Electronic Supplementary Information (ESI) To:

Hidden Aryl-Exchange Processes in Stable 16e Rh^{III} [RhCp*Ar$_2$] Complexes, and their Unexpected Transmetalation Mechanism†

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† ***Dedicated to Prof. Peter M. Maitlis on occasion of his forthcoming 85th birthday***

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Experimental general section

All reactions were performed under N_2 atmosphere. Solvents were purified according to standard procedures.[1] $Ag(C_6F_5)$ and the analogous $Ag(C_6Cl_2F_3)$[2] were prepared according to the literature procedure for the former.[3] The dimeric complex $(\mu\text{-Cl})_2[Cp^*RhCl]_2$ was obtained using microwave techniques.[4] The rest of the reactants are commercially available. The NMR spectra were recorded with Bruker Avance 400 Ultrashield and Agilent 500 NMR instruments equipped with One NMR and Cryo probes. ^1H NMR and ^{19}F NMR spectra are referred to TMS and $CFCl_3$, respectively. The elemental analyses were performed with a Carlo Erba 1108 microanalyser (by Vigo University, Spain).

Synthesis and characterization of the complexes

Experimental procedure for X-ray crystallography: Each suitable crystal was attached to a glass fibre and transferred to an Agilent Supernova diffractometer with an Atlas CCD area detector. Data collection was performed with Mo-Kα radiation (λ = 0.71073 Å) or Cu-Kα (λ = 1.54184 Å). Data integration, scaling and empirical absorption correction was carried out using the CrysAlisPro program package.[5] The crystal was kept at 294 K during data collection. The structure was solved using Olex2[6] with the olex2.solve,[7] and refined with Shelx program.[8] The non-hydrogen atoms were refined anisotropically and hydrogen atoms were placed at idealized positions and refined using the riding model. Refinement proceeded smoothly to give the residuals shown in Tables ESI1 and ESI2. CCDC 1582590-1582594 contain the supporting crystallographic data for this paper. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: (internat.) +44-1223/336-033; E-mail: deposit@ccdc.cam.ac.uk].

Synthesis of $[RhCp^*(C_6Cl_2F_3)_2]$ (2): Excess of $Ag(C_6Cl_2F_3)$ (440 mg, 1.44 mmol) was added to a suspension of $(\mu\text{-Cl})_2[Cp^*RhCl]_2$ (150 mg, 0.24 mmol) in dry Et_2O (100 mL) and the mixture was stirred for 3 hours at room temperature, shielded from the light. The deep red solution was then filtered on dry Celite, concentrated in vacuum and cooled to 253 K. A microcrystalline deep red solid was obtained, which was filtered, washed with *n*-hexane (3 × 5 mL) and vacuum dried. Yield: 0.190 g (62 %). Suitable single crystals for X-ray crystallography were obtained by layering hexane in a dichloromethane solution of **2** (Figure ESI1).

^1H NMR (400.14 MHz, $CDCl_3$, 293 K): δ 1.58 (s, 15H, Cp*).

^{19}F NMR (376.47 MHz, $CDCl_3$, 293 K): δ –91.22 (d, $^3J_{F\text{-}Rh}$ = 9.6 Hz, $4F_o$), –118.38 (s, $2F_p$).

Analysis for $C_{22}H_{15}Cl_4F_6Rh$: Calcd.:C, 41.41; H, 2.37. Found: C, 41.73; H, 2.16

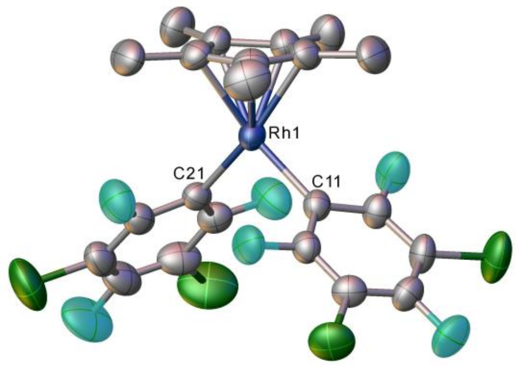


Figure ESI1. X-ray structure of [RhCp*Rf$_2$] (**2**). Selected bond lengths: (Å): Rh(1)–C(11) = 2.062(4); Rh(1)–C(21) = 2.072(4). Selected bond angles (°): C(11)–Rh(1)–C(21) = 93.74(15).

Synthesis of [RhCp*(C$_6$F$_5$)$_2$(NCMe)] (3): Excess of Ag(C$_6$F$_5$) (400 mg, 1.44 mmol) was added to a suspension of (μ-Cl)$_2$[Cp*RhCl]$_2$ (150 mg, 0.24 mmol) in dry Et$_2$O (100 mL) and the mixture was stirred for 3 hours at room temperature, shielded from the light. The red solution was then filtered on dry Celite. The solution was concentrated in vacuum and cooled down to 253 K. The microcrystalline yellow solid obtained was filtered, washed with *n*-hexane (3 × 5 mL) and vacuum dried. Yield: 120 mg (42 %). Suitable single crystals of **3** for X-ray crystallography were obtained by layering hexane in a dichloromethane solution of the compound in the presence of 10 eq of MeCN (see Figure 1 left).

Addition of CDCl$_3$ to the yellow crystals at room temperature leads to a red solution. ^{1}H and ^{19}F NMR spectra show an equilibrium between **3** and [Cp*Rh(C$_6$F$_5$)$_2$] (**4**) (the chemical shifts of both species are averaged to one signal at room temperature). In the presence of an excess of MeCN, the solution turns yellow and the NMR spectrum shows only complex **3** as the unique species in solution.

^{1}H NMR (499.72 MHz, CDCl$_3$, 293 K): δ 1.61 (s, 15H, Cp*).

^{19}F NMR (470.15 MHz, CDCl$_3$, 293 K): δ –113.40 (m, 4F$_o$), –162.51 (t, $^3J_{Fm\text{-}Fp}$ = 20.5 Hz, 2F$_p$), –164.57 (m, 4F$_m$).

Analysis for C$_{24}$H$_{18}$F$_{10}$NRh: Calcd.: C, 47.00; H, 2.96; N, 2.28. Found: C, 46.87; H, 2.88; N, 2.18

Synthesis of [RhCp*(C$_6$F$_5$)$_2$] (4): [RhCp*(C$_6$F$_5$)$_2$(NCMe)] (**3**) (100 mg, 0.16 mmol) was heated at 353 K under vacuum for 24 hours. The solid obtained was recrystallized in CH$_2$Cl$_2$/*n*-hexane leading to a microcrystalline deep red solid, which was filtered, washed with *n*-hexane (3 × 5 mL) and vacuum dried. Yield: 80 mg (86 %). Suitable single crystals of **4** (Figure 1 right) for X-ray crystallography were obtained by layering hexane in a dichloromethane solution of **4**.

^{1}H NMR (400.14 MHz, CDCl$_3$, 293 K): δ 1.57 (s, 15H, Cp*).

^{19}F NMR (376.47 MHz, $CDCl_3$, 293 K): δ –116.82 (m, 4F_o), –159.87 (t, $^3J_{Fm-Fp}$ = 20.0 Hz, 2F_p), –162.69 (m, 4F_m).

Analysis for $C_{22}H_{15}F_{10}Rh$: Calcd.: C, 46.18; H, 2.64. Found: C, 45.94; H, 2.43.

The refinement of the X-ray structures of **2**, **3** and **4** give the residuals shown in Table ESI1.

Table ESI1. Crystal data and structure refinements for complexes **2**, **3** and **4**.

	[RhCp*Rf$_2$] (2)	**[RhCp*Pf$_2$(NCMe)] (3)**	**[RhCp*Pf$_2$] (4)**
Empirical formula	$C_{22}H_{15}F_6Cl_4Rh$	$C_{24}H_{18}F_{10}NRh$	$C_{22}H_{15}F_{10}Rh$
Formula weight	638.05	613.30	572.25
Temperature/K	294	294	294
Crystal system	orthorhombic	triclinic	orthorhombic
Space group	$P2_12_12_1$	P-1	Pnma
a/Å	8.6634(2)	8.8736(4)	12.1906(2)
b/Å	13.9649(4)	9.2267(3)	18.7742(3)
c/Å	19.5079(6)	16.5011(7)	9.17539(17)
α/°	90	85.672(4)	90
β/°	90	75.218(4)	90
γ/°	90	61.708(4)	90
Volume/Å^3	2360.15(12)	1148.61(9)	2099.96(6)
Z	4	2	4
ρ_{calc}g/cm^3	1.796	1.773	1.810
μ/mm^{-1}	1.233	6.899	7.480
F(000)	1256.0	608.0	1128.0
Crystal size/mm^3	0.2947 × 0.2086 × 0.198	0.2505 × 0.0998 × 0.0601	0.1811 × 0.1146 × 0.0272
Radiation	MoKα (λ = 0.71073)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2θ range for data collection/°	4.176 to 59.84	5.546 to 152.19	9.422 to 152.252
Index ranges	-11 ≤ h ≤ 11, -18 ≤ k ≤ 19, -27 ≤ l ≤ 23	-11 ≤ h ≤ 11, -7 ≤ k ≤ 11, -19 ≤ l ≤ 20	-10 ≤ h ≤ 15, -14 ≤ k ≤ 23, -11 ≤ l ≤ 11
Reflections collected	20500	8234	6431
Independent reflections	5933 [R_{int} = 0.0290, R_{sigma} = 0.0308]	4673 [R_{int} = 0.0251, R_{sigma} = 0.0334]	2249 [R_{int} = 0.0601, R_{sigma} = 0.0622]
Data/restraints/parameters	5933/0/303	4673/0/331	2249/0/157
Goodness-of-fit on F^2	1.029	1.048	1.057
Final R indexes [I>=2σ (I)]	R_1 = 0.0311, wR_2 = 0.0588	R_1 = 0.0309, wR_2 = 0.0780	R_1 = 0.0449, wR_2 = 0.1161
Final R indexes [all data]	R_1 = 0.0420, wR_2 = 0.0651	R_1 = 0.0337, wR_2 = 0.0805	R_1 = 0.0536, wR_2 = 0.1249
Largest diff. peak/hole / e Å^{-3}	0.35/-0.32	0.51/-0.96	0.73/-1.37

Characterization of (μ-OH)$_2$[RhCp*Rf]$_2$ (6) and (μ-OH)$_2$[RhCp*Pf]$_2$ (7)

Hydroxo complexes **6** and **7** could be isolated as by-products during the synthesis of **2** or **3** respectively, only when the reaction time was around 10 hours. They could be separated from **2** or **3** by extraction of the bisarylated major product in acetone, in which (μ-OH)$_2$[RhCp*R]$_2$ is only very sparingly soluble. The signals of **6** and **7**, as well as RfH or PfH were also observed in old solutions of **2** or **4**. Single crystals of **6** (Figure 3) and **7** (Figure ESI2) suitable for X-ray crystallography were obtained by slow hydrolysis (one week) in wet acetone solutions of [RhCp*R_2].

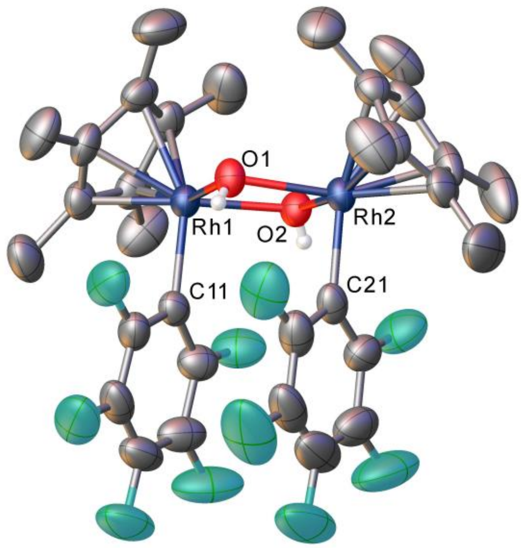


Figure ESI2. X-ray structure of *syn*-(μ-OH)$_2$[RhCp*Pf]$_2$ (**7**). Selected bond lengths (Å) and angles (°): Rh(1)–C(11) = 2.075(3), Rh(1)–O(1) = 2.109(2), Rh(1)–O(2) = 2.100(3), Rh(2)–C(21) = 2.071(4), Rh(2)–O(1) = 2.113(2), Rh(2)–O(2) = 2.108(3); C(11)–Rh(1)–O(1) = 92.13(12), C(11)–Rh(1)–O(2) = 93.74(13), O(1)–Rh(1)–O(2) = 75.72(10), C(21)–Rh(2)–O(1) = 92.94(13), C(21)–Rh(2)–O(2) = 89.67(13), O(1)–Rh(2)–O(2) = 75.44(10).

