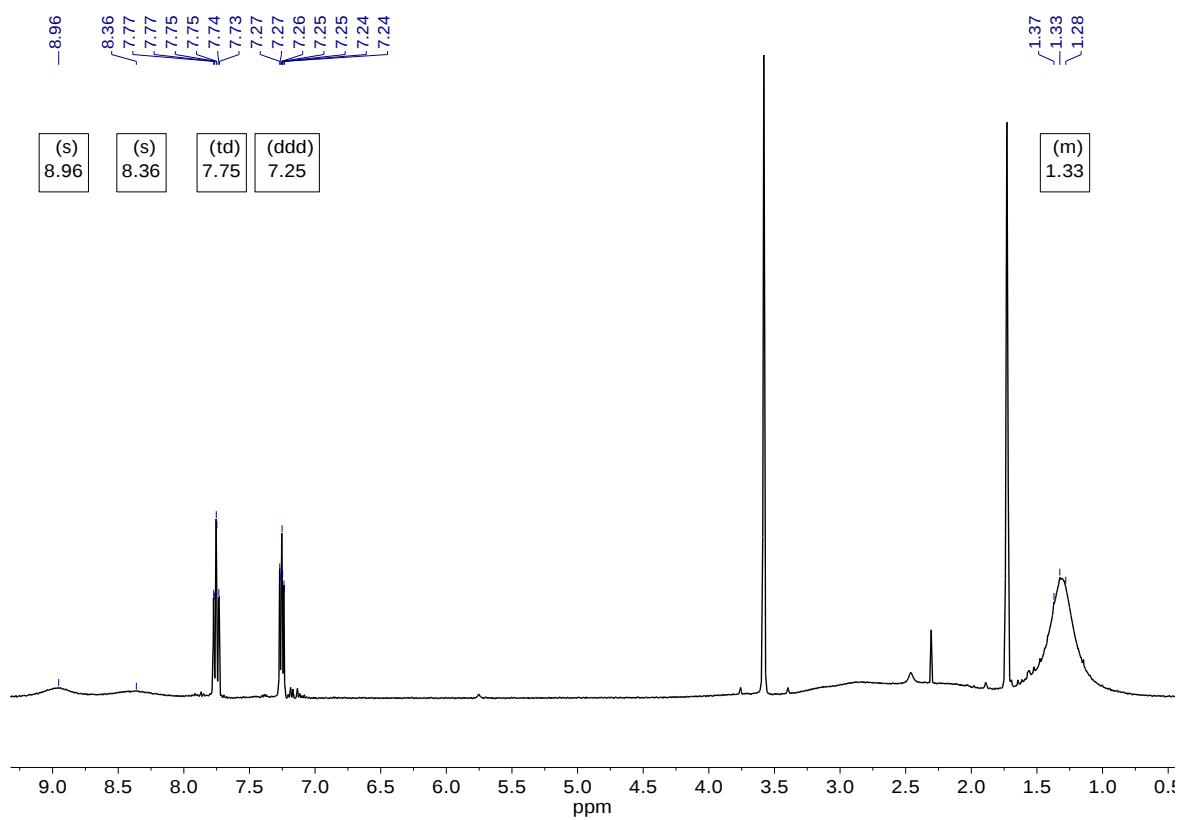


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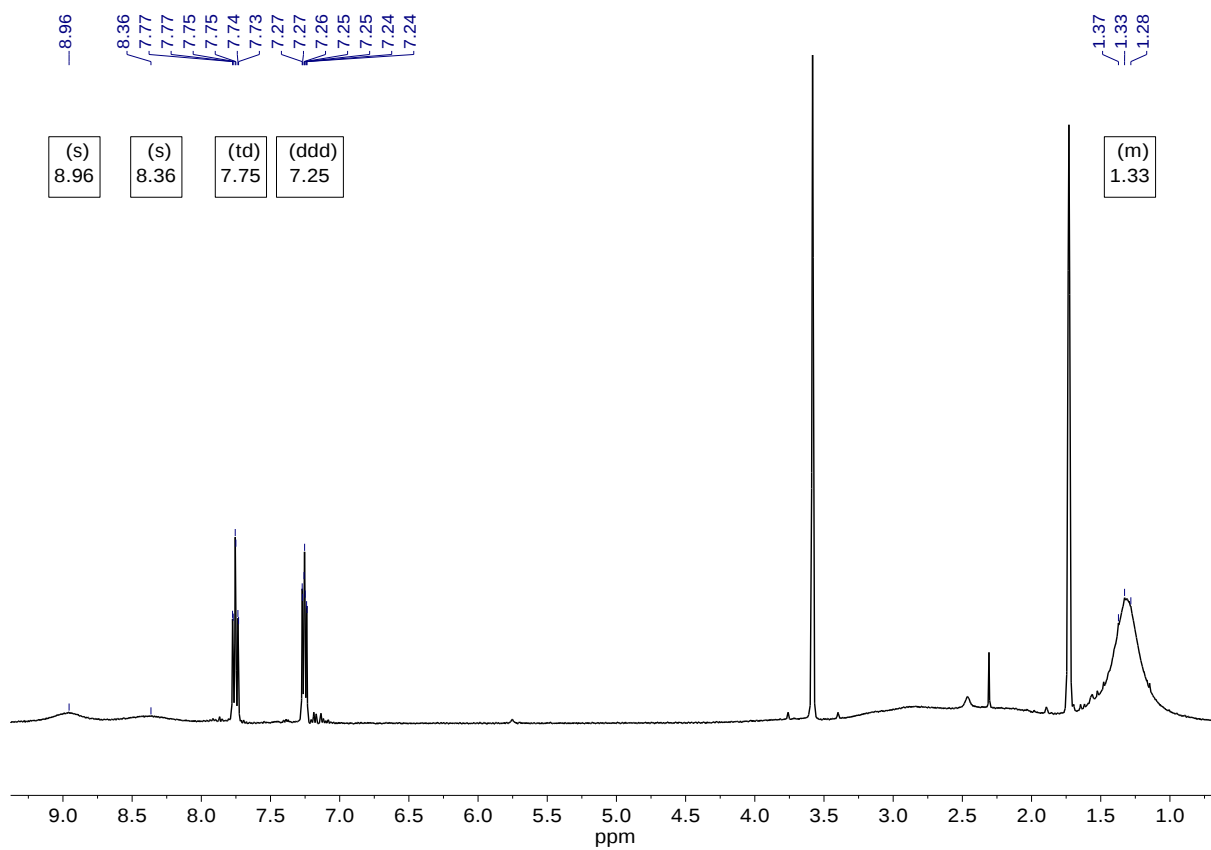
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1. NMR Spectra of 1 and 2 (THF-d₈, r.t.)

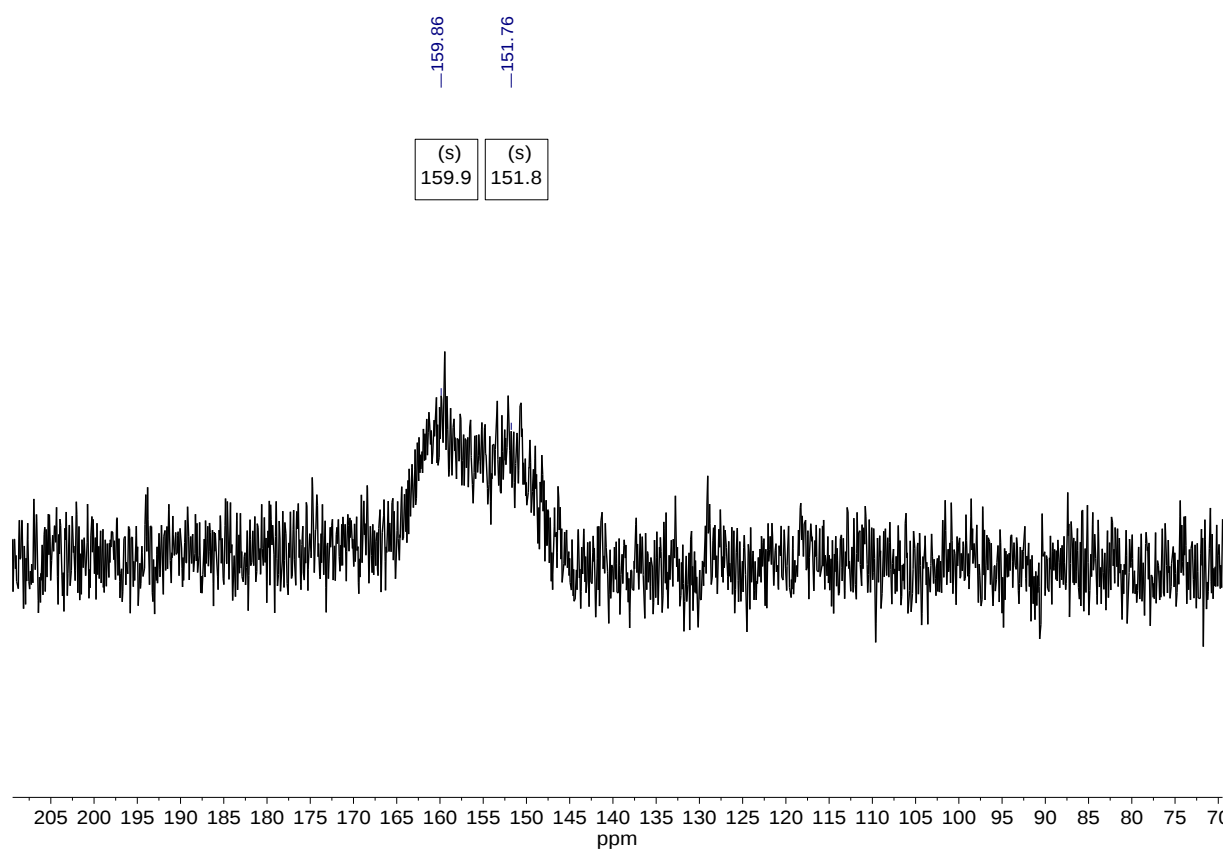
¹H NMR spectrum of 1



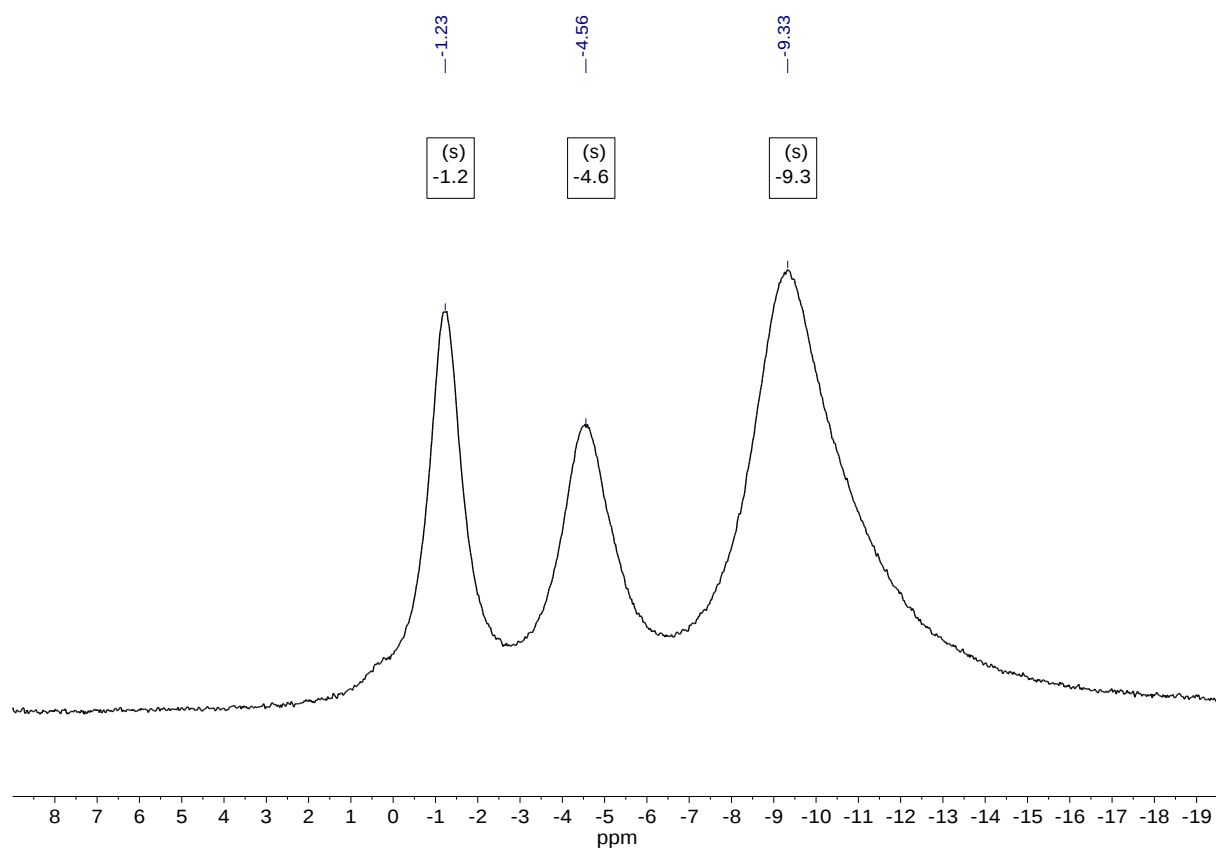
¹H{¹¹B} NMR spectrum of 1



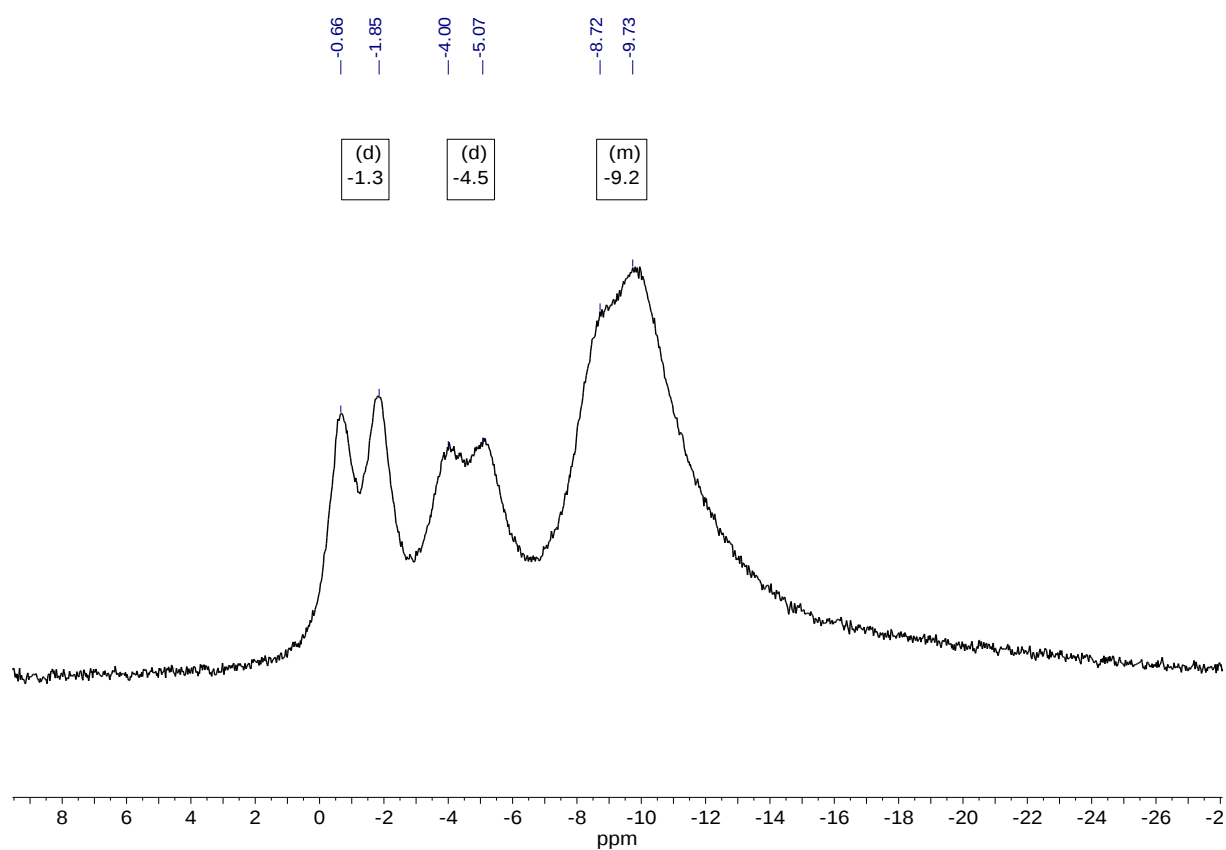
$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **1**



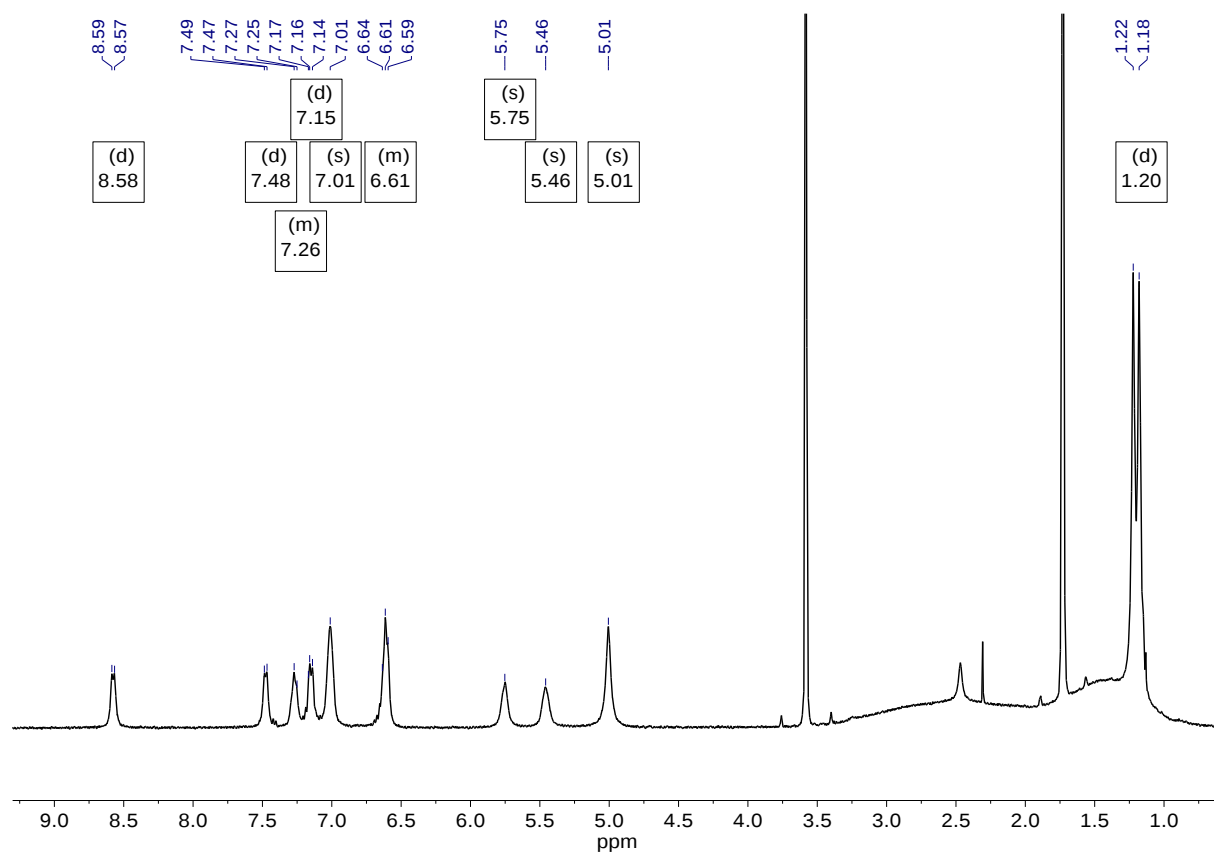
$^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of **1**



