Electronic Supplementary Material (ESI) for ChemComm.

VCD Spectra of Chiral Metal Complexes containing a Carbon Monoxide Vibrational Chromophore

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Supporting information

Contents

1. General methods

All commercially available compounds were purified by distillation or crystallization before use. ^{1}H, ^{13}C, and ^{31}P NMR spectra were recorded in $CDCl_3$ on Bruker DRX Advance 300 MHz equipped with a non-reverse probe or Bruker DRX Avance 400 MHz. Chemical shifts (in ppm) were referenced to residual solvent proton/carbon peak or using external standard 85% H_3PO_4 for ^{31}P NMR. IR and VCD spectra were taken on a Jasco FVS6000 apparatus. Elemental analyses were recorded in the analytical laboratories of Milan University on Perkin Elmer Series II CHNS/O Analyzer 2400.

2. Synthesis of the complexes

The complexes were synthetized as reported in reference[S1] with freshly distilled n-heptane as reaction solvents and separated by flash chromatography (silica gel; cyclohexane/ethylacetate, 9/1, 1psi). $(S)_{Ru}$ is the first eluted complex.

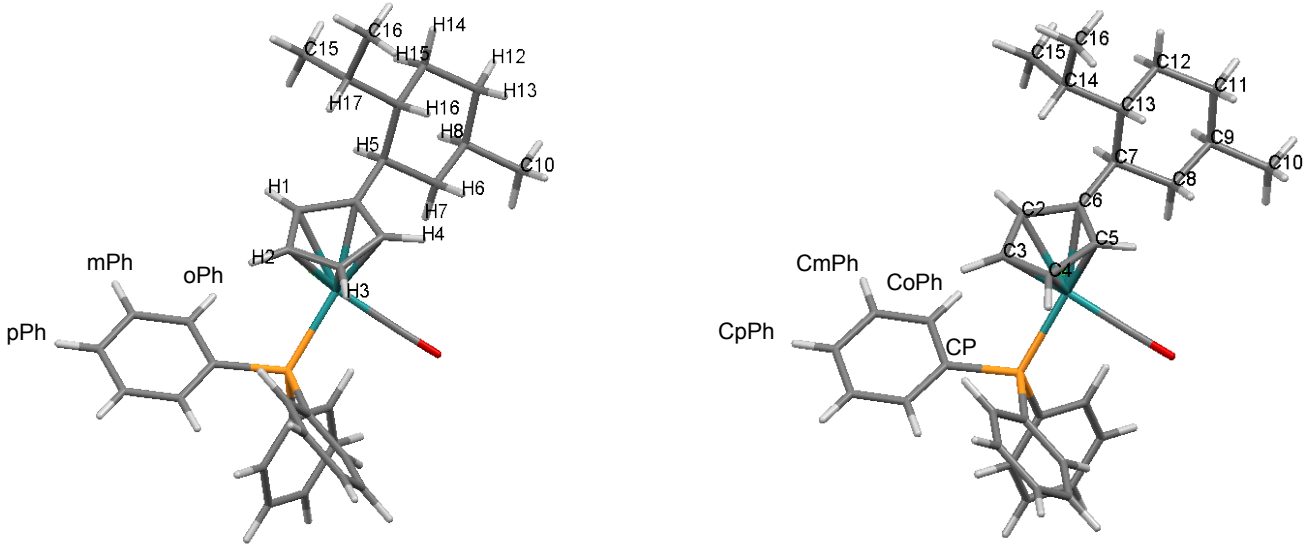

Figure 1SI. Proton (left) and carbon (right) labels referred to the crystallographic structure[S1]. For $(R)_{Ru}$ were retained the same labels.

2.1. T-4-S-η5-[(1R,2S,5R)-menthyl)-C_5H_4)Ru(CO)($P(C_6H_5)_3$)Cl] ($(S)_{Ru}$)

Yellow powder. **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.65 – 7.52 (m, 6H,oPh), 7.46 – 7.34 (m, 9H,mPh/pPh), 5.15 (s, 1H,H1), 4.72 (s, 1H,H4), 4.68 (s, 1H,H2), 3.78 (s, 1H,H3), 2.34 – 2.18 (m, 2H,H7/H5), 1.94 – 1.62 (m, 3H,H17/H12/H15), 1.56 – 1.41 (m, 1H,H8), 1.16 – 0.97 (m, 2H,H14/H16), 0.95 (d, *J* = 6.5 Hz, 3H,C10), 0.90 (m, 2H,H6/H13), 0.86 (d, *J* = 6.9 Hz, 3H,C16), 0.82 (d, *J* = 6.8 Hz, 3H,C15); **^{31}P{^{1}H}-NMR**(121MHz, $CDCl_3$) δ 49.08 (s,1P); **^{13}C{^{1}H}-NMR** (75 MHz, $CDCl_3$) δ 204.78 (d, *J* (C,P)= 21.1 Hz, CO), 135.47 (dd, *J* (C,P)= 47.3 Hz, CP), 134.03 (d, *J* (C,P)= 10.8 Hz, oPh), 130.54 (s,pPh), 128.62 (d, *J* (C,P)= 10.2 Hz, mPh), 114.27 (d, *J* (C,P)= 8.0 Hz, C6), 94.79 (s,C2), 89.86 (s,C3), 79.82 (d, *J* (C,P)= 2.3 Hz, C5), 75.14 (s,C4), 50.89 (s, C13), 43.53 (s, C8), 38.42 (s, C7), 35.64 (s, C11), 33.34 (s, C9), 27.84 (s, C14), 25.15 (s, C12), 22.85 (s, C10), 22.07 (s, C16), 16.04 (s, C15); **IR IR** 1959 cm^{-1} vs(CO stretching),1482,1457,1436 cm^{-1} m (aromatics and HCH bendings),1386,1370, 1349, 1261, cm^{-1} w (methyl and aromatic deformations) 1187,1095 cm^{-1} s (PPh3 CC stretchings); **EA** $C_{34}H_{38}ClOPRu$ calculated C: 64.81%, H: 6.04% found: C: 65.12%, H: 6.11%.

2.2. T-4-S-η5-[(1R,2S,5R)-menthyl)-C_5H_4)Ru(CO)($P(C_6H_5)_3$)Cl] ($(R)_{Ru}$)

Yellow powder. ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.68 – 7.47 (m, 6H,oPh), 7.42 (m, 9H,mPh/pPh), 5.23 (s, 1H,H4), 4.80 (s, 1H,H3), 4.50 (s, 1H,H2), 4.22 (s, 1H,H1), 2.14 (m, 1H,H7), 1.93-1.75(m,1H,H5), 1.73 – 1.53 (m, 3H, H17/H12/H15), 1.49 – 1.34 (m, 1H,H8), 1.19 – 0.98 (m, 1H,H6), 0.94 (d, *J* = 6.4 Hz, 3H, C10), 0.98 – 0.86 (m, 3H,H14/H16/H13), 0.83 (d, *J* = 6.8 Hz, 3H, C16), 0.69 (d, *J* = 6.7 Hz, 3H, C15).; **^{31}P{^{1}H}-NMR**(121MHz, $CDCl_3$) δ 49.18 (s,1P); **^{13}C{^{1}H}-NMR** (75 MHz, $CDCl_3$) δ 204.80 (d, *J* (C,P)= 21.3 Hz, CO), 135.60 (d, *J* (C,P)= 47.4 Hz, CP), 134.00 (d, *J* (C,P)= 10.8 Hz, oPh), 130.96 (s, pPh), 128.64 (d, *J* (C,P)= 10.2 Hz, mPh), 113.83 (d, *J* (C,P)= 4.2 Hz, C6), 91.01 (d, *J* (C,P)= 4.9 Hz, C5), 86.95 (s, C4), 84.80 (s, C3), 78.89 (s, C2), 51.12 (s, C13), 43.32 (s, C8), 39.31 (s, C7), 35.55 (s,C11), 33.38(s, C9), 33.18(s, C14), 27.48 (s, C12), 22.74 (s, C10), 21.93(s, C16), 15.92 (s, C15); **IR** 1959 cm^{-1} vs(CO stretching),1482,1457,1436 cm^{-1} m (aromatics and HCH bendings),1386,1370, 1349, 1261, cm^{-1} w (methyl and aromatic deformations) 1187,1095 cm^{-1} s (PPh3 CC stretchings); **EA** $C_{34}H_{38}ClOPRu$ calculated C: 64.81%, H: 6.04% found: C:65.08%, H: 5.93%.

3. VCD Experimental data

VCD spectra have been taken for CCl_4 solutions in the range 2100-850 cm^{-1}. In the range 2100-1800 cm^{-1} we set 8 cm^{-1} resolution (concentration 0.036M), while in the range 1700-850 cm^{-1} we set 4 cm^{-1} resolution with concentrations 0.09M for R_{Ru} and 0.073 S_{Ru}. In both

frequency regions 2000 scans were accumulated and averaged, a 200 µm pathlength BaF_2 cell was employed. The region between 1800 and 2400 cm^{-1} has been calibrated by running the spectra of (3*R*)-methylcyclopentanone-d_4[S2].

4. NOE structure analysis

The spin-lattice relaxation times (T_1) were measured at 300 K, after the analysis of the NOE build-up curves the mixing time (τ_m) (Figure 2SI) was choose at 1.3 s as a mean value between the aliphatic and the aromatic moieties and sufficiently apart of the NOE maximum enhancement. For a first order multispin system the peak intensities are given by

$I = M^0 \exp(-R\,\tau_m)$ (1)

Using the matrix method equation[S3] (1) could be solved as

$R = -\tau_m^{-1} \ln A = -\tau_m^{-1} X (\ln \Lambda) X^{-1}$ (2)

in the fast tumbling regime, $\sigma_{ij} = k r_{ij}^{-6}$ and *k* is $k = \left(\frac{\mu_0}{4\pi}\right)^2 \frac{\hbar^2 \gamma^4}{10} \left(\frac{6\tau_c}{1+4\omega^2\tau_c^2} - \tau_c \right)$ since *k* relate to parameters fixed for a given experiment and assuming τ_c comparable for each spin pair, than the internuclear distance r_{ij} could be estimated using a reference known distance (r_{ref}) as

$$r_{ij} = r_{ref} \sqrt[6]{\frac{\sigma_{ref}}{\sigma_{ij}}} \quad (3)$$

As reference distance were used the reported distance for germinal proton (1.68Å) considering the cross-peak between H_6 and H_7. The obtained values were compared to them obtained in crystallographic data, referring to the rigid moieties of the complexes they fit well with an average absolute error of 3.7%(0.09 Å) with a standard deviation of 2.4%(0.05 Å). For what concerned the distances between different moieties all the $\langle r_{ij} \rangle$ were increased by 10% in order to correct for overestimation of the short distances[S4].

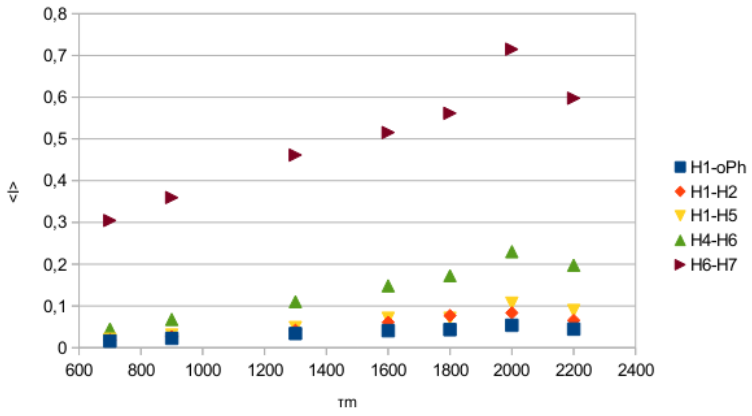

Figure 2SI. Build-up curves for selected cross-peaks of S_{Ru}.

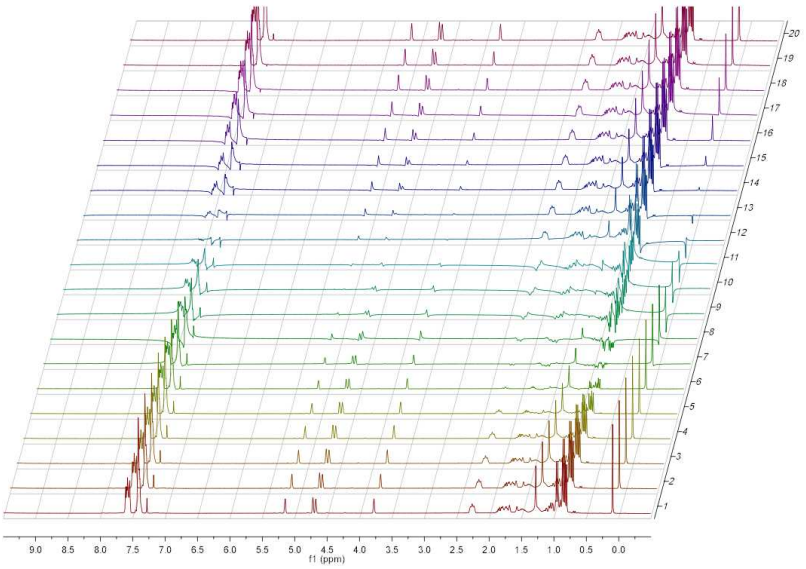

Figure 3SI. t1 determination for S_{Ru}.

4.1 Intensity matrices

Table 1SI. the matrix of peak intensities of $(S)_{Ru}$

	oPh[a]	mPh[a]	H_1	H_4	H_2	H_3	H_5	H_7	H_{17}	H_{12}	H_8	C_{10}[b]	H_6	H_{13}	C_{15}[b]
oPh[a]	107,11	9,72	0,58	0,13	0,77	0,75	0	0,04	0	0	0	0	0	0	0
mPh[a]	3,77	159,89	0	0	0	0	0	0	0	0	0	0	0	0	0
H_1	0,67	0	17,45	0	0,84	0	0,5	0	0,55	0	0	0	0	0	0,5
H_4	0,16	0	0	15,81	0	0,82	0	0,04	0,06	0	0	0	0,97	0	0
H_2	0,96	0	0,83	0	16,88	0,81	0	0	0,03	0	0	0	0	0	0
H_3	0,75	0	0	0,83	0,81	16,57	0	0	0	0	0	0	0	0	0
H_5	0	0	0,51	0	0	0	8,53	0	0	0	0	0	0	0	0,45
H_7	0,04	0	0	0,05	0	0	0	8,53	0	0	1,47	0	3,44	0	0
H_{17}	0	0	0,53	0,09	0,03	0	0	0	9,43	0	0	0	0	0	1,14
H_{12}	0	0	0	0	0	0	0	0	0	9,43	0,22	0	0	3,23	0
H_8	0	0	0	0	0	0	0	1,08	0	0,43	12,14	0,53	0	0	0
C_{10}	0	0	0	0	0	0	0	0	0	0	0,47	19,44	0	0	0
H_6	0	0	0	0,89	0	0	0	3,5	0	0	0	0	7,85	0	0
H_{13}	0	0	0	0	0	0	0	0	0	3,66	0	0	0	7,85	0
C_{15}	0	0	0,57	0	0	0	0,45	0	1,47	0	0	0	0	0	23,55

Table 2SI. the matrix of peak intensities of $(R)_{Ru}$

	oPh	mPh	H_1	H_2	H_3	H_4	H_7	H_5	H_{17}	H_8	H_6	C_{15}
oPh	130,09	5,26	0,22	0,81	0,9	0,67	0,16	0	0	0	0	0
mPh	4,79	163,94	0,01	0,08	0,08	0,04	0	0	0	0	0	0
H_1	0,22	0,02	16,1	0,78	0	0	0	0	0	0	1,01	0
H_2	0,81	0,07	0,75	17,69	0,68	0	0	0	0	0	0	0

