.950984
C	3.556558	1.217255	-0.623957	C	-3.605509	-1.712058	-0.169796
C	4.113440	1.456781	1.878842	C	-3.737301	-2.278405	2.321054
C	4.427090	0.996407	0.478645	C	-4.318183	-1.681525	1.062565
C	-4.271007	-1.169918	2.401475	C	3.892215	2.196716	2.070061
C	-5.521826	-1.101527	-0.665476	C	5.820848	0.652509	-0.147004
C	1.049818	1.489745	-0.216773	C	-1.074986	-1.756679	-0.030065
C	0.288954	-3.455315	-0.101845	C	-1.781592	3.848104	0.791364
C	5.647594	0.325527	0.241683	C	-5.599974	-1.101094	1.078279
C	6.046229	-0.102218	-1.037240	C	-6.203739	-0.584064	-0.085953
C	5.190219	0.184819	-2.119340	C	-5.503984	-0.705615	-1.300747
C	7.346699	-0.845752	-1.244221	C	-7.5656531	0.069309	-0.026156
C	-1.257395	2.491209	-0.717822	C	1.264091	-2.694067	0.233141
C	0.873853	3.675353	-1.143924	C	-0.769072	-4.104967	-0.067190
C	3.099390	-2.570204	0.050410	C	-2.985065	2.468503	-1.545592
C	3.609106	-3.796971	-0.715381	C	-3.618905	3.773122	-2.046549
C	-2.064932	3.158990	0.240520	C	1.725271	2.550393	1.565904
C	-3.456641	3.222286	0.010392	C	3.115505	-2.614469	1.793494
C	-4.059718	2.696946	-1.145192	C	4.037192	-2.837950	0.753331
C	-4.171217	-1.482561	-0.883770	C	4.585274	0.796923	-0.830936
C	-6.532911	-1.468293	-1.568014	C	7.033315	0.577079	-0.851776
C	-3.223118	2.092028	-2.104396	C	3.538825	-2.979738	-0.557901
C	-1.833147	1.990452	-1.920214	C	2.162851	-2.913370	-0.844630
C	-1.940048	-0.495823	0.201392	C	1.643716	1.372402	1.496051
C	-1.481673	3.865297	1.438433	C	0.766333	-2.345035	2.713708
C	-5.551826	2.786450	-1.370755	C	5.520350	-2.948957	1.027219
C	-0.983114	1.412524	-3.027990	C	1.662535	-3.054995	-2.263836
C	-4.070203	-0.961462	3.787253	C	3.365542	2.743162	3.263831
C	-2.826335	-0.531340	4.271834	C	2.004752	2.599444	3.567828
C	1.367056	-1.703880	-2.172049	C	-0.249087	3.495685	-1.675242
C	1.087991	-2.896645	-3.098514	C	1.004530	4.075381	-1.010407
C	0.097134	-4.000878	1.316350	C	-3.073700	3.638900	1.501628
C	-3.881235	-2.245060	-2.046765	C	4.617706	0.860651	-2.249761
C	-1.782860	-0.823968	-0.304780	C	2.092540	0.393714	-0.600506
C	3.963622	0.853125	-1.942913	C	4.218705	-1.285452	-1.378373
C	3.151916	1.235364	-3.161805	C	3.574684	-1.502769	-2.726691
H	3.376950	2.279822	1.902971	H	3.432209	-3.336666	2.173675
H	3.658740	0.636280	2.476214	H	2.838107	-1.708027	2.636906
H	5.040399	1.773575	2.398120	H	4.475021	-2.251869	3.146716
H	3.438020	2.247378	-3.527025	H	3.593118	-2.580236	-3.004585
H	3.332636	0.535021	-4.001683	H	4.127248	-0.957721	-3.517471
H	2.065604	1.261348	-2.955390	H	-2.516221	-1.167843	-2.750221
H	-0.571041	2.212920	-3.682652	H	1.108726	-4.007880	-2.418249
H	-0.119625	0.843269	-2.633574	H	0.967315	-2.229569	-2.530699
H	-1.576587	3.793807	-3.678463	H	2.506966	-3.051799	-2.980762
H	-2.246102	3.991339	2.230563	H	1.304684	-2.334353	3.681215
H	-0.618662	3.317664	1.868890	H	0.205048	-1.390748	2.617687
H	-1.138173	4.887613	1.158609	H	0.003650	-3.151902	2.761565
H	8.117588	-0.531751	-0.511612	H	-8.258761	-0.490494	0.636559
H	7.204548	-1.941457	-1.115747	H	-7.496916	1.101629	0.382101
H	7.752738	-0.687065	-2.263834	H	-8.032256	0.140829	-1.029505
H	5.495018	-0.102074	3.140338	H	-5.979306	-0.359908	-2.234366
H	6.316465	0.149222	1.100980	H	-6.148211	-1.063240	2.034695
H	-6.058749	3.332853	-0.550752	H	5.883806	-3.984979	0.850897
H	-5.786219	3.307069	-2.323955	H	6.103921	-2.282941	0.357678
H	-6.005128	1.774343	-1.440184	H	5.764267	-2.682289	2.074893
H	3.665189	1.689251	3.031207	H	4.245039	-3.141656	-1.389611
H	-4.085911	3.722767	0.765449	H	3.485057	-2.501604	2.826582
H	0.068091	-3.307728	-2.955855	H	1.601786	3.291762	-0.504256
H	1.163874	-2.577451	-4.160142	H	1.656226	4.546595	-1.775804
H	1.805601	-3.728918	-2.955127	H	0.761889	4.856141	-0.260327
H	2.358666	-1.257770	-2.395277	H	-0.831392	4.299000	-2.176956
H	2.952175	-4.682450	-0.587764	H	-3.916426	4.447815	-1.217708
H	3.717256	3.604969	-1.802805	H	-2.939770	4.340016	-2.716078
H	4.613115	-4.085062	-0.337267	H	-4.536023	3.549336	2.631474
H	-0.580886	-4.880246	1.289859	H	-3.176385	4.432787	2.361590
H	1.054390	-4.320845	1.773894	H	-3.976858	3.685261	0.948611
H	-0.342303	-3.239903	1.989361	H	-3.061353	2.657030	2.103483
H	-0.694161	-3.164709	-0.529709	H	-0.902286	3.837319	1.470524
H	3.098508	-2.742854	1.147105	H	-3.704260	1.888150	-0.927632
H	-0.757916	0.002404	3.762620	H	0.064015	1.819706	2.908157
H	-2.681513	-0.377165	5.352918	H	1.601589	3.023262	4.501565
H	-4.898702	-1.151508	4.488528	H	4.031572	3.287995	3.952232
H	-5.240217	-1.547772	2.041897	H	4.955011	2.342916	1.825085
H	-5.772251	-0.483405	0.208943	H	5.825255	0.563400	0.949205
H	-7.572095	-1.155343	-1.377235	H	7.978432	0.458485	-0.297617
H	-7.020586	-2.520594	-3.414488	H	7.997899	0.596793	-2.806983
H	-4.640601	-3.213588	-3.834406	H	5.826483	0.849230	-4.051151
H	-2.846165	-2.575534	-2.226029	H	3.673348	0.994856	-2.799701
H	-1.397382	-0.834883	-1.331521	H	1.947300	-0.113389	-1.558736
H	0.488377	4.603496	-0.676679	H	-0.688077	-4.586200	0.934149
H	0.691890	3.745990	-2.241227	H	-0.247990	-4.754809	-0.798047
H	2.675944	3.972571	0.096305	H	-2.964923	-4.348334	0.138217
H	3.036895	3.625717	-1.629612	H	-2.416440	-3.995550	-1.536350
H	3.768800	-1.699251	-0.113432	H	-2.708190	1.805510	-2.393149
H	0.627405	-0.901259	2.363012	H	0.018928	2.741884	-2.446182
H	0.705044	-4.239676	-0.769443	H	-1.779650	4.842065	0.289444

L=P ^t Pr ₃ in <i>cis</i>				L=P ^t Pr ₃ in <i>trans</i>			
Ru	-0.772139	0.363401	0.961734	Ru	-0.739778	0.166504	0.002495
Cl	-0.896396	-0.927905	3.024971	Cl	-1.643553	-0.005632	2.255848
Cl	-1.350812	2.178661	2.442503	Cl	-0.520392	0.277552	-2.436734
P	-1.091042	2.043246	-0.813479	P	-1.026714	2.628501	0.190047
N	-0.167522	-2.594745	0.165048	N	-0.237326	-2.834404	-0.580376
N	-2.322482	-2.086589	0.244798	N	-2.377180	-2.321238	-0.720633
C	-2.277262	-3.523498	0.593981	C	-2.312297	-3.679048	-1.306907
C	1.102357	0.472314	0.827131	C	1.114634	0.263211	0.323672
C	6.622899	0.919949	-2.753466	C	6.918929	1.487095	-2.537724
C	3.296388	0.705674	-0.004727	C	3.379694	0.701418	-0.192040
C	3.332025	0.979187	1.457216	C	3.278807	0.524545	1.280251
C	1.739691	1.052200	3.326076	C	1.552893	0.035075	2.944251
C	5.322718	1.255843	-3.175136	C	5.673752	2.021341	-2.918690
C	-3.620524	-1.542200	-0.087508	C	-3.678408	-1.722960	-0.547132
C	-4.127644	-0.828960	2.342323	C	-3.718477	-2.715151	1.810870
C	-4.499959	-1.000921	0.891144	C	-4.352682	-1.930438	0.689059
C	4.364464	1.420144	2.294682	C	4.242931	0.651664	2.288229
C	5.754786	0.429074	-0.527733	C	5.862879	0.447037	-0.601815
C	-1.047737	-1.530100	0.205822	C	-1.142649	-1.831189	-0.384725
C	0.388502	3.277762	-0.878835	C	0.147084	3.447311	1.468877
C	-5.800362	-0.624979	0.485986	C	-5.653343	-1.411127	0.835694
C	-6.270876	-0.790088	-0.827693	C	-6.312993	-0.734690	-0.209273
C	-5.400201	-1.386255	-1.760306	C	-5.645841	-0.616777	-1.443142
C	-7.660618	-0.346381	-1.225596	C	-7.694958	-0.153166	-0.011151
C	1.245525	-2.655288	-0.128396	C	1.149183	-2.892871	-0.202339
C	-0.849362	-3.907439	0.212922	C	-0.866843	-4.102111	-1.016954
C	-2.581490	3.165363	-0.424670	C	-2.766978	2.983251	0.843558
C	-2.881615	-1.471761	4.251254	C	-3.168250	4.466282	0.896078
C	2.192023	-2.846576	0.915489	C	1.477799	-3.150857	1.156357
C	3.547761	-3.019829	0.566090	C	2.832753	-3.320725	1.491474
C	3.990974	-3.056832	-0.768143	C	3.855882	-3.255500	0.522867
C	4.437102	0.769544	-0.932593	C	4.599258	0.979360	-0.969515
C	6.831043	0.503279	-1.426669	C	7.005499	0.696104	-1.378702
C	3.022103	-2.923973	-1.780604	C	3.490398	-3.019558	-0.815377
C	1.656949	-2.745859	-1.489496	C	2.146721	-2.844456	-1.207814
C	2.006387	0.808586	1.972610	C	1.911766	0.237036	1.605619
C	1.788946	-2.948118	2.363947	C	0.402494	-3.248476	2.211194
C	5.450005	-3.247624	-1.111046	C	5.302732	-3.439452	0.923852
C	0.669053	-2.754508	-2.633348	C	1.793269	-2.622958	-2.659528
C	4.089647	1.647786	3.665285	C	3.865249	0.441962	3.635621
C	2.797543	1.458352	4.174150	C	2.537613	0.127223	3.956364