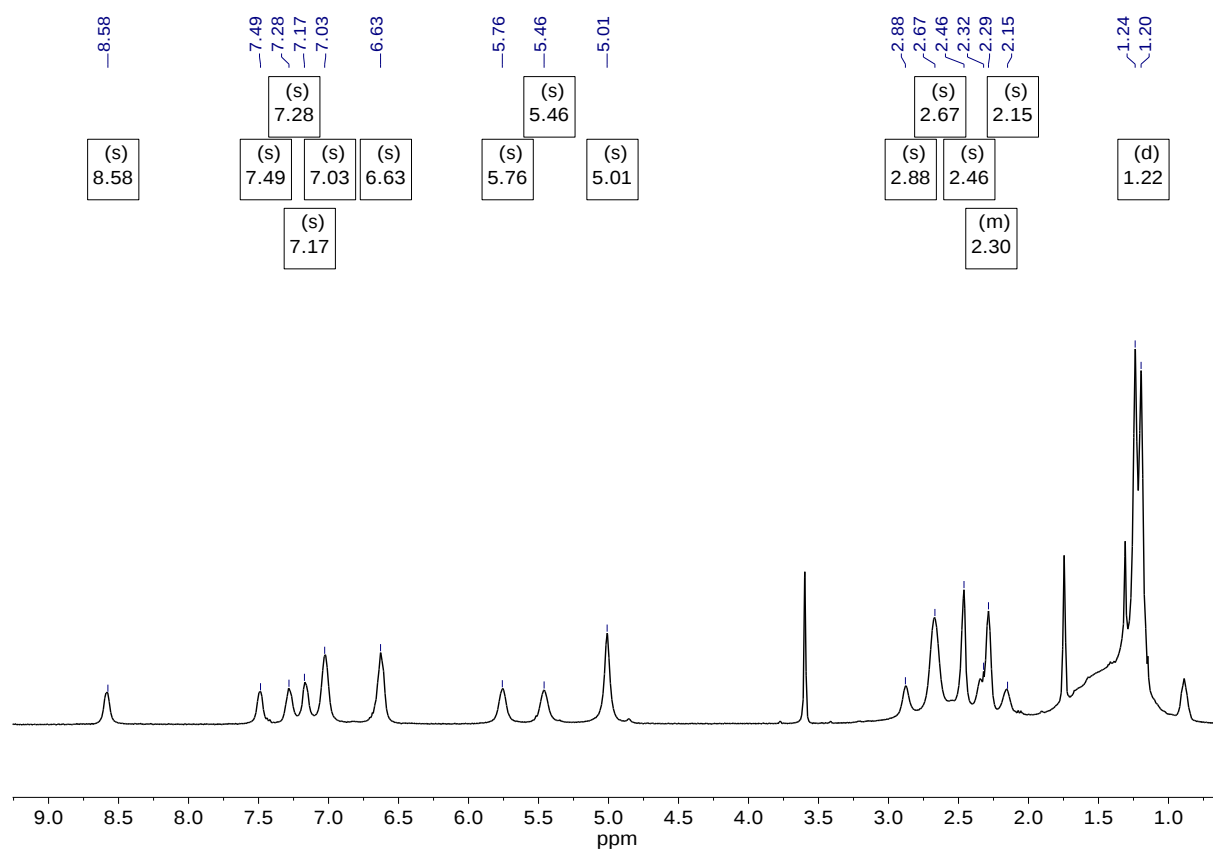
^{11}B NMR spectrum of **1**



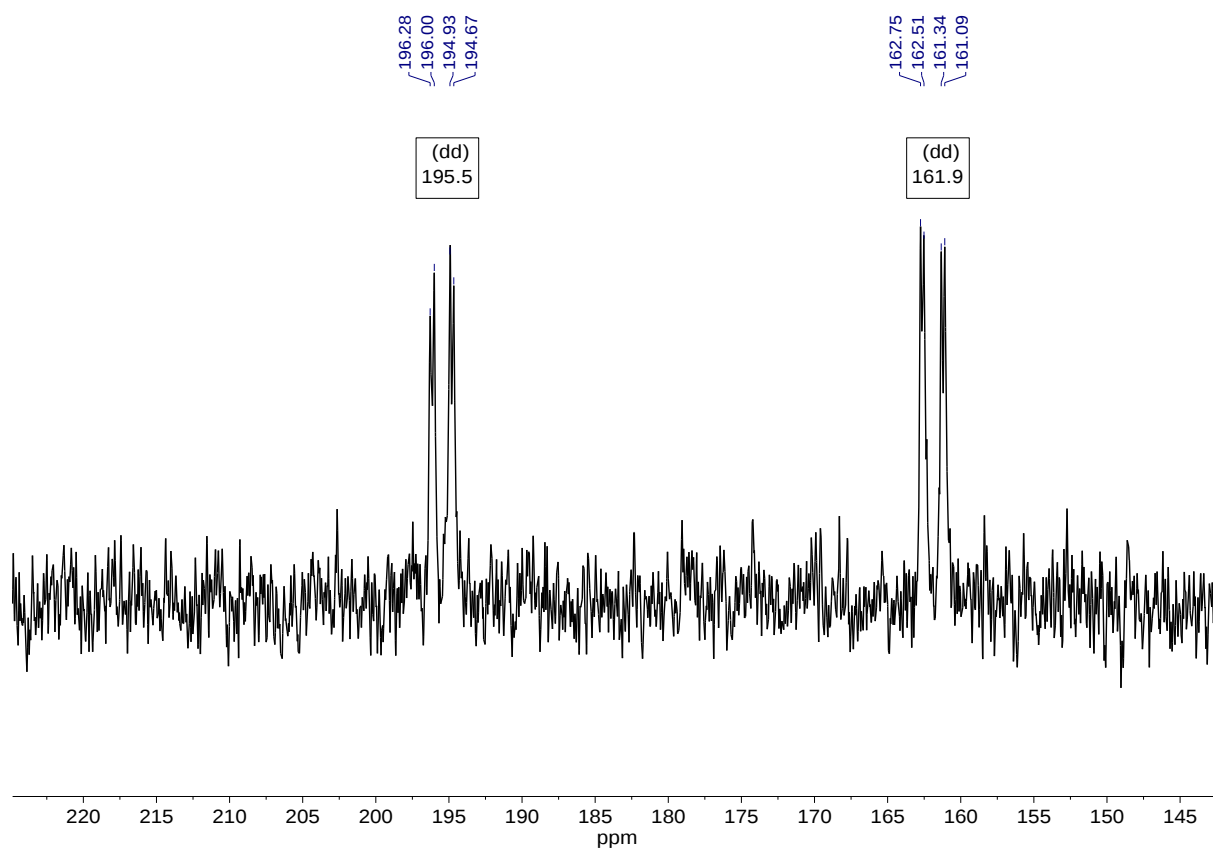
^1H NMR spectrum of **2**



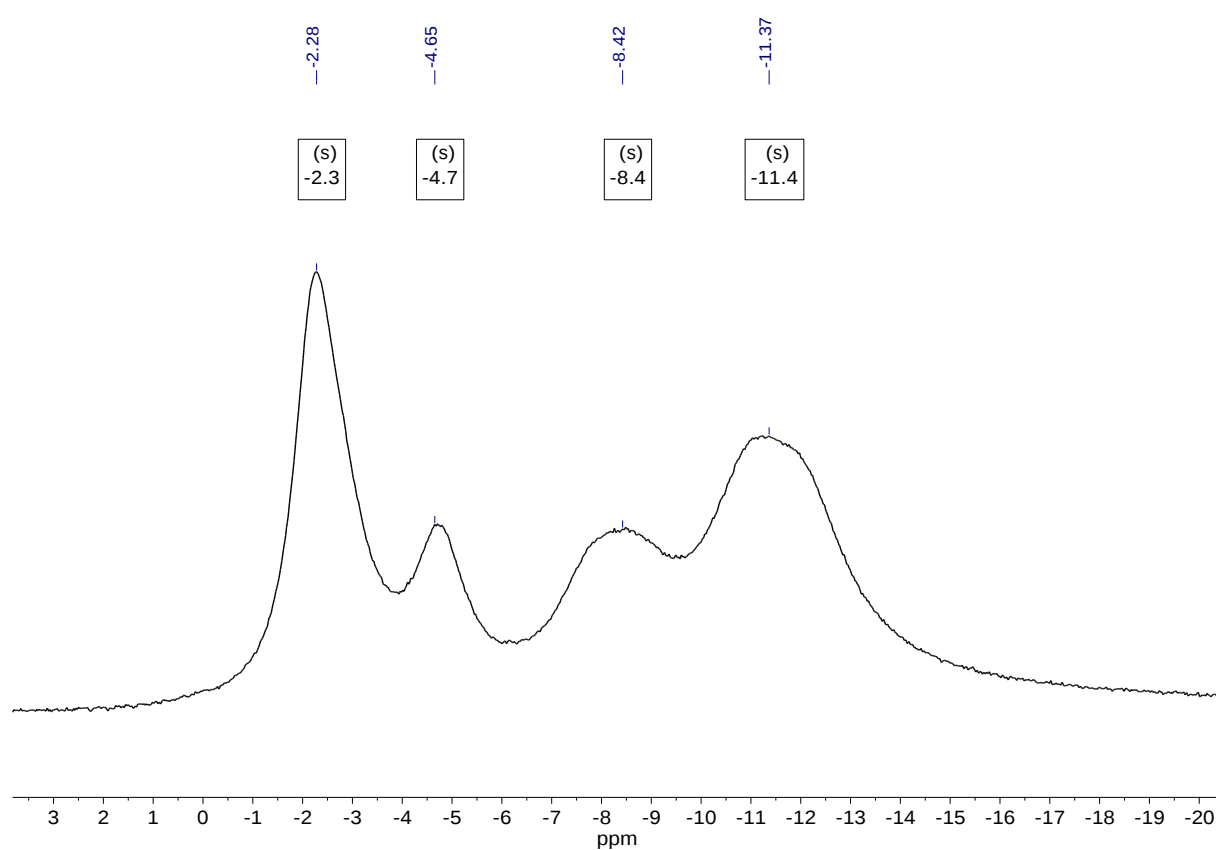
$^1\text{H}\{^{11}\text{B}\}$ NMR spectrum of **2**



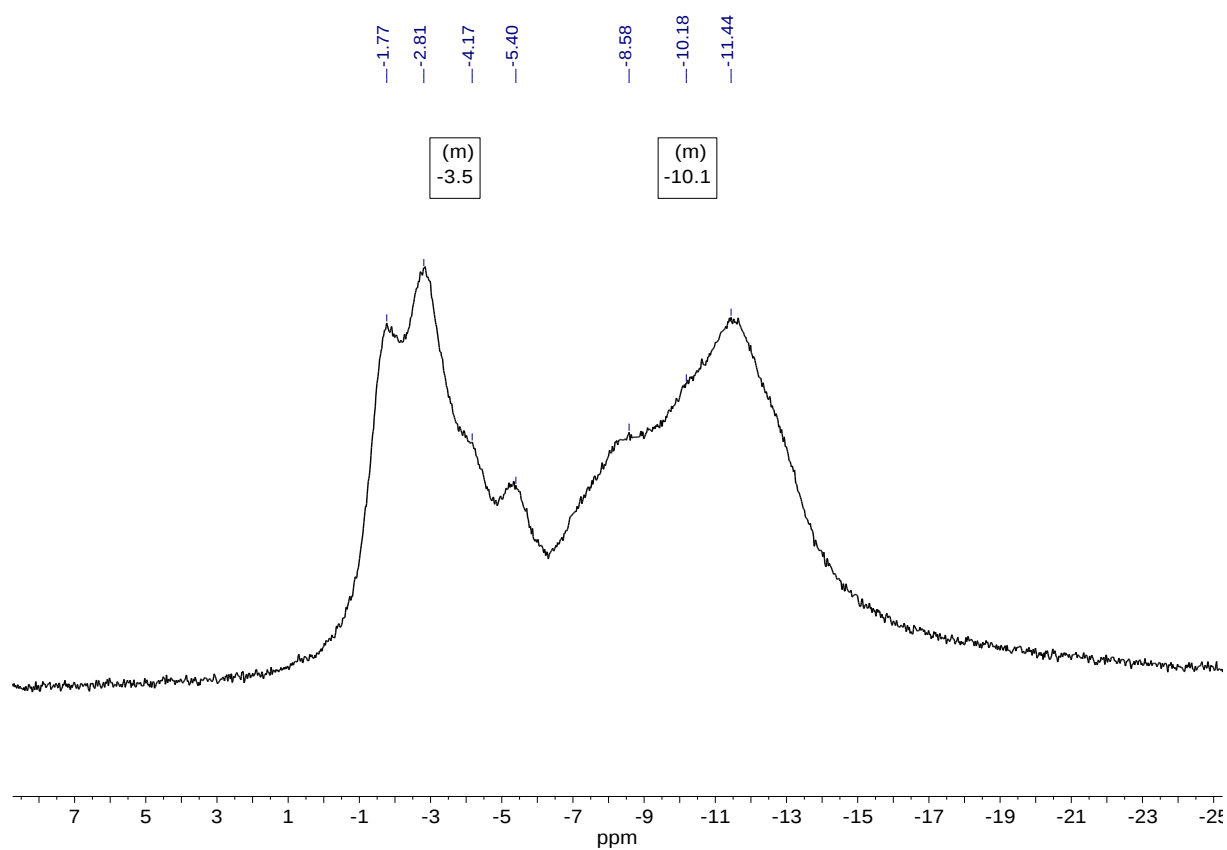
$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **2**



$^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of **2**



$^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of **2**



2. Comparison of Molecular Structures of Rhodium(I) Complexes Containing Two P, One Cl and One N Donor Atom

Table S2: Comparison of solid-state molecular structures of square-planar Rh^I complexes with two phosphorus, one nitrogen and one chlorine donor atom. τ was calculated according to the formula of Yang *et al.*^[1]

CSD identifier	α [°]	β [°]	τ	<i>cis</i> P–Rh–P	chelating P–Rh–P
1	156.06	165.09	0.273	yes	yes
2	160.48	166.21	0.233	yes	yes
UQEHEF ^[2]	162.14	171.77	0.183	yes	yes
NIRSUD ^[3]	166.62	171.5	0.153	yes	no
FORZUI	167.94	171.22	0.145	yes	yes
SERFOK ^[4]	169.26	170.48	0.141	yes	no
PIPMUW ^[5]	165.35	174.52	0.140	yes	yes
FORZOC	168.02	172.23	0.138	yes	yes
KONDIA ^[6]	166.69	174.36	0.132	yes	no
CASVEZ ^[7]	170.13	174.1	0.109	yes	no
SAZNAL ^[8]	173.5	174.78	0.081	yes	yes
GEFDUT ^[9]	173.97	174.55	0.079	yes	yes
VOHDAY ^[10]	172.79	177.7	0.065	yes	no
VOMDAC ^[11]	173.26	177.57	0.063	yes	no
GEFFIJV ^[9]	175.35	177.61	0.048	yes	yes
BESDOT ^[12]	155.28	169.98	0.243	no	yes
BESDIN ^[12]	155.41	171.59	0.231	no	yes
MOWWUS ^[13]	153.11	176.71	0.211	no	yes
RUDCOK ^[14]	162.19	169.65	0.197	no	yes

UMUHUH ^[15]	162.61	171.32	0.182	no	yes
HIPSUV ^[16]	161.58	175.82	0.158	no	yes
UMUHIV ^[15]	161.83	178.33	0.138	no	yes
PAZMOS ^[17]	163.53	178.11	0.128	no	yes
ZUFZIL ^[18]	165.33	177.14	0.122	no	yes
EMIJIV ^[19]	163.27	179.76	0.118	no	yes
PIKVAY ^[20]	164.6	180	0.107	no	yes
DOGNIY ^[21]	166.57	180	0.093	no	yes
JIVJEE ^[22]	166.57	180	0.093	no	yes
GAMED ^[23]	172.15	174.56	0.092	no	no
JIVJII ^[22]	168.32	178.65	0.090	no	yes
UTEROB ^[24]	174.36	177.6	0.055	no	yes
ELEDAA ^[25]	175.83	176.91	0.049	no	no
VAYLAX ^[26]	177.96	179.95	0.012	no	yes

3. Temperature-dependent NMR Spectroscopic Investigations on **1** and **2**

Figure S1 shows the temperature-dependent $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of **1** and **2**. While the spectrum of **1** exhibits a very strong temperature dependence, only line-broadening is observed for **2** when increasing the temperature from $-5\text{ }^{\circ}\text{C}$ to $25\text{ }^{\circ}\text{C}$. This may be explained with the higher activation energy for the isomerisation processes in **2** (*vide infra*). However, it has to be taken into account that the coalescence point/temperature also depends on the chemical shift difference of the interchanging species (at slow exchange rates). Since the chemical shift difference in **1** is significantly smaller than in **2** (**1**: $\Delta\delta(^{31}\text{P}\{^1\text{H}\}) = 8.3\text{ ppm}$ at $-40\text{ }^{\circ}\text{C}$, **1**: $\Delta\delta(^{31}\text{P}\{^1\text{H}\}) = 33.6\text{ ppm}$ at r.t.), a higher isomerisation barrier cannot be derived unambiguously from the $^{31}\text{P}\{^1\text{H}\}$ NMR data. However, the isomerisation barriers can be compared by looking at the temperature-dependent ^1H NMR spectra (Figure S2): Here, both complexes exhibit strong changes in their spectra upon variation of the temperature. While **1** requires cooling to $-40\text{ }^{\circ}\text{C}$ to show two distinctive sets of pyridine resonances, **2** only needs to be cooled to $0\text{ }^{\circ}\text{C}$. Furthermore, while the ^1H NMR spectrum of **1** shows coalescence at about $0\text{ }^{\circ}\text{C}$, coalescence is not reached for **2** even at $60\text{ }^{\circ}\text{C}$. Altogether, these experiments clearly show the higher isomerisation barrier of **2** as was found also by DFT calculations (*vide infra*).

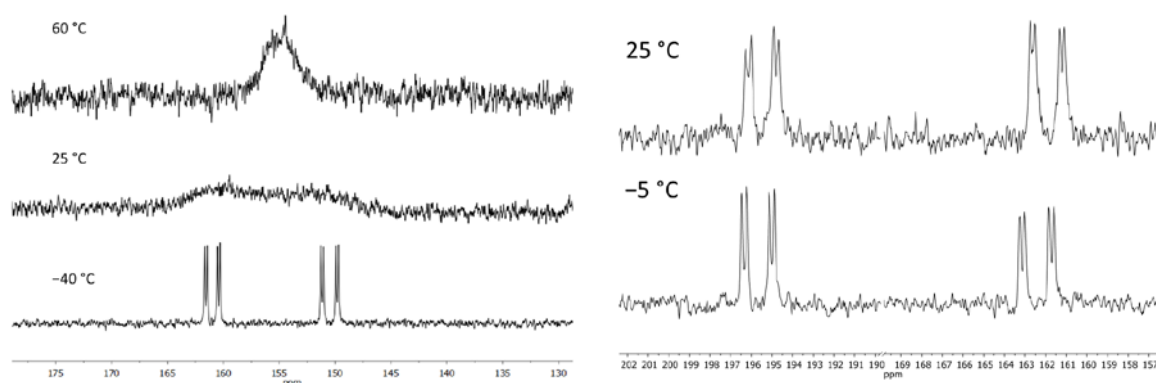


Figure S1. Temperature-dependent $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of **1** (left) and **2** (right).

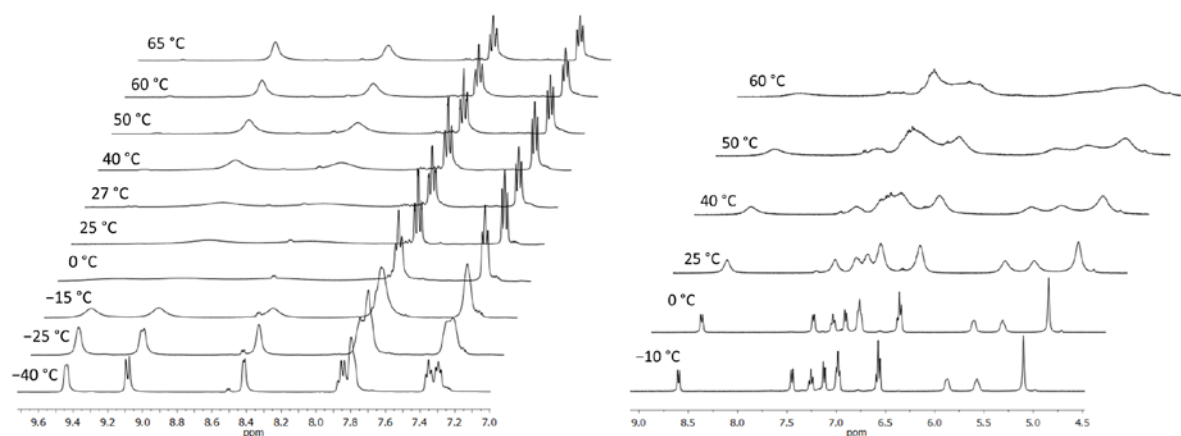


Figure S2. Temperature-dependent ^1H NMR spectra of **1** (left) and **2** (right). For clarity, only the resonances accounting for the pyridine protons in **1** and the aniline protons in **2** are shown.

4. Cyclic Voltammetry (CV)

Cyclic voltammetric measurements on $1.0 \text{ mmol}\cdot\text{L}^{-1}$ analyte solutions in freshly distilled and oxygen-free tetrahydrofuran, containing $0.1 \text{ mol}\cdot\text{L}^{-1}$ tetrabutylammonium tetrafluoroborate as supporting electrolyte, have been conducted in a three-electrode setup (GAMRY Instruments, SP-50 potentiostat by BioLogic Science Instruments) under a blanket of nitrogen at room temperature. The glassy-carbon working electrode (ALS; surface area 0.07 cm^2) and the counter electrode (neoLab; platinum wire, 99.9%) were immersed in the analyte solution, while the reference electrode (ALS; Ag/AgNO_3 ($0.01 \text{ mol}\cdot\text{L}^{-1}$) in $0.1 \text{ mol}\cdot\text{L}^{-1}$ tetrabutylammonium hexafluorophosphate in dry, oxygen-free acetonitrile) was connected to the cell via a bridge tube (filled with the supporting electrolyte) through Vycor tips. The reference electrode was calibrated against decamethylferrocene as an internal standard at the end of the CV experiment,^[27] and the results were converted to the $\text{FcH}/[\text{FcH}]^+$ scale in accordance with the IUPAC requirements.^[28]

In the following text, all potentials are referenced against $\text{FcH}/[\text{FcH}]^+$. Unless stated otherwise, whenever a potential range is given, the first potential refers to the starting potential of the respective measurement. Both **1** and **2** show a fairly complex redox behaviour. In the range of -950 to -200 mV , **1** undergoes a quasi-reversible oxidation event ($E_{1/2} = -588 \text{ mV}$, $E_{\text{peak}(\text{anodic}/\text{cathodic})} = -446/-730 \text{ mV}$, Figure S3). Similarly, **2** undergoes an irreversible oxidation event in the range of -1500 to 80 mV ($E_{\text{peak}(\text{anodic}/\text{cathodic})} = -27/-612 \text{ mV}$). When the range is expanded to larger potentials, both complexes show a second irreversible oxidation event (**1**: -950 to -200 mV , $E_{\text{peak}(\text{anodic})} = -296 \text{ mV}$, **2**: -1500 to 500 mV , $E_{\text{peak}(\text{anodic})} = 149 \text{ mV}$). Based on our calculations (see the main text and the Computational Details below) and the existing literature, these oxidation events can be assigned to the $\text{Rh}^{\text{I}}/\text{Rh}^{\text{II}}$ and the $\text{Rh}^{\text{II}}/\text{Rh}^{\text{III}}$ redox couples.

Only the onset of a reduction of **1** is observed in the range of -700 to -1700 mV (Figure S4). However, in the range of -700 to -2300 mV , **1** undergoes an irreversible reduction event ($E_{\text{peak}(\text{cathodic})} = -1880 \text{ mV}$). An oxidation event at $E_{\text{peak}(\text{anodic})} = -964 \text{ mV}$ is observed as well, which indicates an ECE mechanism. Further reduction and oxidation events can be seen in the second cycle indicating subsequent reactions of the species formed in the first cycle. The situation is similar for complex **2**. No reduction is observed in the range of -250 to -1450 mV . However, in the range of -600 to -2250 mV , **2** undergoes an irreversible reduction event ($E_{\text{peak}(\text{cathodic})} = -1950 \text{ mV}$). An oxidation event at $E_{\text{peak}(\text{anodic})} = -1030 \text{ mV}$ is observed as well. This oxidation event is not observed in the range of -1500 to 80 mV and must therefore be linked to the previous reduction event. Altogether, this indicates an ECE mechanism. Overall, the observed cathodic reduction events are in the range of those published for a variety of carborane-containing compounds and can thus be assigned to reductions of the carborane cluster in **1** and **2**. This is further underpinned by DFT calculations (*vide infra*).

When the cyclic voltammetry experiments are carried out over a wide range (**1**: -2250 to 800 mV, starting potential: -650 mV, going to lower potentials first; **2**: -2250 to 1250 mV, starting potential: -650 mV, going to lower potentials first) the voltammograms exhibit more redox events than the sum of redox events observed in the respective two previously discussed ranges for each complex (Figure S5). This indicates subsequent reactions/decompositions of the species formed within each potential range.