H_3	0,86	0,1	0	0,68	16,32	0,67	0	0	0	0	0	0
H_4	0,61	0,06	0	0	0,67	14,71	0	0,62	0,78	0	0	0,53
H_7	0,16	0	0	0	0	0	8,54	0,59	0	0,8	2,91	0
H_5	0	0	0	0	0	0,65	0,61	19,21	0	0,8	0	0,75
H_{17}	0	0	0	0	0	0,78	0	0	15,04	0	0	0,82
H_8	0	0	0	0	0	0	0,84	0,8	0	21,03	0	0
H_6	0	0	0,95	0	0	0	2,88	0	0	0	11,79	0
C_{15}	0	0	0	0	0	0,52	0	0,8	0,085	0	0	22,95

5. NMR spectra

5.1. T-4-S-η^5-[(1R,2S,5R)-menthyl)-C_5H_4)Ru(CO)($P(C_6H_5)_3$)Cl] ($(S)_{Ru}$)

5.1.1. ^{1}H-NMR

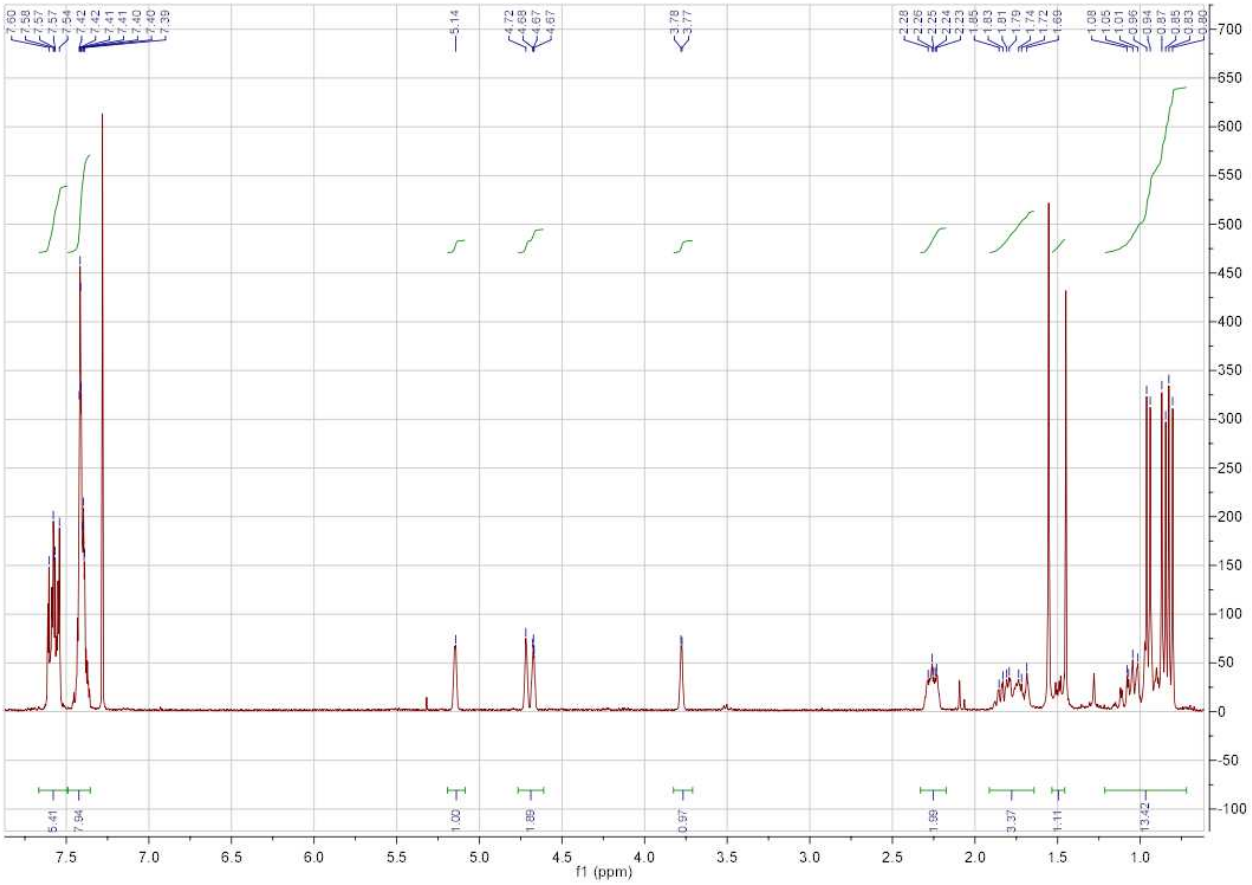

Figure 5SI. ^{1}H-NMR spectrum (300 MHz) of $(S)_{Ru}$ in $CDCl_3$ at 300 K.

5.1.2. ^{31}P-NMR

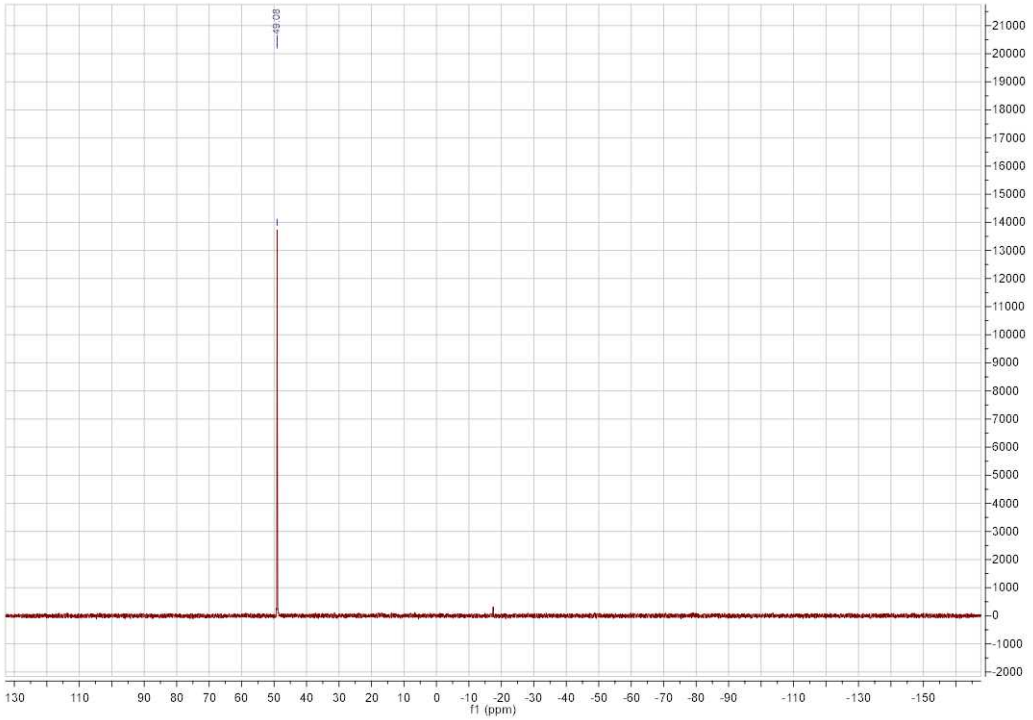

Figure 6SI. ^{31}P-NMR spectrum (121.49 MHz) of $(S)_{Ru}$ in $CDCl_3$ at 300 K.

5.1.3. *^{13}C-NMR*

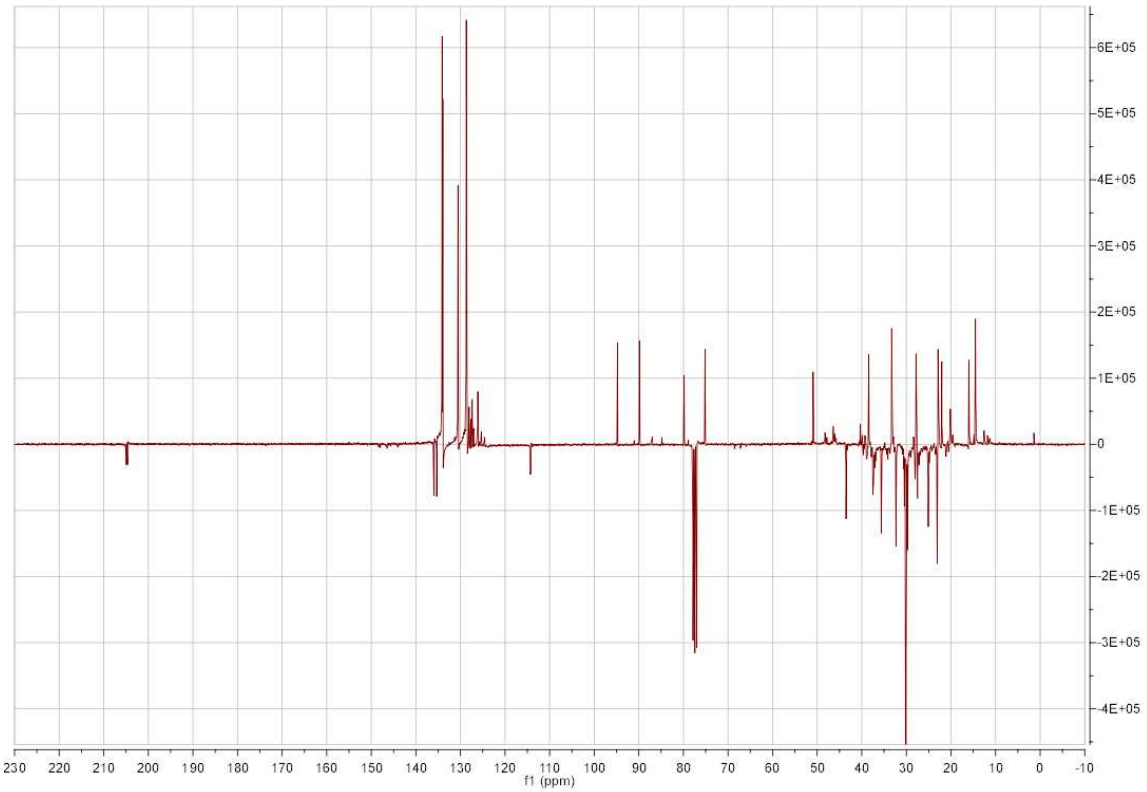

Figure 7SI. ^{13}C-NMR spectrum (75.47 MHz) of $(S)_{Ru}$ in $CDCl_3$ at 300 K.

5.1.4. *COSY*

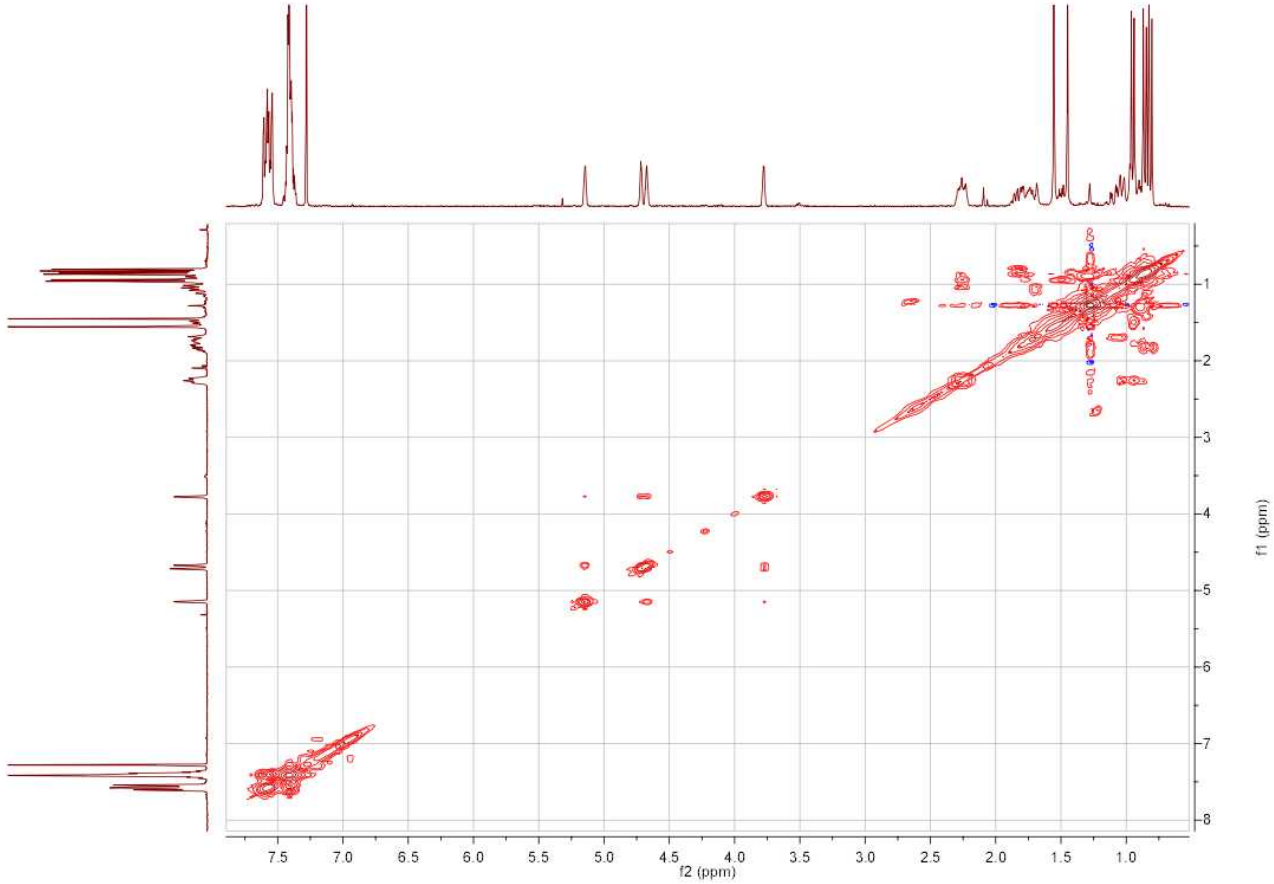

Figure 8SI. COSYGPQF spectrum (300 MHz) of $(S)_{Ru}$ in $CDCl_3$ at 300 K.

5.1.5. HSQC

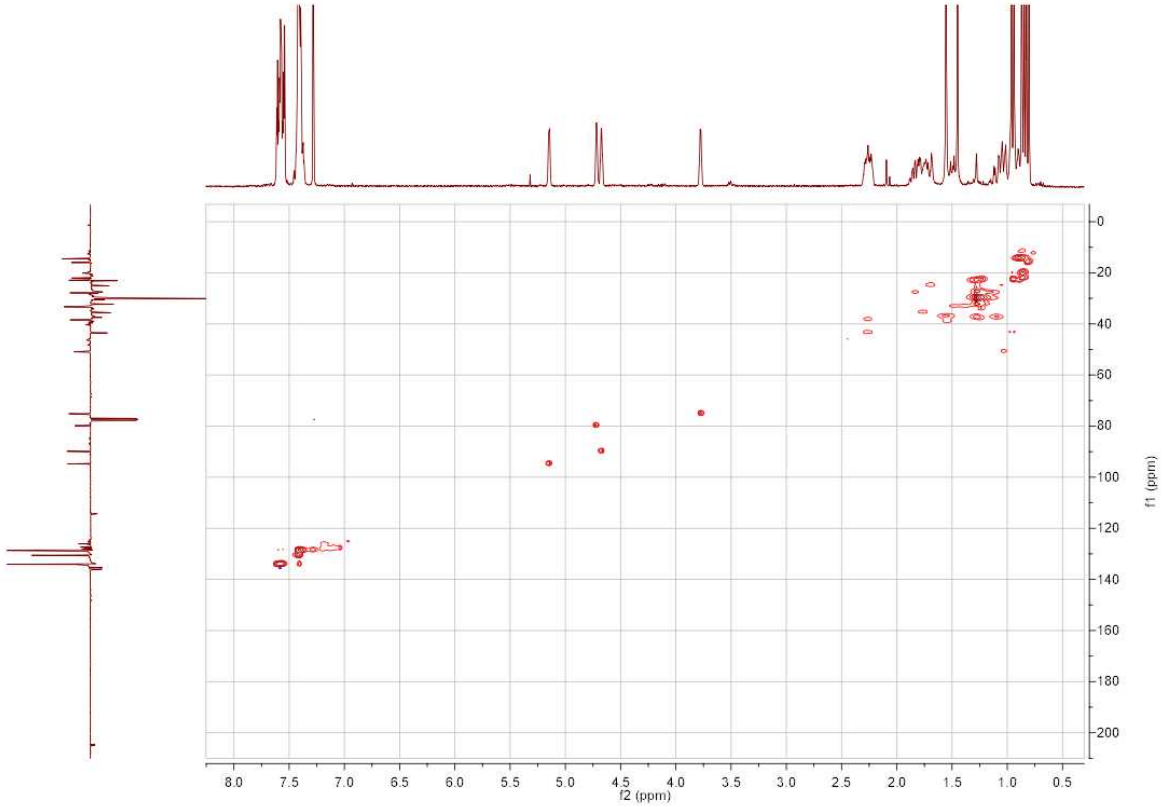

Figure 9SI. HSQCetgpsi ^{13}C-^{1}H spectrum of $(S)_{Ru}$ in $CDCl_3$ at 300 K.