C	-1.326435	1.642914	-2.659221	C	-0.811520	3.732508	-1.333675
C	-0.190821	0.780237	-3.221945	C	0.598745	3.595415	-1.938121
C	-3.848077	2.391171	-0.020701	C	-3.833244	2.119744	0.148313
C	-2.692895	1.017535	2.967915	C	-1.887459	3.538180	-2.417204
C	0.396361	4.266713	0.300687	C	-0.304642	3.187569	2.917814
C	0.635874	4.027267	-2.202952	C	0.468526	4.941413	1.271975
C	4.248053	1.182665	2.278347	C	4.530669	1.770269	-2.147184
C	1.983267	0.419920	-0.344230	C	2.114395	0.547895	-0.722012
C	-4.094280	-1.779540	-1.413370	C	-4.342198	-1.115112	-1.647839
C	-3.244057	-2.492338	-2.440675	C	-3.721102	-1.044307	-3.022290
H	-3.469842	-1.636292	2.712614	H	-3.330790	-3.694907	1.459567
H	-3.554821	0.107829	2.519431	H	-2.862703	-2.152898	2.241048
H	5.039460	-0.784220	2.970192	H	-4.450570	-2.908232	2.619319
H	3.063758	-3.553675	2.163883	H	-3.771652	-2.032636	-3.532192
H	-3.738913	-2.490813	-3.431468	H	-4.268792	-0.325893	-3.663916
H	-2.248492	-2.020704	2.558043	H	-2.654774	-0.737458	-2.985161
H	0.438872	-3.797684	-2.945751	H	1.398408	-3.552407	-3.129168
H	-0.289168	-2.275474	2.363740	H	1.017429	-1.836933	-2.776166
H	1.078045	-2.239268	-3.525338	H	2.687892	-2.325866	-3.241650
H	2.641033	-2.703029	3.028127	H	0.841103	-3.463335	3.204807
H	0.938069	-2.283816	2.615595	H	-0.185183	-2.308356	2.285944
H	1.478693	-3.989846	2.609118	H	-0.323787	-4.058731	1.982830
H	-8.370107	-0.411172	-0.375848	H	-8.270522	-0.714664	0.752594
H	-7.658731	0.712798	-1.565989	H	-7.636453	0.902143	0.336442
H	-8.062844	-0.955832	-2.060262	H	-8.278817	-0.152085	-0.954080
H	-5.751628	-1.569144	-2.789952	H	-6.158649	-0.130547	-2.290265
H	-6.475635	-0.199761	1.247565	H	-6.172934	-1.558476	1.797467
H	6.029155	3.618265	-0.241579	H	5.476063	-4.443966	1.367030
H	5.580798	-3.967913	-1.945436	H	5.985412	-3.329444	0.058018
H	5.909284	-2.288150	-1.434200	H	5.601777	-2.695778	1.693293
H	3.333113	-2.983449	2.837649	H	4.275990	-2.963969	-1.587383
H	4.280049	-3.155238	1.379838	H	3.095573	-3.508664	2.545959
H	-9.202561	0.149400	-2.315712	H	-2.903017	3.802637	-2.062795
H	-3.525734	1.734385	2.837595	H	-1.658974	4.203600	-3.278422
H	-2.720820	0.667012	-4.022572	H	-1.895222	2.493574	-2.787649
H	-0.170516	-0.213152	2.734244	H	0.697854	2.616066	-2.445757
H	-0.338071	0.619511	-4.312024	H	0.760287	4.397763	-2.690541
H	0.807609	1.241628	-3.087020	H	1.407737	3.675188	-1.184328
H	-1.284535	2.638651	-3.150640	H	-0.921064	4.759384	-0.919866
H	-3.640489	1.690054	0.802301	H	-3.570681	1.043031	0.177738
H	-4.616029	3.108241	0.336366	H	-4.803209	2.227942	0.679339
H	-4.296184	1.819033	-0.862912	H	-3.998231	2.405005	-0.909141
H	-2.010519	4.902398	-1.678955	H	-2.455177	5.083961	1.477095
H	-3.233816	3.834290	-2.438502	H	-3.261614	4.914145	-0.115347
H	-3.694306	4.908121	-1.091592	H	-4.161655	4.564551	1.385975
H	1.387529	4.766572	0.350447	H	0.533323	3.417569	3.609991
H	-0.365000	0.565909	0.172934	H	-1.153312	3.846130	3.200941
H	0.208297	3.769221	1.271730	H	-0.613377	2.137312	3.084826
H	0.782103	3.360164	-3.074993	H	0.923379	5.172371	0.289721
H	-0.174904	4.741711	2.453678	H	-0.423215	5.589032	1.401393
H	1.566761	4.625768	-2.098219	H	1.202793	5.248973	2.048010
H	1.243805	2.584332	-0.731142	H	1.084832	2.874739	1.302497
H	-2.218878	3.656112	0.503178	H	-2.680912	2.595399	1.882101
H	0.718075	0.929226	3.711365	H	0.504862	-0.178848	3.197685
H	2.594271	1.641532	5.241186	H	2.249120	-0.036590	5.007002
H	4.900135	1.987089	4.330388	H	4.620397	0.533786	4.432998
H	5.373962	1.614865	1.902219	H	5.280640	0.927673	2.046779
H	5.927078	0.067299	0.496179	H	5.939529	-0.202203	0.282414
H	7.842863	0.228698	-1.087431	H	7.973062	0.262738	-1.078157
H	7.469310	0.985198	-3.455419	H	7.817739	1.686514	-3.142692
H	5.147649	1.589547	-4.210544	H	5.594355	2.645407	-3.823277
H	3.240201	1.476147	-2.610061	H	3.563458	2.205983	-2.441527
H	1.643481	0.135945	-1.345234	H	1.862841	0.585515	-1.786871
H	-0.364390	-4.562877	0.963935	H	-0.789660	-4.862269	-0.207052
H	-0.782381	-4.414995	-0.777438	H	-0.347367	-4.507213	-1.908789
H	-2.461627	-3.644368	1.684794	H	-3.067717	-4.341239	-0.835632
H	-3.053170	-4.091569	0.042949	H	-2.530286	-3.633240	-2.396362

L=PCy ₃ in cis			L=PCy ₃ in trans				
Ru	0.530073	-0.331757	-1.203480	Ru	0.505973	-0.444539	0.030726
Cl	0.448838	-1.955945	-3.013598	Cl	1.253331	-0.721115	-2.271439
Cl	1.229092	1.139794	-2.982828	Cl	0.410009	-0.297196	2.469263
P	1.037302	1.604034	0.259871	P	1.079416	1.975851	-0.185289
N	-0.279476	-3.051484	0.075923	N	-0.337801	-3.387276	0.544751
N	1.905935	-2.761332	-0.123199	N	1.837332	-3.110454	0.765599
C	1.736350	-4.228459	-0.186675	C	1.615958	-4.478588	1.288864
C	-1.323120	-0.034138	-1.048400	C	-1.332241	-0.116284	-0.217399
C	-6.646508	1.447446	2.551223	C	-6.799486	1.947308	2.817078
C	-3.461318	0.503018	-0.212282	C	-3.498522	0.622023	0.370834
C	-3.540415	0.501387	-1.698014	C	-3.519903	0.262524	-1.070731
C	2.022347	0.127676	3.593114	C	1.968345	-0.582088	-2.762466
C	-5.309740	1.755504	2.866123	C	-5.495982	2.421219	3.056943
C	3.255821	-2.282570	0.073688	C	3.206565	-2.666828	0.652801
C	3.707516	-2.072920	-2.458584	C	3.200546	-3.536106	-1.753202
C	4.129273	-1.996208	-1.012826	C	3.894360	-2.907319	-0.570504
C	-4.578693	0.845370	-2.573035	C	-4.534845	0.377915	-2.029870
C	-5.908913	0.501300	0.427534	C	-5.957461	0.618401	0.958484
C	0.685889	-2.093454	-0.156069	C	0.674263	-2.483755	0.401066
C	5.467915	-1.651931	-0.722727	C	5.263861	-2.584697	-0.642708
C	5.978119	-1.602609	0.586178	C	5.973081	-2.068318	0.459829
C	5.110589	-1.960331	1.635990	C	5.275040	-1.897326	1.669912
C	7.406946	-1.189072	0.857788	C	7.440456	-1.718045	0.351361
C	-1.677163	-2.930057	0.410523	C	-1.714020	-3.298938	0.134875
C	0.275799	-4.414448	0.224298	C	0.126694	-4.715460	1.008416
C	-2.679482	-3.262636	-0.538139	C	-2.046167	-3.631248	-1.205971
C	-4.025286	-3.271282	-0.110585	C	-3.405932	-3.682123	-1.560328
C	-4.403058	-3.007397	1.217140	C	-4.430703	-3.415759	-0.628747
C	-4.555123	0.812106	0.722775	C	-4.636620	1.086829	1.181413
C	-6.938388	0.815633	1.329429	C	-7.022800	1.041160	1.765581
C	-3.380541	-2.722011	2.144799	C	-4.063082	-3.101408	0.692968
C	-2.025752	-2.694382	1.771887	C	-2.714973	-3.047760	1.105439
C	-2.248888	0.150998	-2.210761	C	-2.214679	-0.203887	-1.436749
C	-2.355824	-3.679616	-1.951258	C	-0.970255	-3.919047	-2.226380
C	-5.851262	-3.035536	1.647926	C	-5.881422	-3.454278	-1.053980
C	-0.968871	-2.491601	2.832286	C	-2.358801	-2.755403	2.543159
C	-4.347104	0.797440	-3.969244	C	-4.270813	-0.010087	-3.364289
C	-3.088798	0.437195	-4.470959	C	-3.003018	-0.490370	-3.722527
C	-4.281471	1.443004	1.966080	C	-4.429864	1.996373	2.252222
C	-2.153834	0.201468	0.135400	C	-2.214374	0.416897	0.836737
C	3.771418	-2.325962	1.404132	C	3.905924	-2.209507	1.803495
C	2.951097	-2.853650	2.560476	C	3.253730	-2.130487	3.162336
H	2.954012	-2.860512	-2.641376	H	2.690144	-4.482484	-1.473606
H	3.224142	-1.133264	-2.804129	H	2.426717	-2.851159	-2.161673
H	4.588299	-2.251455	-3.106847	H	3.925112	-3.765837	-2.558741
H	3.050868	-3.959782	2.640701	H	3.238258	-3.131289	3.650296
H	3.299221	-2.433385	3.524573	H	3.823064	-1.457446	3.833846
H	1.872713	-2.636091	2.452296	H	2.211367	-1.757516	3.099385
H	-0.538944	-3.463194	3.164328	H	-2.037436	-3.678411	3.076656
H	-0.126601	-1.874820	2.464978	H	-1.523450	-2.027539	2.619882
H	-1.392947	-2.004668	3.732382	H	-3.232288	-2.351666	3.091804
H	-3.164074	-3.374330	-2.645473	H	-1.413516	-4.133448	-3.212894
H	-1.403693	-3.244205	-2.314399	H	-0.272475	-3.061096	-2.336121
H	-2.278202	-4.788921	-2.019599	H	-0.351639	-4.798376	-1.941886
H	8.064499	-1.393640	-0.011185	H	7.948481	-2.319014	-0.429938
H	7.473135	-0.098462	1.066844	H	7.579078	-0.647775	0.080078
H	7.825940	-1.714342	1.740406	H	7.971654	-1.878108	1.311745
H	5.494326	-1.985091	2.670313	H	5.816845	-1.533045	2.559238
H	6.139904	-1.431232	-1.569184	H	5.797700	-2.769939	-1.589994
H	-6.493204	-3.530127	0.891167	H	-6.120189	-4.388672	-1.604716
H	5.977694	-3.572241	2.611443	H	-6.566402	-3.384514	-0.185453