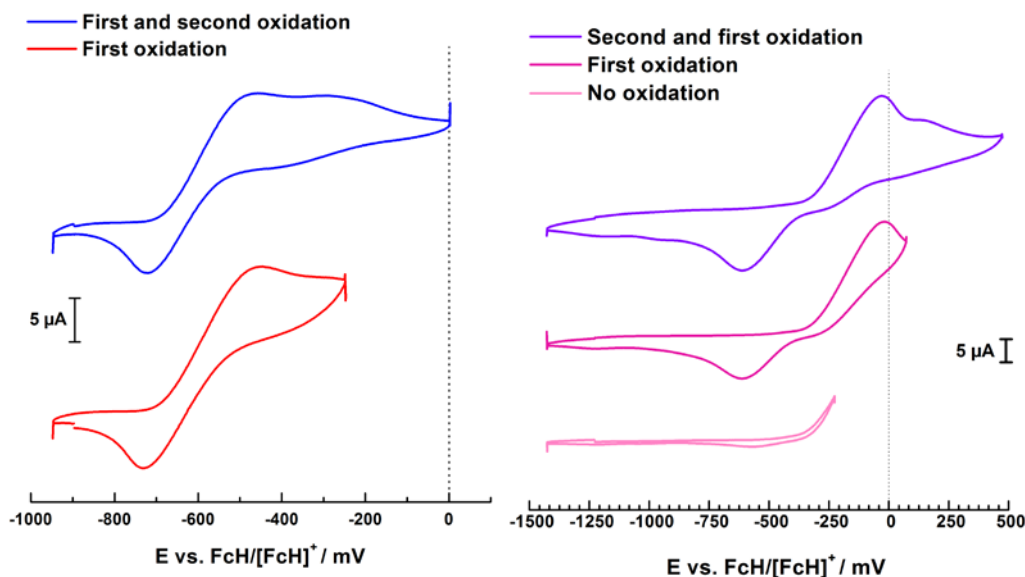


Figure S3. Cyclic voltammograms of **1** (left) and **2** (right) showcasing the oxidation events of both complexes.

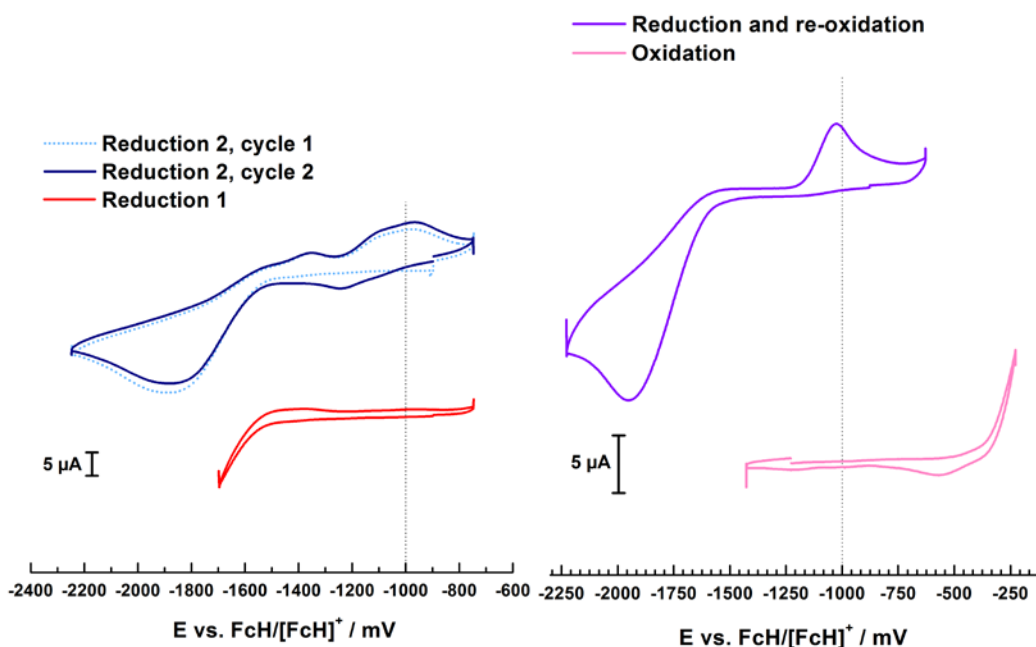


Figure S4. Cyclic voltammograms of **1** (left) and **2** (right) showcasing the reduction event of both complexes.

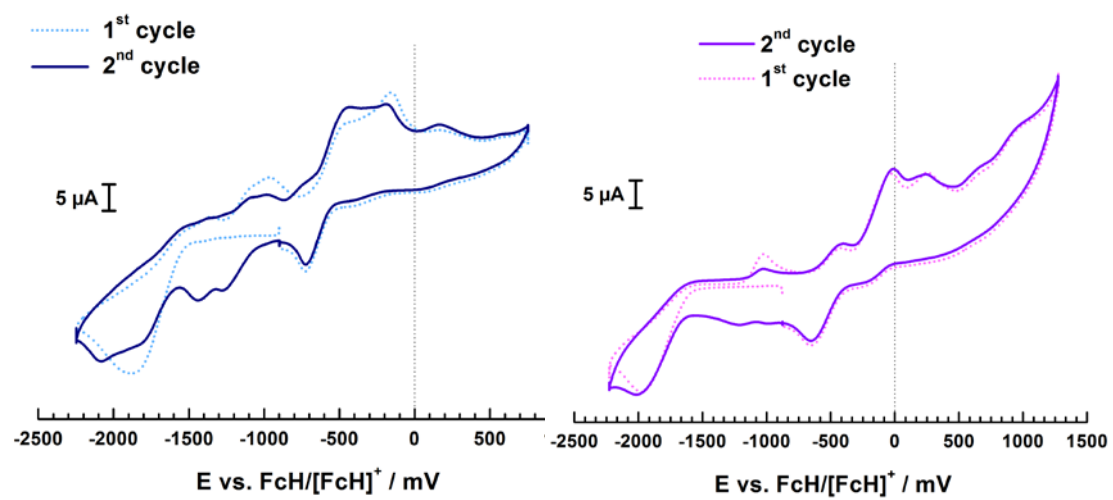


Figure S5. Cyclic voltammograms of **1** (left) and **2** (right) from -2300 mV to 1200 mV vs. FcH/[FcH]⁺.

5. Catalytic activity of **1** and **2** in the Dehydrocoupling of Dimethylamine-Borane

Dehydrocoupling reactions of dimethylamine-borane were carried out as follows: The respective rhodium complex (**1**: 5.1 mg, 2 mol%; **2**: 5.4 mg, 2 mol%, $[\{\text{RhCl}(\text{cod})\}_2]$: 1.9 mg, 1 mol%)^a was dissolved in 2 mL of toluene- d_8 and dimethylamine-borane (0.5 mL of a 0.75 M solution in toluene- d_8 , 0.38 mmol) was added. The mixtures were stirred at 800 rpm at room temperature and ambient pressure and monitored by $^{11}\text{B}\{^1\text{H}\}$ NMR spectroscopy. To determine yields, 1,2,4,5-tetramethylbenzene (50.1 mg, 0.38 mmol) was added to the reaction mixtures before preparing the NMR samples. Hereby, the intensities of the signals of the methyl protons of the cyclic product of the reaction, 1,1,3,3-tetramethyl-1,3,2,4-diazadiboretidine (**N₂B₂**) (2.16 ppm), were compared to the intensities of the methyl protons of 1,2,4,5-tetramethylbenzene (2.01 ppm, Figure S6). When $[\{\text{RhCl}(\text{cod})\}_2]$ is used as the catalyst, the desired tetracyclic product **N₂B₂** is the only species observed in the ^{11}B NMR spectrum after 24 h. In accordance with the literature,^[29] the yield is also quite high (88 %). Using complex **1** as catalyst, full conversion of the starting material is observed after 24 h as well. However, two additional species, besides **N₂B₂**, were detected in the ^{11}B NMR spectrum of the reaction mixture (Figure S7). While the species accounting for the doublet at 29.0 ppm can be identified as dimethylaminoborane, no matching boron compound could be found for the broad singlet at 20.1 ppm. Further investigations by ESI-MS also did not allow to unambiguously identify the respective species. However, the two species at 29.0 and 20.1 ppm are further converted under the given conditions leading to the formation of a colourless precipitate. In addition, the formation of gaseous products could not be excluded. Thus, after 72 h, **N₂B₂** was the only species detectable by ^{11}B NMR spectroscopy; the yield was determined as 35 %. Due to signal overlap with two by-products in the ^1H NMR spectrum, the yield could not be determined after 24 h and 48 h. Using **2** as catalyst, full conversion of the starting material was observed after 24 h. The formation of the two boron species accounting for the signals at 29.0 and 20.1 ppm was observed as well (Figure S8). However, their amount is significantly smaller compared to the reaction where **1** was used as catalyst. Similar to the reaction with **1**, these species are further converted under the given conditions as well. Subsequently, they could only be detected in traces after 48 h, and the yield of **N₂B₂** was determined as 77 %. Altogether, all three rhodium complexes are able to fully convert the starting material within 24 h. Hereby, $[\{\text{RhCl}(\text{cod})\}_2]$ is the most selective catalyst for the formation of **N₂B₂**, followed by **2** and **1**.

^a Only 1 mol% of $[\{\text{RhCl}(\text{cod})\}_2]$ was used to ensure the same substrate/Rh ratio in all reactions.

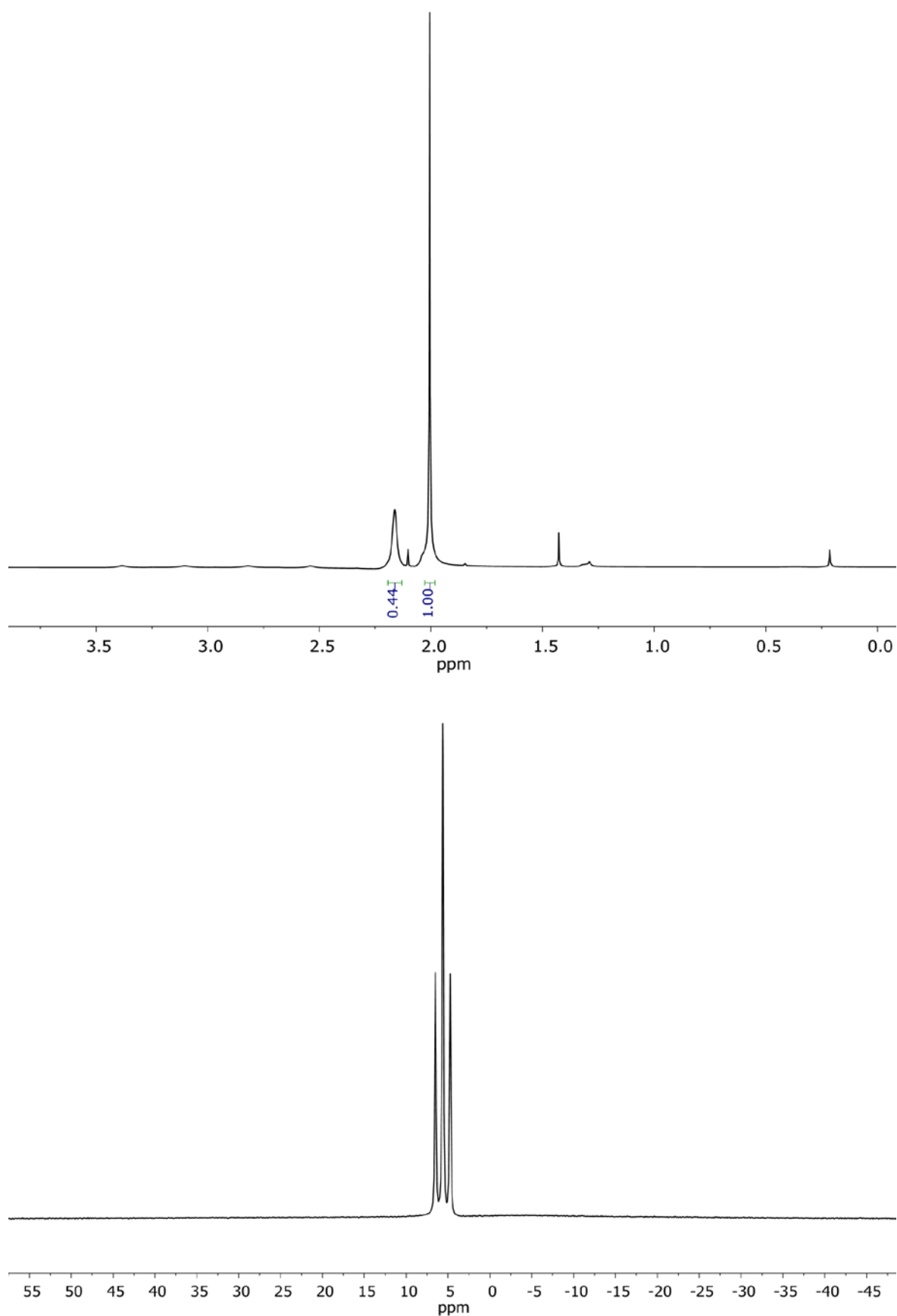


Figure S6: ^1H NMR (top) and ^{11}B NMR (bottom) spectrum of the catalytic dehydrocoupling of dimethylamine borane complex with $[\{\text{RhCl}(\text{cod})\}_2]$ in toluene- d_8 after 24 h at r.t.

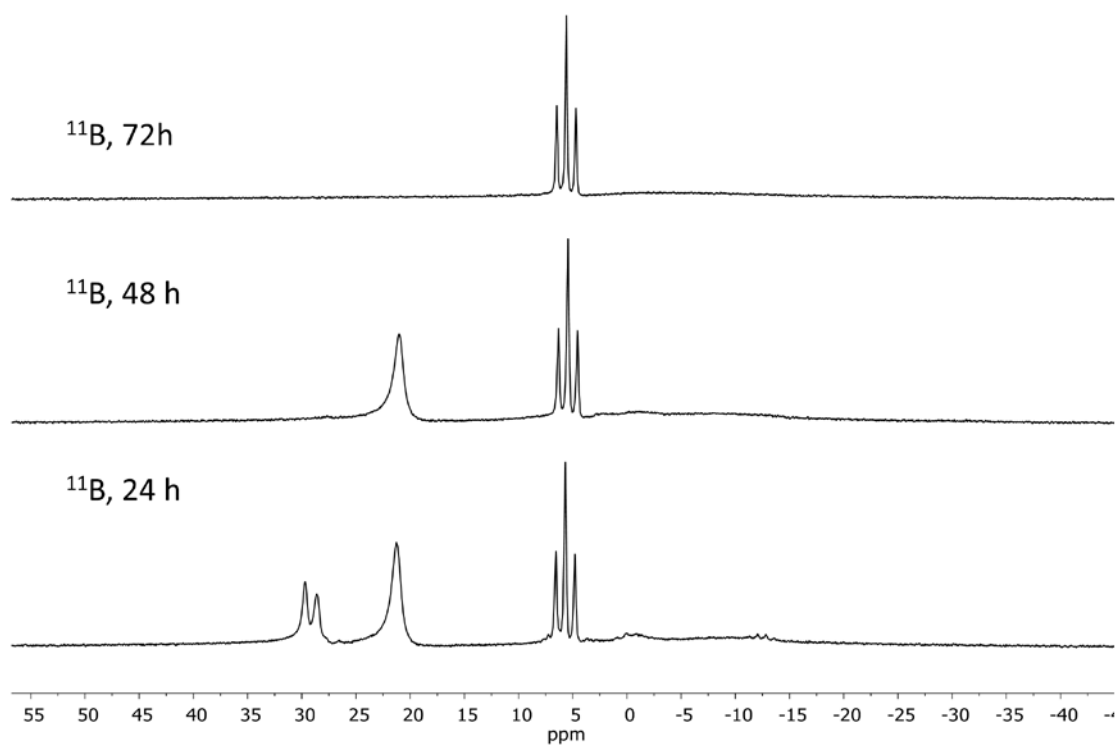


Figure S7: ^{11}B NMR spectra of the catalytic dehydrocoupling of dimethylamine-borane with **1** in toluene- d_8 after 24, 48 and 72 h at r.t.

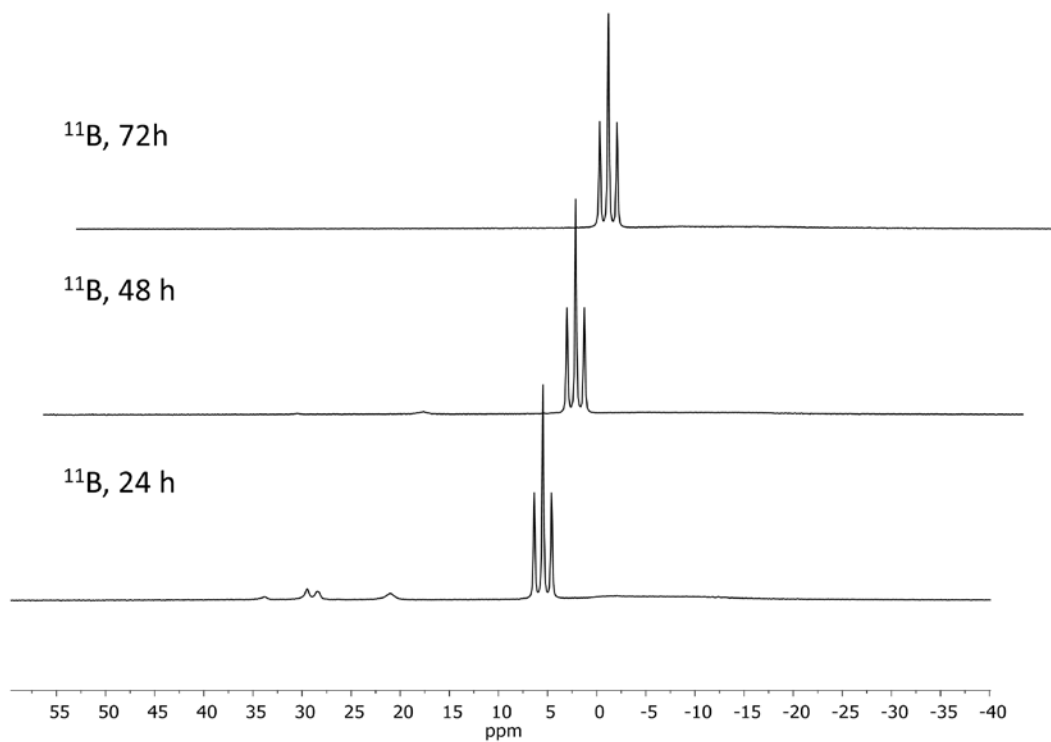


Figure S8: ^{11}B NMR spectra of the catalytic dehydrocoupling of dimethylamine-borane with **2** in toluene- d_8 after 24, 48 and 72 h at r.t. For clarity, the spectra have been plotted with a stacked angle of 10° .

6. Computational Details

6.1. General Methods

All calculations were carried out with the ORCA program package.^[30,31] All calculations were carried out in the gas phase unless stated otherwise. Frequency calculations were carried out to confirm the nature of stationary points found by geometry optimisations. All geometry optimisations were performed at the TPSS-D3BJ/ZORA-def2-TZVP^[32–36] (old-ZORA-TZVP on Rh) level of theory. Density fitting techniques, also called resolution-of-identity approximation (RI),^[37] were used for *meta*-GGA calculations, whereas the RIJCOSX^[38] approximation was used for all other calculations. Relaxed surface scans were carried out to find approximate minima and transition states for the investigation of the dynamic behaviour of **1** and **2**. Subsequent geometry optimisations were performed to locate the minima and transition states.

6.2. Dynamic Behaviour of **1** and **2**

Figure S10 shows the located minima and transition states for the dynamic coordination of the ligand in **1**. Energies were obtained at the M06-D3(0)/ZORA-def2-TZVP^[33–36,39,40] (old-ZORA-TZVP on Rh) level of theory in the gas phase. In the case of complex **2**, the conformation of the C₂SPRhN chelate ring needs to change (**2** to **2-RC** via **TS0**) in order to undergo an isomerisation mechanism similar to **1**. However, the formation of the five-coordinate complex (**TS1-2**) is still the rate-determining step of the whole isomerisation process like in the case of **1** (Figure S11).

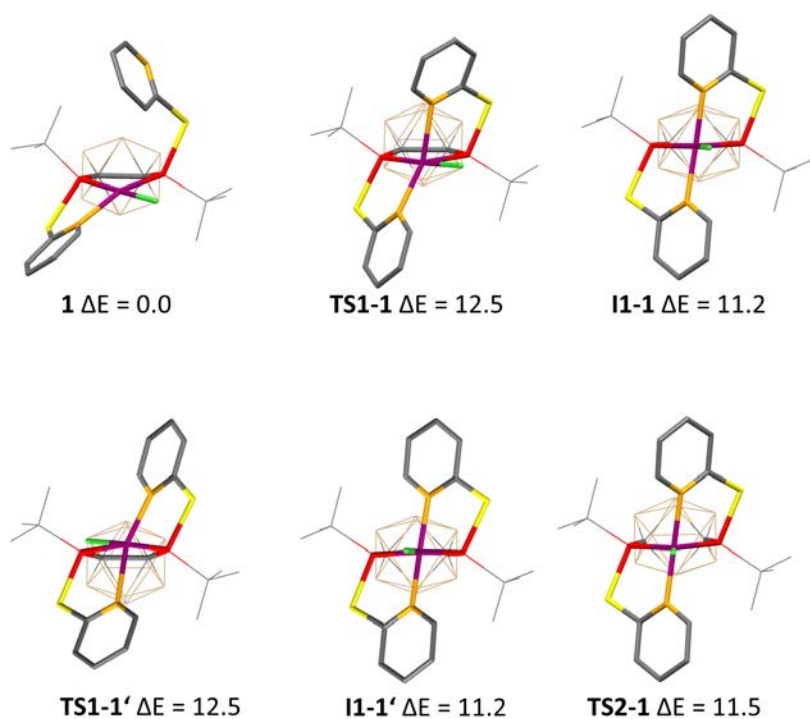


Figure S10. Located minima and transition states of the dynamic coordination in **1**. Energy differences are given in kcal·mol⁻¹.

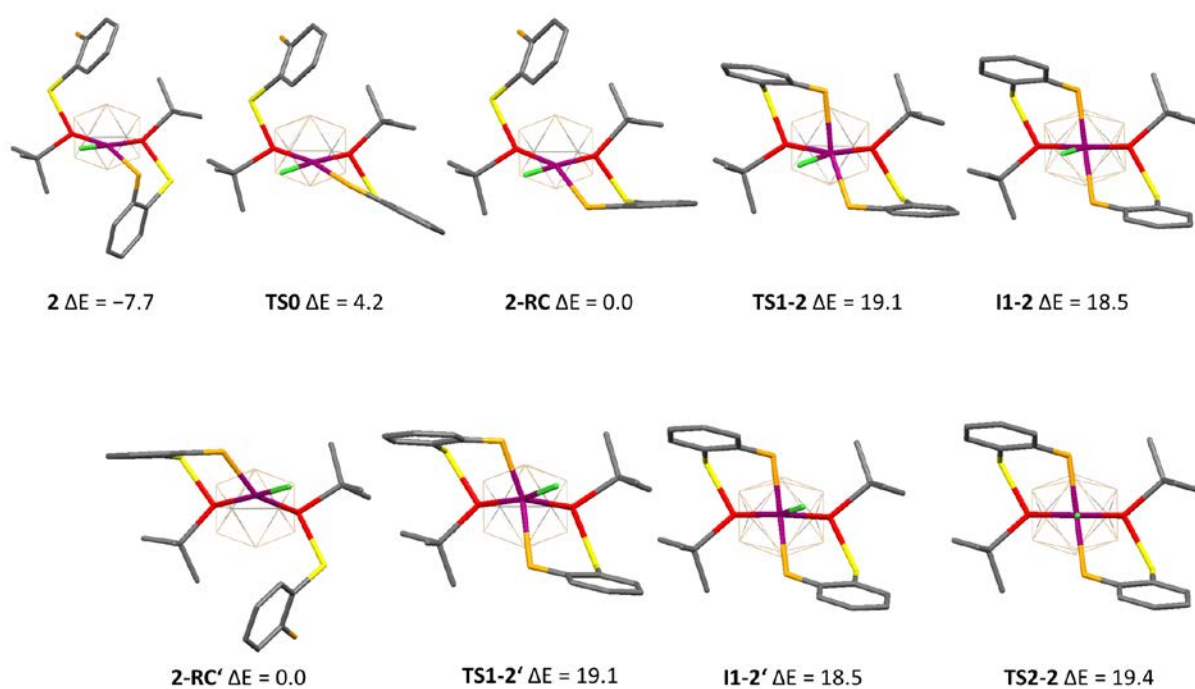


Figure S11. Located minima and transition states of the dynamic coordination in **2**. Energy differences are given in kcal·mol⁻¹.