<u>NMR data for *syn*-(μ-OH)$_2$[RhCp*Rf]$_2$ (**6**)</u>

^{1}H NMR (499.72 MHz, $CDCl_3$, 293 K): δ 1.43 (s, 30H, 2Cp*), –1.52 (t, $^2J_{H\text{-}Rh}$ = 5.2 Hz, 2O*H*).

^{19}F NMR (470.15 MHz, $CDCl_3$, 293 K): δ –95.10 (m, 4F_o), –119.74 (s, 2F_p).

The *anti* isomer could be observed in solutions of **6** as a minor product (about 12%). Figure ESI3 shows the OH signals in the ^{1}H NMR spectrum for both isomers.

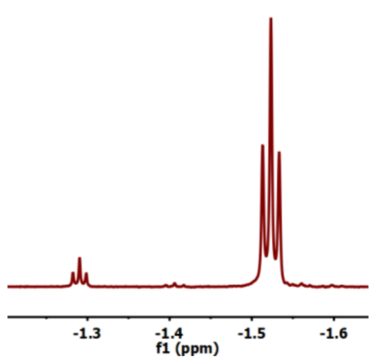


Figure ESI3. μ-OH signals of (μ-OH)$_2$[RhCp*Rf]$_2$ (**6**): *anti* isomer (left, –1.29 ppm) and *syn* isomer (right, –1.52 ppm). Both are triplets by coupling with two ^{103}Rh.

NMR data for *syn*-(μ-OH)$_2$[RhCp*Pf]$_2$ (**7**)

^{1}H NMR (499.72 MHz, $CDCl_3$, 293 K): δ 1.44 (s, 30H, 2Cp*), –1.50 (t, $^2J_{H\text{-}Rh}$ = 5.2 Hz, 2O*H*).

^{19}F NMR (470.15 MHz, $CDCl_3$, 293 K): δ –121.07 (m, 4F_o), –161.65 (t, $^3J_{Fm\text{-}Fp}$ = 20.0 Hz, 2F_p), –163.67 (m, 4F_m).

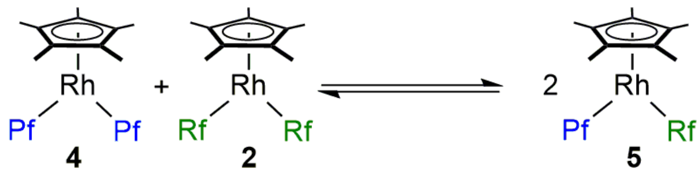
The *anti* isomer could be also observed in solutions of **7** as minor product (about 15 %).

Refinement of the X-ray structures of **6** and **7** give the residuals shown in Table ESI2.

Table ESI2. Crystal data and structure refinement for complexes **6** and **7**.

	(μ-OH)$_2$[RhCp*Rf]$_2$ (6)	**(μ-OH)$_2$[RhCp*Pf]$_2$ (7)**
Empirical formula	$C_{32}H_{32}O_2F_6Cl_4Rh_2$	$C_{32}H_{32}O_2F_{10}Rh_2$
Formula weight	910.19	844.39
Temperature/K	294	294
Crystal system	triclinic	monoclinic
Space group	P-1	$P2_1/n$
a/Å	11.1207(9)	10.8682(5)
b/Å	11.2919(8)	16.2215(7)
c/Å	16.0905(10)	18.4548(8)
α/°	89.827(6)	90
β/°	70.323(7)	92.287(4)
γ/°	65.775(8)	90
Volume/Å^3	1713.4(2)	3251.0(3)
Z	2	4
ρ_{calc}g/cm^3	1.764	1.725
μ/mm^{-1}	1.337	1.101
F(000)	904.0	1680.0
Crystal size/mm^3	0.3352 × 0.1289 × 0.0865	0.445 × 0.198 × 0.107
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2θ range for data collection/°	4.174 to 59.182	4.276 to 58.994
Index ranges	$-15 \le h \le 15$, $-15 \le k \le 11$, $-21 \le l \le 20$	$-14 \le h \le 11$, $-20 \le k \le 22$, $-25 \le l \le 22$
Reflections collected	12210	17945
Independent reflections	7832 [R_{int} = 0.0251, R_{sigma} = 0.0548]	7851 [R_{int} = 0.0327, R_{sigma} = 0.0487]
Data/restraints/parameters	7832/0/433	7851/0/433
Goodness-of-fit on F^2	1.070	1.043
Final R indexes [I>=2σ (I)]	R_1 = 0.0372, wR_2 = 0.0720	R_1 = 0.0389, wR_2 = 0.0739
Final R indexes [all data]	R_1 = 0.0561, wR_2 = 0.0849	R_1 = 0.0662, wR_2 = 0.0882
Largest diff. peak/hole / e Å^{-3}	0.54/-0.85	0.52/-0.50

Kinetic experiments for aryl exchange (Scheme ESI1)



Scheme ESI1. Aryl/Aryl' exchange reaction (Pf = C_6F_5; Rf = $C_6Cl_2F_3$)

The kinetic experiments were monitored by ^{19}F NMR. The NMR tube (5mm), placed in a cold bath at 195 K, was charged with [RhCp*($C_6Cl_2F_3$)$_2$] (**2**) (3.06 mg, 5.00×10^{-3} mmol) and [RhCp*(C_6F_5)$_2$] (**4**) (2.86 mg, 5.00×10^{-3} mmol). Subsequently, freshly distilled $CDCl_3$ (0.50 mL) was added (concentration of 1.0×10^{-2} M for **2** and **4**).

^{19}F NMR spectra were recorded at fixed time intervals depending on the temperature imposed by a thermostated probe: 15 min at 261 K, 10 min at 271 K, 5 min at 280 K, and 3 min at 289 K. Concentration-time data were obtained from the integrated areas of the Rf F_{ortho} signals of [RhCp*($C_6Cl_2F_3$)$_2$] (**2**) and [RhCp*($C_6Cl_2F_3$)(C_6F_5)] (**5**).[9]

The initial rate was obtained by linear fitting of the concentration-time curves in the interval 0-15% of consumption of the starting reagents. When the equilibrium was reached, the concentration of the three species was close to the statistical values (**2**:**4**:**5** = 1:1:2 for a 1:1 mixture or **2** and **4**).

The temperature of the sample was determined using methanol as chemical shift thermometer.[10]

Kinetic experiment for aryl exchange in the presence of 5 mol% of complex (μ-OH)$_2$[RhCp*Rf]$_2$ (6) as catalyst: 25 μL of a 1.0×10^{-2} M solution of **6** in distilled $CDCl_3$ was added to the NMR tube (placed in a cold bath at 195 K) with a solution of **2** and **4** in concentration 1.0×10^{-2} M for both complexes. The reaction was monitored at 280 K.

Figures ESI4 and ESI5 display all the kinetic fits obtained from the NMR data.

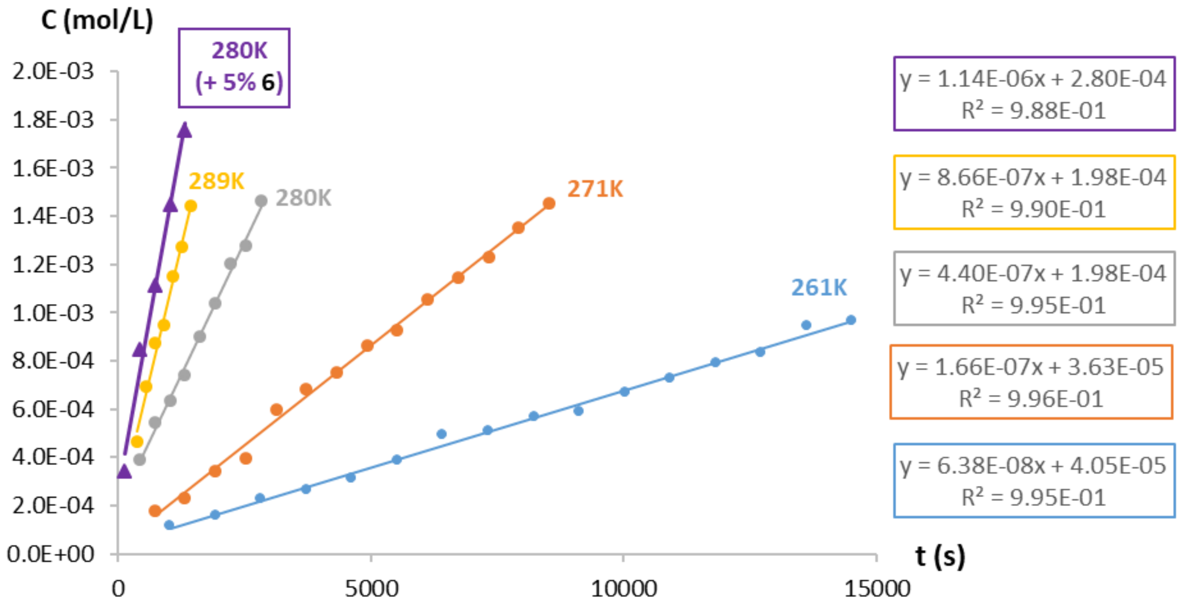


Figure ESI4. Representation of half of the concentration of complex [RhCp*RfPf] (**5**) formed *vs* time.[11] The slope of each line corresponds to the initial rate, r_0 (in mol × L^{-1} × s^{-1}).

Rate constants (k) are obtained from initial rates (r_0) as follows: $k = \frac{r_0}{[\mathbf{2}]_0 \cdot [\mathbf{4}]_0}$ ($[\mathbf{2}]_0 = [\mathbf{4}]_0 = 1.0 \times 10^{-2}$ M).

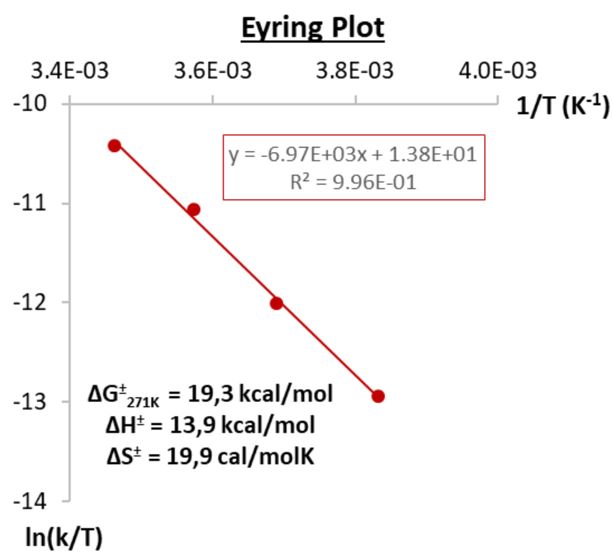


Figure ESI5. Eyring plot based on the results obtained without 5 mol% of extra catalyst $(\mu\text{-OH})_2[RhCp^*Rf]_2$ (**6**) added (lines blue, orange, grey and yellow of Figure ESI4). From the Eyring equation,[12] the *apparent* values for $\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$ were calculated.

^{19}F NMR data for [RhCp*($C_6Cl_2F_3$)(C_6F_5)] (**5**)

Complex **5** was characterized from the reaction mixture shown in Scheme ESI1.

^{19}F NMR (376.47 MHz, $CDCl_3$, 271 K): δ –91.36 (dt, $^{3}J_{F\text{-}Rh} \approx J_{F\text{-}FoPf} \approx 9$ Hz, 2F_o, Rf), –118.44 (s, 1F_p, Rf), –159.83 (t, $^{3}J_{Fm\text{-}Fp} = 20.2$ Hz, 1F_p, Pf). The signals for F_o of the Pf group and F_m of the Pf group were overlapped with the corresponding signals of [RhCp*Pf_2] (**4**). Figure ESI6 shows the overlapped triplets for F_p of the Pf groups of **4** and **5**.

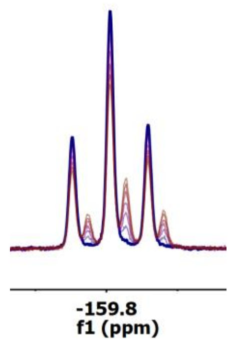


Figure ESI6. Appearance of the F_p signal of Pf in complex **5** during the kinetically monitored experiment registered at 271 K.

