Pt^{II}-N-Heterocyclic Carbene Complexes in Solvent-Free Alkene Hydrosilylation

Author approved version of the manuscript

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https://doi.org/10.1002/chem.202301259

Abstract: Herein, we report the catalytic activity of a series of platinum(II) pre-catalysts, bearing *N*-heterocyclic carbene (NHC) ligands, in the alkene hydrosilylation reaction. Their structural and electronic properties are fully investigated using X-ray diffraction analysis and nuclear magnetic resonance spectroscopy (NMR). Next, our study presents a structure-activity relationship within this group of pre-catalysts and gives mechanistic insights into the catalyst activation step. An exceptional catalytic performance of one of the complexes is observed, reaching a turnover number (TON) of 970 000 and a turnover frequency (TOF) of 40 417 h^{-1} at 1 ppm catalyst loading. Finally, an attractive solvent-free and open-to-air alkene hydrosilylation protocol, featuring efficient platinum removal (reduction of residual Pt from 582 ppm to 5.8 ppm), is disclosed.

Introduction

Olefin hydrosilylation, the addition of silicon-hydrogen bonds across unsaturated carbon-carbon bonds, is a highly sustainable transformation, not only utilizing reagents which are inexpensive, stable, and comprised of earth abundant elements, but also fully atom-economical. Moreover, the reaction can oftentimes be carried out under mild and solvent-free conditions. The main hydrosilylation products are silicone release coatings, silicone rubbers and functional silanes,[1] however, the potential of this transformation expands beyond the production of bulk commodities. Numerous attractive transformations utilizing organosilanes, including the Fleming-Tamao-Kumada oxidation[2] and the Hiyama coupling,[3] have been developed and show silicon chemistry highly useful in fine chemicals synthesis.[4]

A significant amount of platinum is consumed each year by the silicon industry, which significantly contributes to the price of silicone commodities,[5a] and research in recent years has focused on replacing platinum with other, more earth-abundant and cheaper transition metals, namely iron, nickel, and cobalt.[1a,5] However, for many hydrosilylation products, such as volatile and soluble organosilanes, the valuable residual platinum can be separated by simple distillation of the product[6] or using other techniques (e.g., membrane-assisted nanofiltration),[7] thus the use of platinum for such processes is still justified, since the activity and selectivity both play a more important role than the cost of the catalyst, which can, in the end, be recycled.[1b]

Historically, the first widely used form of platinum in the catalytic hydrosilylation was hexachloroplatinic acid in isopropanol, introduced in 1957 and known as the Speier catalyst.[8] Significant improvement was made in 1973, when Karstedt described a platinum catalyst obtained from the reaction of hexachloroplatinic acid with 1,3-divinyltetramethyldisiloxane (dvtms),[9] although its structure was only solved several years later. The new complex gradually replaced Speier's catalyst in industrial applications due to its higher activity and shorter induction period. Up to this day, it is commonly used and serves as a standard for any new catalyst in the hydrosilylation of olefins.[5a] However, this catalyst possesses a number of important drawbacks. The Karstedt catalyst is not sufficiently selective and in a benchmark reaction between 1-octene (a model terminal alkene) and bis(trimethylsilyloxy)methylsilane (MD'M; a polymethylhydrosiloxane mimic) large amounts of undesired side-products are formed, especially isomerized and reduced alkenes.[10a] Furthermore, the low stability of this Pt(0) complex results in its degradation to platinum colloidal species, associated with the appearance of a yellow to dark brown color in the reaction mixture.[10a,7b]

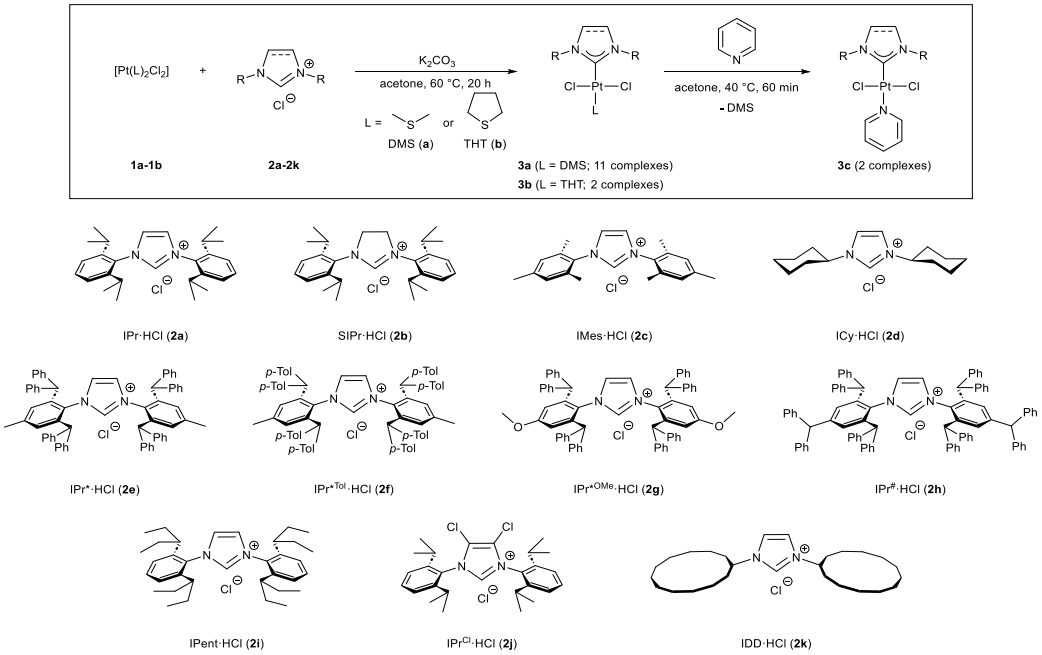
More recently, outstanding results were achieved by Markó and co-workers with Pt(0)-*N*-heterocyclic carbene complexes as pre-catalysts.[10] Compared to Karstedt's complex, the Pt(0)-NHC complexes were shown to be much more selective, presumably because of the increased steric protection around the platinum atom, enhancing the addition of platinum to the less hindered side of the olefin. What is equally important, due to the strength of the NHC-Pt bond, is that this new generation of catalysts is remarkably stable under the reaction conditions and no formation of platinum colloids was observed during the benchmark hydrosilylation reactions.[10a] In addition, Markó-type [Pt(NHC)(dvtms)] pre-catalysts are effective in hydrosilylation of olefins functionalized with Lewis

acid-sensitive groups, such as tetrahydropyranyl ethers and epoxides, which are not tolerated in reactions using Karstedt's catalyst.[10b]

Despite the long history and importance of platinum-catalyzed hydrosilylation, reflected in numerous research publications published over the past 65 years, some of the very basic principles of this transformation have been unraveled only recently, or still remain unknown.[11] One of the reasons behind this, is the highly elusive nature of the reactive platinum intermediates, including the active form of the catalyst.[12] Furthermore, much less attention has been devoted to Pt(II) hydrosilylation pre-catalysts. The existing literature reports suggest not only Pt(0)/Pt(II),[13] but also Pt(II)/Pt(IV)[14] variations of the widely accepted Chalk-Harrod mechanism,[15] and to the best of our knowledge the hypothesized Pt(II) → Pt(0) reduction in the pre-catalyst activation step has not yet been supported by convincing scientific evidence. In this contribution, we aim to explore the catalytic activity of a recently disclosed family of easily accessible well-defined Pt(II)-NHC pre-catalysts and explain their performance based on structural and spectroscopic descriptors.

Results and Discussion

In the course of recent studies, we have developed a sustainable and facile synthetic route to Pt(II)-NHC complexes (Scheme 1).[16] The operationally simple protocol, involving a weak-base-mediated[17] reaction between platinum precursors (**1**) and azolium salts (**2**) under mild and open-to-air conditions, allowed us to obtain a series of air- and moisture-stable complexes of general formula [Pt(NHC)(L)Cl_2] (**3**; L: DMS = dimethyl sulfide or THT = tetrahydrothiophene). Moreover, the use of [Pt_2(dvtms)$_3$] as a Pt(0) metal precursor allowed us to access the known Markó-type [Pt(NHC)(dvtms)] pre-catalysts. Some limitations were encountered, since some of the tested Pt(II) precursors, including [Pt(DMSO)$_2Cl_2$] (DMSO = dimethyl sulfoxide) and [Pt(Py)$_2Cl_2$] (Py = pyridine), as well as certain azolium salts, proved incompatible with the weak-base protocol, most likely due to solubility issues, and an alternative route to Pt-PEPPSI-type[18] [Pt(NHC)(Py)Cl_2] complexes, relying on simple DMS/Py ligand substitution, was proposed.



Scheme 1. The weak-base route to Pt(II)-NHC complexes and the precursors of NHC ligands used in this study.

All complexes used in this work were synthesized during the course of our previous studies,[16] except for **3ca** and **3be**, whose synthesis and characterization are presented in the experimental section. Having access to 15 complexes of the general formula [Pt(NHC)(L)Cl_2] (L: DMS, THT or Py), we next examined the impact of the NHC and sacrificial ligands L on the structure of the Pt(II)-NHC complexes, reflected by various structural and spectroscopic descriptors, and catalytic activity, to explore the structure-activity relationship and possibly gain new insights into the mechanism of Pt(II)-mediated catalytic hydrosilylation.

X-ray diffraction analyses

Single-crystal X-ray structures for all complexes, except for **3ca** and **3be**, have been previously disclosed as part of several reported studies.[16] In this section, we compare data of all existing and new complexes for a better understanding, and later in attempts to correlate their catalytic activity in the hydrosilylation reaction. Suitable single crystals were grown by slow diffusion of *n*-pentane into saturated solutions of Pt(II)-NHC complexes **3** in CH_2Cl_2 at 4 °C, or in case of the *n*-pentane-soluble **3ai** by slow evaporation of the solvent from a saturated solution in ^{i}PrOH at 4 °C.[19] All synthesized 16-electron d^8-Pt(II)-NHC complexes exhibit the expected square planar geometry. In **3ah**, bearing the bulkiest IPr$^{\#}$ ligand, the S-Pt-C2 angle (171.28(9)°) shows the highest deviation from the idealized 180° and the least bent angle is found in **3aa** (177.8°). The distances d(Pt-S) presented in Table 1 do not vary significantly within the series of *trans*-dimethyl sulfide and tetrahydrothiophene complexes (from 2.335(1) Å in **3ae** to 2.375(3) Å in **3ab**), however, they are slightly shortened in *cis*- complexes (2.2695(9) Å in ***cis*-3ad** and 2.261(1) Å in ***cis*-3ak**). The values for the pyridine analogues are clearly smaller (2.10(1)/2.070(6) Å in **3ca** and 2.110(4) Å in **3ce**), suggesting a stronger coordinate covalent bond, which explains the observed DMS/Py substitution reaction, occurring easily under mild conditions. The d(Pt-C2) distances vary from 1.960(6) Å (**3ca**) to 2.009(8) Å (**3ab**).

The steric impact of NHC ligands was quantified by the percent buried volume (%V_{bur})[20] and the values obtained from crystallographic data using the Samb*V*ca software[20c] are included in Table 1. Surprisingly, in contrast with the results based on the [Au(NHC)Cl] model,[21] the metal center of the bulkiest IPr$^{\#}$ complex (%V_{bur} of 38.6%) is noticeably less hindered than in the IPr*-type complexes (IPr*, IPr*^{OMe} and IPr*^{Tol}; %V_{bur} ranging from 41.2% to 43.4%). The lowest values were found for the *N*-alkyl substituted NHCs, IDD (%V_{bur} of 32.3%) and ICy (%V_{bur} of 27.1%). Figure 1 shows the molecular structures of the selected complexes and the topographic steric maps of the corresponding metal centers obtained using Samb*V*ca.

Table 1. Selected structural descriptors of the [Pt(NHC)(L)Cl_2] complexes.

Entry	[Pt]	d(Pt-C2) [Å]	d(Pt-L) [Å]	L-Pt-C2 angle [°][a]	NHC %V_{Bur} [%]
1	*trans*-[Pt(IPr)(DMS)Cl_2] (**3aa**)[16a]	1.987	2.343	177.8	33.7
2	*trans*-[Pt(IPr)(THT)Cl_2] (**3ba**)[16b]	1.980(3)	2.3519(9)	176.44(8)	35.5
3	*trans*-[Pt(IPr)(Py)Cl_2] (**3ca**)[b]	1.960(7)/ 1.960(6)	2.10(1)/ 2.070(6)	173.9(4)/ 178.0(2)	34.6/ 36.8
4	*trans*-[Pt(IPr*)(DMS)Cl_2] (**3ae**)[16a]	1.987(4)	2.335(1)	172.1(1)	42.3

5	*trans*-[Pt(IPr*)(THT)Cl_2] (**3be**)	1.995(3)	2.3505(8)	176.78(8)	41.2
6	*trans*-[Pt(IPr*)(Py)Cl_2] (**3ce**)[16b]	1.970(4)	2.110(4)	177.3(2)	43.1
7	*trans*-[Pt(SIPr)(DMS)Cl_2] (**3ab**)[16a][b]	1.98(1)/	2.352(3)/	175.7(3)/	35.7/
		2.00(1)/	2.358(3)/	174.4(3)/	36.2/
		2.009(8)	2.375(3)	174.0(3)	35.4
8	*trans*-[Pt(IMes)(DMS)Cl_2] (**3ac**)[16a]	1.998(5)	2.352(1)	173.2(2)	33.8
9	*cis*-[Pt(ICy)(DMS)Cl_2] (***cis*-3ad**)[16a]	1.984(4)	2.2695(9)	176.3(1)	27.1
10	*trans*-[Pt(IPr*^{Tol})(DMS)Cl_2] (**3af**)[16b][b]	1.983(3)/	2.336(1)/	177.7(1)/	41.2/
		1.988(3)	2.3411(9)	174.7(1)	43.4
11	*trans*-[Pt(IPr*^{OMe})(DMS)Cl_2] (**3ag**)[16b]	1.990(4)	2.339(2)	172.5(1)	41.8
12	*trans*-[Pt(IPr$^{\#}$)(DMS)Cl2] (**3ah**)[16b]	1.985(3)	2.3442(8)	171.28(9)	38.6
13	*trans*-[Pt(IPent)(DMS)Cl_2] (**3ai**)[16b][b]	1.976(4)/	2.340(1)/	173.6(1)/	41.3/
		1.985(4)	2.349(1)	175.8(1)	40.9
14	*trans*-[Pt(IPr^{Cl})(DMS)Cl_2] (**3aj**)[16b]	1.987(2)	2.3487(9)	172.93(7)	34.3
15	*cis*-[Pt(IDD)(DMS)Cl_2] (***cis*-3ak**)[16b]	1.972(6)	2.261(1)	177.3(2)	32.3

[a] Cl-Pt-C2 angle in case of the *cis*- complexes (***cis*-3ad** and ***cis*-3ak**). [b] Complexes **3ca**, **3ab**, **3af** and **3ai** contain 2-3 different molecules within the asymmetric unit.

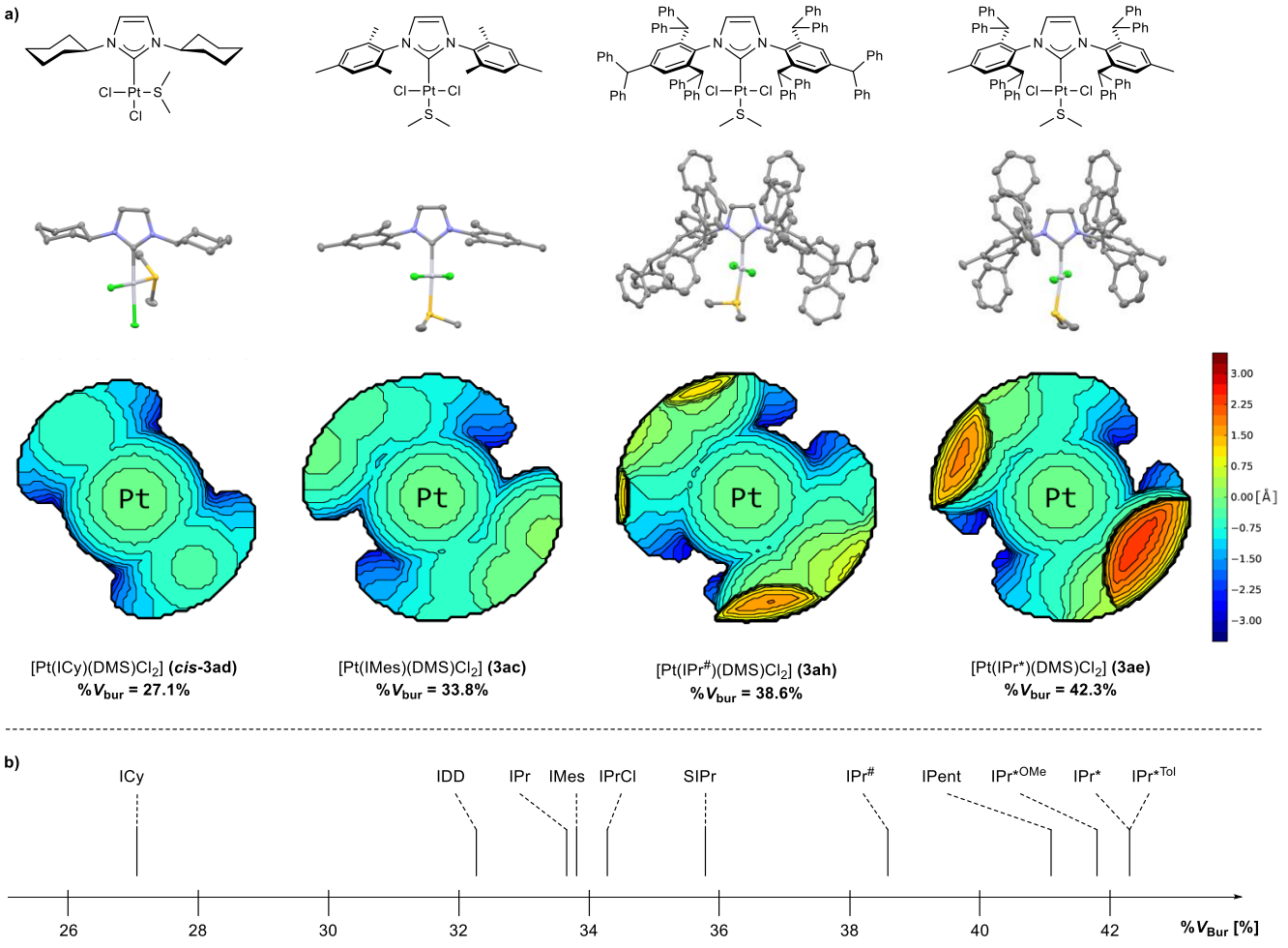


Figure 1. a) Molecular structures of the selected complexes, showing thermal displacement ellipsoids at the 50% probability level, and the corresponding steric maps. Hydrogen atoms and solvent molecules are omitted for clarity and excluded in calculating %V_{bur}; b) Percent buried volumes of the NHC ligands in [Pt(NHC)(DMS)Cl_2] complexes.

^{1}H, ^{13}C and ^{195}Pt NMR spectroscopic studies

Nuclear magnetic resonance spectroscopy, especially ^{13}C NMR, is an invaluable tool for understanding and quantifying the unique properties of NHC ligands.[22] A characteristic feature in ^{1}H NMR spectra of the dimethyl sulfide complexes are very distinct platinum satellites associated with $S(CH_3)_2$ proton signals at around 2.00-2.50 ppm. Despite that both short- and long-range Pt-C couplings are clearly visible in the ^{13}C NMR spectra of Pt(0) [Pt(NHC)(dvtms)] complexes,[10d] the Pt satellites could not be easily detected in the carbon spectra of our Pt(II)-NHC compounds. The most interesting peak in the ^{13}C NMR spectra, the C2 carbene signal, provides insightful information on the new pre-catalysts.[22b] These values in Table 2 vary from 139.3 ppm (**3ce**) to 179.7 ppm (**3ab**). The C2 signal for most of the SR_2-based *trans*-complexes appears within a narrow range of values, between 147.8 ppm (***trans*-3ak**) and 152.4 ppm (**3aa**), except for the backbone-substituted **3aj** (IPr^{Cl}; 156.1 ppm) and imidazolidinium-derived **3ab** (SIPr; 179.7 ppm), which clearly stand out (Table 2 and Figure 2). Almost no difference is observed between DMS and THT complexes bearing the same NHC ligands, however, the pyridine analogues are shifted upfield by roughly 10 ppm (143.3 ppm for **3ca** and 139.3 ppm for **3ce**). A similar effect is observed for the *cis*-isomers (141.7 ppm for ***cis*-3ad** and 142.6 ppm for ***cis*-3ak**). The ^{195}Pt signals appear within the wide range of values reported for neutral Pt(II) tetracoordinate complexes,[23] and the values for *trans*-

[Pt(NHC)(DMS)Cl_2] complexes vary from -3325 ppm for **3ab** to -3232 ppm for **3ac**. The shifts reported in Table 2 reveal a considerable difference between Py complexes and their THT and DMS analogues. The ^{195}Pt signals of the Pt-PEPPSI-type **3ca** and **3ce** are shifted downfield by about 400 ppm. The platinum chemical shift also depends significantly on the geometry of the complexes;[23] i.e. the *cis*-isomer of **3ak** is shifted upfield by some 200 ppm relative to that found for the ***trans*-3ak**.

Table 2 also includes the experimental values of the widely used Tolman electronic parameter (TEP), quantifying the electron-donating properties of the ligands based on the IR stretching frequencies of the carbonyl ligands in Ni(0)-, Ir(I)- or Rh(I)-NHC-carbonyl complexes, with lower values indicating increased electron density on the metal centre.[24a,b,c] The δ_{C2}/δ_{Pt}/TEP trends across the series of *trans*-[Pt(NHC)(DMS)Cl_2] complexes are presented in Figure 2. Unfortunately, for the most part, no direct correlation between the different spectroscopic parameters is observed, even when the considered series is narrowed down to only a few closely related complexes (e.g., **3aa**, **3ac**, **3ae**, **3ah**, **3ai**). In particular, the diagnostic C2 carbene signal shifts of the *trans*-[Pt(NHC)(DMS)Cl_2] complexes do not correlate with the TEP parameters of the corresponding NHC ligands. When comparing IDD and ICy, the only ligands to afford cis-complexes, to the rest of the series, we observe that they are the most electron-donating ligands based on the TEP.

Table 2. Selected spectroscopic descriptors of the [Pt(NHC)(L)Cl_2] complexes.

Entry	[Pt]	δ_{C2} [ppm][a,b]	δ_{Pt} [ppm][b]	TEP_{NHC} [cm^{-1}]
1	*trans*-[Pt(IPr)(DMS)Cl_2] (**3aa**)	152.4	-3278	2051.5[24c]
2	*trans*-[Pt(IPr)(THT)Cl_2] (**3ba**)	152.4[c]	-3268	2051.5[24c]
3	*trans*-[Pt(IPr)(Py)Cl_2] (**3ca**)	143.3[c]	-2878	2051.5[24c]
4	*trans*-[Pt(IPr*)(DMS)Cl_2] (**3ae**)	148.9	-3315	2052.7[24d]
5	*trans*-[Pt(IPr*)(THT)Cl_2] (**3be**)	148.8	-3295	2052.7[24d]
6	*trans*-[Pt(IPr*)(Py)Cl_2] (**3ce**)	139.3	-2928	2052.7[24d]
7	*trans*-[Pt(SIPr)(DMS)Cl_2] (**3ab**)	179.7	-3325	2052.2[24c]
8	*trans*-[Pt(IMes)(DMS)Cl_2] (**3ac**)	151.0	-3232	2050.7[24c]
9	*cis*-[Pt(ICy)(DMS)Cl_2] (***cis*-3ad**)	141.7	-3489	2049.6[24c]
10	*trans*-[Pt(IPr*^{Tol})(DMS)Cl_2] (**3af**)	148.5	-3315	-
11	*trans*-[Pt(IPr*^{OMe})(DMS)Cl_2] (**3ag**)	149.6	-3318	2051.1[24d]
12	*trans*-[Pt(IPr$^{\#}$)(DMS)Cl_2] (**3ah**)	149.7	-3315	2051.8[21]
13	*trans*-[Pt(IPent)(DMS)Cl_2] (**3ai**)	150.6	-3276	2049.3[24e]
14	*trans*-[Pt(IPr^{Cl})(DMS)Cl_2] (**3aj**)	156.1	-3261	2055.1[24f]
15	*cis*-[Pt(IDD)(DMS)Cl_2] (***cis*-3ak**)	142.6	-3481	2049.0[24g]
16	*trans*-[Pt(IDD)(DMS)Cl_2] (***trans*-3ak**)	147.8	-3281	2049.0[24g]

[a] Taken from Ref. 16. [b] The NMR spectra were recorded in $CDCl_3$. [c] The carbene signals could not be located in the ^{13}C NMR spectra and were misassigned in the original synthetic reports. See experimental section for the correct NMR data.

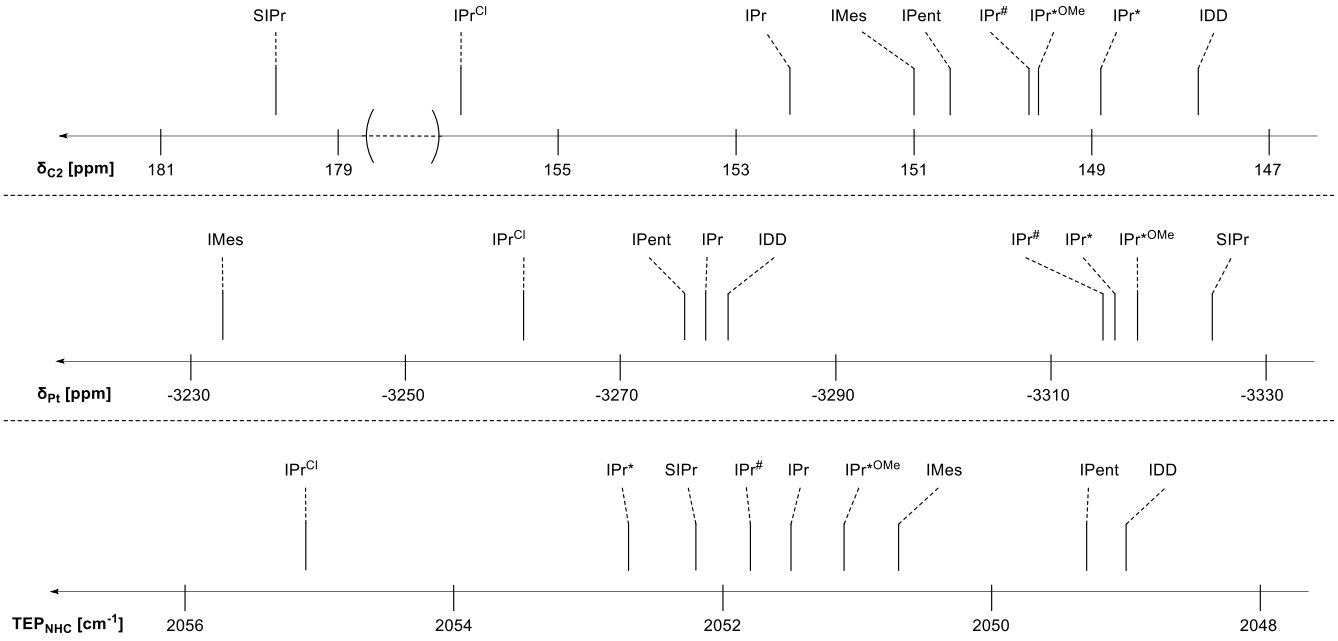
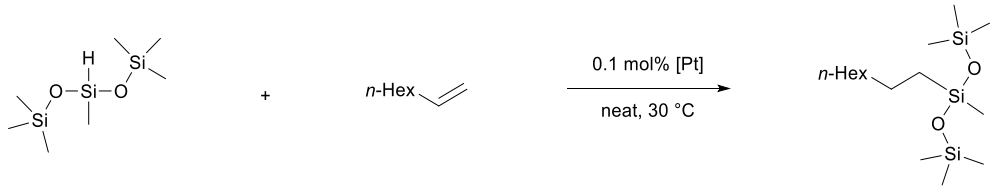


Figure 2. Spectroscopic descriptors of the *trans*-[Pt(NHC)(DMS)Cl_2] complexes and the TEP values for the corresponding NHC ligands.

Catalytic activity in a model hydrosilylation reaction

In our recent reports, we have demonstrated the catalytic activity of two of the novel [Pt(NHC)(DMS)Cl_2] complexes in a solventless model reaction between 1,1,1,3,5,5,5-heptamethyltrisiloxane (**4a**) and 1-octene (**5b**). During the initial attempts, the SIPr complex (**3ab**) appeared to be the most active of all pre-catalysts,[16a] however, subsequent optimization of the procedure revealed that much shorter reaction times can be achieved when the pre-catalyst is added in a solid form, instead of as a solution in toluene. Further developments were made during parallel studies on a membrane-integrated continuous hydrosilylation process,[7b] when we unexpectedly discovered that the complex bearing bulky IPr* ligand (**3ae**) allows the model reaction to proceed rapidly even at room temperature. Herein, we examined the catalytic activity of all the analogous Pt(II)-NHC pre-catalysts under similar reaction conditions (Table 3).

Table 3. Pre-catalyst screening.



4a **5b** **6ab**

Entry	[Pt]	Yield [%][a]					TON/TOF [h^{-1}][b]
		5 min	60 min	150 min	300 min	24 h	
1	[Pt(IPr)(DMS)Cl_2] (**3aa**)	1	7	49	72	94	720/144
2	[Pt(IPr)(THT)Cl_2] (**3ba**)	0	0	0	0	1	0/0

3	[Pt(IPr)(Py)Cl_2] (**3ca**)	0	0	0	0	0	0/0
4	[Pt(IPr*)(DMS)Cl_2] (**3ae**)	97	97	97	98	99	980/196
5	[Pt(IPr*)(THT)Cl_2] (**3be**)	97	97	97	97	98	970/194
6	[Pt(IPr*)(Py)Cl_2] (**3ce**)	0	0	0	0	1	0/0
7	[Pt(SIPr)(DMS)Cl_2] (**3ab**)	0	0	96	97	97	970/194
8	[Pt(IMes)(DMS)Cl_2] (**3ac**)	0	0	0	0	17	0/0
9	[Pt(ICy)(DMS)Cl_2] (***cis*-3ad**)	0	1	1	2	98	20/4
10	[Pt(IPr*^{Tol})(DMS)Cl_2] (**3af**)	85	95	97	98	99	980/196
11	[Pt(IPr*^{OMe})(DMS)Cl_2] (**3ag**)	94	97	97	97	97	970/194
12	[Pt(IPr$^{\#}$)(DMS)Cl_2] (**3ah**)	9	93	97	97	97	970/194
13	[Pt(IPent)(DMS)Cl_2] (**3ai**)	0	0	1	1	25	10/2
14	[Pt(IPr^{Cl})(DMS)Cl_2] (**3aj**)	0	0	0	1	4	10/2
15	[Pt(IDD)(DMS)Cl_2] (***cis*/*trans*-3ak**)[c]	1	2	3	6	95	60/12
16	[Pt(IPr)(dvtms)]	0	0	1	18	93	180/36
17	[Pt(ICy)(dvtms)]	0	12	51	74	89	740/148
18	[Pt(IPr*)(dvtms)]	0	0	2	19	80	190/38
19	[Pt_2(dvtms)$_3$]	85	87	88	88	88	880/176

[a] Determined by GC (average of at least two runs). See experimental section for details. [b] Based on GC yield after 300 min at 0.1 mol% catalyst loading. [c] The pre-catalyst was used in form of a mixture of two isomers (*cis*/*trans* ratio = 66:34).

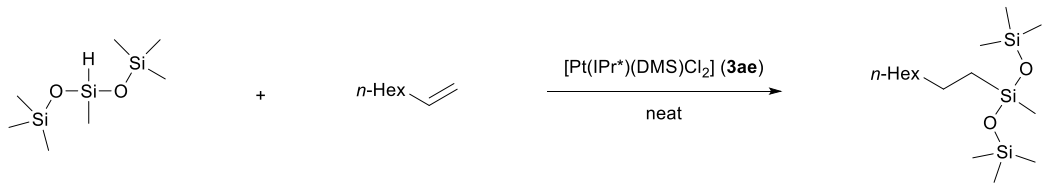
While many of the tested Pt(II) pre-catalysts did not exhibit any significant catalytic activity within 5 hours at 30 °C, the complexes closely related to the sterically congested **3ae**, the tetrahydrothiophene IPr* analogue (**3be**), as well as the IPr*^{OMe} pre-catalyst (**3ag**), displayed similar and exceptional performance (94-97% yield of **6ab** after just 5 min). The IPr*^{Tol} complex (**3af**) performed almost as well (85% yield after 5 min), and the somewhat less sterically hindered IPr$^{\#}$ complex (**3ah**) required 60 min to reach 93% yield of the desired product. SIPr (**3ab**) and IPr (**3aa**) dimethyl sulfide complexes turned out to be less active (respectively 97% and 49% yield of **6ab** after 150 min), and a significant induction time was observed in reactions with the *N*-alkyl substituted complexes ICy (***cis*-3ad**) and IDD (***cis*/*trans*-3ak**), both being the least sterically hindered complexes in this study (based on the %V_{bur}) while also featuring the most electron-donating NHC ligands (based on TEP values). Nonetheless, in both cases, the reaction reached completion after 24 hours. These results suggest a correlation between %V_{bur} and the catalytic performance, but the poor catalytic activity of **3ba**, **3ac**, **3ai** and **3aj** remains unclear. Replacing DMS or THT with pyridine leads to a significant decrease in catalyst efficiency and no conversion was observed in the reactions with **3ca** and **3ce**. The presence of a sterically congested IPr*-type *N*-heterocyclic carbene and a thioether sacrificial ligand appears to be the optimal combination.

Interestingly, all three tested Markó-type [Pt(NHC)(dvtms)] were much less efficient than **3ae** at 30 °C, with the ICy-based complex being the most active of the three. The %V_{Bur}/activity trend for the three dvtms-based

complexes, being the opposite to the one observed with our Pt(II)-NHC pre-catalysts, displayed the least activity for the bulky [Pt(IPr*)(dvtms)] complex. We also tested the Karstedt catalyst ([Pt_2(dvtms)$_3$]) under these reaction conditions, and while the reaction reached full conversion of the substrates within approximately the same amount of time as with the most active Pt(II)-NHC pre-catalyst, the conversion of the substrates was less selective and resulted in 88% GC yield of **6ab**. The Karstedt catalyst is known to produce significant amount of isomerized alkene as a byproduct, however, based on the previously published results, we were expecting the yield of the desired product to be somewhat lower (<80%).[10a] It is worth mentioning that all hydrosilylation reactions carried out with Pt-NHC complexes (Table 3, Entries 1-18) resulted in colorless post-reaction mixtures, and no coloration of the product, characteristic of [Pt_2(dvtms)$_3$], was observed. Encouraged by the initial results, we explored the catalytic activity of **3ae** in more detail (Table 4).

The model reaction proceeds rapidly at room temperature using 10-times lower amount of the catalyst (Table 4, Entry 2), and takes just a few hours with 0.001 mol% (10 ppm) of [Pt] (Table 4, Entry 3). We also carried out a reaction at RT using 1 ppm of [Pt] and even though initially the reaction did not appear to proceed, a sample taken two weeks later revealed complete conversion of the model substrates. Increasing the temperature to 80 °C allowed us to obtain the desired hydrosilylation product within approximately 24 hours at this loading (97% GC purity; TON = 970 000, TOF = 40 417 h^{-1}; Table 4, Entry 4).

Table 4. Optimization of the reaction conditions.



4a **5b** **6ab**

Entry	Cat. loading [mol%]	Additive	T [°C][a]	Time	1-Octene conversion [%][b]
1	0.1	-	RT	5 min	>99
2	0.01	-	RT	15 min	>99
3	0.001	-	RT	6 h	>99
4	0.0001	-	80	24 h	>99
5	0.1	0.06 equiv. Py	RT	60 min	0
6	0.1	2.0 equiv. DMS	RT	60 min	0
7	0.1	0.02 equiv. HCl[c]	RT	60 min	0
8	0.1	0.34 equiv. Hg[d]	RT	15 min	45

[a] Room temperature (RT): 18-22 °C. [b] Determined by ^{1}H NMR. [c] Dioxane solution of HCl was used (4.0 M). [d] Mercury drop test. The reaction reached completion after 60 min.

Mechanistic considerations

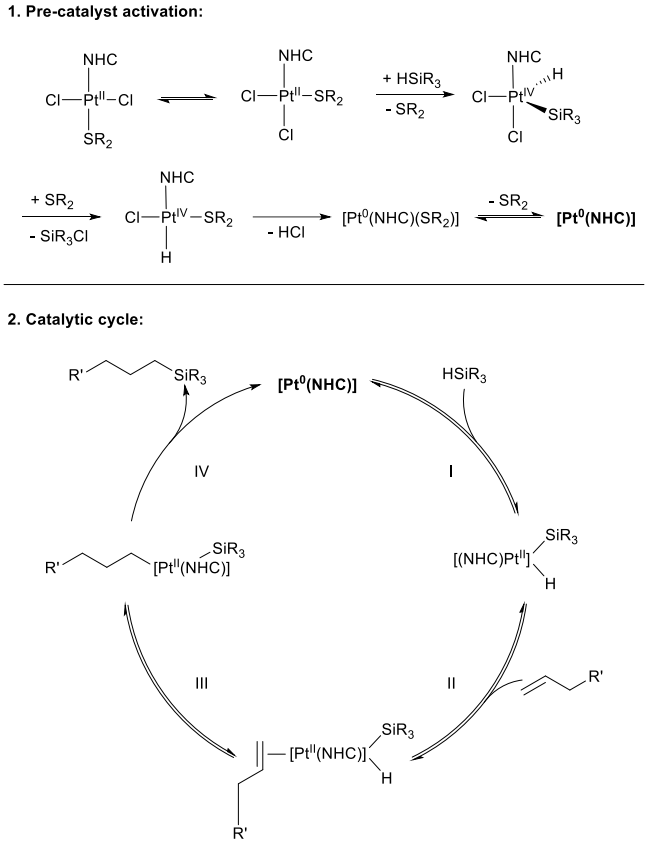
Entries 5-8 in Table 4 show that the studied catalytic system is sensitive to certain inhibitors. Entries 5-6 suggest that the sacrificial ligand needs to decoordinate at an early stage along the reaction pathway, which also explains why the pyridine-Pt(II)-NHC complex **3ce** does not match the activity of **3ae**. Dimethyl sulfide, a soft Lewis donor, is a superior sacrificial ligand for the soft acidic Pt-centre. It provides the essential stability to the Pt(II)-NHC pre-catalysts, while also being labile enough to be easily displaced during catalysis to facilitate the catalyst activation step. The model reaction is also inhibited by small amounts of HCl as seen in entry 7 (Table 4). Reacting **3ae** separately with up to 8.0 equivalents of HCl at 70 °C did not lead to any change or decomposition in the NMR spectrum, which suggests that the HCl inhibition pathway is not directly related to the Pt(II)-pre-catalyst, but most likely is associated with an unfavorable shift of the reaction equilibrium at a stage involving reductive elimination of HCl from the envisioned Pt(II)-hydride intermediate, leading to a Pt(0) active form of the catalyst (see Scheme 2). In addition, a decreased catalytic activity was observed in a mercury drop test (Table 4, Entry 8). A similar effect has already been reported for Pt(0)-NHC complexes,[10g] however, the mercury test is known to be inconclusive in assessing the contribution of platinum nanoclusters and nanoparticles in an overall reaction mechanism.[25]

Furthermore, we carried out a series of stoichiometric reactions involving **3ae** and the model silane **4a** in various NMR solvents ($CDCl_3$, benzene-d_6, toluene-d_8) with the ratios **3ae**/**4a** ranging from 1:1 to 1:20, however, we were unable to detect any shifts for the pre-catalyst signals or to detect the appearance of a hydride peak.[11] [Pt] intermediates are known to be elusive,[12] and the appearance of a faint dark yellow tint in the measured NMR samples over the course of 2-3 weeks at room temperature was observed, suggesting a slow reaction resulting in a formation of platinum colloidal species, which was confirmed in a reaction between **3ae** and **4a** in toluene at 80 °C by UV-VIS spectroscopy (see Supporting Information). These results support the assumption that the activation step involves a reaction between the pre-catalyst and **4a**, however, the exact reaction pathway remains unclear. Even though Pt colloids were not visibly detected in hydrosilylation mixtures when using Pt-NHC complexes as pre-catalysts,[10a,g,i] the observed slow formation of Pt colloids in our case, when reacting **3ae** and **4a** stoichiometrically, indicates the possible "cocktail" nature of the studied catalytic system. This is similar to the recently described system by Ananikov and co-workers,[12c] involving multiple platinum active species (both nanoclusters/nanoparticles and molecular complexes). Unfortunately, in the case of our neat protocol utilizing [Pt(IPr*)(DMS)Cl_2], the contribution of platinum colloidal species to the overall reaction mechanism has proven challenging to assess. On the other hand, the excellent selectivity of the model reaction suggests a low contribution of Pt-colloids, which often cause undesired side reactions.[10a,i]

In silico studies, focusing on *cis*-*trans* isomerization and DMS decoordination energies across the series of [Pt(NHC)(DMS)Cl_2] complexes, provide further insights into the activation step (Table 5). The theoretical energy barriers associated with DMS dissociation are quite similar across the studied series of pre-catalysts, ranging from only 16.3 to 18.5 kcal mol^{-1}, and do not correlate well with the catalytic performance, however, they are much lower than the values calculated for dvtms-dissociation in the Pt(0)-dvtms complexes (43.5 kcal mol^{-1} for [Pt(IPr)(dvtms)] and 35.3 kcal mol^{-1} for [Pt(ICy)(dvtms)]).

Although the calculated *cis*-*trans* isomerization processes show that the *trans*-isomer is the energetically favored form for almost all of the studied complexes, the results unexpectedly suggest an exceptional, isoenergetic character of the IPr*-type complexes (Table 5, Entries 4, 8, 9 and 10). To confront the theoretical values with experiments, *trans*-**3ae** (IPr*) and **3ak** (IDD; *cis*/*trans* ratio = 66:34) were dissolved in $CDCl_3$ and heated to 70 °C. In line with the *in silico* results, ^{1}H NMR spectra of the IDD complex revealed a slow *cis*-*trans* isomerization occurring at high temperature (Figure 3; *cis*/*trans* ratio = 37:63 after 144 h) and no isomerization was observed for the IPr* complex (see experimental section). Even though the thermodynamics included in Table 4 between the 2 isomers of [Pt(NHC)(DMS)Cl_2], *cis* and *trans*, do not exactly correlate to the experimental observations regarding the hydrosilylation performance, some trends can be extrapolated allowing us to present a proposal for

the reaction mechanism in Scheme 2. Based on experimental and theoretical evidence as well as previous postulations,[12b] we suggest that both *cis*/*trans* isomerization and reductive elimination of HCl are key steps in the pre-catalyst activation, considering that the most efficient reactions were obtained with the sterically hindered and *cis*/*trans*-isoenergetic complexes **3ae**, **3af**, **3ag** and **3ah** (all with *cis*/*trans* ΔG difference lower than 0.8 kcal mol^{-1}). Taking into account that the *trans*-isomer is the more thermodynamically stable isomer for all other complexes, these high performing *cis*/*trans*-isoenergetic complexes point towards a possible correlation between the ease of DMS-dissociation/association to generate the *cis*-isomer and a faster precatalyst activation and/or initiation time. Once the [Pt^0(NHC)] active species is formed, it enters the catalytic cycle similar to previously postulated systems.[13] In addition, DMS stabilization of the Pt(0) active species or its involvement in the catalyst resting state cannot be dismissed at this point. DFT calculations and kinetic trials are still ongoing in our groups to better illustrate the mechanism, but so far no clear or publishable conclusions can be reached.



Scheme 2. Proposed hydrosilylation mechanism. Steps I-IV in the catalytic cycle: I - oxidative addition of the silane; II – olefin coordination; III – olefin insertion of the olefin into the Pt-H bond; IV – reductive elimination of alkylsilane. NHC = IPr*.

Table 5. Relative Gibbs free energies in kcal mol^{-1} for the *cis* and *trans* isomers of [Pt(NHC)(DMS)Cl_2] complexes, and their corresponding DMS-dissociated species.[a]

Entry	NHC	ΔG [kcal mol^{-1}]		
		trans-[Pt(NHC)(DMS)Cl_2]	*cis*-[Pt(NHC)(DMS)Cl_2]	*trans*-[Pt(NHC)Cl_2]
1	ICy	0.0	5.1	17.1
2	IPr	0.0	4.4	17.5
3	SIPr	0.0	3.4	16.3
4	IPr*	0.0	0.1	17.2
5	IPent	0.0	4.1	17.3
6	IMes	0.0	3.5	16.8
7	IDD	0.0	8.0	18.3
8	IPr*^{Tol}	0.0	0.4	16.5
9	IPr$^{\#}$	0.0	-0.1	17.1
10	IPr*^{OMe}	0.0	0.8	17.0
11	IPr^{Cl}	0.0	4.0	18.5

[a] Calculated in 1-octene as a solvent. See Supporting Information for additional details.

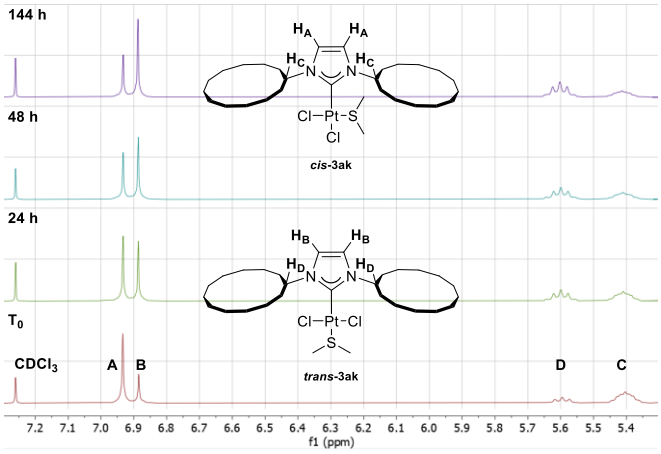
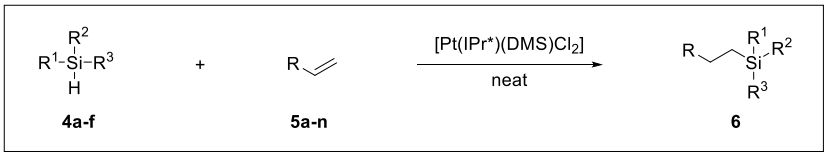


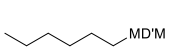
Figure 3. Stacked ^{1}H NMR spectra of **3ak** in $CDCl_3$, showing *cis*/*trans* isomerization occurring at 70 °C.

Substrate scope studies

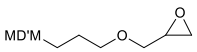
Next, we investigated the substrate scope of our optimized hydrosilylation reaction conditions (Scheme 3). The simple protocol, featuring a solventless and open-to-air reaction, allowed us to obtain a series of organosilanes in very good to excellent yields; however, many of the substrates required increased reaction temperature. Nonetheless, reactions which were carried out at 110 °C highlighted the thermal stability of the catalyst (**6ad** and **6ae**). Some of the examples demonstrating the scope of compatible alkenes included bromo- and ester-functionalized derivatives (**6al** and **6am**, respectively). The developed protocol was also compatible with sensitive epoxy-functionalized olefins (**6af** and **6ag**) and allowed us to obtain the desired hydrosilylation products with natural allylbenzene-derived estragole (**6ah**) and eugenol (**6ai**). In addition, increasing the catalyst loading to 0.5 mol% allowed us to obtain full conversion of styrene (**6an**), with the ratio of linear and branched hydrosilylation products comparable with other Pt(II)-NHC pre-catalysts.[10i,j] The scope of compatible silanes includes industrially relevant 2,4,6,8-tetramethylcyclotetrasiloxane (**6fb**).