6.3. Energy Decomposition Analyses of **1** and **2**

Table S3 summarises the results of the energy decomposition analyses on complexes **1** and **2** and selected key intermediates of their respective isomerisation processes at the M06-D3(0)/ZORA-def2-TZVP (old-ZORA-TZVP on Rh) level of theory in the gas phase. The interaction energy of the ligand with the RhCl fragment is slightly higher in **1** compared to **2** indicating a slightly stronger metal-ligand interaction. **2-RC** exhibits a slightly lower interaction energy of the ligand with Rh when compared to **2** as indicated by their different coordination energies. However, the main contribution to their energy difference (7.7 kcal·mol⁻¹) is the higher preparation energy in **2-RC**, indicating that steric reasons play a major role. Comparing **TS1-1** and **TS1-2** to their respective ground states (**1** and **2-RC**), a similar decrease in coordination energy can be observed (15.7 kcal·mol⁻¹ for **TS1-1** and 15.6 kcal·mol⁻¹ for **TS2-2**). Furthermore, the preparation energy in **TS1-1** is reduced by 4.2 kcal·mol⁻¹ when compared to **1**, indicating that the ligand adopts a more relaxed conformation in **TS1-1**. In contrast, the preparation energy in **TS1-2** is increased by 2.4 kcal·mol⁻¹ when compared to **2-RC**, indicating that the ligand adopts a less favoured conformation in **TS1-1**. These different preparation energy changes are the major contributions for the energy difference of the transition states **TS1-1** and **TS1-2** relative to their respective ground states (12.5 kcal·mol⁻¹ for **TS1-1** and 19.1 kcal·mol⁻¹ for **TS1-2**). Thus, steric factors are the main reasons for the slower isomerisation of **2** compared to **1**.

Table S3: Summary of energy decomposition analyses on **1**, **2**, **2-RC**, **TS1-1** and **TS1-2**. Energies are given in kcal·mol⁻¹. [a]: energy difference between the ligand fragment and the free ligand. [b]: Energy difference of the RhCl fragments in each complex relative to the one in **1**. [c]: Energy difference between the complex, and the sum of the energies of the ligand fragment and the RhCl fragment. [d]: Energy difference between the complex, and the sum of the energies of the free ligand and the RhCl fragment.

	$E_{\text{prep}}^{[a]}$	$\Delta E_{\text{RhCl}}^{[b]}$	$E_{\text{coordination}}^{[c]}$	$E_{\text{complexation}}^{[c]}$
1	+13.0	0.0	-149.0	-136.0
2	+13.5	+0.3	-146.8	-133.3
2-RC	+18.7	0.0	-144.0	-125.3
TS1-1	+8.8	+1.0	-133.3	-124.5
TS1-2	+21.1	+1.1	-128.4	-107.3

6.4. *Ab initio* Calculations on **1** and **2**

CASSCF-NEVPT2 calculations with the ZORA-def2-TZVP basis (old-ZORA-TZVP on Rh) were carried out on **1** and **2**. Hereby, the active space was chosen to consist of only the 4d orbitals on Rh, resulting in an active space of eight electrons in five orbitals. Furthermore, all possible roots (15 singlets and 10 triplets) were calculated for the active space. The resulting energies for the d-d transitions were corrected for spin-orbit coupling effects. Selected transitions are given for both complexes in Table S4. The calculated values deviate from the experimental absorption spectra of **1** and **2** (e.g. observed λ_{max} for **2**: 471 nm). These deviations from the

experimental values might be explained by the lack of solvent effects, basis set incompleteness and the treatment of dynamic correlation by perturbative methods. The choice of the active space allowed us to calculate ligand field theory parameters utilising the AILFT (*ab initio* ligand field theory)^[41,42] module of ORCA. Hereby the d-orbital splittings (given in the main text) and the calculated Racah parameters B (**1**: 647 cm⁻¹, **2**: 659 cm⁻¹) and C (**1**: 2056 cm⁻¹, **2**: 2030 cm⁻¹) are very similar. However, the slightly smaller value of B indicates higher covalency within the metal-ligand bonds in **1**, thus corroborating the assumption of stronger metal-ligand interactions.

Table S4: First ten energetically lowest calculated d–d transitions for **1** and **2**.

d–d transition	1		2	
	λ [nm]	$f_{\text{osc.}} \cdot 10^3$	λ [nm]	$f_{\text{osc.}} \cdot 10^3$
1	544.7	0.0004	557.6	0.0004
2	543.2	0.0082	556.1	0.0029
3	542.2	0.0091	555.5	0.0087
4	437.8	0.5840	431.2	1.9845
5	433.8	0.0180	425.8	0.0113
6	428.7	0.0136	420.6	0.2388
7	416.4	3.3021	417.1	3.4210
8	404.5	0.0530	400.8	0.0581
9	398.2	0.0093	394.2	0.0057
10	382.5	5.0615	383.8	3.6593

6.5. TDDFT Calculations on **1** and **2**

To get further insight into the absorption spectra of both **1** and **2**, TDDFT (time-dependent density functional theory) calculations were carried out at the ω B97X-D3/ZORA-def2-TZVP^[35,36,43] (old-ZORA-TZVP on Rh) level of theory in the gas phase. As commonly observed for range-separated hybrid functionals, the calculated spectra are blue-shifted compared to the experimental ones. However, the overall shapes of the theoretical spectra are in very good agreement with the experiment (Figure S11). This allowed identifying the nature of the transitions by analysing the respective difference densities (Figure S12 and Figure S13). As

already discussed in the main text, the spectrum of **1** is dominated by d- π^* transitions, while the spectrum of **2** is dominated by d- σ^* transitions (Table S5). Notably, only 4 d-d transitions are obtained for both complexes, while the CASSCF calculations yielded the correct number of 44 possible transitions. This can be explained by the exclusion of triplets and therefore spin-flip transitions in the calculations as well as the conceptual limitations of TDDFT which is not able to treat double-excitations and spin-orbit coupling effects. However, since the agreement between the experimental and theoretical spectra predicted by TDDFT is rather good for both complexes, we assume that these effects have a rather small impact on the overall spectra.

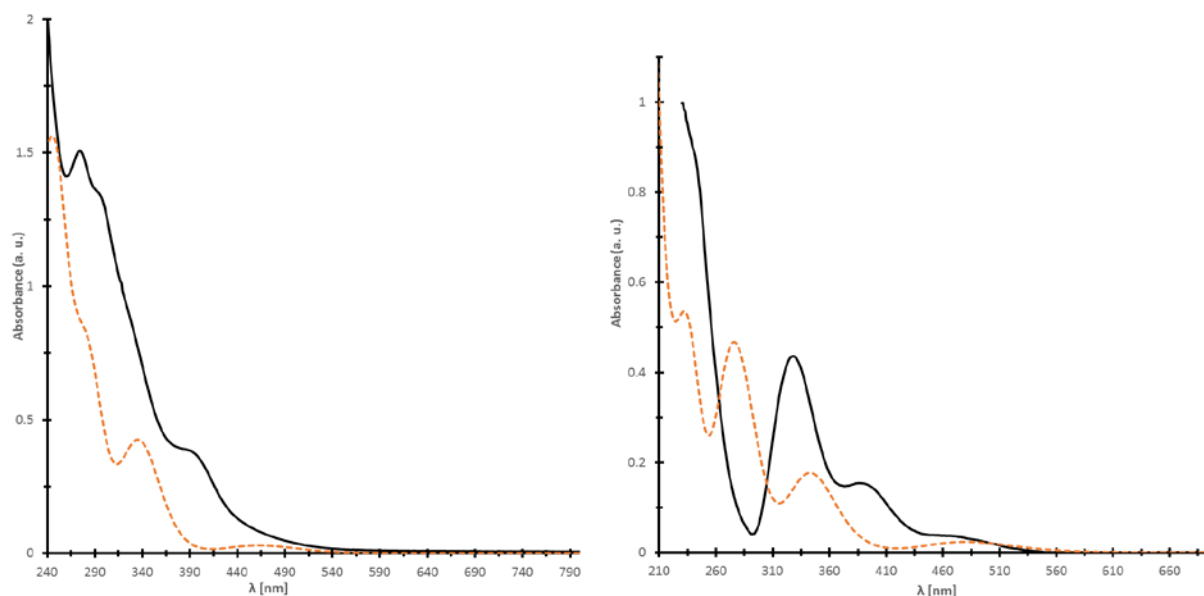


Figure S11: Comparison of experimental (black) and calculated (dotted, orange) absorption spectra of **1** (left) and **2** (right). Calculated spectra were plotted with a full width at half maximum of 4500 cm^{-1} .

Table S5: Comparison of calculated transitions in **1** and **2**. d- π^* : transitions from d orbitals on Rh to antibonding orbitals of the aromatic systems. d- σ^* : transitions from d orbitals on Rh to P-C and P-S antibonding orbitals.

state	1			2		
	λ [nm]	$f_{\text{osc.}}$	character	λ [nm]	$f_{\text{osc.}}$	character
1	462.5	0.0053	d-d	479.7	0.0096	d-d
2	375.6	0.0012	d-d	382.5	0.0007	d-d
3	363.6	0.0009	d-d	376.5	0.0031	d-d
4	339.1	0.0629	MLCT (d- π^*)	343.4	0.0677	MLCT (d- σ^*)
5	323.7	0.0089	d-d	321.8	0.0058	d-d
6	322.0	0.0094	MLCT (d- π^* , d- σ^*)	287.8	0.0783	MLCT (d- σ^*)

7	293.5	0.0199	MLCT (d- π^*)	280.6	0.0093	MLCT (d- π^* , d- σ^*)
8	283.4	0.0961	MLCT (d- π^*)	275.0	0.0319	MLCT (d- σ^*)
9	274.1	0.0068	MLCT (d- π^* , d- σ^*)	269.9	0.1059	n- π^* , π - π^*
10	270.8	0.0053	MLCT (d- π^* , d- σ^*)	254.7	0.0063	MLCT (d- π^*)
11	266.6	0.0361	MLCT (d- π^*)	249.6	0.0065	MLCT (d- σ^*)
12	261.6	0.0114	MLCT (d- σ^*)	244.6	0.0020	MLCT (d,S- σ^*)
13	259.9	0.0146	MLCT (d- π^*)	242.8	0.0226	MLCT (d,S- σ^*)
14	253.9	0.0484	MLCT (d,S- π^*)	239.1	0.0236	MLCT (d- σ^*)
15	247.8	0.1291	MLCT (d,S- π^*)	235.0	0.0908	MLCT (d,S- σ^*)

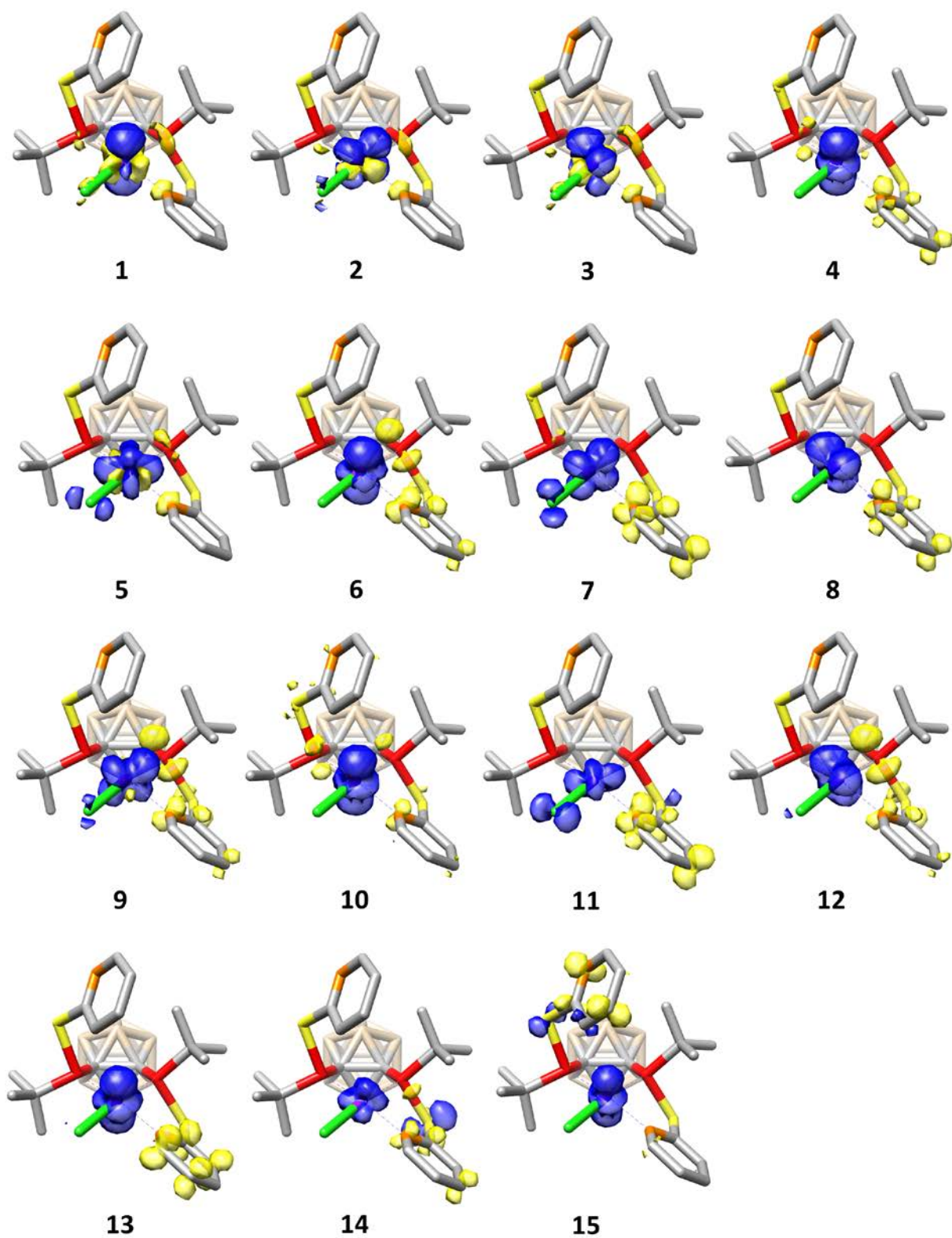


Figure S12: Difference densities of the first 15 excited states of **1**. Surface isovalue: 0.05. Transitions proceed from blue to yellow.

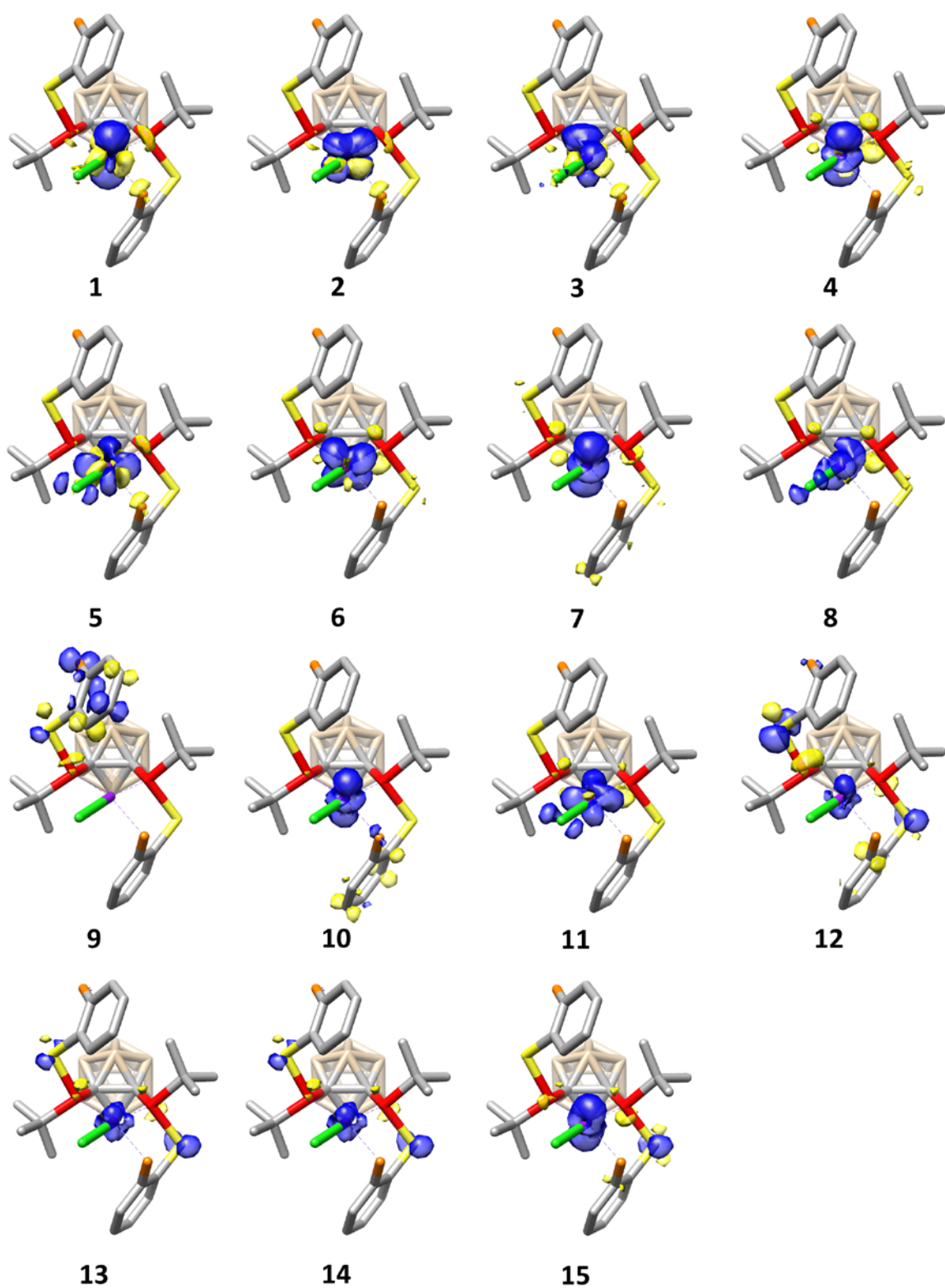


Figure S13: Difference densities of the first 15 excited states of **2**. Surface isovalue: 0.05, except for 12 (0.03). Transitions proceed from blue to yellow.

6.6. Calculation of Redox Potentials of **1** and **2** in Solution

The one-electron redox potentials of **1** and **2** were calculated employing a commonly used procedure.^[44–46] Hereby, the geometries of the reduced/oxidised species as well as the neutral complexes were optimised including solvent effects (TPSS-D3BJ/ZORA-def2-TZVP (old-ZORA-TZVP on Rh) CPCM(THF), see the main text for a graphical representation) and final single point energies were calculated at the M06-D3(0)/ ZORA-def2-TZVP (old-ZORA-TZVP on Rh) CPCM(THF) level of theory. Subsequently, the calculated energy differences were referenced to the FcH/[FcH]⁺ couple which was calculated at the same level of theory (Table S6). Hereby, the deviations of the calculated potentials from the measured peak potentials are in the range typically reported in the literature for this procedure. It is noteworthy, that these good agreements could only be achieved when the ligands in **1**[−], **1**⁺ and **2**⁺ act as tetradentate ligands.

Table S6: Calculated redox potentials of ferrocene, **1** and **2**.