5.1.6. HMBC

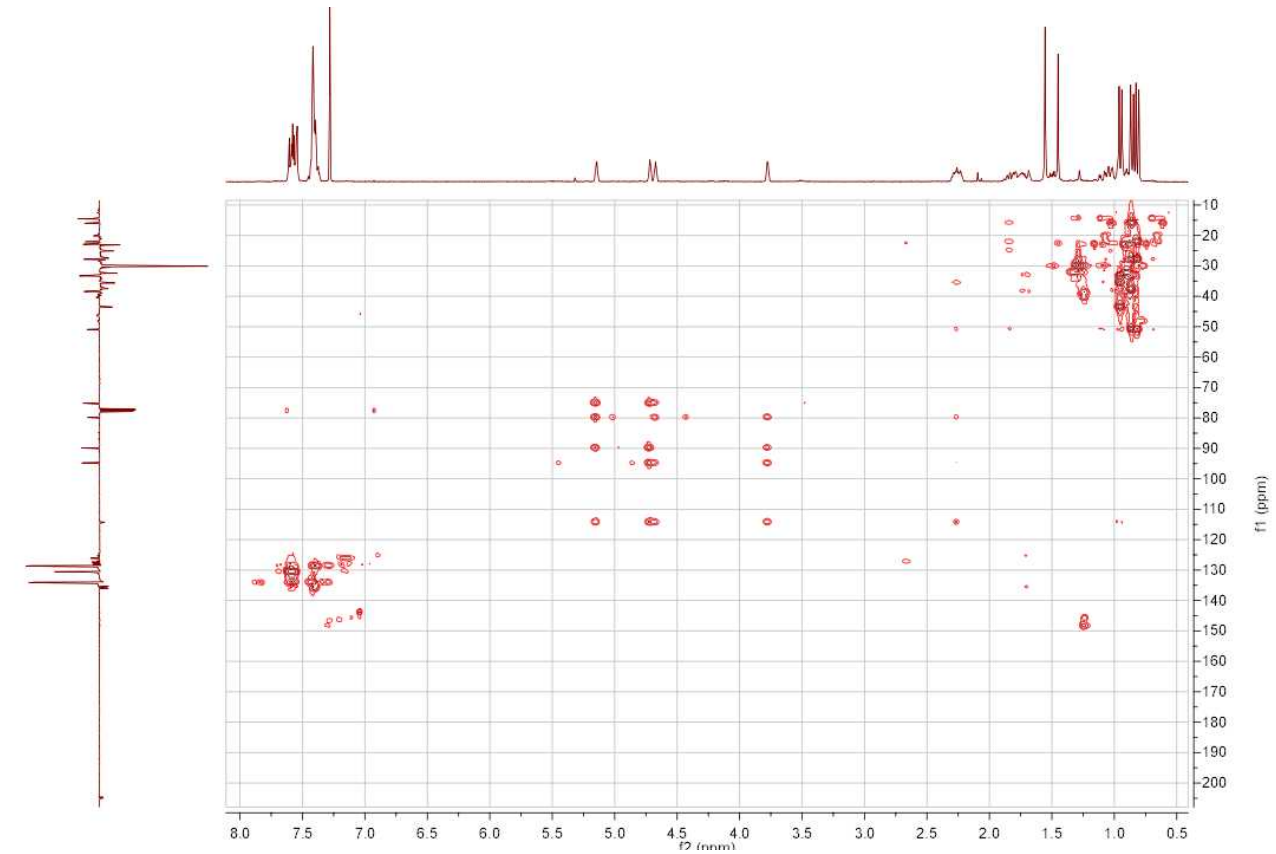

Figure 10SI. HMBC long range ^{13}C-^{1}H spectrum of $(S)_{Ru}$ in $CDCl_3$ at 300 K.

5.1.7. *^{31}P-INVBTP*

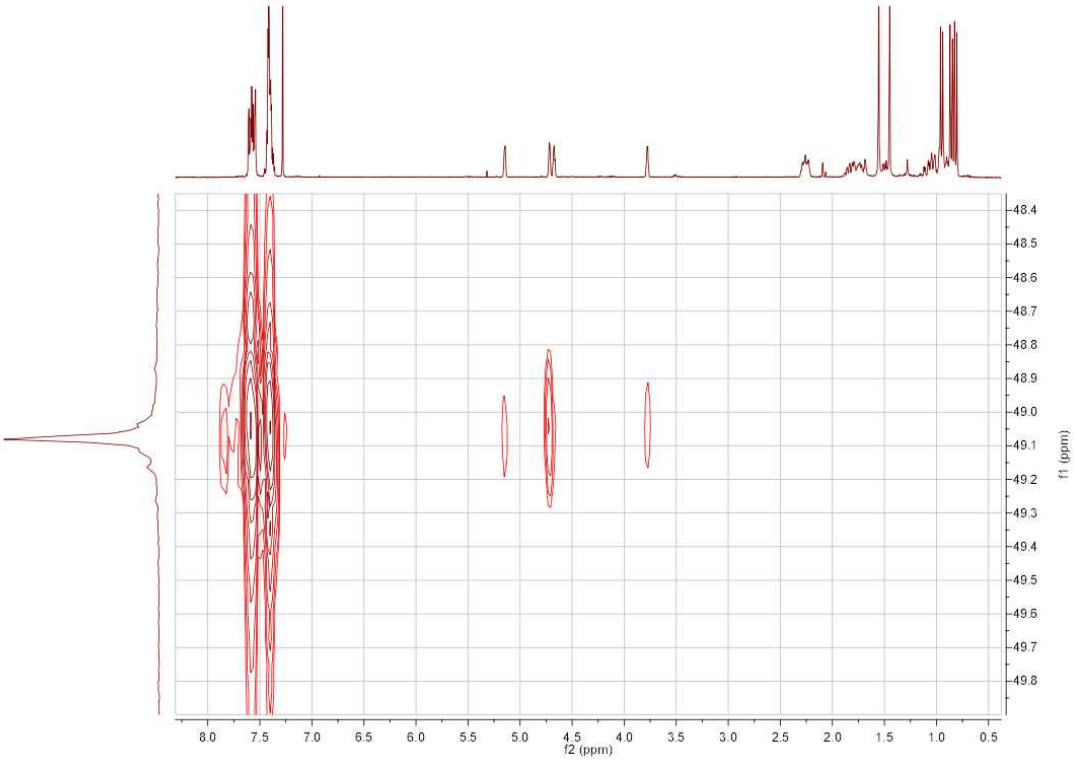

Figure 11SI. ^{31}P-INVBTP spectrum of $(S)_{Ru}$ in $CDCl_3$ at 300 K.

5.1.8. *NOESYGPPH mixingtime=1.3 s d1=3 s*

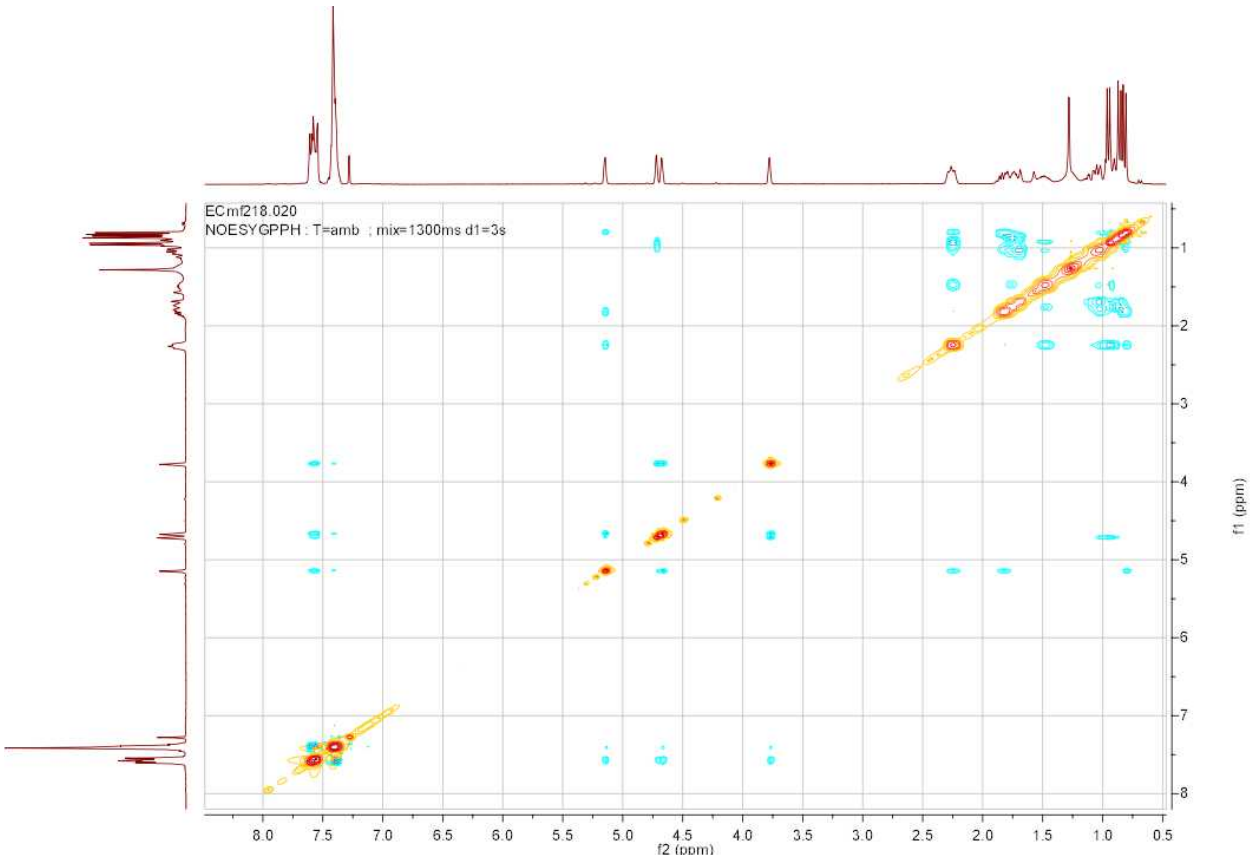

Figure 12SI. NOESY spectrum (300 MHz, mixing time: 1.3 s, time delay 3 s) of $(S)_{Ru}$ in $CDCl_3$ at 300 K.

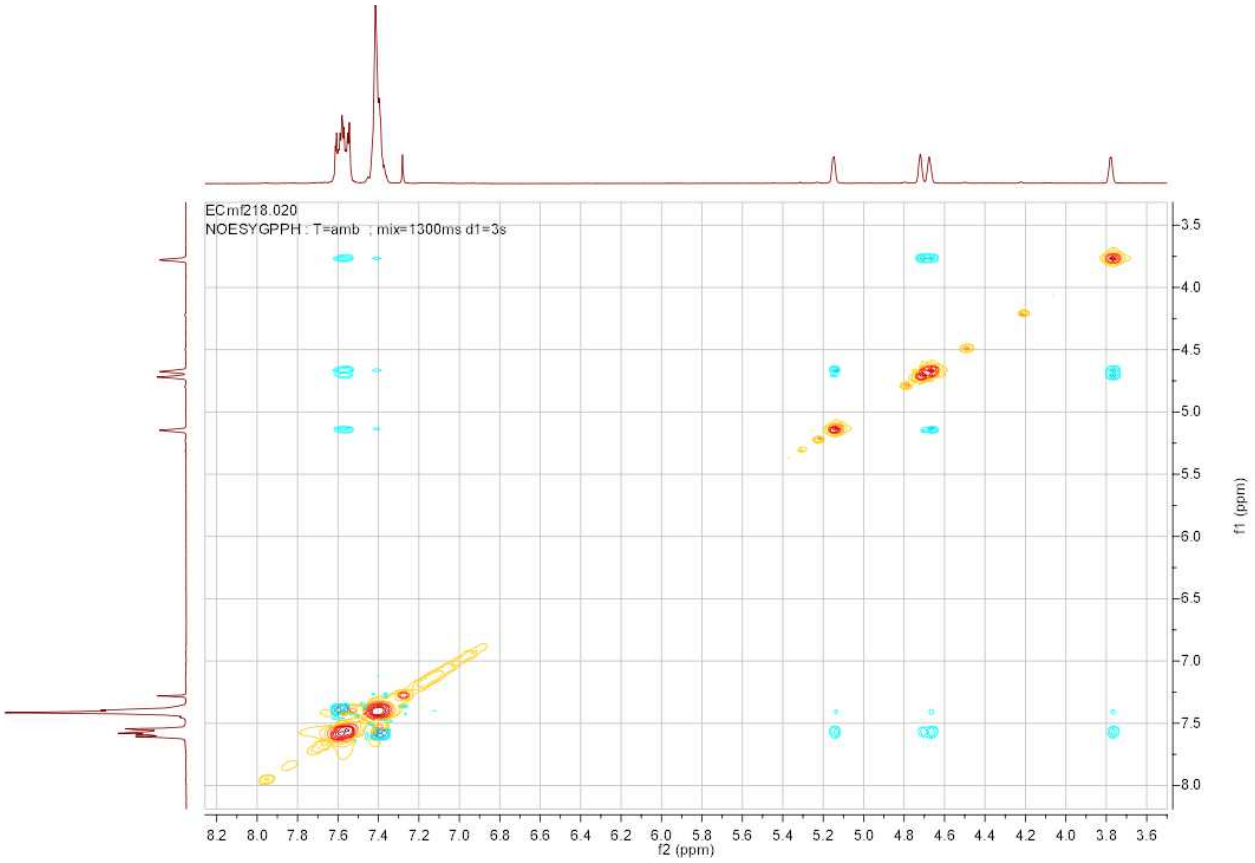

Figure 13SI. NOESY of $(R)_{Ru}$: expansion from 8.5ppm to 3.5ppm.