Detection of (μ-OH)$_2$[RhCp*Rf]$_2$ (**6**) as a contamination in a solution of [RhCp*Rf_2] (**2**)

[RhCp*($C_6Cl_2F_3$)$_2$] (**2**) (3.06 mg, 5.00 × 10^{-3} mmol) was dissolved in distilled $CDCl_3$ (0.50 mL) and a ^{19}F NMR spectrum was registered at 280 K in an Agilent 500 NMR instrument equipped with a Cryo probe. Figure ESI7 highlights the position of the F_o signal of the impurity **6**, which is expanded in the figure.

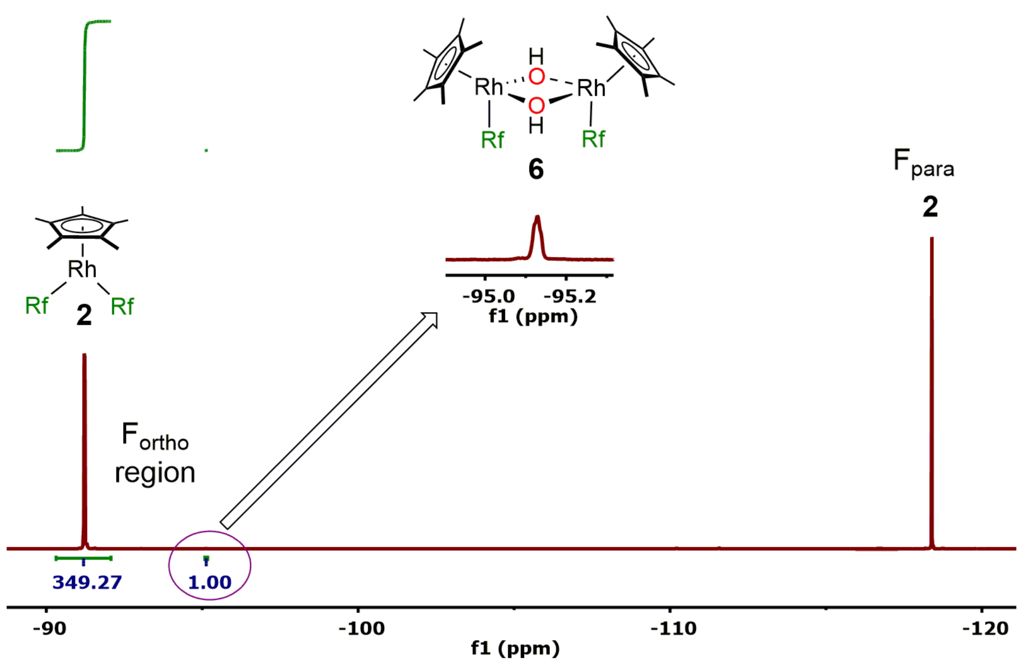


Figure ESI7. ^{19}F NMR spectrum of complex **2** (crystalline fraction used for all the kinetic experiments).

Calculations of the concentration of non measurable [RhCp*Rf(OH)] (8) and [RhCp*Pf(OH)] (9) needed for the kinetic behavior observed.

Kinetic data for the formation of the aryl exchange product [RhCp*RfPf] (**5**)

- Initial rate (r_0) at 271 K = 1.66×10^{-7} mol × L^{-1} × s^{-1}

It is assumed that the formation of **5** is produced by reaction of [RhCp*Rf_2] (**2**) with **9**, or [RhCp*Pf_2] (**4**) with **8** (catalytic cycle, Scheme 3). The rate constants (k) were obtained with the following mathematical expressions (first kinetic order for both reactants).

$$k = \frac{r_0}{[\mathbf{4}]\cdot[\mathbf{8}]} \qquad [\mathbf{4}]_0 = 0.010 \text{ mol} \times \text{L}^{-1} \qquad k' = \frac{r_0}{[\mathbf{2}]\cdot[\mathbf{9}]} \qquad [\mathbf{2}]_0 = 0.010 \text{ mol} \times \text{L}^{-1}$$

- Solving the equation:

$$\Delta G^{\ddagger} = -R \cdot T \cdot \ln\left(\frac{k \cdot h}{k_B \cdot T}\right)$$

h = 6.63×10^{-34} J × s $\quad$ $k_B = 1.38 \times 10^{-23}$ J × K^{-1} $\quad$ T = 271 K $\quad$ R = 1.98×10^{-3} kcal × mol^{-1} × K^{-1}

a) $\Delta G^{\ddagger}$ = 10.7 kcal × mol^{-1} (calculated Gibbs energy profile, Figure 4).

$$[\mathbf{8}] = 1.3 \times 10^{-9} \text{ M}$$

b) $\Delta G^{\ddagger}$ = 7.8 kcal × mol^{-1} (calculated Gibbs energy profile, Figure ESI8).

$$[\mathbf{9}] = 5.0 \times 10^{-12} \text{ M}$$

Calculations of the concentration of non-detected [RhCp*Rf(OH)] (8) and [RhCp*Pf(OH)] (9) from the DFT calculated K_{dis} of the corresponding dimer.

In order to estimate the concentration of the dissociated species **8** and **9,** the ΔG_0 values for the dissociation of (μ-OH)$_2$[RhCp*Rf]$_2$ (**6**) and (μ-OH)$_2$[RhCp*Pf]$_2$ (**7**) were calculated respectively (DFT, ωB97X-D) in $CHCl_3$ at 271 K.

Using the formula: $K_{eq} = e^{\frac{-\Delta G_0}{RT}}$ the equilibrium constants for the dissociation (K_{dis}) can be obtained.

a) For complex **6**: $\quad$ ΔG_{dis} = 22.3 kcal × mol^{-1} $\quad$ $K_{dis} = 8.9 \times 10^{-19}$

In the equilibrium: $\quad$ $complex\mathbf{6} \rightleftharpoons 2\ complex\mathbf{8}$ $\quad$ with $[\mathbf{6}]_0 = 3 \times 10^{-5}$ mol × L^{-1}*

* In the kinetic experiments **6** is a contaminant of complex **2** (0.3 mol% in a solution 0.01 M, Figure ESI7).

$$K_{dis} = \frac{(2 \cdot [\mathbf{8}]_{eq})^2}{[\mathbf{6}]_0} \qquad [\mathbf{8}] = 2.6 \times 10^{-12} \text{ mol} \times \text{L}^{-1}$$

b) For complex **7**: ΔG_{dis} = 22.7 kcal × mol^{-1} K_{dis} = 4.2 × 10^{-19}

In the equilibrium: $complex\mathbf{7} \rightleftharpoons 2\ complex\mathbf{9}$ with [**7**]$_0$ = 3 × 10^{-5} mol × L^{-1}

$$K_{dis} = \frac{(2 \cdot [\mathbf{9}]_{eq})^2}{[\mathbf{7}]_0}$$ [**9**] = 1.8 × 10^{-12} M

Considerations about these figures

The calculated values using both methods have very different sources of error because the mathematical expressions used are exponential (1.5 kcal mol^{-1} means roughly one order of magnitude difference in rate). In systems where DFT methods results can be contrasted with experimental values differences in the order 2-4 kcal mol^{-1} are common. Thus, the exponential range 10^{-9}-10^{-12} in concentrations corresponds essentially to the same order of magnitude 2-4 kcal mol^{-1} in ΔG values (ΔG_0 or $\Delta G^{\ddagger}$), and is within the expected range of uncertainty (in theoretical calculations the concept *error* cannot be applied) when calculations (particularly those containing entropy changes) are involved. It must be considered acceptable. Whatever the exact value, the range of values obtained confirms that concentration of the catalytic species is minuscule.

Computational Section

Density functional theory (DFT) calculations reported in this work were carried out using the dispersion corrected hybrid functional ωB97X-D developed by Head-Gordon and Chai,[12] and the Gaussian09 software.[13] The choice of this level of theory is based on the satisfactory results obtained in previous theoretical studies on related Pd/Au and Au/Sn transmetalations.[14-16] C and H atoms were described using the double-ζ basis set 6-31G(d,p), whereas the same basis set plus diffuse functions was employed to describe the more electronegative O, Cl and F atoms. The Rh metal was described using the effective core potential LANL2DZ[17,18] including f-polarization functions (exponent = 1.350).[19] Geometry optimizations in vacuum were performed without imposing any constraint and the nature of all the stationary points was further verified through vibrational frequency analysis. Furthermore, for transition states, geometry relaxations along the reaction coordinate were carried out to confirm that they connect the corresponding reaction energy minima.

The effect of the same solvent employed in experiments ($CHCl_3$, ε = 4.711) was introduced through single-point calculations at the optimized geometries in vacuum using the SMD solvation model.[20] The reported Gibbs energies in $CHCl_3$ were obtained by adding to the potential energies in solution the Gibbs energy corrections of the solute in vacuum calculated at the experimental temperature of 271 K and 1 atm.

Profile for the Rf/OH exchange (Figure ESI8)

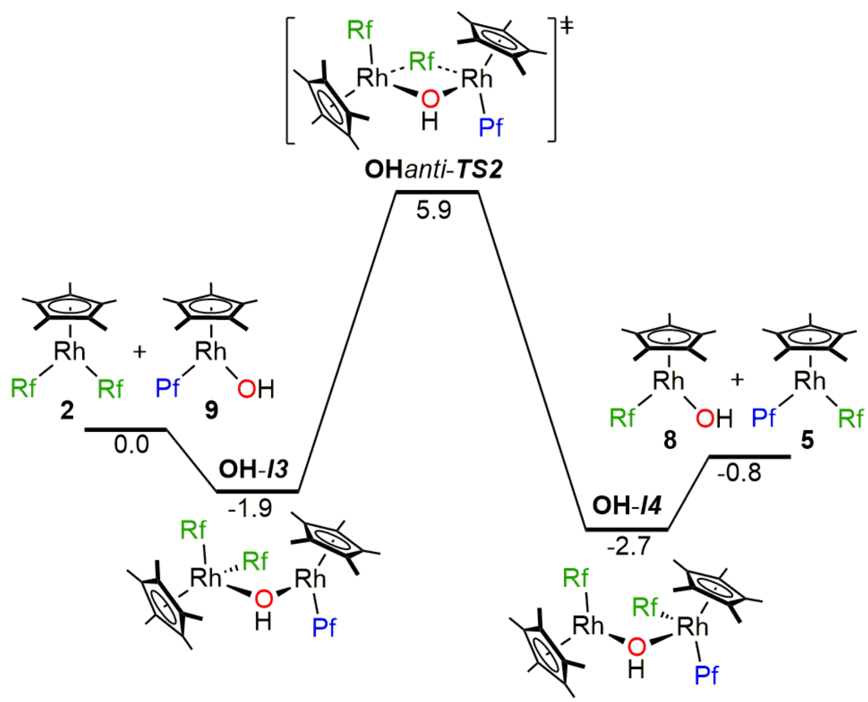


Figure ESI8. Calculated Gibbs energy profile (in kcal × mol^{-1}), in $CHCl_3$ at 271K, for the exchange between **2** and **9** (Scheme 2).