	FcH/[FcH] ⁺	1/1 ⁺	1/1 [−]	2/2 ⁺	2/2 [−]
E _{ox.} − E _{red.} [kcal·mol ^{−1}]	118.9	100.3	69.1	115.4	70.7
Potential vs. FcH/[FcH] ⁺ [eV]	0.00	−0.80	−2.14	−0.15	−2.07

7. Cartesian Coordinates of Calculated Molecular Structures

Cartesian coordinates of **1** (TPSS-D3BJ/ZORA-def2-TZVP (old-ZORA-TZVP on Rh))

C	-0.21088929994568	1.77686912323714	13.96447746461900
H	0.86183242296942	1.88650910692307	13.84609877708232
C	-0.80170602810878	1.56280854724715	15.19847560899447
H	-0.17581956513244	1.47331346688625	16.07952385253355
C	-1.11361428821280	-0.92343166100979	11.08959093874316
H	-1.08827052397069	-2.01579191117698	10.99968533926034
H	-1.68427383843698	-0.67110091491400	11.98808146927252
H	-0.08961150247824	-0.55508459662292	11.20657489223199
C	2.44384916061129	-0.91096282968154	7.35092008902639
H	2.41144811257379	-1.60170585197539	6.51107861667251
C	2.38608722002360	5.41480017874816	9.79691739380412
H	3.09753456286220	4.85051424251652	9.18792811272482
H	2.40297822536085	5.02156472859499	10.81272244928458
H	2.70510522234427	6.46443401238046	9.81391438813389
C	2.83307355460519	-0.41168235787425	9.66027283737271
H	3.11779744228669	-0.70283692731475	10.66741099228677
C	0.97397062061163	5.38181984771024	9.18362769220693
C	-2.93074517620395	1.57242514147955	14.10567135848013
H	-4.01115752434752	1.47923089137522	14.11083836362952
C	-2.19166774702858	1.47209125678503	15.27484542249131
H	-2.69204276482164	1.31146905220027	16.22500808386060
C	2.53001287000394	0.91882482847823	9.38584476074734
H	2.59219034621916	1.68136158485590	10.15504592961252
C	-2.27030363264106	1.78445624485636	12.88883643893177
C	-2.29703142848999	2.38888690465023	8.53819118539412
C	-0.92100693849538	-0.75885625139558	8.60271192459498
H	-1.39884875750742	-0.49235492955526	7.65937048612888
H	-0.79126515022375	-1.84734507100311	8.62513978494373
H	0.06863730471058	-0.29968830619573	8.64027203264985
C	2.15982909535886	1.24067749002903	8.07457987404179
C	-1.76833784796126	-0.35142395023935	9.81596678777320
C	-3.20220451950914	-0.88375784709875	9.69408743884590
H	-3.73764160476610	-0.44633758192588	8.84968438138600
H	-3.77396408764906	-0.69509947679959	10.60591119361415
H	-3.15150748105412	-1.96827756214957	9.53729750732893

C	1.07484688379887	6.04741626049312	7.79929137772025
H	1.85401006155151	5.57004199862321	7.19712918266632
H	1.37243447874103	7.09151589036672	7.95606107113731
H	0.14598637412606	6.04346904671691	7.23418796044988
C	-1.22400716047446	3.61275864660200	8.07028011810229
C	0.00490302974792	6.11562816326018	10.12621010087211
H	0.37073323379650	7.13910603635772	10.27195603337596
H	-0.02707626364026	5.61674522548277	11.09982063352535
H	-1.00914572763491	6.17191172608844	9.72725627851652
C	2.78891360801675	-1.34873406730626	8.62750618769395
H	3.02724964399314	-2.39340285470902	8.80276527261695
B	-4.09833224688938	3.09818695708259	6.58331819543105
H	-5.13998350629298	2.89310878309977	6.05760420256227
B	-3.91116054394026	2.85995598665215	8.32876473507904
H	-4.69770497913946	2.45298030671256	9.11343531800943
B	-2.67436297652091	4.01483660603501	8.91094360944070
H	-2.57955503218277	4.35353418335402	10.03494004225115
B	-2.13290622795865	4.95801100063275	7.51983317821507
H	-1.73849491365600	6.04720860079362	7.72518358313076
B	-3.83248524081037	4.49491753425664	7.66248951839111
H	-4.66121787975247	5.30274617987094	7.91362809932015
B	-2.99536331097089	4.39229230759301	6.08517880814232
H	-3.23092891466054	5.13693691922781	5.19444224866864
B	-1.40659227875363	2.22261304453169	7.08120864903125
H	-0.51444941381625	1.46051959912227	7.03980067866140
B	-2.53903424354322	2.69232763547254	5.80788028793384
H	-2.45216333341057	2.20067477475837	4.73444565770701
B	-1.33085281262037	3.85544100105579	6.39084314507205
H	-0.33967045409722	4.15843408273214	5.82634305512491
B	-3.11865026970194	1.75728168756494	7.19104993919280
H	-3.37211581169058	0.60583434791369	7.17675359217284
P	0.42267395363032	3.57348902819176	9.08481167034203
P	-1.66871417861227	1.51541237735563	10.05256277703590
N	2.11736887181614	0.36093169799035	7.06985772313018
N	-0.91749544618908	1.91191410579320	12.81713946678547
S	-3.27898744084562	1.87425979993808	11.44667331879726
S	1.80192967672226	2.92448533904033	7.58532704428160
Cl	1.97803825223780	3.11334005724426	12.16711315010186

Rh	0.03937708606992	2.44709836198691	10.95232922060618
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Cartesian coordinates of **TS1-1** (TPSS-D3BJ/ZORA-def2-TZVP (old-ZORA-TZVP on Rh))

Rh	3.44892587311032	11.35987972030698	0.11620823568438
S	2.02175364739935	12.85899534583315	-2.67375684910202
S	1.77603165849196	9.67220765788836	2.79690442117390
P	1.98351935362794	11.11251629240541	-1.46402098146450
P	1.79900190669700	11.48933425289342	1.68913135989291
Cl	5.31447700224874	11.46904234112130	1.63912232152889
N	3.59244154862838	9.20467717123591	0.78918115251312
N	4.17194135087973	13.00438086229025	-0.99804007919397
C	0.09363884052068	11.38010943701772	0.85528094723042
C	0.20280844337596	11.11595749273194	-0.84684497287562
C	3.06980963334029	8.79091423975942	1.95728346648451
C	4.60554633634397	8.48298579289119	0.25581384768180
H	5.00977077341516	8.86441875848265	-0.67288918918021
C	3.80950376618533	14.85062063916495	-2.53752093006706
H	3.18027910991265	15.28145320475468	-3.30944032020053
C	1.89887878341547	8.38330114800341	-2.16122575976910
H	0.84553375802288	8.21912261727383	-1.93221344659612
H	2.47900337750841	8.24224799210602	-1.24751299872042
H	2.21154377599282	7.62356004265968	-2.88764257672804
C	3.45492963970278	13.61615403436813	-1.98824766571121
C	4.95719955747222	15.49641840627076	-2.09934919261553
H	5.24686426412405	16.45468419604425	-2.51796720404691
C	1.41921222724793	14.11882623761037	2.47642604982352
H	2.19051769580274	14.30810390664493	1.72219972668812
H	1.51933356678260	14.87447235308208	3.26488657841545
H	0.43934928388276	14.24015119012312	2.01323553147479
C	4.54276302655897	6.88987836160416	2.03408172645516
H	4.90735542942849	5.99303414536043	2.52562889069832
C	3.51202825521431	7.62409569370078	2.59718985161064
H	3.05111829225411	7.32652691597679	3.53353953160924
C	2.14675639818191	9.76962331223043	-2.77728869456714
C	1.61283906982454	12.72892040093993	3.10888601519511
C	1.25497565847447	10.00419491541189	-4.00619518854531
H	1.50039494623713	10.95214462686943	-4.49350437469270
H	0.19182389746829	9.99645615114754	-3.76572305837957
H	1.44671309749937	9.19830296464655	-4.72542271543790

C	0.52579315288620	12.38879210190177	4.13720192065385
H	-0.47031723658203	12.30978742011216	3.70283560073500
H	0.50400769432855	13.18104779129930	4.89711244640205
H	0.76123133834734	11.44865948454649	4.64594761002533
C	5.11115051406899	7.33463883787676	0.83798338318283
H	5.92751193743005	6.80271039870868	0.36181632338160
C	5.30850212598247	13.65112122999242	-0.60103179860339
H	5.86543947022056	13.13792852161558	0.17399867606174
C	3.62129039986525	9.88180418367036	-3.21734146019263
H	3.82940820144852	9.08532867449852	-3.94157209337203
H	4.30250304873687	9.78226568840564	-2.36825964943826
H	3.81825017804977	10.84586807848024	-3.69528514194028
C	2.98101353000867	12.70991678705469	3.81622717998833
H	3.79518120089156	12.970644446784341	3.13703927131200
H	3.20019988097542	11.72637846483962	4.24071943112003
H	2.94434980884801	13.44104824345012	4.63355511736713
C	5.72118693316684	14.86514135125764	-1.11508882344291
H	6.63917133393584	15.30477745609443	-0.73930610577578
B	-2.06730266210269	12.61369857494826	-0.38487817152526
H	-2.65779746093295	13.62099653590874	-0.58337179906056
B	-1.29971675049806	12.30688788483546	1.17482965611536
H	-1.27518595015806	13.08606217840606	2.05611293484159
B	-0.29968630824552	12.63583166636118	-0.25096135254100
H	0.44710212375170	13.54164260034656	-0.34332629135322
B	-2.54673027579270	11.03440541828872	-1.06179812551276
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B	-2.02215098215481	9.76081970510944	0.08338645595758
H	-2.57823398175167	8.72177010155451	0.20190941679122
B	-0.25324514169697	9.83689221168698	0.19263771618040
H	0.51948063816551	8.96764711534776	0.37387411469847
B	-2.67001457911779	11.30808372735841	0.68141899561860
H	-3.70425372846266	11.38577140294879	1.25432324513000
B	-1.08983450400195	11.85818758600807	-1.65188720768325
H	-0.86875281149134	12.30279520486574	-2.72546698135400
B	-1.26183157397490	10.56282201456344	1.46782066098044
H	-1.17520243793622	10.12222930052814	2.56062978166981
B	-1.07141509128513	10.11459556058805	-1.35962485896662
H	-0.87366820825043	9.34400897399795	-2.22731032389325

Cartesian coordinates of **11-1** (TPSS-D3BJ/ZORA-def2-TZVP (old-ZORA-TZVP on Rh))

Rh	3.53220547278936	11.20254369886794	0.09082007219382
S	2.26738761401914	12.54223604984854	-2.86484570831255
S	1.91062893417775	9.77641442871544	2.85669336479768
P	2.01524674663826	10.86964003417723	-1.57721231998096
P	1.84683043086840	11.52689227820423	1.66069893253848
Cl	5.84583203604651	11.28669674925399	0.75207227548374
N	3.65591934182216	9.26964139940833	0.82246779172018
N	3.75413761803885	13.12654957232793	-0.66107904709856
C	0.18316895492333	11.47579778426831	1.08201411626251
C	0.29123628918385	11.00243531526535	-1.15570075817989
C	3.01260473198419	8.79237773014136	1.91614858245412
C	4.57182860985153	8.46791491725903	0.22038591173725
H	5.10998858267838	8.92599274195127	-0.59698408335854
C	3.39583794402141	14.89982245617996	-2.26126336604350
H	2.92202007800865	15.21354180908842	-3.18481968313120
C	1.87169280958344	8.14234473717954	-2.11048834707180
H	0.82586265329966	8.10609544666543	-1.80210114124254
H	2.50028123794495	7.97897168100930	-1.23240567860544
H	2.05044820298294	7.32080772178685	-2.81483325952066
C	3.21240085061127	13.57930332137710	-1.82445483468686
C	4.17218377133567	15.77004302267606	-1.51698472843800
H	4.32442862180429	16.79167114038709	-1.85062481790088
C	1.79087197600243	14.23031036558707	2.25580344764997
H	2.50251223268147	14.37697547478303	1.44063190362538
H	1.94655535070765	15.02898632916983	2.99124402292180
H	0.77971617522120	14.32539215943673	1.85650225574463
C	4.11780753109466	6.65814645249699	1.71343991804011
H	4.28023830078134	5.64103698431055	2.05607812297170
C	3.21419904524050	7.47716971706416	2.36552715355669
H	2.65772464245340	7.13001058178176	3.22914498273233
C	2.21382819542420	9.46533056116790	-2.81603896750906
C	2.00193022647016	12.87904261133407	2.95861552496318
C	1.30500583605208	9.67978588521683	-4.03602053184170
H	1.57453822297659	10.59320994058779	-4.57641929846028
H	0.25089654340230	9.73212677700014	-3.75910632598746
H	1.43885249727841	8.83648970568610	-4.72534689858047
C	0.97307761666315	12.68699382257058	4.08124755941036

H	-0.05118777282989	12.71757736178662	3.70428919471658
H	1.09570163177619	13.49393310738932	4.81524878520643
H	1.12951478412718	11.73750913657001	4.60365767451143
C	4.82463673945493	7.17165482254256	0.62302663947470
H	5.56493122842408	6.58446180862688	0.09216144881347
C	4.51552237534097	13.99778371533365	0.05523862888891
H	4.95676901468818	13.58288170410770	0.95005971574869
C	3.68254623480478	9.46435834173314	-3.26942511655137
H	3.84527185598626	8.61379796151640	-3.94224479499827
H	4.36602704945390	9.37587347450603	-2.42203807295028
H	3.93053640445556	10.38360087140660	-3.80721462246005
C	3.42626478130653	12.78104975377794	3.52748281397058
H	4.18571614236872	12.78949598408897	2.74076336722255
H	3.55708123911615	11.85805618681797	4.09957180966127
H	3.59864645413185	13.63105782570982	4.19841990912704
C	4.74882646062209	15.30206417874301	-0.33419501894662
H	5.37058660898722	15.93492526717720	0.28875448614735
B	-1.81649503042838	12.68993149731550	-0.47757222735480
H	-2.33360221937820	13.72955946003313	-0.71881140946339
B	-1.11925732665790	12.45977348335229	1.13107132484778
H	-1.11966169755081	13.34771110373815	1.91455042118674
B	-0.03320459781455	12.47497682998154	-0.34709902764959
H	0.73817910124387	13.36387604881756	-0.48950000737180
B	-2.44616955397460	11.11840732718134	-1.06558183407511
H	-3.42763122839161	11.00767352055466	-1.72279539651367
B	-1.92519357512132	9.89384445925825	0.13824287138126
H	-2.51691127772392	8.88233733954885	0.32033654039343
B	-0.12561113390079	10.01890886038036	0.20477316489677
H	0.57409525742817	9.08909099862435	0.42722464002103
B	-2.53058247276782	11.49561363769117	0.65327626987320
H	-3.56925859855561	11.65993077472212	1.20265761156166
B	-0.98261593604486	11.82857459132593	-1.77876793120485
H	-0.85488027578812	12.28889320393184	-2.86334046595228
B	-1.19407656120195	10.70811962609719	1.52382379168406
H	-1.22042969145324	10.24345143725404	2.61399663088836
B	-1.04415878209712	10.08487177107962	-1.38368574687423
H	-0.99469155709942	9.19082112304605	-2.15785221071057

Cartesian coordinates of **TS2-1** (TPSS-D3BJ/ZORA-def2-TZVP (old-ZORA-TZVP on Rh))

Rh	3.53041916412395	11.20764506671153	0.14769921661291
S	2.26053613639407	12.59685151277414	-2.79741163726913
S	1.90061513257575	9.82991860353077	2.91600464134954
P	2.02499191963526	10.88499317486691	-1.56322290639284
P	1.83026455579605	11.54304574515079	1.66329307704217
Cl	5.93043165395068	11.19860444664302	0.29948956836095
N	3.64402407984384	9.27852622900355	0.89669656949303
N	3.75007564545871	13.13542664284047	-0.58110644586921
C	0.16661096687135	11.45919802112390	1.06469014731609
C	0.30144248558265	10.98190947386748	-1.17127407004356
C	2.98259844771260	8.81600196509318	1.98903792478715
C	4.52041639782605	8.43832499317150	0.28516963186169
H	5.06223007888260	8.87079099486314	-0.54303958093015
C	3.45565064176360	14.91979921961553	-2.17504567696692
H	2.99775014444046	15.25202267766127	-3.10017829941357
C	1.95670754986395	8.16893372207297	-2.13278413746895
H	0.90692424590673	8.10630769964100	-1.84173423855595
H	2.57417894779167	8.01046649690749	-1.24616762884313
H	2.16523036852227	7.35879977234795	-2.84214543008776
C	3.22937898957269	13.60285974350802	-1.74520997534327
C	4.25616581241720	15.76117332390570	-1.42362437669180
H	4.43947751276086	16.77969617576207	-1.75117107960909
C	1.71441561427534	14.25982303672768	2.22092583574730
H	2.43622502497640	14.41267552672502	1.41586968243963
H	1.84166321414736	15.06887443838229	2.95047094636694
H	0.70827733822800	14.33046753108271	1.80454492750110
C	4.02505213617487	6.65003650340966	1.79425785715679
H	4.15986221509706	5.63050057549018	2.14160876754037
C	3.14549980303594	7.49782054499053	2.44309820291377
H	2.57645299705828	7.16971414939800	3.30591274675570
C	2.27876031853355	9.50669477990653	-2.81928569375250
C	1.94015093414283	12.92012803251393	2.94127588744870
C	1.38360336923756	9.71120733930825	-4.04999619951103
H	1.62745008110975	10.64483374955498	-4.56754596966984
H	0.32415244417685	9.71993658932889	-3.78741812526909
H	1.55810734303385	8.88712238177138	-4.75360632868522
C	0.90040942123617	12.72340456635721	4.05391776217885
H	-0.11926622703295	12.72260818329352	3.66438018757156

H	0.99434584064973	13.54661292951043	4.77374364320538
H	1.07228138227170	11.78828183590447	4.59704298423228
C	4.73560579617924	7.13716148495718	0.69478052139193
H	5.44920074202141	6.52390944128313	0.15666660918862
C	4.55173155899523	13.96937488967086	0.13298531442506
H	4.98588593569701	13.53306898524186	1.02048904772258
C	3.75656433161163	9.55547031275715	-3.23992928652250
H	3.96899753426092	8.70039408819857	-3.89272822677485
H	4.42633813195627	9.51577140451523	-2.37708541171630
H	3.97828371394370	10.47421602607487	-3.79016622880939
C	3.35548128738106	12.86013564638697	3.53829505426082
H	4.12539547992222	12.89400470192372	2.76320347883245
H	3.50155068456225	11.94007452893003	4.11115024633065
H	3.49371648528743	13.71397485775233	4.21229257799658
C	4.82448195260077	15.26888649965941	-0.24647367235251
H	5.47187049709653	15.87695022229168	0.37482778986918
B	-1.85024242520752	12.62693701778012	-0.49328147307115
H	-2.38747133655152	13.65466293132837	-0.74151668536890
B	-1.15807858783998	12.41527147414222	1.12041971905664
H	-1.17722518586687	13.30679698012322	1.89935508410867
B	-0.06174431138035	12.44921038841253	-0.35082348003013
H	0.68887500357545	13.35580944830968	-0.49053356390799
B	-2.44063507463352	11.04157017959638	-1.07890433564193
H	-3.41423821603078	10.90748290636835	-1.74351801586132
B	-1.89914958969894	9.83053414289848	0.12851762276238
H	-2.47055291803045	8.80711195498335	0.30897523571309
B	-0.10528596273316	9.99432928553520	0.20513035129247
H	0.61560626534387	9.08198424068818	0.43490113541612
B	-2.54416877851338	11.42068923878338	0.63854794264441
H	-3.59041003767823	11.56262741011371	1.17968296834111
B	-0.98891703936521	11.78420859908677	-1.78654840357069
H	-0.87031549766194	12.24547241524470	-2.87191809170975
B	-1.19529632450493	10.66711361803240	1.51747645510566
H	-1.21350538541388	10.20540780082368	2.60896628346420
B	-1.01392510939542	10.03607615560447	-1.38873615062233
H	-0.94487174797414	9.14433732778358	-2.16459181947176
Cartesian coordinates of 2 (TPSS-D3BJ/ZORA-def2-TZVP (old-ZORA-TZVP on Rh))			
B	7.59466285418682	7.31011317489373	1.67330094279377

H	7.36619916457908	6.20171226390143	1.34196641543494
B	6.65966287839547	8.76636542287115	1.30760623095529
H	5.68573726549161	8.70409675764699	0.63555462582981
C	6.63978860687095	8.31330521843347	7.56421022533982
H	5.71898562640943	8.47680423486714	7.01357017602526
B	6.77302781913048	9.85075511134601	2.72151827300599
H	5.90290383756195	10.57541058551062	3.06971724483910
C	9.33616671628584	8.87865193379007	3.18478452265879
B	6.65606807973302	8.10116982925834	2.94844029658159
H	5.79434432498672	7.52411136545087	3.51202011039375
C	12.67942723052254	6.14971526735027	1.38460116756892
B	7.79505780397700	9.06131764775315	3.93349131139282
H	7.75503271428933	9.10848128145368	5.10953742074391
C	8.68462314651733	7.05192482841487	7.87207314059797
B	8.30202704897780	8.55579135190498	0.63559190982167
H	8.52017880090955	8.34548533620619	-0.50944211917926
B	8.46650641326411	10.32460180462453	2.88995956755344
H	8.81894159114298	11.32698654758235	3.39600247496615
C	8.24948372159211	7.58157591350191	3.22133854386668
B	9.29426921989050	7.78073367573794	1.87746082937215
H	10.20354445372323	7.05111377072763	1.76251032937131
B	9.40819859422509	9.53271744326938	1.61886643624931
H	10.44862736882687	9.96678253385813	1.26642517453504
B	7.77903134146721	10.13806458769190	1.27183107233208
H	7.62786008035273	11.08172601362893	0.57126062700595
C	12.73656196641218	6.70437217262852	2.68505409341032
H	12.31011954371857	7.90965711353341	0.40973323250965
H	12.61348536379264	6.58352681475796	-0.61781102927612
C	9.63944831960483	4.54520009933126	2.63626060548155
H	9.78455601837191	3.48876752903769	2.38153424992078
H	10.61645437711322	4.96997125605012	2.87967014135057
H	9.23824756283342	5.05257954840461	1.75875522349795
C	7.47616663057975	7.26322352889509	7.18142669825958
C	11.31097686144087	10.26118051899057	5.01886833959063
C	9.24167398822320	3.71413793301656	4.95004352918064
H	9.30734691511910	2.69101719504604	4.56238350014309
H	8.57567962082718	3.69641227814197	5.82008911581615
H	10.24442761219083	4.03377616830384	5.25339531617796

C	12.95828697270476	4.77707595827818	1.24167080898914
H	12.91324210397426	4.33419297092718	0.24943713290038
C	13.06237886042134	5.90649725562732	3.78662904928366
H	13.11957774762963	6.36195144767355	4.77002291037163
C	8.68441186773545	4.62298465062490	3.83649707124333
C	9.04668508054017	7.90083706921331	8.91947669068697
H	9.99810765918969	7.74721894901369	9.42007653671983
C	11.59297137580891	11.31888425947378	3.93668627256508
H	12.51238584644760	11.07893639824234	3.39418336815960
H	11.74589210489027	12.28235727930194	4.43843577257772
H	10.78537213184125	11.43759685365173	3.21651079488848
C	13.31073996076733	4.54651397087230	3.62619770791225
H	13.55789659268599	3.93735821525265	4.48964379739503
C	13.26474259702878	3.99064144457534	2.34439532057822
H	13.47113785634342	2.93355641465764	2.20048241847256
C	12.59264270560871	10.09812177416422	5.85567049640969
H	13.42244014927296	9.72069512601115	5.25235995031920
H	12.44628815240024	9.42396199306756	6.69984679516309
H	12.86372344058763	11.09183122600242	6.23374736562627
C	10.16550119736146	10.67189230670732	5.96090468198459
H	9.24534888364378	10.91194439759218	5.42731864567891
H	10.47959940922073	11.56371100552744	6.51667158407431
H	9.95530575607926	9.87287326020623	6.67938941269423
C	6.99717927843312	9.15147844888521	8.61965670174176
H	6.34279510680649	9.96924566156888	8.90411169241207
C	7.27038634629086	4.15906592982228	3.45612247662761
H	6.79544969401088	4.82445353947435	2.73337450926821
H	6.62510195712669	4.07822016957722	4.33602305243113
H	7.34333543629643	3.16285493069558	3.00257930808648
C	8.20473003200321	8.94739427883171	9.28801915949606
H	8.49784644880163	9.60583014515542	10.09995562854258
N	9.56185817412168	6.00303016688258	7.45038434018779
H	9.05877408660570	5.13845077708223	7.24629473256127
H	10.34622465869466	5.85132748770366	8.08959295931336
N	12.29993889067048	6.90375500918614	0.28793220571504
P	10.88419280342128	8.57177116117624	4.28845307217314
P	8.73138752263970	6.36065056332584	4.56441754772020
S	6.98752205938374	6.20494226438061	5.84149286672094

S	12.49483457272091	8.45725908710041	2.87745650297344
Cl	12.33651571764219	7.02080718179743	7.18929518360809
Rh	10.45638727860935	6.96583291287662	5.71447350960761

Cartesian coordinates of **TS0** (TPSS-D3BJ/ZORA-def2-TZVP (old-ZORA-TZVP on Rh))