To examine the possibility of a more challenging hydrosilylation, involving selectively only one of the terminal alkene groups, a reaction between 1,7-octadiene and 1.0 equiv. of MD'M was attempted (**6aj'**), however, a mixture of mono- and dihydrosilylated products was obtained (**6aj'**/**6aj** = 60:40). On the other hand, **6aj** can be selectively obtained if the amount of MD'M is increased accordingly. In all other cases, except for **6an**, the reactions proceeded with great selectivity and the post-reaction mixtures consisted of NMR-pure colorless products. Depending on the used catalyst loading, the only potentially problematic impurity appears to be the residual catalyst. Herein, we report that a facile workup, consisting of a simple filtration through a mixture of florisil/celite/$MgSO_4$ (1:1:1 m/m/m), allows the reduction of residual Pt from 582 ppm to 5.8 ppm, when **3ae** is used as pre-catalyst (see experimental section). An alternative and sustainable approach based on membrane nanofiltration technology that allows for continuous processing/purification has been demonstrated in our previous report.[7b]

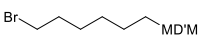




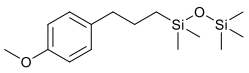
6aa
89% (0.01 mol% [Pt], RT, 15 min)



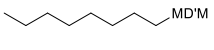
6ag
95% (0.01 mol% [Pt], 80 °C, 6 h)



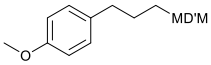
6al
98% (0.1 mol% [Pt], 80 °C, 6 h)



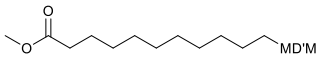
6bh
99% (0.01 mol% [Pt], 80 °C, 20 h)



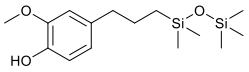
6ab
99% (0.01 mol% [Pt], RT, 15 min



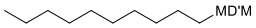
6ah
98% (0.01 mol% [Pt], 80 °C, 20 h)



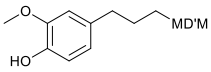
6am
99% (0.1 mol% [Pt], 80 °C, 20 h)



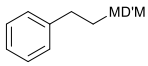
6bi
99% (0.01 mol% [Pt], 80 °C, 20 h)



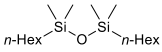
6ac
96% (0.01 mol% [Pt], 80 °C, 6 h)



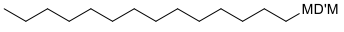
6ai
95% (0.01 mol% [Pt], 80 °C, 18 h)



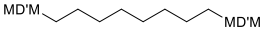
6an
>99%[b] (0.5 mol% [Pt], 80 °C, 22 h)



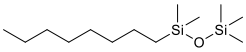
6ea
96% (0.01 mol% [Pt], 60 °C, 24 h)



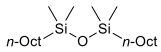
6ad
98% (0.01 mol% [Pt], 110 °C, 160 min)



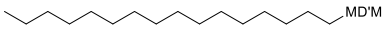
6aj
93% (0.01 mol% [Pt], 80 °C, 24 h)



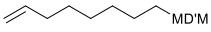
6bb
99% (0.01 mol% [Pt], 80 °C, 4 h)



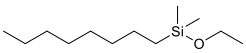
6eb
98% (0.01 mol% [Pt], 60 °C, 24 h)



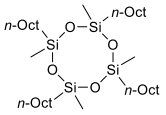
6ae
95% (0.01 mol% [Pt], 110 °C, 6 h)



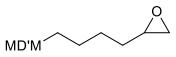
6aj'
43%[a] (0.1 mol% [Pt], 80 °C, 24h)



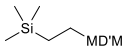
6cb
96% (0.01 mol% [Pt], 60 °C, 4 h)



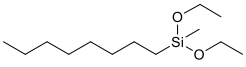
6fb
97% (0.01 mol% [Pt], 80 °C, 22 h)



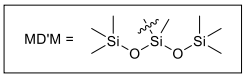
6af
94% (0.01 mol% [Pt], 80 °C, 6 h)



6ak
94% (0.01 mol% [Pt], 80 °C, 24 h)



6db
97% (0.01 mol% [Pt], 60 °C, 4 h)



Scheme 3. Substrate scope. The reaction conditions are listed in brackets and the yields refer to isolated products. See experimental section for details. [a] Determined by GC; a mixture of products and unreacted diene was isolated (**6aj'**/**6aj** = 60:40). [b] Styrene conversion (determined by ^{1}H NMR). A mixture of linear (***l***) and branched (***b***) products was isolated (***l***/***b*** ratio = 84:16); total isolated yield of both hydrosilylation products: 92%.

Conclusion

In summary, we have examined the structure/activity of a group of Pt(II)-NHC pre-catalysts. The experimental and theoretical evidence provide insights into the pre-catalyst activation step and information about the optimal elements for the catalyst design: the sterically hindered IPr*-type complexes, bearing weakly coordinating thioether-based DMS ligand are the most active in the model alkene hydrosilylation reaction and prove superior to the Markó-type Pt(0)-NHC complexes. The [Pt(IPr*)(DMS)Cl$_2$] pre-catalyst was also used to obtain a series of alkylsilanes, following a sustainable, neat, and open-to-air protocol. Furthermore, we have shown that the use of **3ae** allows easy platinum removal and a 100-fold reduction in the residual Pt levels can be achieved by a simple filtration, using widely available and inexpensive filter aids.

Experimental Section

General information

All chemical syntheses were performed in glass vials under air. Solvents and all other reagents were purchased and used as received without any additional purification, except for K_2CO_3, which was finely grinded (using a mortar and pestle) and dried under high vacuum before use. ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ using Bruker 300 and 400 MHz spectrometers. All chemical shifts are quoted in parts per million referenced to the $CHCl_3$ solvent residue (δ_H = 7.26 ppm, δ_C = 77.16 ppm). ^{1}H NMR splitting patterns are abbreviated as follows: broad signal (br), singlet (s), doublet (d), triplet (t), doublet of doublets (dd), doublet of triplets (dt), triplet of triplets (tt), quartet (q), quintet (quint), heptet (hept), multiplet (m). ^{195}Pt NMR spectra were recorded in $CDCl_3$ on a Bruker AVANCE NEO 400 MHz spectrometer (^{1}H = 400 MHz, ^{195}Pt = 86 MHz) equipped with a z-gradiented 5 mm TBI ^{1}H/^{13}C/broad-band probe at 300 K. The standard 1D-^{195}Pt{^{1}H} experiment settings were 2 s recycling delay, 2 s acquisition time, with a 30° pulse (90° being 18.5 µs at 100 W), and 512, 1000 (compounds **3aa**, **3ab** and **3ce**), 3000 (compound **3ag**) or 16000 (compounds **3ae** and **3ak**) scans according to the ^{195}Pt peak width. The spectra were processed with a 10 Hz exponential apodization function. The ^{195}Pt chemical shifts values were referenced using an external reference, [Pt(IPr*)(dvtms)], with δ(^{195}Pt) = -5320.94 ppm,[10g] recorded with 512 scans. The spectrum reference frequency (Bruker sr parameter) determined in the reference spectrum was applied on the spectra recorded on the compounds of interest. Previously reported Pt(0)- and Pt(II)-NHC complexes were synthesized following the procedures described in the literature.[16] The general hydrosilylation procedure (**A**) was used for catalyst screening (Table 3) and the general hydrosilylation procedure (**B**) was used to synthesize the products presented in Scheme 3. The platinum content after the simple filtration was determined by ICP analysis of a sample obtained by digestion of **6ab** with 3 mL of HCl, 1 mL of HNO_3 and 2 mL of HF for 120 min at 105 °C.

Synthesis of [Pt(IPr*)(THT)Cl_2] (3be)

A vial was charged with [Pt(THT)$_2$$Cl_2$] (113 mg, 0.256 mmol, 1.0 equiv.), IPr*·HCl (243 mg, 0.256 mmol, 1.0 equiv.), freshly dried and crushed K_2CO_3 (142 mg, 1.024 mmol, 4.0 equiv.) and acetone (5.0 mL). The vial was closed with a septum screw cap and the reaction mixture was stirred at 60 °C for 20 h. After this time, the reaction volatiles were removed under vacuum, 3.0 mL of CH_2Cl_2 was added and the resulting mixture was filtered through a layer of silica gel (2-3 cm) in a Pasteur pipette. The silica gel was washed with 10.0 mL of CH_2Cl_2 and the filtrate was concentrated to dryness under reduced pressure. The obtained residue was sonicated for 1 min at room temperature with 5.0 mL of *n*-pentane to induce precipitation of the product. The resulted solid was washed with *n*-pentane (3x5.0 mL) and dried under high vacuum, affording 290 mg (89%) of the product as a pale yellow microcrystalline solid. The crystals for single-crystal X-ray diffraction analysis were grown by slow diffusion of *n*-pentane into a concentrated solution of **3be** in CH_2Cl_2 at 4 °C. **^{1}H NMR** (400 MHz, $CDCl_3$): δ (ppm) = 7.47 – 7.36 (m, 8H, C**H**$_{Ar}$), 7.29 – 7.13 (m, 12H, C**H**$_{Ar}$), 7.09 – 6.95 (m, 12H, C**H**$_{Ar}$), 6.77 – 6.65 (m, 12H, C**H**$_{Ar}$), 6.21 (s, 4H, C**H**(Ph)$_2$), 4.80 (s, 2H, NC**H**=C**H**N), 3.66 – 2.86 (br, 4H, S(C**H**$_2$)$_2$), 2.20 (s, 6H; C**H**$_3$), 2.10 – 1.97 (br, 4H, S(CH$_2$)(C**H**$_2$)). **^{13}C NMR** (101 MHz, $CDCl_3$): δ (ppm) = 148.8 (N-**C**-N), 144.6 (**C**^{IV}$_{Ar}$), 144.5 (**C**^{IV}$_{Ar}$), 141.7 (**C**^{IV}$_{Ar}$), 138.2 (**C**^{IV}$_{Ar}$), 135.2 (**C**^{IV}$_{Ar}$), 130.6 (**C**H$_{Ar}$), 130.5 (**C**H$_{Ar}$), 129.5 (**C**H$_{Ar}$), 128.2 (**C**H$_{Ar}$), 127.9 (**C**H$_{Ar}$), 126.2 (**C**H$_{Ar}$), 126.1 (**C**H$_{Ar}$), 123.0 (N**C**H=**C**HN), 50.8 (**C**H(Ph)$_2$), 34.9 (S(**C**H$_2$)$_2$), 30.2 (S(CH$_2$)(**C**H$_2$)), 22.0 (**C**H$_3$). **Elemental analysis:** expected [%]: C 69.18, H 5.09, N 2.21; found: C 68.73, H 4.95, N 2.35. **CCDC number:** 2204029.

NMR characterization of [Pt(IPr)(THT)Cl_2] (3ba)

^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 7.48 (t, *J* = 7.8 Hz, 2H, C**H**$_{Ar}$), 7.31 (d, *J* = 7.7 Hz, 4H, C**H**$_{Ar}$), 7.09 (s, 2H, N**H**C=C**H**N), 3.70 – 2.29 (br, 4H, S(C**H**$_2$)$_2$), 3.11 (hept, *J* = 6.6 Hz, 4H, C**H**(CH$_3$)$_2$), 1.95 – 1.61 (br, 4H, S(CH$_2$)(C**H**$_2$)), 1.41 (d, *J* = 6.7 Hz, 12H, CH(C**H**$_3$)$_2$), 1.10 (d, *J* = 6.9 Hz, 12H, CH(C**H**$_3$)$_2$). **^{13}C NMR** (75 MHz, $CDCl_3$): δ (ppm) = 152.4 (N-**C**-N), 146.7 (**C**^{IV}$_{Ar}$), 135.4 (**C**^{IV}$_{Ar}$), 130.0 (**C**H$_{Ar}$), 124.2 (NH**C**=**C**HN), 123.9 (**C**H$_{Ar}$), 34.9 (S(**C**H$_2$)$_2$), 29.7 (S(CH$_2$)(**C**H$_2$)), 28.8 (**C**H(CH$_3$)$_2$), 26.4 (CH(**C**H$_3$)$_2$), 23.1 (CH(**C**H$_3$)$_2$).

NMR characterization of [Pt(IPr)(Py)Cl_2] (3ca)

^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 8.57 (dt, *J* = 5.1, 1.6 Hz, 2H, C**H**$_{Py}$), 7.56 (tt, *J* = 7.6, 1.6 Hz, 1H, C**H**$_{Py}$), 7.49 (t, *J* = 7.8 Hz, 2H, C**H**$_{Ar}$), 7.32 (d, *J* = 7.5 Hz, 4H, C**H**$_{Ar}$), 7.17 – 7.09 (m, 2H, C**H**$_{Py}$), 7.09 (s, 2H, N**H**C=C**H**N), 3.19 (hept, *J* = 6.7 Hz, 4H, C**H**$(CH_3)_2$), 1.47 (d, *J* = 6.6 Hz, 12H, CH(C**H**$_3)_2$), 1.14 (d, *J* = 6.9 Hz, 12H, CH(C**H**$_3)_2$). **^{13}C NMR** (75 MHz, $CDCl_3$): δ (ppm) = 151.5 (**C**H$_{Py}$), 146.7 (**C**$^{IV}_{Ar}$), 143.3 (N-**C**-N), 137.4 (**C**H$_{Py}$), 135.5 (**C**$^{IV}_{Ar}$), 130.1 (**C**H$_{Ar}$), 124.5 (**C**H$_{Py}$), 124.2 (NH**C**=**C**HN), 124.0 (**C**H$_{Ar}$), 28.8 (**C**H$(CH_3)_2$), 26.3 (CH(**C**H$_3)_2$), 23.2 ((CH(**C**H$_3)_2$)). **CCDC number:** 2240569.

***Cis*/*trans* isomerization experiment (Figure 3)**

A sample of **3ak** (*cis*/*trans* ratio = 66:34) was dissolved in $CDCl_3$, transferred to an NMR tube, closed with a rubber cap and sealed with parafilm. The tube was placed in an oil bath set at 70 °C and *cis*/*trans* isomerization was monitored by ^{1}H NMR (300 MHz; the spectra were recorded at room temperature). No isomerization was observed in an analogous experiment with **3ae**.

General hydrosilylation procedure (A)

A 4.0 mL vial was charged with a platinum catalyst (2.0 µmol, 0.1 mol%) and dodecane (internal standard, 138 µL, 0.605 mmol). 1,1,1,3,5,5,5-heptamethyltrisiloxane (**4a**) (546 µL, 2.0 mmol, 1.0 equiv.) and 1-octene (**5b**) (318 µL, 2.0 mmol, 1.0 equiv.) were added, the vial was closed with a septum screw cap and the resulted mixture was stirred at 30 °C. The reaction aliquots were analyzed by gas chromatography (GC), calibrated on a commercial sample of the product (**6ab**).

General hydrosilylation procedure (B)

A 4.0 mL vial was charged with solid pre-catalyst **3ae**. Silane (2.0 mmol, 1.0 equiv.) and subsequently terminal alkene (2.0 mmol, 1.0 equiv.) were added, the vial was closed with a septum screw cap and the resulted mixture was stirred at temperature ranging from RT to 110 °C (see Scheme 3). After confirming the completion of the reaction by ^{1}H NMR spectroscopy, the reaction mixture was cooled down to room temperature, filtered through a layer of florisil/celite/$MgSO_4$ (300 mg of a mixture 1:1:1 m/m/m) in a Pasteur pipette using 10.0 mL of *n*-pentane, and the volatiles were removed under vacuum, affording the desired alkylsilane **6**, without the need of any additional purification steps. Caution: the hydrosilylation reactions are strongly exothermic and on a larger scale the reaction temperature must be carefully controlled. In case of **6aj'**, 2.0 mmol of the bifunctional substrate and 2.0 mmol of the monofunctional substrate was used. In case of all other reactions using bi- and tetrafunctional substrates (**6aj**, **6ea**, **6eb** and **6fb**), the exact amounts of the substrates are listed in the detailed procedures below. The amount of pre-catalyst was calculated based on the number of Si-H groups involved in hydrosilylation (e.g., 0.20 µmol of the catalyst was used in case of **6aa** and 0.40 µmol in case of **6fb**).

3-hexyl-1,1,1,3,5,5,5-heptamethyltrisiloxane (6aa) CAS 1873-90-1

Following the general procedure (**B**), **6aa** was obtained as a colorless oil (574 mg, 94%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ (ppm) = 1.36 – 1.21 (m, 8H), 0.88 (t, *J* = 6.8 Hz, 3H), 0.45 (t, *J* = 7.5 Hz, 2H), 0.08 (s, 18H), -0.01 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ (ppm) = 33.1, 31.8, 23.2, 22.8, 17.8, 14.3, 2.0, -0.1. Analytical data match the values reported in the literature.[26]

1,1,1,3,5,5,5-heptamethyl-3-octyltrisiloxane (6ab) CAS 17955-88-3

Following the general procedure (**B**), **6ab** was obtained as a colorless oil (664 mg, 99%). **^{1}H NMR** (300 MHz, $CDCl_3$): δ (ppm) = 1.38 – 1.17 (m, 12H), 0.88 (t, *J* = 6.6 Hz, 3H), 0.45 (t, *J* = 7.7 Hz, 2H), 0.09 (s, 18H), 0.01 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ (ppm) = 33.4, 32.1, 29.5, 29.4, 23.2, 22.8, 17.8, 14.3, 2.0, -0.1. Analytical data match the values reported in the literature.[10e]

3-decyl-1,1,1,3,5,5,5-heptamethyltrisiloxane (6ac) CAS 54253-66-6

Following the general procedure (**B**), **6ac** was obtained as a colorless oil (696 mg, 96%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ (ppm) = 1.40 – 1.14 (m, 16H), 0.88 (t, *J* = 6.8 Hz, 3H), 0.45 (t, *J* = 7.6 Hz, 2H), 0.09 (s, 18H), -0.00 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ (ppm) = 33.4, 32.1, 29.8, 29.8, 29.6, 29.5, 23.2, 22.8, 17.8, 14.3, 2.0, -0.1. Analytical data match the values reported in the literature.[27]

1,1,1,3,5,5,5-heptamethyl-3-tetradecyltrisiloxane (6ad) CAS 286938-65-6

Following the general procedure (**B**), **6ad** was obtained as a colorless oil (821 mg, 98%). **^{1}H NMR** (300 MHz, $CDCl_3$): δ (ppm) = 1.33 – 1.23 (m, 24H), 0.88 (d, *J* = 6.6 Hz, 3H), 0.45 (t, *J* = 7.5 Hz, 2H), 0.09 (s, 18H), -0.01 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ (ppm) = 33.4, 32.1, 29.9, 29.82, 29.76, 29.5, 29.5, 23.2, 22.8, 17.8, 14.3, 2.0, -0.1.

3-hexadecyl-1,1,1,3,5,5,5-heptamethyltrisiloxane (6ae) CAS 286938-67-8

Following the general procedure (**B**), **6ae** was obtained as a colorless oil (849 mg, 95%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ (ppm) = 1.37 – 1.18 (m, 28H), 0.88 (t, *J* = 6.6 Hz, 3H), 0.45 (t, *J* = 7.5 Hz, 2H), 0.09 (s, 18H), -0.01 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ (ppm) = 33.4, 32.1, 29.9, 29.83, 29.77, 29.6, 29.5, 23.2, 22.9, 17.8, 14.3, 2.0, -0.1.

1,1,1,3,5,5,5-heptamethyl-3-(4-(oxiran-2-yl)butyl)trisiloxane (6af) CAS 2123611-86-7

Following the general procedure (**B**), **6af** was obtained as a colorless oil (603 mg, 94%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ (ppm) = 2.95 – 2.84 (m, 1H), 2.74 (dd, *J* = 5.1, 3.9 Hz, 1H), 2.46 (dd, *J* = 5.0, 2.7 Hz, 1H), 1.59 – 1.32 (m, 6H), 0.52 – 0.42 (m, 2H), 0.08 (s, 18H), 0.00 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ (ppm) = 52.5, 47.3, 32.4, 29.5, 23.1, 17.7, 2.0, -0.1.

1,1,1,3,5,5,5-heptamethyl-3-(3-(oxiran-2-ylmethoxy)propyl)trisiloxane (6ag) CAS 7422-52-8

Following the general procedure (**B**), **6ag** was obtained as a colorless oil (639 mg, 95%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ (ppm) = 3.69 (dd, *J* = 11.5, 3.2 Hz, 1H), 3.51 – 3.35 (m, 3H), 3.18 – 3.10 (m, 1H), 2.85 – 2.76 (m, 1H), 2.60 (dd, *J* = 5.1, 2.7 Hz, 1H), 1.65 – 1.54 (m, 2H), 0.51 – 0.41 (m, 2H), 0.08 (s, 18H), 0.01 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ (ppm) = 74.4, 71.6, 51.0, 44.5, 23.4, 13.6, 2.0, -0.2. Analytical data match the values reported in the literature.[10e]

3-(3-(4-methoxyphenyl)propyl)-1,1,1,3,5,5,5-heptamethyltrisiloxane (6ah) CAS 1851415-14-9

Following the general procedure (**B**), **6ah** was obtained as a colorless oil (726 mg, 98%). **^{1}H NMR** (300 MHz, $CDCl_3$): δ (ppm) = 7.14 – 7.05 (m, 2H), 6.88 – 6.79 (m, 2H), 3.79 (s, 3H), 2.56 (t, *J* = 7.7 Hz, 2H), 1.66 – 1.53 (m, 2H), 0.56 – 0.44 (m, 2H), 0.08 (s, 18H), 0.00 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ (ppm) = 157.8, 135.0, 129.5, 113.8, 55.4, 38.7, 25.5, 17.5, 2.0, -0.1. Analytical data match the values reported in the literature.[27]

4-(3-(1,1,1,3,5,5,5-heptamethyltrisiloxan-3-yl)propyl)-2-methoxyphenol (6ai) CAS 889894-43-3

Following the general procedure (**B**), **6ai** was obtained as a colorless oil (735 mg, 95%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ (ppm) = 6.93 – 6.75 (m, 1H), 6.75 – 6.59 (m, 2H), 5.44 (s, 1H), 3.88 (s, 3H), 2.54 (t, *J* = 7.7 Hz, 2H), 1.69 – 1.57 (m, 2H), 0.58 – 0.43 (m, 2H), 0.08 (s, 18H), 0.00 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ (ppm) = 146.4, 143.7, 134.9, 121.2, 114.2, 111.2, 56.0, 39.3, 25.6, 17.5, 2.0, -0.1.

1,8-bis(1,1,1,3,5,5,5-heptamethyltrisiloxan-3-yl)octane (6aj) CAS 1688709-56-9

The synthesis was carried out with 4.0 mmol of **4a** and 2.0 mmol of diene **5j**. Following the general procedure (**B**), **6aj** was obtained as a colorless oil (1033 mg, 93%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ (ppm) = 1.37 – 1.20 (m, 12H), 0.45 (t, *J* = 7.5 Hz, 4H), 0.09 (s, 36H), -0.01 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ (ppm) = 33.4, 29.4, 23.2, 17.8, 2.0, -0.1.

1,1,1,3,5,5,5-heptamethyl-3-(2-(trimethylsilyl)ethyl)trisiloxane (6ak) CAS 18077-53-7

Following the general procedure (**B**), **6ak** was obtained as a colorless oil (607 mg, 94%). **^{1}H NMR** (300 MHz, $CDCl_3$): δ (ppm) = 0.44 – 0.29 (m, 4H), 0.09 (s, 18H), 0.00 (s, 3H), -0.03 (s, 9H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ (ppm) = 9.7, 8.1, 2.0, -1.0, -2.1.

3-(6-bromohexyl)-1,1,1,3,5,5,5-heptamethyltrisiloxane (6al)

Following the general procedure (**B**), **6al** was obtained as a colorless oil (756 mg, 98%). **^{1}H NMR** (300 MHz, $CDCl_3$): δ (ppm) = 3.41 (t, *J* = 6.9 Hz, 2H, Br(C**H**$_2$)), 1.85 (quint, *J* = 6.9 Hz, 2H, Br(CH$_2$)(C**H**$_2$)), 1.47 – 1.27 (m, 6H, C**H**$_2$), 0.55 – 0.39 (m, 2H, Si(C**H**$_2$)), 0.09 (s, 18H, Si(C**H**$_3$)$_3$), -0.00 (s, 3H, Si(C**H**$_3$)). **^{13}C NMR** (75 MHz, $CDCl_3$): δ (ppm) = 34.2 (Br(**C**H$_2$)), 33.0 (Br(CH$_2$)(**C**H$_2$)), 32.4 (**C**H$_2$), 28.1 (**C**H$_2$), 23.1 (**C**H$_2$), 17.7 (Si(**C**H$_2$)), 2.0 (Si(**C**H$_3$)$_3$), -0.1 (Si(**C**H$_3$)).

methyl 11-(1,1,1,3,5,5,5-heptamethyltrisiloxan-3-yl)undecanoate (6am) CAS 60728-44-1

Following the general procedure (**B**), **6am** was obtained as a colorless oil (838 mg, 99%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ (ppm) = 3.67 (s, 3H, O(C**H**$_3$)), 2.31 (t, *J* = 7.5 Hz, 2H, CO(C**H**$_2$)), 1.68 – 1.53 (m, 2H, CO(CH$_2$)(C**H**$_2$)), 1.39 – 1.06 (m, 14H, C**H**$_2$), 0.52 – 0.35 (m, 2H, Si(C**H**$_2$)), 0.09 (s, 18H, Si(C**H**$_3$)$_3$), -0.00 (s, 3H, Si(C**H**$_3$)). **^{13}C NMR** (101 MHz, $CDCl_3$): δ (ppm) = 174.5 (**C**=O), 51.6 (O(**C**H$_3$)), 34.3 (CO(**C**H$_2$)), 33.4 (**C**H$_2$), 29.7 (**C**H$_2$), 29.6 (**C**H$_2$), 29.5 (**C**H$_2$), 29.4 (**C**H$_2$), 29.3 (**C**H$_2$), 25.1 (CO(CH$_2$)(**C**H$_2$)), 23.2 (**C**H$_2$), 17.8 (Si(**C**H$_2$)), 2.0 (Si(**C**H$_3$)$_3$), -0.1 (Si(**C**H$_3$)).

1,1,1,3,5,5,5-heptamethyl-3-phenethyltrisiloxane (6an) CAS 3439-16-5

Following the general procedure (**B**), **6an** was obtained as a colorless oil (601 mg). The isolated product contains 16% of the branched side product (see Supporting Information). **^{1}H NMR** (400 MHz, $CDCl_3$): δ (ppm) = 7.34 – 7.06 (m, 5H), 2.70 – 2.62 (m, 2H), 0.89 – 0.81 (m, 2H), 0.14 (s, 18H), 0.05 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ (ppm) = 145.3, 128.4, 127.9, 125.6, 29.4, 19.9, 2.0, -0.2. Analytical data match the values reported in the literature.[5d]

1,1,1,3,3-pentamethyl-3-octyldisiloxane (6bb) CAS 180006-15-9

Following the general procedure (**B**), **6bb** was obtained as a colorless oil (516 mg, 99%). **^{1}H NMR** (300 MHz, $CDCl_3$): δ (ppm) = 1.38 – 1.18 (m, 12H), 0.89 (t, *J* = 6.6 Hz, 3H), 0.50 (t, *J* = 7.5 Hz, 2H), 0.06 (s, 9H), 0.03 (s, 6H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ (ppm) = 33.6, 32.1, 29.5, 29.4, 23.4, 22.8, 18.5, 14.3, 2.1, 0.5. Analytical data match the values reported in the literature.[28]

ethoxydimethyl(octyl)silane (6cb) CAS 87281-31-0

Following the general procedure (**B**), **6cb** was obtained as a colorless oil (416 mg, 96%). **^{1}H NMR** (300 MHz, $CDCl_3$): δ (ppm) = 3.66 (q, *J* = 7.0 Hz, 2H), 1.41 – 1.23 (m, 12H), 1.19 (t, *J* = 7.0 Hz, 3H), 0.89 (t, *J* = 6.8 Hz, 3H), 0.61 (t, *J* = 7.6 Hz, 2H), 0.09 (s, 6H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ (ppm) = 58.4, 33.6, 32.1, 29.5, 29.4, 23.4, 22.8, 18.7, 16.5, 14.2, -1.9. Analytical data match the values reported in the literature.[5b]

diethoxy(methyl)(octyl)silane (6db) CAS 2652-38-2

Following the general procedure (**B**), **6db** was obtained as a colorless oil (478 mg, 97%). **^{1}H NMR** (300 MHz, $CDCl_3$): δ (ppm) = 3.76 (q, *J* = 7.0 Hz, 4H), 1.43 – 1.16 (m, 12H), 1.21 (t, *J* = 7.0 Hz, 6H), 0.88 (t, *J* = 6.8 Hz, 3H), 0.69 – 0.51 (m, 2H), 0.10 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ (ppm) = 58.2, 33.5, 32.1, 29.4, 29.4, 23.0, 22.8, 18.6, 14.2, 14.0, -4.7. Analytical data match the values reported in the literature.[29]

1,3-dihexyl-1,1,3,3-tetramethyldisiloxane (6ea) CAS 18546-93-5

The synthesis was carried out with 2.0 mmol of **4e** and 4.0 mmol of **5a**. Following the general procedure (**B**), **6ea** was obtained as a colorless oil (581 mg, 96%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ (ppm) = 1.37 – 1.24 (m, 16H), 0.90 (t, *J* = 6.7 Hz, 6H), 0.56 – 0.44 (m, 4H), 0.03 (s, 12H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ (ppm) = 33.3, 31.8, 23.4, 22.8, 18.6, 14.3, 0.5. Analytical data match the values reported in the literature.[30]

1,1,3,3-tetramethyl-1,3-dioctyldisiloxane (6eb) CAS 18642-94-9

The synthesis was carried out with 2.0 mmol of **4e** and 4.0 mmol of **5b**. Following the general procedure (**B**), **6eb** was obtained as a colorless oil (703 mg, 98%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ (ppm) = 1.41 – 1.16 (m, 24H), 0.88 (t, *J* = 6.6 Hz, 6H), 0.50 (t, *J* = 7.7 Hz, 4H), 0.03 (s, 12H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ (ppm) = 33.6, 32.1, 29.5, 29.4, 23.4, 22.8, 18.6, 14.3, 0.5. Analytical data match the values reported in the literature.[31]

1-(3-(4-methoxyphenyl)propyl)-1,1,3,3,3-pentamethyldisiloxane (6bh)

Following the general procedure (**B**), **6bh** was obtained as a colorless oil (588 mg, 99%). **^{1}H NMR** (300 MHz, $CDCl_3$): δ (ppm) = 7.15 – 7.03 (m, 2H, C**H**$_{Ar}$), 6.89 – 6.79 (m, 2H, C**H**$_{Ar}$), 3.79 (s, 3H, OC**H**$_3$), 2.57 (t, *J* = 7.7 Hz, 2H, Ar(C**H**$_2$)), 1.68 – 1.53 (m, 2H, Ar(CH_2)(C**H**$_2$)), 0.63 – 0.49 (m, 2H, Si(C**H**$_2$)), 0.06 (s, 9H, Si(C**H**$_3$)$_3$), 0.04 (s, 6H, Si(C**H**$_3$)$_2$). **^{13}C NMR** (75 MHz, $CDCl_3$): δ (ppm) = 157.8 (**C**$^{IV}_{Ar}$), 135.0 (**C**$^{IV}_{Ar}$), 129.5 (**C**H$_{Ar}$), 113.8 (**C**H$_{Ar}$), 55.4 (O**C**H$_3$), 38.9 (Ar(**C**H$_2$)), 25.8 (Ar(CH_2)(**C**H$_2$)), 18.3 (Si(**C**H$_2$)), 2.1 (Si(**C**H$_3$)$_3$), 0.5 (Si(**C**H$_3$)$_2$).

2-methoxy-4-(3-(1,1,3,3,3-pentamethyldisiloxaneyl)propyl)phenol (6bi) CAS 4515-16-6

Following the general procedure (**B**), **6bi** was obtained as a colorless oil (616 mg, 99%). **^{1}H NMR** (300 MHz, $CDCl_3$): δ (ppm) = 6.88 – 6.79 (m, 1H, C**H**$_{Ar}$), 6.76 – 6.57 (m, 2H, C**H**$_{Ar}$), 5.45 (s, 1H, O**H**), 3.88 (s, 3H, OC**H**$_3$), 2.55 (t, *J* = 7.7 Hz, 2H, Ar(C**H**$_2$)), 1.67 – 1.56 (m, 2H, Ar(CH_2)(C**H**$_2$)), 0.63 – 0.46 (m, 2H, Si(C**H**$_2$)), 0.06 (s, 9H, Si(C**H**$_3$)$_3$), 0.04 (s, 6H, Si(C**H**$_3$)$_2$). **^{13}C NMR** (75 MHz, $CDCl_3$): δ (ppm) = 146.4 (**C**$^{IV}_{Ar}$), 143.7 (**C**$^{IV}_{Ar}$), 134.9 (**C**$^{IV}_{Ar}$), 121.2 (**C**H$_{Ar}$), 114.2 (**C**H$_{Ar}$), 111.2 (**C**H$_{Ar}$), 56.0 (O**C**H$_3$), 39.5 (Ar(**C**H$_2$)), 25.8 (Ar(CH_2)(**C**H$_2$)), 18.3 (Si(**C**H$_2$)), 2.1 (Si(**C**H$_3$)$_3$), 0.5 (Si(**C**H$_3$)$_2$).

2,4,6,8-tetramethyl-2,4,6,8-tetraoctyl-1,3,5,7,2,4,6,8-tetraoxatetrasilocane (6fb) CAS 15147-32-7

The synthesis was carried out with 1.0 mmol of **4f** and 4.0 mmol of **5b**. Following the general procedure (**B**), **6fb** was obtained as a colorless oil (667 mg, 97%). **^{1}H NMR** (300 MHz, $CDCl_3$): δ (ppm) = 1.43 – 1.17 (m, 48H), 0.88 (t, *J* = 6.3 Hz, 12H), 0.52 (t, *J* = 7.3 Hz, 8H), 0.06 (s, 12H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ (ppm) = 33.4, 32.1, 29.5, 23.2, 23.1, 22.9, 17.4, 14.3, -0.5. Analytical data match the values reported in the literature.[31]

Supporting Information

The authors have cited additional references within the Supporting Information.[32-38]

Acknowledgements

We gratefully acknowledge the VLAIO (SBO project CO2PERATE) and the Special Research Fund (BOF) of Ghent University. Funding of the iBOF project C3 (BOF20/IBF/010) is also gratefully acknowledged. K. V. H and M. B. thank the Research Foundation – Flanders (FWO) (projects AUGE/11/029 and G099319N) for funding. The FWO is also gratefully acknowledged for the PhD fellowship to B. P. M. (1SB5321N). A. P. thanks ICREA Academia Prize 2019, the Spanish Ministerio de Ciencia e Innovación for project PID2021-127423NB-I00 and the Generalitat de Catalunya for project 2021SGR623. Umicore AG and Johnson Matthey are thankfully acknowledged for the generous gifts of materials.

Keywords: alkenes • hydrosilylation • *N*-heterocyclic carbenes • platinum • solvent-free catalysis

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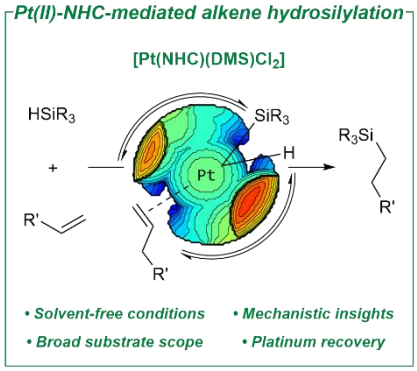

Pt(II)-NHC complexes are used in alkene hydrosilylation reactions. Some of the examined compounds display excellent catalytic activity, outperforming Pt(0)-NHC pre-catalysts. Our study explores the catalyst structure-activity relationship and provides new mechanistic insights into this industrially important transformation. A sustainable protocol, featuring efficient platinum removal, allows us to access a series of organosilanes in very good to excellent yields.

Institute and/or researcher Twitter usernames: @Nahra_Chem

Supporting Information

Pt(II)-N-heterocyclic carbene complexes in solvent-free alkene hydrosilylation

Benon P. Maliszewski, Dr. Tahani A. C. A. Bayrakdar, Perrine Lambert, Lama Hamdouna, Dr. Xavier Trivelli, Prof. Dr. Luigi Cavallo, Dr. Albert Poater, Marek Beliš, Prof. Dr. Olivier Lafon, Prof. Dr. Kristof Van Hecke, Dr. Dominic Ormerod, Prof. Dr. Catherine S. J. Cazin, Prof. Dr. Fady Nahra,* and Prof. Dr. Steven P. Nolan*

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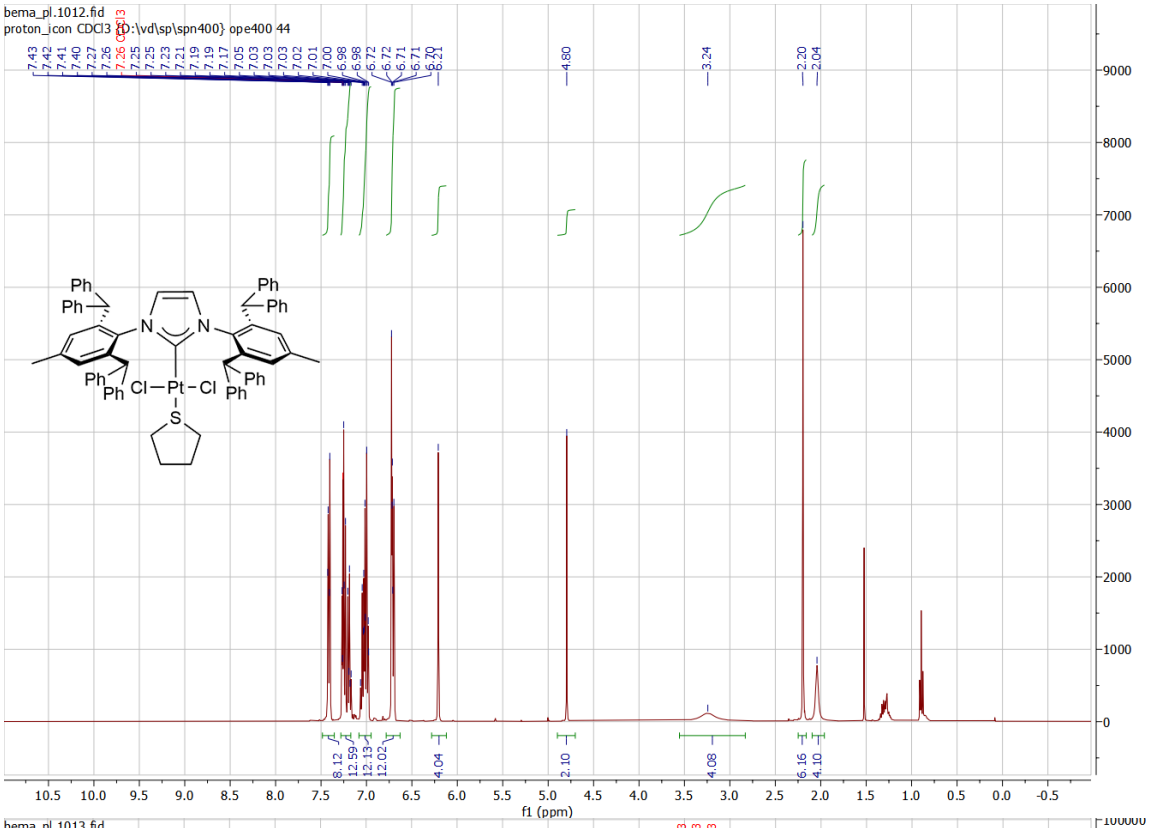
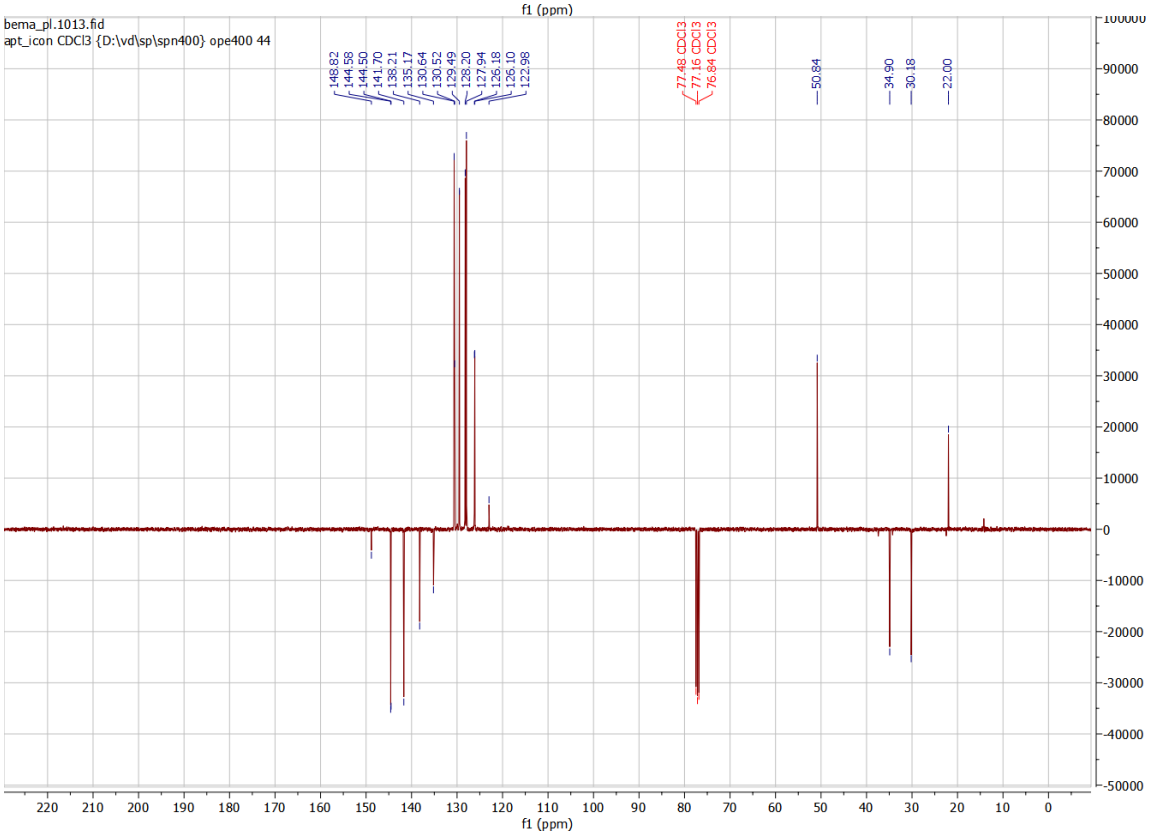
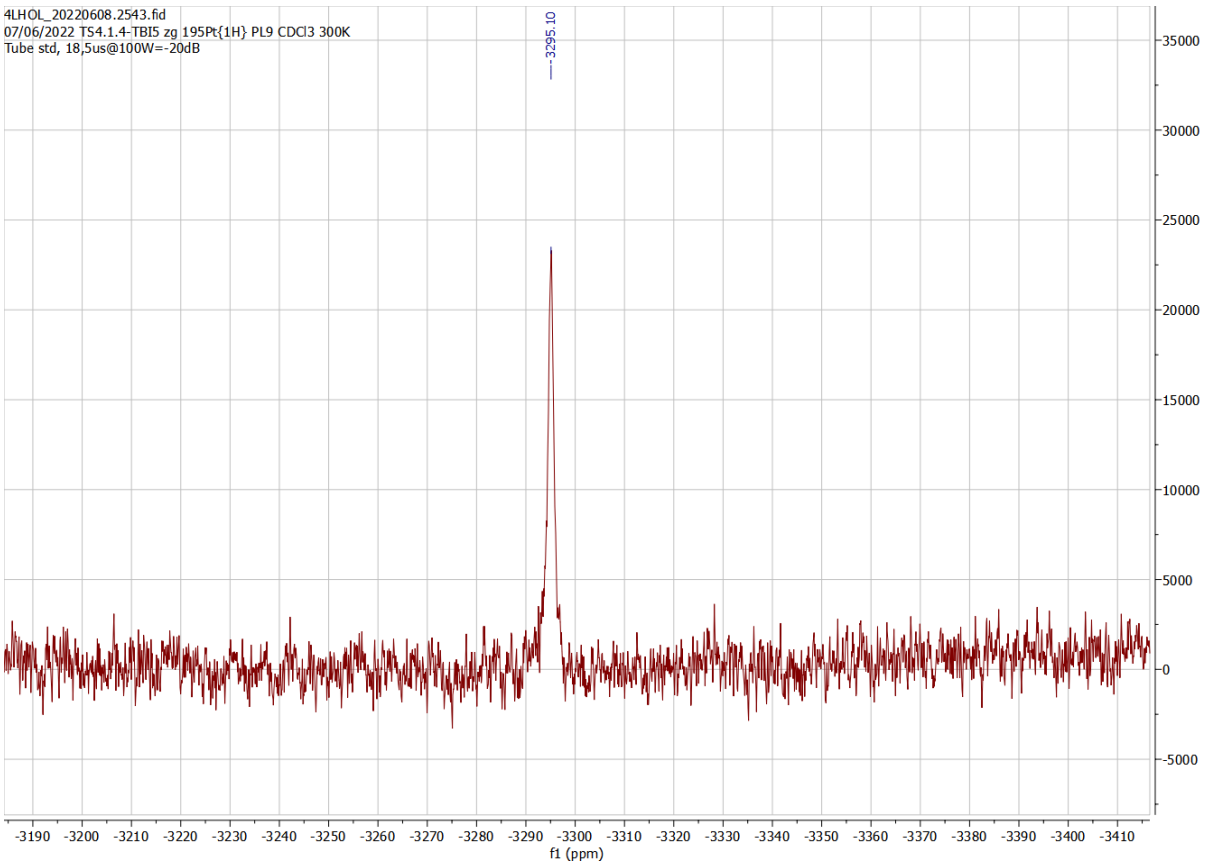
1. NMR spectra of the Pt(II)-NHC complexes