Relevant Calculated Structures

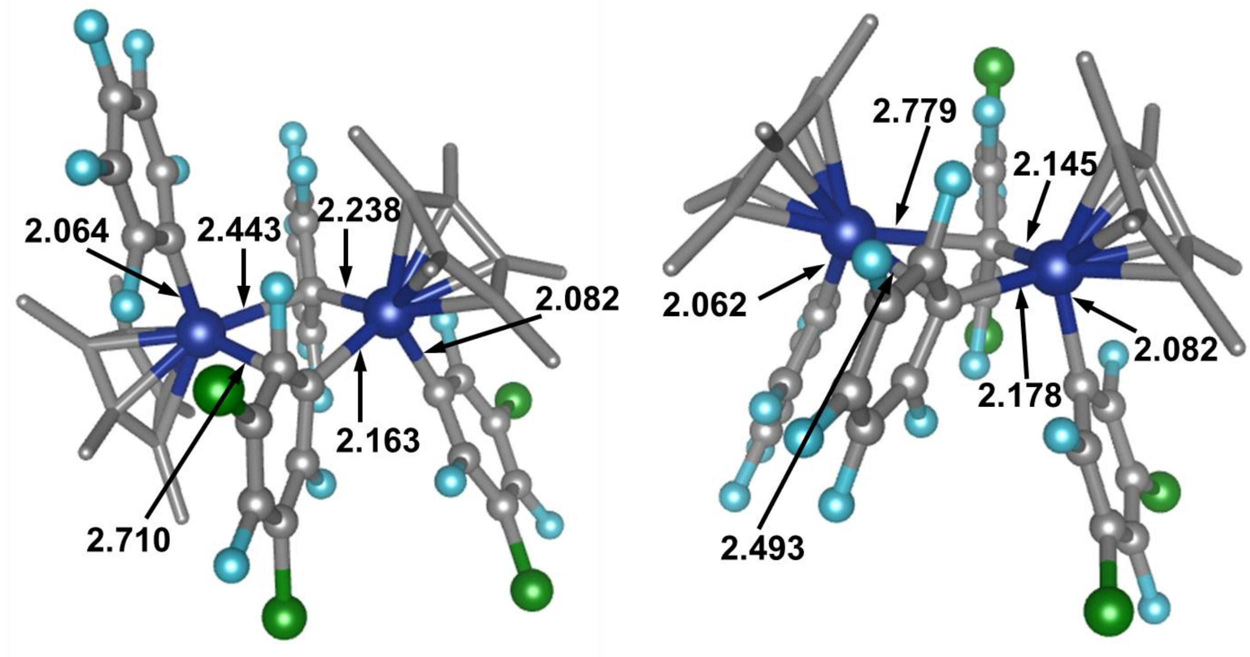


Figure ESI9. Direct mechanism: **Dir*anti*-*TS*** (left) and **Dir*syn*-*TS*** (right). Bond distances in Å.

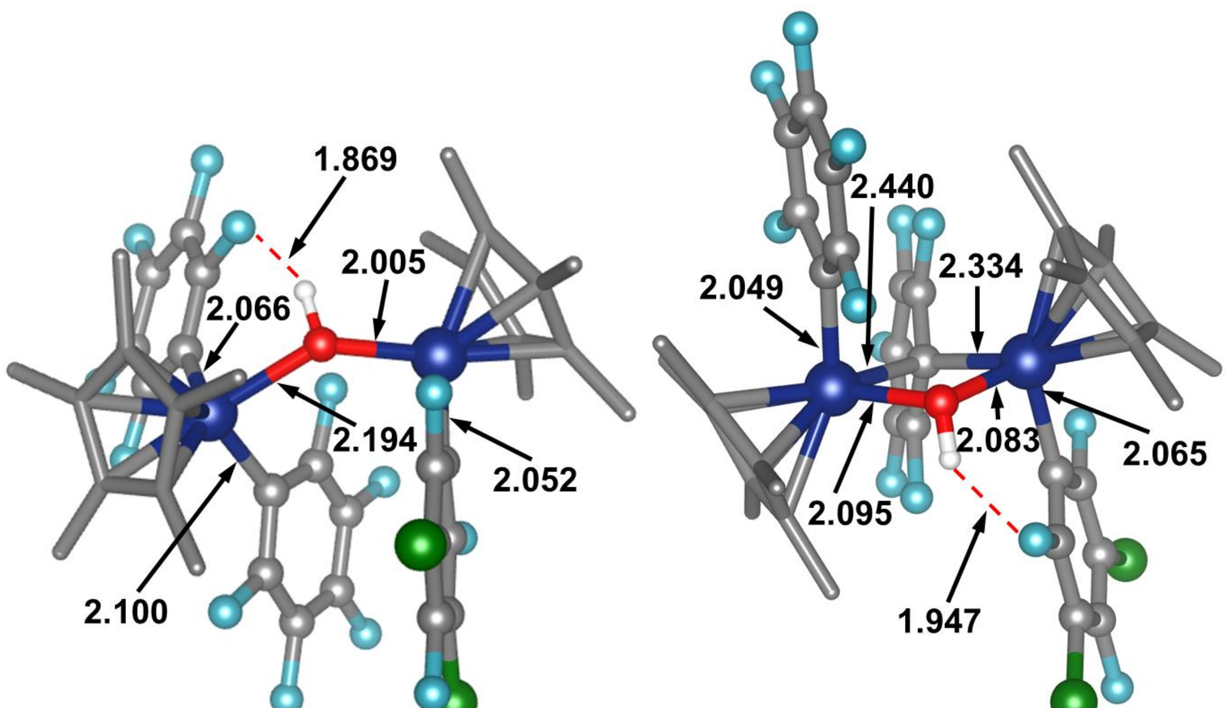


Figure ESI10. OH-*I1* (left) and **OH*anti*-*TS1*** (right). **OH-*I2***, **OH-*I3*** and **OH-*I4*** are similar to **OH-*I1***. Selected bond distances (Å). The hydrogen O–H····F bond is indicated with a red dashed line

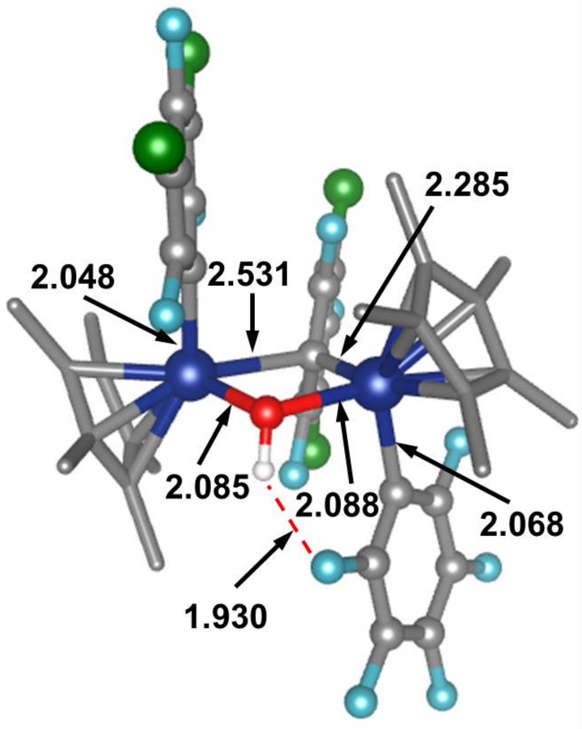


Figure ESI11. OH*anti*-*TS2*. Selected bond distances (Å). The hydrogen bond is indicated with a red dashed line

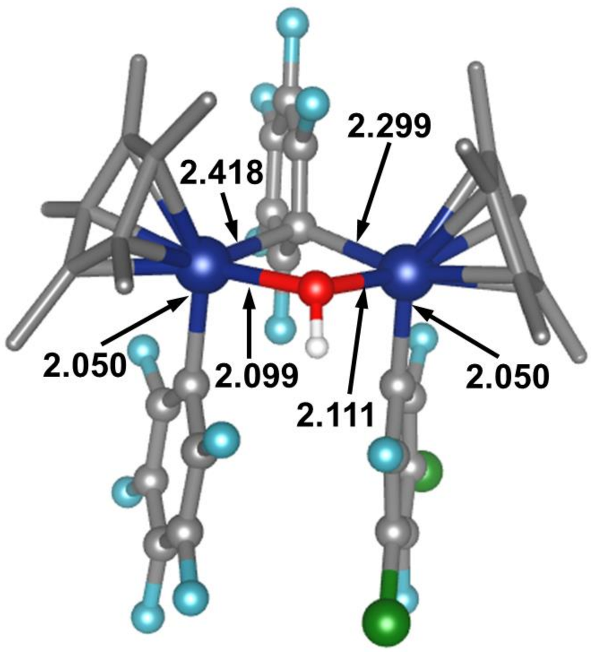


Figure ESI12. OH*syn*-*TS1*, with selected bond distances (Å).

Cartesian coordinates of all the calculated species

[RhCp*Rf$_2$] (**2**)

45	-0.087441	1.333304	0.107015
17	4.489197	-1.708281	-1.888174
17	2.918391	-2.148428	3.277662
17	-2.237924	-3.287546	-2.633149
17	-4.473869	-1.687852	2.031260
9	2.241340	0.141299	-2.053767
9	4.564666	-2.678980	0.887256
9	0.856238	-0.218961	2.418220
9	-0.445055	-1.036317	-2.138879
9	-4.120206	-3.351927	-0.372866
9	-2.389312	0.369688	1.907809
6	0.375747	3.490997	0.488281
6	-1.083327	3.293425	0.477863
6	-1.465061	2.824137	-0.785999
6	-0.236189	2.600801	-1.541994
6	0.882835	3.139414	-0.768290
6	1.136847	4.012782	1.663834
1	0.836468	3.503380	2.583383
1	0.945544	5.082878	1.798775
1	2.210971	3.871565	1.536141
6	-1.961067	3.585652	1.650396
1	-2.960641	3.171669	1.517931
1	-2.047740	4.667858	1.796046
1	-1.543757	3.156198	2.564881
6	-2.844216	2.520701	-1.277888
1	-2.858289	1.593693	-1.855216
1	-3.204825	3.329305	-1.922023
1	-3.545587	2.402839	-0.450258
6	-0.172757	2.162133	-2.966102
1	0.757118	1.632570	-3.171095
1	-0.232146	3.038996	-3.621544
1	-0.998940	1.492801	-3.209332
6	2.295039	3.254089	-1.243750
1	3.003914	3.139993	-0.421398
1	2.455547	4.236911	-1.699784
1	2.522654	2.490913	-1.987528
6	1.482312	0.014833	0.177529
6	2.369217	-0.369318	-0.812117
6	3.413246	-1.271872	-0.608165
6	3.572184	-1.817643	0.660920
6	2.714147	-1.472709	1.701440
6	1.698509	-0.568071	1.415578
6	-1.337585	-0.278790	-0.094979
6	-1.349485	-1.173867	-1.153519
6	-2.269557	-2.214112	-1.279606
6	-3.226811	-2.366465	-0.282260
6	-3.271095	-1.499656	0.804605
6	-2.323440	-0.481071	0.858595

[RhCp*Pf$_2$] (**4**)

45	-0.078045	1.062838	-0.150417
9	-0.495682	-1.269096	2.152549
9	2.212209	-0.064919	2.118287
9	-2.324682	0.023035	-2.021463
9	0.965043	-0.540240	-2.417924
9	-4.080270	-2.012032	-1.867086
9	3.016199	-2.279261	-2.789083
9	-2.263240	-3.280326	2.292933
9	4.229310	-1.781043	1.739981
9	-4.064691	-3.677900	0.290925
6	-1.319592	-0.556880	0.045070
6	1.509254	-0.239152	-0.146646
6	0.379258	3.213751	-0.571445
6	-1.076599	2.998937	-0.604781
6	-1.352775	-1.426311	1.124934
6	2.367688	-0.587156	0.881739
6	-0.292322	2.369083	1.460251
6	-2.265265	-0.793382	-0.941879
6	1.769053	-0.842809	-1.367293
6	0.846853	2.899284	0.709952
6	-1.496606	2.558504	0.657994
6	-3.188412	-1.828902	-0.887831
6	2.806798	-1.735074	-1.586565
6	-2.261836	-2.472805	1.227505
6	3.422498	-1.478667	0.717527
6	-0.267190	1.963614	2.895189
6	1.174997	3.713529	-1.733467
6	-1.920735	3.251142	-1.810517
6	-3.184114	-2.678165	0.210271
6	3.643662	-2.056283	-0.524880
6	2.240544	3.040124	1.230491
6	-2.891682	2.253602	1.101883
1	-1.093978	1.292236	3.130046
1	-0.352296	2.854745	3.527991
1	0.660514	1.446405	3.138315
1	0.988272	4.781100	-1.892839
1	-2.031180	4.328719	-1.973702
1	0.901672	3.187876	-2.652240
1	-1.461949	2.821188	-2.704476
1	2.244868	3.574536	-1.571980
1	-2.912822	2.812079	-1.704396
1	2.977691	2.921975	0.434064
1	-3.533379	2.009889	0.253367
1	2.452651	2.291970	1.993987
1	-2.908113	1.400068	1.782502
1	2.373599	4.032182	1.675280
1	-3.322435	3.114799	1.622958
9	4.657807	-2.906371	-0.700799

[RhCp*RfPf] (**5**)