P	8.77721905809758	7.06070739555637	4.70074703157978
S	7.06948718170942	7.56461102430723	5.91100570434037
N	9.89537348375266	6.91466520065574	7.57404141760083
C	8.60121532306489	6.52506037447857	8.11337647795801
Rh	10.55326886531586	7.77544328971191	5.66993675298883
C	7.37884659595439	6.73015389778672	7.45183676021370
N	12.15884933535319	6.23179163342207	0.42470835445441
B	7.51195104085104	7.54994082406004	1.77710495455260
H	7.15792119763153	6.42755095813664	1.70836343681204
B	6.68686841390285	8.98430960907561	1.15341582040345
H	5.66740794608907	8.88034500304081	0.55868623068926
C	6.19748939839407	6.29704501595448	8.08364754092957
H	5.25583254643971	6.44145724476366	7.56259801249540
B	6.99417693655079	10.32258039895353	2.29385841642002
H	6.21716090002377	11.18728993521669	2.52015713797094
C	9.48732711510552	9.21681272934024	2.82991703538061
B	6.74009552412422	8.68157346236746	2.89676052504487
H	5.86591137604681	8.32232518011982	3.60488095088472
C	12.51463696404813	5.74930765023625	1.67220191629973
B	8.02615245274540	9.70877264755912	3.59666065278023
H	8.07618920867382	10.01334615892438	4.73269342190520
B	8.25382327459248	8.47243338407427	0.46308080997161
H	8.37118419895983	8.00536679715576	-0.61907978091128
B	8.72854220525501	10.64788135910357	2.27108989058651
H	9.19905039602379	11.69319820157048	2.53573387875455
C	8.29667986693782	8.06641482176785	3.19540697319317
B	9.25908464164317	7.88008195117406	1.78997844180692
H	10.09306523751426	7.05718680573669	1.78353340310211
B	9.50842132172584	9.51693542299906	1.15725978326658
H	10.55710210086871	9.75559272825620	0.66879709014661
B	7.91757821187823	10.19703524017826	0.76765798100989
H	7.80022343046148	10.98405563063649	-0.11032424285601
C	12.64600575700290	6.60639279762940	2.79006871325522
H	12.24744195338456	7.23179592375304	0.28753395106481

H	12.41935166498559	5.67017954305106	-0.37407500110870
C	9.35486113648897	4.84324959526185	3.06997103136495
H	9.39913300017551	3.74895454265480	3.01363107107469
H	10.37953256801428	5.21476289466950	3.13796210346424
H	8.89954648719829	5.21209177814821	2.15129300102500
C	11.72207750147679	10.76276997900082	4.16650495756132
C	9.18455873992051	4.47174825685424	5.51013736462188
H	9.14074687103720	3.39706284308792	5.29738505165438
H	8.64975084803238	4.65026769491570	6.44544441017352
H	10.23641786819289	4.75475422274632	5.62235426844511
C	12.68892530304229	4.36712578046308	1.87696480558529
H	12.58678719256306	3.69482013242097	1.02831509856851
C	12.93453965314430	6.08673066902627	4.05636173159683
H	13.05481899886259	6.76999115965030	4.89149485919608
C	8.54683712621604	5.21747500292072	4.32064791420511
C	8.60704740330872	5.89541438950891	9.36289184830222
H	9.56435085679413	5.73821250695982	9.85449631671420
C	11.98964898269463	11.48985684105430	2.83629638469634
H	12.80158691279944	11.00327652860637	2.28726228189594
H	12.31642327014809	12.50981263356194	3.07376106999211
H	11.12098339339509	11.55728955741626	2.18504521026045
C	13.07127774661922	4.71413647659640	4.24251827447364
H	13.29391247996303	4.32172652188419	5.22974104770065
C	12.95589872664097	3.86010117456067	3.14165798312063
H	13.07857463918815	2.78789297705060	3.26804678764988
C	13.06835834790056	10.66574759410847	4.90844482595513
H	13.79934432723558	10.08631077010183	4.33884281175933
H	12.96090789026594	10.21829226727195	5.89615231862129
H	13.44975198582223	11.68861375052907	5.01960311085344
C	10.72550119407017	11.51818009706599	5.06306808639725
H	9.76572039145509	11.69254300926551	4.57512375046176
H	11.15974876628070	12.49224779577735	5.31864491468527
H	10.55332433642343	10.96172787455099	5.98986808706294
C	6.21651471593059	5.69142674654878	9.33306970713343
H	5.28450378147771	5.37119414615343	9.78869336943924
C	7.07542179469495	4.80967311964137	4.18110333212555
H	6.55730155985522	5.38540489240030	3.41162659080570
H	6.53654731333214	4.93337071765833	5.12344087190619

H	7.03818766896964	3.75036145192425	3.89768424851799
C	7.43308116510991	5.48071388770233	9.98088126891437
H	7.47110063782786	4.99587894708989	10.95115521881368
H	10.54897797082193	6.13456855869039	7.67785435330759
H	10.31191615140798	7.66157982702221	8.14395006469468
P	11.05698982080234	9.00739470269482	3.92408015758096
S	12.55094867557544	8.36255845384256	2.52732522327376
Cl	12.41131567371512	8.23438999018665	7.11542937136084

Cartesian coordinates of **2-RC** (TPSS-D3BJ/ZORA-def2-TZVP (old-ZORA-TZVP on Rh))

C	-1.16507436348028	1.33220859525844	14.79907637020592
H	-0.21908575531914	1.63676694436158	15.23876686574537
C	-1.92079213200266	0.31637964330522	15.37860039212381
H	-1.55701182897971	-0.17674951122337	16.27473245497600
C	-0.81455935737679	-0.49222950705204	11.43456236859997
H	-0.64579719545992	-1.57256978805677	11.35148734651358
H	-1.31824185754636	-0.30013807597653	12.38196018691239
H	0.16107971604887	0.00588158974249	11.43593026558410
C	2.31458832018544	-0.98091319723836	7.56637139822160
H	2.23303197162512	-1.77650892839567	6.82944356440634
C	2.36676356529351	5.64864935199439	9.68349812696931
H	3.10085225111915	5.04931789632529	9.13888490552255
H	2.35173611370175	5.32335326820175	10.72408091049885
H	2.68145536263371	6.69902894172527	9.64344747967501
C	2.78704443107931	-0.25931564683500	9.82963787289233
H	3.07931114476032	-0.48482024474176	10.85015285440316
C	0.97547008297156	5.56409903441564	9.02941340794158
C	-3.58718683775342	0.56770033235533	13.65404026880352
H	-4.52346895812718	0.27121035309869	13.19168797647827
C	-3.14424563182707	-0.05424592400876	14.81868788598258
H	-3.74406515580499	-0.83477578222970	15.27589279213758
C	2.54243560489515	1.05860823242535	9.45444339018867
H	2.63951806018111	1.86254398545178	10.17764377719299
C	-2.82567722869111	1.57286387514280	13.04716400041135
C	-2.30051162296626	2.54750117717653	8.67159697726549
C	-0.89256413769351	-0.50834350390560	8.96008619255081
H	-1.47062346260989	-0.35689804597910	8.04817736113249
H	-0.69725700739001	-1.58186038255845	9.06610679847001
H	0.07096092065258	-0.00401938975648	8.86939531580481

C	2.15446034810862	1.36076547822184	8.14486111793869
C	-1.64969618840379	-0.04924270255288	10.21349407783765
C	-3.04727224048118	-0.67578070441726	10.25125972089234
H	-3.67861632475498	-0.31865535876404	9.43445282823918
H	-3.55547373352300	-0.47241103059321	11.19504315875723
H	-2.93710928602304	-1.76249430472783	10.14745029071212
C	1.10868860222594	6.11599792048025	7.59806826549989
H	1.92273257329640	5.61656848662563	7.06464517247219
H	1.36694037477083	7.17950808131534	7.67426912479050
H	0.20021063018442	6.03192965633187	7.00525696281129
C	-1.22204471684646	3.70567943255494	8.06419660982654
C	-0.01632773981246	6.37813534951200	9.87679180868526
H	0.35586499518706	7.40679079785641	9.95418264732787
H	-0.08390338117423	5.95762346985499	10.88529726492479
H	-1.01624080754809	6.41072151847920	9.44164229299847
C	2.67398516855320	-1.27469856993381	8.87552094090663
H	2.87235771635061	-2.30656976906228	9.15218523901776
B	-4.09505815432884	3.04360552291258	6.63876120380229
H	-5.13762212213670	2.78648825742530	6.13840756678893
B	-3.91413169052273	3.00680902248754	8.39820408666218
H	-4.71418508113439	2.69992673647920	9.21054329014055
B	-2.66928679968109	4.20729826209055	8.85188142574188
H	-2.57726061759077	4.67202343413138	9.93063370889163
B	-2.11962539765723	4.98762193421829	7.36247187537910
H	-1.71384760083659	6.08938866256230	7.44074392584918
B	-3.82122507837074	4.55427759189888	7.55144650427160
H	-4.64652031638617	5.38893853076494	7.70866871713556
B	-2.98516996013881	4.26704711714649	5.99859874288485
H	-3.21333094208410	4.90561999107650	5.02713426347483
B	-1.41324289200336	2.22196266317158	7.24135525891163
H	-0.51602184911489	1.46891231993347	7.28941610023656
B	-2.53924323678024	2.54176188650963	5.92015326050150
H	-2.44991914320739	1.92928815713128	4.90971898873864
B	-1.32712201383473	3.75971464135358	6.36806344488917
H	-0.33132614677976	3.99176563744145	5.77655778031419
B	-3.12666925155987	1.77310712070603	7.40366007973418
H	-3.39553592832990	0.63097864312200	7.52818811830465
P	0.43015351845536	3.74922835252919	9.06512181900501

P	-1.67600356096126	1.84628805771613	10.29051587683981
C	2.03841475369166	0.34095386707624	7.17150740369225
C	-1.61984749861163	1.97764186105029	13.64820242620029
S	-3.41618067719745	2.30644779774562	11.53497014994390
S	1.86848487450552	3.03874327008250	7.63489456442062
Cl	1.97733295252415	3.54560281372711	12.29722073918191
Rh	0.07266989535315	2.86719656880993	11.03736443936640
N	1.71885375261953	0.63482804993119	5.85355572184604
H	1.28811658683901	-0.11640670300767	5.32922551006592
H	1.26791372901402	1.53509186647812	5.71600882068220
H	-1.41678524557525	3.81274457916653	12.80244404063614
H	-0.03567065782434	3.29592023248494	13.60747420817217
N	-0.84090920258326	3.00311020944280	13.04568890604524

Cartesian coordinates of **TS1-2** (TPSS-D3BJ/ZORA-def2-TZVP (old-ZORA-TZVP on Rh))

N	-0.88876273352855	2.67011963873537	12.51451110514278
Rh	-0.02353605058395	1.94812680221913	10.67718080513169
N	1.17987321886943	0.38606633742176	9.35548553386674
C	-0.99285597559403	1.06819786293359	14.37659304341698
H	0.01201090399221	1.35478903374445	14.67278202402598
C	-1.70138468066485	0.10135373279533	15.08265538804943
H	-1.24347005955338	-0.36767703263358	15.94837895928788
C	-1.81672566815754	-1.18835297074611	10.72481858100241
H	-1.98653255994462	-2.25703191918668	10.54433716330082
H	-2.23753973284673	-0.93340427428053	11.69936193791077
H	-0.74019365919125	-1.00073841605271	10.77427571989115
C	3.57375917404957	0.22477332449354	9.81067898825568
H	3.36296853769946	-0.53969326704242	10.55316090662361
C	2.42331614008775	4.91343565458468	9.71421295697567
H	3.09504802492330	4.43320339044171	8.99965529872244
H	2.36775743802969	4.28694819840491	10.60948533940012
H	2.85520756418892	5.88463853489671	9.98716159731763
C	5.14068949332020	1.62921815710831	8.62701163880578
H	6.16004689627053	1.94566538617157	8.42901037565126
C	1.03661438294709	5.16770546265583	9.08936242689037
C	-3.57208148278663	0.33412967201446	13.57292533701251
H	-4.56672556299369	0.04978629914830	13.24319271326724
C	-2.99652997129469	-0.25804257255167	14.69567526809949
H	-3.54978008881296	-1.00400247321000	15.25731387303523

C	4.08413296807322	2.23601080712269	7.95672868602965
H	4.26782023591255	3.03018740290683	7.23944399215797
C	-2.86534933754872	1.29554717269543	12.84566412492622
C	-2.58520594089161	2.50088142338695	8.53691990255392
C	-1.91885727814815	-0.87362457834307	8.24183932794531
H	-2.40401561787324	-0.39957105418714	7.38946042569145
H	-2.09767494482144	-1.95420620491391	8.17764783041739
H	-0.84147402095714	-0.71995416876170	8.15410235704491
C	2.76131662785833	1.84212583880357	8.19500930010527
C	-2.48225438109528	-0.38617569948367	9.58688870722318
C	-3.99856554941178	-0.63141716513969	9.62165032617601
H	-4.53870638588649	-0.00110065197358	8.91288755158613
H	-4.40545882904610	-0.45240747255069	10.61823171461739
H	-4.18168378651981	-1.67995757144263	9.35473741692272
C	1.23669439239663	5.94324294137448	7.78315147166444
H	1.87532758422186	5.37566878972699	7.10061096312070
H	1.74411812743946	6.88880462395936	8.01595123237349
H	0.30506383083562	6.17859259808842	7.27042050767021
C	-1.34123777002918	3.61612408041349	8.01351593993145
C	0.18044902983156	5.93339099740883	10.11146929936049
H	0.69353143372095	6.86792557250773	10.36971271722049
H	0.06886421982553	5.34543675935574	11.02952503685064
H	-0.81109771078074	6.18348543805946	9.73103772513496
C	4.87997627951845	0.62958257248277	9.56714122225546
H	5.69496402657069	0.16803069759218	10.11608536885926
B	-4.35458021138948	3.54466200854452	6.68975546626036
H	-5.44101723160004	3.50452667726053	6.21882980489379
B	-4.11482750398825	3.22605158842776	8.41637518607331
H	-4.92023820745674	2.92766658083873	9.22780515413798
B	-2.68160147690559	4.15416686635553	8.95020041548060
H	-2.48507214296305	4.46148296196606	10.07071276394502
B	-2.09434869358393	5.07005236081773	7.55108891395083
H	-1.54286094771166	6.08708723809923	7.75893249932632
B	-3.82741671773901	4.85019060414400	7.78603431783243
H	-4.51412301116964	5.76135835535657	8.10382137616430
B	-3.10706909233951	4.67817703170299	6.15656003004448
H	-3.28243608988553	5.47677714601218	5.29911488053627
B	-1.79775275428147	2.28248562139838	7.03681917859124

H	-1.03777190552907	1.39314575796081	6.92274110616963
B	-2.91145536592808	2.93890831636860	5.82293533238426
H	-2.95285789216534	2.46584747373619	4.73788968435817
B	-1.52049124094186	3.90259473443442	6.35334642526974
H	-0.52847709247442	4.07976890517915	5.73505630281179
B	-3.55305324727470	2.06051155643407	7.21588365277869
H	-3.97972770067040	0.96240607499422	7.17679470702516
P	0.31000437616903	3.41453122586967	8.93891927441341
P	-2.01427751190639	1.42260479165657	9.97119633386195
C	2.51256536606963	0.80481657384778	9.11177914841069
C	-1.57683496009581	1.67588666804616	13.26117281558939
S	-3.56442688666085	2.03425852239511	11.39267923843083
S	1.46223197521680	2.62333492656508	7.25785303230139
Cl	1.96426756636073	2.21397237853613	12.01231414735657
H	1.13788892382210	-0.55506960795975	9.73685434397871
H	0.63413882051421	0.45272314469771	8.49589645769658
H	-1.51245421139624	3.43243495418984	12.24374281224395
H	-0.04092868371589	3.00732585096924	12.98022406875950

Cartesian coordinates of **11-2** (TPSS-D3BJ/ZORA-def2-TZVP (old-ZORA-TZVP on Rh))

N	-0.83227382249346	2.85909764415474	12.07249638855278
Rh	-0.01190623888399	1.76946401946628	10.47292418311836
N	1.00378915191265	0.50768540520670	9.07700237316514
C	-0.68106897130514	1.68283216930395	14.23329094940910
H	0.30416493177443	2.11133582311958	14.38365981705759
C	-1.24287861714595	0.82398460682940	15.17529935517776
H	-0.69359292127199	0.59555511717436	16.08320249358654
C	-1.95895815510675	-1.35727070952838	10.65939348141033
H	-2.13888342700709	-2.42698251211063	10.49617834493932
H	-2.42034840465475	-1.07299302706116	11.60891069613087
H	-0.87983845676537	-1.19145984637812	10.75746849141587
C	3.35998646830965	-0.00700596739281	9.56135674007042
H	3.03956009698140	-0.85148369708826	10.16410770048618
C	2.24699609063930	4.84897339575842	10.22962928358550
H	3.00589729876478	4.42929927135995	9.56330233081694
H	2.08523494152476	4.13110642889805	11.04003837896197
H	2.64315699416505	5.78059546920251	10.65202670444107
C	5.11052941419780	1.40169216644489	8.67697017379714
H	6.16436980638834	1.64067131563782	8.57290882998533

C	0.95440859102420	5.16547691788291	9.46257760294145
C	-3.19471978660526	0.54443292704560	13.77973833435543
H	-4.16844347774049	0.10410440331578	13.58886561250802
C	-2.50058591769730	0.26099440150823	14.95465406943867
H	-2.93778462994420	-0.40712783003371	15.69023382344680
C	4.15534004349488	2.21485377810624	8.07328434143967
H	4.45163814321697	3.08593182371915	7.49711768446789
C	-2.63699607938315	1.39754261400905	12.82341321870447
C	-2.79875934436280	2.25426247560777	8.50826277262738
C	-1.92041864129529	-1.02481397181444	8.16365548349852
H	-2.30121232466488	-0.46854639841833	7.30666147577849
H	-2.17007897400680	-2.08372288433007	8.02395938780785
H	-0.83051147768372	-0.95095329625101	8.16817706429709
C	2.79397454791751	1.91823449388143	8.19927944042309
C	-2.55158908690080	-0.55821925647407	9.48600441461894
C	-4.07016594216493	-0.77741871051138	9.42090415379645
H	-4.53200017743635	-0.17948950988239	8.63221453341183
H	-4.54720341291730	-0.53055589304174	10.37151727658235
H	-4.25864496591689	-1.83628663293523	9.20311385618684
C	1.26511180470060	6.08057953820212	8.27119556878298
H	2.00489292602279	5.62314291561689	7.60974983317570
H	1.68308800466747	7.02024326866987	8.65499698307052
H	0.37079925215517	6.31420126623930	7.69055064676282
C	-1.15982059598553	3.79902093823361	7.89184887492930
C	-0.06114288661452	5.84217232492759	10.39546046526443
H	0.36557425534008	6.79404958316604	10.73404360496682
H	-0.25820583252719	5.24149504944509	11.28739047881312
H	-1.00803713642872	6.05080177762964	9.89496073634913
C	4.71186835884587	0.29269730660087	9.42424304834101
H	5.45168536090245	-0.33379219038728	9.91200277028187
B	-4.31747635786564	3.46190895265596	6.57747356725627
H	-5.37509531293987	3.43947806243388	6.04050333905620
B	-4.19839701775021	3.08180429284513	8.30772991732097
H	-5.08838829219847	2.85633085855317	9.05832837780142
B	-2.63675974894155	3.91542294651705	8.84644745664291
H	-2.50820307809437	4.23500694956032	9.98325317511599
B	-2.10743690778850	5.07932549693035	7.53206464692217
H	-1.69777345499169	6.16288280115592	7.77709649398138

B	-3.82243374810514	4.72161609806537	7.75455228686947
H	-4.53130283549499	5.61048442200857	8.09218523454273
B	-3.09013118530847	4.63852687307212	6.11939571512467
H	-3.29127700158793	5.44270674536981	5.27047676705635
B	-1.74617555546005	2.34319398886917	7.15475760165704
H	-0.96251415835671	1.46134432586267	7.01281128255673
B	-2.79964576573533	2.90372594258590	5.79643093187792
H	-2.77157533642584	2.44043079789084	4.70502073238841
B	-1.46054867080284	3.94520732048230	6.29327679888910
H	-0.52678094331159	4.13470006242841	5.58692723526656
B	-3.54746150651213	1.95170477834602	7.08556990059043
H	-3.94098408452374	0.85599493041736	6.86960497394847
P	0.25828402454328	3.50110263326376	8.88367133455259
P	-2.12759034619100	1.25906564764581	9.82087913601685
C	2.40788880952587	0.79596507472933	8.94059874121066
C	-1.38332328270582	1.97425345925131	13.06555073204361
S	-3.54193508956453	1.80089523608283	11.35153121722554
S	1.60359180150547	2.91044606579966	7.32956160965215
Cl	1.87017180735297	1.61255330873505	11.97531002808437
H	0.86776067604955	-0.46304172450886	9.35600134684174
H	0.53549856602347	0.67079081545382	8.17824105970306
H	-1.55764779649939	3.48831930243164	11.71202081141288
H	-0.04149298588027	3.37996923234050	12.45487927521415

Cartesian coordinates of **TS2-2** (TPSS-D3BJ/ZORA-def2-TZVP (old-ZORA-TZVP on Rh))

N	-0.77354202359375	2.84975957696776	12.02935214974461
P	-2.14160488204802	1.24998056942303	9.80140461136974
Rh	0.03223331338632	1.74090154187828	10.41331816502607
Cl	1.53173038764556	0.81258762518436	12.04538575861186
N	1.04836032686449	0.50746495887034	9.02120861056653
C	-0.66966942314610	1.77381710518637	14.24382061256075
H	0.31530793785753	2.20291342383215	14.39383480539514
C	-1.24863254479701	0.96358343194476	15.21709503603619
H	-0.71276830719070	0.77319215779896	16.14146864168085
C	-1.95275856513110	-1.35392663003718	10.66468515336652
H	-2.11151304720322	-2.42730844262640	10.50401081004085
H	-2.42982049517528	-1.07556140278821	11.60848935934065
H	-0.87853216521100	-1.16682353427450	10.77518323980907
C	3.42199211843513	0.05377964974269	9.50592126754871

H	3.12557597156402	-0.80072094659427	10.10486710145025
C	2.17958878989715	4.73305485609232	10.33626763417417
H	2.94930094242626	4.27304533657712	9.71041372499945
H	1.94508562885265	4.02363253192942	11.13809007920467
H	2.59842736852339	5.64459164134610	10.77996076755944
C	5.13289536129903	1.51117299531077	8.61630726197954
H	6.17987221706354	1.77765118973906	8.50900928904870
C	0.93435792831594	5.09849570237751	9.51093495314828
C	-3.17891630540982	0.62844961201223	13.80528573986598
H	-4.15303496507793	0.18644375482549	13.62034886322725
C	-2.50359269401531	0.39325098626157	15.00044960475538
H	-2.95400234432994	-0.24145823534839	15.75739183969875
C	4.15479057806397	2.29706096010030	8.01179406025245
H	4.42541341773059	3.17369694190744	7.43149174348313
C	-2.60628792918849	1.44150398007408	12.82139804718635
C	-2.82633728525800	2.23199632513839	8.50699094766430
C	-1.91645818169064	-1.03694597064279	8.16469142571205
H	-2.30346674853439	-0.48725846427111	7.30574689320157
H	-2.15260522701963	-2.09932546157589	8.02793556285115
H	-0.82745248745271	-0.94883926640721	8.17250744241082
C	2.80257616053042	1.96508901689519	8.14674891051938
C	-2.55314787215497	-0.57255484846736	9.48393976451749
C	-4.07011439039197	-0.79736801557349	9.41994305025839
H	-4.52980779572189	-0.21998956609025	8.61468701973940
H	-4.54990115084168	-0.52695375964635	10.36307906988320
H	-4.25698257794988	-1.86206636780893	9.22999455505787
C	1.32424793436786	6.02343755660004	8.34978121699798
H	2.09855580755084	5.57094889295914	7.72646605119398
H	1.71922291776326	6.95850787643375	8.76716595942895
H	0.46476028816014	6.26533732723600	7.72056030152274
C	-1.18807724314250	3.77837204884500	7.88159235561597
C	-0.09842253965841	5.80977281147012	10.39915172969338
H	0.35104870776189	6.74102810781927	10.76499105687735
H	-0.37184840616461	5.21942335841336	11.27688977699712
H	-1.00792590562470	6.06104559955730	9.85192046736731
C	4.76528300687624	0.39262441779539	9.36524824336951
H	5.52293670495633	-0.21553811122277	9.84895139147977
B	-4.32538692966559	3.47405356133158	6.57271143579090