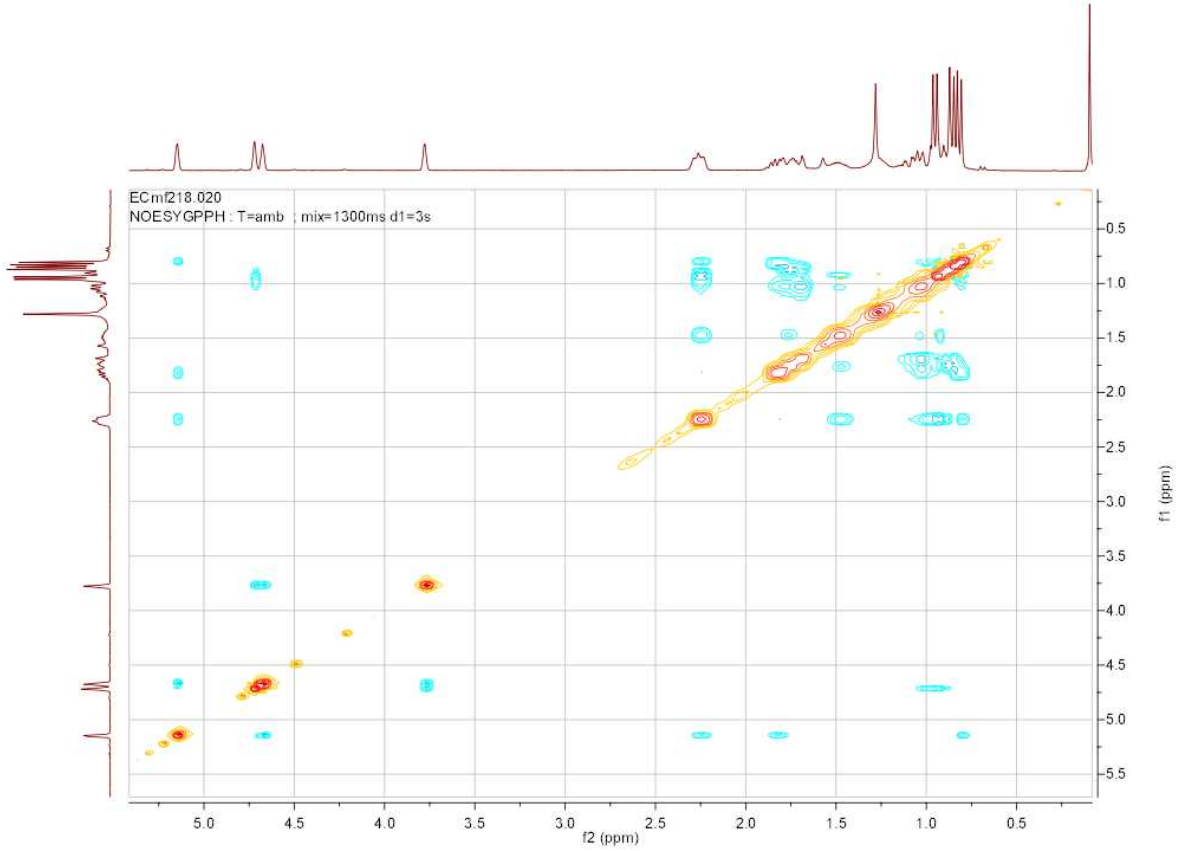

Figure 14SI. NOESY of $(R)_{Ru}$: expansion from 6ppm to 0ppm.

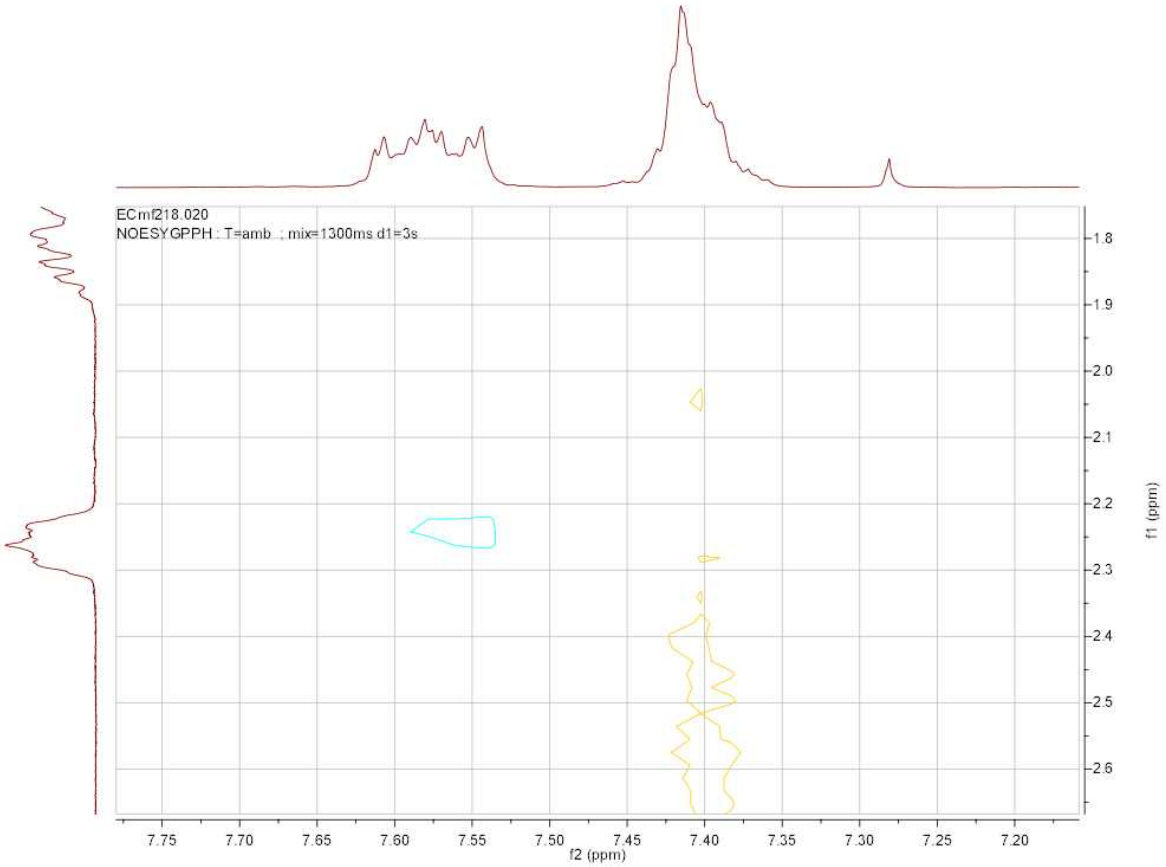

Figure 15SI. NOESY of $(R)_{Ru}$ cross-peak between oPh and H_7.

5.2. T-4-R-η^5-[(1R,2S,5R)-menthyl)-C_5H_4)Ru(CO)($P(C_6H_5)_3$)Cl] ($(R)_{Ru}$)

5.2.1. ^{1}H-NMR

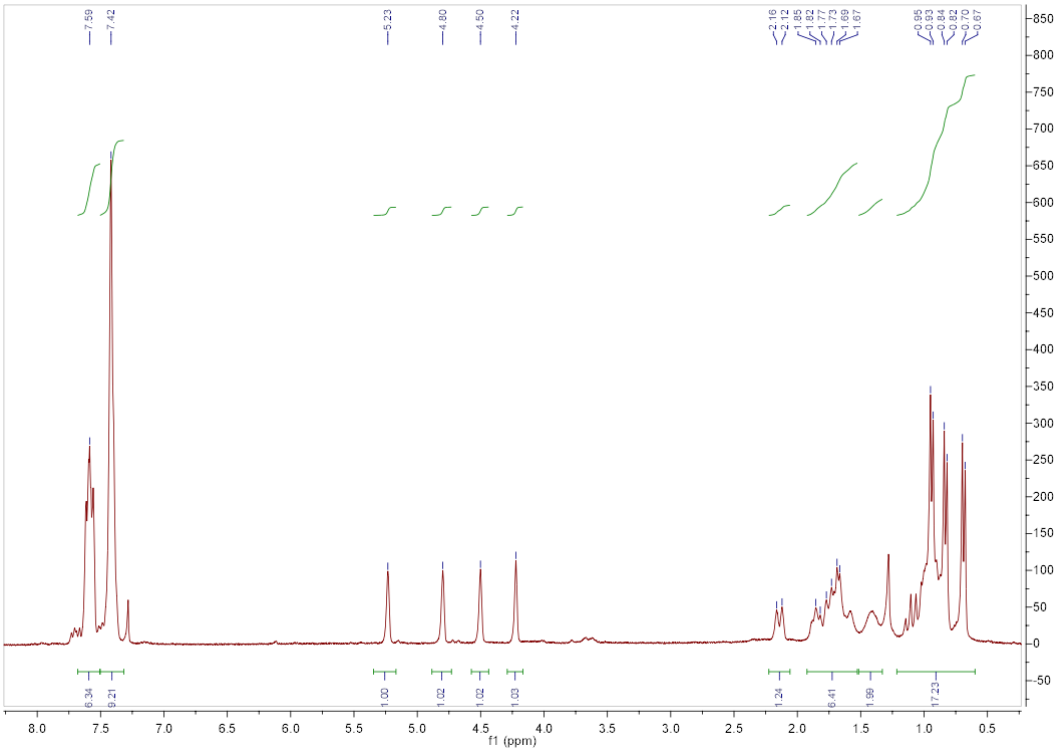

Figure 16SI. ^{1}H-NMR spectrum (300 MHz) of $(R)_{Ru}$ in $CDCl_3$ at 300 K.

5.2.2. ^{31}P-NMR

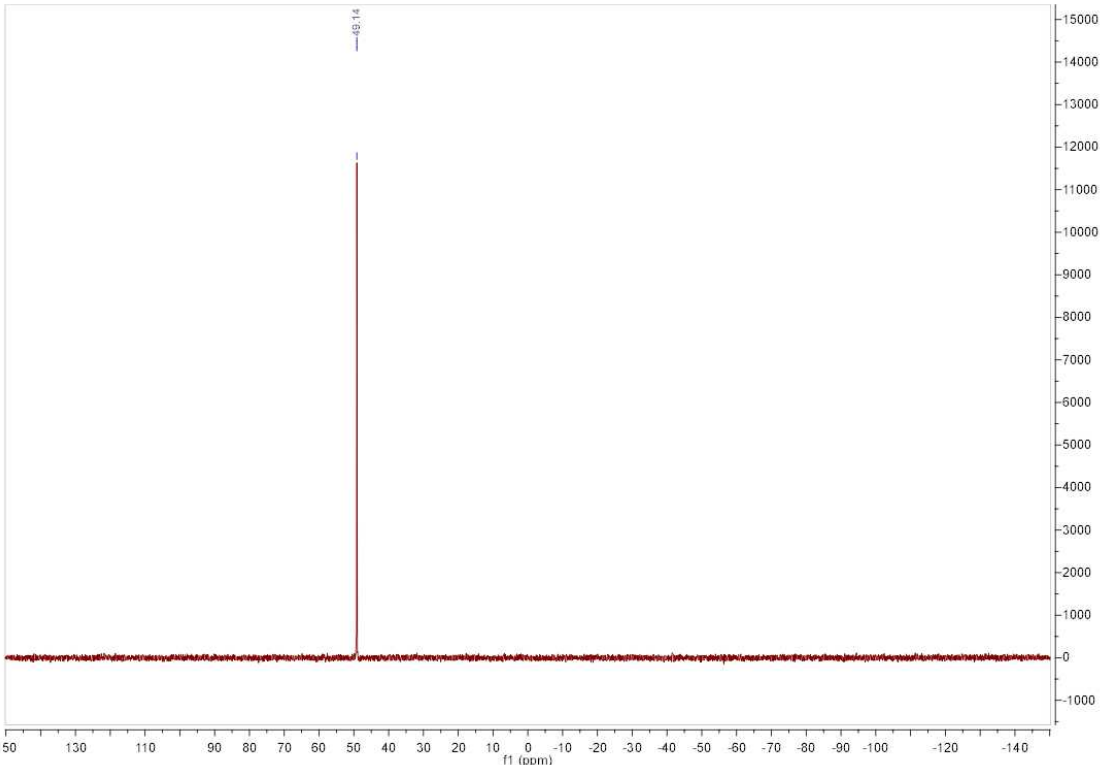

Figure 17SI. ^{31}P-NMR spectrum (121.49 MHz) of $(R)_{Ru}$ in $CDCl_3$ at 300 K.

5.2.3. *^{13}C-NMR*

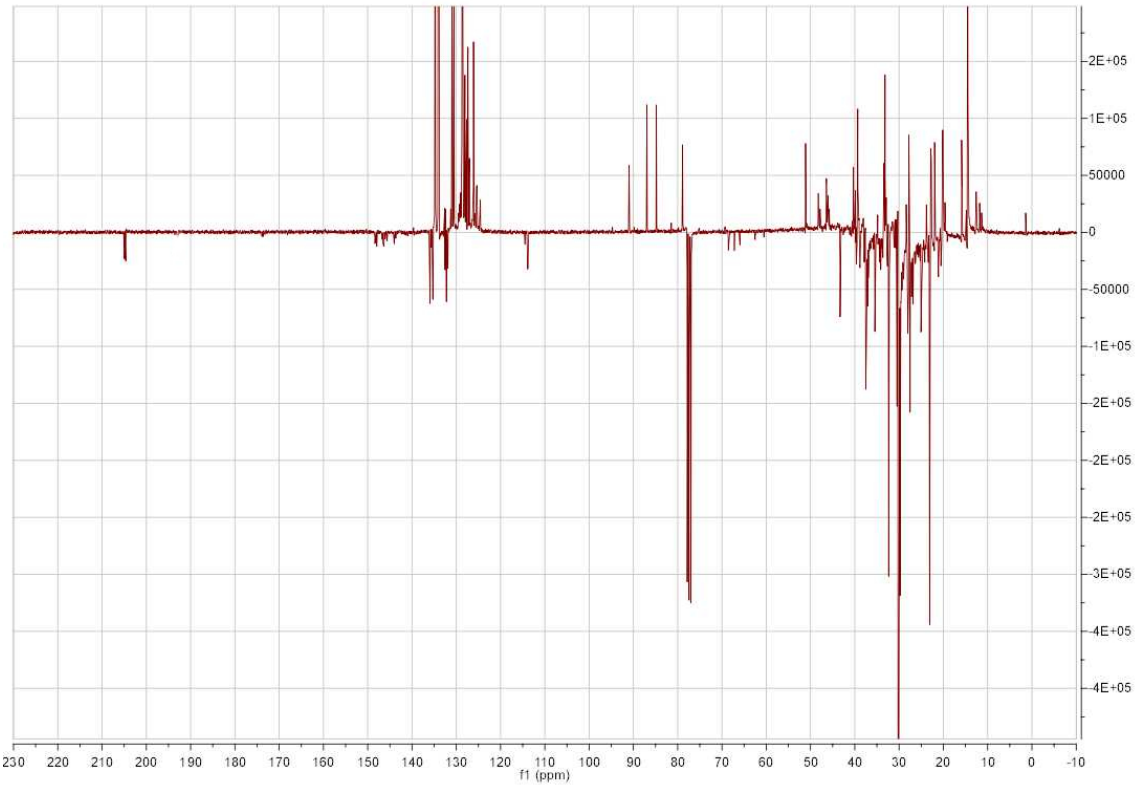

Figure 18SI. ^{13}C-NMR spectrum (75.47 MHz) of $(R)_{Ru}$ in $CDCl_3$ at 300 K.