1.1. ^{1}H, $^{13}C\{^{1}H\}$ apt and ^{195}Pt NMR of 3be



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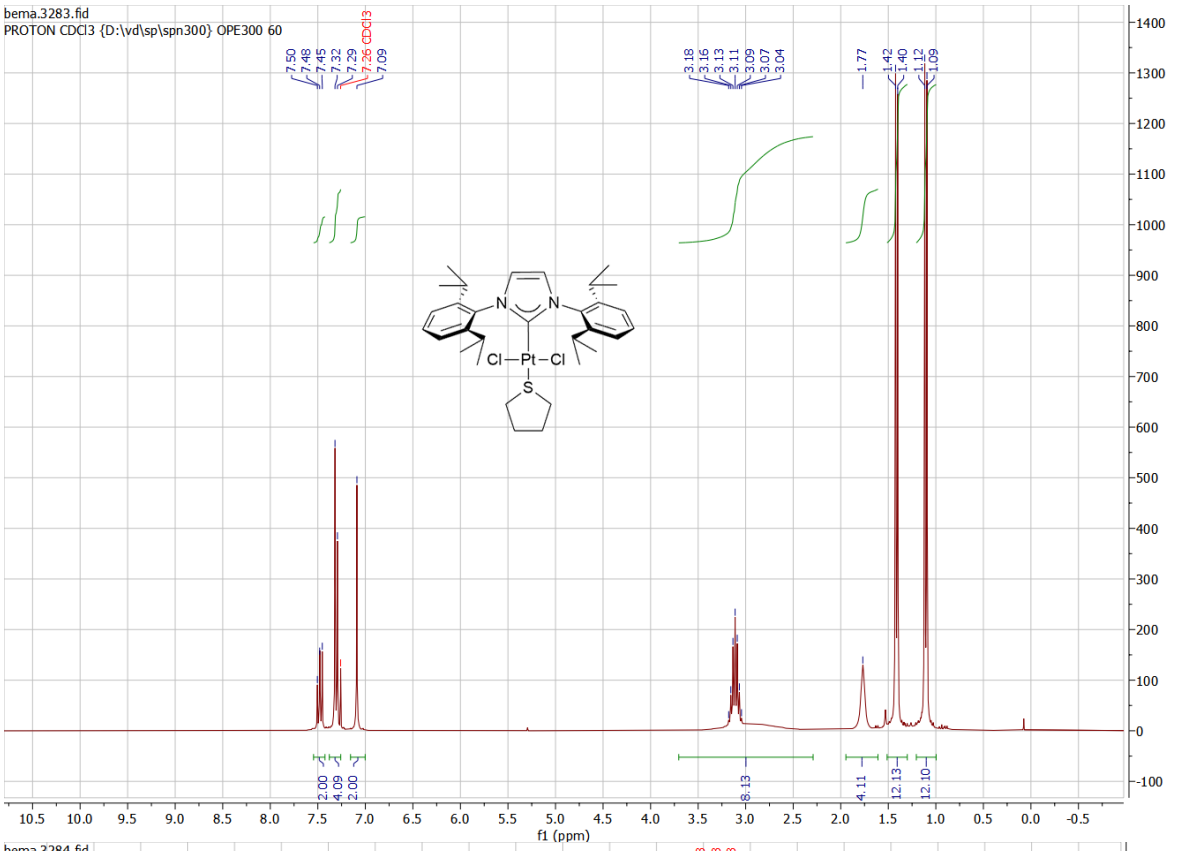
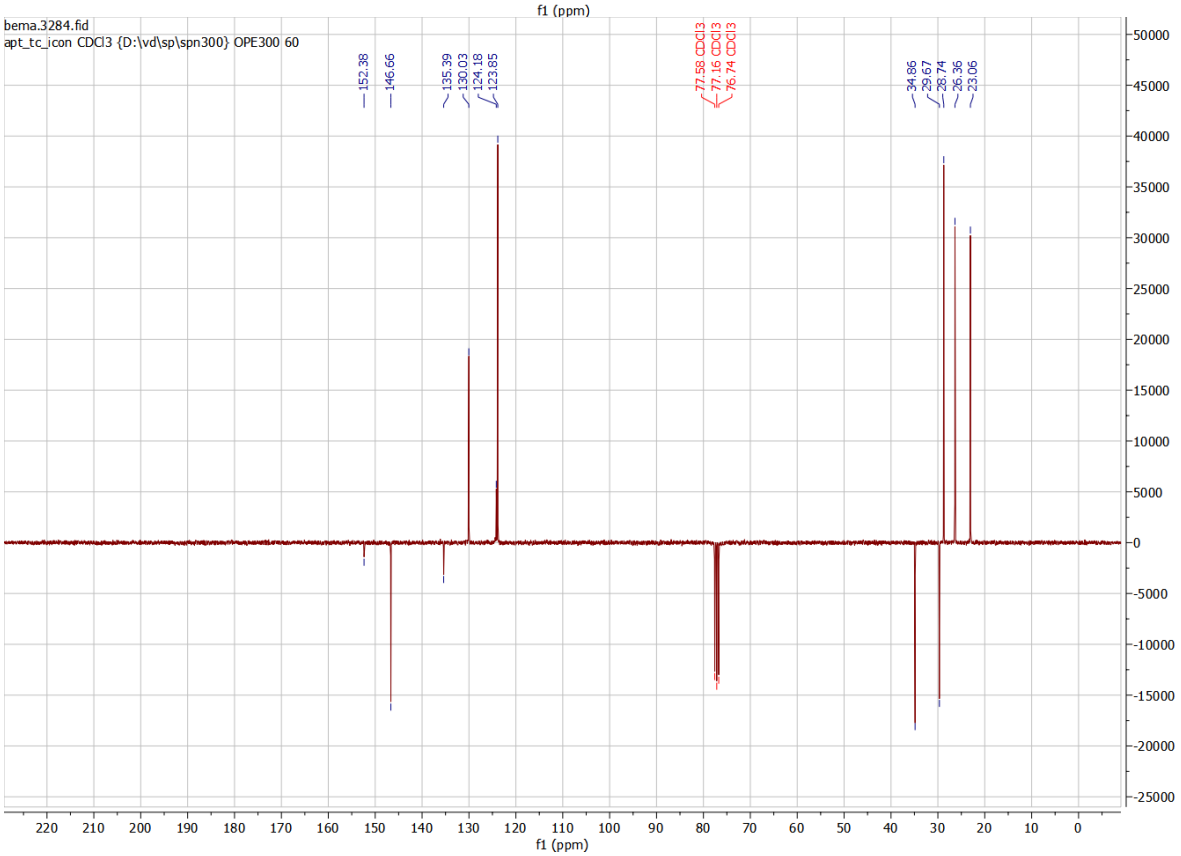
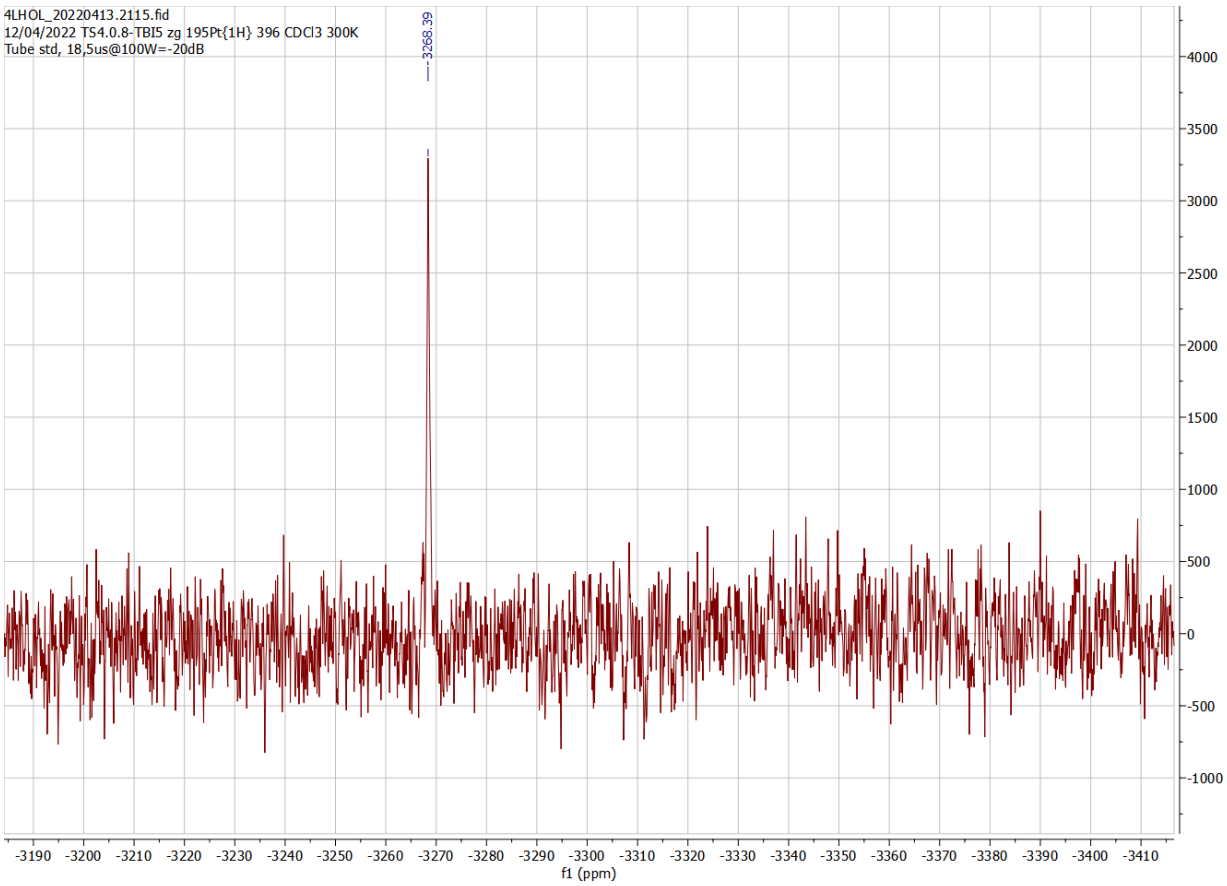
f1 (ppm)

1.2. ^{1}H, $^{13}C\{^{1}H\}$ apt and ^{195}Pt NMR of 3ba



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3000
2500
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1000
500
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-1000
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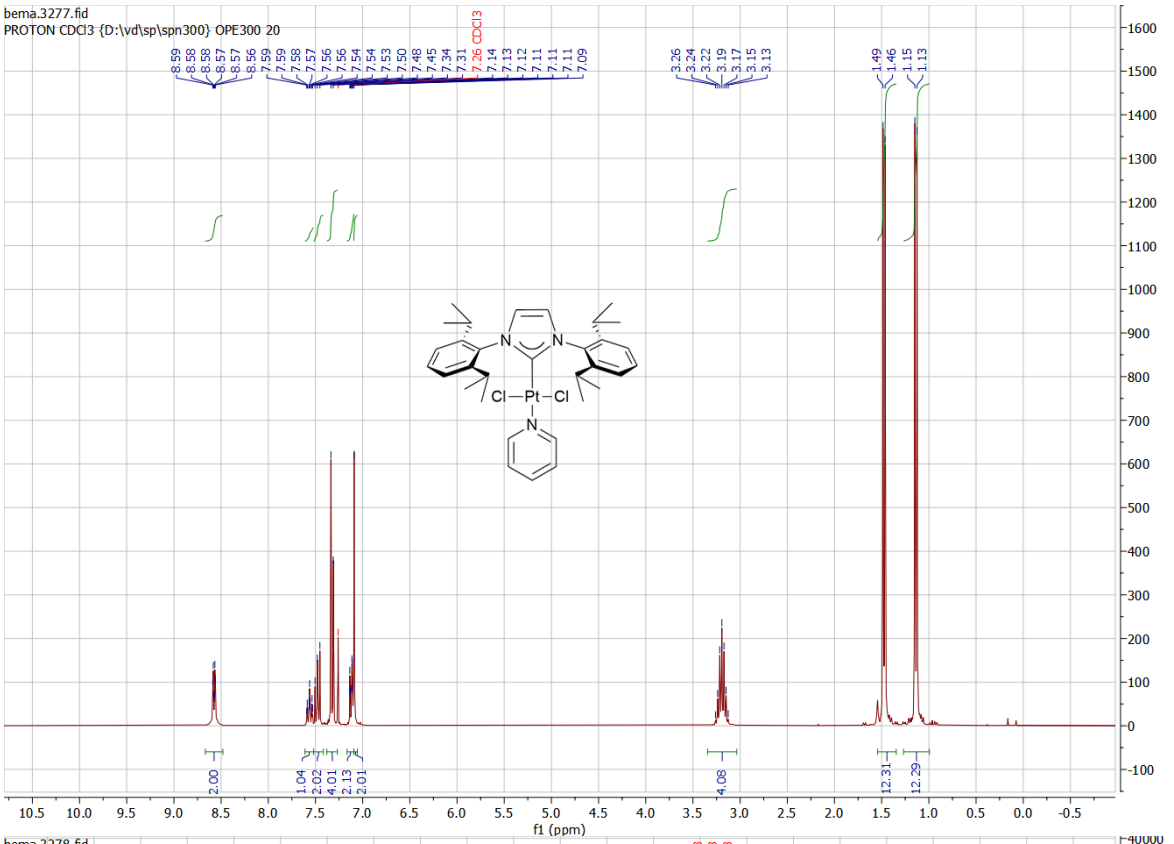
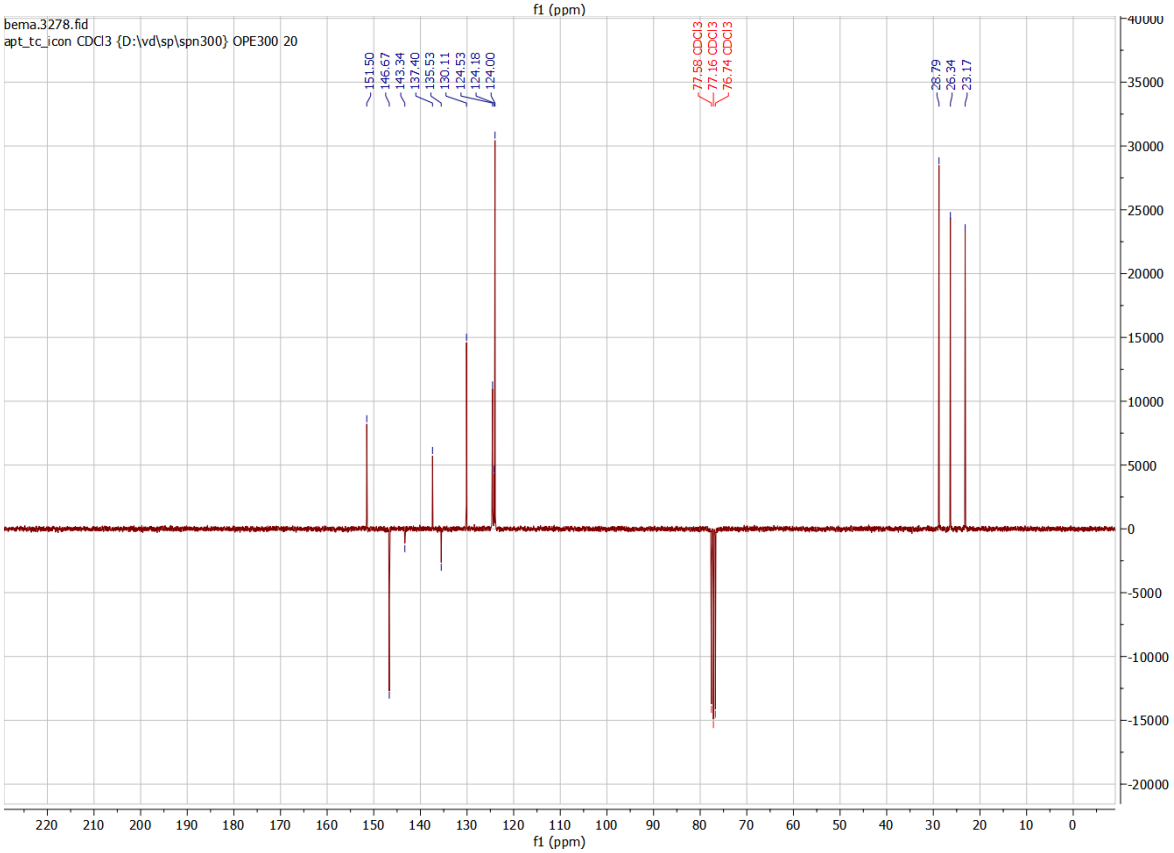
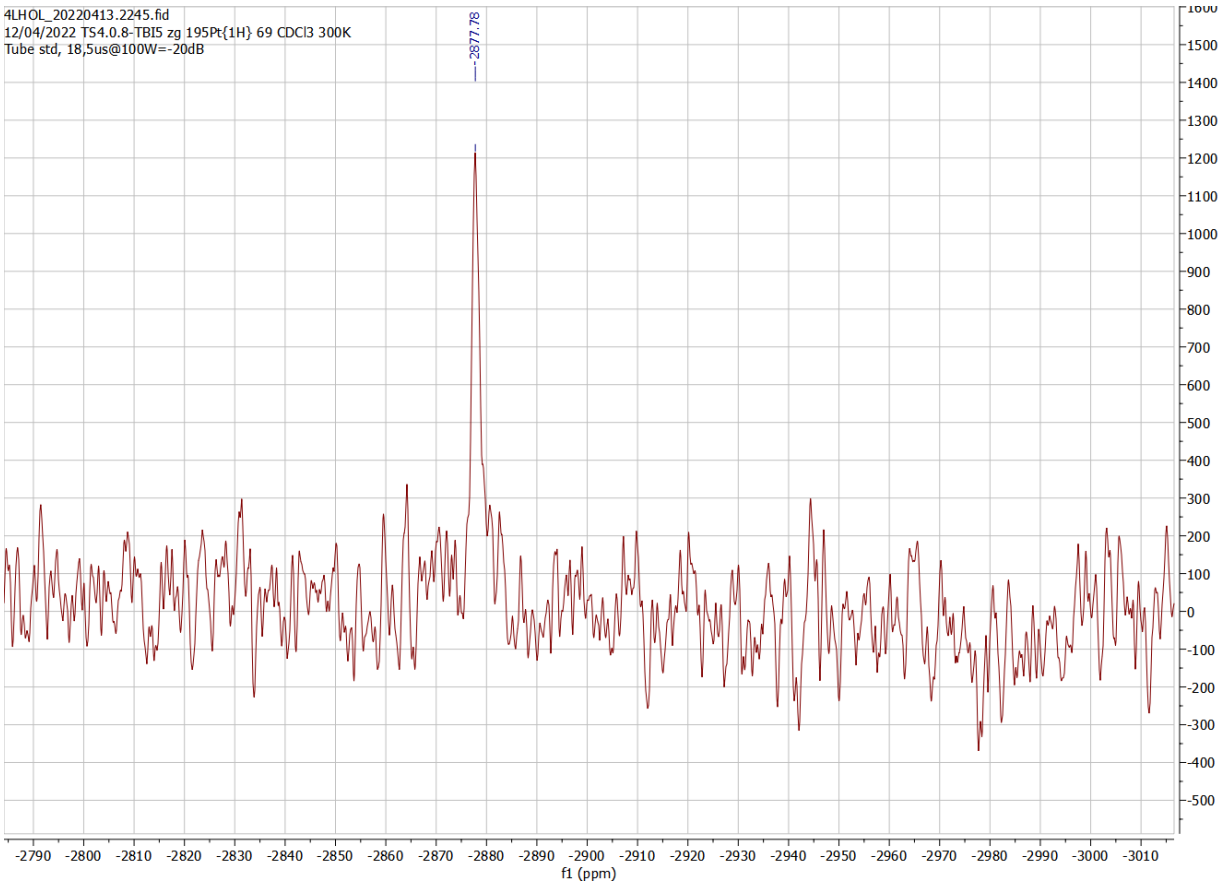
f1 (ppm)

1.3. ^{1}H, $^{13}C\{^{1}H\}$ apt and ^{195}Pt NMR of 3ca



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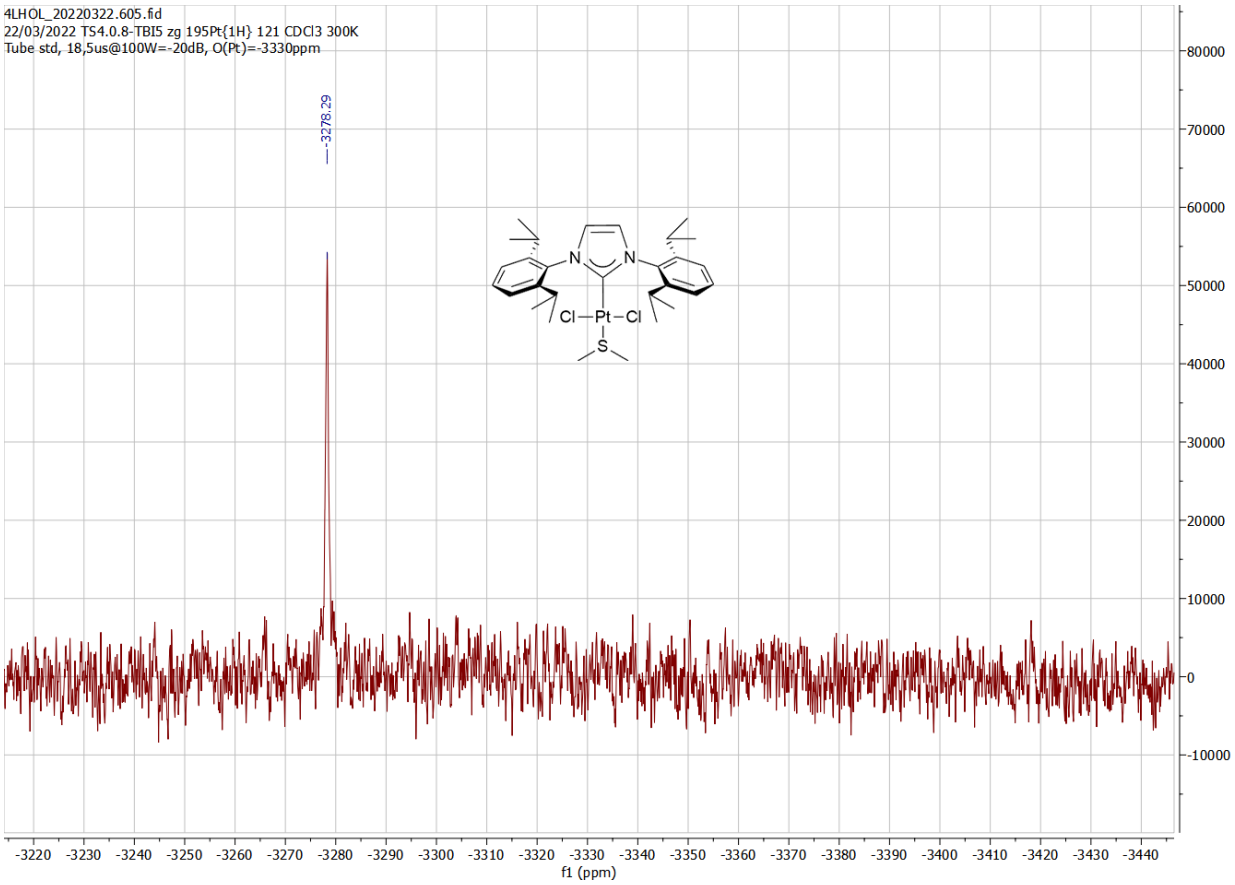
f1 (ppm)

1.4. ^{195}Pt NMR of 3aa



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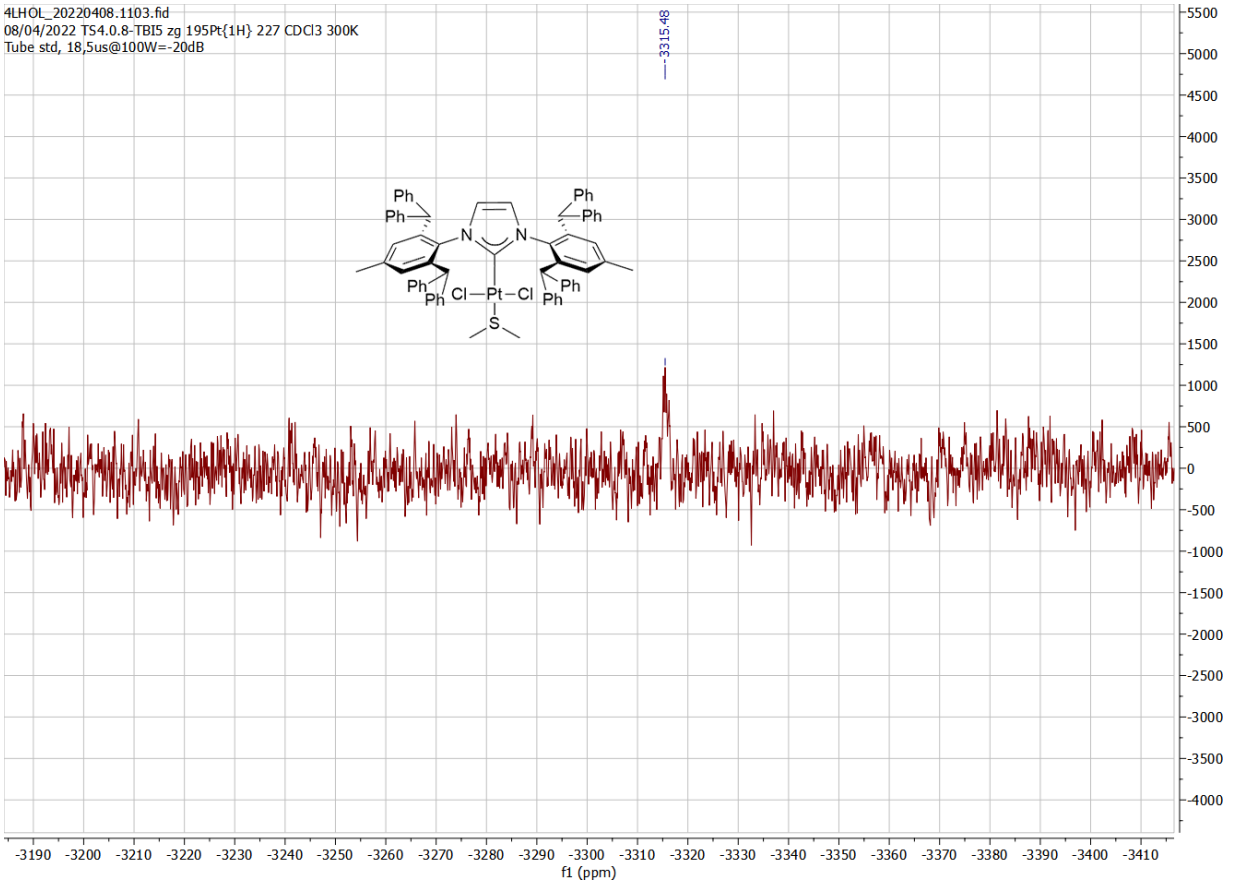
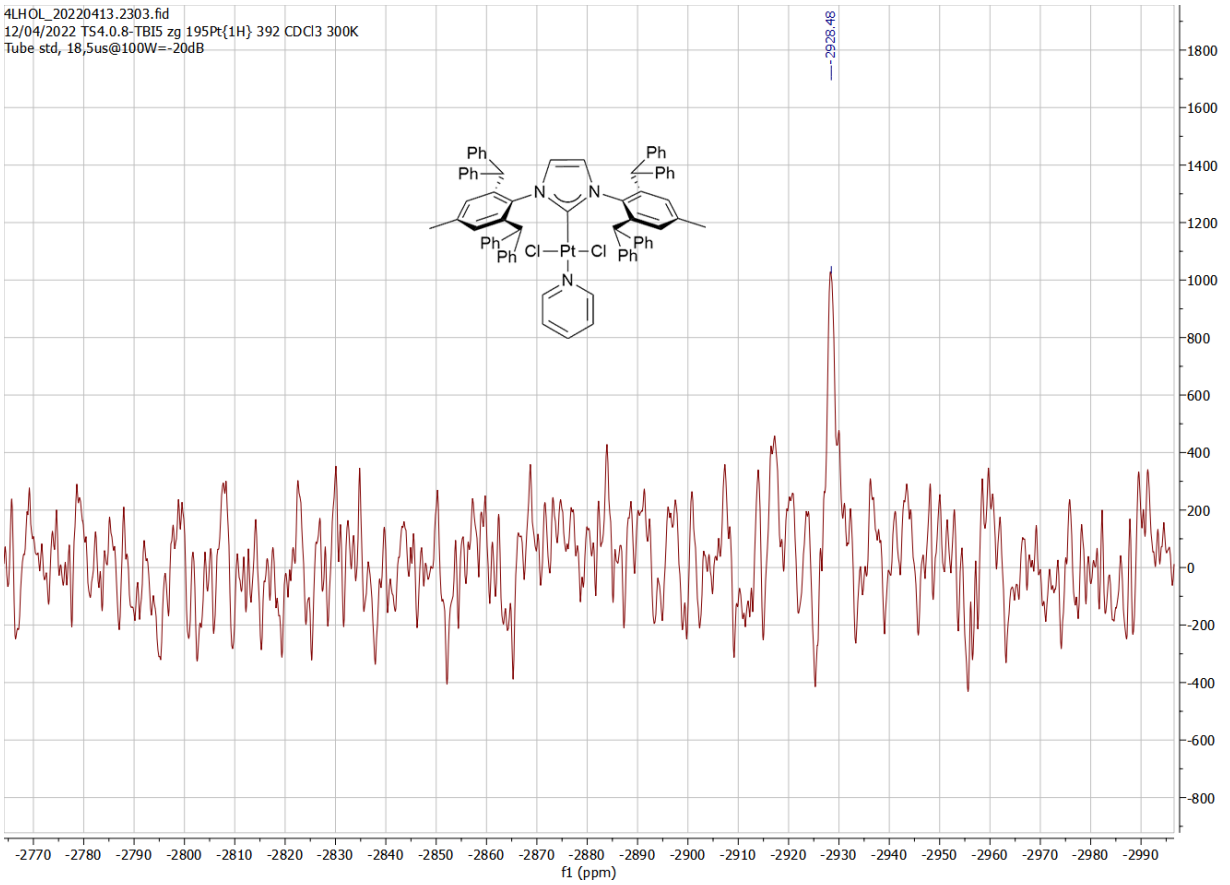
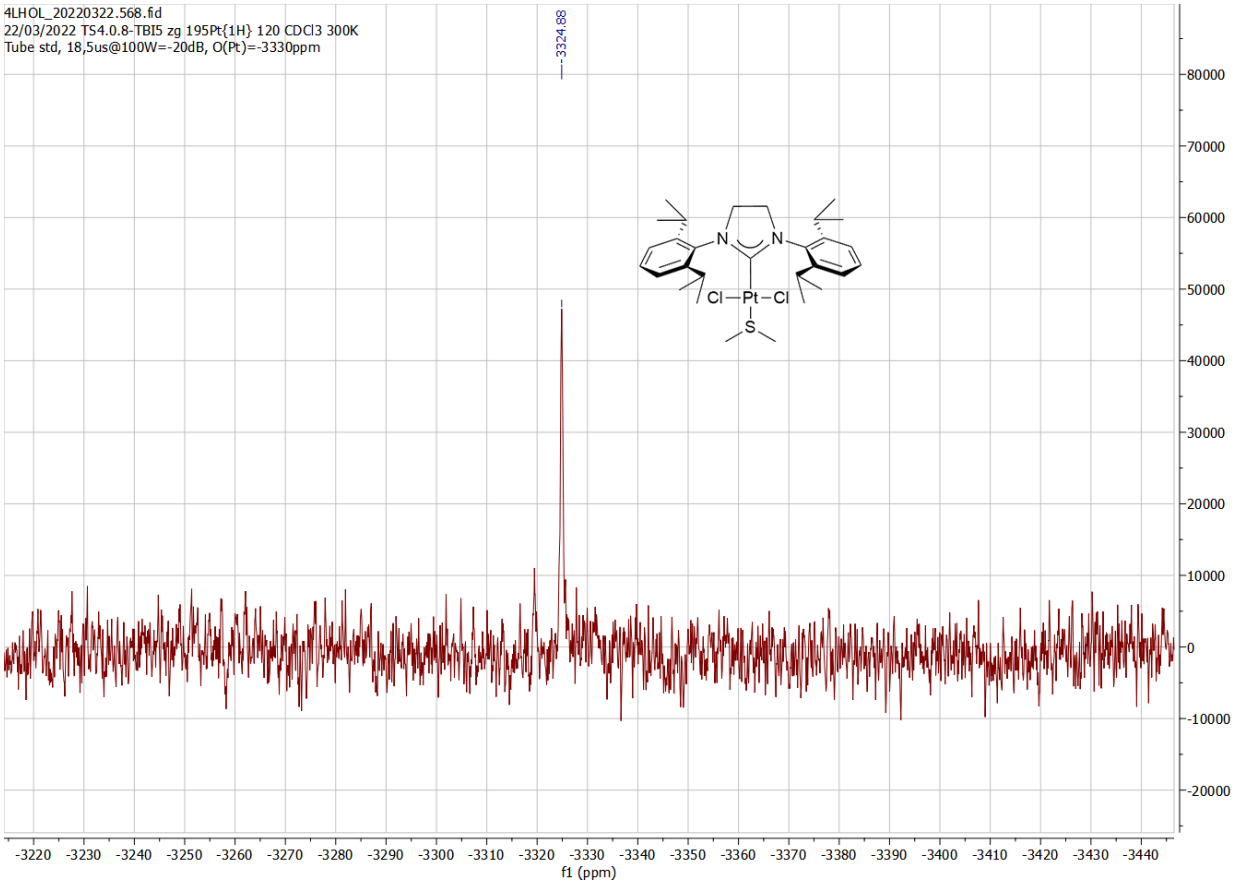