H	-5.38655560783526	3.45529556342486	6.04231806473315
B	-4.20348481610373	3.09260913999299	8.30396036326154
H	-5.09771930704004	2.87838956605353	9.05295567819041
B	-2.63560574124971	3.91067328011240	8.83288273312441
H	-2.50418325619487	4.22971642794760	9.96995874011142
B	-2.10514982679945	5.08051885524678	7.51429592786499
H	-1.67662683274581	6.15756747520562	7.75877367865926
B	-3.82206772281957	4.72905059084612	7.74800342173505
H	-4.52865594965693	5.61760089082459	8.09146998359613
B	-3.09497375979103	4.64600443144114	6.10906754217696
H	-3.30074314773753	5.44941948720287	5.26057581632355
B	-1.76365517469469	2.33818654611399	7.13674334414648
H	-0.98285666430325	1.45412909439421	6.99252534490464
B	-2.81548869339503	2.90618670005625	5.78573945120087
H	-2.79673407645841	2.44361422649893	4.69374337913982
B	-1.47056675043212	3.94589553923166	6.27833892084827
H	-0.53459547611622	4.13431829993809	5.57478050623294
B	-3.56288940871689	1.95424948857900	7.07458477010627
H	-3.97006843463714	0.86402690809492	6.85332869239318
P	0.23129626896742	3.45667980029465	8.87657478888265
C	2.44669981855732	0.83435765850398	8.89068948035416
C	-1.35201203312195	2.01686497098184	13.05458082545972
S	-3.52092910037908	1.80641968755389	11.34493302311149
S	1.57559391324839	2.92300843558407	7.29438155868799
H	0.93957178074779	-0.45318194977334	9.34495212272390
H	0.58095345951938	0.62881442920995	8.11562536020519
H	-1.49410796198029	3.46854913627249	11.64072844585196
H	-0.00855688193454	3.40253091366538	12.41500047669166

Cartesian coordinates of **VIIa** (TPSS-D3BJ/ZORA-def2-TZVP)

S	6.91902587531264	14.77061979153123	0.91705735075054
S	7.24808879817111	8.77245051209371	1.21191651490356
P	7.71681219524213	13.02384454638928	1.80931788304571
P	6.74808296226819	10.52628572929217	0.13597062106837
C	8.46418501264285	11.10285231334919	-0.39383705828586
C	6.93965200304506	9.31429946289627	2.89165166875511
C	8.98175938256783	12.52069566263554	0.50349289708488
C	8.65714319597500	13.78224265067267	3.26138246079642
C	5.30084387239281	14.18131279642226	0.42249948626518

C	7.51684937834492	14.23867423290724	4.19807176175598
H	7.96058899613181	14.61090762327715	5.12927606237114
H	6.85142619056094	13.40492014642080	4.44777642137517
H	6.92452725580741	15.04155184314020	3.75059784575533
C	9.42099023655509	12.64657298902214	3.96802589834493
H	10.26191440642590	12.27768706096240	3.38066415048187
H	8.75587156677019	11.80487658334436	4.18738487039700
H	9.81162691538366	13.02820558877995	4.91949702124513
C	9.55648759166961	14.97952206129036	2.93740008975466
H	10.00499012529539	15.35340250198584	3.86704050806437
H	8.97431775712794	15.79466846167830	2.49541175598371
H	10.36380740292411	14.71924084674158	2.25198680465079
C	5.92591085400127	10.21911032906794	3.22931387239415
H	5.29354808980818	10.64082781787785	2.45669087515258
C	5.57384389404396	10.91642731651509	-2.34907738436951
H	6.46294267890909	11.32781398739463	-2.82709708229435
H	5.04911756710612	11.72891279051172	-1.83576137976419
H	4.91373850585301	10.52812071840694	-3.13458445623049
C	7.56372548202139	9.05875555794998	5.08013689568788
H	8.23154633036017	8.56604735637368	5.78359748048066
C	5.90175936239596	9.77011106574131	-1.37392311952510
C	4.57523638845695	13.23434204076283	1.15539692094318
H	4.99459748417743	12.80826141562275	2.05942450694607
C	6.60466303972243	9.96700336952220	5.52017226927520
H	6.51264578892582	10.20354515848699	6.57536759484831
C	4.56944882406467	9.25283313399810	-0.78796624951959
H	3.95109377814330	8.87604037482018	-1.61153501117575
H	4.01765724480306	10.05672697011587	-0.28839201254305
H	4.73129199096974	8.43954000495806	-0.07519082319857
C	3.62068968546978	14.40925311105218	-1.11675951102085
H	3.27645799453353	14.90903669929538	-2.01971263983598
C	6.63799708215948	8.61309093298827	-2.05698591506547
H	6.02331910311888	8.23518808733888	-2.88434909316933
H	6.79977344213565	7.78755171504010	-1.35623957994607
H	7.60344787735160	8.91703410992274	-2.46298269954514
C	5.76782260388152	10.55274181897641	4.56854226593691
H	4.99500384508136	11.25557284579894	4.86796207605223
C	2.82848536070037	13.45855836120340	-0.47885458920961

H	1.85420112263097	13.19536543447866	-0.87805158331175
C	3.32127095585604	12.86546710586684	0.68494326313623
H	2.73111776172544	12.12957411308852	1.22443332127875
B	8.47246780141899	12.65576305383959	-1.12928021974473
H	7.43347196671786	13.16223403272357	-1.35803723794779
B	9.05898256921938	11.20586934156086	-1.97737048024458
H	8.40251470599640	10.77303793090043	-2.85396862290453
B	9.69725053845553	10.98560812446088	0.79329126946844
H	9.45228077228090	10.44750540250766	1.81250071171927
B	9.96913508919896	12.71494318852590	-2.07827200247588
H	10.00597719949133	13.33237282215501	-3.08834549819733
B	9.89414588325016	13.52986952407968	-0.50806428717911
H	9.79220632418612	14.69456499123427	-0.33352880893059
B	10.66621070908253	12.47372363666360	0.68366626146009
H	11.13813495816188	12.90211385636659	1.67385397138164
B	11.21927563122858	11.00066949183332	-0.11634261198228
H	12.15938108578928	10.40728331833570	0.29221663942918
B	10.81702235791808	11.15392006535550	-1.84513350394975
H	11.46776741646925	10.65403434446936	-2.70022628364250
B	9.81322670250723	10.14929824291636	-0.77465805768265
H	9.65315527005056	8.97815409821378	-0.78792200232994
B	11.33672068899354	12.58545553072959	-0.94384159373398
H	12.37465021205590	13.12690281000687	-1.12843328291865
N	7.74259390218873	8.73725091359074	3.78930922108204
N	4.84128295631702	14.76563813152140	-0.68691680764771

Cartesian coordinates of **VIIb** (TPSS-D3BJ/ZORA-def2-TZVP)

S	6.92030504725094	14.71852654765369	1.08321606819974
S	7.08873228904565	8.84902023793958	1.16880136558858
P	7.79195481366038	12.95113979271394	1.86707900479075
P	6.74072889528576	10.62579755084815	0.06424938685789
N	5.54892147615154	15.21626568882925	-1.54318837735984
H	5.34683912243365	15.10098776920122	-2.52862755157724
H	6.54308435589993	15.27978745772054	-1.34198850131480
N	8.80500805907572	8.37110961560862	3.58839541485688
H	9.08597588918899	8.33264420162585	2.61247155053207
H	9.58238433453675	8.50312982737373	4.22358837522889
C	8.49831727431109	11.12568034781332	-0.42165565408553
C	6.75715488016527	9.45200843754216	2.81877824114757

C	9.04418404416209	12.51128586293817	0.52041407861415
C	8.75964059010564	13.70073501101730	3.31095534324314
C	5.32201958382890	14.07768220605015	0.60316299777483
C	4.83556305290854	14.39030901481180	-0.68555712969898
C	7.63528787185867	14.12412203488372	4.28321267359661
H	8.09763156458211	14.45618997187176	5.22078467346271
H	6.97076091426770	13.28297703865439	4.50963851243037
H	7.04003249693428	14.94679980590606	3.87879549294797
C	9.55104294832258	12.56719862245354	3.98989055439427
H	10.37798050798219	12.20520244042716	3.37877664927324
H	8.89240376713181	11.72554735765563	4.22568645535791
H	9.96602509492697	12.94940115673509	4.93108572709864
C	7.68731349010298	9.15491671392241	3.83937113441611
C	9.63830047848942	14.91242604443000	2.98523447027991
H	10.09452811517435	15.28477195213932	3.91190430247782
H	9.03993413078929	15.72393140866954	2.55833902676236
H	10.44034914899469	14.66887567406811	2.28700531543854
C	5.60159270255935	10.18059413550906	3.10568325854840
H	4.90823833744992	10.39588499259711	2.29854411968172
C	5.65011622120281	11.02122314660750	-2.46617345333321
H	6.56123618362724	11.41823704847859	-2.91385012833128
H	5.11355539028480	11.83904547123813	-1.97516125976185
H	5.01588320889966	10.63363461776700	-3.27344230678999
C	7.41716051626478	9.62809228293968	5.13710480266543
H	8.12565969678725	9.40861473009781	5.93256731045360
C	5.92375953818699	9.87816263591957	-1.47081947541008
C	4.55789024363646	13.30465654139851	1.47889060238499
H	4.96154790844226	13.07820404975833	2.46088738439287
C	6.27369811491579	10.36871922685748	5.40687385749731
H	6.09701427257202	10.72555908312086	6.41757037185352
C	4.55711118788612	9.40555343396140	-0.92527345695671
H	3.94567320459590	9.06998307779406	-1.77180282688998
H	4.02705070264269	10.22326838185469	-0.42450018683467
H	4.66750279454436	8.57363558309079	-0.22495202111301
C	3.57416008659651	13.88708287011410	-1.05516426499423
H	3.18780674457126	14.11813177495690	-2.04523778264460
C	6.65091716575941	8.69773851782035	-2.12212953993157
H	6.04764699006957	8.32156062586654	-2.95881921138715

H	6.77945731801699	7.87765926006154	-1.40814659570972
H	7.63168183101283	8.97635403024911	-2.51021962589065
C	5.35595616061795	10.65211281617426	4.39111953559677
H	4.45762363851963	11.22480828968714	4.59996121850252
C	2.83102001974770	13.10288668360114	-0.18244360107464
H	1.86373946354057	12.72385396788009	-0.49987187489876
C	3.31856589565743	12.80423583145494	1.09324367626235
H	2.73725585028211	12.19728056375413	1.78048083141824
B	8.54723535904225	12.69479289063126	-1.10868022875632
H	7.51430770901791	13.21869823278125	-1.32724507851307
B	9.10693139556567	11.25760912527365	-1.99706745174332
H	8.45100287643089	10.85894449709830	-2.88929886381653
B	9.72288199067849	10.95683990614004	0.76421941094203
H	9.45884497358287	10.40676591823611	1.77265425727154
B	10.04611277245685	12.75087293208871	-2.05432143280622
H	10.09954615843854	13.39379458331119	-3.04837348345046
B	9.97939643663482	13.52722832683209	-0.46370908844294
H	9.90062687632115	14.68975053111194	-0.26112060441661
B	10.72635360954358	12.42551078499187	0.70062090291242
H	11.20638615150556	12.82038340470838	1.70012881207397
B	11.25163725160623	10.96173694743259	-0.13402922523231
H	12.17795844784997	10.33854788719735	0.26334193275991
B	10.86196686037790	11.16726071666342	-1.85951716401881
H	11.50666348180807	10.67766208227541	-2.72512534285832
B	9.83101300232302	10.15542194252781	-0.81886785846251
H	9.64919517636963	8.98763054165638	-0.86268180971310
B	11.40613363359173	12.56488855170527	-0.91977513599845
H	12.45618221039651	13.08861673522182	-1.08628950577105

Cartesian coordinates of FcH (TPSS-D3BJ/ZORA-def2-TZVP (old-ZORA-TZVP on Rh), CPCM(THF))

Fe	0.00000019545236	0.00000424879531	-0.00000627809310
C	-1.62800387913260	0.00000755290331	1.21892366379600
C	-1.62805260220899	1.15922244444461	0.37667690626673
C	-1.62804161285039	-1.15921775146178	0.37669014439672
H	-1.59519491033346	0.00001152508973	2.30053858502918
C	-1.62808025514210	0.71642889214105	-0.98606737305167
H	-1.59516563895187	2.18788892307725	0.71091901266008
C	-1.62807265737547	-0.71644034222571	-0.98605957026116

H	-1.59514043182165	-2.18788021986494	0.71094269263959
H	-1.59496847878095	1.35226374797843	-1.86103198667001
H	-1.59495230542804	-1.35228376303410	-1.86101755849081
C	1.62805820540559	1.15922138987410	-0.37667665629901
C	1.62806443154425	0.71642900501781	0.98606765731868
C	1.62802340293693	0.00000671132265	-1.21892177346041
H	1.59517494648623	2.18788778327367	-0.71091889803302
C	1.62805678121633	-0.71644059882949	0.98606064802441
H	1.59493944116689	1.35226325305543	1.86103222769175
C	1.62804660338366	-1.15921878899782	-0.37668878748825
H	1.59523040763837	0.00001188766668	-2.30053726666202
H	1.59492406664153	-1.35228485721465	1.86101769068901
H	1.59515429015337	-2.18788103803093	-0.71094308000271

Cartesian coordinates of [Fch]⁺ (TPSS-D3BJ/ZORA-def2-TZVP (old-ZORA-TZVP on Rh), CPCM(THF))

Fe	-0.00000307141719	0.00000152474355	0.00000075098835
C	-1.70264033474372	0.02071746706289	1.22002724600894
C	-1.72856498118551	1.16991736520749	0.38032147668796
C	-1.66465255136240	-1.14042004078422	0.38433121458927
H	-1.66416112772026	0.02793340741687	2.30086848713298
C	-1.70227717809638	0.73379235905106	-0.97455757231530
H	-1.69588776352274	2.19831422176235	0.71439415981083
C	-1.66441186887388	-0.69688949291246	-0.98095964859791
H	-1.62144440906512	-2.16641780252338	0.72268582049057
H	-1.66333078136339	1.37522129658781	-1.84448495674422
H	-1.62080720398755	-1.32823593923212	-1.85758976248567
C	1.66464963742850	1.14041798122980	-0.38433458572743
C	1.66441335663070	0.69689235357663	0.98095406998314
C	1.70262883221968	-0.02071763686016	-1.22003057833634
H	1.62144063936399	2.16641452558438	-0.72269075379782
C	1.70227485328789	-0.73378784829420	0.97456237750566
H	1.62082010675730	1.32824226169928	1.85758196663783
C	1.72855632044504	-1.16991755366171	-0.38031906196220
H	1.66413454506640	-0.02794051078845	-2.30087287411792
H	1.66335522225461	-1.37521549794972	1.84449335910762
H	1.69590675788402	-2.19832144091571	-0.71437913485833

Cartesian coordinates of **1** (TPSS-D3BJ/ZORA-def2-TZVP (old-ZORA-TZVP on Rh), CPCM(THF))

C	-0.15911208124464	1.57108994306609	13.88058204583784
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H	0.90948832846471	1.68635782788682	13.75237916159070
C	-0.71548638685437	1.20046199266503	15.09395311742195
H	-0.06575792497045	0.99444421440538	15.93703673973852
C	-1.10937417708782	-0.90952701404186	11.05577943243532
H	-1.07250085027932	-1.99812742226160	10.93679551131342
H	-1.67287875095048	-0.68808998701578	11.96604053105341
H	-0.08801095034405	-0.53338227130711	11.16822432531829
C	2.55017947708702	-0.95935644688611	7.66318253104674
H	2.59359866838602	-1.70292470831749	6.87119169238697
C	2.45285300143877	5.40971344229929	9.59668852198631
H	3.12907623416441	4.89436824730897	8.90986503604582
H	2.51593346727786	4.94536612560981	10.58090952648376
H	2.77283178434031	6.45564756262086	9.67753171794061
C	2.77443199449973	-0.30252193418889	9.95556032072765
H	3.00106952502343	-0.52374562904836	10.99436695463673
C	1.01012934710134	5.41928873148024	9.05260992715922
C	-2.87850091200903	1.34412610228727	14.07176546366597
H	-3.95738300215860	1.24110337063288	14.09727429227756
C	-2.10345504646025	1.10535214837141	15.19890722554984
H	-2.57571237170977	0.82734362402476	16.13567318149759
C	2.45789249994222	0.99907055595929	9.57513927703675
H	2.45663061854389	1.81235700626144	10.29301193101569
C	-2.25020033526764	1.70078707127547	12.87465820651600
C	-2.32085463544213	2.43221922714069	8.54000346426408
C	-0.97161325351693	-0.72617430582567	8.56718793389470
H	-1.47283382426863	-0.45793472320322	7.63636897394864
H	-0.84668820343185	-1.81460217930217	8.58742147918855
H	0.02060273998243	-0.27110992865419	8.58146564464710
C	2.15744030059001	1.22782236390559	8.22749856993822
C	-1.78861377629565	-0.32139009934186	9.80215990862870
C	-3.22845142490235	-0.84380365289136	9.70903403118188
H	-3.78318554401395	-0.39518306830334	8.88297812970765
H	-3.77534623453572	-0.66429755316978	10.63755934453625
H	-3.18194987097509	-1.92592890094885	9.53862087136650
C	1.07374000400210	6.04133217275685	7.64709230438984
H	1.74407089783678	5.47085253613173	6.99638340863184
H	1.49664234599185	7.04738742481480	7.75529865033376
H	0.10593884093879	6.13376543386772	7.16035899832671

C	-1.24631228169060	3.64936122421100	8.04988537381456
C	0.11119931227985	6.21932260725203	10.01107438856504
H	0.49307510343176	7.24526932068288	10.06949971003660
H	0.13690337761336	5.77854821349866	11.01210906792702
H	-0.92611339677254	6.26240135791570	9.67341687220798
C	2.81732316278892	-1.30456204138310	8.98558251570098
H	3.06458412338284	-2.32903941864340	9.24407212960683
B	-4.14347157714084	3.15239124412697	6.60888506308954
H	-5.19455469372516	2.95590120491240	6.09647032616127
B	-3.93390195058082	2.91842017486582	8.35246630686641
H	-4.71577584212808	2.52343363082047	9.14700891111246
B	-2.67896730341618	4.06501408611606	8.91132593673427
H	-2.56269699243994	4.41330640823175	10.03012657426951
B	-2.14982225836952	4.99967166398883	7.50848798403662
H	-1.74526735549673	6.08590372423629	7.70594059865963
B	-3.84973113882999	4.54983561691914	7.67720839145201
H	-4.66887535735269	5.36646000262270	7.93451751535481
B	-3.03660851667166	4.43458777954867	6.08891166564810
H	-3.28106574066664	5.17713138481473	5.19724530489328
B	-1.45621064168601	2.25509762083678	7.07158911386745
H	-0.57281665693852	1.48484162709946	7.01886510198108
B	-2.60044574573402	2.73006843740784	5.81300661533932
H	-2.53424929128658	2.23494459045599	4.73862673237446
B	-1.37290809523364	3.88414182397290	6.37301747719633
H	-0.38741295229896	4.17513698668275	5.79158084845220
B	-3.16937972071118	1.80358632888645	7.20755023666362
H	-3.43391888798071	0.65556315642483	7.19957908910410
P	0.39843112957146	3.62863481800722	9.06044109200427
P	-1.67984805272300	1.54381999360860	10.04584194219990
N	2.20871209405827	0.28465080025072	7.27988995713472
N	-0.90193635076862	1.85195808577941	12.78386949735341
S	-3.27151984533491	1.92918918027427	11.45311919338682
S	1.76347934258339	2.85540721353424	7.60078731978075
Cl	1.71425694435340	3.53988399239151	12.30591186136320
Rh	-0.00934346297861	2.54910685958463	10.95649990199430
Cartesian coordinates of 1^+ (TPSS-D3BJ/ZORA-def2-TZVP (old-ZORA-TZVP on Rh), CPCM(THF))			
Rh	3.63847562148671	11.19538701204148	0.07026945473785
S	2.29627915370172	12.49864231256303	-2.84970322366934

S	1.97720999302996	9.80200458312300	2.79169913416368
P	2.10397858818360	10.85871207606038	-1.54083340321753
P	1.96608396203107	11.54843022050707	1.61299770471431
Cl	5.77778373628800	11.35563057049604	1.12215741303892
N	3.72555689639555	9.24181169692872	0.76460325481815
N	3.82013161827414	13.14770650616554	-0.68180256427549
C	0.28180900900009	11.45000689384596	0.78939636978318
C	0.35325204236920	11.04118667253056	-0.88368467394481
C	3.04093911997773	8.77500649798826	1.83361174714830
C	4.62468493601667	8.42282712365592	0.16379558347284
H	5.19324333728078	8.86419750296385	-0.64363211101725
C	3.33725557942238	14.90178229586561	-2.26756566855384
H	2.83014817276760	15.19937363142366	-3.17828774011194
C	1.82806309869912	8.11554580734576	-2.07131302028275
H	0.78325214682062	8.06048616285420	-1.76657129403654
H	2.46015866412077	7.94326673233761	-1.19761146332249
H	2.01678653492177	7.30794746448677	-2.78658527009025
C	3.22463804582198	13.58066827571007	-1.82343219387337
C	4.09273439570023	15.80490546317245	-1.53509828145563
H	4.19066386191944	16.83221784235505	-1.86948066113251
C	1.75859805143744	14.25074616052224	2.26666303008731
H	2.51526061396662	14.42412406813792	1.49766286537888
H	1.88331318875999	15.01762699800706	3.03874803686845
H	0.77120861225804	14.37433924781212	1.82248615037719
C	4.07419412573417	6.61274218221881	1.62388528964523
H	4.19267963760899	5.58646597931646	1.95469852697890
C	3.18187017651310	7.45283491661542	2.27156578111967
H	2.59798873525541	7.10990748044505	3.11820835112670
C	2.16925977849076	9.44238550842203	-2.76981303776200
C	1.94322625199441	12.87908772544968	2.93815508444030
C	1.26062334554488	9.69671275329316	-3.98464903555048
H	1.57133516274328	10.59083564823398	-4.53404128719104
H	0.20813286264492	9.79067865122421	-3.71863460077748
H	1.36770379495828	8.84127853525643	-4.66122414218538
C	0.88984282270354	12.62003507752744	4.02598405948726
H	-0.12895572738510	12.62187158944854	3.63858858597767
H	0.97499300192408	13.42067492197916	4.76999682848578
H	1.07509170942247	11.67085082835878	4.53861213763299