5.2.4. *COSY*

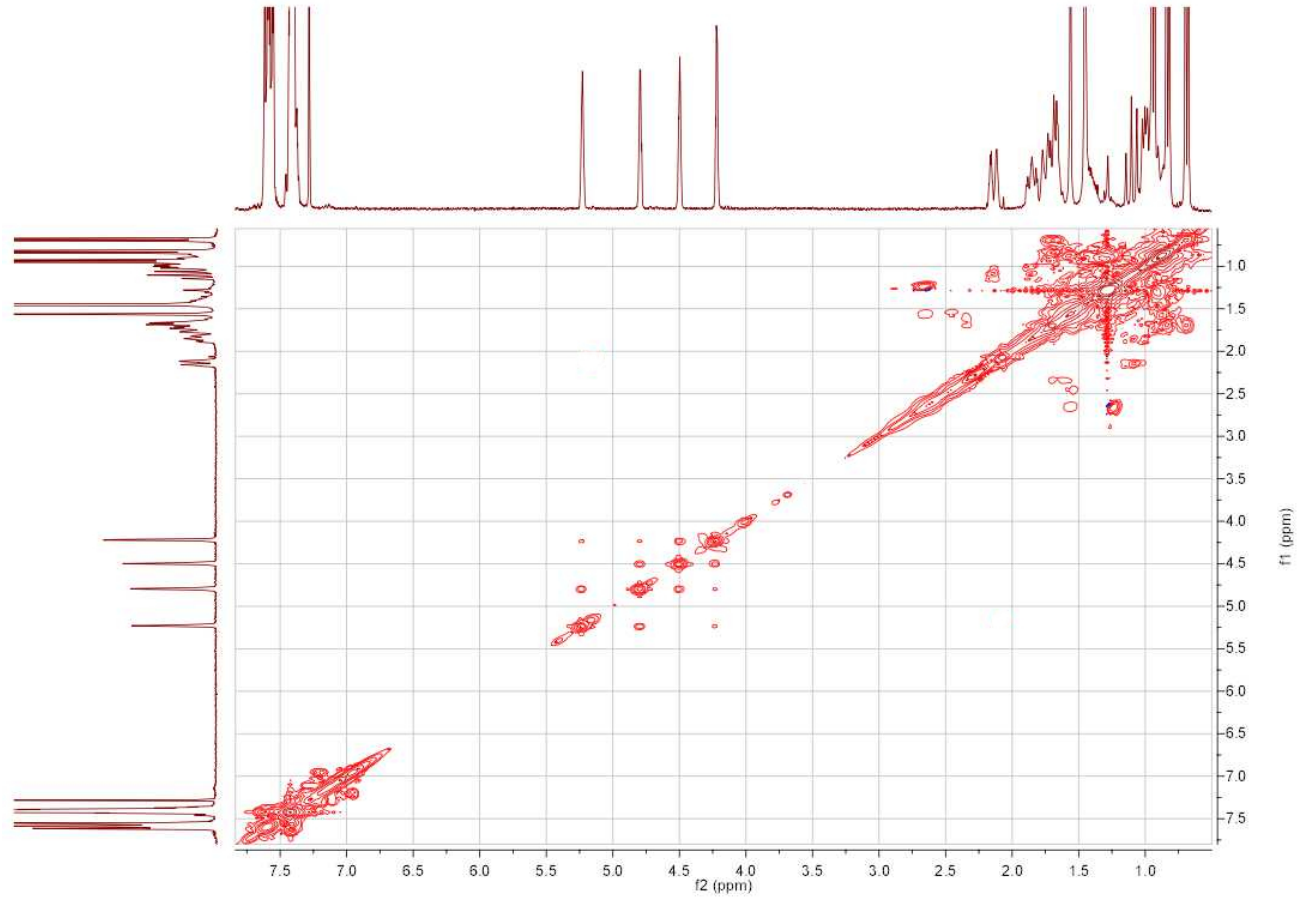

Figure 19SI. COSYGPQF spectrum (300 MHz) of $(R)_{Ru}$ in $CDCl_3$ at 300 K.

5.2.5. HSQC

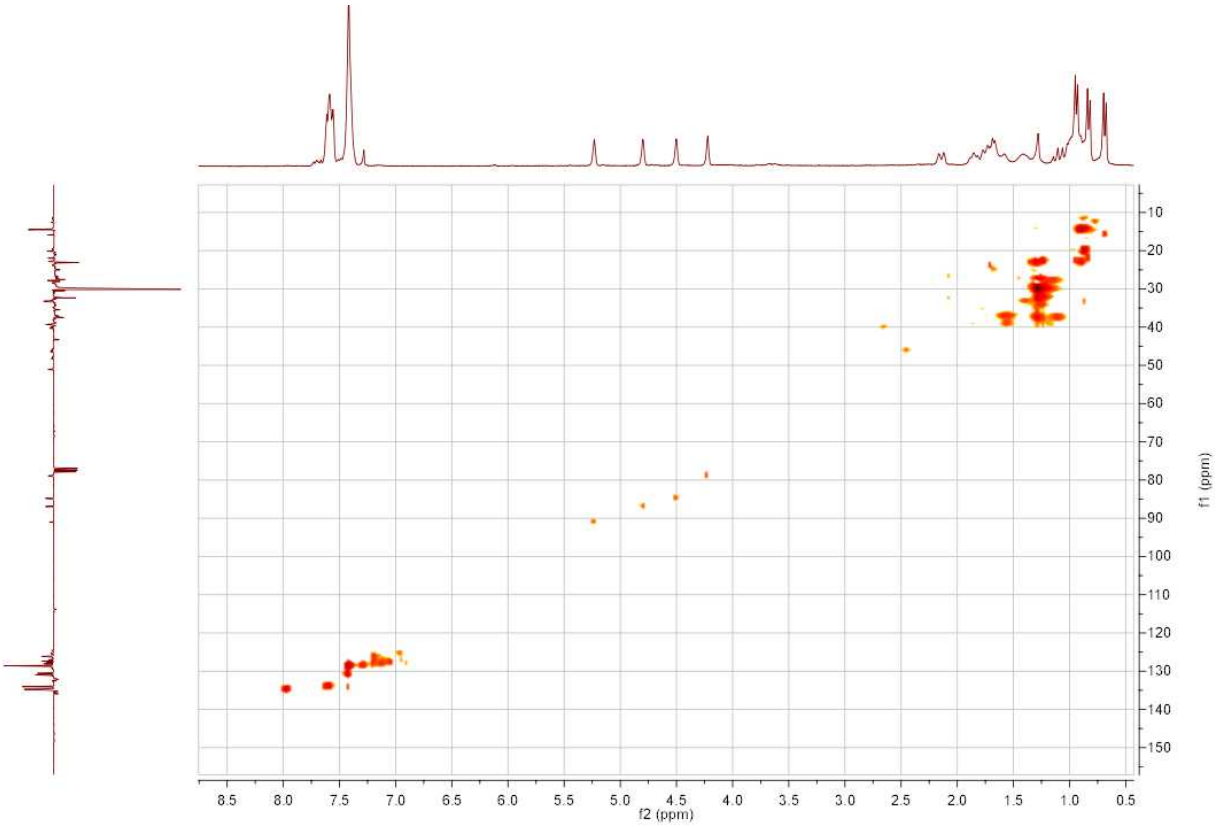

Figure 20SI. HSQCetgpsi ^{13}C-^{1}H spectrum of $(R)_{Ru}$ in $CDCl_3$ at 300 K.

5.2.6. HMBC

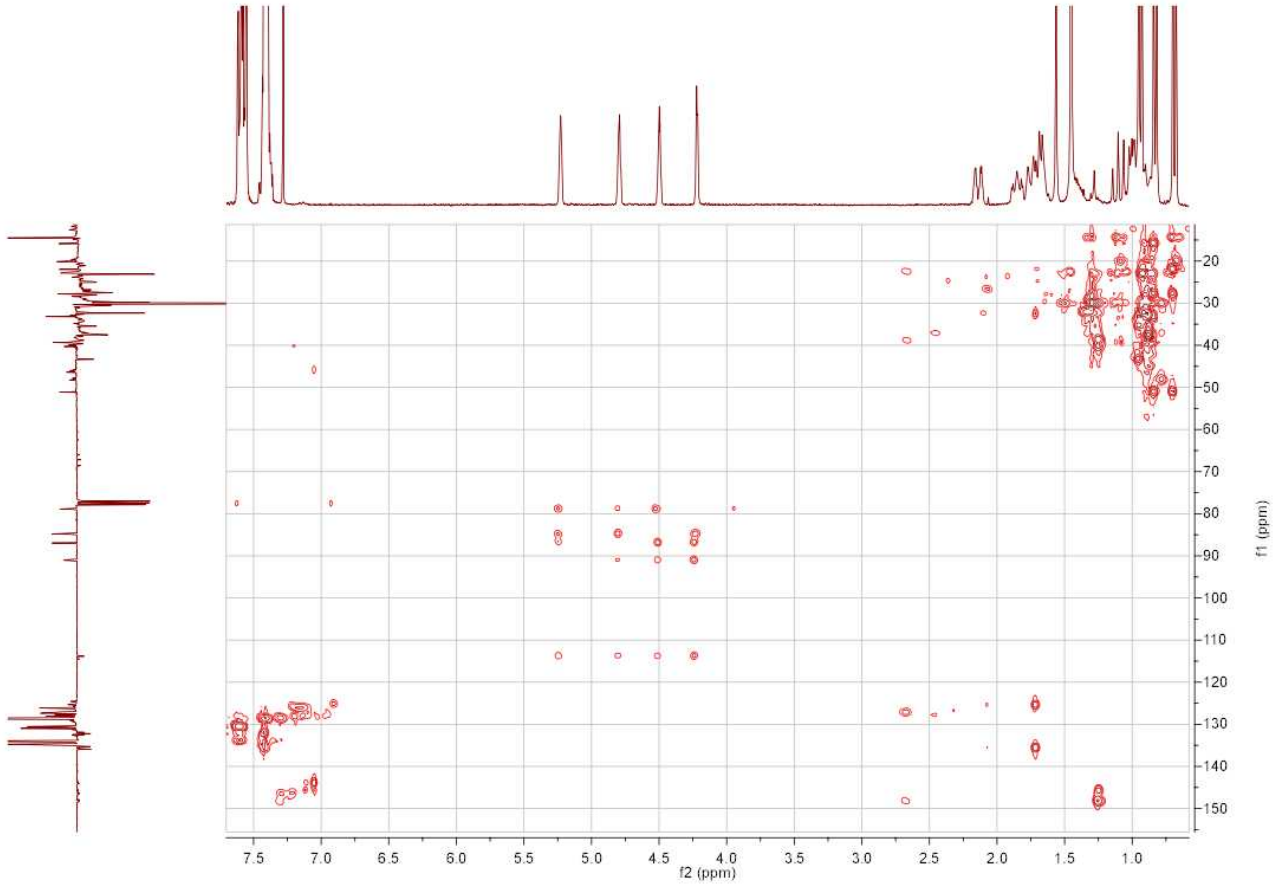

Figure 21SI. HMBC long range ^{13}C-^{1}H spectrum of $(R)_{Ru}$ in $CDCl_3$ at 300 K.

5.2.7. *^{31}P-INVBTP*

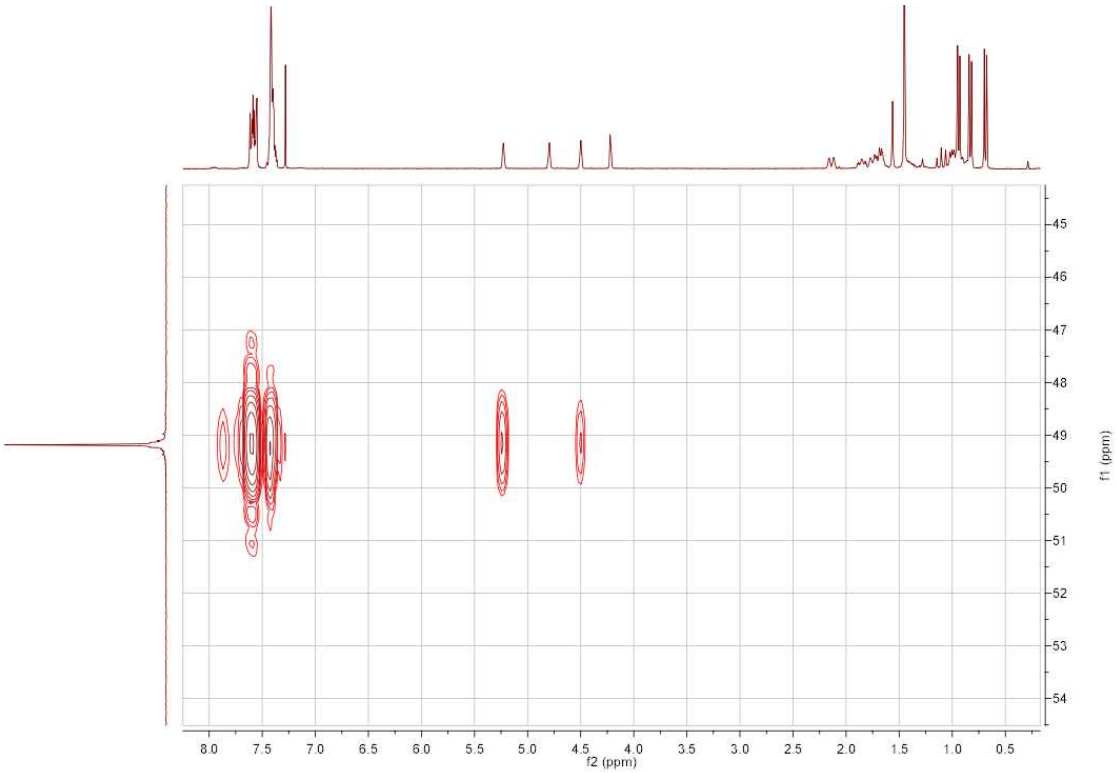

Figure 22SI. ^{31}P-INVBTP spectrum of $(R)_{Ru}$ in $CDCl_3$ at 300 K.

5.2.8. *NOESYGPPH mixingtime=1.3 s d1=3 s*

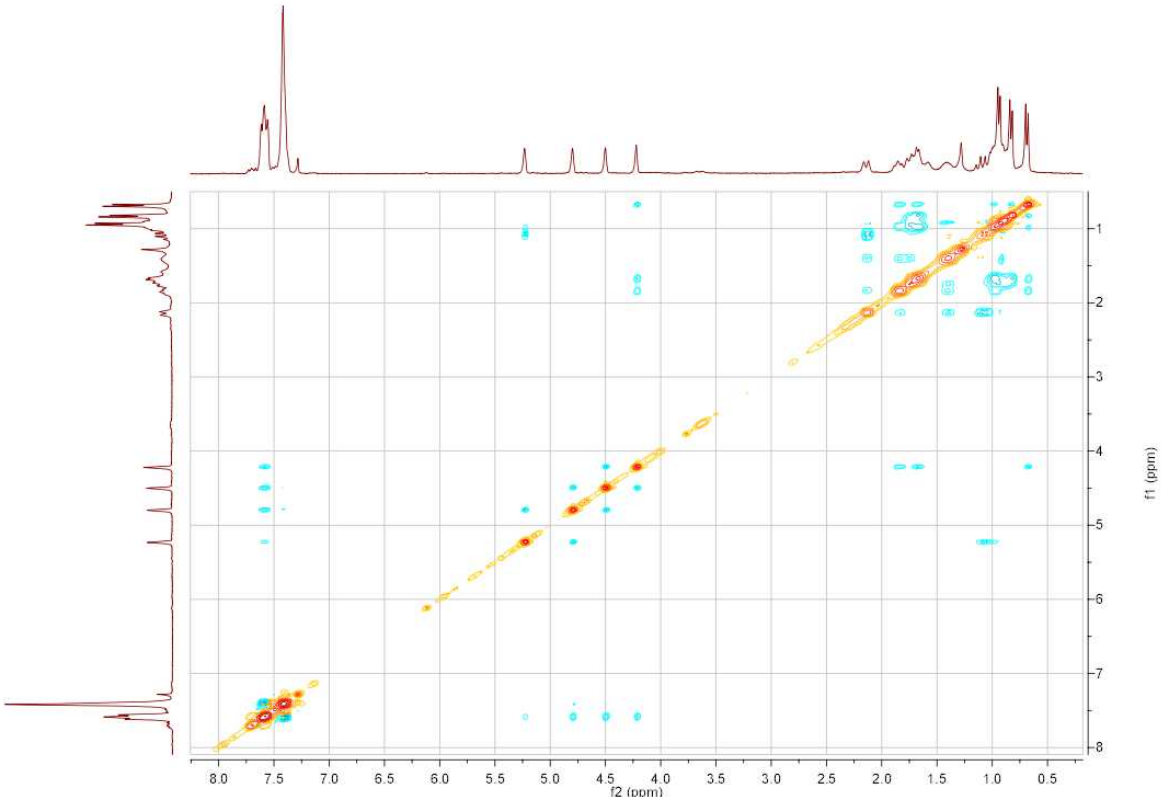

Figure 23SI. NOESY spectrum (300 MHz, mixing time: 1.3 s, time delay 3 s) of $(R)_{Ru}$ in $CDCl_3$ at 300 K.