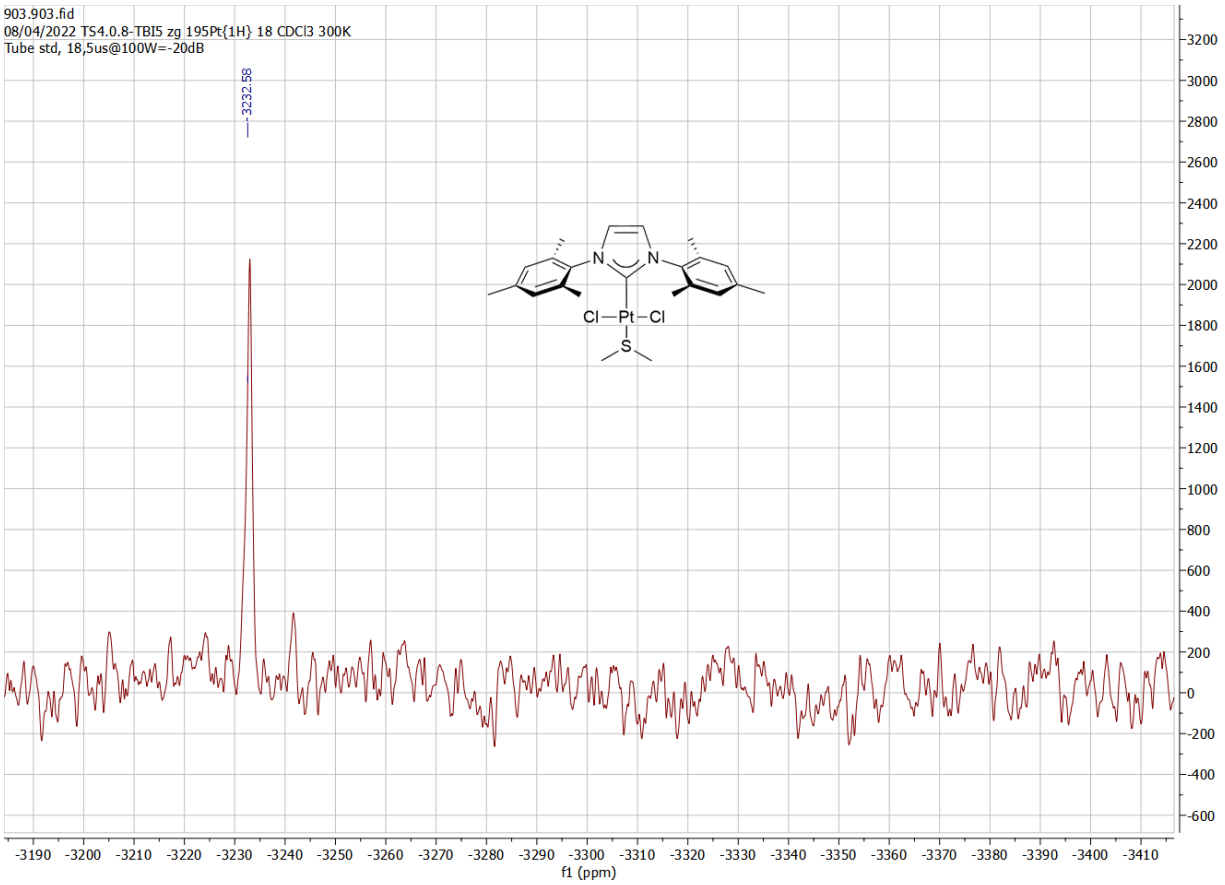
1.6. ^{195}Pt NMR of 3ce



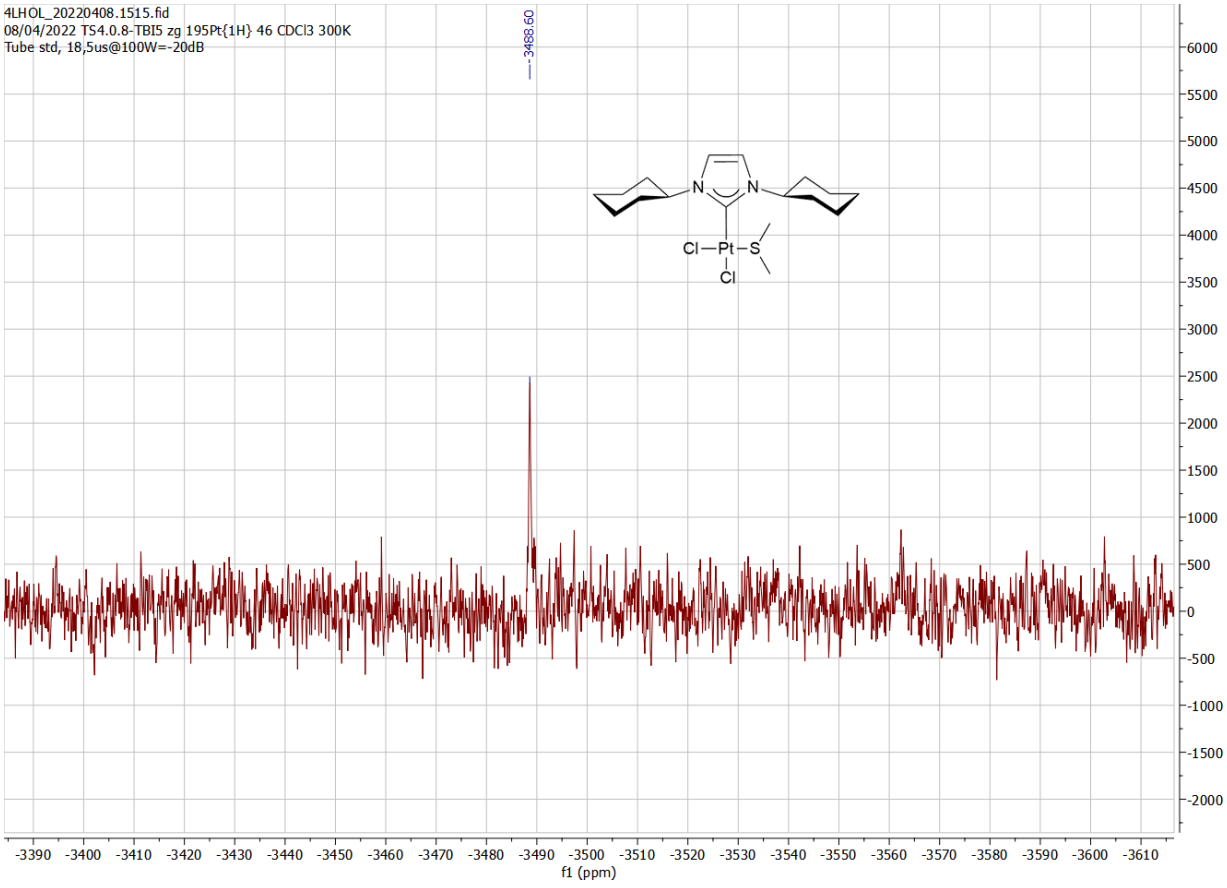
1.7. ^{195}Pt NMR of 3ab



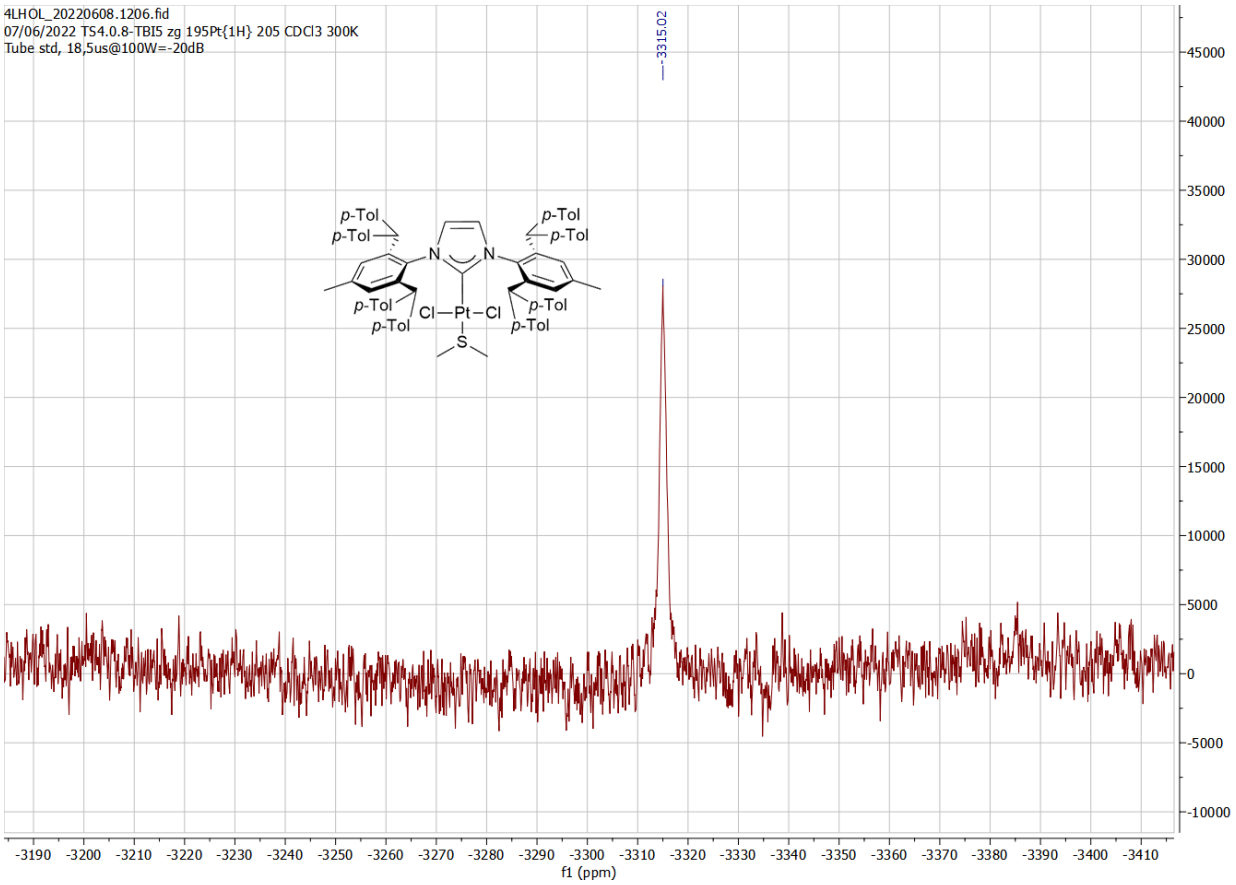
1.8. ^{195}Pt NMR of 3ac



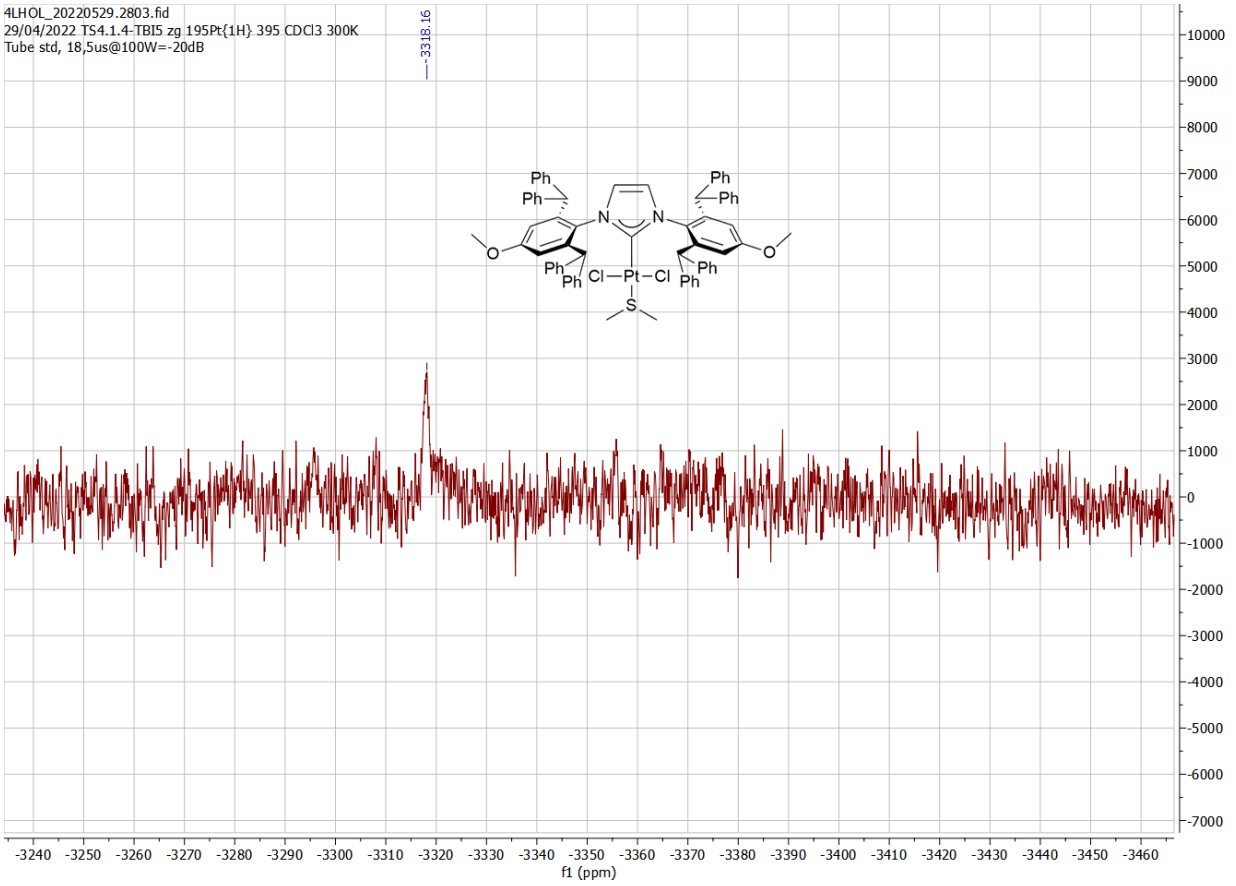
1.9. ^{195}Pt NMR of *cis*-3ad



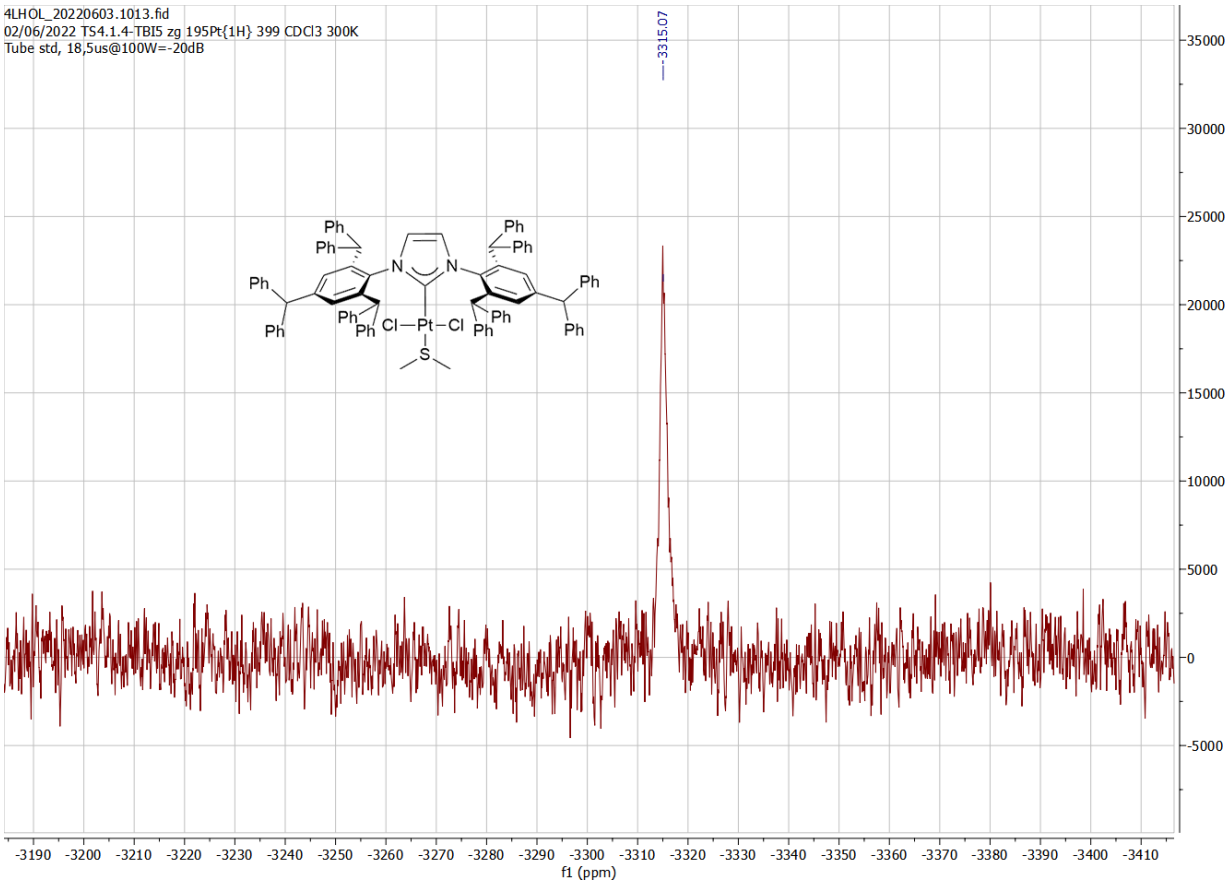
1.10. ^{195}Pt NMR of 3af



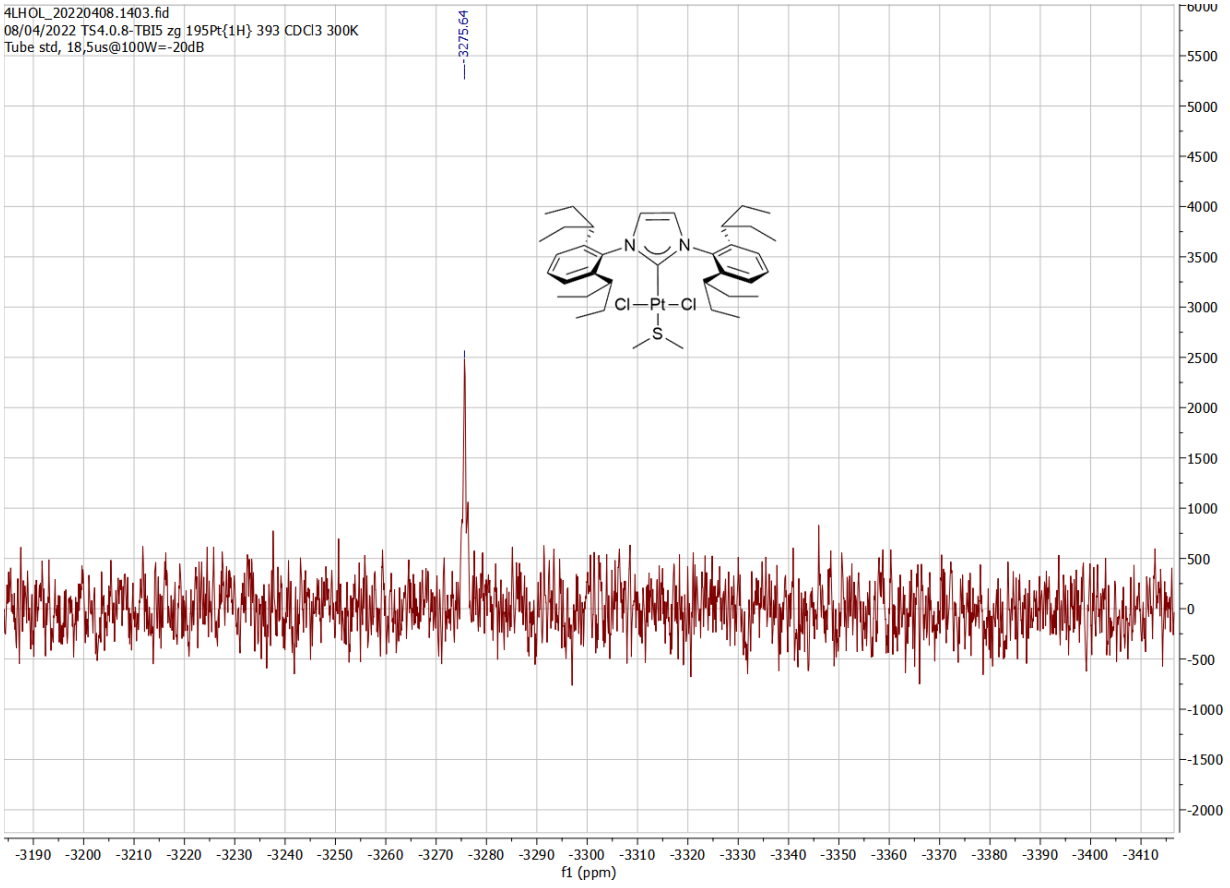
1.11. ^{195}Pt NMR of 3ag



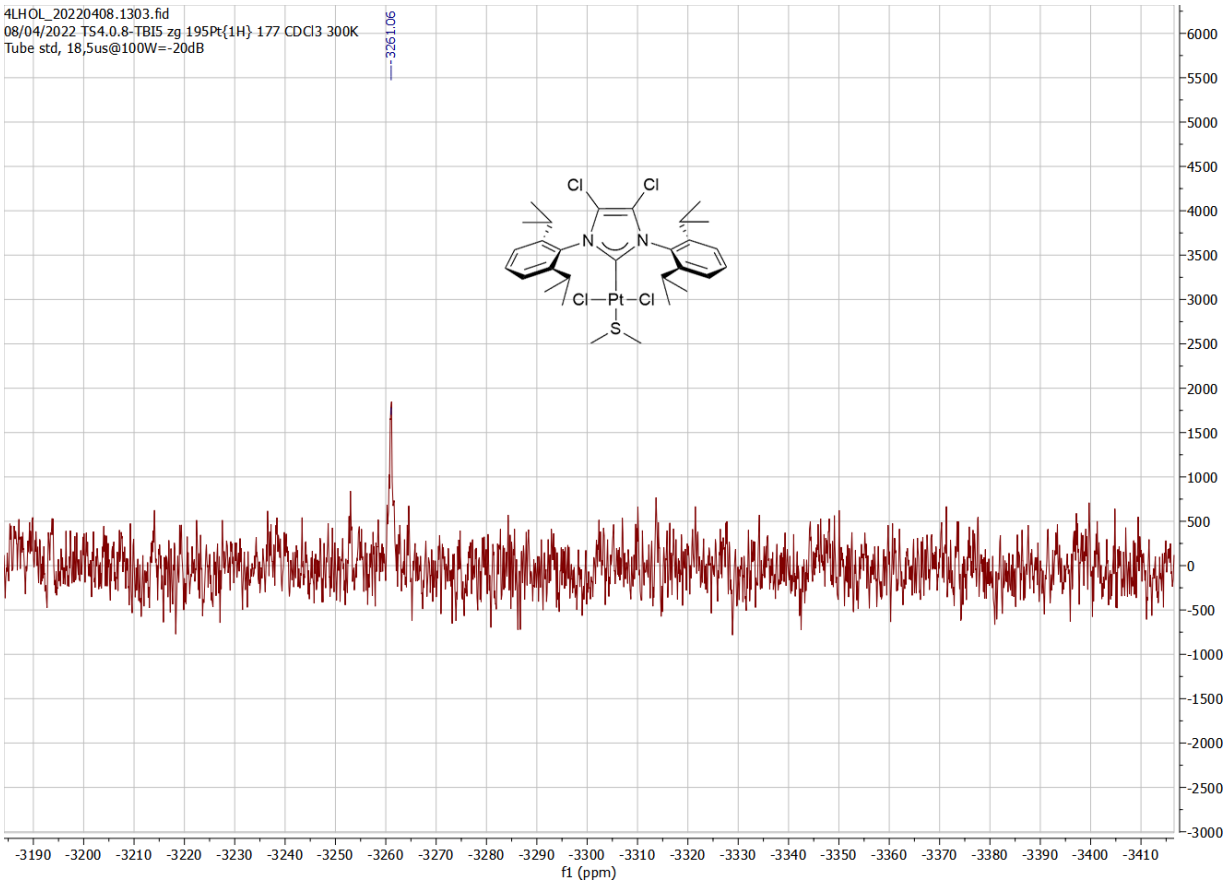
1.12. ^{195}Pt NMR of 3ah



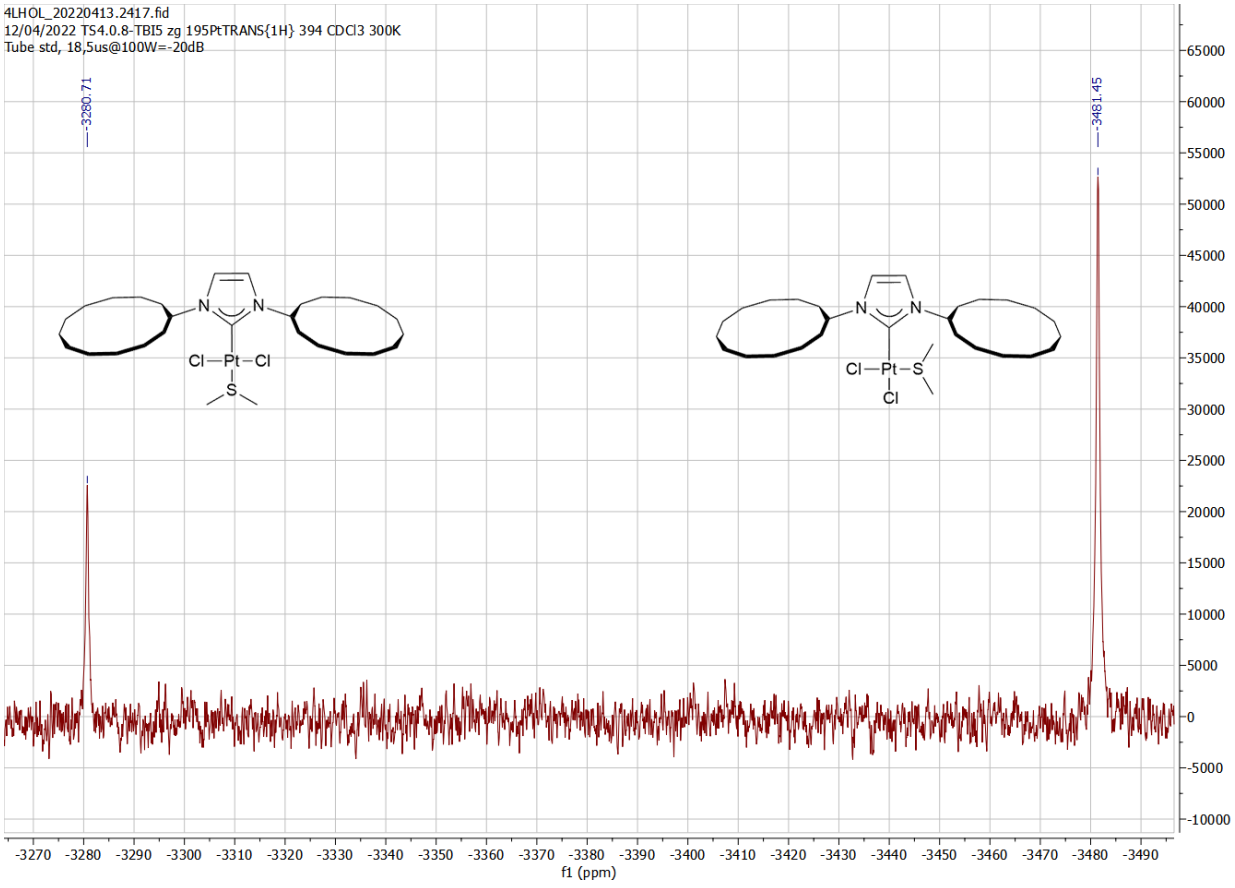
1.13. ^{195}Pt NMR of 3ai



1.14. ^{195}Pt NMR of 3aj

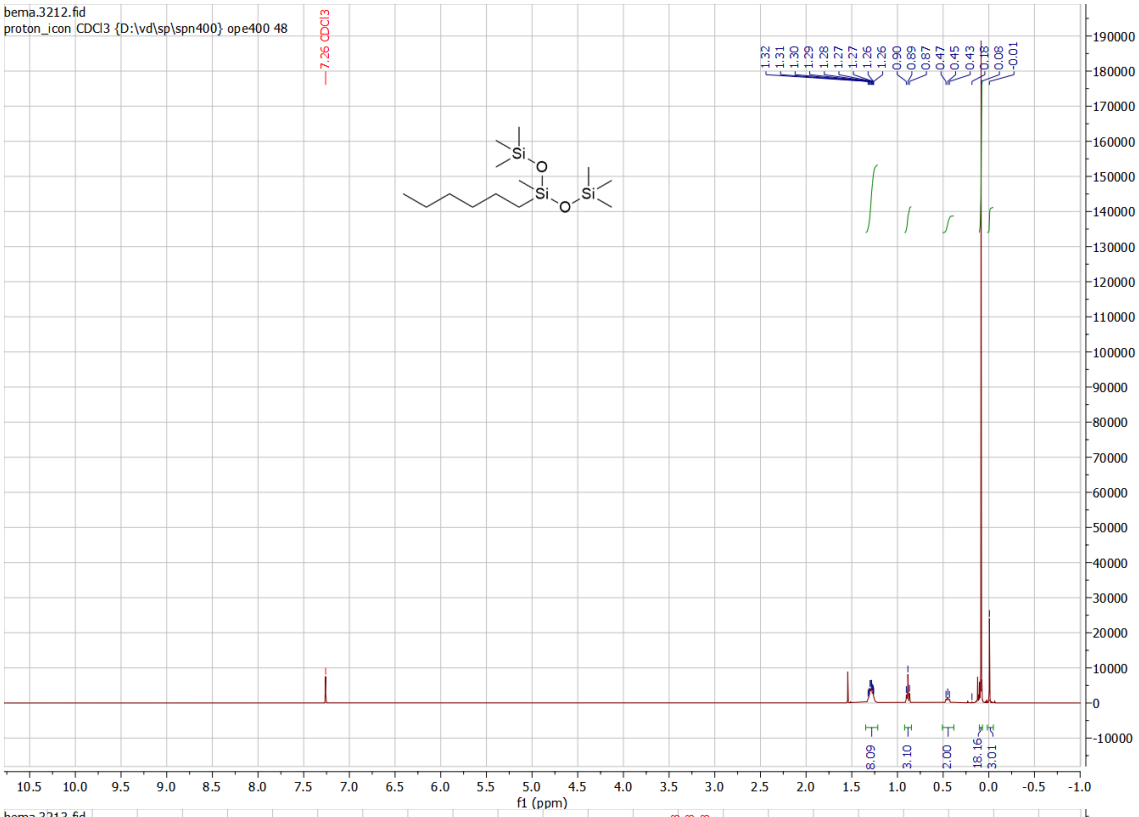


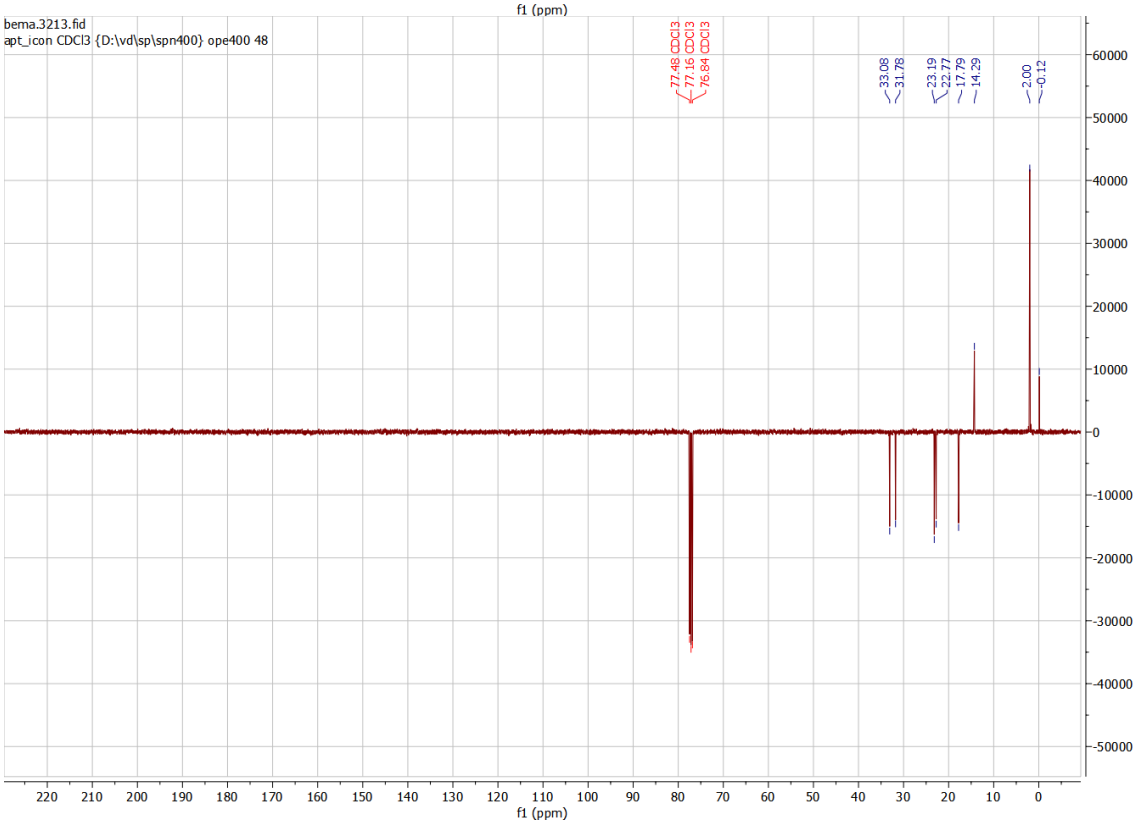
1.15. ^{195}Pt NMR of *cis*/*trans*-3ak



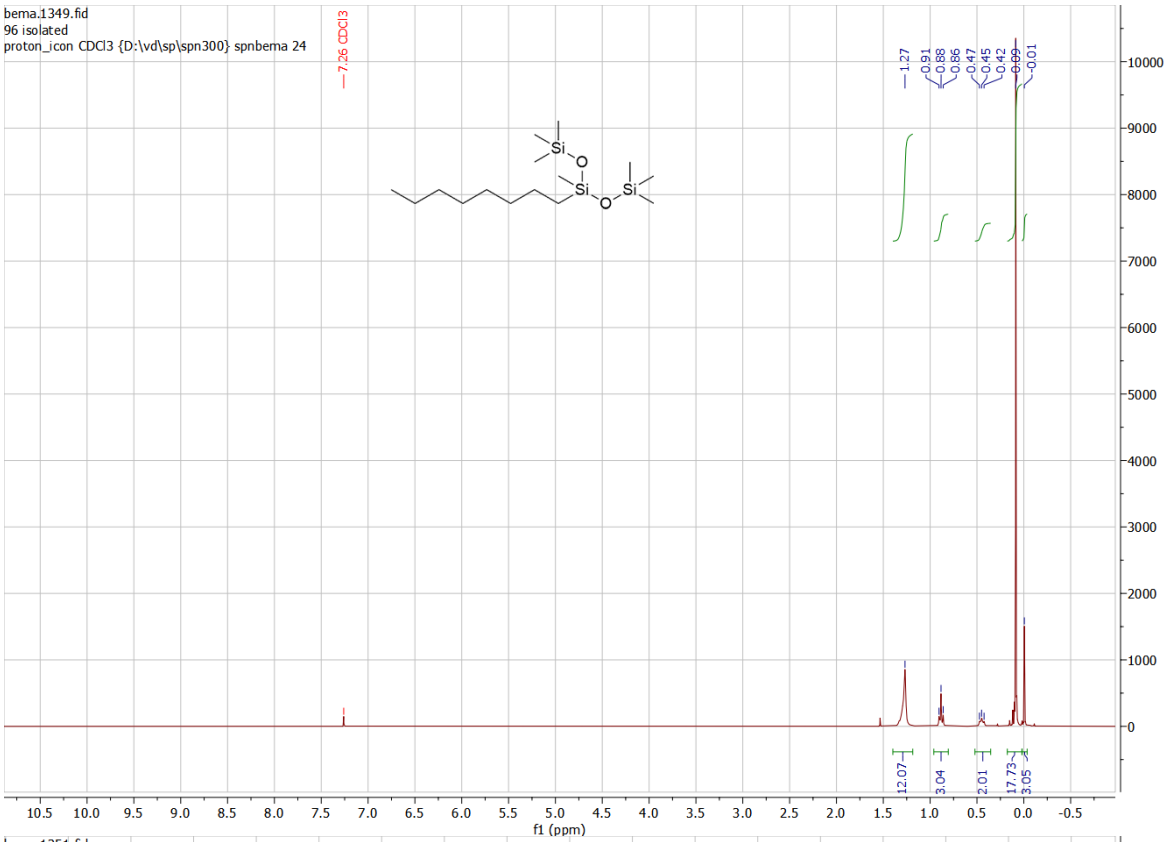
2. NMR spectra of the hydrosilylation products

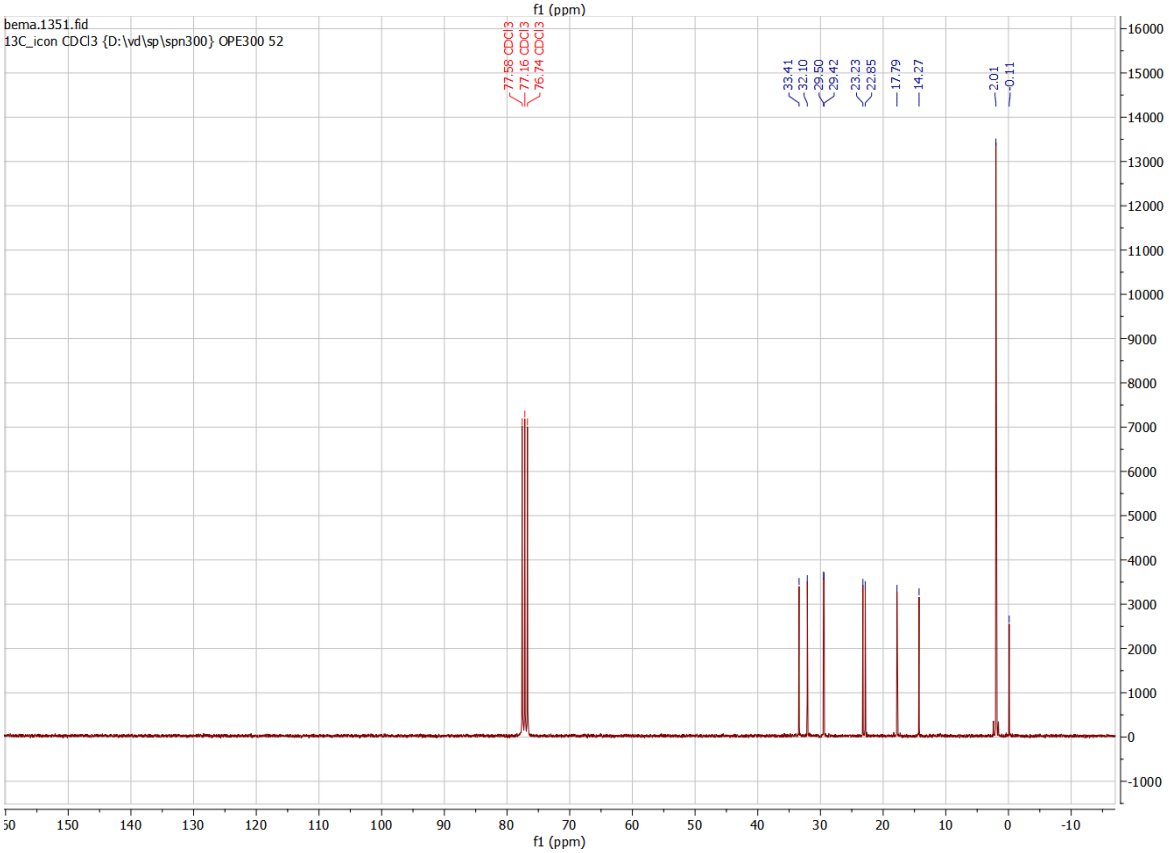
2.1. ^{1}H and $^{13}C\{^{1}H\}$ apt NMR of 6aa



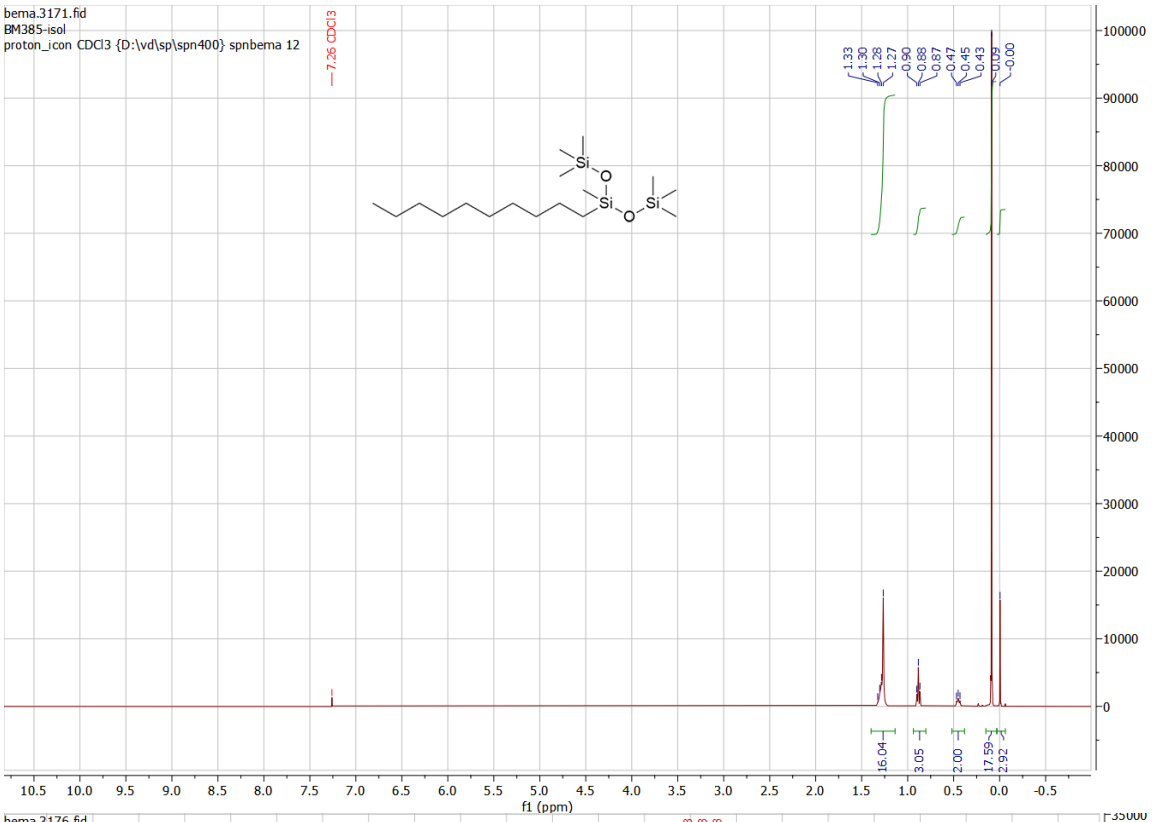


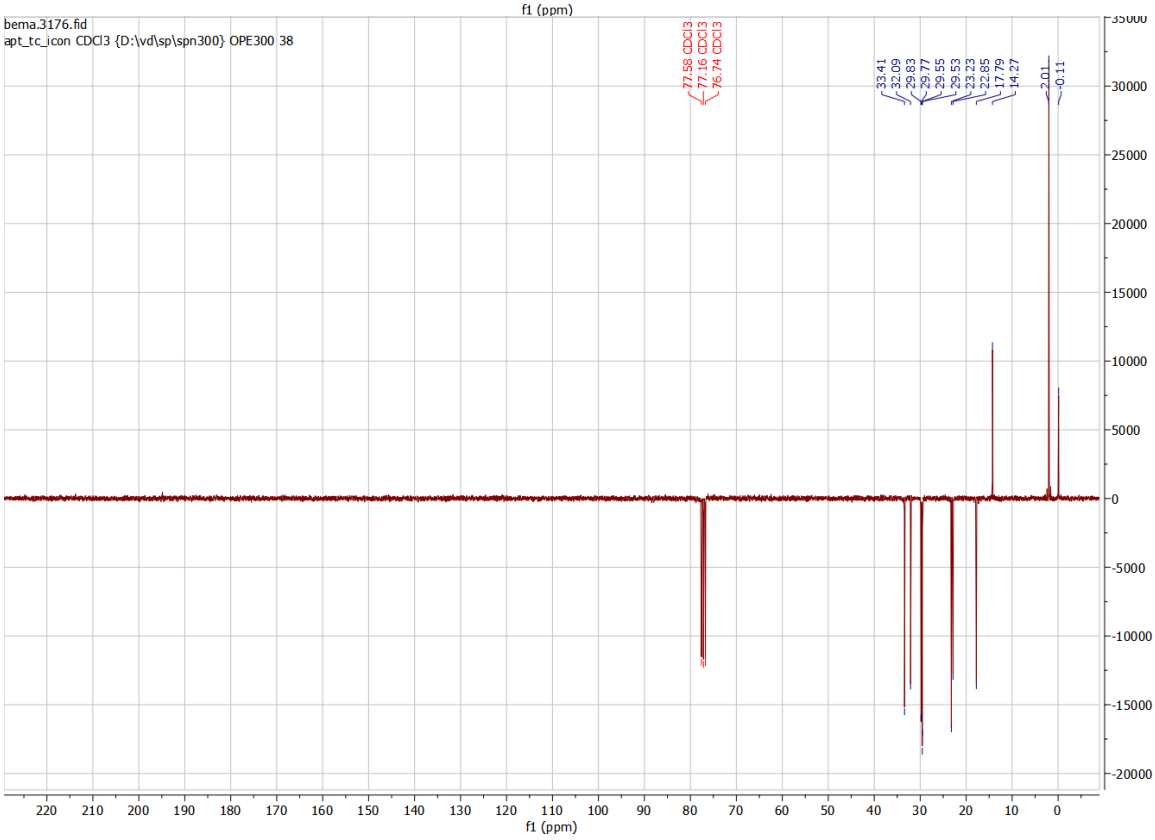
2.2. ^{1}H and $^{13}C\{^{1}H\}$ NMR of 6ab



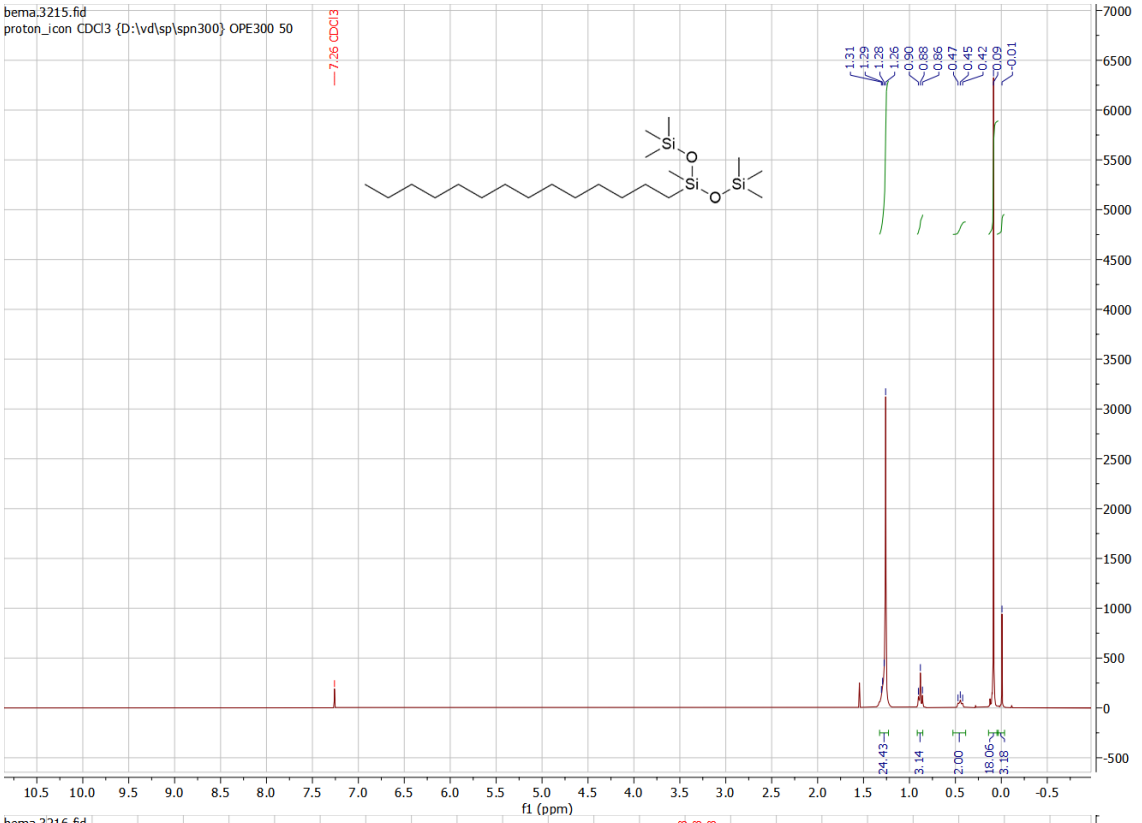


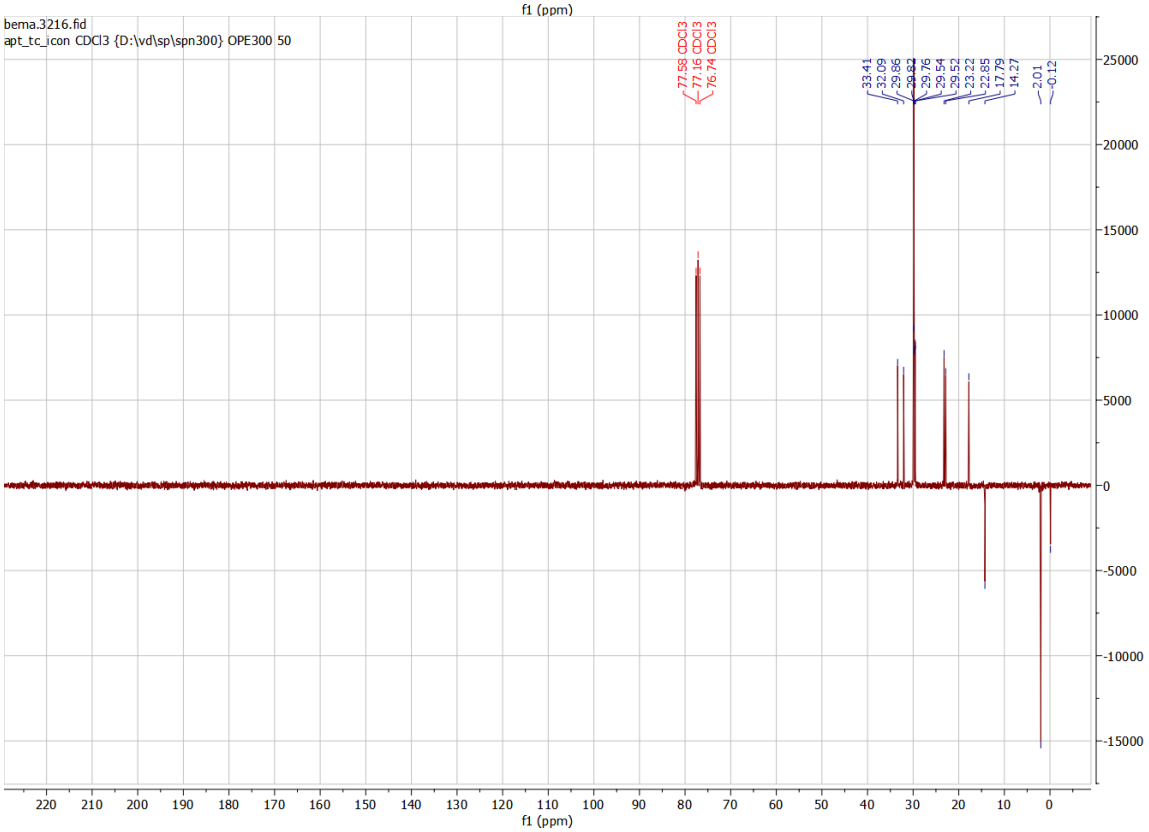
2.3. ^{1}H and $^{13}C\{^{1}H\}$ apt NMR of 6ac



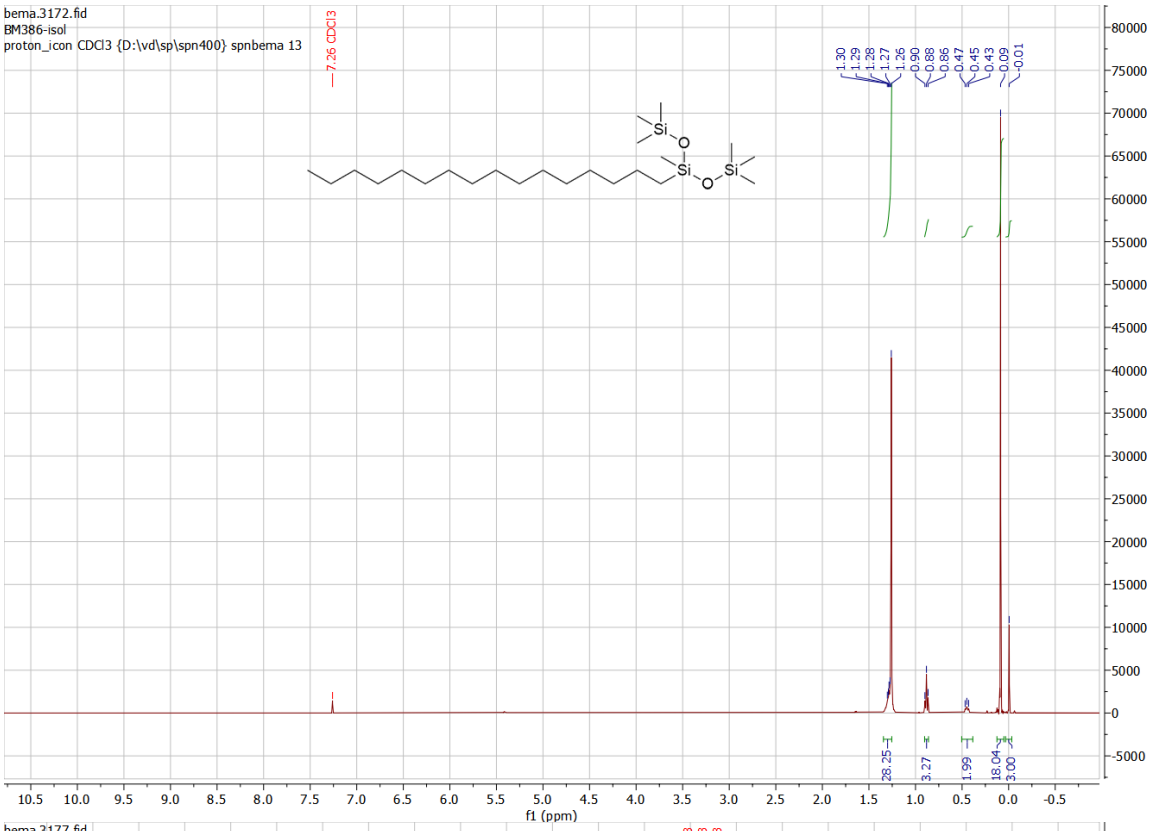


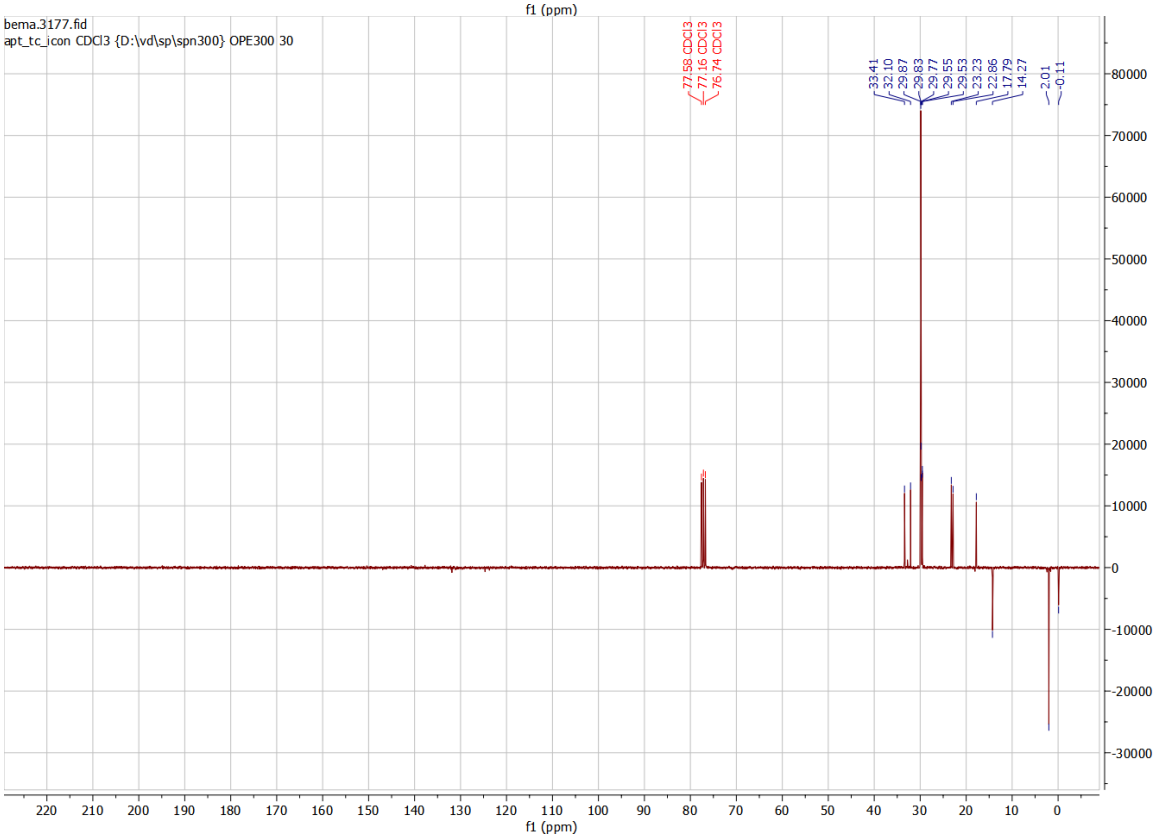
2.4. ^{1}H and $^{13}C\{^{1}H\}$ apt NMR of 6ad



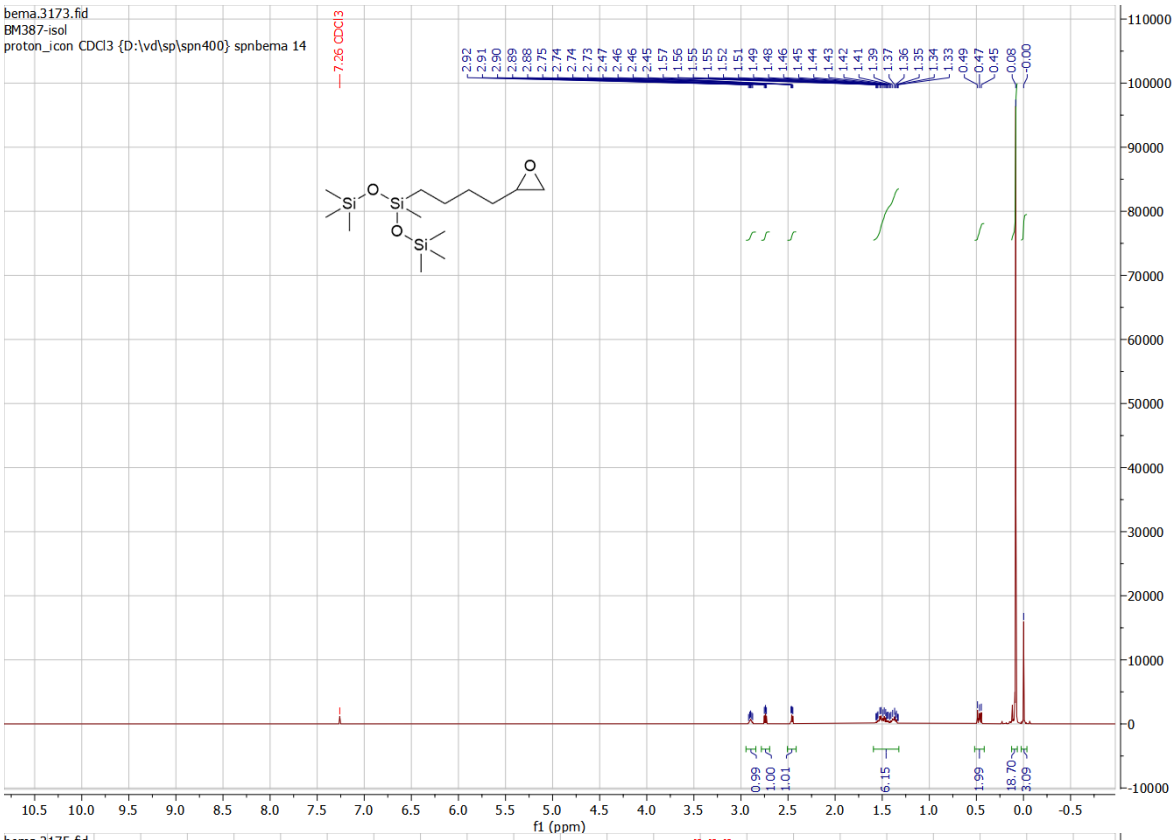


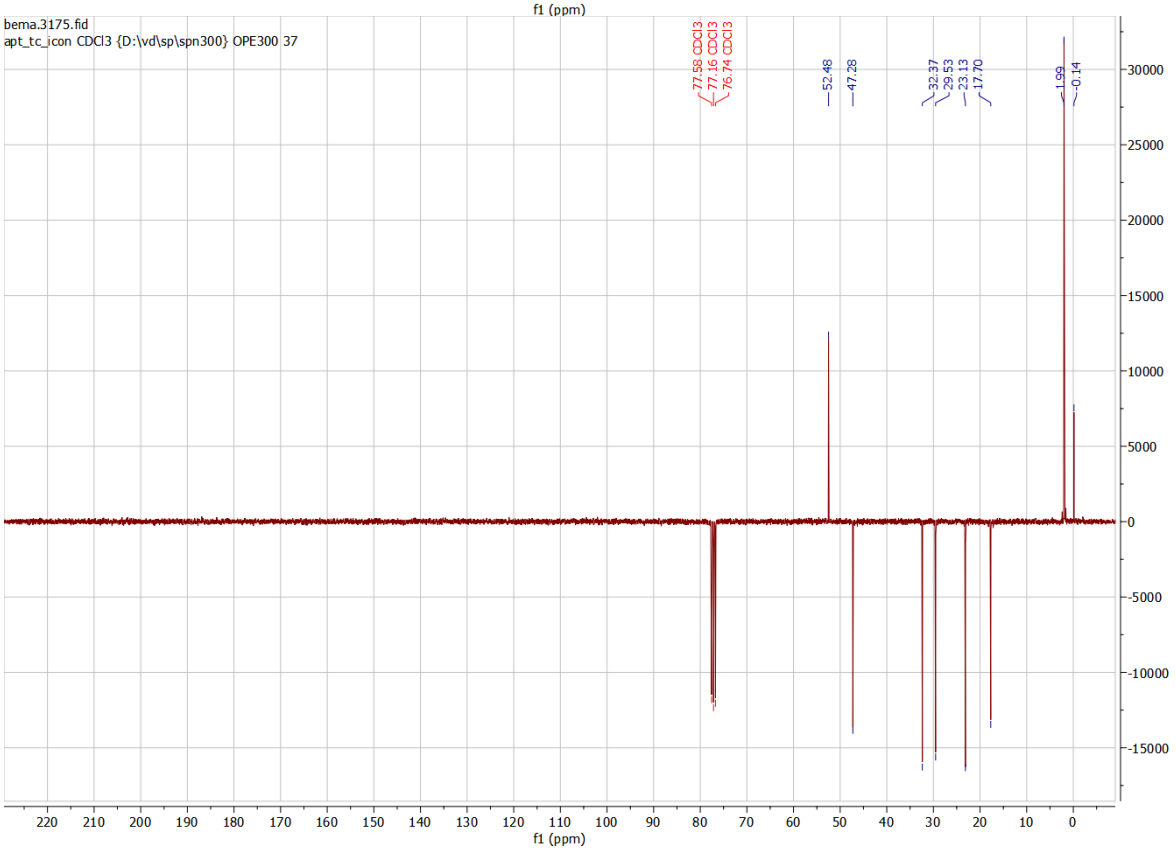
2.5. ^{1}H and $^{13}C\{^{1}H\}$ apt NMR of 6ae