45	-0.594687	-1.055659	0.184415
9	-0.432735	1.155183	-2.264481
9	1.861800	-0.681296	-2.128383
9	-2.439556	0.661315	1.996648
9	0.856114	0.303275	2.351365
9	-3.589776	3.079028	1.720716
17	3.416696	1.614316	3.012818
9	-1.599042	3.554986	-2.525198
17	4.541219	0.464906	-2.159732
9	-3.179786	4.544858	-0.541494
6	-1.367605	0.820043	-0.111024
6	1.278009	-0.220125	0.111925
6	-0.710534	-3.223047	0.731952
6	-2.061975	-2.639664	0.737430
6	-1.192990	1.599167	-1.244627
6	2.186770	-0.156996	-0.929173
6	-1.149263	-2.352067	-1.351212
6	-2.191166	1.362632	0.864572
6	1.710566	0.345755	1.300258

6	-0.182697	-3.113962	-0.559726
6	-2.358787	-2.178626	-0.552337
6	-2.803604	2.603357	0.749243
6	2.951837	0.940780	1.492160
6	-1.789555	2.843746	-1.409398
6	3.450593	0.423748	-0.819751
6	-1.029078	-2.055802	-2.807929
6	-0.069852	-3.847672	1.928845
6	-2.938907	-2.597715	1.945558
6	-2.598172	3.351642	-0.401758
6	3.819186	0.971881	0.403783
6	1.124799	-3.639007	-1.058358
6	-3.629071	-1.551611	-1.031081
1	-1.643743	-1.199739	-3.089054
1	-1.361035	-2.926563	-3.385465
1	0.002046	-1.827801	-3.075802
1	-0.550837	-4.804000	2.161043
1	-3.336439	-3.596642	2.155921
1	-0.167261	-3.204176	2.807336
1	-2.379077	-2.266859	2.824012
1	0.992377	-4.031095	1.762107
1	-3.776346	-1.913079	1.810016
1	1.863580	-3.698195	-0.257047
1	-4.189909	-1.111356	-0.204743
1	1.532004	-2.998238	-1.840379
1	-3.425776	-0.757321	-1.752117
1	0.988776	-4.643083	-1.474323
1	-4.263308	-2.299659	-1.517941
9	5.023014	1.528978	0.539620

(μ-OH)$_2$[RhCp*Rf]$_2$ (6)

45	-1.363736	-1.626394	0.246899
45	-1.362307	1.627293	-0.246913
17	3.436306	2.709392	2.650050
9	1.003345	1.000134	-2.368546
8	-1.421742	-0.193574	-1.317725
8	-1.421813	0.194536	1.317828
6	0.685111	1.660703	-0.124378
6	1.534596	1.383542	-1.184227
6	3.505040	1.874645	0.069772
6	2.715873	2.174520	1.173896
9	0.595738	2.342022	2.133702
6	1.334923	2.048163	1.039004
9	1.002387	-1.001150	2.368719
6	-1.925366	-3.176426	1.596219
6	-3.405971	-2.501744	-0.060035
6	-2.354278	-3.304906	-0.673123
6	-3.887287	-1.657352	2.358655
1	-3.251314	-0.835491	2.707534
1	-4.809937	-1.229845	1.961778
1	-4.140876	-2.291754	3.213214
6	-1.356160	-3.417868	2.958814
1	-1.484675	-2.537526	3.592393
6	-3.151967	-2.441581	1.321739
6	-4.488022	-1.822567	-0.836368
1	-5.122096	-1.212696	-0.189895
1	-4.045550	-1.167812	-1.593384
1	-5.122787	-2.554929	-1.345876
6	-2.305203	-3.643467	-2.128130
1	-2.446901	-2.743530	-2.732241
1	-3.098925	-4.355737	-2.379875
6	-3.149918	2.443952	-1.321759
6	-3.403749	2.504491	0.059995
6	-2.351311	3.306808	0.672969
6	-1.922629	3.177649	-1.596344
6	-1.493690	3.783525	-0.363497
6	-4.486167	1.826164	0.836565
1	-5.121014	1.216992	0.190198
1	-4.044003	1.170876	1.593297
1	-5.120097	2.559002	1.346435
6	-3.886009	1.660353	-2.358598
1	-3.250736	0.838052	-2.707695
1	-4.808873	1.233461	-1.961542
1	-4.139356	2.295064	-3.213005
6	-0.359521	4.746069	-0.208177
1	0.081743	4.686360	0.788256
1	0.429956	4.547341	-0.935571
1	-0.718684	5.768887	-0.364235
6	-1.353154	3.418089	-2.959013
1	-0.283645	3.629724	-2.905548
1	-1.481475	2.537223	-3.591901
1	-1.846937	4.266942	-3.445980
6	-2.301916	3.645338	2.127973
1	-2.442685	2.745255	2.732096
1	-1.343423	4.085740	2.402990
1	-3.096065	4.356994	2.380077
1	-0.652170	0.280526	1.888329
1	-0.652217	-0.280361	-1.888248
6	0.683696	-1.661510	0.124568
6	2.924240	1.471642	-1.127858
9	4.830819	1.978518	0.157265
6	1.533387	-1.384835	1.184371
6	-1.497007	-3.782486	0.363252
1	-1.849985	-4.267143	3.445002
1	-0.286626	-3.629383	2.905448
1	-1.346480	-4.083134	-2.403511
6	1.333259	-2.049333	-1.038835
17	3.910967	1.102692	-2.496870
6	2.922983	-1.473639	1.127943
6	-0.364003	-4.746348	0.207658
6	2.714131	-2.176432	-1.173795
9	0.593875	-2.342717	-2.133542
6	3.503512	-1.876953	-0.069714
17	3.909950	-1.105127	2.496890
1	-0.724797	-5.768849	0.362079
1	0.425118	-4.549730	0.935996
1	0.078174	-4.685990	-0.788329
17	3.434227	-2.711643	-2.649995
9	4.829232	-1.981500	-0.157271

(μ-OH)$_2$[RhCp*Pf]$_2$ (7)

45	-1.068297	1.641396	0.133412
45	-1.068656	-1.641201	-0.133542
8	-1.125735	0.102973	-1.327548
8	-1.125820	-0.102721	1.327410
9	1.291599	-1.172857	-2.326797
9	0.928749	-2.176136	2.300440
9	1.291500	1.172841	2.326904
9	0.929474	2.175242	-2.300571
9	3.591756	-2.303592	2.465333
9	5.141045	-1.851698	0.264148
9	3.952320	-1.284673	-2.121282
6	0.978856	-1.661942	-0.020347

9	3.952278	1.284441	2.121818
6	-2.865291	2.522005	1.137694
6	-3.105728	2.499417	-0.247177
6	-2.044171	3.259995	-0.897510
9	3.592519	2.302450	-2.465057
9	5.141428	1.850913	-0.263540
6	0.979184	1.661533	0.020346
6	-2.045138	-3.259362	0.897400
6	-1.639279	3.269738	1.379631
6	1.637734	-1.945832	1.168168
6	-3.106382	-2.498593	0.246761
6	-1.199704	-3.800951	-0.117873
6	1.814337	-1.453921	-1.107580
6	1.638263	1.945106	-1.168136
6	-2.865690	-2.521467	-1.138065
6	-1.198770	3.801191	0.118007
6	1.814476	1.453636	1.107732
6	-1.639837	-3.269548	-1.379683
6	3.811170	-1.794071	0.174837
6	3.019492	-2.017595	1.292244
6	3.200875	1.506820	1.038725
6	3.200721	-1.507205	-1.038350
6	-3.615592	1.807028	2.213290
1	-4.524419	1.340726	1.828639
1	-3.895174	2.500614	3.011894
1	-2.980217	1.021030	2.636611
6	3.811536	1.793383	-0.174423
6	3.020047	2.016742	-1.291997
6	-0.063510	-4.751784	0.085101
1	0.715222	-4.603560	-0.665548
1	-0.425583	-5.782136	0.002492
1	0.391260	-4.625550	1.069177
6	-0.062298	4.751742	-0.084653
1	0.716296	4.603179	0.666074
1	-0.424056	5.782204	-0.001922
1	0.392568	4.625532	-1.068682
6	-1.979965	-3.510202	2.369514
1	-1.015432	-3.925783	2.661787
1	-2.766075	-4.211300	2.671428
1	-2.121975	-2.576773	2.920071
6	-1.083776	3.593523	2.730547
1	-1.225149	2.756666	3.418020
1	-1.577235	4.474846	3.156113
1	-0.012206	3.794410	2.676102
6	-4.183446	1.779161	-0.991460
1	-3.737407	1.095910	-1.720373
1	-4.824611	2.483973	-1.531001
1	-4.811679	1.192084	-0.318567
6	-3.615560	-1.806373	-2.213892
1	-4.524364	-1.339822	-1.829489
1	-3.895122	-2.499926	-3.012534
1	-2.979834	-1.020578	-2.637064
6	-4.184139	-1.778076	0.990723
1	-3.738114	-1.095080	1.719890
1	-4.825769	-2.482734	1.529924
1	-4.811896	-1.190664	0.317667
6	-1.084172	-3.593623	-2.730465
1	-1.225336	-2.756847	-3.418076
1	-1.577686	-4.474944	-3.155969
1	-0.012644	-3.794645	-2.675858
6	-1.978725	3.511070	-2.369574
1	-1.014111	3.926618	-2.661648
1	-2.764740	4.212281	-2.671493
1	-2.120739	2.577761	-2.920309
1	-0.357871	-0.149791	1.904302
1	-0.357708	0.149873	-1.904493

[RhCp*Rf(OH)] (8)

45	-1.305362	-0.017571	-0.517369
17	3.715654	2.709793	0.015929
17	3.730967	-2.704882	0.013273
9	0.834624	2.347859	-0.345998
9	4.870112	0.005607	0.154779
9	0.847413	-2.358399	-0.348409
6	-2.253386	-1.104193	1.047449
6	-3.324265	-0.731455	0.114083
6	-3.359234	0.664718	0.041542
6	-2.307067	1.181262	0.923756
6	-1.712706	0.085260	1.620341
6	-1.924532	-2.508723	1.433294
1	-1.936301	-3.169047	0.563728
1	-2.663413	-2.878039	2.153588
1	-0.936076	-2.575962	1.889146
6	-4.152475	-1.715303	-0.646749
1	-4.676931	-1.238798	-1.475725
1	-4.892205	-2.182083	0.012383
1	-3.524917	-2.505789	-1.065436
6	-4.230972	1.528054	-0.812249
1	-3.625999	2.201736	-1.424811
1	-4.892719	2.137499	-0.187908
1	-4.846531	0.930822	-1.485771
6	-2.048696	2.634127	1.151765
1	-1.056853	2.804121	1.571282
1	-2.794291	3.037631	1.846420
1	-2.116064	3.192600	0.215861
6	-0.659139	0.165783	2.679836
1	0.045875	-0.664489	2.600612
1	-1.113856	0.137124	3.675223
1	-0.084920	1.090255	2.593383
6	0.745430	-0.005566	-0.369414
6	1.481202	1.165079	-0.277206
6	2.863228	1.210137	-0.100877
6	3.546894	0.001919	-0.015443
6	2.869995	-1.210020	-0.101733
6	1.487564	-1.172632	-0.278145
8	-1.193730	-0.077025	-2.442193
1	-0.286584	-0.080456	-2.764120

[RhCp*Pf(OH)] (9)

45	-1.002631	-0.018031	-0.514758
9	3.818742	2.357986	0.000585
9	3.831640	-2.355841	-0.003462
9	1.151510	2.363755	-0.327707
9	5.180737	0.004593	0.165940
9	1.164051	-2.375063	-0.333154
6	-1.963252	-1.102368	1.044738
6	-3.026368	-0.729622	0.102732
6	-3.059764	0.666581	0.028700
6	-2.013671	1.182999	0.918010
6	-1.425608	0.087077	1.620153
6	-1.638749	-2.507024	1.433744
1	-1.642929	-3.167238	0.564038
1	-2.384501	-2.875863	2.147177

1	-0.654668	-2.575060	1.898761
6	-3.850481	-1.713520	-0.662455
1	-4.369931	-1.237374	-1.494763
1	-4.594284	-2.179477	-0.007316
1	-3.220937	-2.504654	-1.076892
6	-3.925407	1.529726	-0.831418
1	-3.316241	2.201913	-1.441422
1	-4.589963	2.140728	-0.211586
1	-4.537878	0.932329	-1.507577
6	-1.754704	2.635673	1.146291
1	-0.763560	2.804659	1.567822
1	-2.501529	3.040023	1.839140
1	-1.819268	3.193960	0.210110
6	-0.380159	0.167982	2.687545
1	0.321473	-0.665912	2.617505
1	-0.842772	0.146118	3.679443
1	0.198712	1.089503	2.600925
6	1.047393	-0.006030	-0.355531
6	1.779519	1.167674	-0.263151
6	3.157836	1.198102	-0.089350
6	3.855768	0.001105	-0.003153
6	3.164369	-1.199496	-0.091359
6	1.785764	-1.176339	-0.265428
8	-0.878632	-0.078054	-2.438422
1	0.030687	-0.081854	-2.754102