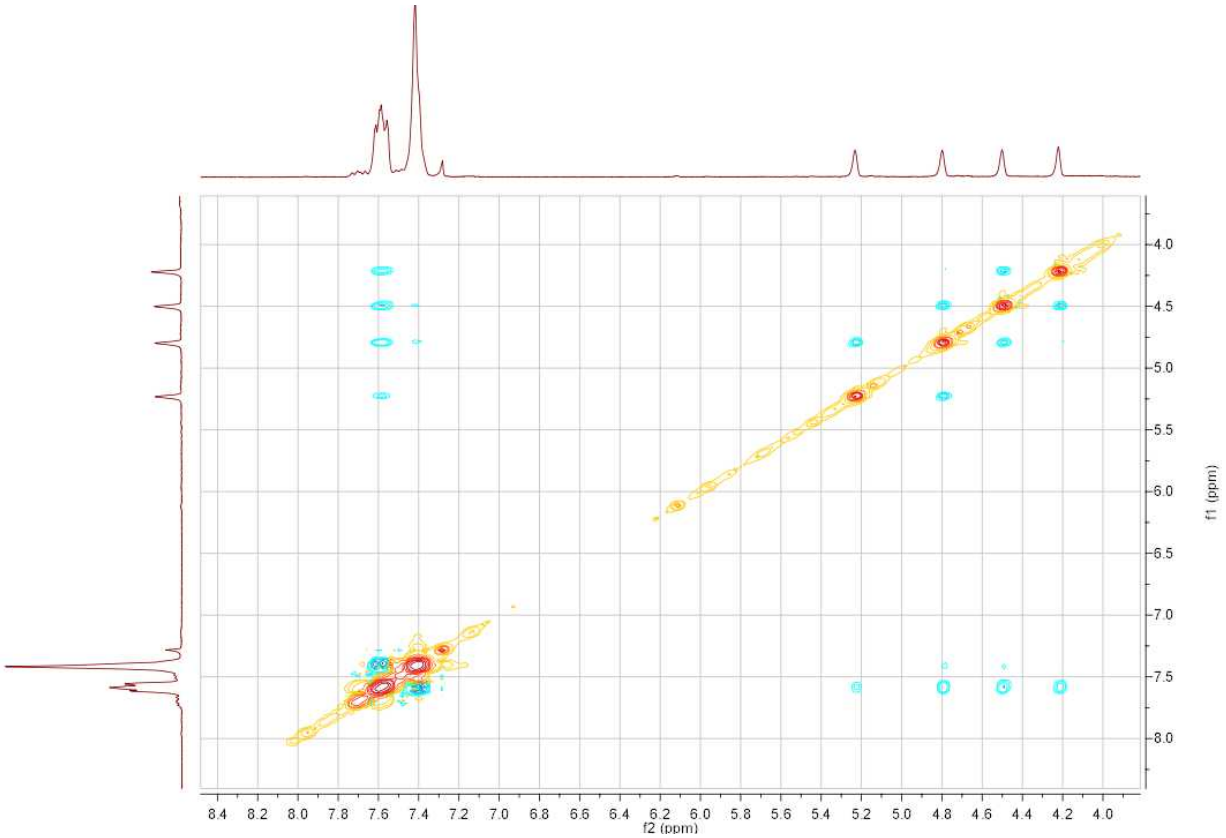

Figure 24SI. NOESY of $(R)_{Ru}$: expansion from 8.5ppm to 4ppm.

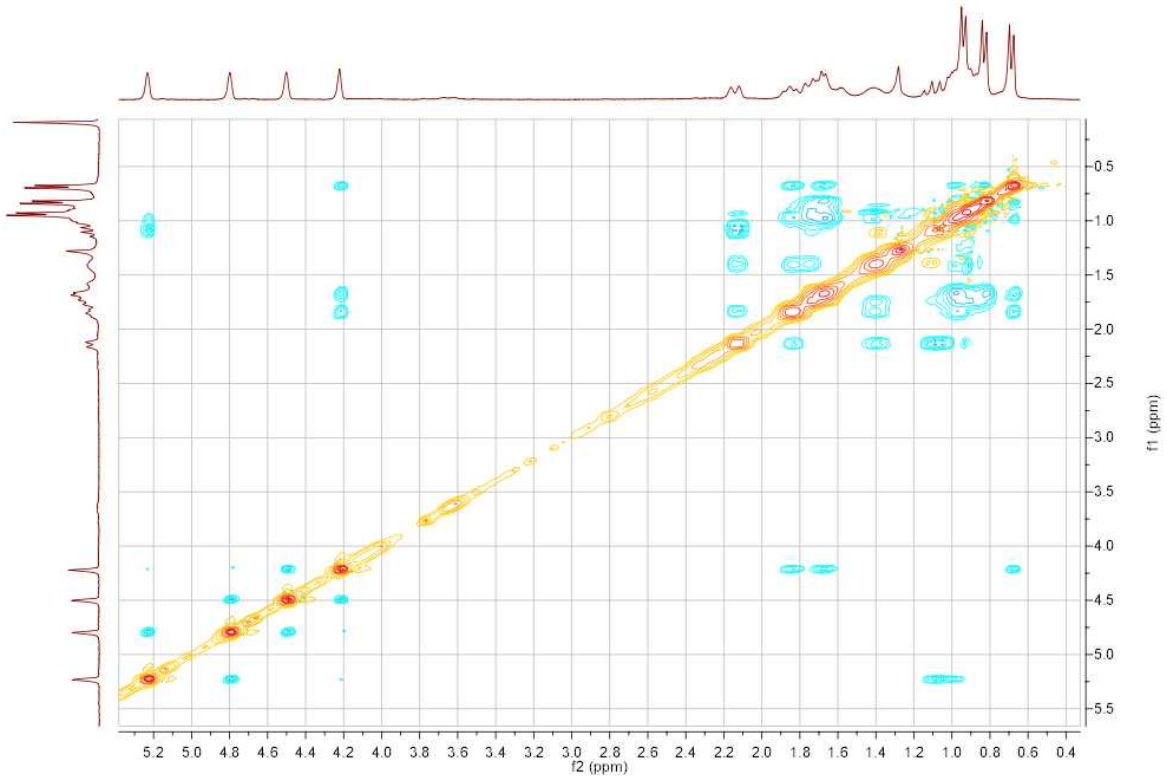

Figure 25SI. NOESY of $(R)_{Ru}$:expansion from 5.5ppm to 0ppm.

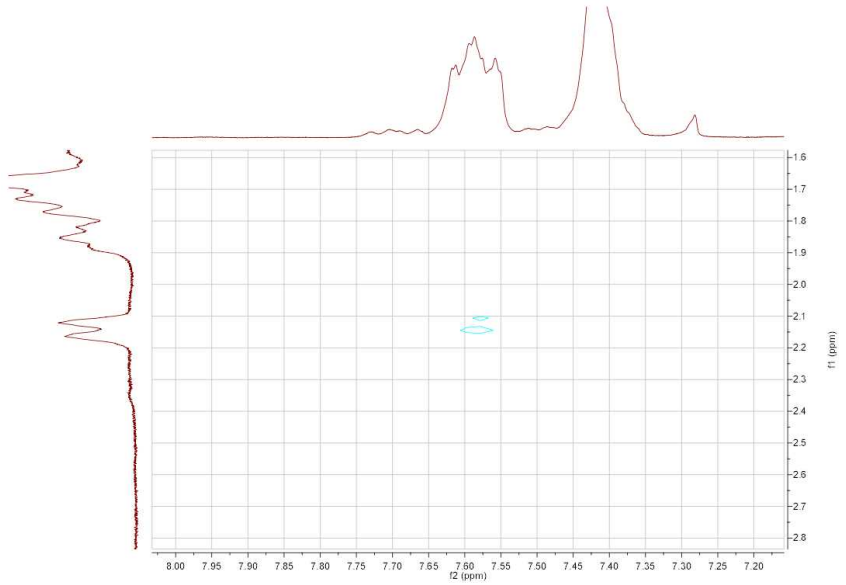

Figure 26SI. NOESY of $(R)_{Ru}$ cross-peak between oPh and H_7.

6. DFT CALCULATIONS

DFT calculations were conducted with Gaussian09[S5]; the complex was treated in vacuo with a choice of functional and basis functions analogous to ref. [S6]: B97D[S7]/SVP[S8]. The conformational search was carried out by first starting from the conformer of $(S)_{Ru}$ determined by x-ray, introducing a pseudo atom PSu at the center of the cyclopentadienyl ring, and drawing a line PSu-Ru around which the ring was rotated in five successive steps. For each one of the five positions thus reached, the menthyl moiety was allowed to rotate to avoid steric hindrance and the two orientations ~0° and ~180°of the menthyl moiety (referring to dihedral angle Ru-PSu-menthyl-isopropyl) have been tested. The lowest energy four conformers optimized at B97D[S7]/SVP[S8] level for both $(R)_{Ru}$ and $(S)_{Ru}$, are shown in Figure 4SI and most representative distances are reported in Table 1.

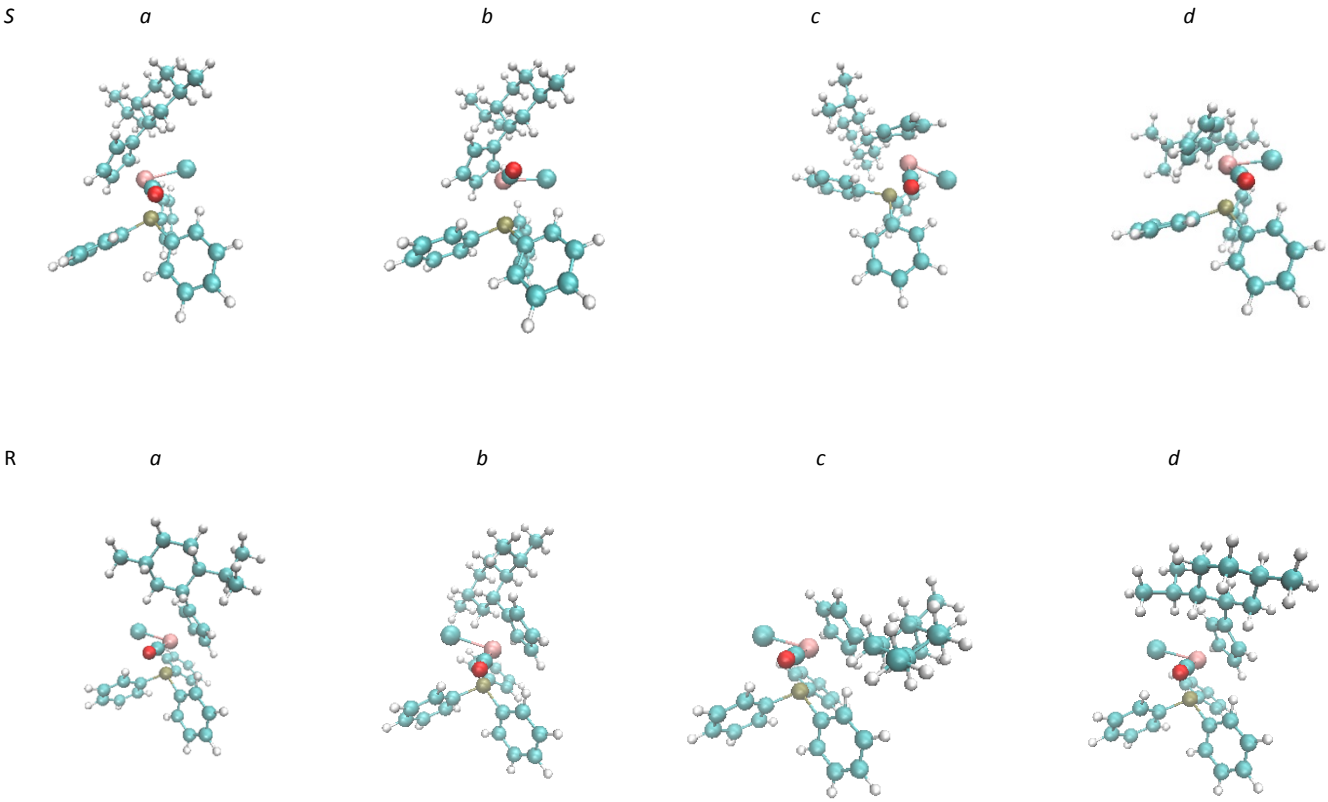

Figure 4SI. For each diastomers, $(S)_{Ru}$ and $(R)_{Ru}$, the four structure relative to table 1 in the text are reported

7. DFT optimized geometries

7.1. $(S)_{Ru}$

Coordinates of optimized structures of $(S)_{Ru}$ commented in the text (B97D/SVP level).

7.1.1. (S) conformer a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.790209	-0.005892	2.101861
2	1	0	-2.221259	0.804210	2.693298
3	6	0	-0.606240	-0.762927	2.441778
4	6	0	-0.388480	-1.716256	1.389805
5	6	0	-1.388530	-1.516622	0.392286
6	1	0	-0.018727	-0.676040	3.358348

7	1	0	0.428235	-2.441175	1.352619
8	1	0	-1.496588	-2.075544	-0.537386
9	6	0	-3.433471	0.108825	0.060024
10	6	0	-4.746054	-0.709925	0.271326
11	6	0	-3.664158	1.599073	0.381687
12	6	0	-5.872119	-0.085025	-0.581073
13	6	0	-4.786204	2.212927	-0.468625
14	6	0	-6.082850	1.406245	-0.278476
15	1	0	-3.158246	0.051486	-1.010083
16	1	0	-5.025612	-0.587231	1.340118
17	1	0	-5.610897	-0.199718	-1.651970
18	1	0	-6.815159	-0.640345	-0.419058
19	1	0	-6.886659	1.817324	-0.921762
20	1	0	-6.421374	1.524239	0.773387
21	1	0	-4.478068	2.119375	-1.531516
22	1	0	-2.717979	2.142341	0.212443
23	1	0	-3.934537	1.706178	1.453696
24	6	0	-4.579477	-2.234754	0.026488
25	1	0	-3.742933	-2.568787	0.670525
26	6	0	-4.213644	-2.578828	-1.428873
27	1	0	-3.346573	-1.993394	-1.786983
28	1	0	-3.965860	-3.653913	-1.523085
29	1	0	-5.059909	-2.370105	-2.111350
30	6	0	-5.821255	-3.025955	0.475111
31	1	0	-6.696609	-2.802450	-0.164888
32	1	0	-5.633142	-4.115460	0.412877
33	1	0	-6.092245	-2.781766	1.521039
34	6	0	-4.980321	3.700028	-0.146785
35	1	0	-4.043086	4.266096	-0.310263
36	1	0	-5.772748	4.147420	-0.778392
37	1	0	-5.276885	3.830881	0.913937
38	6	0	0.432959	2.008445	1.324105
39	8	0	0.723695	2.980577	1.897661
40	15	0	2.033623	-0.044070	-0.137101
41	6	0	2.201824	-1.037849	-1.680818
42	6	0	3.476129	-1.314483	-2.222359
43	6	0	1.047217	-1.530676	-2.318213
44	6	0	3.592145	-2.101998	-3.378195
45	1	0	4.375779	-0.910632	-1.741681
46	6	0	1.168161	-2.316754	-3.477104
47	1	0	0.064357	-1.256520	-1.922033
48	6	0	2.437464	-2.608033	-4.004312
49	1	0	4.584587	-2.316315	-3.795295
50	1	0	0.265118	-2.691668	-3.975810
51	1	0	2.529388	-3.219634	-4.911277
52	6	0	2.884101	-1.050398	1.157960
53	6	0	3.051386	-0.462194	2.431988
54	6	0	3.271070	-2.390302	0.959325
55	6	0	3.612456	-1.200043	3.484177
56	1	0	2.738122	0.576446	2.596280
57	6	0	3.821250	-3.132383	2.021523
58	1	0	3.140918	-2.856966	-0.023919
59	6	0	3.995409	-2.540212	3.282689
60	1	0	3.747004	-0.730507	4.467135
61	1	0	4.115667	-4.177090	1.857833
62	1	0	4.426878	-3.119568	4.108941
63	6	0	3.173398	1.380262	-0.405689
64	6	0	2.662748	2.531745	-1.043484
65	6	0	4.531841	1.332529	-0.025536
66	6	0	3.511759	3.620045	-1.300174
67	1	0	1.605993	2.567750	-1.337509
68	6	0	5.373662	2.427640	-0.283768
69	1	0	4.930528	0.445974	0.481881
70	6	0	4.865346	3.572032	-0.922048
71	1	0	3.109299	4.513410	-1.794585
72	1	0	6.428176	2.386129	0.018436
73	1	0	5.523274	4.428081	-1.120389
74	6	0	-2.265282	-0.443421	0.829897
75	44	0	-0.111966	0.397400	0.571230
76	17	0	-0.701049	1.375242	-1.618909