H	6.240975	-2.005009	1.796384	H	6.114366	-2.609969	-1.739003
H	-3.643940	-2.533752	3.199456	H	-4.849896	-2.895529	1.437907
H	-4.803619	-3.520609	-0.851495	H	-3.672079	-3.932950	-2.600743
H	-1.025346	-0.127794	-3.979127	H	-0.965549	-0.928562	-3.048777
H	-2.918449	0.407858	-5.558877	H	-2.801727	-0.788162	-4.763983
H	-5.163243	0.558225	-4.662271	H	-5.064861	0.075734	-4.123617
H	-5.558525	1.173741	-2.194887	H	-5.521875	0.784743	-1.762132
H	6.149214	-0.025539	-0.507156	H	-6.140237	-0.117064	0.157854
H	-7.979839	0.559509	1.076318	H	-8.037241	0.654354	1.577062
H	-7.455914	1.700376	3.254284	H	-7.637409	2.283121	3.448517
H	-5.068359	2.254818	3.818221	H	-5.310324	3.133424	3.876889
H	-3.242561	1.711978	2.211438	H	-3.415232	2.382335	2.435208
H	-1.790030	0.089537	1.161647	H	-1.881630	0.555993	1.870761
H	-0.267920	-5.122058	-0.433720	H	-0.051568	-5.477282	0.217312
H	0.157508	-4.767843	1.274619	H	-0.440879	-5.028364	1.909067
H	1.928063	-4.581702	-1.224420	H	2.280817	-5.200817	0.770201
H	2.451772	-4.738644	0.488677	H	1.857400	-4.514737	2.373216
C	2.643908	2.451754	-0.317117	C	2.733008	2.138305	-1.085606
C	3.212468	3.583549	0.570826	C	3.303364	3.567239	-1.224101
C	3.770511	1.460825	-0.681857	C	3.821378	1.162061	-0.581925
C	2.299899	2.895503	-1.278521	C	2.446702	1.772647	-2.097755
C	4.374398	4.309143	-0.140738	C	4.531834	3.585457	-2.156745
C	3.590090	3.160833	1.529480	C	3.603048	3.952112	-0.223147
C	2.432802	4.323150	0.839568	C	2.534563	4.266533	-1.611937
C	4.928751	2.179054	-1.396482	C	5.038730	1.181401	-1.525392
C	4.156931	0.956132	0.230757	C	4.148642	1.438641	0.443768
C	3.371912	0.666151	-1.340029	C	3.415267	0.130798	-0.522095
C	5.490529	3.337834	-0.556545	C	5.614328	2.597656	-1.692797
C	4.776682	5.108526	0.519709	C	4.942404	4.617061	-2.219567
C	3.977918	4.822794	-1.046440	C	4.206360	3.314781	-3.187496
H	5.730990	1.448598	-1.638024	H	5.816221	0.485841	-1.144843
H	4.557823	2.570338	-2.371041	H	4.727206	0.785341	-2.518759
H	6.286501	3.878212	-1.114175	H	6.465592	2.591882	-2.408250
H	5.976044	2.926985	0.359460	H	6.029481	2.943102	-0.717266
C	-0.307927	2.969652	0.105157	C	1.209203	3.078344	1.347013
C	-0.257879	4.162553	1.093485	C	-0.127256	3.157859	2.121620
C	-0.501031	3.508094	-1.330098	C	2.362750	2.718245	2.311957
H	-1.222731	2.381199	0.347014	H	1.427317	4.088851	0.927547
C	-1.544590	5.009399	0.999372	C	-0.046369	4.170546	3.278743
H	0.607124	4.816473	0.847851	H	-0.343309	2.147259	2.526033
H	-0.114581	3.834040	2.142769	H	-0.967508	3.420859	1.445284
C	-1.771819	4.373310	-1.439488	C	2.438989	3.722171	3.480183
H	0.384125	4.122713	-1.613696	H	2.194645	1.691123	2.701523
H	-0.540252	2.679137	2.061949	H	3.333577	2.708700	1.775712
C	-1.778235	5.529079	-0.427352	C	1.106215	3.830932	4.238465
H	-1.487932	5.854032	1.720865	H	-1.013859	4.194395	3.826382
H	-2.415078	4.388193	1.313587	H	0.104077	5.197239	2.868939
H	-1.865879	4.761425	-2.476694	H	3.257163	3.426032	4.172509

H	-2.663416	3.727848	-1.269594		H	2.716818	4.727032	3.083252
H	-2.732766	6.096666	-0.483150		H	1.179888	4.591335	5.046491
H	-0.969776	6.251436	-0.687250		H	0.889588	2.858776	4.736551
C	1.251760	1.546652	2.149216		C	-0.171069	2.929421	-1.281043
C	-0.030818	1.193646	2.929432		C	-0.267733	4.465896	-1.117392
C	2.412269	0.645653	2.608290		C	-0.026531	2.573307	-2.778812
H	1.521326	2.596310	2.404597		H	-1.138579	2.449503	-0.933559
C	0.185216	1.290284	4.452810		C	-1.448166	5.028322	-1.937817
H	-0.333337	0.158124	2.666752		H	0.674047	4.945381	-1.465620
H	-0.872544	1.852477	2.631964		H	-0.394563	4.758739	-0.056061
C	2.637197	0.739639	4.129629		C	-1.202857	3.132578	-3.601396
H	2.180884	-0.401978	2.326679		H	0.921854	3.010583	-3.167575
H	3.350418	0.901851	2.077194		H	0.056800	1.476345	-2.913288
C	1.359433	0.414698	4.919433		C	-1.350023	4.652119	-3.424677
H	-0.748898	1.007659	4.985752		H	-1.493513	6.132712	-1.815112
H	0.387962	2.352099	4.725027		H	-2.400682	4.629585	-1.518834
H	3.466236	0.062583	4.431272		H	-1.062609	2.875971	-4.673919
H	2.975119	1.770708	4.385509		H	-2.141244	2.624950	-3.282125
H	1.530052	0.540713	6.010783		H	-2.237969	5.027978	-3.978423
H	1.098627	-0.657736	4.766515		H	-0.465136	5.161966	-3.872286

L=PPh ₃ in <i>cis</i>			L=PPh ₃ in <i>trans</i>				
Ru	0.588572	-0.554682	-1.084459	Ru	-0.608485	-0.314246	-0.037991
Cl	1.241331	0.609510	-3.073748	Cl	-0.418625	0.004045	-2.443423
Cl	0.603626	-2.496461	-2.540366	Cl	-1.534835	-0.591931	2.166994
P	1.130628	1.534523	-0.023546	P	-1.077503	2.090396	0.156465
N	-0.249611	-2.892769	0.812022	N	0.203406	-3.198915	-0.878463
N	1.932330	-2.643978	0.575423	N	-1.976353	-2.864981	-0.945977
C	-1.983604	-0.689830	-3.492149	C	1.700177	-0.944993	2.787868
C	-3.053679	-0.595307	-4.414921	C	2.694160	-1.067942	3.787890
C	-1.263851	-0.208143	-0.992879	C	1.217768	-0.052521	0.333259
C	-4.520458	0.303546	-2.674540	C	4.361619	-0.082985	2.293933
C	3.252560	-2.065701	0.581617	C	-3.323812	-2.445771	-0.643698
C	-3.376087	0.589782	-0.323810	C	3.433148	0.643754	-0.055757
C	0.314234	-4.134096	1.390700	C	-0.317638	-4.448197	-1.481081
C	-3.971933	-3.188259	0.432156	C	3.288497	-3.820282	1.133339
C	-4.443409	1.184661	0.495414	C	4.628936	1.166022	-0.735643
C	5.497344	-1.821765	-0.317617	C	-5.242885	-2.550193	0.846613
C	-2.198296	-0.317853	-2.159414	C	2.041245	-0.406440	1.541325
C	-3.477373	0.180810	-1.749393	C	3.384906	0.025772	1.296568
C	-3.479637	-2.064260	2.507754	C	3.938488	-3.012614	-1.049578
C	-5.802206	0.798696	0.356545	C	5.898810	0.549236	-0.586717
C	3.866425	-3.226967	-1.629621	C	-3.088692	-3.620195	1.618429
C	-2.599226	-3.282900	0.115667	C	1.927835	-3.693765	0.802794
C	5.909989	-1.081677	0.804617	C	-6.047590	-1.881271	-0.098496
C	-2.167764	-4.041385	-1.113838	C	0.857483	-4.086687	1.793674
C	-4.132365	2.180674	1.458851	C	4.530120	2.292566	-1.594110
C	1.793114	-4.052438	0.999789	C	-1.800574	-4.125143	-1.703810
C	3.664887	-1.391183	1.767726	C	-4.117081	-1.813869	-1.637058
C	4.190456	-2.344068	-0.450332	C	-3.893452	-2.857670	0.595761
C	4.977823	-0.893051	1.845705	C	-5.465434	-1.529559	-1.328730
C	0.715258	-2.034874	0.340092	C	-0.784209	-2.311481	-0.557634
C	-6.803586	1.379254	1.150671	C	7.022874	1.039589	-1.269731
C	-1.665156	-2.706422	1.014524	C	1.588879	-3.201353	-0.486643
C	-1.115748	-1.599996	3.254942	C	2.235091	-2.432954	-2.836047
C	-2.101808	-2.117978	2.235355	C	2.588500	-2.878252	-1.437737
C	-2.072679	0.362990	0.082038	C	2.151144	0.631014	-0.573014
C	-5.909966	-2.541234	1.951895	C	5.764296	-3.604821	0.623665
C	2.738451	-1.278371	2.953458	C	-3.586292	-1.498467	-3.015281
C	-4.436689	-2.592952	1.617742	C	4.311155	-3.479515	0.224546
C	-5.133802	2.758546	2.251792	C	5.656434	2.783304	-2.269324
C	-4.303336	-0.103680	-0.013830	C	4.009235	-0.646050	3.544108
C	-6.475769	2.361643	2.102018	C	6.908851	2.160818	-2.110579
C	7.306275	-0.510051	0.900990	C	-7.500715	-1.584018	0.200727
H	2.483754	-4.278294	1.838327	H	-2.041181	-3.960591	-2.776789
H	2.041681	-4.731493	0.154574	H	-2.484867	-4.907771	-1.315668
H	0.155559	-4.152749	2.493008	H	0.222575	-4.678169	-2.422101
H	-0.196299	-5.020049	0.962166	H	-0.159501	-5.301943	-0.784529
H	2.843977	-3.050966	-0.022616	H	-2.364701	-2.936551	2.113332
H	4.592462	-3.068045	2.451082	H	-3.746920	-4.054258	2.396481
H	3.931737	-4.300379	-1.341735	H	-2.506025	-4.445264	1.158245
H	1.844883	-0.665280	2.723449	H	-2.543758	-1.119861	-2.989778
H	2.370562	-2.276380	3.274223	H	-3.603073	-2.404008	-3.663024
H	3.251990	-0.811248	3.815168	H	-4.219632	-0.737984	-3.513515
H	7.714329	-0.589894	1.929123	H	-8.083884	-2.520775	0.335412
H	8.006267	-1.016727	0.206700	H	-7.612422	-1.004293	1.142018
H	7.309863	0.572424	0.644433	H	-7.978203	-1.006343	-0.615661
H	-2.993068	-4.099985	-1.850358	H	1.302880	-4.353454	2.771639
H	-1.285800	-3.580921	-1.603607	H	0.129857	-3.265625	1.957837
H	-1.891718	-5.088896	-0.852999	H	0.274579	-4.967583	1.444352
H	-1.615812	-0.944517	3.994877	H	3.128732	-2.046691	-3.364398
H	-0.646259	-2.430987	3.827354	H	1.838569	-3.279282	-3.441103