Dir_anti_**-_TS_**

45	0.886843	-0.053255	-1.375154
17	5.613525	-2.858758	0.295470
17	5.760791	2.552583	0.309009
17	-2.248585	4.625429	-1.233371
17	1.742491	4.261703	2.393977
9	2.903305	-2.436836	-0.599050
9	6.795241	-0.182978	0.684992
9	3.025699	2.284344	-0.567898
9	-1.681043	1.815827	-1.610374
9	-0.375410	5.561520	0.837139
9	1.741845	1.480083	1.598775
6	0.355528	0.979843	-3.428401
6	-0.309749	-0.275326	-3.405374
6	0.712536	-1.294029	-3.306579
6	1.977872	-0.657718	-3.241242
6	1.757229	0.766550	-3.254638
6	-0.211422	2.313357	-3.805965
1	-1.297739	2.300709	-3.872459
1	0.194631	2.591397	-4.785520
1	0.082204	3.098498	-3.104603
6	-1.770435	-0.483574	-3.683250
1	-2.393802	-0.155953	-2.848608
1	-1.990298	-1.535324	-3.870432
1	-2.071602	0.082725	-4.570599
6	0.566890	-2.775346	-3.489942
1	1.065311	-3.324663	-2.686852
1	1.044099	-3.068075	-4.431574
1	-0.474674	-3.089711	-3.524181
6	3.299809	-1.334119	-3.422595
1	4.116167	-0.757542	-2.984475
1	3.499438	-1.436158	-4.496029
1	3.310854	-2.331243	-2.981548
6	2.807043	1.812438	-3.460006
1	2.509503	2.769973	-3.031264
1	2.975529	1.955905	-4.534407
1	3.758538	1.526000	-3.009331
6	2.796828	-0.071176	-0.545544
6	3.506424	-1.249870	-0.350217
6	4.832132	-1.332435	0.068954
6	5.522708	-0.147827	0.284474
6	4.897950	1.073049	0.068954
6	3.567061	1.068646	-0.346453
6	0.101271	1.510216	-0.103809
6	-0.874054	2.331651	-0.672704
6	-1.063842	3.685201	-0.401137
6	-0.242183	4.268756	0.552434
6	0.704541	3.509555	1.232394
6	0.823032	2.159989	0.906085
45	-1.446362	-0.178699	1.343310
9	1.672028	-1.174757	1.808713
9	-3.474198	2.014353	0.180138
9	-1.450824	-2.329328	-1.560211
9	-3.235171	-2.700347	0.193644
9	-1.315603	-4.858954	-0.805134
9	-5.257962	-2.799796	-1.504086
9	1.808431	-3.716990	2.526342
9	-5.488485	1.903824	-1.537336
9	0.308655	-5.589897	1.255938
6	0.098637	-1.573391	0.065135
6	-3.075261	-0.325795	0.083924
6	-2.950770	-0.037200	2.867299
6	-2.170614	-1.234576	3.047824
6	0.888011	-2.027624	1.133814
6	-3.785831	0.800732	-0.318064
6	-0.782897	0.546668	3.536853
6	-0.641476	-2.601453	-0.528818
6	-3.670147	-1.523594	-0.299064
6	-2.047390	1.062718	3.010708
6	-0.870137	-0.837328	3.584322
6	-0.590248	-3.938265	-0.166236
6	-4.765257	-1.609520	-1.150783
6	0.981131	-3.349883	1.540207
6	-4.880878	0.772151	-1.170713
6	0.313148	1.366868	4.126114
6	-4.437937	0.041538	2.736410
6	-2.675644	-2.639248	3.085846
6	0.235231	-4.316690	0.881943
6	-5.366550	-0.449166	-1.612346
6	-2.392957	2.513162	2.971494
6	0.094914	-1.755026	4.254022
1	1.292801	0.927717	3.936802
1	0.164797	1.421536	5.211430
1	0.314537	2.386106	3.743084
1	-4.867540	0.068718	3.744142
1	-2.794866	-2.954398	4.128888
1	-4.849424	-0.823139	2.215081
1	-3.633446	-2.741377	2.578815
1	-4.754491	0.942561	2.210788
1	-1.968761	-3.320733	2.605738
1	-3.340773	2.691592	2.466937
1	-0.055242	-2.793680	3.961128
1	-1.618969	3.082994	2.454082
1	1.131437	-1.481763	4.058491
1	-2.459448	2.897650	3.995721
1	-0.072215	-1.690485	5.335970
9	-6.419113	-0.507364	-2.428331

Dir*syn*-*TS*

45	1.316547	-0.504698	1.289040
17	4.143099	4.233517	-0.437560
17	5.321375	-0.482850	-2.816930
17	-0.682016	4.743017	0.170735
17	-2.805752	1.922499	4.270977
9	2.242111	2.629120	1.018908
9	5.519396	2.416392	-2.307460
9	3.285024	-1.491783	-1.041589
9	0.323561	2.159687	-0.621737
9	-2.197964	4.305364	2.656106
9	-1.440319	-0.292799	2.986088
6	2.423685	-2.207161	2.416455
6	1.327564	-1.826065	3.267297
6	1.524023	-0.461758	3.625491
6	2.698800	0.021457	2.981272
6	3.277789	-1.084762	2.259842
6	2.783735	-3.581622	1.937062
1	1.999153	-4.308286	2.144262
1	3.697656	-3.917034	2.439596
1	2.980785	-3.586892	0.861664
6	0.356378	-2.747367	3.936792
1	-0.616725	-2.271970	4.063489
1	0.726648	-3.018227	4.932855
1	0.218213	-3.670692	3.374044
6	0.793033	0.311224	4.679253
1	0.591083	1.337589	4.362810
1	1.423808	0.367198	5.574124
1	-0.150284	-0.155725	4.958910
6	3.389576	1.305924	3.317218
1	4.103549	1.598490	2.546101
1	3.943418	1.185401	4.256458
1	2.681079	2.125301	3.442823
6	4.665081	-1.129932	1.701313
1	4.752050	-1.851114	0.887518
1	5.355679	-1.434574	2.496930
1	4.991581	-0.156311	1.332637
6	2.588035	0.521385	-0.000813
6	2.891173	1.873242	0.111336
6	3.854810	2.541168	-0.643334
6	4.590070	1.810420	-1.566504
6	4.375892	0.446111	-1.705970
6	3.399545	-0.147364	-0.910304
6	-0.349725	0.844108	1.221520
6	-0.305499	2.073908	0.549988
6	-0.874727	3.253398	1.018106
6	-1.629654	3.199610	2.184724
6	-1.833876	1.992124	2.837673
6	-1.208463	0.861856	2.316258
45	-1.939352	-0.904858	-0.239469
9	0.049325	-3.458303	1.070914
9	-3.228572	1.987254	-0.007437
9	0.821626	-0.019567	-2.102181
9	-1.355029	-0.629821	-3.477917
9	1.082772	-1.838065	-3.988471
9	-1.650736	1.398726	-5.151364
9	0.522453	-5.269517	-0.818063
9	-3.553828	3.992604	-1.713456
9	0.976743	-4.487774	-3.380428
6	0.448108	-1.610621	-0.373888
6	-2.111178	0.629185	-1.606761
6	-4.038771	-1.159621	-0.615188
6	-3.291388	-2.282224	-1.113991
6	0.344669	-2.995243	-0.161460
6	-2.728798	1.823826	-1.254110
6	-3.168342	-2.371592	1.196742
6	0.661872	-1.285550	-1.719731
6	-1.806824	0.526721	-2.957782
6	-3.835203	-1.132709	0.801989
6	-2.887903	-3.087033	0.038522
6	0.834348	-2.224390	-2.739621
6	-1.985117	1.561135	-3.869985
6	0.558350	-3.962650	-1.119334
6	-2.940882	2.881397	-2.126068
6	-2.995627	-2.863946	2.594283
6	-4.991366	-0.310351	-1.392877
6	-3.239393	-2.773560	-2.523307
6	0.799017	-3.569250	-2.435311
6	-2.545440	2.757033	-3.449698
6	-4.493130	-0.197445	1.758658
6	-2.448070	-4.505997	-0.061417
1	-2.114618	-3.501000	2.678661
1	-3.873610	-3.452887	2.884736
1	-2.893172	-2.041562	3.301052
1	-5.957435	-0.826778	-1.423951
1	-3.938157	-3.608382	-2.650455
1	-4.656659	-0.152361	-2.418550
1	-3.501983	-1.990060	-3.233072
1	-5.143419	0.661770	-0.924099
1	-2.235802	-3.125550	-2.774456
1	-4.602454	0.801385	1.339549
1	-1.931364	-4.708235	-0.999326
1	-3.937834	-0.122957	2.693047
1	-1.812499	-4.811429	0.767696
1	-5.491488	-0.586665	1.992607
1	-3.349832	-5.130708	-0.048302
9	-2.740143	3.754600	-4.310672

OH-*I1* (Figure 5)

45	1.071357	-1.085329	-1.038968
9	3.354752	-2.147947	0.982310
9	6.482685	1.336520	0.956485
9	2.663675	1.714016	-1.727141
6	0.102782	-1.709772	-3.002141
6	-0.062232	-2.783272	-2.096339
6	1.261142	-3.176169	-1.657772
6	2.219971	-2.377703	-2.381886
6	1.508800	-1.435240	-3.175778
6	-0.979637	-0.944769	-3.683254
1	-1.964062	-1.364987	-3.471633
1	-0.825317	-0.950679	-4.767110
1	-0.972471	0.093035	-3.336420
6	-1.374506	-3.445116	-1.792989
1	-2.028805	-2.797179	-1.206966
1	-1.234291	-4.365920	-1.227373
1	-1.891415	-3.695547	-2.725143
6	1.638819	-4.387406	-0.860832
1	2.331246	-4.127038	-0.058278
1	2.131303	-5.117193	-1.513409
1	0.768258	-4.859657	-0.409708
6	3.699714	-2.592010	-2.369037
1	4.242391	-1.660748	-2.542911
1	3.969553	-3.298303	-3.162289

1	4.031901	-3.011127	-1.418040
6	2.081309	-0.430753	-4.125933
1	1.448878	0.459473	-4.175832
1	2.158647	-0.846648	-5.137191
1	3.078271	-0.112263	-3.813786
6	2.853052	-0.266415	-0.389345
6	3.687261	-0.928846	0.506315
6	4.893277	-0.417435	0.969360
6	5.327823	0.822580	0.524065
6	4.545916	1.514688	-0.386787
6	3.354230	0.952043	-0.822716
8	0.097503	0.871283	-1.233567
45	-1.079752	2.071158	-0.141381
9	1.370359	1.019582	1.489957
9	-3.037667	0.878528	-2.327656
9	-0.451617	-3.338476	0.870722
9	-2.170006	0.221863	2.243133
9	-0.778098	-3.543678	3.470186
9	1.050597	0.755026	4.080180
9	-0.041355	-1.512882	5.147898
6	0.541425	-1.175095	0.991177
6	-2.461823	0.556588	-0.066382
6	-2.311377	3.577175	0.775678
6	-1.051954	3.505202	1.441889
6	0.854934	-0.170452	1.903520
6	-3.176689	0.169351	-1.187014
6	-0.594919	4.153938	-0.729524
6	-0.039206	-2.282002	1.603515
6	-2.748409	-0.155498	1.085435
6	-2.032520	3.881101	-0.598205
6	0.003933	3.927702	0.515073
6	-0.239612	-2.425069	2.971724
6	-3.624076	-1.237718	1.142119
6	0.688377	-0.261759	3.278378
6	-4.070032	-0.899808	-1.211916
6	0.076990	4.540942	-2.006886
6	-3.655752	3.343132	1.387757
6	-0.835043	3.188533	2.881742
6	0.136731	-1.404601	3.828538
6	-4.274539	-1.605858	-0.030566
6	-3.031073	4.061217	-1.692214
6	1.450423	4.061556	0.866087
1	1.151994	4.359550	-1.963507
1	-0.083135	5.605214	-2.209113
1	-0.330023	3.976281	-2.849453
1	-4.058438	4.278914	1.788772
1	-0.837189	4.119528	3.460237
1	-3.594037	2.619494	2.202351
1	-1.619932	2.538288	3.268546
1	-4.361660	2.951968	0.653022
1	0.122204	2.692040	3.039767
1	-3.960531	3.534444	-1.474275
1	1.752314	3.299812	1.585211
1	-2.646547	3.681260	-2.640607
1	2.089158	3.962733	-0.013270
1	-3.255000	5.126999	-1.813518
1	1.633675	5.044338	1.313611
9	-5.115843	-2.639596	-0.021399
1	0.828321	1.409809	-1.552890
17	-4.908017	-1.348249	-2.656667
17	-3.909429	-2.092379	2.612940
9	4.943087	2.714679	-0.834985
9	5.644761	-1.107156	1.833609