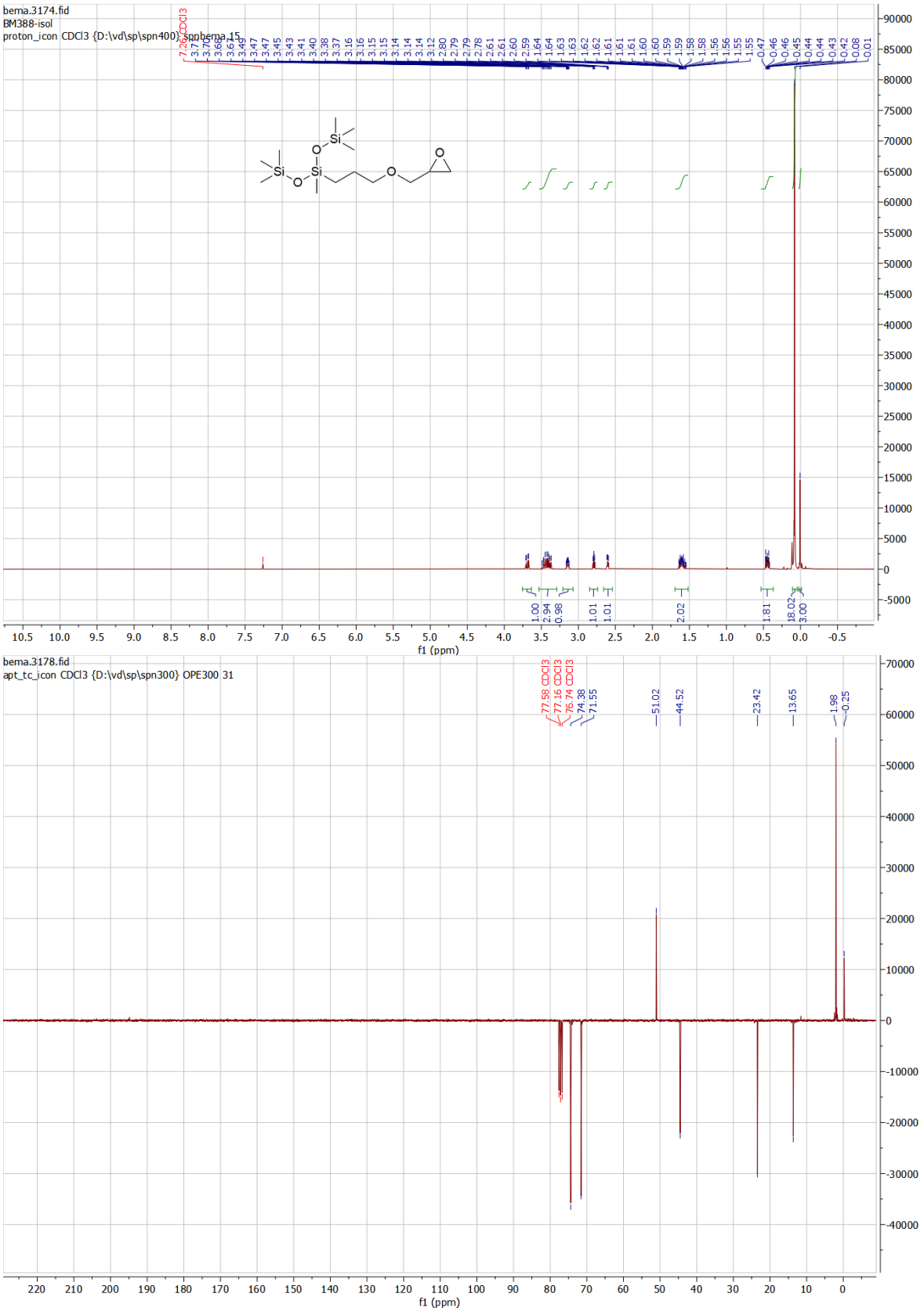


2.6. ^{1}H and $^{13}C\{^{1}H\}$ apt NMR of 6af

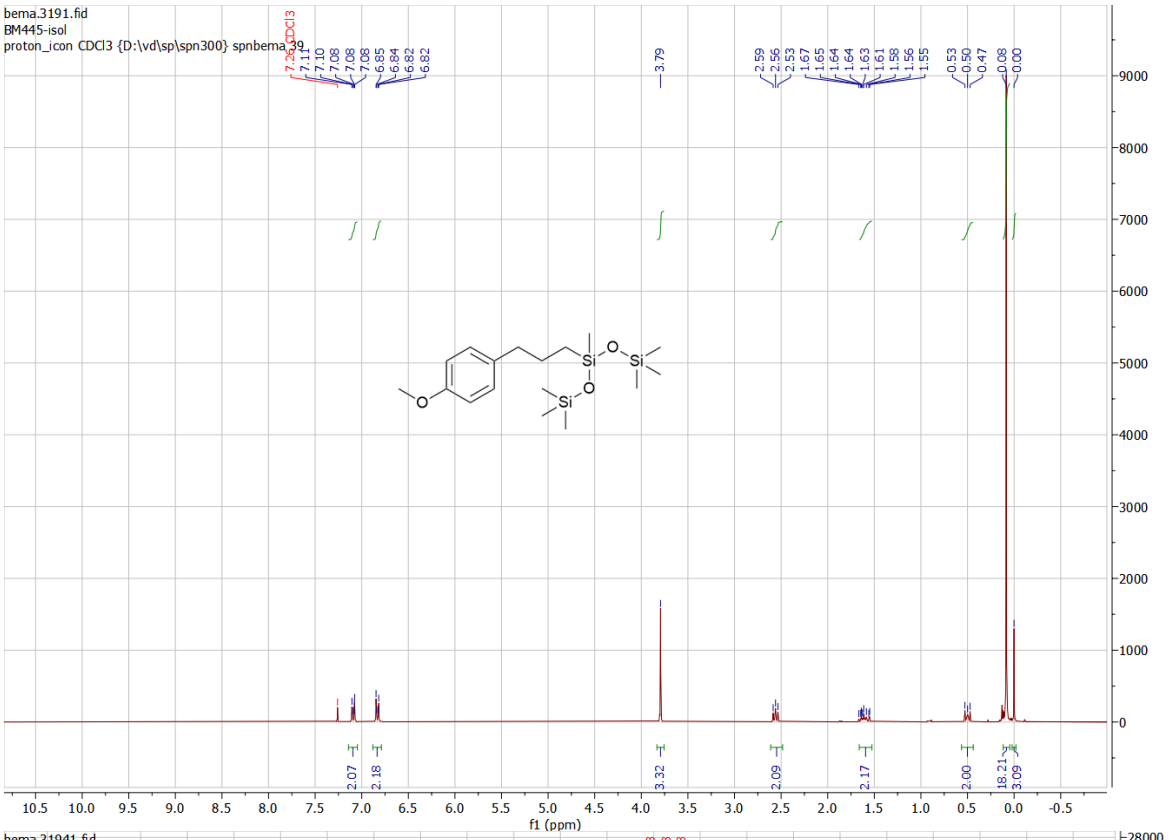


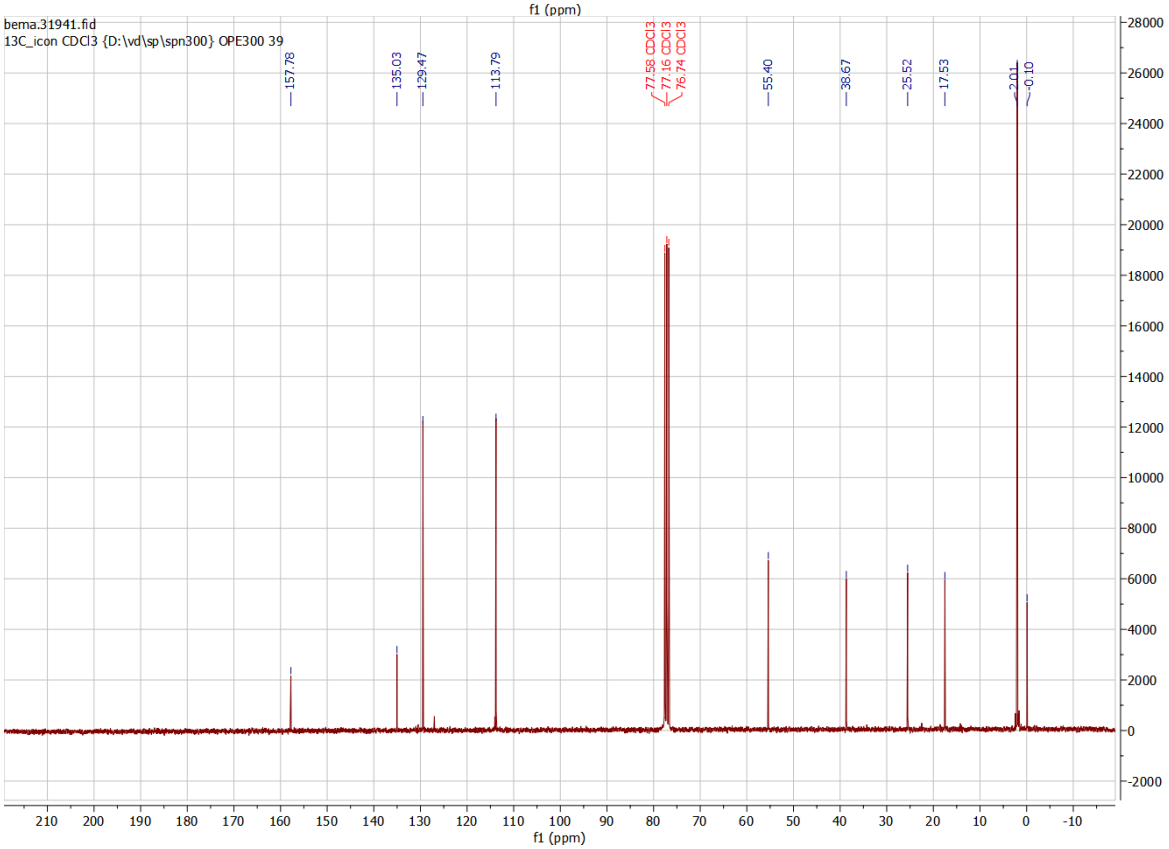


2.7. ^{1}H and $^{13}C\{^{1}H\}$ apt NMR of 6ag

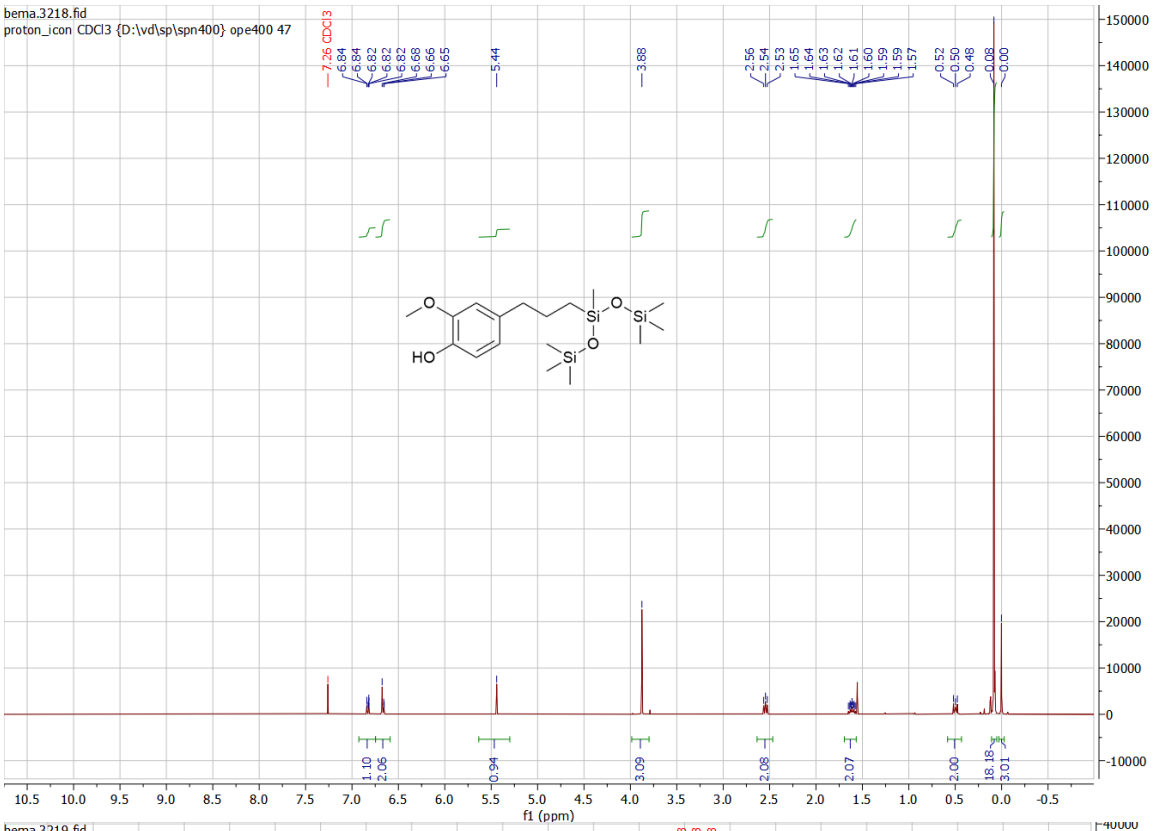


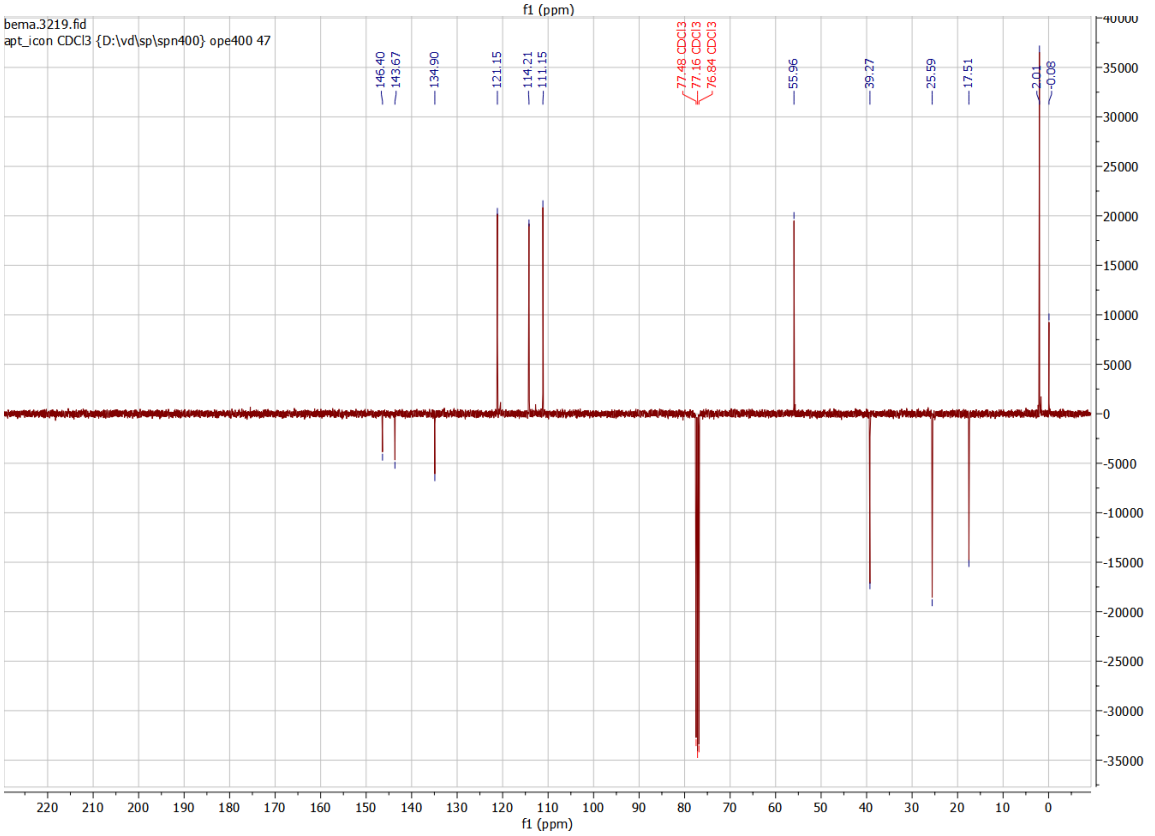
2.8. ^{1}H and $^{13}C\{^{1}H\}$ NMR of 6ah



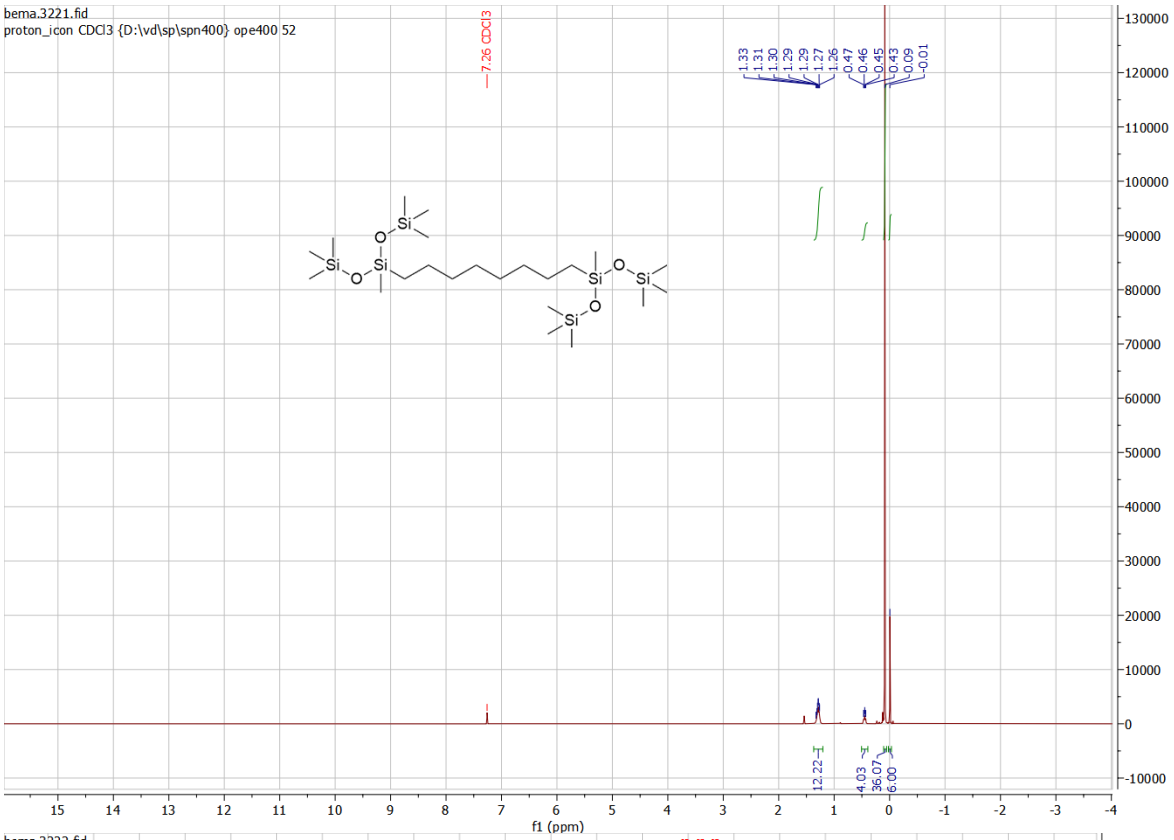


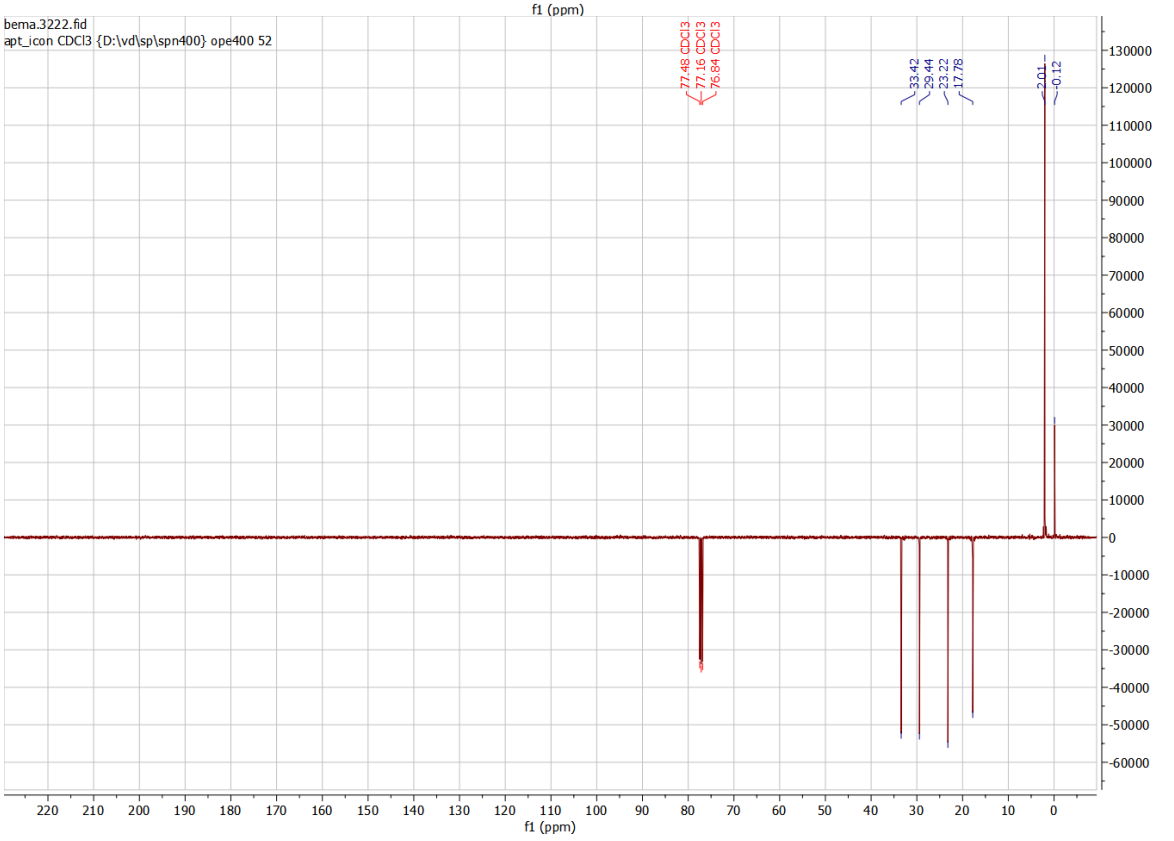
2.9. ^{1}H and $^{13}C\{^{1}H\}$ apt NMR of 6ai



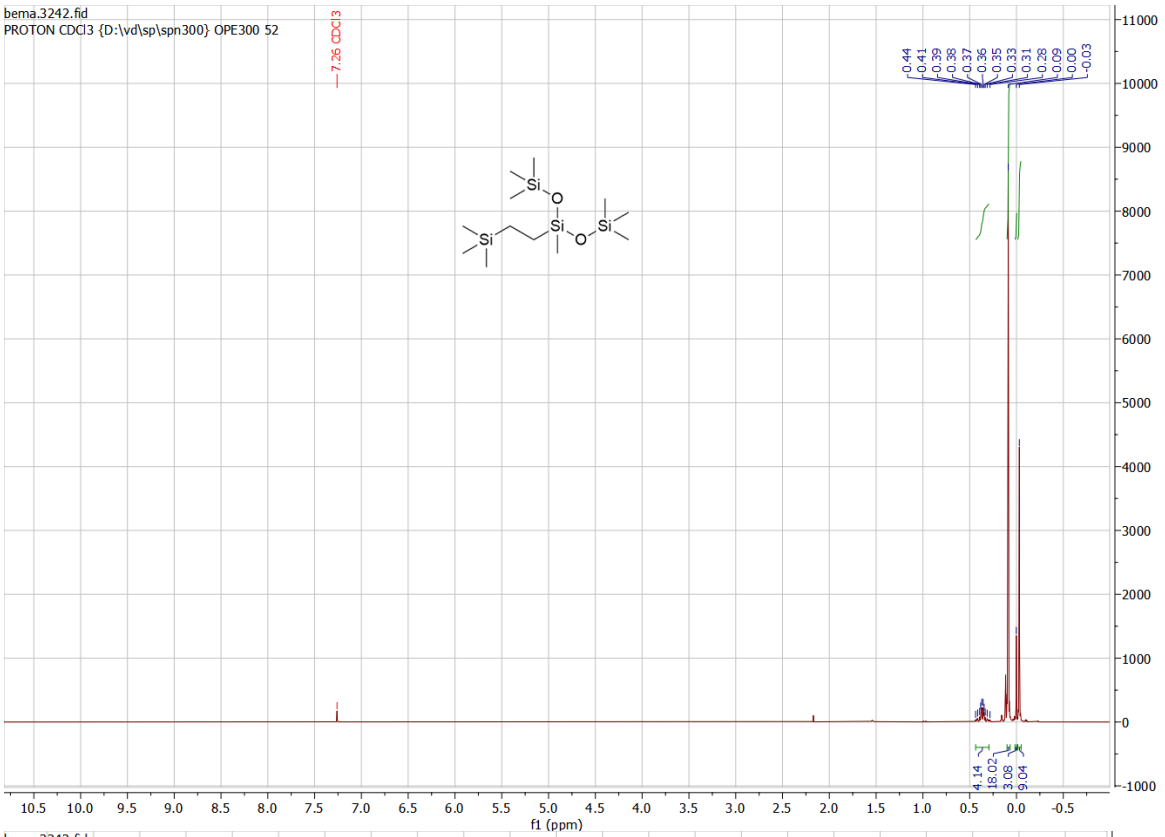


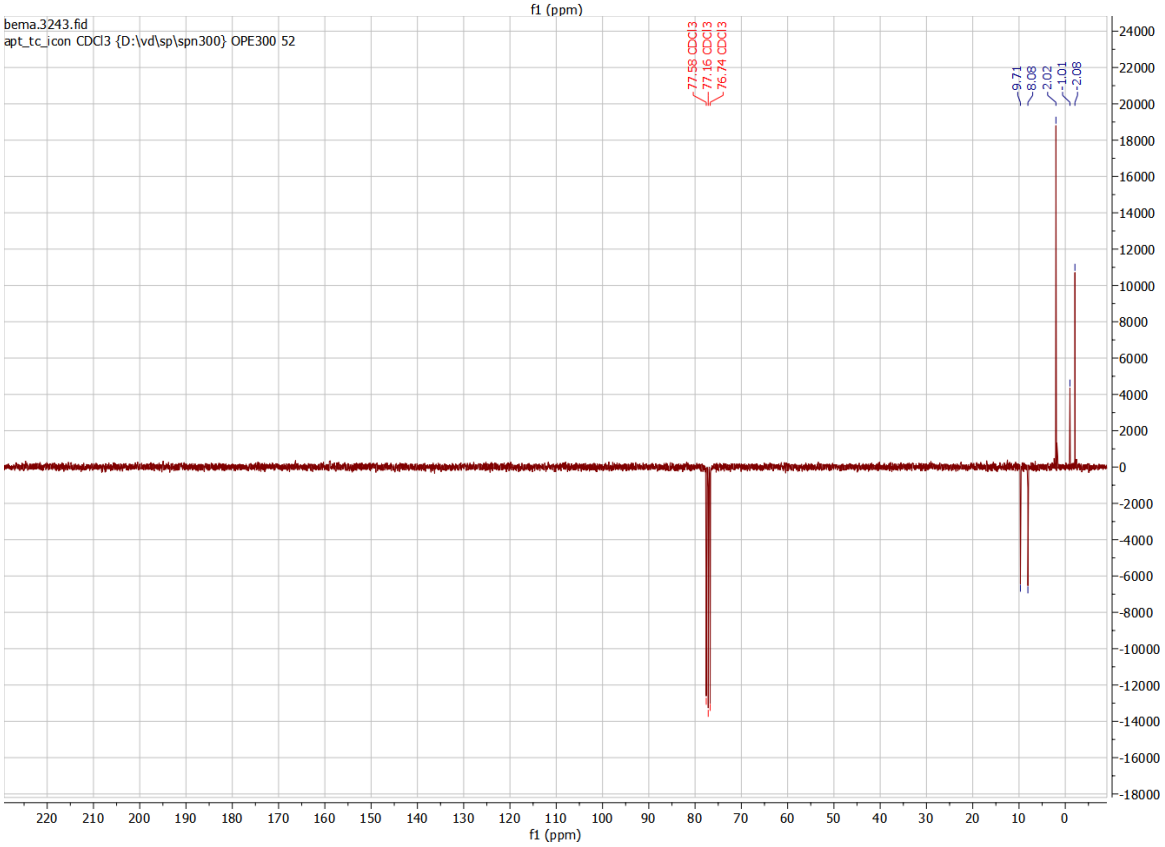
2.10. ^{1}H and $^{13}C\{^{1}H\}$ apt NMR of 6aj



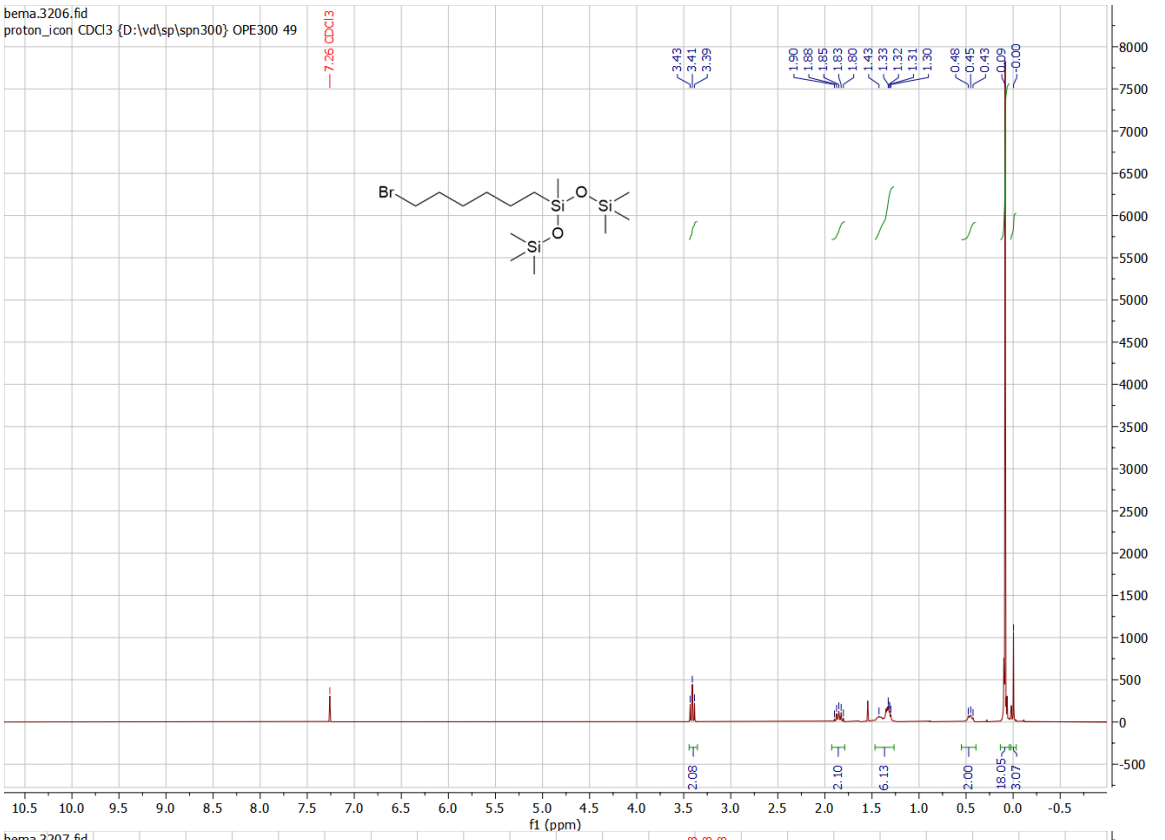


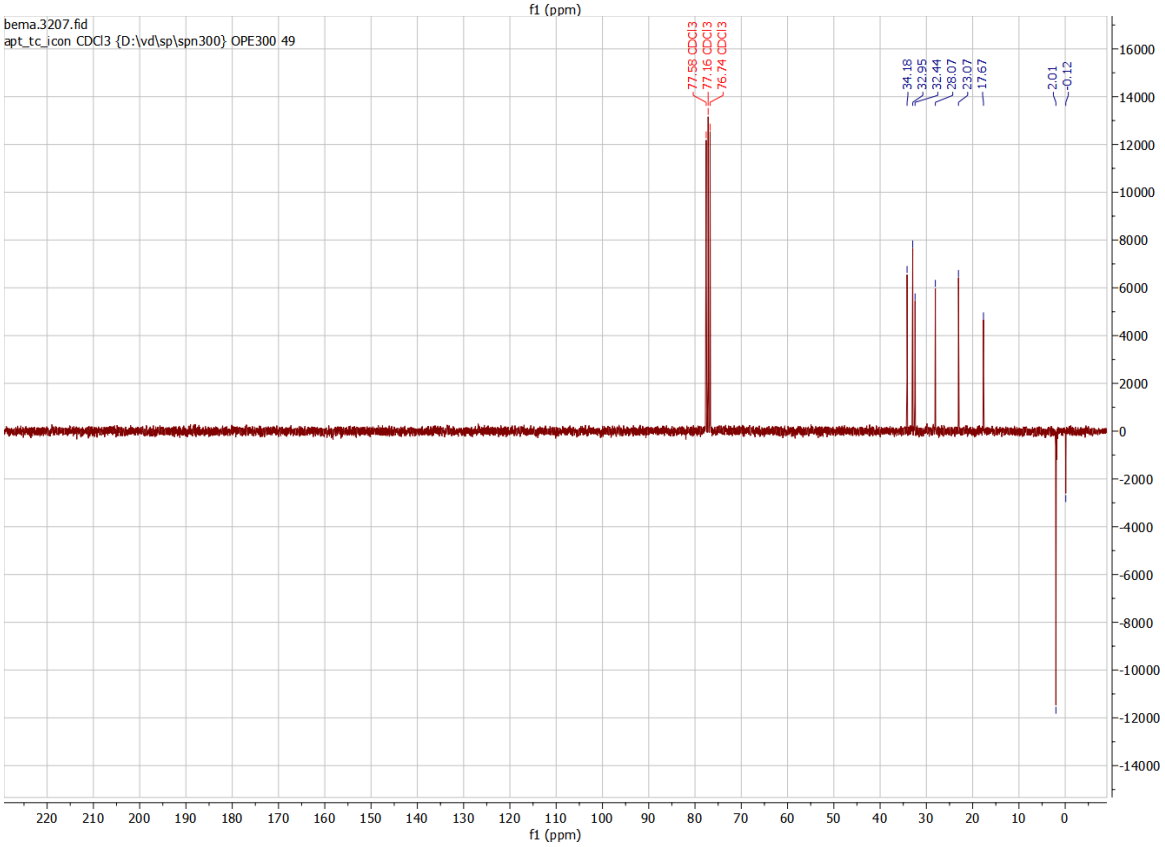
2.11. ^{1}H and $^{13}C\{^{1}H\}$ apt NMR of 6ak



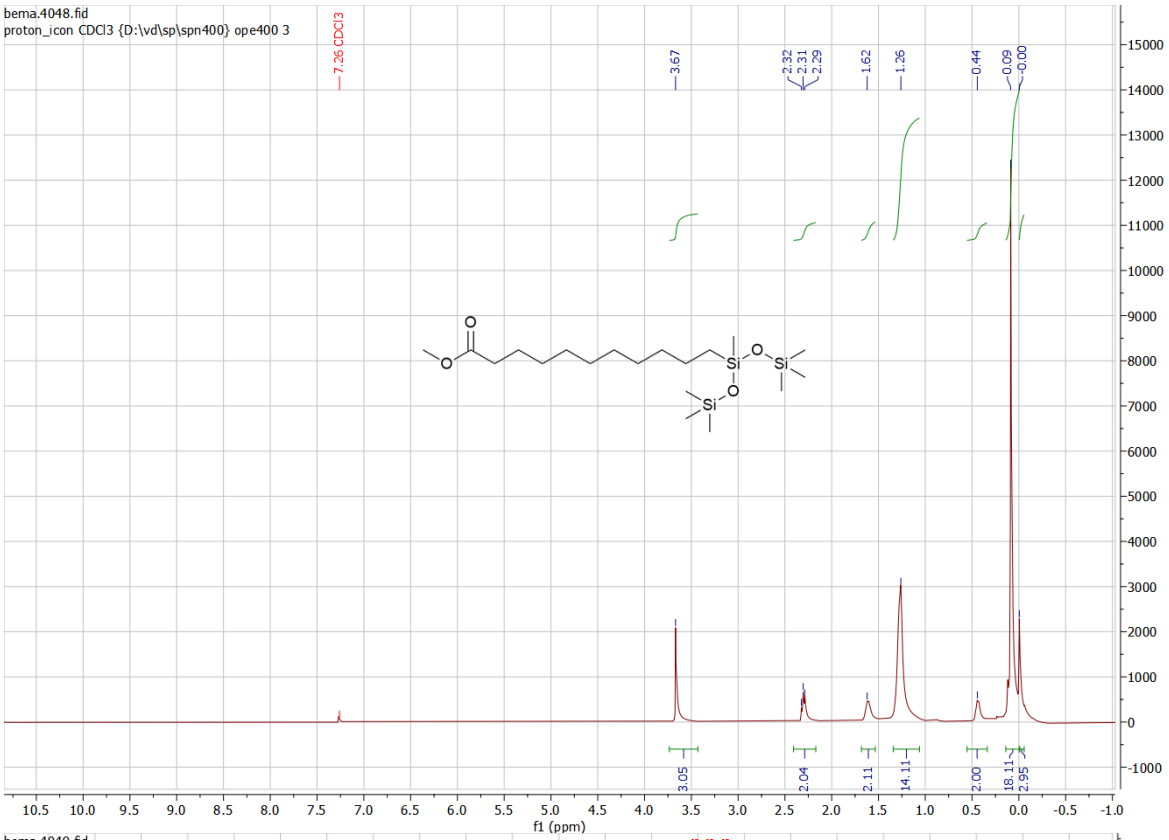


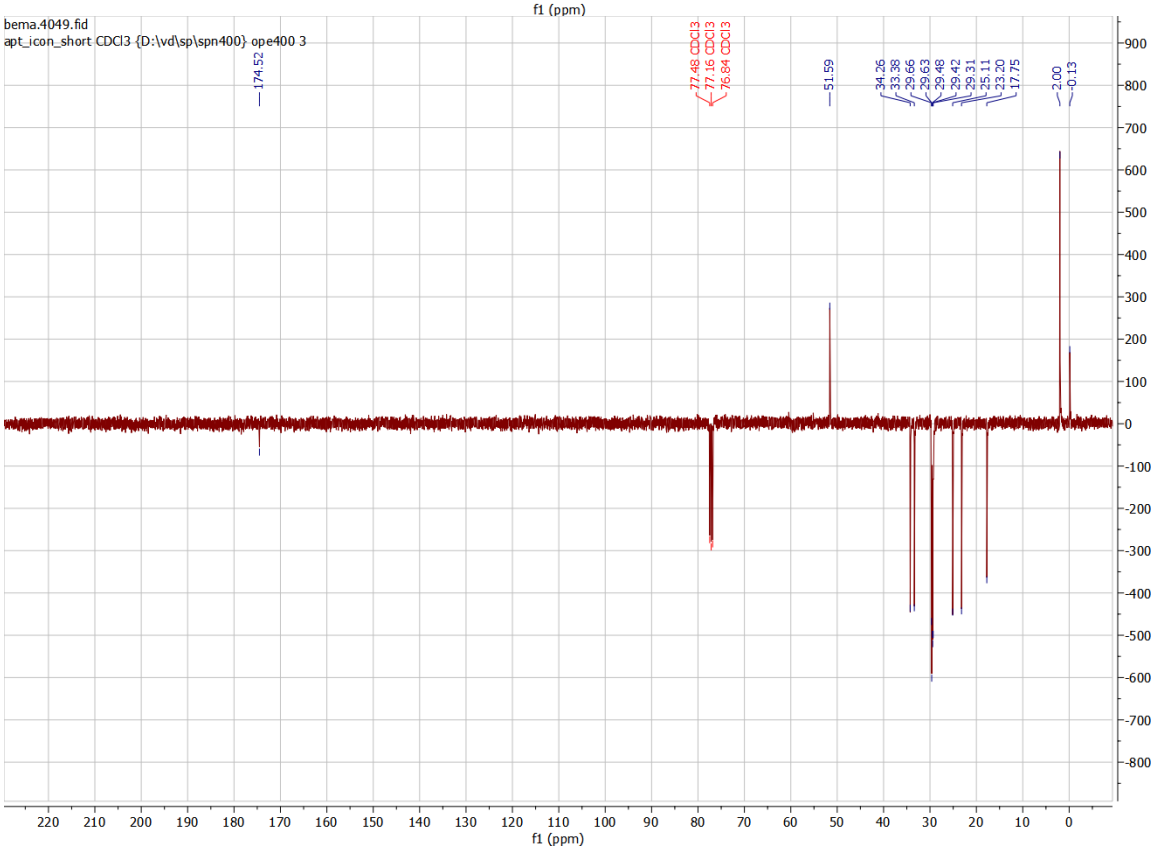
2.12. ^{1}H and $^{13}C\{^{1}H\}$ apt NMR of 6al



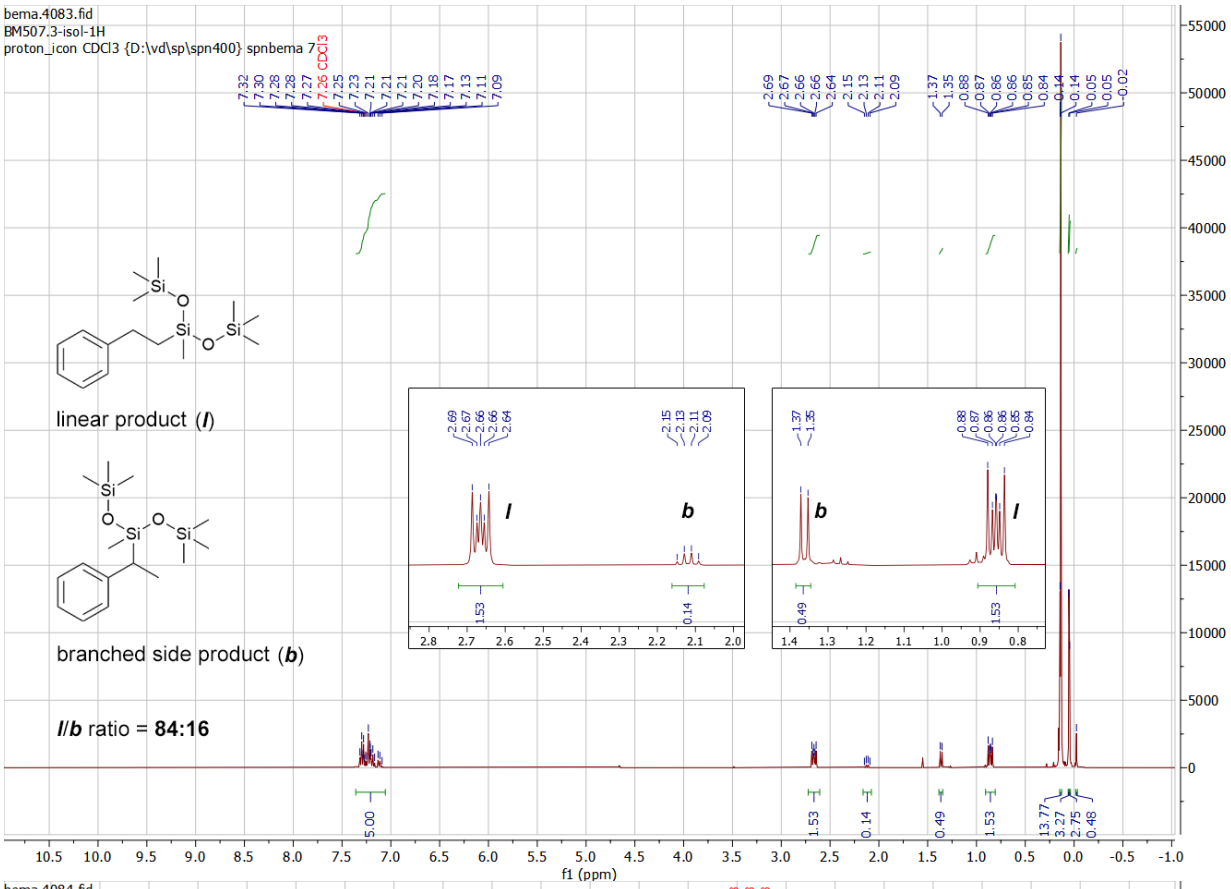


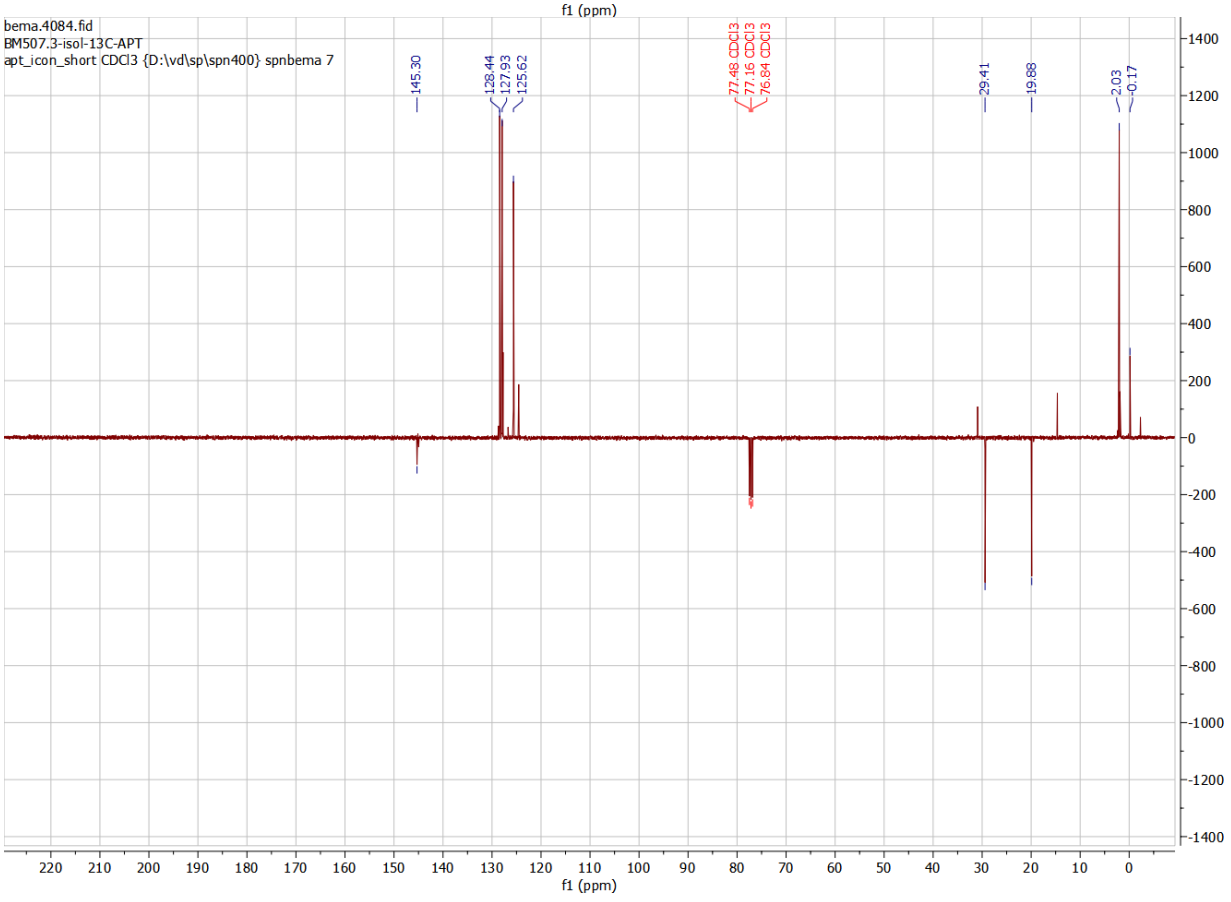
2.13. ^{1}H and $^{13}C\{^{1}H\}$ apt NMR of 6am