H	-0.289849	-1.030532	2.787321	H	1.452603	-1.644735	-2.833076
H	-6.258319	-1.492960	2.068335	H	6.027093	-2.855069	1.401742
H	-6.525333	-3.019290	1.163941	H	5.983296	-4.603657	1.057025
H	-6.122935	-3.060973	2.910805	H	6.442722	-3.450516	-0.239007
H	-3.815367	-1.602807	3.451847	H	4.722727	-2.748574	-1.778604
H	-4.700224	-3.622763	-0.273059	H	3.556369	-4.191712	2.136562
H	6.221117	-2.025415	-1.124835	H	-5.683275	-2.861386	1.809038
H	5.288019	-0.363713	2.762230	H	-6.080256	-1.022849	-2.091312
H	-0.992277	-1.046645	3.806841	H	0.658636	-1.235823	2.987753
H	-2.892150	-0.899086	-5.461358	H	2.425238	-1.489137	4.769652
H	-5.122527	-0.016921	-4.745829	H	4.772178	-0.734769	4.334415
H	-5.490728	2.734227	-2.383696	H	5.384454	2.288620	2.127625
H	-6.066821	0.009025	-0.362889	H	5.992111	-0.348914	0.041646
H	-7.850635	1.058420	1.027823	H	7.996482	0.537995	-1.148149
H	-7.263586	2.812086	2.719963	H	7.793140	2.548900	-2.640835
H	-4.867831	3.538055	2.983770	H	5.557697	3.664977	-2.922690
H	-3.091532	2.528343	1.549416	H	3.557812	2.796794	-1.706681
H	-1.698348	0.540914	1.094779	H	1.857458	0.989971	-1.565978
C	2.716910	2.237561	-0.714361	C	-2.836299	2.427128	-0.331763
C	3.801483	1.372552	-0.974045	C	-3.219443	3.505160	-1.160144
C	2.867686	3.618172	-0.964913	C	-3.834428	1.592309	0.222348
C	5.012643	1.880304	-1.472003	C	-4.578455	3.740156	-1.434868
C	3.703653	0.290175	-0.799819	C	-2.456723	4.173029	-1.587169
C	4.080471	4.122696	1.466996	C	-5.190670	1.840455	-0.047468
C	2.030149	3.407869	-0.782974	C	-3.546227	0.757896	0.883847
C	5.156561	3.256415	-1.722561	C	-5.566855	2.910619	-0.878056
H	5.842245	1.186604	-1.681000	H	-4.863534	4.584416	-2.083069
H	4.177421	5.201721	-1.667916	H	-5.957049	1.186930	0.396244
H	6.103125	3.651324	-2.125186	H	-6.631470	3.100365	-1.089693
C	1.441365	1.765760	1.813344	C	-0.071059	3.282349	-0.854123
C	0.379137	1.646447	2.740522	C	-0.153568	3.272545	-2.268219
C	2.721820	2.102538	2.307889	C	0.823600	4.182065	-0.230653
C	0.586652	1.858476	4.113595	C	0.633415	4.152208	-3.031527
H	-0.635666	1.413007	2.387671	H	-0.822284	2.560451	-2.771934
C	2.930546	2.310601	3.683755	C	1.612275	5.055249	-1.000414
H	3.566101	2.212070	1.612307	H	0.905117	4.208068	0.865996
C	1.866456	2.190379	4.592537	C	1.517741	5.046389	-2.402720
H	-0.261238	1.770539	4.811676	H	0.553295	4.133080	-4.130251
H	3.937325	2.577679	4.043394	H	2.301092	5.750622	-0.494735
H	2.030148	2.361519	5.668427	H	2.130243	5.736797	-3.004699
C	-0.073663	2.934562	-0.347129	C	-0.993684	2.851748	1.850175
C	-0.757144	2.979916	-1.583368	C	0.014206	2.436103	2.746327
C	-0.274134	3.983076	0.580538	C	-1.886532	3.873106	2.243721
C	-1.631684	4.039966	-1.874359	C	0.136888	3.042543	4.008136
H	-0.584303	2.188408	2.329469	H	0.702934	1.628089	2.461170
C	-1.153120	5.041540	0.284854	C	-1.765485	4.471781	3.509645
H	0.261748	3.986403	1.540921	C	-2.684255	4.203641	1.560717
C	-1.837870	5.071257	-0.941405	C	-0.753078	4.059736	4.393949
H	-2.157792	4.053001	-2.841907	H	0.927829	2.705004	4.696359

H -1.296894	5.849089	1.020867		H -2.470306	5.265390	3.805493
H -2.528687	5.898368	-1.170756		H -0.661826	4.528439	5.386996

L=py in cis				L=py in trans			
Ru	-0.913461	-0.185789	1.049080	Ru	-0.926409	0.465560	0.033489
Cl	-1.705773	0.472704	3.188066	Cl	-0.758516	0.405768	-2.395238
Cl	-1.069741	-2.473159	1.809988	Cl	-1.660962	0.633558	2.323526
N	-0.512877	-1.838375	-1.542504	N	-0.261358	-2.553449	0.407747
N	-2.618589	-1.311658	-1.094816	N	-2.398615	-2.117425	0.082137
C	1.784301	-1.503782	3.039880	C	1.366670	1.735434	2.680495
C	2.908403	-1.845377	3.828409	C	2.334541	2.362648	3.503024
C	0.961921	0.003336	1.023606	C	0.929572	0.686696	0.264875
C	4.332611	-0.360082	2.507638	C	4.003001	2.164054	1.730959
C	-3.792607	-0.507850	-0.843151	C	-3.645961	-1.463035	-0.229812
C	3.083198	0.925614	0.584896	C	3.161546	0.968294	-0.451495
C	-1.296805	-2.626250	-2.520449	C	-0.897183	-3.889871	0.459300
C	3.099031	-2.838703	-1.570815	C	3.169618	-2.400848	1.874113
C	4.153952	1.708427	-0.051778	C	4.352265	0.963365	-1.317135
C	-5.735332	0.143908	0.463080	C	-5.746545	-0.455297	0.460718
C	1.944933	-0.616828	1.967418	C	1.716066	1.315403	1.389852
C	3.232027	-0.042922	1.701015	C	3.061927	1.506457	0.930779
C	2.843240	-0.792282	-2.822978	C	3.348685	-2.834114	-0.498991
C	5.470632	1.195794	-0.192357	C	5.661486	0.787912	-0.796610
C	-4.305245	-1.704484	1.381221	C	-4.277396	-1.431874	2.261902
C	1.722391	-2.862849	-1.260108	C	1.764442	-2.326794	1.784775
C	-6.127107	1.084542	-0.503715	C	-6.116260	-0.231972	-0.879684
C	1.144220	-4.018903	-0.481557	C	0.919034	-2.092414	3.013868
C	3.889591	3.004226	-0.570265	C	4.211186	1.109207	-2.723118
C	-2.726463	-2.483945	-1.989389	C	-2.396542	-3.561054	0.393750
C	-4.201662	0.393669	-1.873600	C	-4.037661	-1.352475	-1.594649
C	4.594879	-0.677617	0.316997	C	-4.538303	-1.088450	0.814615
C	-5.352193	1.178033	-1.677585	C	-5.260290	-0.714321	-1.888136
C	-1.304741	-1.069747	-0.729606	C	-1.149984	-1.547604	0.161229
C	6.475554	1.945786	-0.824129	C	6.779220	0.757864	-1.646214
C	0.914274	-1.797144	-1.732609	C	1.170201	-2.500378	0.510329
C	0.603154	0.339399	-3.106397	C	1.307174	-2.926854	-2.003732
C	1.466921	-0.762447	-2.536671	C	1.952231	-2.756403	-0.647628
C	1.742223	0.963784	0.239769	C	1.917715	0.487132	-0.806059
C	5.153162	-1.838738	-2.695099	C	5.480710	-2.782454	0.875600
C	-3.458293	0.494659	-3.189224	C	-3.207724	-1.935890	-2.711010
C	3.681027	-1.822592	-2.349452	C	3.977976	-2.664913	0.751986
C	4.894436	3.751624	-1.200293	C	5.329158	1.081560	-3.568451
C	4.164880	-1.279216	3.570306	C	3.632800	2.589149	3.029841
C	6.194448	3.227381	-1.329735	C	6.620174	0.907538	-3.035156
C	-7.332418	1.972482	-0.292370	C	-7.400450	0.490296	-1.221217
H	-3.477304	-2.310902	2.785379	H	-2.934229	-4.129989	-0.393542
H	-3.045202	-3.373352	-1.401096	H	-2.914013	-3.748364	1.360132
H	-1.166016	-2.207182	-3.545180	H	-0.555180	-4.510842	-0.398038
H	-0.947802	-3.677885	-2.538401	H	-0.607718	-4.417822	1.391486
H	-3.657272	-2.522204	1.018045	H	-3.207822	-1.330883	2.527662
H	-3.763125	-1.248853	2.238093	H	-4.851955	-0.765191	0.934707
H	-5.252516	-2.128741	1.771366	H	-4.608234	-2.473211	2.477040
H	-2.366880	0.344034	-3.076458	H	-2.303357	-1.314507	-2.895453
H	-3.813337	-0.272795	-3.912936	H	-2.856165	-2.960825	-2.469889
H	-3.625357	1.480477	-3.667330	H	-3.795840	-1.987280	-3.648494
H	-7.859774	2.183789	-1.245200	H	-7.750478	0.244233	-2.244074
H	-8.057654	1.517057	0.411523	H	-8.212801	0.241105	-0.507828
H	-7.031276	2.953018	0.138205	H	-7.260669	1.593139	-1.177672
H	1.948270	-4.602866	0.007778	H	1.554791	-1.891769	3.898170
H	0.428047	-3.675313	0.294767	H	0.221338	-1.238242	2.881570
H	0.596662	-4.720721	-1.151203	H	0.291830	-2.980681	3.250279
H	1.225443	1.135743	-3.559552	H	2.072451	-2.945023	-2.804309
H	-0.073400	-0.040086	-3.904165	H	0.737571	-3.879966	-2.076605
H	-0.039585	0.803704	-2.331204	H	0.593114	-2.104228	-2.223489
H	5.627331	-0.857246	-2.484585	H	5.997289	-2.128743	0.141657
H	5.699256	2.615352	2.123376	H	5.832146	-2.506652	1.889843
H	5.309188	-2.046775	-3.776315	H	5.819196	-3.822223	0.674037
H	3.273709	0.016739	3.436769	H	3.965950	-3.025065	-1.392959
H	3.733912	-3.657059	-1.191699	H	3.643592	-2.258618	2.859682
H	-6.347231	0.021412	1.372561	H	-6.429239	-0.141728	1.268583
H	-5.656283	1.880894	-2.472081	H	-5.560164	-0.615000	-2.945103
H	0.792069	-1.927238	3.253236	H	0.342851	1.565401	3.046508
H	2.785946	-2.552587	4.664152	H	2.053979	2.682424	4.519357
H	5.027475	-1.536861	4.205849	H	4.373297	3.098951	3.666394
H	5.312502	0.114123	2.344434	H	5.018273	2.367326	1.358288
H	5.695115	0.182664	0.171942	H	5.798209	0.637784	0.284322
H	7.488103	1.5222972	-0.925462	H	7.784410	0.612164	-1.218620
H	6.985256	3.817672	-1.819333	H	7.498495	0.890702	-3.699928
H	4.665664	4.758657	-1.584815	H	5.193330	1.205874	-4.654834
H	2.882855	3.433518	-0.447975	H	3.206752	1.270112	-3.144953
H	1.330307	1.577040	-0.570415	H	1.668772	0.038362	-1.772003