OH*anti*-*TS1* (Figure 5)

45	-0.556042	1.492416	-0.089208
17	-5.706469	-0.045283	1.867830
17	-4.823737	-0.478120	-3.455231
9	-2.956633	0.873176	1.895878
9	-6.351292	-0.660842	-0.941472
9	-2.212346	0.561575	-2.762955
6	0.535380	3.355523	-0.770092
6	0.866634	3.194502	0.588702
6	-0.377579	3.177896	1.344413
6	-1.451134	3.417446	0.441006
6	-0.903723	3.429430	-0.892960
6	1.472134	3.377752	-1.929428
1	2.511373	3.442104	-1.602452
1	1.257695	4.231753	-2.578831
1	1.354889	2.456802	-2.509746
6	2.260415	3.224355	1.135795
1	2.873183	2.430976	0.708150
1	2.272001	3.108187	2.218754
1	2.729425	4.183896	0.893163
6	-0.508561	3.135175	2.834661
1	-1.404799	2.585880	3.129214
1	-0.586170	4.152693	3.233980
1	0.353053	2.654697	3.298270
6	-2.864115	3.740632	0.806989
1	-3.568117	3.401745	0.044843
1	-2.967148	4.827591	0.900215
1	-3.147284	3.290604	1.758565
6	-1.646000	3.720595	-2.158511
1	-1.164331	3.236417	-3.010541
1	-1.675841	4.799896	-2.347234
1	-2.674065	3.356142	-2.105832
6	-2.457816	0.754077	-0.411443
6	-3.358387	0.593064	0.636252
6	-4.663170	0.129196	0.501645
6	-5.109671	-0.204302	-0.772207
6	-4.272301	-0.060075	-1.869929
6	-2.984347	0.426856	-1.650528
8	0.295663	0.380452	-1.630835
45	1.155956	-1.298376	-0.719675
9	-1.842979	-1.788036	0.331631
9	2.893633	0.670920	-2.591034
9	1.564385	0.819045	2.362269
9	3.186774	-1.123602	1.788029
9	1.000226	-0.284421	4.691219
9	5.429792	0.253714	2.184253
9	-2.381696	-2.873742	2.673251
9	5.112947	2.064545	-2.154006
9	-0.975912	-2.150849	4.892230
6	-0.089782	-0.409963	1.180851
6	2.838212	-0.182486	-0.367177
6	2.432967	-2.803851	-1.579700
6	1.860550	-3.344183	-0.382090
6	-1.088684	-1.368858	1.369465
6	3.421923	0.606047	-1.352391
6	0.114438	-2.977912	-1.872235
6	0.586649	-0.101706	2.361029
6	3.581467	-0.293001	0.801699
6	1.348730	-2.489505	-2.469229

6	0.443701	-3.530058	-0.621919
6	0.315063	-0.654056	3.604443
6	4.771422	0.388245	1.028729
6	-1.405890	-1.961956	2.581086
6	4.608229	1.308689	-1.170229
6	-1.227902	-2.934742	-2.532487
6	3.891464	-2.676715	-1.883394
6	2.602659	-3.920917	0.782226
6	-0.694040	-1.598668	3.715446
6	5.286531	1.208625	0.035527
6	1.458239	-1.926364	-3.848639
6	-0.440660	-4.310914	0.292919
1	-2.031455	-3.075580	-1.808935
1	-1.307346	-3.716624	-3.295595
1	-1.396160	-1.975321	-3.029482
1	4.249037	-3.613910	-2.323684
1	2.707740	-5.005870	0.666835
1	4.472772	-2.480291	-0.981095
1	3.598949	-3.487619	0.872815
1	4.086662	-1.871808	-2.593509
1	2.078753	-3.725605	1.720135
1	2.408886	-1.414564	-3.996713
1	-0.229445	-4.093729	1.341666
1	0.661397	-1.204665	-4.043690
1	-1.498637	-4.133734	0.108085
1	1.373005	-2.731286	-4.587062
1	-0.236487	-5.376274	0.135574
9	6.425687	1.877452	0.229923
1	-0.400999	0.092337	-2.226386

OH-*I2* (Figure 5)

45	0.773079	-1.128815	-1.108060
17	5.603256	-1.210269	1.987063
17	4.583997	3.204050	-0.975989
9	3.105062	-2.128786	0.848370
9	6.074499	1.489879	0.903595
9	2.234336	1.721672	-1.765283
6	-0.185917	-1.763156	-3.077184
6	-0.305165	-2.855317	-2.187019
6	1.033853	-3.202318	-1.757723
6	1.958520	-2.359284	-2.475585
6	1.207556	-1.433436	-3.253264
6	-1.300235	-1.027511	-3.739716
1	-2.266627	-1.492624	-3.539367
1	-1.146423	-0.997712	-4.823163
1	-1.336335	-0.000187	-3.364567
6	-1.589285	-3.574017	-1.893081
1	-2.268335	-2.962394	-1.296399
1	-1.412070	-4.498165	-1.343559
1	-2.095881	-3.830114	-2.829260
6	1.455278	-4.407359	-0.974019
1	2.181212	-4.137835	-0.204993
1	1.922528	-5.137496	-1.644672
1	0.608728	-4.881890	-0.481369
6	3.445283	-2.519269	-2.478764
1	3.953076	-1.566289	-2.639847
1	3.733041	-3.200429	-3.287610
1	3.802451	-2.944179	-1.539443
6	1.738673	-0.397819	-4.194245
1	1.068032	0.464245	-4.239922
1	1.836324	-0.802515	-5.208311
1	2.720096	-0.038331	-3.877428
6	2.528462	-0.249750	-0.465961
6	3.399555	-0.888869	0.411135
6	4.588903	-0.342265	0.889802
6	4.946934	0.930077	0.461252
6	4.141317	1.618536	-0.435640
6	2.974847	0.997090	-0.874666
8	-0.285490	0.782478	-1.257557
45	-1.443592	1.913021	-0.069259
9	1.054016	0.928920	1.470551
9	-3.381445	0.711240	-2.298214
9	-0.706326	-3.440148	0.764197
9	-2.502659	-0.026654	2.291692
9	-1.027073	-3.702642	3.356408
9	-4.104397	-2.175641	2.246502
9	0.774933	0.593731	4.056430
9	-4.984779	-1.441324	-2.327264
9	-0.282940	-1.710822	5.079441
6	0.266044	-1.270081	0.926459
6	-2.791923	0.367665	-0.026080
6	-2.706849	3.375484	0.873087
6	-1.449198	3.326402	1.540179
6	0.569221	-0.282043	1.860289
6	-3.488274	-0.013658	-1.161451
6	-1.002466	4.014309	-0.622665
6	-0.297188	-2.396938	1.518031
6	-3.057674	-0.376462	1.111086
6	-2.432652	3.704040	-0.498958
6	-0.401811	3.786414	0.620700
6	-0.490844	-2.572361	2.883265
6	-3.899660	-1.481401	1.125138
6	0.418699	-0.408667	3.234473
6	-4.346394	-1.105297	-1.199302
6	-0.334048	4.429726	-1.893055
6	-4.047755	3.105318	1.477721
6	-1.226075	2.990462	2.974959
6	-0.115423	-1.570255	3.762045
6	-4.544840	-1.853976	-0.046506
6	-3.437376	3.877025	-1.588211
6	1.039933	3.955048	0.975284
1	0.744314	4.269186	-1.846870
1	-0.514730	5.492450	-2.085517
1	-0.726017	3.864916	-2.742743
1	-4.472854	4.028584	1.884536
1	-1.256652	3.909566	3.571331
1	-3.972846	2.376446	2.286535
1	-1.992208	2.309623	3.346943
1	-4.741755	2.704866	0.736568
1	-0.254867	2.519511	3.126607
1	-4.336479	3.290743	-1.395909
1	1.359692	3.202717	1.696361
1	-3.031574	3.560799	-2.550734
1	1.683697	3.870760	0.097665
1	-3.719382	4.933310	-1.663261
1	1.198056	4.943309	1.420528
9	-5.361356	-2.909033	-0.062467
1	0.408476	1.355740	-1.597048

OH*syn*-*TS1*

45	-0.504016	-1.626840	-0.876951
17	3.602461	-2.760079	2.933756
17	5.025721	-0.292735	-1.663893

9	0.960361	-2.673262	1.747854
9	5.419093	-1.466167	1.006903
9	2.181955	-0.451478	-2.222131
6	-1.774835	-2.643969	-2.482456
6	-2.259597	-3.146748	-1.270120
6	-1.139838	-3.709591	-0.529557
6	0.002697	-3.692563	-1.386432
6	-0.346686	-2.931764	-2.552510
6	-2.514070	-1.883266	-3.532628
1	-3.545350	-1.685459	-3.235498
1	-2.522509	-2.430675	-4.480899
1	-2.015540	-0.921248	-3.693745
6	-3.682533	-3.279020	-0.831636
1	-4.348993	-2.607970	-1.371513
1	-3.802334	-3.095352	0.237472
1	-4.007123	-4.309131	-1.019829
6	-1.292061	-4.431086	0.772729
1	-0.326721	-4.644255	1.229959
1	-1.823373	-5.377959	0.622383
1	-1.867273	-3.830209	1.482388
6	1.299981	-4.399779	-1.156204
1	2.144059	-3.852085	-1.578626
1	1.256028	-5.382400	-1.638708
1	1.492490	-4.553579	-0.093615
6	0.505536	-2.682574	-3.755333
1	0.324349	-1.683691	-4.159223
1	0.277825	-3.413867	-4.539473
1	1.567299	-2.757666	-3.516980
6	1.429807	-1.452502	-0.218593
6	1.856379	-2.031026	0.971506
6	3.172474	-2.039577	1.423342
6	4.145799	-1.469747	0.611708
6	3.805353	-0.929947	-0.621098
6	2.460970	-0.944509	-0.992870
8	-0.563483	0.238804	-1.861942
45	-1.088008	1.666362	-0.414590
9	0.448839	-0.218107	2.300636
9	0.456196	2.301516	2.353563
9	-3.458170	-0.536979	-0.362610
9	1.496339	2.165004	-2.266796
9	-4.893679	-1.020411	1.833648
9	3.995973	2.867062	-1.704657
9	-1.012547	-0.610489	4.476326
9	3.005998	2.831618	2.898715
9	-3.688811	-1.038579	4.273093
6	-1.408742	-0.381524	0.831097
6	0.880485	2.026102	0.029928
6	-1.345691	3.817177	-0.446866
6	-1.733848	3.225544	-1.700611
6	-0.858678	-0.397700	2.114299
6	1.324269	2.285130	1.321538
6	-3.257798	2.533511	-0.115034
6	-2.789481	-0.579522	0.812769
6	1.834577	2.247404	-0.956142
6	-2.208536	3.285077	0.558753
6	-2.957645	2.467558	-1.479911
6	-3.570059	-0.820891	1.929378
6	3.147518	2.623097	-0.702209
6	-1.594914	-0.608135	3.276170
6	2.637062	2.618316	1.631935
6	-4.499124	2.068302	0.572531
6	-0.291335	4.859480	-0.251476
6	-1.158640	3.493172	-3.053014
6	-2.960661	-0.829128	3.179215
6	3.563056	2.781486	0.611494
6	-2.248149	3.660718	2.007085
6	-3.700650	1.757084	-2.563439
1	-4.993512	1.254325	0.043977
1	-5.196780	2.911643	0.631414
1	-4.296149	1.747283	1.595627
1	-0.750773	5.849534	-0.345512
1	-1.825967	4.152247	-3.619691
1	0.499513	4.779496	-0.998706
1	-0.177905	3.963845	-2.989713
1	0.168633	4.788945	0.735207
1	-1.047403	2.558112	-3.607711
1	-1.303913	4.096212	2.332566
1	-3.024336	1.080856	-3.094397
1	-2.435835	2.786120	2.635004
1	-4.525317	1.166383	-2.162608
1	-3.046880	4.388896	2.189979
1	-4.105189	2.471940	-3.288136
9	4.820251	3.131162	0.887193
1	0.308292	0.443065	-2.213803