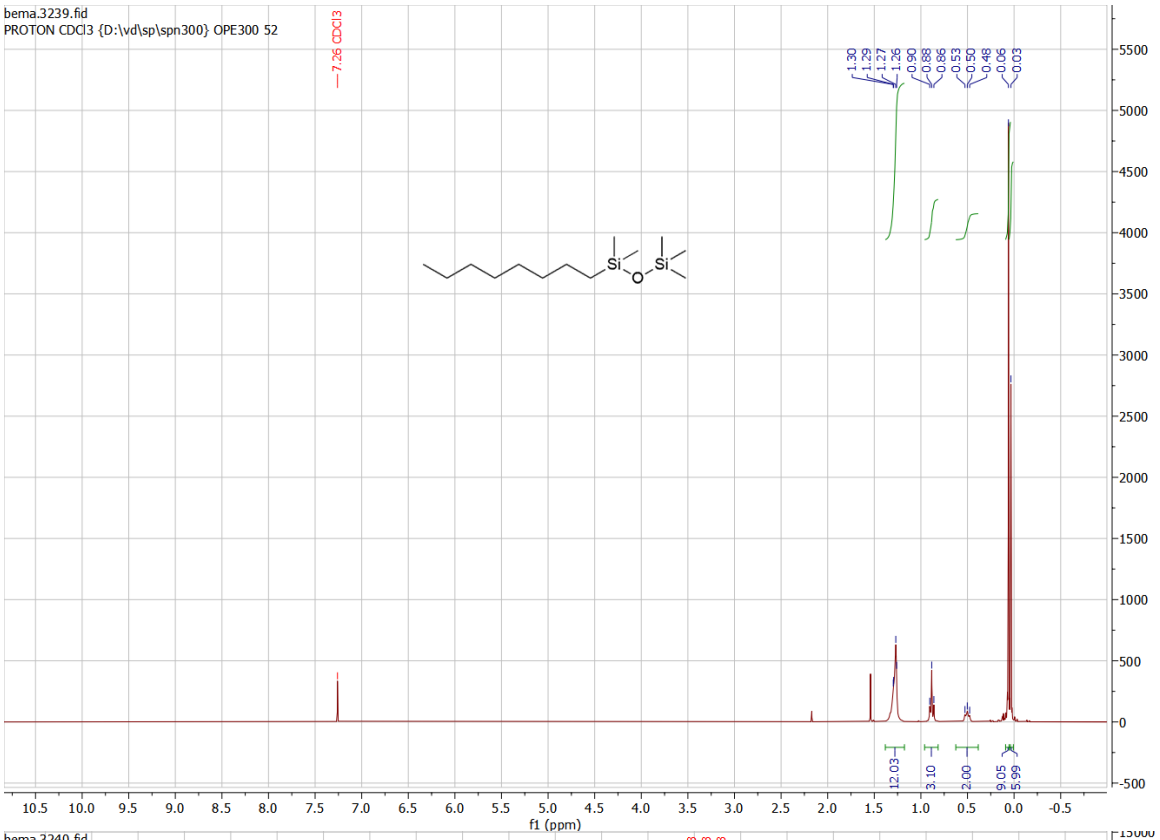


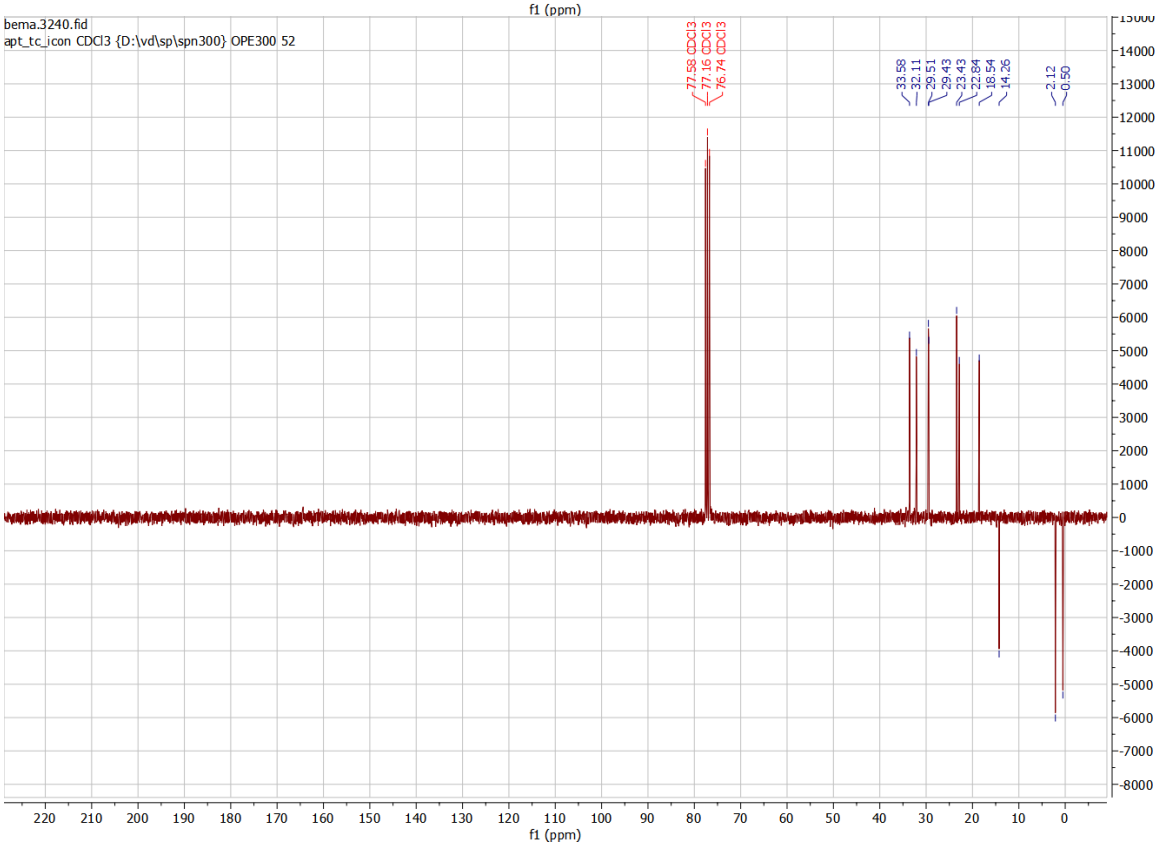
2.14. ^{1}H and $^{13}C\{^{1}H\}$ apt NMR of 6an



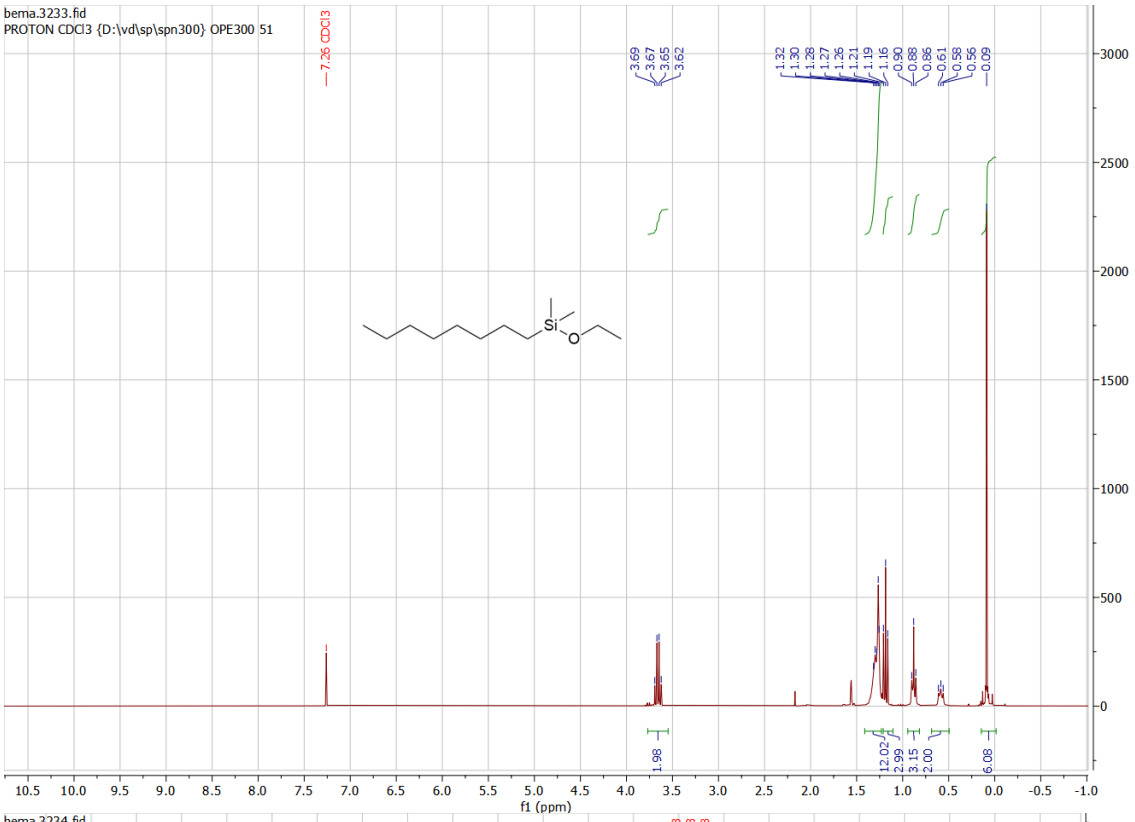


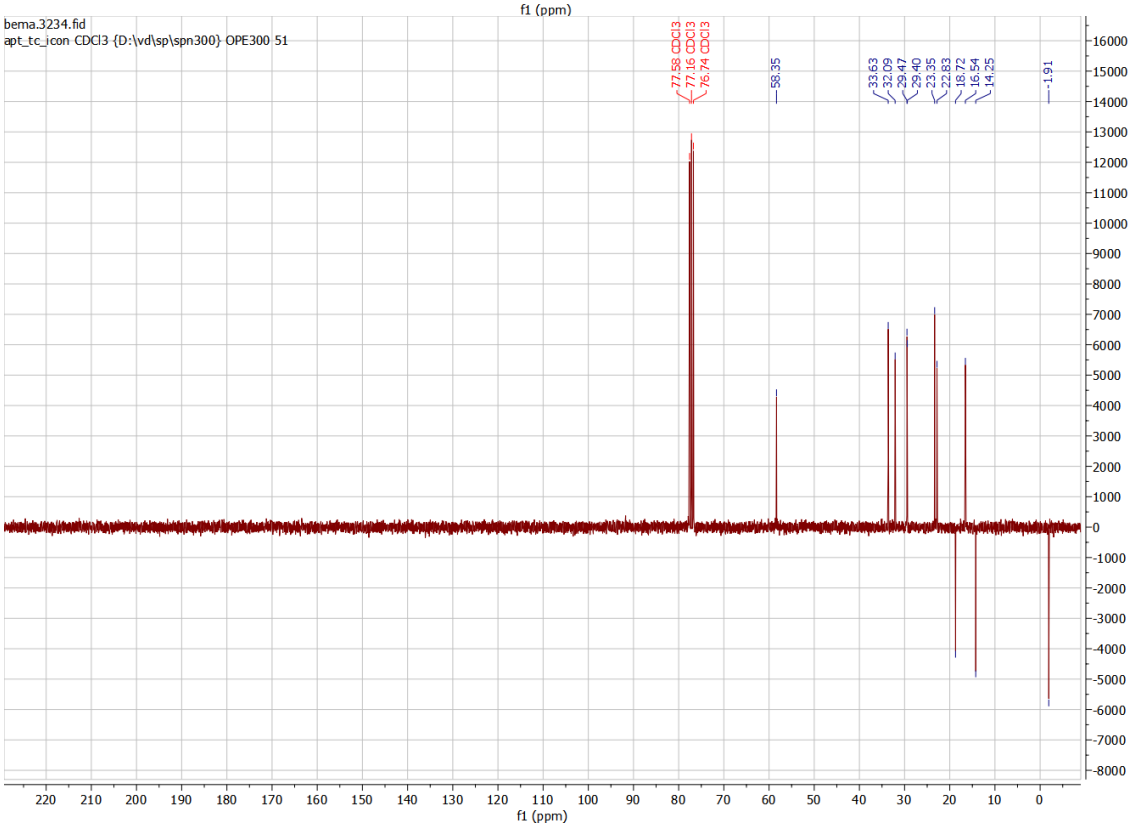
2.15. ^{1}H and $^{13}C\{^{1}H\}$ apt NMR of 6bb



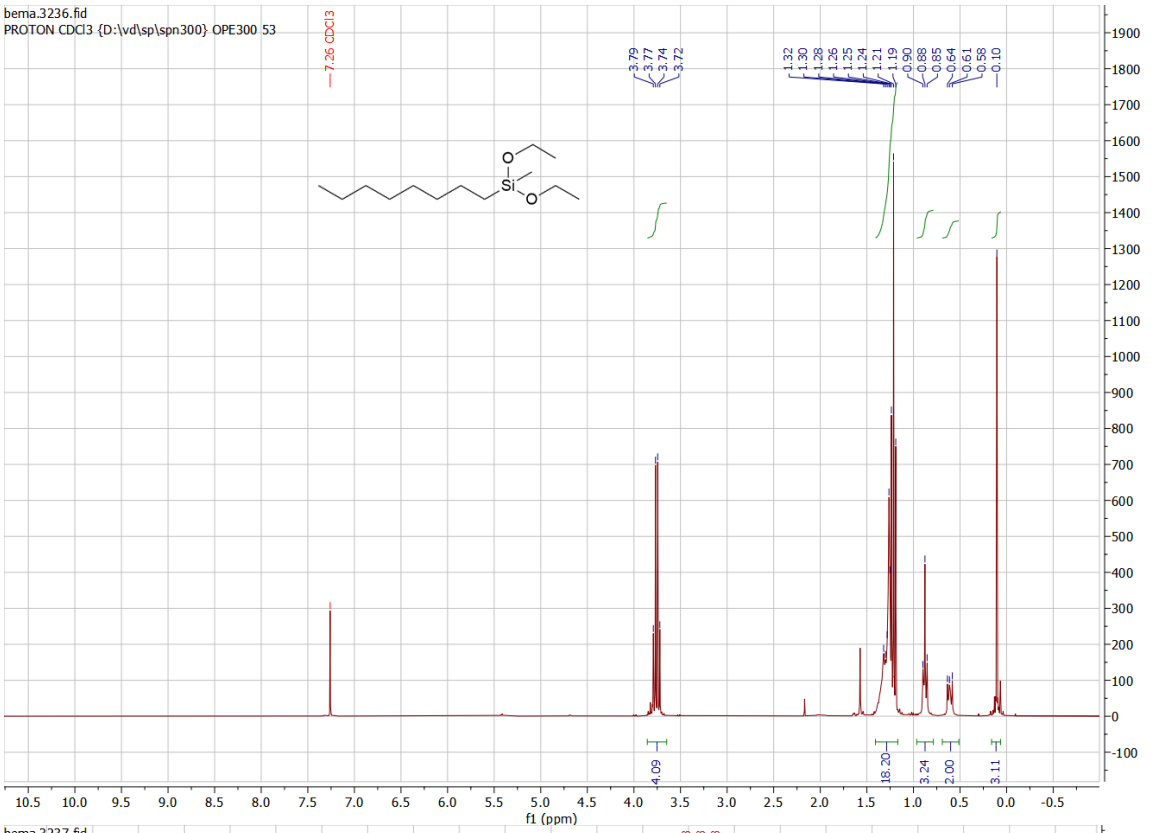


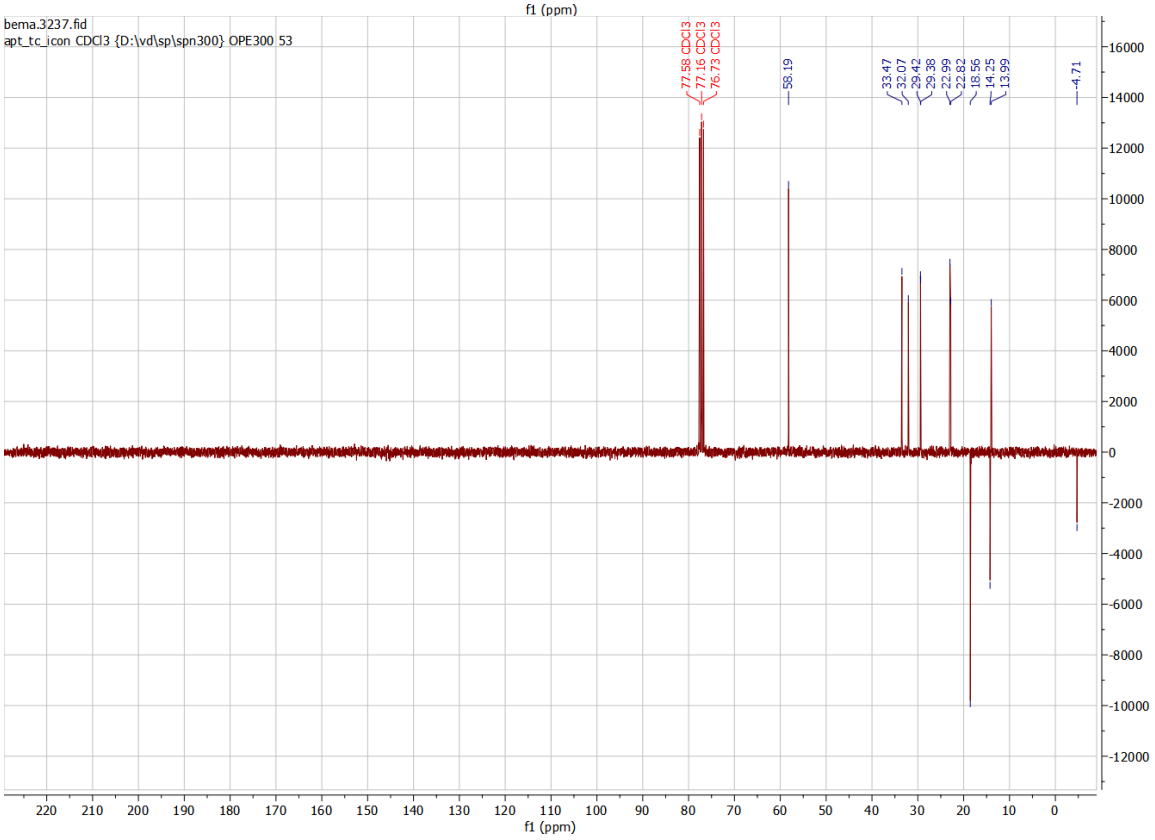
2.16. ^{1}H and $^{13}C\{^{1}H\}$ apt NMR of 6cb



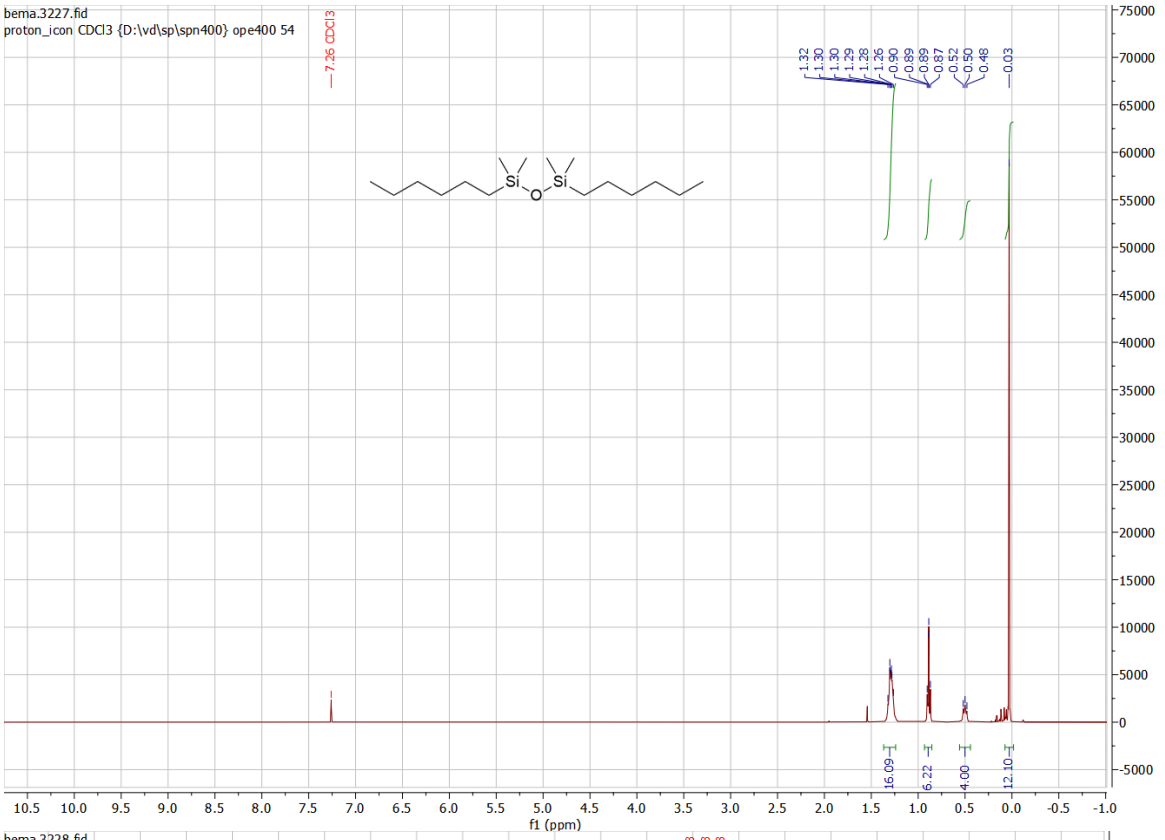


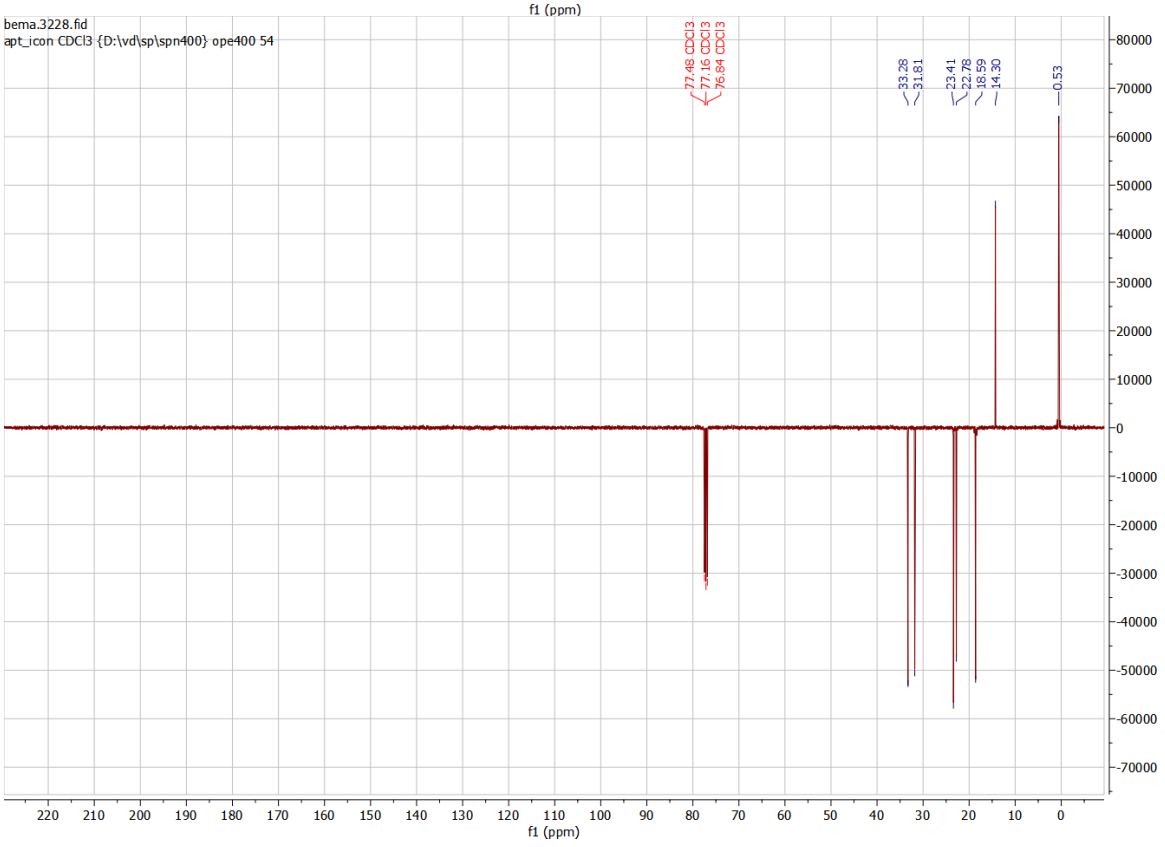
2.17. ^{1}H and $^{13}C\{^{1}H\}$ apt NMR of 6db



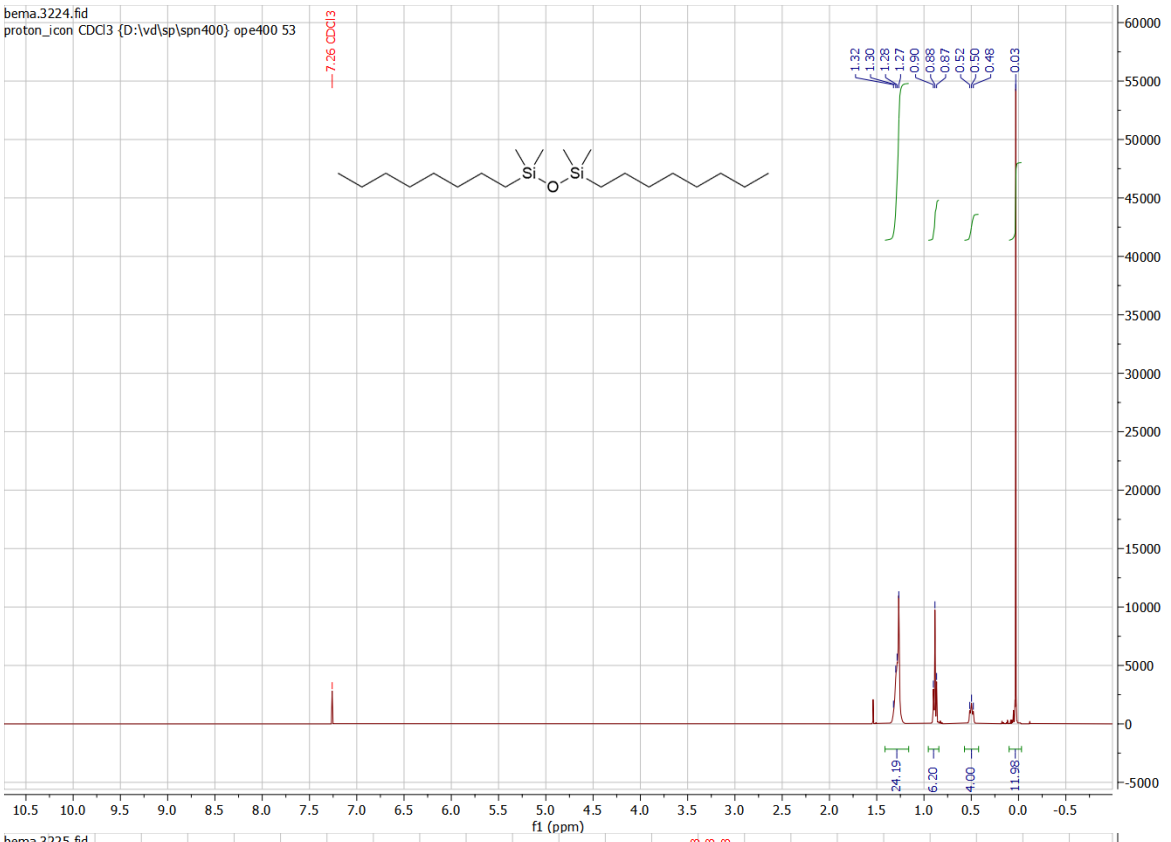


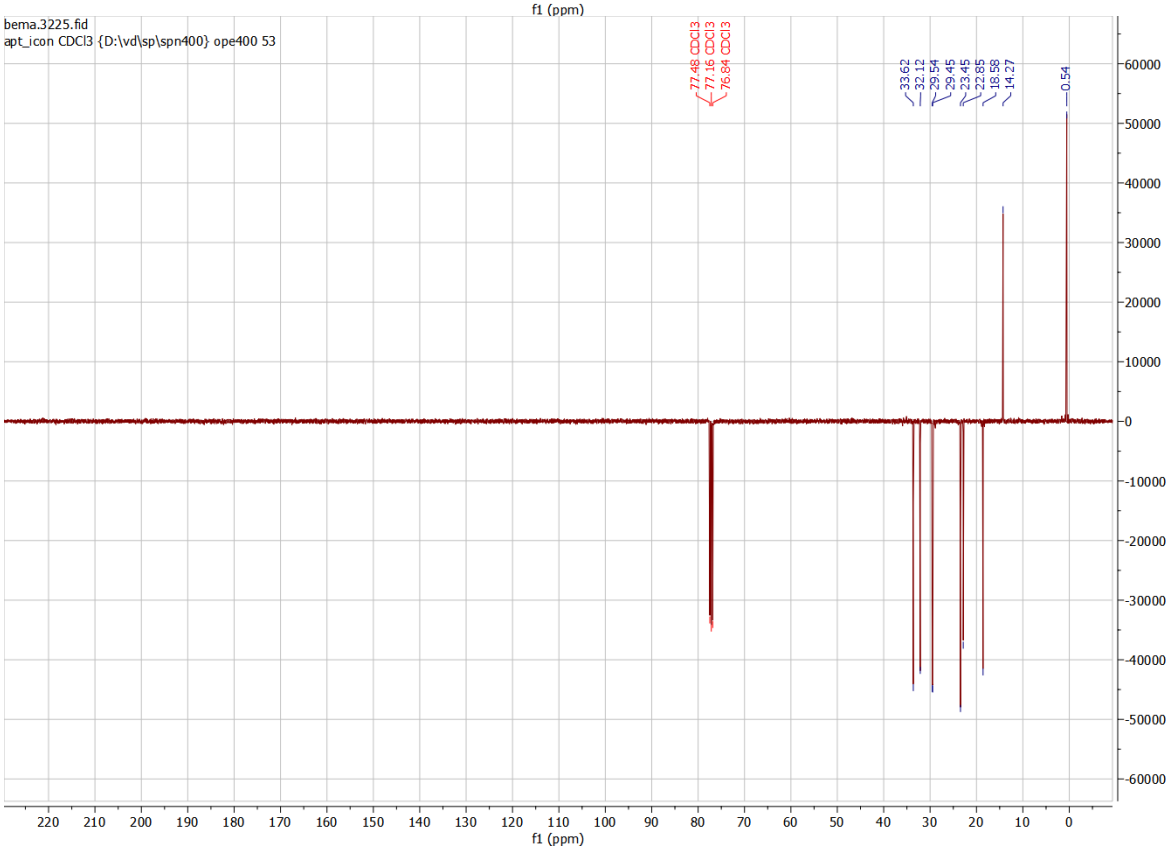
2.18. ^{1}H and $^{13}C\{^{1}H\}$ apt NMR of 6ea



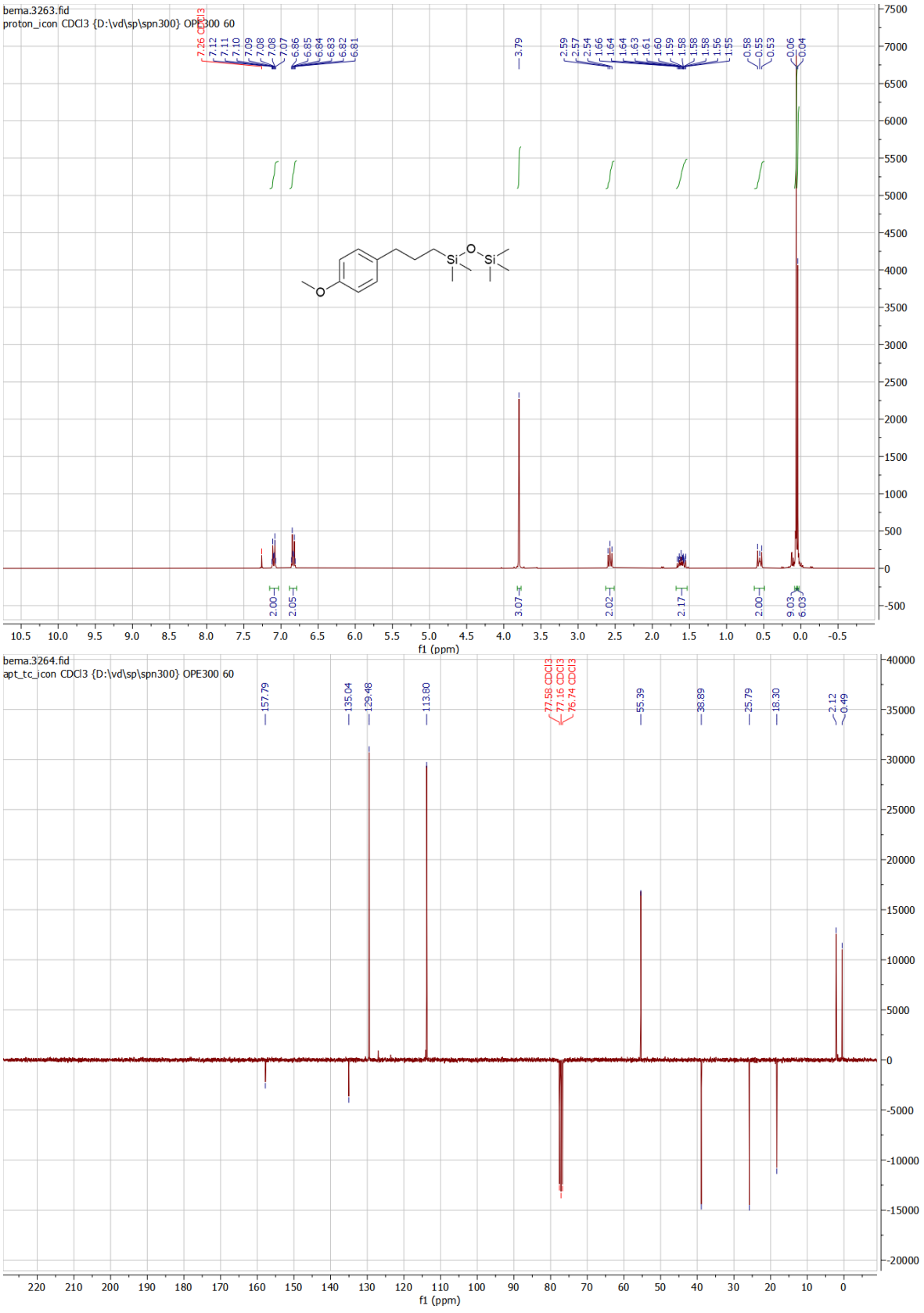


2.19. ^{1}H and $^{13}C\{^{1}H\}$ apt NMR of 6eb

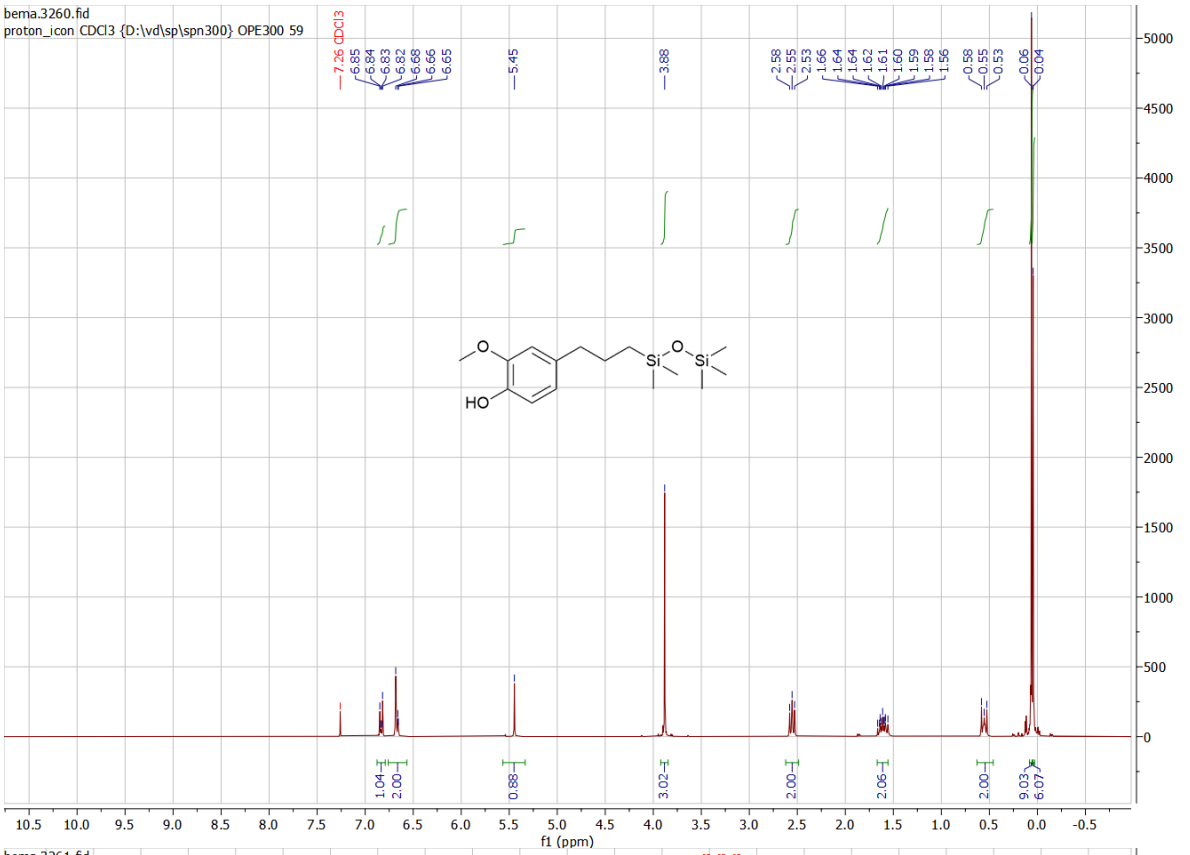


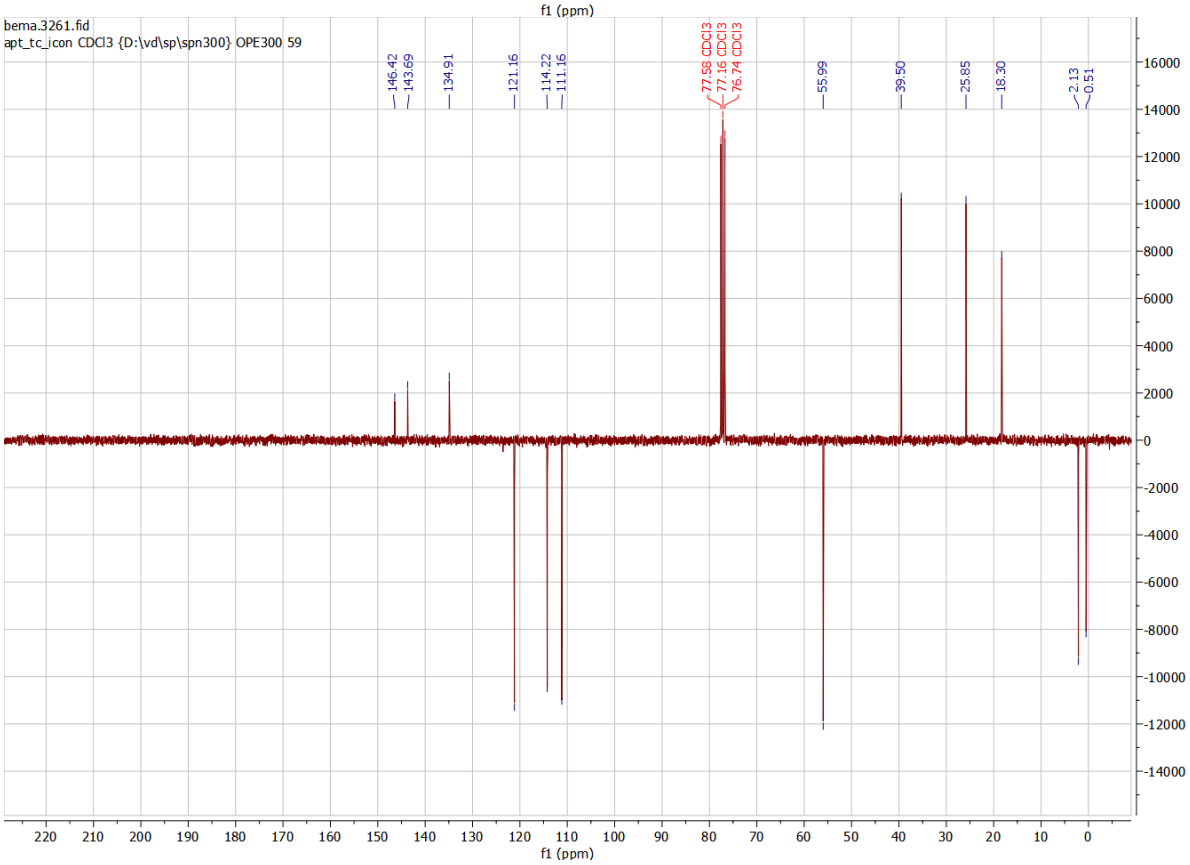


2.20. ^{1}H and $^{13}C\{^{1}H\}$ apt NMR of 6bh

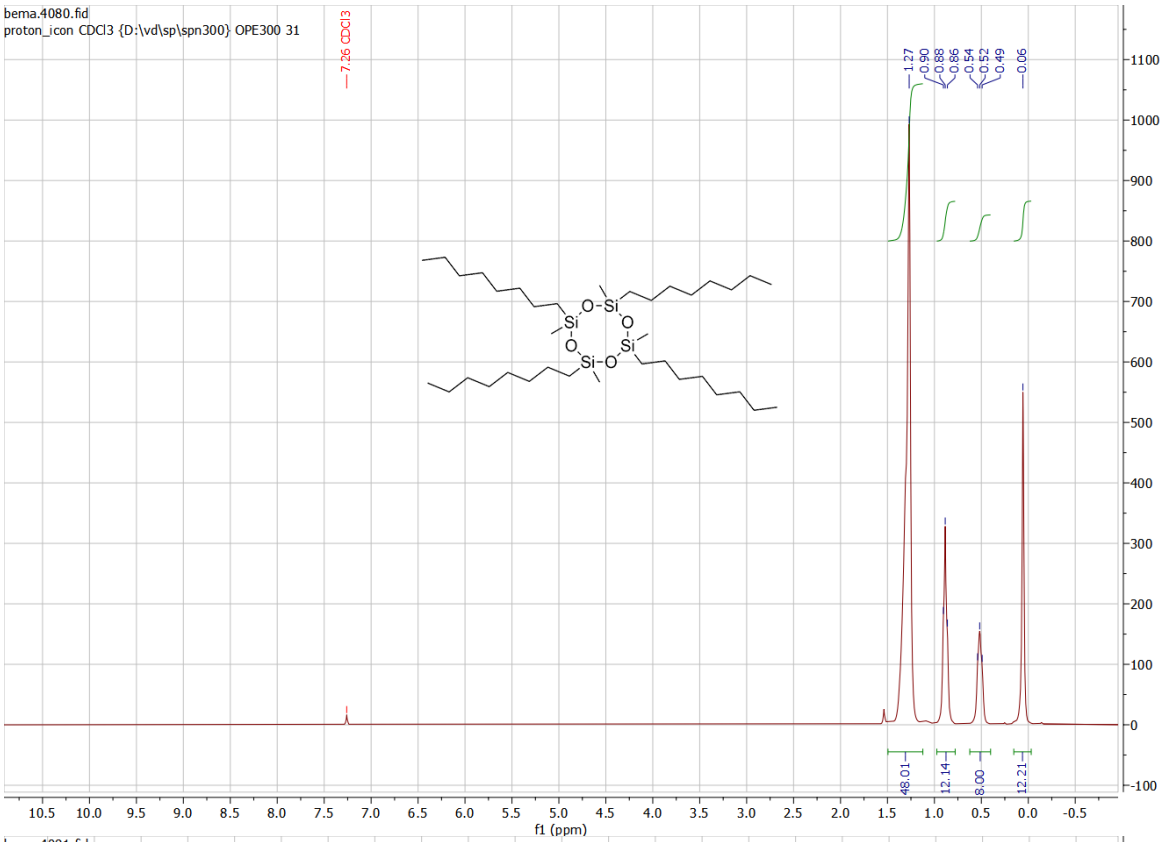


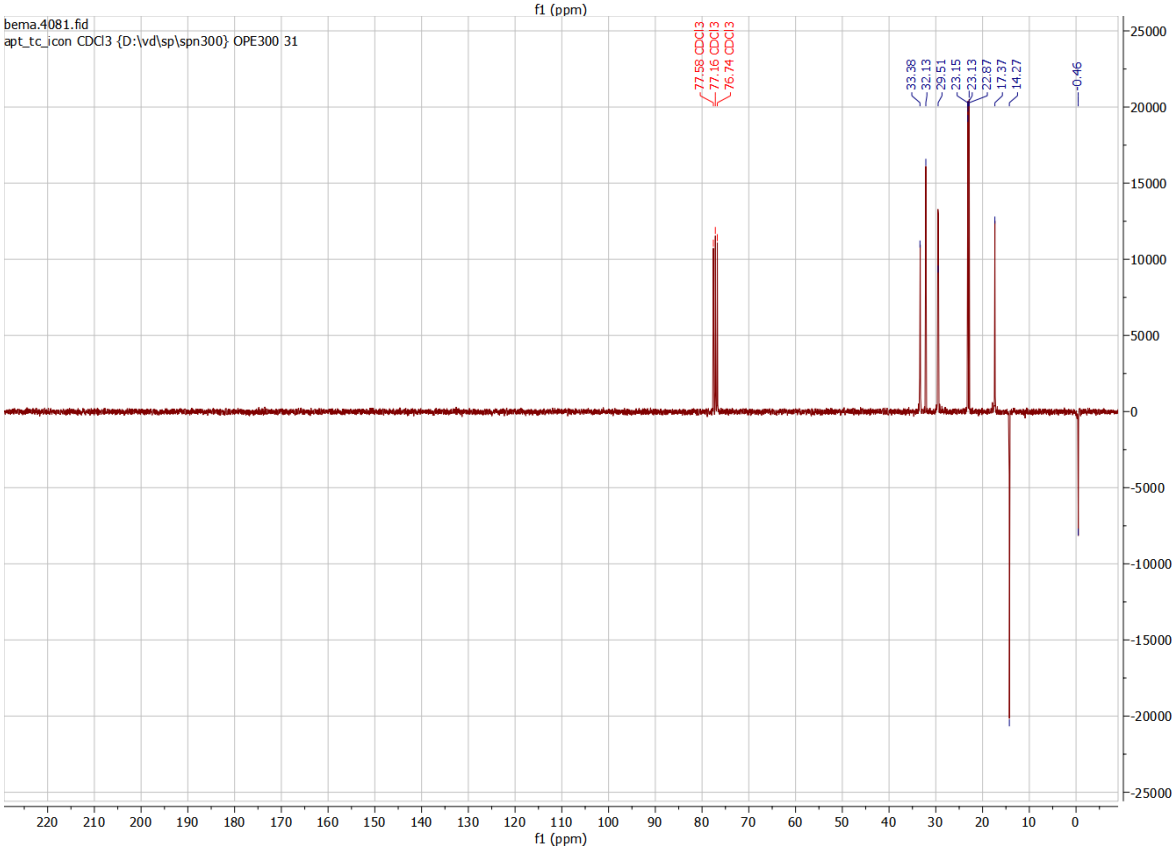
2.21. ^{1}H and $^{13}C\{^{1}H\}$ apt NMR of 6bi





2.22. ^{1}H and $^{13}C\{^{1}H\}$ apt NMR of 6fb





3. Colloidal Pt detection and UV-VIS spectra

A 4.0 mL vial was charged with solid pre-catalyst **3ae** (5.00 mg, 4.0 µmol, 1.0 eqiuv.). MD'M (**4a**, 9.0 mg, 40.0 µmol, 10.0 equiv.) and toluene (4.0 mL) were added, the vial was closed with a septum screw cap and the resulted mixture was stirred at 80 °C. The UV-VIS spectra were measured at RT on a Perkin Elmer Lambda 900 spectrometer in quartz cuvettes at T_0 and after 96 h (Figure S1). A parallel control experiment, without adding **4a**, was also conducted (Figure S2). The baseline in all experiments was measured on a sample of pure toluene.