C	4.82320629278191	7.11361981519959	0.55718047493246
H	5.55207805496218	6.50653236356934	0.03377085022495
C	4.54577940536504	14.05029292178056	0.02900905053318
H	5.01292965262951	13.66349605421339	0.92381562419406
C	3.63552261448138	9.41445956929639	-3.24843093081387
H	3.73862248781037	8.58092733452661	-3.95115746279620
H	4.33307328206193	9.25481357033685	-2.42410733540122
H	3.90962066099187	10.33842643965913	-3.76355744271793
C	3.35034291839148	12.80681901007331	3.56566004126636
H	4.13980675096280	12.94283718564917	2.82255378221166
H	3.51652718552037	11.85358283241064	4.07393280682806
H	3.42254196525363	13.61185969012422	4.30471964961470
C	4.70929625524919	15.36555529950991	-0.36385735554568
H	5.30705433367833	16.02793640105766	0.25119562270259
B	-1.80923283199437	12.71784622044714	-0.50533553472441
H	-2.34033834879799	13.74086047465844	-0.77457924721519
B	-1.03650626299532	12.48616200551362	1.06543543241968
H	-0.93609915172634	13.31829069356090	1.88968180011946
B	-0.04299113323212	12.63985195404102	-0.40283202229817
H	0.76244329211990	13.48477633796008	-0.56494501984540
B	-2.39652865106629	11.12359027082684	-1.04817506650700
H	-3.35832339100567	10.99868144101942	-1.72819824052884
B	-1.93332258906342	9.90942589448409	0.18425640193239
H	-2.55107457415606	8.92170570344813	0.39392118435669
B	-0.16443784756081	9.87683395147712	0.26074975246339
H	0.56038467639931	8.98019662824967	0.49765487504836
B	-2.47052696377629	11.53808597144896	0.67001384444835
H	-3.48669261452038	11.72526502479801	1.24925221342170
B	-0.90471111313559	11.80544490921317	-1.72589375411382
H	-0.67846355951098	12.15115127229262	-2.83194011697595
B	-1.09924523647333	10.76557185468896	1.49277603409670
H	-1.00710437678812	10.40803183921972	2.61462097326464
B	-0.99144714897032	10.08721318585633	-1.29878664936723
H	-0.85651869269019	9.24410426269944	-2.10691595226187

Cartesian coordinates of 1^- (TPSS-D3BJ/ZORA-def2-TZVP (old-ZORA-TZVP on Rh), CPCM(THF))

Rh	3.48409916558951	11.20547638474691	0.06495567278409
S	2.33468149465337	12.50914007658636	-2.95832337724840
S	1.97577927273706	9.81535604751368	2.93076860908380

P	2.05340772358398	10.82689136830846	-1.65417065137996
P	1.88699802768996	11.59092607456492	1.73241163861901
Cl	5.88282785012606	11.30285597725851	0.81328466528173
N	3.59799443002428	9.27303427940878	0.80082178999795
N	3.70286339934932	13.11926802724274	-0.69107081975766
C	0.22116675485474	11.53317617255790	1.14216622467131
C	0.33590003448043	10.95979280977767	-1.24540954649086
C	3.01952032117770	8.81569135954525	1.94076469072540
C	4.46834415498874	8.45243127181501	0.15714930654393
H	4.93963363727577	8.88462066419704	-0.71401678575580
C	3.45174340321215	14.87410014980653	-2.33283904657415
H	3.04575219132633	15.17781690091354	-3.29145434567058
C	1.87712394300186	8.11274536515046	-2.19517070597368
H	0.84464488187446	8.11932675797016	-1.83994165828446
H	2.53557400469458	7.92378304131867	-1.34425175574293
H	1.99259097634888	7.28577775461912	-2.90690805348923
C	3.23153664783122	13.56028426621620	-1.89068006648571
C	4.17669201188304	15.75517984320275	-1.54853840048614
H	4.35278495315823	16.77196438545956	-1.88480158678933
C	1.77514514079086	14.26160028825314	2.38796264874704
H	2.51525826338399	14.43650334806649	1.60305964910431
H	1.87315047490943	15.06027540739433	3.13398982701101
H	0.77931950953679	14.32501342220328	1.94397177234741
C	4.11477798969079	6.67491115246459	1.71445490327743
H	4.29804852419609	5.66508673911776	2.06762747573122
C	3.25092544260176	7.50853951893328	2.40234731227007
H	2.74994669097679	7.17751355305401	3.30550531073280
C	2.23500628056619	9.42755271458467	-2.90899070147362
C	1.99688602721021	12.90625533666645	3.08232361872609
C	1.29196327086083	9.65836186886886	-4.09990783687336
H	1.56440364032755	10.56376718514391	-4.65317853799945
H	0.25109451721923	9.74070720207451	-3.78034327567477
H	1.37730995719116	8.80877295101189	-4.79009911758481
C	0.93836541070942	12.68610525309998	4.17052136417512
H	-0.07047930074984	12.68516028322690	3.75045150266709
H	1.00534364192469	13.49568869129376	4.91003971309882
H	1.10137580552602	11.73906992160044	4.69644481417977
C	4.75171532169545	7.16561529156014	0.57043262515035

H	5.45308597571932	6.56577011794622	0.00192320026181
C	4.40613350209342	14.00421081286500	0.06712832995252
H	4.77021007556089	13.60646604769899	1.00348786172923
C	3.68816384862535	9.39588664759075	-3.40083365901826
H	3.82063197738539	8.53976816300643	-4.07378407869656
H	4.39377759470014	9.29789967212284	-2.57214048948997
H	3.93644592797818	10.30964386230056	-3.94923473421139
C	3.40921443516508	12.83589767714636	3.67980192802295
H	4.17795950101936	12.86392528463652	2.90078833528190
H	3.54702746849352	11.91140590729333	4.24911783231468
H	3.56046240461752	13.68647529160698	4.35596169283435
C	4.66598431004482	15.30447006431466	-0.31882728047183
H	5.23491143322472	15.94848847556697	0.34222894949842
B	-1.73243725824518	12.67638454693865	-0.49963803928785
H	-2.24909602368083	13.71765383038277	-0.77077203434906
B	-1.09969369408957	12.49824547450230	1.14556824049926
H	-1.16816147833930	13.40180555828607	1.91591078914738
B	0.05809514474049	12.37851945168927	-0.34490387973535
H	0.81443699481409	13.28214493551523	-0.51879885575794
B	-2.39210426128098	11.10225029640614	-1.06014272310901
H	-3.40604970662184	10.98758241331239	-1.67983964950094
B	-1.83199616292228	9.91108686775598	0.16980060823197
H	-2.42116292990971	8.89476272413438	0.38115716532115
B	-0.02173950138651	10.12910979444822	0.20714307149256
H	0.66824754798904	9.19124640203999	0.45516216170191
B	-2.47469431837535	11.51495741545995	0.65975111687262
H	-3.54278545822265	11.67765318129171	1.16773721638411
B	-0.95648098927973	11.78369538384880	-1.82109897015957
H	-0.90807580811539	12.22481381055456	-2.92587530218749
B	-1.16182792012384	10.76921327586625	1.56857257344086
H	-1.25408999455485	10.32929398425968	2.67119030018042
B	-1.02131065317619	10.05598939458464	-1.39719121863269
H	-1.04913787227620	9.15233412782876	-2.16939932375106

Cartesian coordinates of **2** (TPSS-D3BJ/ZORA-def2-TZVP (old-ZORA-TZVP on Rh), CPCM(THF))

B	7.61791108621733	7.28036876482224	1.67431238230978
H	7.38879317741188	6.17044555245425	1.35140579025066
B	6.68729630517956	8.73292565919445	1.28630573042737
H	5.71842052276125	8.66547432945651	0.60506381468984

C	6.66815994670302	8.36249169188481	7.57513626828026
H	5.75082836049405	8.54479920039701	7.02436775120664
B	6.78850254035324	9.83267638960885	2.68815358547651
H	5.91352385555708	10.56184749461807	3.01723005819949
C	9.34565959444404	8.86649665864652	3.18246587250403
B	6.66961268250016	8.08582720325600	2.93312384162784
H	5.80073250179755	7.51634215219385	3.49300271599130
C	12.68939069682789	6.20350009959108	1.33856193529501
B	7.79970328360303	9.05689657976653	3.91707327459100
H	7.74692152921116	9.11723041737875	5.09138913278870
C	8.69027044309542	7.06161318730085	7.88879431203540
B	8.33422252519189	8.51552625796377	0.63041264863742
H	8.55908190652408	8.29551497709147	-0.51247755798112
B	8.47991827557839	10.30981519141107	2.86544356353773
H	8.82775466844097	11.31876192044600	3.36066629549672
C	8.26000889332254	7.56953622222218	3.22507883066940
B	9.31598512750208	7.75412015217864	1.88823709992182
H	10.22644310229323	7.02394100483806	1.78815748985385
B	9.43187765467228	9.50403030191114	1.61055383353438
H	10.47285103469295	9.93592602071276	1.25880654316143
B	7.80605955758313	10.10379978698071	1.24466639991788
H	7.65817043338602	11.03955798089838	0.53055801353831
C	12.73463467369268	6.71887992747428	2.65690419967272
H	12.38327740682755	7.99020925812953	0.38945079259209
H	12.65602402518570	6.67431919471387	-0.65169007566536
C	9.62884652420488	4.52424637206036	2.67082087726949
H	9.76772441084491	3.46393540526870	2.43085286845033
H	10.60764633074840	4.94998688225910	2.90629063312418
H	9.22530975156120	5.02078047218707	1.78788854251794
C	7.48939859760192	7.29983082233787	7.19318934187463
C	11.28616529823701	10.26366905036765	5.03334769100870
C	9.22584141649176	3.71216291589431	4.99409224257426
H	9.28194165895403	2.68776432881191	4.60937597452530
H	8.56248655745189	3.70400816073520	5.86557476863044
H	10.23094919255501	4.02464624868956	5.29690911174433
C	12.95958202784525	4.83087258121347	1.16129508170271
H	12.92685531819529	4.42066511490431	0.15492963462486
C	13.03939558425001	5.88495754890137	3.73831126589619

H	13.07522017778531	6.31219674685154	4.73540166701534
C	8.67624083066772	4.61616438217387	3.87257342941690
C	9.05706202921233	7.89565012486419	8.94674173190796
H	9.99279287622696	7.71158262607373	9.46613050885315
C	11.59056984402281	11.31927678396913	3.95539454196742
H	12.52676961157750	11.08550241760036	3.43941705755128
H	11.71986822215847	12.28509075091975	4.45867464593277
H	10.80193348228492	11.42769516176221	3.21259624917548
C	13.28193313533452	4.52825010279840	3.54357535490289
H	13.50575131689845	3.88882634528838	4.39178916830940
C	13.24652202400701	4.00999434934771	2.24404100321339
H	13.44391458500336	2.95533558069913	2.07189522969330
C	12.54607354049035	10.11014775503296	5.90370484732325
H	13.39227604007082	9.72964654241867	5.32488228141380
H	12.37389349708445	9.44149172026967	6.74749846854419
H	12.80429158411943	11.10652580937480	6.28244146925171
C	10.11805273571620	10.67513390017149	5.94756398045270
H	9.21387570774687	10.92342347185202	5.39116509271563
H	10.42328823799343	11.56261096136413	6.51452498729023
H	9.88354292341168	9.87286774129142	6.65555126589456
C	7.03375912066245	9.18838198704223	8.63880538980433
H	6.39168882219014	10.01572194319546	8.92396009895903
C	7.25817714561928	4.15940816196747	3.49730486439011
H	6.78512543458334	4.82059835993435	2.76916066314595
H	6.61538524875024	4.08792174674852	4.37977438001298
H	7.32858732426097	3.15943733408855	3.05286615675329
C	8.23153991987840	8.95597362884425	9.31691186320634
H	8.52838217839140	9.60055528500796	10.13860723952345
N	9.55407049866301	6.00273041338288	7.46509007598007
H	9.03667176280256	5.14609882983566	7.26101925742531
H	10.30088015754451	5.81299523210072	8.13564892999934
N	12.33592691761545	6.98659107926612	0.25647034939536
P	10.88458040006743	8.56787981083875	4.30222089335076
P	8.72728427263142	6.35612818767882	4.58728124180559
S	6.98240578793354	6.24703214039543	5.85430954963762
S	12.50583708325646	8.46815991441025	2.90061985035518
Cl	12.39845009420465	6.98427215626309	7.16763953871600
Rh	10.45783694914052	6.96364103370341	5.73220410020947

Cartesian coordinates of 2^+ (TPSS-D3BJ/ZORA-def2-TZVP (old-ZORA-TZVP on Rh), CPCM(THF))

N	11.63085398740633	5.25238674036602	4.13198685146176
Rh	10.19999401805114	6.66863029278015	5.25510646082599
N	9.35207742643064	5.41639813175194	6.83100752163914
B	6.98621438731466	7.87890961309842	1.57465318827121
H	6.55435114435493	6.88503867535478	1.11308381854251
B	6.23745649073561	9.48427789738075	1.61453364743694
H	5.17668596875934	9.66320530158590	1.11821070992683
C	6.63704640474311	7.89979595923754	7.46844268017440
H	5.72042834620789	8.23336919919930	6.99343596717618
B	6.72172065447035	10.26995511973471	3.13991225620704
H	6.03551004328983	11.01916964982108	3.74784656397687
C	9.15003446284115	8.92974965317234	2.99009287429280
B	6.37795110657959	8.53697363255265	3.10093747995146
H	5.53345947043357	7.97997297466761	3.70523915821515
C	12.95178326358335	5.74396945616553	3.93127020120837
B	7.78017018596231	9.15790788162285	4.01495092414095
H	7.93972627033505	9.00081239931249	5.17247536523848
C	8.57003813137286	6.42842115121119	7.48048608227802
B	7.70670449052221	9.20472092417995	0.64306630488178
H	7.71686424717361	9.18102759736604	-0.54056547194828
B	8.47086281162203	10.50012858810926	3.08728681581684
H	9.03145693077031	11.33645730704424	3.69109266406213
C	7.90401311304991	7.78088374470456	3.00885812638100
B	8.74429984613630	8.10037029404928	1.53946138002046
H	9.49589895829542	7.30534196123055	1.12306381691399
B	9.08904314677457	9.84366476617696	1.55788846972797
H	10.11868354481505	10.19476484762790	1.10037630382802
B	7.53216288901589	10.69484978130211	1.60408065006048
H	7.41790078186608	11.76130288023875	1.10111802735462
C	13.18439643780615	6.81835330457250	3.05738984616025
H	11.16437494929657	5.11366098062270	3.23552466511714
H	11.64860518885562	4.36818474207555	4.63773232737828
C	8.85162514091424	4.77039643060425	1.74271086271002
H	8.91037934224835	3.75321986113198	1.34241274433626
H	9.87366000852328	5.14621136330430	1.85925379145432
H	8.35014397366537	5.39945443247431	1.00641657146517
C	7.37489238614323	6.86999249202128	6.88125660987402

C	11.61833733272454	9.88682391095500	4.47828479058927
C	8.58639716716522	3.56857396440952	3.94933717902418
H	8.47321575050225	2.63455561053977	3.38976788216611
H	8.00061298991076	3.47977311289192	4.86917925241334
H	9.64118387346404	3.67913349191541	4.20808392620021
C	14.02293486444841	5.16432266914396	4.61526958648964
H	13.82962118931099	4.35351766492588	5.31161745467233
C	14.49514843805053	7.24378269141162	2.81699978834160
H	14.66586091906263	8.06456418081868	2.12789711927748
C	8.06515869655135	4.71729749943366	3.06299401571393
C	9.01464434388642	7.02813888931941	8.66171165440570
H	9.94019835344751	6.68889381327666	9.11340503615030
C	11.78131033521919	10.97512237055638	3.40583259239401
H	12.26458874923241	10.56626945941286	2.51359234712786
H	12.44421094049477	11.74027507164349	3.82629150876157
H	10.85029538819450	11.45696091252404	3.11864867695937
C	15.56260509345879	6.63431086746649	3.46989881361492
H	16.57540074167351	6.97309722749582	3.27753075674474
C	15.32132210250938	5.60736051836798	4.38629993951296
H	16.14648918142650	5.14257786223927	4.91642774615000
C	13.04248256339005	9.45838266262730	4.88805847158778
H	13.67662771707507	9.34034841734256	4.00908025755650
H	13.05942740140358	8.54158797727557	5.47837298447698
H	13.45383788630512	10.27029575641714	5.49867189007340
C	10.84672469872101	10.36086368584120	5.72468315389114
H	9.81642972699713	10.64472186031643	5.50318630766499
H	11.36270193922980	11.24028118229445	6.12636717580910
H	10.84448828491758	9.58078771800934	6.49189090776764
C	7.08513968018356	8.49153343141204	8.64830320815722
H	6.51045076284685	9.29404260247493	9.09900432527280
C	6.57357066473635	4.46643188119100	2.77333794922984
H	6.10280357622582	5.29695590101065	2.24631910874477
H	6.01577006653596	4.26298203518241	3.69136784343377
H	6.50519170404944	3.57611469362870	2.13799611345202
C	8.27248561908886	8.05449557484757	9.23993545949577
H	8.62564837514932	8.51359559733199	10.15769768166278
H	8.77703185383122	4.63543635182863	6.50845813889408
H	10.10615006824531	5.07521496296740	7.42861724743773

P	10.73257086979371	8.34625952156634	3.85575622638682
P	8.33394754767046	6.28516418649914	4.06511260848158
S	6.72644969770754	6.06541744757016	5.43747062220553
S	11.85669490956485	7.62435741100301	2.17894803869599
Cl	11.91700898523175	6.95878832476245	6.90969295635363

Cartesian coordinates of 2^- (TPSS-D3BJ/ZORA-def2-TZVP (old-ZORA-TZVP on Rh), CPCM(THF))

B	7.60105034653205	7.20366056766308	1.63772467608955
H	7.36403438265285	6.13000839710830	1.19059271162904
B	6.76398056838592	8.70407969182412	1.20800379849468
H	5.82343691674504	8.68646413158295	0.47667832140507
C	6.66041591812620	8.35476879625456	7.59878026160781
H	5.72138786484758	8.52380212629544	7.08086654470356
B	6.89667382619137	9.80600856860472	2.61377434532404
H	6.03069614036086	10.56411496456323	2.91993021163918
C	9.56239428616010	9.08875255613186	3.13113151560393
B	6.62491889335988	8.07216865985497	2.85640949138764
H	5.63741107671009	7.66572721090895	3.37513160239418
C	12.66134354084398	6.31899437577784	1.33566053525359
B	7.96586792915876	8.94519713905331	3.79094002825679
H	7.83497864144322	9.08217200884505	4.96013106908136
C	8.70186670513115	7.07365331706062	7.84787518125073
B	8.44594642435345	8.41474780403843	0.65940319634558
H	8.71232094989090	8.13928438902866	-0.46831465330742
B	8.57384925716834	10.34852200589607	2.77259150587769
H	8.79993303494400	11.42156839074579	3.22316669493319
C	8.03680636885123	7.33576559764272	3.20734395287441
B	9.30151643120059	7.75205680041071	2.10550074378160
H	10.19896285163266	6.99397493109381	1.99513819664393
B	9.54219698950281	9.49079140678524	1.54760608876417
H	10.55077377258549	9.88151625304099	1.05483530100191
B	7.91002221210854	10.04902842756467	1.15576179869901
H	7.75061637751283	10.94730105604985	0.38929583208911
C	12.79469305392194	6.78917110247123	2.66371792841199
H	11.91621223223784	8.04317732347195	0.58502394241263
H	11.92076155579844	6.75641757941976	-0.50467572005809
C	9.62805139902331	4.45585819841933	2.74620664176459
H	9.76743495352380	3.39809377239427	2.48970637440818
H	10.60304152566224	4.88100487065868	2.99714251100322

H	9.23390782965989	4.97234224235420	1.86940676856904
C	7.46612895290148	7.28460537804122	7.20343761844096
C	11.32487542177357	10.28816670202682	5.13277985173020
C	9.20727110501124	3.66015770626956	5.07297550170755
H	9.30201266669526	2.63050513363965	4.70755955463089
H	8.52610622015396	3.64640597920612	5.93162680038282
H	10.19581117897475	4.00660108160248	5.39440338039717
C	12.87009505256018	4.94852952961283	1.09283710876805
H	12.76805862240383	4.57656935897259	0.07590635505039
C	13.10534389826165	5.90343911272435	3.69988112497531
H	13.17627412300563	6.28874351819044	4.71197456515909
C	8.66220638373935	4.54169785967909	3.93856049038165
C	9.10962608383076	7.93187281351746	8.87364661247224
H	10.07076477674155	7.76510047162016	9.35138396058622
C	11.65582878588842	11.36915808535493	4.08986738758227
H	12.59302494234903	11.13998730658446	3.57222788645068
H	11.78834953977368	12.32610962733404	4.61125159076216
H	10.86672448685926	11.49063520409713	3.34672696683986
C	13.29621162649465	4.54683934694826	3.44291265571673
H	13.52630335469334	3.86682205197409	4.25781138065638
C	13.18359984872922	4.07742276471687	2.13064814011638
H	13.32938873289550	3.02240673696413	1.91317765239879
C	12.53564628176390	10.11576671438723	6.05780408429158
H	13.40874690615558	9.75041997820931	5.50841910599490
H	12.32418943439571	9.41531673635946	6.86679276916489
H	12.77968765566542	11.09694646025186	6.48578834639318
C	10.10271299026072	10.68599112914047	5.97968467976620
H	9.23473030834437	10.92080739452375	5.36075479053682
H	10.35875946452112	11.57748689635370	6.56686346570912
H	9.82897056597590	9.87799574466440	6.66640956867307
C	7.06673426755296	9.20632456668459	8.62712669750183
H	6.43384187356541	10.03829871607909	8.92064063304393
C	7.25841354292967	4.07112406206059	3.53161922040323
H	6.82299767796798	4.71879710149433	2.76671896111085
H	6.58233366506650	4.03715875971047	4.39221883480832
H	7.33036890000026	3.05571505119923	3.12117447999689
C	8.29524686631004	8.99477197191224	9.25800934087010
H	8.62443806118624	9.65975807964986	10.05112281656077

N	9.53998627439796	6.00365229172258	7.41559584154182
H	9.00299461937009	5.15853489700472	7.21411449082152
H	10.30208757622100	5.80424941603410	8.06508524585436
N	12.38544135599207	7.18961117126795	0.28651574041986
P	10.89477719495269	8.64869325864664	4.28867312609562
P	8.64312161415160	6.32335081031751	4.55098319073837
S	6.92619457428756	6.20453814677918	5.90571139196856
S	12.62177191619014	8.53240294960971	2.97436864526084
Cl	12.40821078288461	6.91125877679900	7.08353859779141
Rh	10.41072756992676	6.98040148704598	5.66967095114021

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