OH-*I3* (Figure ESI8)

45	0.752337	-0.882802	-1.379822
9	3.177204	-2.197870	0.262804
9	6.175740	1.363831	0.757806
9	2.214346	2.023680	-1.646713
6	-0.334377	-1.193446	-3.351430
6	-0.408910	-2.415684	-2.645093
6	0.950038	-2.829919	-2.367535
6	1.836953	-1.883984	-3.000373
6	1.048969	-0.842748	-3.566132
6	-1.479448	-0.363311	-3.821533
1	-2.436534	-0.846436	-3.619908
1	-1.401246	-0.187479	-4.899359
1	-1.471229	0.604642	-3.311739
6	-1.680220	-3.165154	-2.376861
1	-2.340056	-2.606429	-1.710542
1	-1.486617	-4.131013	-1.912020
1	-2.215139	-3.341503	-3.316084
6	1.405994	-4.145104	-1.814656
1	2.193946	-4.005584	-1.072447
1	1.804150	-4.767848	-2.623909
1	0.590129	-4.682506	-1.334427
6	3.319025	-2.045689	-3.118491
1	3.825515	-1.081488	-3.193299
1	3.548854	-2.622223	-4.021747
1	3.730132	-2.582412	-2.261939
6	1.521290	0.336963	-4.356626
1	0.910010	1.217116	-4.140031
1	1.457016	0.139830	-5.432978
1	2.557734	0.586108	-4.119533
6	2.557763	-0.133566	-0.707559
6	3.463013	-0.905240	0.014353
6	4.678209	-0.442643	0.517918
6	5.025506	0.882033	0.283362
6	4.183511	1.706200	-0.450649
6	2.994534	1.162664	-0.929391
8	-0.288023	1.032670	-1.162218
45	-1.488271	1.947600	0.165589

9	1.153202	0.797550	1.401480
9	-3.555331	1.199668	-2.160823
9	-0.600787	-3.430900	0.220310
9	-2.378235	-0.447771	2.114801
9	0.044814	-2.306987	4.706410
6	0.359205	-1.312523	0.638624
6	-2.823000	0.405718	-0.047830
6	-2.862620	3.309370	1.093773
6	-1.750184	3.101515	1.952030
6	0.704684	-0.451933	1.677980
6	-3.602141	0.264403	-1.183593
6	-0.908994	4.097999	0.030986
6	-0.164000	-2.514117	1.105157
6	-3.020126	-0.552857	0.933050
6	-2.337940	3.834087	-0.144592
6	-0.547253	3.645012	1.304021
6	-0.292261	-2.883827	2.443730
6	-3.886175	-1.629808	0.786732
6	0.636834	-0.753996	3.036762
6	-4.485691	-0.789915	-1.377197
6	-0.016388	4.682493	-1.016190
6	-4.298941	3.013573	1.387523
6	-1.775018	2.536543	3.332154
6	0.131846	-1.988401	3.413734
6	-4.621927	-1.751530	-0.384961
6	-3.128985	4.227475	-1.346324
6	0.810797	3.691789	1.923304
1	1.035914	4.497846	-0.794113
1	-0.168457	5.764594	-1.086117
1	-0.231914	4.252816	-1.998258
1	-4.793395	3.903690	1.789584
1	-1.643207	3.340099	4.065098
1	-4.393069	2.208300	2.117817
1	-2.716631	2.028237	3.539070
1	-4.829067	2.702221	0.485529
1	-0.967221	1.816294	3.475434
1	-4.082130	3.700875	-1.388927
1	0.937323	2.901701	2.663743
1	-2.583027	4.009415	-2.266195
1	1.598128	3.576525	1.175692
1	-3.326001	5.305111	-1.311528
1	0.949465	4.657583	2.421628
9	-5.461132	-2.775489	-0.551360
1	0.407359	1.657635	-1.388470
17	4.603002	3.362265	-0.738708
17	5.735174	-1.474353	1.414997
17	1.191640	0.362929	4.243893
17	-0.944639	-4.418171	2.900231
9	-4.031585	-2.532710	1.757983
9	-5.205900	-0.888901	-2.501351

OH*anti*-*TS2* (Figure ESI8)

45	-0.792018	-1.305034	-0.833082
9	-5.858355	0.481343	-1.215957
9	-4.963334	-2.214717	2.544771
9	-3.315923	0.296380	-1.974786
9	-6.726848	-0.746734	1.061007
9	-2.435452	-2.476215	1.793740
6	0.393645	-3.112343	-1.496838
6	0.732946	-2.081375	-2.398970
6	-0.498175	-1.622802	-3.016960
6	-1.566655	-2.438037	-2.543682
6	-1.033431	-3.314833	-1.531358
6	1.322074	-3.859798	-0.601427
1	2.365268	-3.629123	-0.824237
1	1.174256	-4.938166	-0.713334
1	1.131298	-3.585660	0.441052
6	2.134135	-1.706963	-2.775554
1	2.704112	-1.360092	-1.913872
1	2.152539	-0.919114	-3.527660
1	2.646214	-2.581989	-3.190076
6	-0.621284	-0.610092	-4.112436
1	-1.553013	-0.048593	-4.018345
1	-0.622508	-1.111533	-5.086714
1	0.206507	0.099406	-4.099924
6	-2.949535	-2.504937	-3.107916
1	-3.686421	-2.762037	-2.344835
1	-2.978299	-3.284410	-3.877545
1	-3.246947	-1.562456	-3.567511
6	-1.765395	-4.406213	-0.816450
1	-1.324113	-4.587547	0.165797
1	-1.720861	-5.339712	-1.389316
1	-2.816368	-4.149541	-0.668018
6	-2.731506	-1.104424	-0.142696
6	-3.677286	-0.374862	-0.856517
6	-5.006012	-0.241413	-0.482410
6	-5.453104	-0.861933	0.676302
6	-4.555187	-1.605986	1.424321
6	-3.237535	-1.715370	0.994215
8	0.016096	-1.430677	1.088295
45	0.753354	0.462814	1.555155
9	-2.313359	1.378138	0.816839
9	2.598506	-2.173436	1.724813
9	1.335897	0.844330	-2.117247
9	2.780965	2.071222	-0.300891
17	1.127911	3.403701	-3.415173
17	5.281193	1.677833	-1.722459
17	-3.170293	3.954475	-0.173573
17	5.066111	-3.204602	0.602357
9	-1.221588	4.731140	-2.229378
6	-0.470513	0.945976	-0.606392
6	2.505009	-0.073674	0.639608
6	1.928028	1.192928	3.203824
6	1.225956	2.306568	2.650305
6	-1.502693	1.784738	-0.177937
6	3.135344	-1.291630	0.864431
6	-0.373864	0.850733	3.500483
6	0.307522	1.533750	-1.603568
6	3.239465	0.816552	-0.132399
6	0.941106	0.237677	3.644042
6	-0.186504	2.118656	2.932573
6	0.103216	2.790008	-2.167205
6	4.459496	0.521109	-0.737692
6	-1.800455	3.039508	-0.702998
6	4.356037	-1.657339	0.294275
6	-1.666305	0.229191	3.926790
6	3.408792	1.069036	3.370724
6	1.812936	3.583845	2.137217
6	-0.975503	3.533398	-1.707398
6	5.005034	-0.738400	-0.521672
6	1.196531	-1.067215	4.325078
6	-1.203252	3.193920	2.750382
1	-2.504884	0.629067	3.354253

1	-1.853708	0.415589	4.989880
1	-1.652864	-0.854025	3.782448
1	3.697267	1.504092	4.333713
1	1.743637	4.367294	2.900496
1	3.947149	1.597657	2.582431
1	2.861371	3.460066	1.866155
1	3.730862	0.026631	3.356790
1	1.283050	3.928616	1.246306
1	2.212882	-1.419016	4.150110
1	-1.048314	3.741739	1.819673
1	0.514686	-1.838374	3.959315
1	-2.223215	2.813666	2.764185
1	1.042595	-0.957937	5.404247
1	-1.090733	3.912347	3.570828
9	6.167136	-1.063303	-1.089411
1	-0.691278	-1.656510	1.698414

OH-*I4* (Figure ESI8)

45	-1.029705	-0.792157	1.350873
9	-5.838678	-1.314046	-1.056796
9	-4.933154	2.935611	0.770128
9	-3.469943	-2.192665	-0.240574
9	-6.619290	1.256363	-0.576587
9	-2.566664	2.105621	1.609226
6	0.107966	-1.062616	3.296256
6	0.187993	-2.289383	2.597762
6	-1.169567	-2.733466	2.363195
6	-2.057294	-1.797323	3.010060
6	-1.275897	-0.736878	3.545730
6	1.248273	-0.209916	3.735291
1	2.208502	-0.678891	3.515672
1	1.191473	-0.030042	4.813817
1	1.211324	0.755448	3.222275
6	1.467091	-3.012100	2.295028
1	2.098856	-2.435347	1.616750
1	1.282683	-3.978733	1.828420
1	2.029128	-3.182008	3.219650
6	-1.618290	-4.065616	1.845278
1	-2.389790	-3.950922	1.081945
1	-2.036109	-4.657369	2.667667
1	-0.794557	-4.623286	1.403498
6	-3.532746	-1.985088	3.165143
1	-4.054966	-1.029008	3.236663
1	-3.730653	-2.550939	4.082531
1	-3.952490	-2.542798	2.326364
6	-1.750261	0.443854	4.333340
1	-1.159903	1.331612	4.091112
1	-1.657264	0.261308	5.410144
1	-2.796148	0.671810	4.117232
6	-2.866002	-0.094133	0.709321
6	-3.770225	-0.904375	0.029336
6	-5.019029	-0.479766	-0.409179
6	-5.424174	0.824242	-0.164698
6	-4.567963	1.669280	0.523152
6	-3.335635	1.189479	0.944270
8	-0.039199	1.149437	1.100353
45	1.167094	2.072576	-0.215421
9	-1.480608	0.876821	-1.416655
9	3.273861	1.397892	2.066352
9	0.261608	-3.364749	-0.265226
9	2.033520	-0.336657	-2.120895
17	0.495555	-4.378392	-2.951056
17	3.772785	-2.682587	-2.067766
17	-1.565977	0.443785	-4.260044
17	5.200862	-0.686874	2.759603
9	-0.468833	-2.243138	-4.739489
6	-0.675602	-1.233715	-0.669592
6	2.517925	0.546039	0.003592
6	2.528336	3.426305	-1.177416
6	1.405430	3.200566	-2.018655
6	-1.039014	-0.372758	-1.702173
6	3.329507	0.436306	1.118869
6	0.584452	4.223867	-0.104477
6	-0.178817	-2.443813	-1.143137
6	2.712663	-0.427941	-0.961928
6	2.016780	3.967264	0.057711
6	0.208722	3.752406	-1.366396
6	-0.092296	-2.820841	-2.483265
6	3.600237	-1.494460	-0.829928
6	-0.999338	-0.676886	-3.061468
6	4.240873	-0.597705	1.324176
6	-0.295157	4.821290	0.946202
6	3.961771	3.129978	-1.484874
6	1.416262	2.613410	-3.389597
6	-0.520256	-1.919522	-3.446004
6	4.358002	-1.567856	0.334506
6	2.819514	4.384313	1.243598
6	-1.156104	3.784855	-1.971414
1	-1.350115	4.641901	0.733832
1	-0.135922	5.902881	1.007452
1	-0.073998	4.396354	1.929053
1	4.447172	4.013987	-1.910800
1	1.277015	3.405351	-4.133767
1	4.049621	2.311227	-2.200906
1	2.355847	2.101905	-3.597891
1	4.505888	2.838240	-0.584634
1	0.606947	1.891232	-3.512944
1	3.777337	3.866140	1.282441
1	-1.288172	2.981589	-2.696619
1	2.286564	4.176286	2.173363
1	-1.934157	3.679390	-1.213110
1	3.007307	5.462802	1.189696
1	-1.303821	4.741327	-2.484819
9	5.213032	-2.576643	0.501875
1	-0.753742	1.759924	1.307307

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