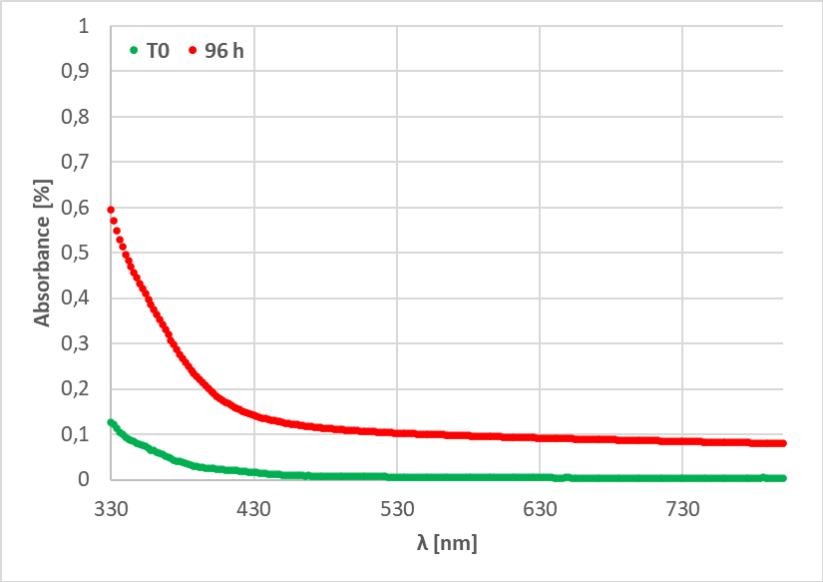


Figure S1. Reaction between **3ae** and **4a** in toluene.

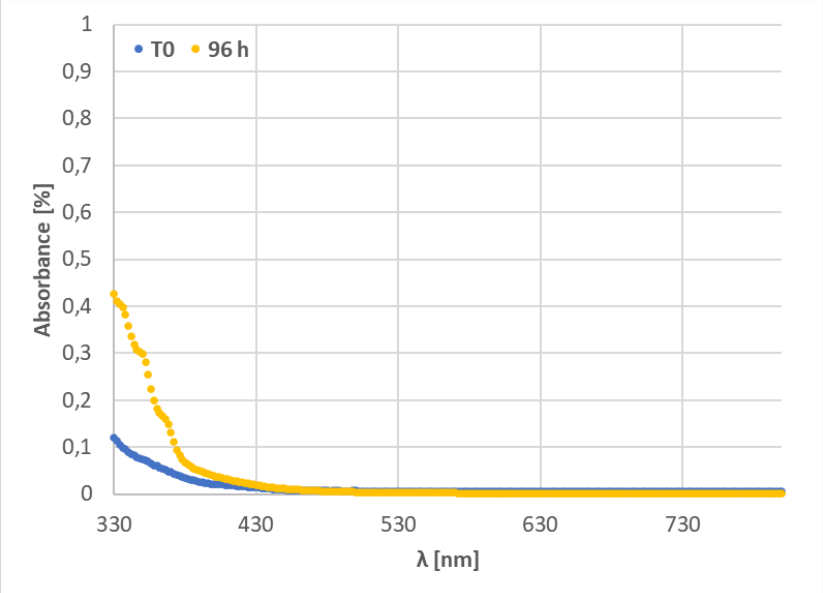


Figure S2. Control experiment.

4. Computational Details

All calculations were conducted at the DFT level with the Gaussian16 set of programs,[1] using the BP86 functional.[2] The electronic configuration of the molecular systems was described with the standard split-valence basis set with a polarization function of Ahlrichs and co-workers for H, C, N, O, S and Cl (Def2SVP keyword in Gaussian).[3] For Ru, the quasi-relativistic Stuttgart/Dresden effective core potential[4] with an associated valence basis set (standard SDD keyword in Gaussian16) was used. Geometry optimizations were carried out without symmetry constraints and normal mode analysis were computed to confirm minima on the potential energy surface. These frequencies were used to calculate unscaled zero-point energies (ZPEs) as well as thermal corrections and entropy effects at 298 K and 1 atm by using the standard statistical mechanics relationships for an ideal gas. Accurate electronic energies were obtained via single-point calculation using the M06 functional of Zhao and Truhlar,[5] on the BP86-optimized geometries. In these calculations, the Def2TZVPP basis set was used for the description of H, C, N, O, S and Cl,[6] whereas for Ru the SDD basis set (and pseudopotential) has been employed, together with the solvent effects of 1-octene estimated with the solvation model based on density (SMD) continuum solvation model in which the quantum mechanical charge density of the solute interacts with the solvent represented by a polarizable continuum with dielectric constant ε.[7] On top of the M06/Def2TZVPP~SDD(SMD,1-octene) electronic energies, we added the thermal and entropy corrections obtained at the BP86/Def2SVP~SDD level in gas phase.

Table S1. XYZ coordinates and absolute energies (in a.u.) of all DFT computed species.

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Dvtms SCF Done: -969.565013984 A.U.

C	-2.537478	2.339667	-0.097472
C	-1.959617	1.310659	-0.753602
Si	1.628903	-0.400285	-0.026888
C	-2.590608	-1.701424	-1.001281
C	-2.099187	-0.449174	1.803221
O	-0.000010	-0.779691	-0.212216
Si	-1.628981	-0.400169	-0.027624
C	2.590971	-1.703312	-0.997732
C	2.097700	-0.446462	1.804394
C	1.960525	1.309286	-0.755370
C	2.538083	2.339232	-0.100451
H	-2.858891	2.255979	0.956671
H	-2.719680	3.320038	-0.574696
H	-1.666454	1.481955	-1.809455
H	-2.368852	-2.721904	-0.623600
H	-2.318112	-1.673179	-2.077116
H	-3.685517	-1.533621	-0.922083
H	-1.856291	-1.442849	2.234923
H	-3.186990	-0.277311	1.947512
H	-1.550934	0.317390	2.389710
H	2.368743	-2.723136	-0.618560
H	3.685855	-1.535596	-0.918022
H	2.319250	-1.676756	-2.073806
H	1.854097	-1.439331	2.237550
H	1.549308	0.321281	2.389212
H	3.185460	-0.274780	1.949223
H	1.668345	1.478892	-1.811770
H	2.858653	2.257176	0.954077
H	2.720861	3.318796	-0.579110

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PtICyCl2cisDIMER SCF Done: -3469.82033467 A.U.

Pt	1.708706	-0.045183	-0.589224
C	3.487348	0.015654	0.211834
N	4.288950	-1.050716	0.520884
N	4.203532	1.132822	0.549252
C	5.497813	-0.603323	1.044897
C	5.444296	0.767715	1.062459
H	6.290384	-1.286072	1.365425
H	6.181580	1.501733	1.401037
C	3.723915	2.512636	0.334575
C	3.704753	3.325227	1.642136
C	4.520704	3.218931	-0.778829
H	2.676801	2.372394	-0.017946
C	3.162585	4.744204	1.389133
H	4.738212	3.395617	2.054004
H	3.088843	2.796019	2.399734
C	3.977296	4.639361	-1.016670
H	5.594969	3.274143	-0.485968
H	4.461914	2.610587	-1.705697
C	3.949899	5.465939	0.281115
H	3.187048	5.329251	2.333245
H	2.090682	4.674255	1.094879
H	4.586174	5.149112	-1.793567
H	2.945853	4.566079	-1.430440
H	3.513940	6.470294	0.090882
H	4.994891	5.641299	0.628047
C	3.917298	-2.457981	0.272794
C	4.779993	-3.081597	-0.840747
C	3.940465	-3.295153	1.564757
H	2.867713	-2.389341	-0.093375
C	4.346071	-4.533231	-1.113251
H	5.851212	-3.063813	-0.532490
H	4.690467	-2.461634	-1.757348
C	3.508610	-4.745159	1.277679
H	4.970552	-3.296166	1.990890
H	3.276369	-2.827635	2.322211
C	4.362181	-5.384903	0.168374
H	5.001422	-4.981439	-1.890269
H	3.317689	-4.527845	-1.540810
H	3.563911	-5.345104	2.211083
H	2.438503	-4.749114	0.968917
H	4.004212	-6.414611	-0.047233
H	5.412458	-5.489693	0.527649
Cl	2.703298	0.040782	-2.707734
Cl	-0.586978	-0.133493	-1.542991
Pt	-1.708740	-0.045067	0.589263
C	-3.487367	0.016241	-0.211805
N	-4.289194	-1.049934	-0.520976
N	-4.203247	1.133589	-0.549243
C	-5.497963	-0.602212	-1.044944
C	-5.444095	0.768809	-1.062483

H	-6.290687	-1.284763	-1.365513
H	-6.181190	1.503034	-1.401025
C	-3.723252	2.513261	-0.334526
C	-3.703782	3.325880	-1.642063
C	-4.519914	3.219749	0.778849
H	-2.676201	2.372717	0.018062
C	-3.161241	4.744702	-1.388992
H	-4.737195	3.396562	-2.053996
H	-3.087965	2.796520	-2.399629
C	-3.976134	4.640025	1.016758
H	-5.594147	3.275254	0.485930
H	-4.461354	2.611366	1.705709
C	-3.948429	5.466625	-0.281005
H	-3.185481	5.329779	-2.333090
H	-2.089376	4.674449	-1.094671
H	-4.584923	5.149922	1.793629
H	-2.944737	4.566453	1.430593
H	-3.512212	6.470856	-0.090719
H	-4.993352	5.642274	-0.628001
C	-3.917914	-2.457304	-0.272950
C	-4.780640	-3.080707	0.840687
C	-3.941475	-3.294451	-1.564923
H	-2.868265	-2.388971	0.093095
C	-4.347058	-4.532454	1.113117
H	-5.851890	-3.062643	0.532549
H	-4.690836	-2.460775	1.757280
C	-3.509956	-4.744572	-1.277923
H	-4.971625	-3.295201	-1.990906
H	-3.277374	-2.827093	-2.322472
C	-4.363545	-5.384111	-0.168515
H	-5.002426	-4.980503	1.890212
H	-3.318621	-4.527338	1.540548
H	-3.565536	-5.344489	-2.211329
H	-2.439808	-4.748810	-0.969301
H	-4.005806	-6.413911	0.047033
H	-5.413895	-5.488636	-0.527656
Cl	-2.703323	0.040643	2.707778
Cl	0.586928	-0.133937	1.543016

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PtICyCl2SMe2cis SCF Done: -2212.78854748 A.U.

Pt	0.945895	0.381343	0.000000
C	-0.922282	-0.299703	0.000000
N	-1.719653	-0.533930	1.090776
N	-1.719653	-0.533930	-1.090776
C	-3.000671	-0.897784	0.685731
C	-3.000671	-0.897784	-0.685731
H	-3.801669	-1.129091	1.394227
H	-3.801669	-1.129091	-1.394227
C	-1.295169	-0.293129	-2.483727
C	-1.533641	-1.518923	-3.384142
C	-1.946211	0.981393	-3.055807
H	-0.200105	-0.108612	-2.396386
C	-1.043621	-1.243551	-4.818358
H	-2.622160	-1.756647	-3.411132
H	-1.024384	-2.408319	-2.953873
C	-1.458411	1.243045	-4.491713
H	-3.054391	0.860139	-3.051467
H	-1.702057	1.835126	-2.389231
C	-1.686420	0.025823	-5.404942
H	-1.252661	-2.124100	-5.462931
H	0.063873	-1.121901	-4.807731
H	-1.966691	2.141183	-4.902414
H	-0.372509	1.488968	-4.465008
H	-1.285862	0.223221	-6.422433
H	-2.781451	-0.142868	-5.528862
C	-1.295169	-0.293129	2.483727
C	-1.946211	0.981393	3.055807
C	-1.533641	-1.518923	3.384142
H	-0.200105	-0.108612	2.396386
C	-1.458411	1.243045	4.491713
H	-3.054391	0.860139	3.051467
H	-1.702057	1.835126	2.389231
C	-1.043621	-1.243551	4.818358
H	-2.622160	-1.756647	3.411132
H	-1.024384	-2.408319	2.953873
C	-1.686420	0.025823	5.404942
H	-1.966691	2.141183	4.902414
H	-0.372509	1.488968	4.465008
H	-1.252661	-2.124100	5.462931
H	0.063873	-1.121901	4.807731
H	-1.285862	0.223221	6.422433
H	-2.781451	-0.142868	5.528862
Cl	-0.021388	2.536443	0.000000
Cl	3.163369	1.301465	0.000000
S	1.859818	-1.770521	0.000000
C	3.053883	-1.802354	-1.392279
H	3.635799	-2.744004	-1.338127
H	2.461286	-1.774252	-2.325764
H	3.693676	-0.899793	-1.317182
C	3.053883	-1.802354	1.392279
H	2.461286	-1.774252	2.325764
H	3.635799	-2.744004	1.338127
H	3.693676	-0.899793	1.317182

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PtICyCl2SMe2cisDIMER90 SCF Done: -4425.59419713 A.U.

Pt	2.787690	-0.316932	0.019213
C	4.184746	1.087134	-0.088882
N	4.044452	2.448925	-0.137712
N	5.538795	0.859278	-0.070054
C	5.294316	3.062555	-0.140993
C	6.232481	2.064305	-0.097080
H	5.416792	4.149049	-0.174914
H	7.325182	2.117727	-0.084229
C	6.155255	-0.477536	0.036479
C	7.108470	-0.766117	-1.138594
C	6.842449	-0.678231	1.400604
H	5.287203	-1.173267	-0.020584
C	7.701217	-2.182911	-1.022922
H	7.937596	-0.021282	-1.139324
H	6.567197	-0.639170	-2.101081
C	7.440743	-2.092516	1.503767
H	7.650691	0.080076	1.521999
H	6.095028	-0.503203	2.202332
C	8.392957	-2.399453	0.334690
H	8.410618	-2.364069	-1.858786
H	6.883266	-2.930114	-1.140640
H	7.965510	-2.207875	2.476056
H	6.610622	-2.834837	1.510854
H	8.775732	-3.440095	0.408659
H	9.285214	-1.734158	0.400629
C	2.756395	3.175357	-0.121886
C	2.597937	3.987611	1.179552
C	2.598461	4.061291	-1.374001
H	1.980510	2.378241	-0.133801
C	1.265977	4.758820	1.189377
H	3.444834	4.707604	1.267207
H	2.668673	3.297937	2.047168
C	1.268208	4.835656	-1.345275
H	3.445244	4.785400	-1.419215
H	2.670515	3.430462	-2.286075
C	1.119803	5.655848	-0.052064
H	1.190528	5.360150	2.121003

H	0.425382	4.030044	1.205640
H	1.201913	5.493995	-2.238008
H	0.423576	4.115093	-1.416945
H	0.135504	6.170856	-0.038806
H	1.895118	6.457821	-0.026367
Cl	3.161986	-0.326307	2.359893
Cl	1.203004	-2.143041	0.211274
S	2.400472	-0.203699	-2.283200
C	2.699559	-1.894523	-2.926044
H	2.363202	-1.931951	-3.981368
H	3.788255	-2.081913	-2.867939
H	2.150303	-2.616767	-2.290493
C	0.585393	-0.112695	-2.501560
H	0.231191	0.824168	-2.027494
H	0.367071	-0.107681	-3.587459
H	0.116431	-0.969520	-1.983018
Pt	-2.787389	0.316549	-0.018758
C	-4.185433	-1.086563	0.088436
N	-5.539349	-0.858178	0.069303
N	-4.045656	-2.448449	0.136668
C	-6.233522	-2.062962	0.095515
C	-5.295747	-3.061594	0.139220
H	-7.326240	-2.115934	0.082303
H	-5.418693	-4.148054	0.172591
C	-2.757827	-3.175269	0.120701
C	-2.600581	-4.062400	1.372037
C	-2.598963	-3.986292	-1.181448
H	-1.981744	-2.378361	0.133690
C	-1.270367	-4.836839	1.343137
H	-3.447424	-4.786504	1.416181
H	-2.672982	-3.432444	2.284686
C	-1.267074	-4.757619	-1.191435
H	-3.445922	-4.706086	-1.270122
H	-2.669268	-3.295763	-2.048418
C	-1.121499	-5.655834	0.049220
H	-1.204473	-5.496010	2.235284
H	-0.425699	-4.116415	1.415827
H	-1.191270	-5.358069	-2.123598
H	-0.426382	-4.028926	-1.206623
H	-0.137239	-6.170914	0.035884
H	-1.896875	-6.457711	0.022464
C	-6.155236	0.478963	-0.036442
C	-6.842976	0.680503	-1.400156
C	-7.107776	0.767499	1.139204
H	-5.286839	1.174263	0.020507
C	-7.440712	2.095085	-1.502476
H	-7.651618	-0.077384	-1.521503
H	-6.096017	0.505462	-2.202310
C	-7.699997	2.184573	1.024369
H	-7.937179	0.022973	1.140042
H	-6.566070	0.639953	2.101366
C	-8.392270	2.401939	-0.332840
H	-7.965871	2.211062	-2.474479
H	-6.610285	2.837062	-1.509627
H	-8.408944	2.365693	1.860627
H	-6.881693	2.931401	1.142011
H	-8.774653	3.442766	-0.406222
H	-9.284826	1.737034	-0.398643
Cl	-3.162230	0.327954	-2.359378
Cl	-1.200229	2.140576	-0.209984
S	-2.400123	0.201735	2.283605
C	-0.585128	0.109149	2.502038
H	-0.366910	0.103432	3.587953
H	-0.231551	-0.827736	2.027550
H	-0.115406	0.965844	1.983970
C	-2.697779	1.892464	2.927310
H	-3.786298	2.080888	2.869276
H	-2.361427	1.928993	3.982669
H	-2.147798	2.614575	2.292241

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PtICyCl2SMe2cisNOsym SCF Done: -2212.78855006 A.U.

Pt	-0.000015	0.945950	0.381148
C	0.000001	-0.922412	-0.299517
N	1.090824	-1.719851	-0.533141
N	-1.090726	-1.719896	-0.533483
C	0.685844	-3.001130	-0.896253
C	-0.685590	-3.001159	-0.896445
H	1.394448	-3.802197	-1.127025
H	-1.394110	-3.802244	-1.127421
C	-2.483716	-1.295336	-0.293119
C	-3.383902	-1.534294	-1.519005
C	-3.055997	-1.945867	0.981574
H	-2.396412	-0.200204	-0.108983
C	-4.818206	-1.044262	-1.244078
H	-3.410747	-2.622888	-1.756397
H	-2.953479	-1.025298	-2.408466
C	-4.491974	-1.457978	1.242769
H	-3.051625	-3.054094	0.860792
H	-2.389536	-1.701355	1.835290
C	-5.404981	-1.686561	0.025473
H	-5.462618	-1.253709	-2.124639
H	-4.807680	0.063283	-1.122901
H	-4.902820	-1.965872	2.141048
H	-4.465358	-0.371970	1.488229
H	-6.422541	-1.286014	0.222504
H	-5.528782	-2.781673	-0.142771
C	2.483767	-1.295197	-0.292791
C	3.056537	-1.946629	0.981212
C	3.383645	-1.532935	-1.519158
H	2.396267	-0.200233	-0.107733
C	4.492513	-1.458702	1.242364
H	3.052349	-3.054771	0.859640
H	2.390286	-1.702853	1.835303
C	4.817957	-1.042935	-1.244242
H	3.410527	-2.621311	-1.757549
H	2.952861	-1.023198	-2.408021
C	5.405188	-1.686193	0.024610
H	4.903715	-1.967235	2.140119
H	4.465795	-0.372890	1.488663
H	5.462156	-1.251559	-2.125156
H	4.807305	0.064506	-1.122137
H	6.422757	-1.285677	0.221662
H	5.529078	-2.781155	-0.144550
Cl	0.000530	-0.021488	2.536261
Cl	0.000005	3.163516	1.301796
S	-0.000477	1.859892	-1.770233
C	-1.392653	3.053986	-1.801704
H	-1.338355	3.636537	-2.742988
H	-2.326298	2.461588	-1.774210
H	-1.317676	3.693390	-0.898813
C	1.391614	3.054054	-1.802094
H	2.325310	2.461724	-1.774925
H	1.336998	3.636630	-2.743351
H	1.316900	3.693450	-0.899178

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PtICyCl2SMe2transCS SCF Done: -2212.79451303 A.U.

Pt	0.000003	0.903926	0.131245
C	-0.000106	-1.065376	-0.103449
N	1.090124	-1.885587	-0.187716
N	-1.090436	-1.885464	-0.187655
C	0.685755	-3.211139	-0.317990
C	-0.686224	-3.211059	-0.317967

H	1.395049	-4.039898	-0.402333
H	-1.395615	-4.039736	-0.402296
C	-2.484156	-1.407232	-0.110929
C	-3.286316	-1.774925	-1.372683
C	-3.176465	-1.884309	1.179911
H	-2.377223	-0.299734	-0.064846
C	-4.723231	-1.229361	-1.279901
H	-3.320776	-2.883672	-1.482759
H	-2.766847	-1.374939	-2.268839
C	-4.614666	-1.340741	1.257538
H	-3.198288	-2.998740	1.197640
H	-2.578545	-1.553219	2.054838
C	-5.430458	-1.700405	0.003222
H	-5.299744	-1.532951	-2.179809
H	-4.689170	-0.115997	-1.294807
H	-5.113035	-1.724824	2.173111
H	-4.576335	-0.232955	1.368163
H	-6.449364	-1.261067	0.065371
H	-5.570647	-2.805633	-0.039763
C	2.483903	-1.407513	-0.111084
C	3.176131	-1.884366	1.179882
C	3.286046	-1.775604	-1.372731
H	2.377107	-0.299991	-0.065261
C	4.614393	-1.340946	1.257407
H	3.197811	-2.998796	1.197871
H	2.578229	-1.552986	2.054711
C	4.723018	-1.230170	-1.280057
H	3.320403	-2.884381	-1.482531
H	2.766641	-1.375800	-2.269006
C	5.430171	-1.700987	0.003191
H	5.112700	-1.724874	2.173079
H	4.576185	-0.233130	1.367780
H	5.299515	-1.534035	-2.179883
H	4.689077	-0.116806	-1.295227
H	6.449123	-1.261743	0.065256
H	5.570243	-2.806240	-0.039536
Cl	0.000207	0.579295	2.477151
Cl	-0.000145	1.212991	-2.226894
S	0.000301	3.293913	0.508667
C	-1.395401	3.926873	-0.493090
H	-1.359241	5.034229	-0.510684
H	-1.339295	3.495683	-1.512457
H	-2.322491	3.591438	0.009457
C	1.396783	3.925988	-0.492587
H	1.340687	3.494919	-1.512004
H	1.361422	5.033373	-0.510115
H	2.323465	3.589846	0.010236

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PtICyCl2SMe2trans SCF Done: -2212.76301387 A.U.

Pt	0.000000	0.000000	0.862689
C	0.000000	0.000000	-1.094171
N	0.000000	1.092191	-1.915100
N	0.000000	-1.092191	-1.915100
C	0.000000	0.685835	-3.246647
C	0.000000	-0.685835	-3.246647
H	0.000000	1.395460	-4.079283
H	0.000000	-1.395460	-4.079283
C	0.000000	-2.486728	-1.432356
C	-1.278955	-3.234569	-1.852774
C	1.278955	-3.234569	-1.852774
H	0.000000	-2.378707	-0.324095
C	-1.271095	-4.672583	-1.302898
H	-1.343432	-3.264211	-2.965311
H	-2.165503	-2.674690	-1.487899
C	1.271095	-4.672583	-1.302898
H	1.343432	-3.264211	-2.965311
H	2.165503	-2.674690	-1.487899
C	0.000000	-5.435360	-1.716247
H	-2.180580	-5.211029	-1.645277
H	-1.333839	-4.634557	-0.191386
H	2.180580	-5.211029	-1.645277
H	1.333839	-4.634557	-0.191386
H	0.000000	-6.454641	-1.273340
H	0.000000	-5.576940	-2.822161
C	0.000000	2.486728	-1.432356
C	1.278955	3.234569	-1.852774
C	-1.278955	3.234569	-1.852774
H	0.000000	2.378707	-0.324095
C	1.271095	4.672583	-1.302898
H	1.343432	3.264211	-2.965311
H	2.165503	2.674690	-1.487899
C	-1.271095	4.672583	-1.302898
H	-1.343432	3.264211	-2.965311
H	-2.165503	2.674690	-1.487899
C	0.000000	5.435360	-1.716247
H	2.180580	5.211029	-1.645277
H	1.333839	4.634557	-0.191386
H	-2.180580	5.211029	-1.645277
H	-1.333839	4.634557	-0.191386
H	0.000000	6.454641	-1.273340
H	0.000000	5.576940	-2.822161
Cl	2.371613	0.000000	0.818930
Cl	-2.371613	0.000000	0.818930
S	0.000000	0.000000	3.306831
C	0.000000	-1.480342	4.369498
H	0.000000	-1.152121	5.426440
H	-0.908528	-2.081040	4.170820
H	0.908528	-2.081040	4.170820
C	0.000000	1.480342	4.369498
H	-0.908528	2.081040	4.170820
H	0.000000	1.152121	5.426440
H	0.908528	2.081040	4.170820

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PtICyCl2transC2V SCF Done: -1734.88113088 A.U.

Pt	1.351777	-0.000152	0.000000
C	-0.555908	-0.000094	0.000000
N	-1.371310	-0.000085	1.097704
N	-1.371310	-0.000085	-1.097704
C	-2.701185	-0.000062	0.685832
C	-2.701185	-0.000062	-0.685832
H	-3.534075	-0.000004	1.395115
H	-3.534075	-0.000004	-1.395115
C	-0.891397	-0.000049	-2.496201
C	-1.317031	-1.278556	-3.241715
C	-1.316274	1.278938	-3.241356
H	0.217064	-0.000385	-2.392413
C	-0.771877	-1.270732	-4.681778
H	-2.429724	-1.340685	-3.267099
H	-0.952592	-2.167468	-2.685136
C	-0.771170	1.271204	-4.681434
H	-2.428930	1.341738	-3.266668
H	-0.951272	2.167456	-2.684517
C	-1.188047	0.000455	-5.442592
H	-1.117645	-2.180183	-5.217637
H	0.339439	-1.334616	-4.648012
H	-1.116437	2.180994	-5.217045
H	0.340181	1.334464	-4.647672
H	-0.747545	0.000467	-6.462558
H	-2.294246	0.000781	-5.581398
C	-0.891397	-0.000049	2.496201
C	-1.316274	1.278938	3.241356
C	-1.317031	-1.278556	3.241715

H	0.217064	-0.000385	2.392413
C	-0.771170	1.271204	4.681434
H	-2.428930	1.341738	3.266668
H	-0.951272	2.167456	2.684517
C	-0.771877	-1.270732	4.681778
H	-2.429724	-1.340685	3.267099
H	-0.952592	-2.167468	2.685136
C	-1.188047	0.000455	5.442592
H	-1.116437	2.180994	5.217045
H	0.340181	1.334464	4.647672
H	-1.117645	-2.180183	5.217637
H	0.339439	-1.334616	4.648012
H	-0.747545	0.000467	6.462558
H	-2.294246	0.000781	5.581398
Cl	1.586340	2.311684	0.000000
Cl	1.586042	-2.312033	0.000000

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PtICyClSMe2cis+ SCF Done: -1752.41467169 A.U.

Pt	1.011336	0.667614	0.000000
C	-0.683160	-0.285746	0.000000
N	-1.406783	-0.635902	1.100266
N	-1.406783	-0.635902	-1.100266
C	-2.600186	-1.219528	0.685961
C	-2.600186	-1.219528	-0.685961
H	-3.349336	-1.586256	1.394208
H	-3.349336	-1.586256	-1.394208
C	-1.030287	-0.357917	-2.510645
C	-0.991905	-1.645779	-3.354017
C	-1.946902	0.714881	-3.130459
H	-0.001735	0.062343	-2.437805
C	-0.570294	-1.331027	-4.802359
H	-2.002945	-2.112220	-3.361995
H	-0.305098	-2.386023	-2.889201
C	-1.523395	1.014655	-4.580604
H	-2.998227	0.347536	-3.117117
H	-1.914550	1.634336	-2.508948
C	-1.475552	-0.261664	-5.437589
H	-0.582012	-2.264987	-5.402067
H	0.485097	-0.972849	-4.807855
H	-2.219702	1.758237	-5.020886
H	-0.520287	1.499008	-4.574823
H	-1.124689	-0.023810	-6.463419
H	-2.505190	-0.671541	-5.549778
C	-1.030287	-0.357917	2.510645
C	-1.946902	0.714881	3.130459
C	-0.991905	-1.645779	3.354017
H	-0.001735	0.062343	2.437805
C	-1.523395	1.014655	4.580604
H	-2.998227	0.347536	3.117117
H	-1.914550	1.634336	2.508948
C	-0.570294	-1.331027	4.802359
H	-2.002945	-2.112220	3.361995
H	-0.305098	-2.386023	2.889201
C	-1.475552	-0.261664	5.437589
H	-2.219702	1.758237	5.020886
H	-0.520287	1.499008	4.574823
H	-0.582012	-2.264987	5.402067
H	0.485097	-0.972849	4.807855
H	-1.124689	-0.023810	6.463419
H	-2.505190	-0.671541	5.549778
Cl	0.119154	2.771510	0.000000
S	2.243842	-1.325705	0.000000
C	3.411861	-1.165800	-1.407772
H	4.114143	-2.021874	-1.365025
H	2.813097	-1.223156	-2.335830
H	3.962721	-0.206255	-1.366518
C	3.411861	-1.165800	1.407772
H	2.813097	-1.223156	2.335830
H	4.114143	-2.021874	1.365025
H	3.962721	-0.206255	1.366518

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PtICyClSMeDIMER SCF Done: -3505.24004442 A.U.

Pt	-0.829808	1.935550	0.000000
C	0.241177	3.603412	0.000000
N	0.694333	4.324536	1.090062
N	0.694333	4.324536	-1.090062
C	1.424779	5.439903	0.685517
C	1.424779	5.439903	-0.685517
H	1.875692	6.144193	1.391887
H	1.875692	6.144193	-1.391887
C	0.507156	3.872600	-2.475645
C	-0.142862	4.952085	-3.360816
C	1.821005	3.343971	-3.084685
H	-0.196912	3.013063	-2.368858
C	-0.362377	4.428858	-4.792486
H	0.514482	5.851857	-3.398929
H	-1.102813	5.278365	-2.905905
C	1.595850	2.831998	-4.518429
H	2.578202	4.162540	-3.093823
H	2.215240	2.536110	-2.432869
C	0.944487	3.902432	-5.411895
H	-0.801424	5.229589	-5.426052
H	-1.112580	3.605370	-4.767226
H	2.559605	2.492520	-4.955580
H	0.938920	1.933260	-4.480817
H	0.752744	3.496226	-6.428750
H	1.653967	4.752282	-5.544915
C	0.507156	3.872600	2.475645
C	1.821005	3.343971	3.084685
C	-0.142862	4.952085	3.360816
H	-0.196912	3.013063	2.368858
C	1.595850	2.831998	4.518429
H	2.578202	4.162540	3.093823
H	2.215240	2.536110	2.432869
C	-0.362377	4.428858	4.792486
H	0.514482	5.851857	3.398929
H	-1.102813	5.278365	2.905905
C	0.944487	3.902432	5.411895
H	2.559605	2.492520	4.955580
H	0.938920	1.933260	4.480817
H	-0.801424	5.229589	5.426052
H	-1.112580	3.605370	4.767226
H	0.752744	3.496226	6.428750
H	1.653967	4.752282	5.544915
Cl	1.529570	0.425469	0.000000
S	-3.135431	2.645808	0.000000
C	-4.010606	1.827102	-1.392709
H	-5.085440	2.104228	-1.379233
H	-3.540967	2.201538	-2.321959
H	-3.868217	0.731434	-1.325891
C	-4.010606	1.827102	1.392709
H	-3.540967	2.201538	2.321959
H	-5.085440	2.104228	1.379233
H	-3.868217	0.731434	1.325891
Pt	0.829849	-1.935590	0.000000
C	-0.241134	-3.603449	0.000000
N	-0.694328	-4.324552	1.090062
N	-0.694328	-4.324552	-1.090062
C	-1.424744	-5.439940	0.685517
C	-1.424744	-5.439940	-0.685517
H	-1.875656	-6.144230	1.391886
H	-1.875656	-6.144230	-1.391886

C	-0.507186	-3.872597	-2.475642
C	0.142825	-4.952066	-3.360835
C	-1.821052	-3.343974	-3.084652
H	0.196877	-3.013054	-2.368856
C	0.362306	-4.428824	-4.792505
H	-0.514510	-5.851845	-3.398943
H	1.102790	-5.278339	-2.905947
C	-1.595932	-2.831986	-4.518396
H	-2.578242	-4.162550	-3.093782
H	-2.215283	-2.536123	-2.432820
C	-0.944577	-3.902406	-5.411884
H	0.801348	-5.229544	-5.426088
H	1.112500	-3.605327	-4.767253
H	-2.559700	-2.492514	-4.955524
H	-0.939010	-1.933242	-4.480790
H	-0.752859	-3.496189	-6.428739
H	-1.654050	-4.752262	-5.544895
C	-0.507186	-3.872597	2.475642
C	-1.821052	-3.343974	3.084652
C	0.142825	-4.952066	3.360835
H	0.196877	-3.013054	2.368856
C	-1.595932	-2.831986	4.518396
H	-2.578242	-4.162550	3.093782
H	-2.215283	-2.536123	2.432820
C	0.362306	-4.428824	4.792505
H	-0.514510	-5.851845	3.398943
H	1.102790	-5.278339	2.905947
C	-0.944577	-3.902406	5.411884
H	-2.559700	-2.492514	4.955524
H	-0.939010	-1.933242	4.480790
H	0.801348	-5.229544	5.426088
H	1.112500	-3.605327	4.767253
H	-0.752859	-3.496189	6.428739
H	-1.654050	-4.752262	5.544895
Cl	-1.529617	-0.425465	0.000000
S	3.135512	-2.645743	0.000000
C	4.010674	-1.827021	-1.392710
H	5.085515	-2.104120	-1.379232
H	3.541045	-2.201471	-2.321959
H	3.868259	-0.731356	-1.325899
C	4.010674	-1.827021	1.392710
H	3.541045	-2.201471	2.321959
H	5.085515	-2.104120	1.379232
H	3.868259	-0.731356	1.325899

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PtICyClSMe2trans+ SCF Done: -1752.40083517 A.U.

Pt	0.000001	0.960833	-0.266225
C	0.000067	-1.029716	-0.109479
N	-1.095651	-1.852248	-0.030812
N	1.095871	-1.852149	-0.030788
C	-0.689336	-3.170374	0.063108
C	0.689670	-3.170311	0.063114
H	-1.393137	-4.007558	0.108573
H	1.393543	-4.007434	0.108585
C	2.503768	-1.384111	-0.045104
C	3.240612	-1.764716	1.252948
C	3.251681	-1.875149	-1.300235
H	2.415785	-0.274384	-0.092769
C	4.687351	-1.236344	1.227970
H	3.255608	-2.873536	1.356217
H	2.685732	-1.365274	2.128012
C	4.698577	-1.347705	-1.311397
H	3.264151	-2.988895	-1.306089
H	2.704910	-1.556000	-2.213661
C	5.448433	-1.716190	-0.019702
H	5.211362	-1.552073	2.154041
H	4.669574	-0.122614	1.248547
H	5.229740	-1.743730	-2.201968
H	4.682555	-0.239783	-1.429038
H	6.471875	-1.286684	-0.034673
H	5.577427	-2.821543	0.028873
C	-2.503582	-1.384313	-0.045151
C	-3.251459	-1.875455	-1.300263
C	-3.240406	-1.764918	1.252913
H	-2.415682	-0.274584	-0.092861
C	-4.698385	-1.348096	-1.311452
H	-3.263864	-2.989203	-1.306067
H	-2.704703	-1.556314	-2.213701
C	-4.687174	-1.236632	1.227910
H	-3.255334	-2.873736	1.356222
H	-2.685551	-1.365409	2.127963
C	-5.448225	-1.716573	-0.019745
H	-5.229521	-1.744188	-2.202010
H	-4.682426	-0.240178	-1.429137
H	-5.211169	-1.552357	2.153992
H	-4.669465	-0.122900	1.248443
H	-6.471691	-1.287124	-0.034738
H	-5.577156	-2.821930	0.028873
Cl	-0.000364	1.291045	1.995424
S	-0.000173	3.288469	-0.772184
C	1.412677	4.073948	0.082335
H	1.367768	5.165968	-0.094575
H	1.374098	3.837499	1.163558
H	2.333685	3.660297	-0.369568
C	-1.413198	4.073807	0.082168
H	-1.374688	3.837417	1.163407
H	-1.368396	5.165823	-0.094796
H	-2.334113	3.660025	-0.369806

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PtICyClSMetrans SCF Done: -1712.76032893 A.U.

Pt	0.029522	1.182527	0.484136
C	0.041341	-0.594966	-0.242994
N	1.148078	-1.347558	-0.539456
N	-1.045022	-1.371398	-0.555320
C	0.754171	-2.589973	-1.029914
C	-0.616700	-2.605330	-1.039260
H	1.473754	-3.355523	-1.334784
H	-1.314582	-3.387588	-1.351857
C	-2.447432	-0.971052	-0.321892
C	-3.308040	-1.128133	-1.589049
C	-3.051813	-1.714457	0.885147
H	-2.373992	0.110203	-0.065340
C	-4.753425	-0.666859	-1.324091
H	-3.319949	-2.197431	-1.902934
H	-2.854900	-0.553938	-2.425449
C	-4.500873	-1.259314	1.134229
H	-3.030466	-2.811327	0.687137
H	-2.417180	-1.522581	1.775737
C	-5.373713	-1.404700	-0.124512
H	-5.368011	-0.814981	-2.237672
H	-4.754262	0.428785	-1.123000
H	-4.933665	-1.834854	1.979907
H	-4.493405	-0.193899	1.458594
H	-6.400294	-1.026437	0.069641
H	-5.482701	-2.485396	-0.375736
C	2.538363	-0.913375	-0.295175
C	3.181312	-1.708975	0.857222
C	3.388982	-0.957271	-1.577444
H	2.429245	0.146657	0.027690
C	4.613725	-1.213146	1.125735
H	3.204685	-2.790939	0.589781
H	2.549755	-1.609748	1.764993

C	4.819918	-0.462980	-1.294360
H	3.431313	-2.002478	-1.962639
H	2.905646	-0.339934	-2.364029
C	5.478117	-1.249238	-0.146838
H	5.076253	-1.821625	1.931780
H	4.568416	-0.169823	1.512740
H	5.430790	-0.533441	-2.219541
H	4.783215	0.617804	-1.028187
H	6.491963	-0.846167	0.063454
H	5.623866	-2.308379	-0.463135
Cl	-0.302943	0.328507	2.675110
S	0.462567	2.610936	-1.219627
C	-1.128337	3.010910	-2.066350
H	-0.923678	3.858487	-2.751974
H	-1.472659	2.147577	-2.670453
H	-1.917904	3.306071	-1.349463

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PtICyDvtms SCF Done: -1784.22678195 A.U.

Pt	-0.044232	-0.549039	0.000067
N	-2.730095	0.983938	-0.000229
C	-1.355313	1.043450	-0.000055
N	-1.074395	2.389767	0.000027
C	-2.243692	3.147586	-0.000101
C	-3.288724	2.260021	-0.000256
C	-3.485149	-0.279992	-0.000132
C	-4.335703	-0.443325	1.274549
C	-5.077749	-1.792320	1.271003
C	-5.927365	-1.970356	0.000462
C	-5.078492	-1.792124	-1.270548
C	-4.336462	-0.443116	-1.274317
C	0.293781	2.933379	0.000020
C	0.587385	3.749236	1.274386
C	2.033151	4.278343	1.270104
C	2.337635	5.090819	-0.000514
C	2.033449	4.277456	-1.270635
C	0.587701	3.748302	-1.274879
C	0.039184	-0.678912	2.148502
C	0.834072	-1.743107	1.586522
Si	2.716036	-1.778735	-1.556073
C	3.373378	-3.165455	2.664515
C	3.447329	-0.119297	2.113724
O	3.277303	-2.133371	0.000025
Si	2.716462	-1.778103	1.556122
C	3.372796	-3.166447	-2.664114
C	3.446695	-0.120124	-2.114537
C	0.833643	-1.743951	-1.585930
C	0.038511	-0.680141	-2.148308
H	-2.244536	4.242123	-0.000075
H	-4.368710	2.437981	-0.000340
H	-2.685856	-1.057028	-0.000404
H	-5.077727	0.386456	1.334055
H	-3.682707	-0.352809	2.168445
H	-4.331768	-2.617229	1.333573
H	-5.710625	-1.877491	2.180175
H	-6.750542	-1.218568	0.000758
H	-6.417830	-2.967428	0.000530
H	-5.711897	-1.877153	-2.179364
H	-4.332543	-2.617018	-1.333678
H	-3.684030	-0.352428	-2.168612
H	-5.078562	0.386639	-1.333241
H	0.933163	2.020834	0.000422
H	0.399352	3.117744	2.168520
H	-0.120048	4.608666	1.333828
H	2.213233	4.890725	2.179434
H	2.735465	3.416205	1.333403
H	1.718873	6.018223	-0.000908
H	3.397449	5.424586	-0.000506
H	2.735798	3.415291	-1.333182
H	2.213719	4.889206	-2.180352
H	-0.119776	4.607640	-1.335132
H	0.399922	3.116121	-2.168578
H	0.534880	0.199459	2.601580
H	-0.942328	-0.907832	2.603928
H	0.355056	-2.744074	1.559839
H	4.480419	-3.232131	2.606363
H	2.960399	-4.148203	2.353522
H	3.092668	-2.998144	3.726158
H	4.553127	-0.134845	2.013376
H	3.206086	0.097249	3.176264
H	3.061541	0.718895	1.496426
H	4.479865	-3.232945	-2.606313
H	3.091704	-2.999593	-3.725729
H	2.960060	-4.149132	-2.352597
H	4.552455	-0.135396	-2.013689
H	3.060479	0.718470	-1.498060
H	3.205900	0.095563	-3.177354
H	0.354759	-2.744963	-1.558547
H	0.534002	0.197990	-2.602071
H	-0.943124	-0.909413	-2.603298

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PtICy SCF Done: -814.565754365 A.U.

Pt	0.000065	-1.612614	-0.000097
N	1.097360	1.108014	0.000045
C	-0.000055	0.261921	-0.000002
N	-1.097421	1.107979	0.000061
C	-0.685863	2.437178	0.000138
C	0.685771	2.437172	0.000101
C	2.489910	0.632815	-0.000048
C	3.242084	1.056329	-1.276120
C	4.681833	0.510916	-1.270876
C	5.443468	0.927725	-0.000357
C	4.682076	0.511107	1.270370
C	3.242330	1.056527	1.275809
C	-2.489999	0.632768	0.000122
C	-3.242420	1.056619	-1.275678
C	-4.682160	0.511167	-1.270287
C	-5.443550	0.927621	0.000498
C	-4.681887	0.510709	1.270968
C	-3.242144	1.056151	1.276245
H	-1.392150	3.273284	0.000208
H	1.391986	3.273344	0.000124
H	2.373804	-0.477912	0.000041
H	3.269152	2.169151	-1.341217
H	2.685320	0.695076	-2.166800
H	4.648305	-0.600846	-1.331378
H	5.219784	0.854875	-2.180272
H	5.580229	2.034262	-0.000453
H	6.464499	0.488896	-0.000421
H	5.220203	0.855199	2.179611
H	4.648555	-0.600646	1.331042
H	2.685741	0.695426	2.166660
H	3.269429	2.169359	1.340727
H	-2.373873	-0.477958	-0.000086
H	-2.685840	0.695644	-2.166585
H	-3.269546	2.169459	-1.340457
H	-5.220318	0.855348	-2.179477
H	-4.648611	-0.600576	-1.331085
H	-5.580347	2.034152	0.000711
H	-6.464565	0.488756	0.000528
H	-4.648329	-0.601057	1.331360
H	-5.219847	0.854565	2.180398
H	-3.269237	2.168967	1.341437

H	-2.685367	0.694837	2.166890

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PtIMesCl2SMe2cis SCF Done: -2441.25619511 A.U.

N	1.089890	-1.739343	0.549668
N	-1.090201	-1.739217	0.549710
C	-0.000119	-0.958215	0.224929
C	0.683848	-2.977712	1.050951
H	1.407941	-3.739238	1.356896
C	-0.684278	-2.977648	1.050940
H	-1.408447	-3.739084	1.356927
C	2.481448	-1.346610	0.461493
C	3.221517	-1.665646	-0.703509
C	2.598970	-2.406387	-1.859012
H	2.144619	-3.366428	-1.532900
C	4.574625	-1.272549	-0.740512
H	5.160471	-1.503207	-1.645825
C	5.197271	-0.606307	0.333141
C	4.436233	-0.361326	1.493790
H	4.913898	0.123005	2.362136
C	3.079874	-0.730548	1.588170
C	2.308796	-0.506685	2.869149
H	1.959071	-1.465896	3.308343
C	-2.481722	-1.346328	0.461653
C	-3.079856	-0.729761	1.588208
C	-2.308522	-0.505560	2.868971
H	-1.958854	-1.464678	3.308416
C	-4.436181	-0.360393	1.493943
H	-4.913613	0.124346	2.362188
C	-5.197472	-0.605721	0.333535
C	-4.575118	-1.272457	-0.739980
H	-5.161162	-1.503374	-1.645098
C	-3.222050	-1.665701	-0.703089
C	-2.599788	-2.406890	-1.858465
H	-2.145626	-3.366958	-1.532170
Pt	0.000004	0.846801	-0.619296
H	2.938617	-0.001009	3.626873
H	1.402147	0.113808	2.707244
H	-1.401801	0.114739	2.706725
H	-2.938141	0.000449	3.626640
H	-3.356358	-2.632976	-2.634496
H	-1.786109	-1.804358	-2.322010
H	3.355415	-2.632462	-2.635170
H	1.785362	-1.803602	-2.322359
C	6.638682	-0.159594	0.236308
H	6.715769	0.812981	-0.297913
H	7.095368	-0.022506	1.237160
H	7.255510	-0.887573	-0.329298
C	-6.638833	-0.158828	0.236796
H	-7.255872	-0.886916	-0.328440
H	-7.095320	-0.021309	1.237680
H	-6.715863	0.813568	-0.297758
Cl	0.000155	2.981634	-1.719519
Cl	-0.000739	-0.176434	-2.748247
S	0.000748	1.972101	1.422238
C	1.403001	3.149425	1.339611
H	2.327216	2.541180	1.342017
H	1.320953	3.713487	0.388750
H	1.366468	3.805970	2.231848
C	-1.400939	3.150146	1.340330
H	-1.363811	3.806423	2.232738
H	-1.318863	3.714429	0.389599
H	-2.325471	2.542381	1.342840

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PtIMesCl2SMe2trans SCF Done: -2441.26485783 A.U.

N	1.090679	-1.882782	-0.231566
N	-1.090528	-1.882868	-0.231539
C	0.000042	-1.053652	-0.105893
C	0.684242	-3.203785	-0.430675
H	1.409731	-4.013998	-0.552358
C	-0.683994	-3.203839	-0.430660
H	-1.409422	-4.014111	-0.552313
C	2.486166	-1.493497	-0.173209
C	3.154444	-1.168282	-1.379154
C	2.445837	-1.195127	-2.711164
H	1.929129	-2.162883	-2.884999
C	4.517482	-0.819869	-1.295229
H	5.050580	-0.559485	-2.224999
C	5.214536	-0.805550	-0.071112
C	4.518906	-1.181839	1.094946
H	5.052900	-1.207374	2.059620
C	3.156282	-1.540174	1.074419
C	2.449254	-1.959094	2.339376
H	1.926293	-2.931462	2.217921
C	-2.486039	-1.493681	-0.173131
C	-3.156040	-1.540145	1.074547
C	-2.448902	-1.958758	2.339544
H	-1.925843	-2.931091	2.218228
C	-4.518690	-1.181851	1.095122
H	-5.052578	-1.207217	2.059860
C	-5.214429	-0.805830	-0.070939
C	-4.517473	-0.820372	-1.295129
H	-5.050682	-0.560198	-2.224894
C	-3.154438	-1.168724	-1.379097
C	-2.445896	-1.195766	-2.711139
H	-1.929424	-2.163649	-2.884974
Pt	-0.000030	0.913725	0.195079
H	3.167272	-2.059422	3.176441
H	1.678405	-1.209143	2.626315
H	-1.678107	-1.208690	2.626323
H	-3.166869	-2.059019	3.176662
H	-3.162272	-1.037881	-3.540768
H	-1.670493	-0.399751	-2.762618
H	3.162212	-1.037382	-3.540820
H	1.670592	-0.398952	-2.762589
C	6.666789	-0.387366	-0.007206
H	6.757466	0.699660	0.211632
H	7.213659	-0.925369	0.793824
H	7.189790	-0.571402	-0.967476
C	-6.666668	-0.387610	-0.007023
H	-7.189692	-0.571644	-0.967280
H	-7.213553	-0.925541	0.794044
H	-6.757285	0.699432	0.211776
Cl	0.000360	0.644107	2.549351
Cl	-0.000348	1.384203	-2.138347
S	-0.000156	3.287514	0.659007
C	1.399736	3.968187	-0.303132
H	2.322722	3.589753	0.175887
H	1.340754	3.604359	-1.347876
H	1.373402	5.074547	-0.248786
C	-1.400455	3.967914	-0.302738
H	-1.374307	5.074279	-0.248419
H	-1.341704	3.604076	-1.347491
H	-2.323231	3.589317	0.176556

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PtIMesCl2trans SCF Done: -1963.35152216 A.U.