7.1.2. (S) conformer b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.763118	-0.635181	-1.665248
2	1	0	2.134073	-0.014251	-2.484278
3	6	0	0.613313	-1.503291	-1.726657
4	6	0	0.492202	-2.143294	-0.438411
5	6	0	1.512021	-1.631866	0.403779
6	1	0	-0.012936	-1.696773	-2.599905
7	1	0	-0.285906	-2.856481	-0.155122
8	1	0	1.657766	-1.863833	1.460785
9	6	0	3.512854	0.067262	0.172951
10	6	0	4.850096	-0.580141	-0.300618
11	6	0	3.464718	1.560961	-0.213057
12	6	0	6.037504	0.213929	0.283004
13	6	0	4.658214	2.351338	0.345849
14	6	0	5.980319	1.701258	-0.099574
15	1	0	3.474178	0.016801	1.277766
16	1	0	4.878938	-0.457405	-1.405235
17	1	0	6.018699	0.125159	1.387906
18	1	0	6.991387	-0.229952	-0.058828
19	1	0	6.839831	2.245606	0.340636
20	1	0	6.068567	1.799755	-1.202886
21	1	0	4.605968	2.283236	1.453708
22	1	0	2.516893	1.985207	0.160967
23	1	0	3.462338	1.652057	-1.319874
24	6	0	4.928228	-2.106124	-0.023448
25	1	0	4.021445	-2.553732	-0.477505
26	6	0	4.911524	-2.451443	1.475877
27	1	0	4.035693	-2.012251	1.988310
28	1	0	4.876357	-3.548540	1.620456
29	1	0	5.822007	-2.075662	1.981414
30	6	0	6.140448	-2.751120	-0.718232
31	1	0	7.093500	-2.400470	-0.276577
32	1	0	6.110414	-3.853091	-0.613597
33	1	0	6.156264	-2.507014	-1.798617
34	6	0	4.579845	3.830215	-0.054686
35	1	0	3.630295	4.283834	0.288765
36	1	0	5.420338	4.408662	0.376685
37	1	0	4.626165	3.933793	-1.157841
38	6	0	-0.026854	1.732344	-1.205388
39	8	0	-0.096572	2.685948	-1.872871
40	15	0	-2.094760	-0.020384	0.058030
41	6	0	-2.632177	-0.832141	1.623556
42	6	0	-3.996684	-0.874347	1.982122
43	6	0	-1.669940	-1.434021	2.457101
44	6	0	-4.394969	-1.536070	3.154202
45	1	0	-4.745255	-0.385722	1.346143
46	6	0	-2.072780	-2.094033	3.630617
47	1	0	-0.610743	-1.350513	2.194779
48	6	0	-3.433153	-2.150106	3.977970
49	1	0	-5.457207	-1.567794	3.428901
50	1	0	-1.318532	-2.554853	4.281280
51	1	0	-3.745411	-2.662741	4.897064
52	6	0	-2.799806	-1.085884	-1.275658
53	6	0	-2.693326	-0.627561	-2.608319
54	6	0	-3.344137	-2.360729	-1.024904
55	6	0	-3.140362	-1.427313	-3.669743
56	1	0	-2.254688	0.357521	-2.811299
57	6	0	-3.777123	-3.167754	-2.093930
58	1	0	-3.432115	-2.724739	0.005580
59	6	0	-3.680129	-2.703347	-3.415262
60	1	0	-3.062393	-1.057638	-4.700319
61	1	0	-4.195173	-4.161656	-1.888408
62	1	0	-4.021956	-3.332139	-4.247303
63	6	0	-3.108189	1.516858	-0.009796
64	6	0	-2.605067	2.669841	0.632207
65	6	0	-4.366530	1.560387	-0.647504
66	6	0	-3.363513	3.851203	0.635285

67	1	0	-1.625498	2.635057	1.126883
68	6	0	-5.117029	2.748574	-0.642279
69	1	0	-4.756739	0.670607	-1.156214
70	6	0	-4.617305	3.894687	-0.000378
71	1	0	-2.967609	4.745184	1.133873
72	1	0	-6.093165	2.777675	-1.143692
73	1	0	-5.203203	4.822983	0.000810
74	17	0	0.470401	1.271168	1.920423
75	6	0	2.312457	-0.677578	-0.341964
76	44	0	0.182678	0.154077	-0.258788

7.1.3. (S) conformer c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.383754	-1.404628	-2.044169
2	1	0	1.471523	-0.695657	-2.868617
3	6	0	0.915567	-2.768083	-2.153275
4	6	0	0.984493	-3.362820	-0.863923
5	6	0	1.444494	-2.354563	0.063642
6	1	0	0.533076	-3.239673	-3.061128
7	1	0	0.693961	-4.385546	-0.610721
8	1	0	1.641632	-2.496250	1.127122
9	6	0	2.469165	0.053941	-0.154035
10	6	0	4.023288	-0.148628	-0.206805
11	6	0	2.076218	1.329765	-0.920377
12	6	0	4.724377	1.130406	0.302133
13	6	0	2.793858	2.593021	-0.426997
14	6	0	4.314271	2.381266	-0.488113
15	1	0	2.190808	0.185968	0.906268
16	1	0	4.284499	-0.269699	-1.279890
17	1	0	4.462825	1.280296	1.368872
18	1	0	5.820588	0.995196	0.255081
19	1	0	4.840615	3.274677	-0.096260
20	1	0	4.619325	2.266671	-1.550065
21	1	0	2.525028	2.732767	0.638847
22	1	0	0.987866	1.473600	-0.854756
23	1	0	2.312435	1.193761	-1.995809
24	6	0	4.518507	-1.429329	0.520113
25	1	0	3.963065	-2.278989	0.080208
26	6	0	4.231608	-1.416122	2.032351
27	1	0	3.167681	-1.210198	2.249155
28	1	0	4.494055	-2.392022	2.484457
29	1	0	4.831739	-0.638586	2.543262
30	6	0	6.010291	-1.700379	0.252971
31	1	0	6.655205	-0.940842	0.735878
32	1	0	6.302507	-2.688902	0.656799
33	1	0	6.228292	-1.693402	-0.832914
34	6	0	2.335184	3.827662	-1.213308
35	1	0	1.238750	3.963727	-1.140612
36	1	0	2.829526	4.746574	-0.841460
37	1	0	2.586756	3.717841	-2.287597
38	6	0	-1.700864	-2.699673	0.288492
39	8	0	-2.324216	-3.413750	0.966112
40	15	0	-1.405386	0.233891	0.203830
41	6	0	-1.627487	1.723251	-0.865312
42	6	0	-1.157067	1.712453	-2.192968
43	6	0	-2.278891	2.870878	-0.362644
44	6	0	-1.301863	2.854851	-2.997114
45	1	0	-0.706953	0.798421	-2.593032
46	6	0	-2.416480	4.012647	-1.168015
47	1	0	-2.683768	2.867416	0.657015
48	6	0	-1.921754	4.007467	-2.485298
49	1	0	-0.936534	2.839513	-4.031808
50	1	0	-2.918418	4.904010	-0.770087
51	1	0	-2.033705	4.898507	-3.116580
52	6	0	-0.323325	0.779351	1.600996
53	6	0	0.068844	-0.218228	2.521938

54	6	0	0.150745	2.092980	1.768946
55	6	0	0.916981	0.096120	3.593037
56	1	0	-0.284214	-1.246602	2.382501
57	6	0	1.010724	2.404522	2.838162
58	1	0	-0.130496	2.873065	1.054120
59	6	0	1.396511	1.410296	3.750803
60	1	0	1.213211	-0.687437	4.301856
61	1	0	1.384200	3.430260	2.950295
62	1	0	2.070965	1.655047	4.581141
63	6	0	-3.067479	0.085234	0.999485
64	6	0	-3.321544	0.530875	2.313161
65	6	0	-4.113274	-0.478440	0.234915
66	6	0	-4.612248	0.414121	2.858688
67	1	0	-2.514704	0.965482	2.914848
68	6	0	-5.398757	-0.588103	0.786594
69	1	0	-3.912730	-0.833174	-0.784707
70	6	0	-5.652242	-0.144069	2.097181
71	1	0	-4.801781	0.759507	3.883364
72	1	0	-6.206449	-1.029425	0.188667
73	1	0	-6.658712	-0.236713	2.525498
74	6	0	1.747616	-1.158742	-0.682923
75	44	0	-0.561127	-1.688413	-0.765002
76	17	0	-2.172759	-1.494305	-2.616793

7.1.4. (S) conformer d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.630325	0.233695	-2.694065
2	1	0	-2.075398	-0.626739	-3.196714
3	6	0	-0.749012	1.172071	-3.298884
4	6	0	-0.295021	2.073056	-2.262490
5	6	0	-0.936404	1.685435	-1.040293
6	1	0	-0.443042	1.185598	-4.347496
7	1	0	0.377639	2.924522	-2.388702
8	1	0	-0.812088	2.182851	-0.078295
9	6	0	-2.705582	-0.135980	-0.314020
10	6	0	-4.035531	0.649552	-0.065062
11	6	0	-3.030487	-1.576115	-0.763394
12	6	0	-4.887639	-0.120909	0.969364
13	6	0	-3.859052	-2.339296	0.280126
14	6	0	-5.164790	-1.573597	0.551848
15	1	0	-2.184130	-0.195072	0.660530
16	1	0	-4.588084	0.644845	-1.029206
17	1	0	-4.347733	-0.125597	1.937737
18	1	0	-5.842059	0.411573	1.138369
19	1	0	-5.756819	-2.089945	1.334026
20	1	0	-5.778358	-1.581663	-0.374186
21	1	0	-3.276443	-2.348841	1.224766
22	1	0	-2.098698	-2.117301	-1.008226
23	1	0	-3.616456	-1.530358	-1.705313
24	6	0	-3.829137	2.138748	0.321735
25	1	0	-3.216322	2.589989	-0.481790
26	6	0	-3.071090	2.323162	1.648781
27	1	0	-2.120414	1.760526	1.664303
28	1	0	-2.832027	3.391252	1.814928
29	1	0	-3.680398	1.977365	2.505971
30	6	0	-5.157313	2.916695	0.343265
31	1	0	-5.809716	2.584477	1.173927
32	1	0	-4.971675	3.999802	0.479335
33	1	0	-5.714140	2.778565	-0.604205
34	6	0	-4.109975	-3.788647	-0.153795
35	1	0	-3.155180	-4.325326	-0.316936
36	1	0	-4.697531	-4.340249	0.606317
37	1	0	-4.677286	-3.814762	-1.106052
38	6	0	2.131216	0.250162	-2.521801
39	8	0	3.115363	0.496009	-3.094473
40	15	0	1.525856	-0.044156	0.368105
41	6	0	0.809153	-1.073894	1.724130

42	6	0	-0.246338	-1.963000	1.451358
43	6	0	1.349646	-1.006069	3.028312
44	6	0	-0.770054	-2.766452	2.480118
45	1	0	-0.621005	-2.051218	0.428888
46	6	0	0.817289	-1.802109	4.053271
47	1	0	2.188273	-0.331761	3.240507
48	6	0	-0.246647	-2.683042	3.780333
49	1	0	-1.585094	-3.465682	2.255891
50	1	0	1.238230	-1.741877	5.065228
51	1	0	-0.657812	-3.311036	4.581312
52	6	0	1.545686	1.671187	1.054201
53	6	0	2.284522	2.649812	0.351606
54	6	0	0.729375	2.067612	2.131923
55	6	0	2.215697	3.997926	0.731529
56	1	0	2.907313	2.353097	-0.501365
57	6	0	0.651067	3.422904	2.501942
58	1	0	0.140939	1.321469	2.677236
59	6	0	1.393349	4.389899	1.805710
60	1	0	2.799360	4.748149	0.182643
61	1	0	0.002178	3.719309	3.335910
62	1	0	1.331493	5.446734	2.094950
63	6	0	3.298048	-0.558281	0.384716
64	6	0	4.265118	0.100230	1.173329
65	6	0	3.666534	-1.681506	-0.386862
66	6	0	5.592698	-0.359862	1.187373
67	1	0	3.986339	0.977817	1.768704
68	6	0	4.994192	-2.137273	-0.363099
69	1	0	2.912072	-2.192527	-0.999164
70	6	0	5.959042	-1.478915	0.420074
71	1	0	6.341939	0.160487	1.798139
72	1	0	5.276303	-3.009673	-0.966238
73	1	0	6.997141	-1.835611	0.430040
74	6	0	-1.776473	0.541139	-1.290774
75	44	0	0.479057	0.046494	-1.687558
76	17	0	0.468168	-2.406159	-1.948943

7.2. $(R)_{Ru}$

Coordinates of optimized structures of $(R)_{Ru}$ commented in the text (B97D/SVP level).

7.2.1. (R) conformer a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.745864	-0.417663	-1.688764
2	1	0	2.050681	0.350176	-2.402905
3	6	0	0.616535	-1.285884	-1.841870
4	6	0	0.489361	-2.044952	-0.625704
5	6	0	1.544979	-1.639192	0.257929
6	1	0	-0.049566	-1.336203	-2.705124
7	1	0	-0.264574	-2.808377	-0.419496
8	1	0	1.747724	-2.044855	1.251895
9	6	0	3.548493	0.075292	0.161080
10	6	0	4.886129	-0.584179	-0.293866
11	6	0	3.541155	1.577505	-0.191321
12	6	0	6.068309	0.174323	0.346846
13	6	0	4.721599	2.334606	0.435504
14	6	0	6.046623	1.674471	0.012021
15	1	0	3.494177	-0.009088	1.264494
16	1	0	4.947569	-0.433840	-1.393421
17	1	0	6.016128	0.052236	1.447435
18	1	0	7.024959	-0.274453	0.019503
19	1	0	6.900844	2.188734	0.496286
20	1	0	6.170581	1.807307	-1.083948
21	1	0	4.634340	2.236532	1.539495
22	1	0	2.574843	2.020699	0.109113
23	1	0	3.598914	1.687589	-1.293948
24	6	0	4.930966	-2.117577	-0.051753

25	1	0	4.026060	-2.537467	-0.534868
26	6	0	4.879563	-2.499382	1.438294
27	1	0	4.008246	-2.049154	1.949521
28	1	0	4.812732	-3.598300	1.555090
29	1	0	5.791112	-2.160922	1.967468
30	6	0	6.145705	-2.767997	-0.737001
31	1	0	7.095305	-2.442751	-0.269285
32	1	0	6.095637	-3.871274	-0.656792
33	1	0	6.186475	-2.501242	-1.811186
34	6	0	4.680478	3.824701	0.072275
35	1	0	3.726420	4.285819	0.392111
36	1	0	5.514861	4.377348	0.547092
37	1	0	4.766339	3.954136	-1.025432
38	6	0	0.389342	0.807524	1.658699
39	8	0	0.619188	1.164280	2.746400
40	15	0	-2.105081	-0.037170	0.081911
41	6	0	-2.720293	-1.184058	1.393863
42	6	0	-4.098415	-1.310335	1.673873
43	6	0	-1.790832	-1.954012	2.120275
44	6	0	-4.537500	-2.209203	2.658713
45	1	0	-4.826248	-0.699365	1.126429
46	6	0	-2.232452	-2.851425	3.107547
47	1	0	-0.723227	-1.825455	1.908665
48	6	0	-3.605531	-2.983018	3.375222
49	1	0	-5.610110	-2.302106	2.872456
50	1	0	-1.501382	-3.443526	3.673046
51	1	0	-3.951017	-3.681861	4.147941
52	6	0	-2.730210	-0.744208	-1.499982
53	6	0	-2.536432	0.026923	-2.669577
54	6	0	-3.296112	-2.030439	-1.593268
55	6	0	-2.922001	-0.487851	-3.915691
56	1	0	-2.059734	1.013758	-2.593270
57	6	0	-3.670820	-2.544030	-2.849005
58	1	0	-3.446032	-2.631464	-0.688339
59	6	0	-3.488506	-1.774449	-4.009452
60	1	0	-2.772777	0.114991	-4.820826
61	1	0	-4.108920	-3.548286	-2.916384
62	1	0	-3.783952	-2.175734	-4.987474
63	6	0	-3.126731	1.477919	0.320520
64	6	0	-2.648656	2.502807	1.162687
65	6	0	-4.391895	1.610838	-0.289834
66	6	0	-3.440671	3.634481	1.409722
67	1	0	-1.655012	2.425808	1.613986
68	6	0	-5.178785	2.748903	-0.044061
69	1	0	-4.757528	0.831091	-0.968795
70	6	0	-4.705907	3.760323	0.808884
71	1	0	-3.059842	4.429063	2.063749
72	1	0	-6.160592	2.845764	-0.525332
73	1	0	-5.318560	4.651316	0.997847
74	17	0	-0.087194	2.328674	-1.108500
75	6	0	2.338274	-0.622082	-0.400849
76	44	0	0.187736	0.129253	-0.056225