C	-0.501278	2.765514	1.415327	C	-1.179633	3.467051	0.760298
C	-1.717119	2.343389	-0.522135	C	-2.388145	2.878578	-1.148585
C	-0.594116	4.148347	1.214280	C	-1.670189	4.777620	0.713874
H	0.011348	2.349756	2.292473	H	-0.485442	3.141140	1.547339
C	-1.855194	3.710918	-0.785025	C	-2.940011	4.163567	-1.242437
H	-2.167758	1.593854	-1.181247	H	-2.600897	2.094440	-1.8924175
C	-1.281357	4.643606	0.095507	C	-2.574919	5.136422	-0.299192
H	-0.125650	4.823195	1.946331	H	-1.342252	5.501634	1.474657
H	-2.415140	4.029009	-1.677047	H	-3.639214	4.390046	-2.061256
H	-1.371453	5.726077	-0.084443	H	-2.984820	6.157343	-0.353213
N	-1.052059	1.854999	0.557799	N	-1.527919	2.530185	-0.157447

L=PF ₃ in <i>cis</i>				L=PF ₃ in <i>trans</i>			
Ru	0.976629	-0.245549	0.934168	Ru	0.960209	0.587679	0.007165
Cl	1.701907	-1.610165	2.745060	Cl	0.925655	0.176201	2.378603
Cl	1.239712	1.628737	2.427446	Cl	1.486966	0.910925	-2.319258
P	1.205240	-2.039791	-0.288124	P	1.327329	2.768366	0.425006
N	0.463239	2.159233	-1.032176	N	0.456982	-2.428921	-0.874483
N	2.563960	1.485273	-0.907341	N	2.552752	-1.945568	-0.403329
C	-1.557295	0.205078	3.362865	C	-1.272874	2.739407	-2.012340
C	-2.618458	0.239877	4.300568	C	-2.236127	3.591155	-2.608706
C	-0.919615	-0.449292	0.879214	C	-0.906780	0.896593	-0.152332
C	-4.174908	-0.616230	2.620198	C	-3.973159	2.714670	-1.122089
C	3.724425	0.629874	-0.808143	C	3.733888	-1.283699	0.101290
C	-3.087776	-1.125504	0.283748	C	-3.146851	0.831952	0.530826
C	1.198803	3.133537	-1.876939	C	1.179351	-3.681743	-1.215866
C	-3.062940	3.234022	-0.356187	C	-3.046563	-2.291309	-2.176454
C	-4.210045	-1.641807	-0.511212	C	-4.344305	0.513129	1.320429
C	5.766925	-0.081775	0.289029	C	5.744033	0.032548	-0.240310
C	-1.819232	-0.200887	0.2049945	C	-1.668698	1.883130	-0.979648
C	-3.138847	-0.620612	1.680647	C	-3.036585	1.844872	-0.557502
C	3.049125	1.734520	-2.247751	C	-3.087300	-3.052714	0.117940
C	-5.524272	-1.120369	-0.377428	C	-5.645848	0.529114	0.751912
C	4.519413	1.866085	1.298596	C	4.448912	-0.667112	-2.289405
C	-1.667681	3.099018	-0.195160	C	-1.644248	-2.144680	-2.136826
C	6.008102	-1.044540	-0.709807	C	6.041107	-0.009711	1.134527
C	-0.944823	3.912319	0.849602	C	-0.881875	-1.686448	-3.356536
C	-3.996603	-2.675298	-1.462498	C	-4.219929	0.157984	2.690809
C	2.668223	2.788264	-1.598371	C	2.652652	-3.307027	-0.976954
C	3.986581	-0.266825	-1.881608	C	4.062167	-1.439571	1.478278
C	4.654552	0.782971	0.257220	C	4.618822	-0.616337	-0.789532
C	5.119451	-1.098431	-1.799782	C	5.204568	-0.779355	1.967374
C	1.284393	1.201788	-0.513263	C	1.280210	-1.458435	-0.408227
C	-6.577057	-1.608622	-1.166939	C	-6.772953	0.202200	1.522347
C	-0.977748	2.225732	-1.075350	C	-0.981520	-2.451553	-0.923291
C	-0.922705	0.698024	-3.133327	C	-0.973523	-3.228250	1.510613
C	-1.659351	1.555252	-2.128998	C	-1.690848	-2.914699	0.216958
C	-1.772214	-1.041259	-0.142761	C	-1.893099	0.271011	0.717371
C	-5.266983	2.738881	-1.530170	C	-5.288696	-2.897754	-1.135522
C	3.133261	-0.296414	-3.130553	C	3.242783	-2.314965	2.394842
C	-3.773289	2.567699	-1.370911	C	-3.785920	-2.747226	-1.068645
C	-5.051161	-1.364578	-2.245103	C	-5.348165	-0.162037	3.457985
C	-3.908807	-0.164733	3.936889	C	-3.561922	3.590289	-2.160011
C	-6.346937	-2.633179	-2.102280	C	-6.631024	-0.140671	2.878751
C	7.178787	-1.994751	-0.608465	C	7.220984	0.745319	1.702203
H	3.281426	2.694572	-2.517322	H	3.169215	-3.988314	-0.268819
H	3.159300	3.530723	-0.931629	H	3.245461	-3.279985	-1.916139
H	0.915152	2.995027	-2.944057	H	0.828755	-4.511849	-0.564995
H	0.933358	4.170164	-1.588627	H	0.968162	-3.968294	-2.266806
H	3.537259	1.835398	1.814792	H	3.384735	-0.685340	-2.591970
H	5.316606	1.775274	2.061544	H	4.914476	0.215629	-2.770437
H	4.615006	2.874853	0.839741	H	4.957709	-1.567936	-2.701734
H	2.069052	-0.076551	-2.930876	H	2.251838	-1.854413	2.592280
H	3.493327	0.458212	-3.865908	H	3.068469	-3.321515	1.958500
H	3.189334	-1.283841	-3.628545	H	3.757116	-2.452037	3.366034
H	7.518411	-2.337313	-1.606798	H	7.651781	0.230731	2.585176
H	8.040644	-1.530628	-0.087333	H	8.024970	0.878905	0.950336
H	6.896988	-2.901127	-0.028510	H	6.912175	1.760648	2.035606
H	-1.660573	4.345016	1.575841	H	-1.575480	-1.414760	-4.175995
H	-0.200811	3.304878	1.404860	H	-0.236264	-0.810016	-3.133159
H	-0.398852	4.764705	0.385345	H	-0.210645	-2.484910	-3.743416
H	-1.634069	0.106244	-3.741991	H	-1.692650	-3.531540	2.296347
H	-0.328682	1.315807	-3.843258	H	-0.242287	-4.057807	1.395233
H	-0.218359	-0.008522	-2.652204	H	-0.400213	-2.351488	1.885329
H	-5.803331	1.792506	-1.302662	H	-5.791185	-2.118430	-0.522205
H	-5.664353	3.524602	-0.857481	H	-5.664601	-2.805676	-2.173937
H	-5.533902	3.012230	-2.572877	H	-5.615969	-3.880552	-0.736068
H	-3.582277	1.209136	-3.057692	H	-3.648015	-3.405948	0.999581
H	-3.606492	3.902839	0.331939	H	-3.573866	-2.049887	-3.114577
H	6.476202	0.014763	1.127860	H	6.418712	0.577214	-0.922066
H	5.309991	-1.812569	-2.618318	H	5.451348	-0.879519	3.037523
H	-0.536550	0.487503	3.657623	H	-0.228934	2.742235	-2.356902
H	-2.415492	0.572109	5.330807	H	-1.929844	4.268472	-3.421308
H	-4.721482	-0.153763	4.680678	H	-4.297320	4.274339	-2.612837
H	-5.178096	-0.987988	2.362161	H	-5.014198	2.741750	-0.767238
H	-5.710093	-0.300711	0.332092	H	-5.768575	0.764027	-0.315474
H	-7.586855	-1.183068	-1.052475	H	-7.771944	0.213105	1.057715
H	-7.175922	-3.020621	-2.715517	H	-7.517538	-0.387680	3.484136
H	-4.863887	-3.975719	-2.966667	H	-5.227544	-0.420898	4.522004
H	-2.992329	-3.116699	-1.558219	H	-3.222786	0.168494	3.157687
H	-1.430692	-1.323461	-1.145616	H	-1.645539	-0.481054	1.470971
F	0.856780	-2.079786	-1.885308	F	1.443054	3.888597	-0.730997
F	2.650478	-2.738720	-0.407814	F	0.423798	3.624005	1.450207
F	0.376364	-3.371188	0.088532	F	2.764774	3.045482	1.105405

L= P(O<i>i</i>Pr)₃ where C₂H₄ trans trans to SiMes, L=P(O<i>i</i>Pr)₃ trans to Cl⁻	L= P(O<i>i</i>Pr)₃ where C₂H₄ trans trans to SiMes, L=P(O<i>i</i>Pr)₃ trans to Cl⁻ with methylidene
<p>Ru -0.667482 -0.272280 1.124269</p> <p>Cl -1.007009 -2.455379 2.242773</p> <p>Cl -3.134144 0.004750 1.562766</p> <p>P -0.811328 1.833893 0.187892</p> <p>O -2.264121 2.540696 -1.848465</p> <p>O -0.175363 0.2020712 -1.346102</p> <p>O -0.220037 3.158522 1.045069</p> <p>N -0.232609 -2.280816 -1.220962</p> <p>N -2.386717 -1.892037 -1.000894</p> <p>C -2.314405 -2.955803 0.2031246</p> <p>C 1.313446 -0.423702 0.929361</p> <p>C 6.789811 2.341487 -1.561274</p> <p>C 3.519621 0.277809 0.367656</p> <p>C 3.641988 -0.741209 1.436827</p> <p>C 2.180034 -2.187420 2.741837</p> <p>C 5.566795 2.998578 -1.333832</p> <p>C 3.754768 -1.430843 -0.862155</p> <p>C -4.191430 -3.327123 0.796287</p> <p>C -4.664151 -2.199020 -0.084606</p> <p>C 4.763549 -1.198833 2.138297</p> <p>C 5.882948 0.332815 -0.517471</p> <p>C -1.147494 -1.478547 -0.568385</p> <p>C 1.074454 3.408534 1.650866</p> <p>C -6.027747 -1.859269 -0.136093</p> <p>C -6.518789 -0.820445 -0.953306</p> <p>C -5.596221 -0.125981 1.756470</p> <p>C -7.987946 -0.460600 -0.953409</p> <p>C 1.193523 -2.231451 -1.403481</p> <p>C -0.864744 -3.396722 -1.962210</p> <p>C -3.196173 3.180003 0.785454</p> <p>C 2.925857 4.685614 0.831416</p> <p>C 2.017385 -3.198539 -0.769392</p> <p>C 3.371555 -3.277266 -1.160849</p> <p>C 3.908141 -2.477089 -2.184243</p> <p>C 4.639354 0.978055 -0.281178</p> <p>C 6.939683 1.004829 -1.151283</p> <p>C 3.049509 -1.558819 -2.827598</p> <p>C 1.696876 -1.433340 -2.473352</p> <p>C 2.325082 -1.203825 1.753241</p> <p>C 1.472371 -4.185241 0.234320</p> <p>C 5.342861 -2.632227 2.635352</p> <p>C 0.780501 -0.525333 -3.254788</p> <p>C 4.596042 -2.187540 3.137438</p> <p>C 3.318943 -2.686148 3.420882</p> <p>C -0.180261 3.294852 -2.074735</p> <p>C 1.158113 3.407064 -2.804907</p> <p>C -4.604974 2.851776 0.303540</p> <p>C -1.359549 3.371087 -3.044249</p> <p>C 0.860978 3.854916 3.099589</p> <p>C 1.787935 4.500021 0.847441</p> <p>C 4.509301 2.325920 -0.705151</p> <p>C 2.167053 0.435516 0.096893</p> <p>C -4.217849 -0.422285 1.740872</p> <p>C -3.267415 0.333765 -2.633882</p> <p>H -3.793249 -4.181855 0.204322</p> <p>H -3.369971 -2.991836 1.463989</p> <p>H -5.023362 -3.717469 1.414846</p> <p>H -2.620758 -0.343276 -3.231770</p> <p>H -3.820126 0.982836 -3.341391</p> <p>H -2.593618 0.978767 -2.037282</p> <p>H -0.049448 -1.099356 -3.722092</p> <p>H 0.312897 0.247564 -2.611468</p> <p>H 1.333032 -0.017129 -4.069708</p> <p>H 2.253528 -4.470539 0.966118</p> <p>H 0.601763 -3.782459 0.790897</p> <p>H 1.155183 -5.123612 -0.275332</p> <p>H -8.630854 -1.361517 -0.871292</p> <p>H -8.238932 0.193965 -0.089415</p> <p>H -8.277329 0.086177 -1.873797</p> <p>H -5.956168 0.670270 -2.429933</p> <p>H -6.732904 -2.433590 0.488566</p> <p>H 5.933510 -3.243972 -1.924261</p> <p>H 5.395446 -3.132579 -3.627442</p> <p>H 5.842717 -1.647485 2.745595</p> <p>H 3.441467 -0.938405 -3.651018</p> <p>H 4.019424 -4.014284 -0.657329</p> <p>H -2.320158 3.298380 -2.503639</p> <p>H -1.331355 4.338203 -3.589288</p> <p>H -1.306323 2.554788 -3.793764</p> <p>H 1.256799 2.610467 -3.570365</p> <p>H 1.231536 4.388061 3.318537</p> <p>H 2.017724 3.316355 -2.112539</p> <p>H -0.269613 4.107601 -1.321610</p> <p>H -4.749804 1.754923 0.283227</p> <p>H -5.351999 3.298980 0.991967</p> <p>H -4.780237 3.266925 -0.711741</p> <p>H -1.896524 4.896106 1.175878</p> <p>H -3.065658 5.139661 -0.172617</p> <p>H -3.640351 5.174327 1.526752</p> <p>H 1.838401 4.061194 3.582864</p> <p>H 0.258841 4.768764 3.131367</p> <p>H 0.339530 3.086193 3.699709</p> <p>H 1.924868 4.204141 -0.209912</p> <p>Ru -0.177483 -0.061311 -1.273481</p> <p>Cl 0.103171 -2.013858 -2.775027</p> <p>Cl 2.298275 0.397815 -1.529132</p> <p>P -0.308373 1.809939 0.017242</p> <p>O 1.007219 2.524193 0.705923</p> <p>O -1.225454 1.636553 1.391821</p> <p>O -0.906453 3.233275 -0.669326</p> <p>N -0.771968 -2.420284 0.587594</p> <p>N 1.403956 -2.082480 0.595414</p> <p>C 1.225626 -3.325255 1.385442</p> <p>C -2.057152 -0.356744 -1.179147</p> <p>C 2.771728 -1.609828 0.625641</p> <p>C 3.287569 -3.120652 -1.366308</p> <p>C 3.718608 -2.199650 -0.253228</p> <p>C 0.220056 -1.551197 0.169303</p> <p>C -2.167735 3.458532 -1.347547</p> <p>C 5.073476 -1.866243 -0.081766</p> <p>C 5.513241 -0.996689 0.937393</p> <p>C 4.549142 -0.467697 1.814429</p> <p>C 6.976364 -0.635573 1.068977</p> <p>C -2.198280 -2.258252 0.634797</p> <p>C -0.236060 -3.681378 1.140104</p> <p>C 2.017308 3.343302 0.019958</p> <p>C 1.672783 4.821678 0.205445</p> <p>C -3.049613 -2.953641 -0.274082</p> <p>C -4.445410 -2.835942 -0.098734</p> <p>C 5.017184 -2.114247 0.964458</p> <p>C 4.146380 -1.533595 1.912150</p> <p>C -2.749722 -1.618305 1.787298</p> <p>C -2.506319 -3.838068 -1.368007</p> <p>C -6.516196 -1.977509 1.103175</p> <p>C -1.846162 -1.104700 2.879121</p> <p>C -1.450483 2.709348 2.364751</p> <p>C -2.883567 2.564065 2.878084</p> <p>C 3.372257 2.967060 0.607318</p> <p>C -0.427044 2.640058 3.499717</p> <p>C -1.882069 4.192255 -2.661111</p> <p>C -3.101310 4.282070 -0.455169</p> <p>C 3.176676 -0.767118 1.687647</p> <p>C 2.178121 -0.164827 2.645643</p> <p>H 2.789817 -4.039432 -0.984549</p> <p>H 2.551819 -2.617913 -2.030065</p> <p>H 4.157733 -3.442469 -1.971627</p> <p>H 1.410184 -0.895020 2.974520</p> <p>H 2.683275 0.228989 3.549887</p> <p>H 1.638335 0.677563 2.164991</p> <p>H -1.187112 -1.910869 3.267278</p> <p>H -1.198521 -0.288134 2.507833</p> <p>H -2.438738 -0.720539 3.732505</p> <p>H -3.263187 -3.993895 -2.162634</p> <p>H -1.587468 -3.417573 -1.830806</p> <p>H -2.257272 -4.844853 -0.963455</p> <p>H 7.632146 -1.516463 0.907224</p> <p>H 7.268761 0.126093 0.312732</p> <p>H 7.207592 -0.213597 2.067969</p> <p>H 4.870584 0.196802 2.634407</p> <p>H 5.812309 -2.302039 -0.775513</p> <p>H -7.054444 -2.761340 0.533580</p> <p>H -6.835972 -2.038365 2.163999</p> <p>H -6.863649 -0.993302 0.718103</p> <p>H -4.569466 -1.025144 2.794923</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -6.835972 -2.038365 2.163999</p> <p>H -6.863649 -0.993302 0.718103</p> <p>H -4.569466 -1.025144 2.794923</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.545876</p> <p>H -3.616715 2.543265 2.047508</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.545876</p> <p>H -3.616715 2.543265 2.047508</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.545876</p> <p>H -3.616715 2.543265 2.047508</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.545876</p> <p>H -3.616715 2.543265 2.047508</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.545876</p> <p>H -3.616715 2.543265 2.047508</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.545876</p> <p>H -3.616715 2.543265 2.047508</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.545876</p> <p>H -3.616715 2.543265 2.047508</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.545876</p> <p>H -3.616715 2.543265 2.047508</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.545876</p> <p>H -3.616715 2.543265 2.047508</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.545876</p> <p>H -3.616715 2.543265 2.047508</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.545876</p> <p>H -3.616715 2.543265 2.047508</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.545876</p> <p>H -3.616715 2.543265 2.047508</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.545876</p> <p>H -3.616715 2.543265 2.047508</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.545876</p> <p>H -3.616715 2.543265 2.047508</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.545876</p> <p>H -3.616715 2.543265 2.047508</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.545876</p> <p>H -3.616715 2.543265 2.047508</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.545876</p> <p>H -3.616715 2.543265 2.047508</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.545876</p> <p>H -3.616715 2.543265 2.047508</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.545876</p> <p>H -3.616715 2.543265 2.047508</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.545876</p> <p>H -3.616715 2.543265 2.047508</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.545876</p> <p>H -3.616715 2.543265 2.047508</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.545876</p> <p>H -3.616715 2.543265 2.047508</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.545876</p> <p>H -3.616715 2.543265 2.047508</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.545876</p> <p>H -3.616715 2.543265 2.047508</p> <p>H -5.105652 -3.348746 -0.818445</p> <p>H 0.600199 2.750723 3.107616</p> <p>H -0.618074 3.455796 4.228504</p> <p>H -0.502293 1.674609 4.041553</p> <p>H -3.001545 1.625561 3.456400</p> <p>H -3.137886 3.413184 3.5</p>	

H	1.198955	5.440656	0.866116	H	-2.790532	0.170120	-0.527861
H	2.788180	4.708520	1.279620	H	-2.566778	-1.031076	-1.902454
H	1.677402	2.472539	1.622907				
H	-3.048060	2.721285	1.786075				
H	1.176498	-2.574504	2.975986				
H	3.188212	-3.462858	4.191306				
H	5.473534	-2.558122	3.691324				
H	5.764918	-0.789566	1.936740				
H	6.006165	-0.721212	-0.231190				
H	7.890087	0.476606	-1.329993				
H	7.622544	2.869678	-2.052068				
H	5.438745	4.048765	-1.641454				
H	3.568818	2.857038	-0.502965				
H	1.767433	1.100003	-0.678840				
H	-0.733073	-4.343757	-1.394872				
H	-0.390193	-3.520563	-2.956381				
H	-3.034668	-3.762986	-1.794333				
H	-2.598472	-2.532726	-3.021886				
C	0.290701	0.326913	3.342591				
H	0.560314	-0.666136	3.722255				
H	1.121162	1.027144	3.172188				
C	-1.022928	0.721641	3.347042				
H	-1.798665	0.044981	3.728536				
H	-1.322744	1.765618	3.170917				

L= P(O<i>i</i>Pr)₃ where C₂H₄ and P(O<i>i</i>Pr)₃ cis to SiMes (C₂H₄ trans to ylidene group) with methylidene	L= P(O<i>i</i>Pr)₃ where C₂H₄ and P(O<i>i</i>Pr)₃ cis to SiMes (P(O<i>i</i>Pr)₃ trans to ylidene group) with methylidene