7.2.2. (R) conformer b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.176370	-0.686758	1.442029
2	1	0	-1.060301	0.242978	1.999110
3	6	0	-0.347841	-1.859857	1.581607
4	6	0	-0.820383	-2.838483	0.642459
5	6	0	-1.916677	-2.262270	-0.090268
6	1	0	0.450605	-2.000132	2.313787
7	1	0	-0.428538	-3.851509	0.517902
8	1	0	-2.488431	-2.745384	-0.882549
9	6	0	-3.168554	0.049548	-0.087481
10	6	0	-4.621463	-0.265666	0.403616
11	6	0	-2.788706	1.496135	0.285157
12	6	0	-5.587378	0.782395	-0.195102

13	6	0	-3.750502	2.531402	-0.313614
14	6	0	-5.186853	2.225109	0.144502
15	1	0	-3.154109	-0.019005	-1.192224
16	1	0	-4.617309	-0.127514	1.506388
17	1	0	-5.597263	0.665243	-1.296952
18	1	0	-6.616492	0.584714	0.158271
19	1	0	-5.898149	2.938794	-0.317857
20	1	0	-5.247767	2.376028	1.243720
21	1	0	-3.710885	2.416195	-1.417176
22	1	0	-1.761882	1.689792	-0.063088
23	1	0	-2.796764	1.603433	1.390179
24	6	0	-5.089345	-1.722746	0.138792
25	1	0	-4.334770	-2.386783	0.601322
26	6	0	-5.167999	-2.069691	-1.358736
27	1	0	-4.232516	-1.817646	-1.891595
28	1	0	-5.364075	-3.150501	-1.497998
29	1	0	-5.990352	-1.515445	-1.850509
30	6	0	-6.425441	-2.032416	0.838355
31	1	0	-7.262753	-1.468404	0.384050
32	1	0	-6.667038	-3.109723	0.754884
33	1	0	-6.381287	-1.771123	1.913886
34	6	0	-3.322428	3.961488	0.039917
35	1	0	-2.304689	4.174189	-0.340604
36	1	0	-4.016718	4.707720	-0.393591
37	1	0	-3.314015	4.103181	1.139896
38	6	0	0.933954	-2.223741	-1.712563
39	8	0	1.438263	-2.988872	-2.435186
40	15	0	1.931958	0.071208	0.053625
41	6	0	3.263645	-0.913563	0.875902
42	6	0	4.464860	-0.305196	1.301451
43	6	0	3.076927	-2.294582	1.079459
44	6	0	5.457371	-1.069844	1.933708
45	1	0	4.625776	0.766190	1.132980
46	6	0	4.074352	-3.060117	1.707956
47	1	0	2.146209	-2.756201	0.731489
48	6	0	5.263431	-2.448801	2.138859
49	1	0	6.388179	-0.589972	2.262429
50	1	0	3.922335	-4.136926	1.856612
51	1	0	6.043172	-3.045858	2.629107
52	6	0	1.446042	1.339324	1.293476
53	6	0	0.656441	2.419094	0.838604
54	6	0	1.714030	1.196530	2.669248
55	6	0	0.146514	3.347855	1.756768
56	1	0	0.421941	2.502292	-0.230530
57	6	0	1.193516	2.128060	3.585686
58	1	0	2.325061	0.357984	3.024357
59	6	0	0.410987	3.203680	3.132081
60	1	0	-0.475992	4.176806	1.398684
61	1	0	1.402457	2.011655	4.657011
62	1	0	0.004825	3.928753	3.848947
63	6	0	2.841873	1.033188	-1.228870
64	6	0	2.904241	0.536659	-2.546612
65	6	0	3.513642	2.231164	-0.903602
66	6	0	3.651506	1.218927	-3.519453
67	1	0	2.357688	-0.370731	-2.818210
68	6	0	4.255078	2.913940	-1.882148
69	1	0	3.445859	2.640343	0.111645
70	6	0	4.328463	2.406340	-3.190675
71	1	0	3.691544	0.826636	-4.543450
72	1	0	4.771794	3.846557	-1.621077
73	1	0	4.905100	2.941160	-3.956417
74	17	0	-0.495311	0.566292	-2.207103
75	6	0	-2.140700	-0.930237	0.415490
76	44	0	0.050840	-1.128252	-0.508204

7.2.3. (R) conformer c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.873341	0.881476	-2.179729
2	1	0	-2.429476	0.327141	-2.938700
3	6	0	-0.923472	1.912027	-2.425045
4	6	0	-0.412340	2.377751	-1.160349
5	6	0	-1.055571	1.611816	-0.136808
6	1	0	-0.581134	2.247932	-3.406610
7	1	0	0.340862	3.152802	-1.012285
8	1	0	-0.899382	1.718557	0.938671
9	6	0	-2.992612	-0.148839	-0.026554
10	6	0	-4.384025	0.564717	-0.065746
11	6	0	-3.111643	-1.584375	-0.575579
12	6	0	-5.418690	-0.285465	0.701344
13	6	0	-4.156455	-2.426845	0.174267
14	6	0	-5.519821	-1.715060	0.150291
15	1	0	-2.691593	-0.214688	1.036779
16	1	0	-4.691705	0.582093	-1.133160
17	1	0	-5.124616	-0.330597	1.769329
18	1	0	-6.408292	0.206139	0.662444
19	1	0	-6.264327	-2.299594	0.726801
20	1	0	-5.881002	-1.680858	-0.899543
21	1	0	-3.831179	-2.488352	1.236225
22	1	0	-2.130703	-2.086073	-0.527059
23	1	0	-3.387625	-1.541267	-1.649082
24	6	0	-4.337103	2.044123	0.406193
25	1	0	-3.569777	2.549098	-0.211900
26	6	0	-3.920298	2.198359	1.879508
27	1	0	-2.950120	1.710391	2.087967
28	1	0	-3.822259	3.268932	2.143113
29	1	0	-4.675965	1.754407	2.556172
30	6	0	-5.668077	2.769635	0.139635
31	1	0	-6.480480	2.378719	0.782650
32	1	0	-5.569061	3.851923	0.350270
33	1	0	-5.981318	2.651184	-0.916052
34	6	0	-4.234715	-3.849433	-0.394530
35	1	0	-3.248668	-4.351299	-0.353981
36	1	0	-4.964563	-4.465613	0.165953
37	1	0	-4.555988	-3.821774	-1.455063
38	6	0	0.075895	-1.641160	-1.768893
39	8	0	-0.061773	-2.770635	-2.030588
40	15	0	1.748993	-0.103198	0.271372
41	6	0	1.152601	-1.054853	1.738926
42	6	0	2.003705	-1.371286	2.819974
43	6	0	-0.193636	-1.462506	1.775741
44	6	0	1.500974	-2.071659	3.928124
45	1	0	3.059563	-1.076767	2.792362
46	6	0	-0.695893	-2.165580	2.883407
47	1	0	-0.829295	-1.229242	0.917990
48	6	0	0.150366	-2.467468	3.963609
49	1	0	2.167164	-2.315175	4.765804
50	1	0	-1.747279	-2.481072	2.895557
51	1	0	-0.237059	-3.018398	4.830348
52	6	0	2.186516	1.560587	0.932266
53	6	0	2.848507	2.446922	0.052180
54	6	0	1.817157	1.994015	2.220415
55	6	0	3.148297	3.751147	0.472217
56	1	0	3.097817	2.111341	-0.963879
57	6	0	2.112546	3.307431	2.630566
58	1	0	1.301422	1.308323	2.903354
59	6	0	2.780464	4.185047	1.760852
60	1	0	3.665466	4.435870	-0.212322
61	1	0	1.821127	3.641902	3.634665
62	1	0	3.012770	5.207950	2.084224
63	6	0	3.387012	-0.866618	-0.092980
64	6	0	3.472018	-1.906561	-1.041231
65	6	0	4.547123	-0.460040	0.600410
66	6	0	4.699384	-2.546577	-1.272862
67	1	0	2.587509	-2.208212	-1.608973
68	6	0	5.774599	-1.100893	0.361443
69	1	0	4.495927	0.367392	1.318477
70	6	0	5.851724	-2.147357	-0.573142
71	1	0	4.756716	-3.352220	-2.015652
72	1	0	6.672403	-0.776038	0.903093
73	1	0	6.811341	-2.645186	-0.763492
74	17	0	2.052680	0.520067	-2.970864

75	6	0	-1.955101	0.669977	-0.747753
76	44	0	0.195226	0.176534	-1.398561

7.2.4. (R) conformer d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.629978	-0.586627	2.164915
2	1	0	1.998372	-1.587901	2.394861
3	6	0	0.363560	-0.051943	2.593473
4	6	0	0.240082	1.256264	2.023932
5	6	0	1.414401	1.510211	1.238980
6	1	0	-0.374059	-0.559005	3.217784
7	1	0	-0.601673	1.939544	2.158542
8	1	0	1.636912	2.438939	0.711721
9	6	0	3.725599	0.292065	0.813790
10	6	0	3.964298	-0.729112	-0.344602
11	6	0	4.217200	1.694444	0.386804
12	6	0	5.452934	-0.699409	-0.753351
13	6	0	5.693960	1.721031	-0.039023
14	6	0	5.923448	0.701118	-1.166956
15	1	0	4.360664	-0.039186	1.661617
16	1	0	3.375958	-0.357538	-1.206169
17	1	0	6.068201	-1.047965	0.100634
18	1	0	5.618791	-1.415363	-1.579228
19	1	0	6.994763	0.684659	-1.450910
20	1	0	5.356269	1.031643	-2.062723
21	1	0	6.300756	1.398296	0.834480
22	1	0	4.052641	2.414866	1.212226
23	1	0	3.599483	2.037448	-0.469533
24	6	0	3.460046	-2.162254	-0.045060
25	1	0	2.406554	-2.071354	0.255886
26	6	0	4.223560	-2.857900	1.093688
27	1	0	4.258778	-2.235693	2.009565
28	1	0	3.730090	-3.813966	1.353946
29	1	0	5.268351	-3.086192	0.804682
30	6	0	3.436843	-3.033571	-1.311438
31	1	0	4.456576	-3.252095	-1.687074
32	1	0	2.935574	-3.996189	-1.098351
33	1	0	2.867688	-2.530388	-2.116236
34	6	0	6.131029	3.135104	-0.444331
35	1	0	5.979743	3.856555	0.382600
36	1	0	7.200283	3.155974	-0.731576
37	1	0	5.539344	3.485334	-1.314168
38	6	0	0.787552	0.065678	-1.467554
39	8	0	1.168324	0.309241	-2.545140
40	15	0	-1.946918	0.143634	-0.141243
41	6	0	-2.357414	1.828099	-0.781977
42	6	0	-3.665636	2.156418	-1.199829
43	6	0	-1.345990	2.806926	-0.837498
44	6	0	-3.956222	3.452699	-1.652977
45	1	0	-4.455028	1.395923	-1.177854
46	6	0	-1.638785	4.103757	-1.293014
47	1	0	-0.330293	2.531680	-0.533244
48	6	0	-2.944021	4.429430	-1.698012
49	1	0	-4.975037	3.700219	-1.977784
50	1	0	-0.843137	4.858586	-1.337537
51	1	0	-3.172864	5.441205	-2.056852
52	6	0	-2.885871	0.003593	1.438114
53	6	0	-2.913704	-1.264062	2.063400
54	6	0	-3.488552	1.109804	2.069111
55	6	0	-3.554066	-1.417583	3.301694
56	1	0	-2.411851	-2.114041	1.582515
57	6	0	-4.120440	0.949556	3.316185
58	1	0	-3.467738	2.095468	1.588868
59	6	0	-4.157773	-0.312139	3.931980
60	1	0	-3.576358	-2.404634	3.781399
61	1	0	-4.587006	1.815313	3.803758
62	1	0	-4.654211	-0.435451	4.903118

63	6	0	-2.847612	-0.983714	-1.287760
64	6	0	-2.172685	-1.515740	-2.405478
65	6	0	-4.212878	-1.282050	-1.091449
66	6	0	-2.865108	-2.313505	-3.329233
67	1	0	-1.104886	-1.324812	-2.544753
68	6	0	-4.900329	-2.086533	-2.016106
69	1	0	-4.737581	-0.896707	-0.208906
70	6	0	-4.228647	-2.599295	-3.138655
71	1	0	-2.330924	-2.726175	-4.194350
72	1	0	-5.961526	-2.315916	-1.854326
73	1	0	-4.764633	-3.230432	-3.859286
74	17	0	-0.152285	-2.620741	0.069945
75	6	0	2.310346	0.372282	1.352639
76	44	0	0.283510	-0.206245	0.297431

8. Table of interatomic distances

Table 3SI. Atom-atom distances in $(S)_{Ru}$ and $(R)_{Ru}$ as evaluated from NOE spectra; X-Ray diffraction data[S1]; DFT calculated data of the lowest energy structures (the data for calculated geometries which are in best agreement with X-ray and NOE data, are given in blue).

S	XRD[a]	NOE[b]	a[c]	b	c	d	R	NOE	a	b	c	d
H_1 - H_5	2.69	2.8	2.7	2.6	2.8	2.8	H_1 - H_5	2.8	2.7	2.8	2.6	2.9
H_1 -H_{17}	2.92	2.8	2.6	3.1	2.6	2.5	H_1 -H_{17}	2.7	2.9	2.4	3.0	2.2
H_1 - C_{15}	2.77	2.9	2.3	2.6	2.4	2.3	H_1 - C_{15}	2.8	2.5	2.3	2.5	2.4
H_4 - H_6	2.41	2.5	2.3	2.4	2.2	2.3	H_4 - H_6	2.4	2.3	2.3	2.5	2.3
H_4 - H_7	3.21	3.7	2.9	3.3	3.0	2.7	H_4 - H_7	n.d.	3.1	2.6	3.4	2.5
H_1 - oPh	3.18	3.1	2.2	2.4	2.6	3.0	H_1 - oPh	2.9	2.6	4.9	3.0	4.5
H_4- oPh	5.85	4.0	5.0	4.4	2.7	4.2	H_4- oPh	3.7	4.2	3.5	4.5	2.3
H_2 - oPh	2.80	2.9	3.1	2.8	4.5	3.2	H_2 - oPh	2.8	2.6	2.8	3.0	3.0
H_3 - oPh	2.78	3.0	3.1	3.1	4.3	5.2	H_3 - oPh	2.9	3.1	2.4	4.4	2.8
H_7- oPh	4.30	4.6	4.6	4.3	2.5	2.1	H_7- oPh	4.2	4.5	2.3	2.1	4.7

[a] Taken from reference[S1]. [b] This work, see SI. [c] for conformer structures see section 7.

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