Ru -0.001518 -0.045366 -1.093133 Cl 0.163686 -1.868457 -2.792098 Cl -0.553823 1.565456 -2.957077 P -0.494125 1.822926 0.169504 O 0.421687 3.208028 0.047541 O -0.350569 1.646668 1.819085 O -2.026527 2.478686 0.110031 N -0.454977 -2.192038 1.062893 N 1.682762 -1.679178 1.026114 C 1.591914 -2.711609 2.084512 C -1.803495 -0.571042 -1.012872 C 3.040747 -1.336003 0.685254 C 3.059710 -3.249118 -1.016420 C 3.742460 -2.136445 -0.255897 C 0.478040 -1.393721 0.424299 C -3.112144 2.337988 -0.858997 C 5.112172 -1.869122 -0.459980 C 5.798847 -0.864955 0.249953 C 5.079772 -0.122729 1.207781 C 7.258445 -0.577223 -0.021229 C -1.825588 -2.476782 0.731068 C 0.088060 -2.947265 2.209757 C 0.169642 4.351981 -0.827385 C -0.565261 5.439597 -0.041503 C -2.109239 -3.579954 -0.133630 C -3.456355 -3.925052 -0.351882 C -4.520128 -3.262019 0.292597 C -4.202716 -2.249401 1.219327 C -2.873883 -1.861265 1.475782 C -1.009235 -4.368891 -0.789921 C -5.955653 -3.630619 -0.002188 C -2.577960 -0.835320 2.539093 C -0.602142 2.771601 2.730174 C -1.781844 2.427948 3.636932 C 1.514812 4.842530 -1.361650 C 0.680376 3.075116 3.501055 C -3.348354 3.665411 -1.577739 C -4.353584 1.872485 -0.096845 C 3.711115 -0.347841 1.451688 C 2.976043 0.441841 2.507708 H 2.642529 -4.018876 -0.331160 H 2.205657 -2.879908 -1.629975 H 3.775031 -3.759766 -1.690146 H 2.793256 -0.170775 3.419086 H 3.564384 1.324960 2.825287 H 1.984553 0.785691 2.151091 H -2.258791 -1.328528 3.484849 H -1.767198 -0.141492 2.243777 H -3.481340 -0.242236 2.782200 H -1.412504 -5.274347 -1.283620 H -0.490795 -3.744064 -1.555139 H -0.239338 -4.689660 -0.056526 H 7.788845 -1.472510 -0.403875 H 7.369027 0.220846 -0.788282 H 7.783706 -0.226336 0.890471 H 5.598494 0.657343 1.790361 H 5.659982 -2.478085 -1.198696 H -6.065167 -4.714340 -0.211396 H -6.629632 -3.368012 0.837982 H -6.324418 -3.089567 -0.901572 H -5.014639 -1.752191 1.776423 H -3.678142 -4.758396 -1.039210 H 1.503124 3.321241 2.802371 H 0.523846 3.943080 4.175526 H 0.987141 2.208834 4.123321 H -1.565193 1.534291 4.258363 H -1.992368 3.276771 4.321039 H -2.692133 2.233719 3.037673 H -0.867180 3.654840 2.114644 H 2.004747 4.080135 -1.997812 H 1.363697 5.750166 -1.981686 H 2.199402 5.102751 -0.527172 H -1.523368 5.057629 0.359935 H 0.058368 5.800660 0.803766 H -0.786472 6.306968 -0.698043 H -4.192370 3.553881 -2.289599 H -3.606155 4.474289 -0.862566 H -2.458237 3.960810 -2.165161 H -4.182371 0.902894 0.413693 H -4.646785 2.620415 0.669594 H -5.205601 1.742189 -0.795754 H -2.804926 1.588586 -1.619866 H -0.446514 3.996647 -1.680334 H -0.193775 -4.018599 2.140151 H -0.329353 -2.551599 3.161965 H 2.150207 -3.622021 1.772934 H 2.056590 -2.342078 3.021822 C 2.206059 0.173898 -2.186600 H 2.714716 -0.783722 -0.2025729	Ru -0.631467 -0.538271 -0.755828 Cl -1.176468 -1.757719 1.310926 Cl -1.814539 -2.659131 -2.068727 P 1.617794 -1.111424 0.114373 O 2.085202 -0.982604 1.703607 O 2.912603 -0.385334 -0.623715 O 1.981969 -2.732500 -0.047509 N -2.250280 1.803336 0.201548 N -0.177098 2.4336147 -0.230630 C -0.926498 3.707581 -0.095208 C -2.541221 -1.115656 -1.280625 C 1.248937 2.575784 -0.093022 C 0.967435 1.979544 2.367659 C 1.814486 2.431325 1.203445 C -0.999460 1.314741 -0.152415 C 1.403703 -3.676152 -0.989551 C 3.161159 2.791727 1.394075 C 3.950209 3.320222 0.353341 C 3.355938 3.466647 -0.913959 C 5.376573 3.764140 0.595770 C -3.509727 1.128702 0.380556 C -2.263797 3.251883 0.480715 C 1.942937 -2.028053 2.718928 C 3.310555 -2.662827 2.974991 C 3.857091 0.622926 1.663045 C 5.125649 0.032475 1.822962 C -6.063766 -0.036415 0.773288 C 5.717844 0.550207 -0.458354 C -4.462117 1.153432 -0.672443 C 2.915396 0.732571 2.836909 C -7.397182 -0.722441 0.969193 C 4.174061 1.841790 -1.988059 C 4.274850 -0.909030 -0.582571 C 4.859544 -0.728523 -1.983217 C 1.334448 -1.395596 3.967370 C 5.091184 -0.197168 0.494762 C 0.692597 -4.768891 -0.193985 C 2.521797 -4.209720 -1.886807 C 2.010488 3.123942 -1.158096 C 1.409224 3.426583 -2.512969 H 0.120363 2.678250 2.543369 H 0.534954 0.975099 2.191470 H 1.565498 1.934302 3.297705 H 1.117214 4.498007 -2.587325 H 2.140860 3.239104 -3.324879 H 0.507802 2.819833 -2.717479 H -4.320219 2.942710 -1.907254 H -3.133268 1.674810 -2.324764 H 4.859822 1.486373 -2.782626 H -3.405302 0.384826 3.767354 H -2.014181 0.107853 2.663923 H -2.579948 1.777824 3.001330 H 5.769777 3.378095 1.557402 H 6.056326 3.425092 -0.213706 H 5.449079 4.873635 0.629969 H 3.949299 3.889412 -1.743038 H 3.598865 2.679159 2.400035 H -7.839965 -0.480990 1.957754 H -8.126218 -0.435658 0.184934 H -7.284226 -1.828179 0.928412 H -6.450217 0.545108 -1.283450 H -5.390589 -0.380172 2.811040 H 4.599906 -0.294808 1.480969 H 6.109254 -0.636653 0.556393 H 5.186345 0.881400 0.260041 H 4.883339 0.346976 -2.256620 H 5.896757 -1.121872 -2.024190 H 4.254793 -1.264049 -2.742691 H 4.213798 -1.993918 -0.347673 H 0.329974 -0.989756 3.738872 H 1.224992 -2.160024 4.764889 H 1.980164 -0.580766 4.356693 H 3.713034 -3.109400 2.044815 H 4.035286 -1.912629 3.356249 H 3.222137 -3.468380 3.734317 H 0.228615 -5.508486 -0.879012 H 1.411849 -5.304322 0.461451 H -0.105385 -4.323148 0.432709 H 3.003344 -3.392571 -2.461428 H 3.302416 -4.717778 -1.282148 H 2.116212 -4.944964 -2.612619 H 0.652824 -3.142755 -1.611319 H 1.246081 -2.795135 2.324463 H -2.350234 3.439088 1.576515 H -3.134458 3.733254 -0.008555 H -0.381944 4.408285 0.568831 H -1.037683 4.197888 -1.089181 C 0.598681 -0.053137 -2.480780 H 1.387536 0.676765 -2.248398

H	1.842881	0.374707	-3.204964	H	0.979938	-0.986822	-2.934789
C	2.198682	1.154842	-1.230985	C	-0.735841	0.344588	-2.746955
H	2.712670	1.029304	-0.268845	H	-1.001058	1.416299	-2.737243
H	1.855966	2.164576	-1.478728	H	-1.360208	-0.266368	-3.421223
H	-2.166127	-1.301404	-1.766810	H	-3.162616	-1.486350	-0.445365
H	-2.614020	-0.138183	-0.398195	H	-3.143456	-0.658530	-2.084944

L=/ with methylidene			L=P(OMe) ₃ in <i>cis</i> methylidene			L=P(OMe) ₃ in <i>trans</i> methylidene		
Ru -0.081032 0.478650 -1.397947 Cl -0.232716 2.764839 -0.966940 Cl -1.174698 -1.313613 -2.392801 N 1.206885 -0.253480 1.224871 N -1.008123 -0.218210 1.281774 C -0.621373 -0.344767 2.699718 C 1.593180 0.306904 -2.061173 C -2.402555 -0.213431 0.916597 C -2.590970 2.259419 1.580310 C -3.170723 0.976068 1.033342 C 0.084036 -0.065600 0.450399 C -4.536222 0.919331 0.684490 C -5.158170 -0.272975 0.270887 C -4.382722 -1.449759 0.245915 C -6.613248 -0.294962 -0.139683 C 2.583889 -0.273255 0.820199 C 0.878081 -0.658106 2.606998 C 3.356360 0.910918 0.942368 C 4.717495 0.853862 0.587131 C 5.323444 -0.334112 0.127879 C 4.524280 -1.489781 0.021669 C 3.155762 -1.487277 0.363640 C 2.729228 2.200677 1.414521 C 6.791361 -0.355366 -0.235372 C 2.314052 -2.731728 0.194965 C -3.014639 -1.450787 0.572607 C -2.233273 -2.743286 0.571675 H -2.507978 2.213996 2.689254 H -1.586810 2.476572 1.166617 H -3.246350 3.119863 1.340694 H -1.637604 -2.869664 1.500096 H -2.913078 -3.613254 0.482496 H -1.527213 -2.771685 -0.284556 H 1.886807 -3.081924 1.159228 H 1.456657 -2.546881 -0.486852 H 2.913988 -3.563362 -0.222824 H 3.481297 3.011970 1.468209 H 1.913629 2.523568 0.731969 H 2.276062 2.094314 2.423525 H -7.172573 0.564582 0.281208 H -6.711850 -0.242520 -1.246443 H -7.116334 -1.229037 0.184977 H -4.858524 -2.404800 -0.033529 H -5.134350 1.843637 0.753228 H 7.425967 -0.102976 0.641134 H 7.107625 -1.349419 -0.607442 H 7.023720 0.392993 -1.023203 H 4.976543 -2.427079 -0.343099 H 5.324167 1.771354 0.672816 H 1.488123 -0.086721 3.335972 H 1.096802 -1.740584 2.757845 H -0.817240 0.607673 3.242736 H -1.205134 -1.146570 3.196093 H 1.691431 0.649900 -3.124711 H 2.508679 -0.095492 -1.587590	Ru -0.126155 -0.148233 -1.083854 Cl -0.836679 -1.824924 -2.697143 Cl 1.433395 0.529598 -2.771388 P 0.734291 1.596075 0.087178 O 2.334718 1.607565 0.510351 O 0.097275 1.897264 1.591036 O 0.647401 3.107118 -0.605089 N -1.921556 -1.769643 0.867912 N 0.198282 -2.386544 0.861991 C -0.465753 3.459984 1.632328 C -1.782636 0.644819 -1.163873 C 1.633017 2.418192 0.712645 C 1.427563 -4.060551 -1.250114 C 2.236922 -3.231997 -0.284024 C -0.682188 -1.463069 0.371878 C -0.066632 3.512081 -1.810921 C 3.646405 -3.290209 -0.317461 C 4.454530 -2.616928 0.617158 C 3.816317 -1.871181 1.629188 C 5.962614 -2.580375 0.532134 C -3.188159 -1.127139 0.634882 C -1.888680 -2.912623 1.808614 C 3.407224 2.102537 -0.359421 C 3.935706 4.310984 0.227800 C -4.090314 -1.687475 -0.312140 C 5.347191 0.106981 0.475083 C -5.743513 0.047199 0.285273 C -4.853051 0.527924 1.266412 C -3.585166 -0.049106 1.473208 C 3.740074 -2.917860 -1.110228 C -7.083140 0.711666 0.060534 C -2.690082 0.453628 2.578940 C 0.488226 0.308052 2.368318 C -0.761791 3.918994 2.627968 C 4.469021 1.014689 -0.472063 C 1.183962 0.622371 3.648013 C 0.929941 4.204784 -2.737946 C -1.233985 4.4515648 -1.410545 C 2.416076 -1.763124 1.701605 C 1.763291 -0.005639 2.832343 C -0.761791 3.918994 2.627968 C 4.469021 1.014689 -0.472063 C -0.206993 1.230980 3.175724 C -4.544747 -3.161165 -1.831162 C -2.789581 -2.776878 -1.672227 C -3.607375 -3.805921 -0.453162 C 6.306752 3.605779 0.027725 C 6.361356 -1.821887 -0.052512 C 6.433154 -2.636017 1.535706 C 4.425818 -1.363552 2.395150 C 4.123628 -3.907127 -1.097125 H -7.789386 0.041763 -0.469470 H -7.551912 0.220237 0.107247 H -6.973490 1.629755 -0.557862 H -5.158504 3.171155 1.908972 H -6.042883 -1.489897 -1.220764 H 2.096861 0.043930 3.409071 H 1.477960 3.501258 4.259312 H 0.510314 1.987186 4.260410 H -1.505051 3.351603 3.225222 H -0.496330 4.837362 3.192394 H -1.235580 4.225029 1.674969 H 1.201165 3.669967 1.754759 H 4.034426 0.093528 -0.906220 H 5.292672 1.358434 -1.132134 H 4.895790 0.772854 0.523385 H 3.137452 4.179114 0.257293 H 4.322534 3.255963 1.257221 H 4.765996 3.803442 -0.395880 H 0.417539 4.545638 -3.661358 H 1.382620 5.090244 -2.243847 H 1.730583 3.499773 -3.034861 H -1.954078 3.883513 -0.755904 H -0.869226 5.314487 -0.870375 H -1.783911 4.755366 -2.312624 H -0.447349 2.597845 -2.315397 H 2.972876 2.287024 -1.363752 H -2.671930 -3.652304 1.546996 H -2.090143 -2.560751 2.845455 H -0.442210 -4.412203 1.057779 H 0.060462 -3.630992 2.593869 H -2.121403 1.544731 -0.604192 H -2.510134 0.241225 -1.901785	Ru 0.195791 -0.193025 0.110800 Cl -0.028066 -0.207318 -2.321844 Cl 0.240255 -0.152149 2.521410 P -1.560241 -1.808115 0.163772 O -3.062782 -1.167294 -0.065302 O -1.769854 -2.541496 1.603711 O -1.635033 -3.030914 -0.955051 N 2.618806 1.712290 0.124677 N 0.712901 2.818694 0.146367 C 1.723889 3.896032 0.244435 C 1.558149 -1.396604 0.072479 C -0.681973 3.179028 0.079604 C -0.461300 3.298620 -2.466794 C -1.251556 3.464863 -1.192030 C 1.261227 1.572502 0.104931 C -0.475939 -3.653127 -1.581943 C -2.583736 3.921034 -1.235167 C -3.349511 4.111377 -0.067246 C -2.739576 3.852804 1.174938 C -4.788175 4.569978 -0.149984 C 3.626097 0.689268 0.054114 C 3.054030 3.127509 0.152404 C -3.607362 -0.825098 -1.386283 C -4.545414 -1.944796 -1.836222 C 4.090556 0.260114 -1.219088 C 5.130192 -0.689873 -1.259178 C 5.720779 -1.205288 -0.087381 C 5.254142 -0.733374 1.155426 C 4.217802 0.216933 1.256368 C 3.476116 0.782710 -2.494414 C 6.811580 -2.250333 -0.164960 C 3.746099 0.704839 2.603652 C -2.934001 -3.363449 1.939943 C -2.410508 -4.644532 2.584942 C -4.306345 0.522397 -1.242327 C -3.848265 -2.553273 2.857445 C -0.892907 -4.037131 -2.998772 C -0.003150 -4.839221 -0.740406 C -1.406321 3.405180 1.281647 C -0.777120 3.208615 2.638518 H 0.513215 3.830312 -2.425438 H -0.237360 2.224257 -2.654241 H -0.085546 -4.555545 -1.987930 H 1.113065 -1.666033 3.446817 H 2.526878 -0.572657 3.507001 H 1.125983 -0.177954 2.461925 H -2.405722 -0.363223 3.276847 H -3.882417 1.802653 2.716236 H 2.661055 0.497282 2.746698 H 4.310238 0.215247 3.421426 H 4.033531 0.418930 -3.379772 H 2.414265 0.459777 -2.592655 H 3.473049 1.892959 -2.530935 H -4.945427 5.277051 -0.990229 H -5.469849 3.707542 -0.320328 H -5.115525 5.065571 0.786124 H -3.311352 4.022929 2.102659 H -3.031159 4.145507 -2.210895 H 7.453517 -2.106247 -1.057975 H 7.460272 -2.234477 0.734080 H 6.378763 -3.272669 -0.238045 H 5.713819 -1.111037 2.084296 H 5.493738 -1.031558 -2.243145 H -4.195413 -1.636515 2.343365 H -4.734988 -3.154737 3.148582 H -3.304982 -2.256517 3.778084 H -1.826861 -4.408597 3.498650 H -3.255773 -5.304786 2.870266 H -1.754990 -5.201780 1.886932 H -3.471370 -3.611895 0.998138 H -3.594698 1.308859 -0.923568 H -4.746517 0.827491 -2.214355 H -5.123936 0.460385 -0.493827 H -3.997101 -2.902839 -1.917470 H -5.380220 -2.069075 -1.114340 H -4.980694 -1.704257 -2.828834 H -0.038386 -4.495961 -3.537750 H -1.727200 -4.769620 -2.982466 H -2.121915 -3.137389 -3.559941 H 0.293642 -4.516566 0.278125 H -0.805999 -5.600623 -0.645807 H 0.875554 -5.323113 -1.215808 H 0.325778 -2.884931 -1.644108 H -2.757336 -0.729577 -2.097771 H 3.631207 3.369319 -0.766958 H 3.720173 3.310601 1.021627 H 1.587626 4.629871 -0.578028 H 1.607821 4.443725 1.204687 H 1.961794 -1.845913 1.008788 H 2.027095 -1.729758 -0.882496						

L=I	L=P(OMe) ₃ in cis	L=P(OMe) ₃ in trans
Ru -0.177483 -0.061311 -1.273481 Cl 0.103171 -2.013858 -2.775027 Cl 2.298275 0.397815 -1.529132 P -0.308373 1.809939 0.017242 O 1.007219 2.524193 0.705923 O -1.225454 1.636553 1.391821 O -0.906453 3.233275 -0.669326 N -0.771968 -2.420284 0.587594 N 1.403956 -2.082480 0.595414 C 1.225626 -3.325255 1.385442 C -2.057152 -0.356744 -1.179147 C 2.771728 -1.609828 0.625641 C 3.287569 -3.120652 -1.366308 C 3.718608 -2.199650 -0.253228 C 0.220056 -1.551197 0.169303 C -2.167735 3.458532 -1.347547 C 5.073476 -1.866243 -0.081766 C 5.513241 -0.996689 0.937393 C 4.549142 -0.467697 1.814429 C 6.976364 -0.635573 1.068977 C -2.198280 -2.258252 0.634797 C -0.236060 -3.681378 1.140104 C 2.017308 3.343302 0.019958 C 1.672783 4.821678 0.205445 C -3.049613 -2.953641 -0.274082 C -4.445410 -2.835942 -0.098734 C -5.017184 -2.114247 0.964458 C -4.146380 -1.533595 1.912150 C -2.747922 -1.618305 1.787298 C -2.506319 -3.838068 -1.368007 C -6.516196 -1.977509 1.103175 C -1.846162 -1.104700 2.879121 C -1.450483 2.709348 2.364751 C -2.883567 2.564065 2.878084 C 3.372257 2.967060 0.607318 C -0.427044 2.640058 3.499717 C -1.882069 4.192255 -2.661111 C -3.101310 4.282070 -0.455169 C 3.176676 -0.767118 1.687647 C 2.178121 -0.164827 2.645643 H 2.789817 -4.039432 -0.984549 H 2.551819 -2.617913 -2.030065 H 4.157733 -3.442469 -1.971627 H 1.410184 -0.895020 2.974520 H 2.683275 0.228989 3.549887 H 1.638335 0.677563 2.164991 H -1.187112 -1.910869 3.267278 H -1.195821 -0.288134 2.507833 H -2.438738 -0.720539 3.732505 H -3.263187 -3.993895 -2.162634 H -1.587468 -3.417573 -1.830806 H -2.257272 -4.844853 -0.963455 H 7.632146 -1.516463 0.907224 H 7.268761 0.126093 0.312732 H 7.207592 -0.213597 2.067969 H 4.870584 0.196802 2.634407 H 5.812309 -2.302039 -0.775513 H -7.054444 -2.761340 0.533580 H -6.835972 -2.038365 2.163999 H -6.863649 -0.993302 0.718103 H -4.569466 -1.025144 2.794923 H -5.105562 -3.348746 -0.818445 H 0.600199 2.750723 3.107616 H -0.618074 3.455796 4.228504 H -0.502293 1.674609 4.041553 H -3.001545 1.625561 3.456400 H -3.137886 3.413184 3.545876 H -3.616715 2.543265 2.047508 H -1.339229 3.677126 1.828943 H 3.575192 1.893880 0.427057 H 4.171503 3.563131 0.119706 H 3.402427 3.176523 1.697825 H 0.678615 5.053151 -0.220643 H 1.670860 5.092059 1.282833 H 2.432181 5.452553 -0.302530 H -2.826907 4.387658 3.209245 H -1.396937 5.168396 -2.452750 H -1.213632 3.611266 -3.323923 H -3.356584 3.747498 0.478269 H -2.629141 5.250604 -0.188843 H -4.048754 4.498060 -0.991499 H -2.648117 2.475899 -1.556701 H 2.009661 3.063308 -1.054886 H -0.352556 -4.500832 0.396639 H -0.780715 -3.971725 2.061745 H 1.933797 -4.102159 1.036316 H 1.453615 -3.118055 2.455870 C -1.218997 0.747691 -3.346199 H -1.458224 -0.213134 -3.827592 H -2.060035 1.428843 -3.144997 C 0.094753 1.172298 -3.286113 H 0.888591 0.562684 -3.738801 H 0.359863 2.202384 -3.006625 H -2.790532 0.170120 -0.527861 H -2.566778 -1.031076 -1.902454		

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