N	1.097955	0.000426	1.457699
N	-1.098057	0.000429	1.457626
C	-0.000021	0.000109	0.631749
C	0.684241	0.000991	2.792135
H	1.409637	0.001290	3.611448
C	-0.684428	0.001014	2.792089
H	-1.409878	0.001346	3.611354

C	2.489161	0.000212	1.047840
C	3.152559	-1.241589	0.893550
C	2.440986	-2.556368	1.100987
H	1.872850	-2.578221	2.054776
C	4.512376	-1.208922	0.526244
H	5.044035	-2.166407	0.397595
C	5.207332	-0.000007	0.325662
C	4.512214	1.209376	0.525529
H	5.043782	2.166887	0.396382
C	3.152739	1.242209	0.892651
C	2.440784	2.556914	1.099368
H	1.874021	2.579692	2.053964
C	-2.489244	0.000225	1.047694
C	-3.152811	1.242229	0.892501
C	-2.440876	2.556930	1.099303
H	-1.874061	2.579636	2.053870
C	-4.512290	1.209408	0.525392
H	-5.043854	2.166924	0.396266
C	-5.207423	0.000032	0.325535
C	-4.512489	-1.208889	0.526156
H	-5.044175	-2.166368	0.397575
C	-3.152674	-1.241568	0.893466
C	-2.441157	-2.556354	1.101051
H	-1.873105	-2.578163	2.054891
Pt	0.000078	-0.000671	-1.272712
H	3.162374	3.396681	1.110530
H	1.709692	2.741463	0.281319
H	-1.709831	2.741565	0.281232
H	-3.162483	3.396681	1.110577
H	-3.163167	-3.395730	1.114263
H	-1.711200	-2.742338	0.282298
H	3.162967	-3.395768	1.114205
H	1.711086	-2.742271	0.282164
C	6.655263	0.001244	-0.110162
H	6.732816	0.047940	-1.218842
H	7.203774	0.877706	0.290808
H	7.183083	-0.917723	0.215524
C	-6.655366	0.001299	-0.110246
H	-7.183160	-0.917709	0.215362
H	-7.203883	0.877711	0.290828
H	-6.732950	0.048109	-1.218919
Cl	0.000164	2.296514	-1.625215
Cl	0.000012	-2.298135	-1.623385

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PtIPentCl2SMe2cis SCF Done: -2991.17447095 A.U.

Pt	0.046145	0.322643	-1.611641
Cl	-1.520969	2.067381	-1.427212
N	-1.305459	-0.289475	1.066649
N	0.785944	0.303011	1.314098
C	-0.169209	0.040938	0.347274
C	-1.054397	-0.218009	2.437418
C	0.247603	0.163372	2.593743
C	-2.590593	-0.725497	0.541362
C	-3.731458	0.114714	0.681131
C	-4.950971	-0.356116	0.144338
C	-5.045026	-1.598236	-0.488125
C	-3.920020	-2.431599	-0.556289
C	-2.676393	-2.032087	-0.027174
C	-3.748760	1.476943	1.380672
C	-4.627104	1.448811	2.666351
C	-4.185847	0.533177	3.812524
C	-4.278411	2.597903	0.436773
C	-3.838334	4.008770	0.845361
C	-1.510190	-3.023582	0.030391
C	-1.445840	-3.713198	1.429857
C	-2.605557	-4.658307	1.768592
C	-1.511717	-4.039504	-1.137100
C	-0.285551	-4.961847	-1.174877
C	2.178510	0.641960	1.081049
C	3.165085	-0.368812	1.287174
C	4.511416	-0.016425	1.043468
C	4.863824	1.275697	0.632996
C	3.875710	2.256431	0.474315
C	2.511051	1.975742	0.705401
C	2.826255	-1.777006	1.786254
C	2.999212	-1.904504	3.333777
C	4.429649	-1.822089	3.881124
C	3.588750	-2.883144	1.010691
C	3.159579	-4.313559	1.361853
C	1.467309	3.088686	0.619639
C	1.258337	3.755014	2.015720
C	2.438155	4.560591	2.574220
C	1.764933	4.104861	-0.511900
C	0.646843	5.129181	-0.744254
H	-1.829937	-0.443262	3.172247
H	0.837421	0.355318	3.493785
H	-5.845007	0.282083	0.217831
H	-6.004155	-1.930581	-0.915956
H	-4.016838	-3.423012	-1.020869
H	-2.707492	1.744489	1.660036
H	-4.697987	2.490643	3.048348
H	-5.663059	1.174733	2.364686
H	-4.099903	-0.526194	3.487092
H	-4.923441	0.557736	4.641764
H	-3.210710	0.849101	4.240383
H	-3.921355	2.394376	-0.592241
H	-5.390798	2.546756	0.405866
H	-4.145647	4.271049	1.880611
H	-4.278004	4.771745	0.169960
H	-2.734570	4.107099	0.780494
H	-0.570654	-2.438647	-0.070371
H	-0.484229	-4.268459	1.498796
H	-1.379371	-2.921507	2.206768
H	-3.585944	-4.139634	1.723048
H	-2.491765	-5.066881	2.794269
H	-2.655370	-5.525693	1.077085
H	-2.425021	-4.672053	-1.103618
H	-1.586013	-3.466958	-2.088012
H	0.663819	-4.384990	-1.152936
H	-0.281393	-5.579620	-2.096892
H	-0.262886	-5.663348	-0.315142
H	5.298046	-0.774432	1.169625
H	5.920407	1.523371	0.442807
H	4.167353	3.269834	0.163929
H	1.745656	-1.945790	1.587242
H	2.382624	-1.122005	3.823812
H	2.542618	-2.869468	3.645284
H	5.085129	-2.616837	3.466876
H	4.428787	-1.944655	4.984218
H	4.904873	-0.844229	3.659491
H	4.684279	-2.785627	1.173022
H	3.423098	-2.707243	-0.073619
H	3.408168	-4.587116	2.408377
H	3.665586	-5.050276	0.704071
H	2.064745	-4.451845	1.232758
H	0.496723	2.621600	0.352830
H	0.364610	4.412158	1.943253
H	0.977901	2.962217	2.744039
H	3.347527	3.935691	2.700071
H	2.188180	4.983964	3.569579
H	2.707707	5.413422	1.916472
H	1.923673	3.527460	-1.448482

H	2.717970	4.645202	-0.315113
H	-0.312229	4.615846	-0.962321
H	0.885655	5.776112	-1.613658
H	0.496150	5.797801	0.129732
Cl	0.286353	0.853736	-3.940785
S	1.675842	-1.330246	-1.873251
C	1.232644	-2.278956	-3.378257
H	0.321989	-2.857585	-3.140389
H	1.022449	-1.556505	-4.192191
H	2.071173	-2.962930	-3.616868
C	3.135953	-0.438975	-2.532319
H	3.509479	0.212870	-1.720639
H	3.906032	-1.186057	-2.810667
H	2.803631	0.166772	-3.398875

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PtIPentCl2SMe2trans SCF Done: -2991.18288282 A.U.

Pt	-0.018325	-0.079758	1.549253
Cl	-0.943543	-2.262968	1.520223
N	-1.082102	0.232315	-1.282058
N	1.088815	-0.044175	-1.263865
C	-0.010148	0.037414	-0.434880
C	-0.650030	0.277510	-2.608544
C	0.703912	0.093699	-2.597896
C	-2.484001	0.371700	-0.914852
C	-3.375150	-0.706262	-1.181945
C	-4.726040	-0.539707	-0.803464
C	-5.177047	0.638450	-0.201627
C	-4.288602	1.703886	-0.001552
C	-2.929839	1.612904	-0.368999
C	-2.984272	-2.021642	-1.863415
C	-3.714620	-2.194436	-3.226262
C	-3.420339	-1.151995	-4.309966
C	-3.284000	-3.238926	-0.942530
C	-2.606814	-4.545064	-1.375651
C	-2.022151	2.840850	-0.269972
C	-1.962676	3.589411	-1.638721
C	-3.261007	4.262305	-2.102158
C	-2.388187	3.771217	0.913258
C	-1.400997	4.923520	1.138883
C	2.473704	-0.240566	-0.861583
C	3.343752	0.887256	-0.839271
C	4.679437	0.661309	-0.440885
C	5.133925	-0.617658	-0.099637
C	4.263637	-1.713039	-0.168314
C	2.916221	-1.560669	-0.559479
C	2.901687	2.293927	-1.248344
C	3.189856	2.582781	-2.755793
C	4.662868	2.631808	-3.181860
C	3.479834	3.389064	-0.314538
C	2.842641	4.771274	-0.503747
C	2.011737	-2.786119	-0.709821
C	2.006121	-3.298296	-2.184174
C	3.326905	-3.876631	-2.707856
C	2.336224	-3.901304	0.315791
C	1.331313	-5.060054	0.327745
H	-1.350122	0.429876	-3.432852
H	1.428533	0.042469	-3.414648
H	-5.435910	-1.361962	-0.983263
H	-6.232951	0.737580	0.097100
H	-4.662603	2.638397	0.440009
H	-1.888805	-2.012363	-2.051356
H	-3.465339	-3.202486	-3.622420
H	-4.810401	-2.216847	-3.030259
H	-3.651860	-0.121139	-3.965737
H	-4.034448	-1.339197	-5.215479
H	-2.356833	-1.182074	-4.628794
H	-2.950047	-2.985064	0.083726
H	-4.386201	-3.390725	-0.891831
H	-2.925621	-4.884291	-2.384015
H	-2.844872	-5.364717	-0.666253
H	-1.501890	-4.435527	-1.390293
H	-0.991476	2.485864	-0.061999
H	-1.154143	4.350176	-1.576164
H	-1.624697	2.871321	-2.417342
H	-4.093127	3.533616	-2.200642
H	-3.122386	4.744252	-3.092606
H	-3.594083	5.054521	-1.399079
H	-3.408862	4.193526	0.779175
H	-2.433513	3.146733	1.831684
H	-0.373195	4.533605	1.288075
H	-1.675446	5.503696	2.044487
H	-1.382911	5.637083	0.288251
H	5.373422	1.512304	-0.386634
H	6.179505	-0.764459	0.215354
H	4.639108	-2.714347	0.086419
H	1.798929	2.336740	-1.123474
H	2.663997	1.823236	-3.372104
H	2.702173	3.548909	-3.012071
H	5.228579	3.420925	-2.643480
H	4.747173	2.854399	-4.266194
H	5.180274	1.666587	-3.001070
H	4.580420	3.474744	-0.451920
H	3.318678	3.054986	0.731303
H	3.029280	5.194639	-1.513384
H	3.247485	5.495754	0.233115
H	1.743402	4.726655	-0.352929
H	0.972864	-2.464976	-0.485011
H	1.205052	-4.064149	-2.277331
H	1.685604	-2.463249	-2.844189
H	4.152449	-3.135918	-2.655901
H	3.226372	-4.188440	-3.768544
H	3.646785	-4.772464	-2.135075
H	2.364779	-3.434835	1.324027
H	3.355882	-4.309889	0.139391
H	0.304691	-4.686352	0.520786
H	1.580347	-5.788376	1.127685
H	1.321214	-5.621136	-0.630354
Cl	0.956962	2.065063	1.745420
S	-0.001406	-0.117729	3.969210
C	-1.698785	-0.599092	4.454667
H	-2.352854	0.256453	4.200385
H	-2.007766	-1.493018	3.877732
H	-1.725495	-0.781576	5.547194
C	0.895670	-1.646855	4.422726
H	1.954478	-1.483828	4.145470
H	0.813726	-1.804647	5.516370
H	0.480960	-2.500664	3.851447

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PtIPentCl2trans SCF Done: -2513.26996782 A.U.

Pt	0.009805	0.002042	-1.809439
Cl	-0.973939	2.047864	-2.267139
N	-1.129125	-0.128067	0.916760
N	1.048546	0.208170	0.932210
C	-0.032326	0.030012	0.095116
C	-0.725914	-0.052163	2.251482
C	0.622941	0.167957	2.260851
C	-2.514691	-0.332268	0.518929
C	-3.433482	0.743928	0.668958
C	-4.768189	0.512636	0.268760
C	-5.173453	-0.722712	-0.244849
C	-4.255519	-1.778172	-0.335788
C	-2.910687	-1.623188	0.058737

C	-3.083665	2.121496	1.240389
C	-3.873278	2.411825	2.548111
C	-3.618653	1.467873	3.728221
C	-3.340677	3.238640	0.189524
C	-2.736768	4.602742	0.546304
C	-1.965652	-2.826556	0.069925
C	-1.930892	-3.485105	1.485177
C	-3.223841	-4.168897	1.947186
C	-2.261306	-3.838266	-1.065278
C	-1.227212	-4.964139	-1.191188
C	2.438130	0.398094	0.542294
C	3.321894	-0.715936	0.620340
C	4.663479	-0.496363	0.239414
C	5.105902	0.762708	-0.183076
C	4.216663	1.844210	-0.223240
C	2.862177	1.697794	0.143987
C	2.883607	-2.097962	1.109857
C	3.143515	-2.287119	2.638230
C	4.608686	-2.314614	3.091506
C	3.486149	-3.243963	0.255906
C	2.881164	-4.623866	0.542662
C	1.927397	2.908790	0.156592
C	1.890090	3.573485	1.568288
C	3.187752	4.241812	2.039633
C	2.234342	3.912511	-0.983401
C	1.194559	5.029540	-1.135892
H	-1.446039	-0.153771	3.066691
H	1.323356	0.305438	3.088721
H	-5.501635	1.328909	0.357773
H	-6.217054	-0.872081	-0.564447
H	-4.593708	-2.752440	-0.715780
H	-1.998251	2.141880	1.481029
H	-3.642089	3.451531	2.864681
H	-4.960001	2.411302	2.306341
H	-3.832714	0.409532	3.465662
H	-4.267274	1.727735	4.590554
H	-2.568211	1.532787	4.083900
H	-2.922046	2.902217	-0.780817
H	-4.438645	3.346063	0.038142
H	-3.161783	5.035002	1.476679
H	-2.920072	5.335587	-0.266436
H	-1.636358	4.532224	0.680232
H	-0.939127	-2.451781	-0.123630
H	-1.098433	-4.222222	1.497932
H	-1.642306	-2.708627	2.227218
H	-4.080690	-3.463088	1.970316
H	-3.105571	-4.581585	2.970842
H	-3.506760	-5.014834	1.286219
H	-3.269718	-4.288971	-0.932868
H	-2.302078	-3.272531	-2.020976
H	-0.209038	-4.548117	-1.337164
H	-1.453509	-5.607504	-2.066655
H	-1.208443	-5.624007	-0.298286
H	5.371730	-1.336897	0.261697
H	6.156519	0.903919	-0.482885
H	4.580493	2.828096	-0.551709
H	1.782549	-2.159903	0.973270
H	2.611575	-1.484590	3.192168
H	2.645619	-3.231427	2.949860
H	5.177718	-3.141922	2.618035
H	4.672995	-2.463094	4.189660
H	5.135423	-1.366801	2.854771
H	4.587837	-3.294571	0.399248
H	3.322000	-2.988288	-0.811409
H	3.085561	-4.974710	1.576222
H	3.296980	-5.386200	-0.148225
H	1.779738	-4.616732	0.400090
H	0.899186	2.538354	-0.039571
H	1.067599	4.322014	1.571390
H	1.584942	2.803823	2.310749
H	4.033350	3.523382	2.078911
H	3.063716	4.664731	3.058408
H	3.490845	5.077980	1.375219
H	2.292377	3.338447	-1.933036
H	3.238326	4.369500	-0.839517
H	0.183146	4.605313	-1.303754
H	1.435110	5.671953	-2.008261
H	1.149714	5.692103	-0.245883
Cl	1.044466	-2.052670	-2.108149

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PtIPrCl2DIMER SCF Done: -4398.10183646 A.U.

N	4.190610	1.193188	0.511433
C	3.802362	2.536919	0.117276
N	4.240759	-0.959065	0.906060
C	4.393786	3.104546	-1.044269
C	4.040205	4.431607	-1.366243
H	4.475043	4.899437	-2.262740
C	3.145123	5.160341	-0.573167
H	2.881088	6.193837	-0.849348
C	2.588822	4.578487	0.573807
H	1.893501	5.161747	1.195915
C	2.907594	3.258770	0.954486
C	5.415635	2.363090	-1.909358
H	5.324148	1.281196	-1.680030
C	5.146802	2.523541	-3.418777
H	4.108333	2.229903	-3.667245
H	5.835389	1.872824	-3.997269
H	5.317143	3.565596	-3.763934
C	6.855561	2.813491	-1.568889
H	6.996373	3.893461	-1.788662
H	7.594885	2.246587	-2.173330
H	7.105759	2.658962	-0.499352
C	2.361231	2.687618	2.263906
H	2.379212	1.581486	2.185690
C	0.898422	3.081213	2.538367
H	0.788930	4.166466	2.748757
H	0.519238	2.535626	3.426012
H	0.239346	2.820745	1.686597
C	3.273310	3.093208	3.445812
H	4.320524	2.756560	3.298151
H	2.903827	2.647641	4.393480
H	3.291078	4.196904	3.573302
C	3.462835	0.033750	0.347390
C	5.394584	0.922432	1.162805
H	6.108938	1.715681	1.399577
C	5.430024	-0.423559	1.401482
H	6.189623	-1.052535	1.873662
C	3.917234	-2.373192	0.997439
C	4.158208	-3.202885	-0.131680
C	3.871106	-4.576744	0.003801
H	4.037901	-5.245869	-0.853669
C	3.382646	-5.104432	1.206331
H	3.163248	-6.181208	1.285864
C	3.175419	-4.265697	2.308677
H	2.794592	-4.691188	3.249516
C	3.437619	-2.881739	2.236140
C	4.771252	-2.670097	-1.426773
H	4.541660	-1.587060	-1.492910
C	6.308974	-2.833297	-1.400671
H	6.767369	-2.314192	-0.533402
H	6.760717	-2.411913	-2.323520
H	6.596673	-3.904980	-1.339431

C	4.170604	-3.312351	-2.690594
H	4.442299	-4.385357	-2.788887
H	4.552114	-2.792541	-3.593020
H	3.066071	-3.224833	-2.697428
C	3.249253	-2.008557	3.479744
H	3.178625	-0.952948	3.141397
C	1.952528	-2.327299	4.250983
H	1.067225	-2.297666	3.586531
H	1.798004	-1.581022	5.057676
H	1.995020	-3.325267	4.736592
C	4.469595	-2.125587	4.423556
H	4.583862	-3.167539	4.791491
H	4.343825	-1.465921	5.307940
H	5.419052	-1.843874	3.924992
Pt	1.724848	-0.178577	-0.512020
Cl	2.674390	0.094304	-2.631301
Cl	0.514403	-0.486337	1.540121
N	-4.241070	-0.958474	-0.905974
C	-3.917808	-2.372647	-0.997488
N	-4.190396	1.193732	-0.511160
C	-3.438237	-2.881137	-2.236222
C	-3.176253	-4.265131	-2.308896
H	-2.795462	-4.690583	-3.249765
C	-3.383677	-5.103951	-1.206650
H	-3.164449	-6.180754	-1.286286
C	-3.872128	-4.576316	-0.004092
H	-4.039086	-5.245513	0.853291
C	-4.158998	-3.202425	0.131527
C	-3.249760	-2.007826	-3.479723
H	-3.178862	-0.952281	-3.141228
C	-1.953194	-2.326744	-4.251137
H	-1.067822	-2.297322	-3.586768
H	-1.798639	-1.580431	-5.057790
H	-1.995919	-3.324664	-4.736818
C	-4.470251	-2.124422	-4.423405
H	-4.584820	-3.166290	-4.791490
H	-4.344447	-1.464640	-5.307696
H	-5.419568	-1.842578	-3.924650
C	-4.772052	-2.669684	1.426634
H	-4.542315	-1.586684	1.492897
C	-4.171587	-3.312155	2.690427
H	-4.443401	-4.385146	2.788564
H	-4.553131	-2.792428	3.592888
H	-3.067048	-3.224739	2.697368
C	-6.309800	-2.832667	1.400398
H	-6.768054	-2.313412	0.533146
H	-6.761559	-2.411322	2.323257
H	-6.597638	-3.904305	1.339017
C	-3.462834	0.034130	-0.347350
C	-5.430350	-0.422695	-1.401039
H	-6.190187	-1.051480	-1.873091
C	-5.394595	0.923267	-1.162250
H	-6.108861	1.716675	-1.398750
C	-3.801802	2.537365	-0.116985
C	-2.907159	3.259139	-0.954403
C	-2.588017	4.578756	-0.573683
H	-1.892773	5.161945	-1.195940
C	-3.143846	5.160592	0.573526
H	-2.879516	6.194006	0.849737
C	-4.038828	4.431954	1.366799
H	-4.473301	4.899783	2.263474
C	-4.392770	3.105000	1.044798
C	-2.361334	2.688003	-2.264051
H	-2.379147	1.581873	-2.185769
C	-3.273991	3.093465	-3.445558
H	-4.321110	2.756728	-3.297443
H	-2.904889	2.647912	-4.393383
H	-3.291906	4.197155	-3.573060
C	-0.898709	3.081771	-2.539243
H	-0.789480	4.167014	-2.749816
H	-0.519885	2.536138	-3.427013
H	-0.239178	2.821494	-1.687766
C	-5.414481	2.363670	1.910150
H	-5.323225	1.281771	1.680757
C	-5.145156	2.524012	3.419498
H	-4.106653	2.230223	3.667649
H	-5.833640	1.873347	3.998169
H	-5.315264	3.566071	3.764770
C	-6.854430	2.814342	1.570165
H	-6.994962	3.894334	1.790005
H	-7.593665	2.247573	2.174842
H	-7.105025	2.659874	0.500713
Pt	-1.724745	-0.178644	0.511781
Cl	-0.514405	-0.485679	-1.540571
Cl	-2.674105	0.093712	2.631228

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PtIPrCl2Pycis SCF Done: -2447.15928604 A.U.

N	-1.561328	-0.262142	-1.238912
C	-2.787204	0.412431	-0.843440
N	0.455666	-1.084864	-1.382611
C	-3.923517	-0.372440	-0.502322
C	-5.117241	0.313687	-0.194449
H	-6.009975	-0.266856	0.084011
C	-5.186203	1.710768	-0.220732
H	-6.127482	2.222291	0.035945
C	-4.056971	2.459239	-0.578233
H	-4.126826	3.556454	-0.608981
C	-2.838867	1.832499	-0.909156
C	-3.924129	-1.903551	-0.493396
H	-2.866163	-2.236571	-0.482650
C	-4.590388	-2.488664	0.768917
H	-4.150373	-2.052700	1.686464
H	-4.440173	-3.588042	0.801363
H	-5.686751	-2.309838	0.780438
C	-4.610748	-2.467161	-1.759764
H	-5.679760	-2.167070	-1.798454
H	-4.573127	-3.577089	-1.761441
H	-4.137363	-2.113689	-2.698718
C	-1.655078	2.667336	-1.402503
H	-0.729620	2.131705	-1.101548
C	-1.594136	4.071467	-0.773308
H	-2.424037	4.722145	-1.121039
H	-0.651753	4.581474	-1.063803
H	-1.644420	4.027384	0.334553
C	-1.663260	2.766366	-2.946076
H	-1.635485	1.766302	-3.424945
H	-0.784757	3.340965	-3.309789
H	-2.579461	3.284006	-3.302161
C	-0.362000	-0.343659	-0.547520
C	-1.475226	-0.936979	-2.458220
H	-2.320365	-0.978414	-3.150511
C	-0.216976	-1.460511	-2.546195
H	0.261617	-2.065813	-3.321117
C	1.843183	-1.421944	-1.147198
C	2.160902	-2.455977	-0.223301
C	3.527196	-2.763980	-0.046156
H	3.807135	-3.554497	0.666947
C	4.528561	-2.098900	-0.768335
H	5.586581	-2.366155	-0.615701
C	4.183471	-1.103338	-1.692375
H	4.975954	-0.593988	-2.263225
C	2.836892	-0.738598	-1.903070

C	1.094944	-3.275217	0.503623
H	0.138419	-2.717049	0.459070
C	0.889736	-4.629269	-0.214826
H	0.608525	-4.493521	-1.280304
H	0.080732	-5.207485	0.278721
H	1.813306	-5.246998	-0.188054
C	1.405176	-3.471651	1.999416
H	2.314784	-4.087791	2.167029
H	0.557533	-3.989799	2.491720
H	1.531110	-2.496217	2.511520
C	2.499427	0.330978	-2.946634
H	1.422031	0.576595	-2.844631
C	3.283418	1.642124	-2.735226
H	3.120935	2.057787	-1.721144
H	2.959675	2.405469	-3.473512
H	4.376137	1.498794	-2.871404
C	2.721358	-0.207016	-4.378761
H	3.790408	-0.453632	-4.552159
H	2.423327	0.550868	-5.133553
H	2.134920	-1.128298	-4.572549
Pt	0.069801	0.257423	1.299630
Cl	-1.641814	-1.161559	2.041354
Cl	0.534119	0.884094	3.560896
N	1.689184	1.479488	0.907775
C	1.528745	2.820494	0.776834
C	2.942088	0.984469	1.080052
C	2.611556	3.708060	0.804660
C	4.068935	1.814578	1.123983
C	3.908553	3.201908	0.985125
H	0.494130	3.173431	0.677281
H	3.018751	-0.104967	1.202461
H	2.423695	4.787085	0.702501
H	5.059460	1.361512	1.275409
H	4.777253	3.877440	1.024346

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PtIPrCl2Pytrans SCF Done: -2447.17995572 A.U.

N	-1.083104	-1.741178	0.142826
C	-2.471052	-1.353839	0.330053
N	1.082749	-1.741401	-0.142741
C	-2.906963	-0.983423	1.632413
C	-4.268386	-0.650565	1.788776
H	-4.636306	-0.351763	2.781826
C	-5.160125	-0.700914	0.708972
H	-6.219465	-0.436087	0.856943
C	-4.707296	-1.094326	-0.556461
H	-5.416978	-1.137580	-1.396797
C	-3.355885	-1.431555	-0.780523
C	-1.980072	-1.014206	2.848090
H	-0.941863	-0.857999	2.490769
C	-2.258138	0.116106	3.855505
H	-2.246777	1.107027	3.359629
H	-1.469612	0.125331	4.635364
H	-3.232935	-0.009444	4.374202
C	-2.048178	-2.396044	3.539644
H	-3.070927	-2.601029	3.923235
H	-1.347463	-2.435600	4.400363
H	-1.778809	-3.220670	2.847669
C	-2.916136	-1.908552	-2.166928
H	-1.811484	-1.815847	-2.216504
C	-3.488051	-1.043100	-3.307048
H	-4.589278	-1.154044	-3.402839
H	-3.045033	-1.353373	-4.276454
H	-3.247584	0.026106	-3.148082
C	-3.291514	-3.393590	-2.381700
H	-2.849585	-4.057417	-1.610962
H	-2.937702	-3.746324	-3.373569
H	-4.393234	-3.533086	-2.346427
C	-0.000091	-0.899511	0.000060
C	-0.677519	-3.075556	0.093645
H	-1.390527	-3.897560	0.200644
C	0.676888	-3.075691	-0.093584
H	1.389730	-3.897849	-0.200519
C	2.470764	-1.354311	-0.329981
C	3.355561	-1.432021	0.780632
C	4.707006	-1.094953	0.556575
H	5.416662	-1.138187	1.396933
C	5.159912	-0.701718	-0.708892
H	6.219280	-0.437000	-0.856851
C	4.268217	-0.651401	-1.788729
H	4.636199	-0.352754	-2.781803
C	2.906747	-0.984083	-1.632363
C	2.915700	-1.908930	2.167027
H	1.811069	-1.815988	2.216599
C	3.290755	-3.394058	2.381748
H	2.848729	-4.057760	1.610958
H	2.936825	-3.746769	3.373583
H	4.392448	-3.533777	2.346514
C	3.487790	-1.043644	3.307184
H	4.588989	-1.154833	3.402994
H	3.044684	-1.353846	4.276573
H	3.247556	0.025619	3.148241
C	1.979875	-1.014871	-2.848053
H	0.941682	-0.858494	-2.490756
C	2.258106	0.115293	-3.855592
H	2.246892	1.106271	-3.359827
H	1.469590	0.124535	-4.635459
H	3.232892	-0.010456	-4.374263
C	2.047809	-2.396785	-3.539470
H	3.070541	-2.601952	-3.923012
H	1.347116	-2.436327	-4.400206
H	1.778305	-3.221309	-2.847428
Pt	0.000125	1.073709	-0.000001
Cl	0.905023	1.126775	2.188908
Cl	-0.904791	1.126693	-2.188898
N	0.000352	3.195475	-0.000112
C	-1.056410	3.883683	-0.499293
C	1.057257	3.883522	0.498990
C	-1.093566	5.284157	-0.509271
C	1.094692	5.283988	0.508823
C	0.000634	6.001706	-0.000259
H	-1.869248	3.270076	-0.915492
H	1.869977	3.269793	0.915238
H	-1.976652	5.797060	-0.918579
H	1.977882	5.796757	0.918074
H	0.000746	7.103187	-0.000316

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PtIPrCl2SMe2cis SCF Done: -2676.92880524 A.U.

N	1.351774	0.112155	-1.340488
C	2.672934	-0.290233	-0.887403
N	-0.780292	0.555442	-1.515175
C	3.696396	0.692271	-0.793815
C	4.983598	0.252905	-0.418108
H	5.794800	0.991347	-0.327595
C	5.245556	-1.093882	-0.144712
H	6.256734	-1.409064	0.158187
C	4.220996	-2.043410	-0.258573
H	4.442472	-3.100582	-0.051472
C	2.917449	-1.670817	-0.642816
C	3.478043	2.173110	-1.114734
H	2.384024	2.357099	-1.106809
C	4.094671	3.106290	-0.052529
H	3.746608	2.833893	0.962649

H	3.793903	4.156238	-0.250907
H	5.205067	3.077525	-0.068334
C	4.032556	2.526480	-2.514760
H	5.131746	2.370596	-2.557446
H	3.834713	3.592718	-2.754056
H	3.583431	1.912001	-3.321914
C	1.843260	-2.739682	-0.860884
H	0.865961	-2.282503	-0.596805
C	2.018526	-3.976415	0.039163
H	2.908782	-4.577327	-0.243212
H	1.139856	-4.647606	-0.059367
H	2.126810	-3.693503	1.106403
C	1.785032	-3.160104	-2.348305
H	1.586611	-2.297481	-3.016576
H	0.981612	-3.908931	-2.514581
H	2.746853	-3.616800	-2.665405
C	0.184146	0.169188	-0.602613
C	1.111309	0.467955	-2.669017
H	1.912232	0.479422	-3.413133
C	-0.219902	0.754987	-2.777698
H	-0.819374	1.086742	-3.629828
C	-2.198361	0.709808	-1.257058
C	-2.655549	1.865434	-0.564969
C	-4.046443	1.985467	-0.356684
H	-4.430544	2.865081	0.182087
C	-4.944401	1.019322	-0.830606
H	-6.025727	1.140122	-0.657201
C	-4.468158	-0.095099	-1.534642
H	-5.182570	-0.841987	-1.914592
C	-3.088714	-0.279203	-1.767237
C	-1.723160	2.993597	-0.125522
H	-0.685763	2.603776	-0.113889
C	-1.781922	4.153679	-1.146614
H	-1.518841	3.816595	-2.171298
H	-1.069200	4.954992	-0.859536
H	-2.797462	4.602925	-1.192308
C	-2.010226	3.487169	1.304931
H	-3.005406	3.973676	1.393775
H	-1.247195	4.234457	1.602581
H	-1.951618	2.653078	2.033021
C	-2.620512	-1.482775	-2.592512
H	-1.520247	-1.569427	-2.471760
C	-3.234770	-2.815867	-2.118652
H	-3.024791	-2.992644	-1.044916
H	-2.805131	-3.660856	-2.696490
H	-4.334435	-2.845145	-2.269779
C	-2.914990	-1.263873	-4.095081
H	-4.008012	-1.190223	-4.278285
H	-2.527471	-2.111805	-4.698209
H	-2.452974	-0.333230	-4.482541
Pt	-0.067879	-0.054444	1.355198
Cl	1.340293	1.810310	1.651316
Cl	-0.358569	-0.180900	3.734064
S	-1.562443	-1.835528	1.122694
C	-3.088487	-1.274156	1.967866
H	-2.806662	-0.902944	2.973470
H	-3.511845	-0.456363	1.354899
H	-3.796953	-2.125210	2.015126
C	-1.041488	-3.133460	2.307153
H	-1.834835	-3.906147	2.347847
H	-0.103982	-3.568603	1.916043
H	-0.861501	-2.654065	3.290412

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PtIPrCl2SMe2trans SCF Done: -2676.93524681 A.U.

N	0.975892	1.169354	-1.125301
C	2.385426	0.825975	-1.041188
N	-1.192802	1.240776	-0.870651
C	3.236009	1.630826	-0.234413
C	4.607357	1.300334	-0.210442
H	5.292084	1.898966	0.409469
C	5.111391	0.226014	-0.954081
H	6.185834	-0.015169	-0.914046
C	4.251727	-0.537764	-1.755073
H	4.659978	-1.371720	-2.345620
C	2.872128	-0.254555	-1.827966
C	2.737388	2.849021	0.546554
H	1.638940	2.743278	0.663486
C	3.330913	2.934927	1.966371
H	3.155057	1.994717	2.524358
H	2.847813	3.761121	2.528590
H	4.421341	3.146754	1.950956
C	3.021610	4.154288	-0.233288
H	4.113935	4.304468	-0.370293
H	2.626235	5.032646	0.319371
H	2.558544	4.154444	-1.241017
C	1.975122	-1.043503	-2.782288
H	0.937890	-0.996537	-2.392111
C	2.333928	-2.538520	-2.859337
H	3.314378	-2.713993	-3.352029
H	1.567374	-3.078352	-3.451903
H	2.358544	-2.997032	-1.850805
C	1.991723	-0.402913	-4.189995
H	1.664387	0.657021	-4.168190
H	1.311695	-0.951420	-4.875593
H	3.012317	-0.429536	-4.629041
C	-0.065900	0.565675	-0.455620
C	0.501949	2.197605	-1.941680
H	1.174726	2.793523	-2.564478
C	-0.854577	2.246678	-1.776841
H	-1.610843	2.904129	-2.214474
C	-2.562666	0.994613	-0.451005
C	-3.008388	1.548658	0.780779
C	-4.353772	1.326648	1.140121
H	-4.728658	1.733983	2.091025
C	-5.220920	0.605082	0.308971
H	-6.267890	0.444650	0.612655
C	-4.759495	0.092213	-0.909715
H	-5.450192	-0.468162	-1.558166
C	-3.422922	0.272795	-1.323160
C	-2.112031	2.418665	1.662617
H	-1.059325	2.124003	1.474919
C	-2.269512	3.909846	1.283080
H	-2.029394	4.095201	0.215634
H	-1.591807	4.541226	1.895815
H	-3.310171	4.258498	1.457772
C	-2.352302	2.208985	3.168727
H	-3.344486	2.588460	3.495003
H	-1.583644	2.757039	3.750858
H	-2.275497	1.137957	3.442081
C	-2.974577	-0.258014	-2.686866
H	-1.866012	-0.305629	-2.677595
C	-3.479526	-1.686948	-2.967838
H	-3.195904	-2.373966	-2.146941
H	-3.027777	-2.070181	-3.906634
H	-4.581963	-1.721243	-3.100336
C	-3.412685	0.698472	-3.820601
H	-4.520096	0.773748	-3.870174
H	-3.054632	0.327831	-4.804388
H	-3.017214	1.725534	-3.683664
Pt	0.025234	-0.938677	0.829510
Cl	0.848108	0.469525	2.558157
Cl	-0.746780	-2.444691	-0.821643

S	0.113209	-2.650877	2.539414
C	-0.355116	-4.282348	1.865158
H	-1.439084	-4.239721	1.650597
H	0.186354	-4.490339	0.922941
H	-0.150469	-5.049816	2.637463
C	1.905429	-2.912874	2.801415
H	2.051316	-3.665995	3.600872
H	2.392464	-3.231685	1.859657
H	2.303762	-1.930266	3.118094

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PtIPrCl2trans SCF Done: -2199.02270865 A.U.

N	1.098483	0.048787	1.160156
C	2.494526	0.110197	0.758290
N	-1.098481	-0.048709	1.160268
C	3.233375	-1.101991	0.686283
C	4.595762	-1.005345	0.334757
H	5.197418	-1.923890	0.261518
C	5.194131	0.234029	0.074022
H	6.258895	0.282340	-0.204694
C	4.442742	1.412837	0.169902
H	4.925578	2.381007	-0.030604
C	3.077057	1.384995	0.519493
C	2.627560	-2.464943	1.027320
H	1.524959	-2.374184	0.937344
C	3.063068	-3.577903	0.054845
H	2.841694	-3.299824	-0.994049
H	2.510871	-4.513637	0.280999
H	4.145596	-3.809864	0.144170
C	2.959245	-2.857102	2.486405
H	4.055940	-2.962773	2.628813
H	2.488633	-3.828766	2.746098
H	2.600970	-2.102717	3.216593
C	2.301625	2.691771	0.694250
H	1.222940	2.463549	0.568868
C	2.650531	3.751060	-0.367777
H	3.689552	4.128332	-0.257642
H	1.974207	4.624321	-0.264099
H	2.523930	3.350140	-1.392534
C	2.510242	3.255985	2.119383
H	2.200056	2.535583	2.904139
H	1.919200	4.185271	2.261379
H	3.579010	3.502657	2.296218
C	-0.000026	-0.000150	0.331500
C	0.683207	0.032330	2.493122
H	1.403695	0.068345	3.314954
C	-0.683112	-0.031580	2.493175
H	-1.403523	-0.067194	3.315094
C	-2.494544	-0.109697	0.758415
C	-3.077542	-1.384313	0.519725
C	-4.443247	-1.411692	0.170224
H	-4.926460	-2.379690	-0.030165
C	-5.194245	-0.232616	0.074334
H	-6.259055	-0.280581	-0.204266
C	-4.595422	1.006556	0.334912
H	-5.196749	1.925317	0.261634
C	-3.232962	1.102736	0.686317
C	-2.302441	-2.691269	0.694600
H	-1.223791	-2.463448	0.568203
C	-2.510069	-3.254616	2.120247
H	-2.198890	-2.533893	2.904310
H	-1.919263	-4.184051	2.262237
H	-3.578787	-3.500749	2.298133
C	-2.652452	-3.751075	-0.366503
H	-3.691334	-4.128364	-0.255082
H	-1.975981	-4.624253	-0.263117
H	-2.527010	-3.350688	-1.391616
C	-2.626696	2.465580	1.027033
H	-1.524087	2.374341	0.937572
C	-3.061420	3.578272	0.053900
H	-2.839615	3.299626	-0.994750
H	-2.509075	4.513949	0.279929
H	-4.143925	3.810550	0.142640
C	-2.958746	2.858410	2.485857
H	-4.055447	2.964573	2.627862
H	-2.487840	3.829975	2.745381
H	-2.601060	2.104097	3.216409
Pt	0.000007	-0.000637	-1.569614
Cl	0.323425	-2.270996	-1.918050
Cl	-0.323582	2.269287	-1.920486

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PtIPrClSMe2cis+ SCF Done: -2216.56065839 A.U.

N	-1.221390	-0.053219	1.278434
C	-2.587637	-0.317635	0.845604
N	0.943497	0.338651	1.343707
C	-3.508720	0.764647	0.830294
C	-4.831487	0.469111	0.439141
H	-5.575009	1.279668	0.406748
C	-5.215863	-0.831032	0.089275
H	-6.254219	-1.032745	-0.216714
C	-4.286178	-1.879475	0.136262
H	-4.609987	-2.897897	-0.124569
C	-2.949776	-1.653855	0.522513
C	-3.147083	2.186571	1.268112
H	-2.038703	2.268573	1.283300
C	-3.669278	3.268391	0.300634
H	-3.335968	3.081879	-0.738744
H	-3.295201	4.265712	0.611035
H	-4.777579	3.325101	0.304111
C	-3.661076	2.459219	2.702278
H	-4.769403	2.409217	2.740151
H	-3.358062	3.472356	3.038820
H	-3.275232	1.726807	3.440689
C	-1.978507	-2.828087	0.664763
H	-0.946344	-2.428313	0.557070
C	-2.164871	-3.903220	-0.423492
H	-3.114687	-4.462837	-0.297764
H	-1.348897	-4.653726	-0.367852
H	-2.176032	-3.461216	-1.441647
C	-2.087824	-3.454521	2.075060
H	-1.890376	-2.712522	2.875550
H	-1.361983	-4.285859	2.195281
H	-3.105278	-3.864683	2.244703
C	-0.102216	0.072005	0.495071
C	-0.872036	0.138721	2.614484
H	-1.618800	0.077479	3.411368
C	0.471337	0.394414	2.655769
H	1.137732	0.619070	3.493371
C	2.333921	0.564023	0.984373
C	2.689605	1.806822	0.388303
C	4.051695	1.997881	0.070847
H	4.366304	2.945850	-0.391364
C	5.012840	1.017301	0.355245
H	6.070396	1.196298	0.105225
C	4.634723	-0.181555	0.976188
H	5.403570	-0.932242	1.214591
C	3.289240	-0.441708	1.313573
C	1.695730	2.950126	0.176792
H	0.669380	2.535186	0.250832
C	1.854447	4.000571	1.301711
H	1.719723	3.553613	2.308338
H	1.103844	4.809207	1.183889
H	2.861286	4.467734	1.275194

C	1.812187	3.599962	-1.215468
H	2.782302	4.120714	-1.355413
H	1.013179	4.356826	-1.349057
H	1.699161	2.849971	-2.024932
C	2.935351	-1.729607	2.064639
H	1.832046	-1.856714	2.026338
C	3.561703	-2.991322	1.435749
H	3.287942	-3.094629	0.366465
H	3.206138	-3.897869	1.967126
H	4.668836	-2.987981	1.509798
C	3.347511	-1.619122	3.552428
H	4.448691	-1.520985	3.651776
H	3.037721	-2.526524	4.110788
H	2.894631	-0.740384	4.054635
Pt	-0.080625	0.028182	-1.446452
Cl	-1.558095	1.576225	-2.227639
S	1.544285	-1.643455	-1.432552
C	2.930391	-0.908338	-2.381016
H	2.565692	-0.457984	-3.324493
H	3.391802	-0.137812	-1.735020
H	3.660851	-1.715407	-2.588916
C	0.896553	-2.819160	-2.683996
H	1.693404	-3.559419	-2.897479
H	0.023105	-3.325414	-2.233391
H	0.598990	-2.291671	-3.611671

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PtIPrClSMe2trans+ SCF Done: -2216.56506152 A.U.

N	-1.026161	-1.239367	-1.051197
C	-2.422711	-0.936326	-0.772372
N	1.157344	-1.204636	-1.103273
C	-3.122278	-1.751937	0.158796
C	-4.480977	-1.445734	0.381689
H	-5.056011	-2.051081	1.098389
C	-5.113119	-0.390511	-0.289661
H	-6.175480	-0.174452	-0.095989
C	-4.400581	0.380835	-1.217429
H	-4.915345	1.192440	-1.754731
C	-3.040630	0.124138	-1.488538
C	-2.485259	-2.953062	0.860958
H	-1.382851	-2.829615	0.805779
C	-2.854560	-3.040419	2.355262
H	-2.634243	-2.091721	2.883058
H	-2.270631	-3.847801	2.842833
H	-3.927305	-3.283192	2.505148
C	-2.859652	-4.268351	0.136861
H	-3.955833	-4.441440	0.170780
H	-2.366140	-5.134556	0.624518
H	-2.559476	-4.265768	-0.930957
C	-2.321932	0.931446	-2.571406
H	-1.238682	0.689623	-2.513423
C	-2.465786	2.453297	-2.363542
H	-3.515277	2.790029	-2.491035
H	-1.857746	3.009343	-3.107671
H	-2.144148	2.756781	-1.344586
C	-2.805076	0.514734	-3.979441
H	-2.659530	-0.570230	-4.157695
H	-2.251200	1.068013	-4.766498
H	-3.885588	0.731786	-4.111692
C	0.069404	-0.589543	-0.549118
C	-0.618141	-2.245074	-1.928003
H	-1.341867	-2.874879	-2.453731
C	0.751873	-2.225453	-1.962439
H	1.470789	-2.833983	-2.519592
C	2.529842	-0.823279	-0.845604
C	3.367022	-1.702656	-0.113072
C	4.701583	-1.288938	0.092217
H	5.384783	-1.943322	0.655513
C	5.170615	-0.063043	-0.394481
H	6.216658	0.233334	-0.220536
C	4.312085	0.791668	-1.104216
H	4.699091	1.749737	-1.481614
C	2.974045	0.429045	-1.348906
C	2.885399	-3.030094	0.473970
H	1.810567	-3.148290	0.222863
C	3.639313	-4.229931	-0.140133
H	3.550141	-4.256007	-1.246143
H	3.236055	-5.184037	0.257292
H	4.721736	-4.200739	0.104600
C	2.985504	-3.025886	2.015547
H	4.037032	-2.930933	2.358229
H	2.587795	-3.976663	2.426815
H	2.402494	-2.192099	2.456361
C	2.025665	1.374247	-2.092887
H	1.265061	0.758885	-2.619628
C	1.284827	2.305517	-1.104494
H	0.168655	1.945044	-0.804858
H	0.882002	3.211394	-1.612718
H	1.942187	2.655152	-0.287959
C	2.728419	2.233290	-3.166354
H	3.410269	2.988326	-2.723803
H	1.980101	2.780929	-3.774765
H	3.324506	1.598081	-3.851319
Pt	0.158673	1.001431	0.663165
Cl	-0.397461	-0.357009	2.460587
S	0.216681	2.813859	2.300467
C	0.296658	4.443747	1.469867
H	1.311099	4.558053	1.043576
H	-0.471394	4.537055	0.677643
H	0.148228	5.226125	2.239544
C	-1.486588	2.885188	2.968322
H	-1.518153	3.672493	3.746011
H	-2.218019	3.087152	2.162745
H	-1.678964	1.893345	3.417846

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PtIPrDvtms SCF Done: -2249.56280601 A.U.

Pt	0.359694	-0.657817	-0.301440
C	-0.969168	0.870858	0.069034
N	-0.699872	2.193846	0.326782
C	-1.925288	2.978225	0.605053
H	-1.880241	3.978300	0.132947
H	-2.036894	3.124466	1.704713
C	-3.014312	2.080173	0.020725
H	-3.933627	2.044424	0.636868
H	-3.306699	2.381106	-1.012087
N	-2.336737	0.764596	-0.012854
C	0.574803	2.787328	0.638642
C	1.178703	2.541392	1.904124
C	2.403124	3.180881	2.191648
H	2.892697	2.994266	3.160775
C	2.372770	4.318660	0.051824
H	2.841349	5.019723	-0.656902
C	3.001295	4.056154	1.276604
H	3.958109	4.543756	1.522345
C	1.153036	3.701269	-0.292580
C	0.530579	1.662180	2.973596
H	-0.367371	1.190448	2.524838
C	0.070912	2.506163	4.183826
H	-0.451670	1.869156	4.928615
H	-0.622450	3.319119	3.881966
H	0.932987	2.981937	4.698159
C	1.459943	0.514636	3.411158
H	0.945977	-0.149005	4.137794

H	2.382946	0.890800	3.901104
H	1.754431	-0.095345	2.533140
C	0.476256	4.066635	-1.616869
H	-0.342916	3.333600	-1.777649
C	1.423881	3.973582	-2.831124
H	0.862739	4.160919	-3.770783
H	1.897945	2.975826	-2.908457
H	2.232959	4.732614	-2.779874
C	-0.145707	5.482015	-1.547245
H	-0.704798	5.714244	-2.478456
H	0.643623	6.254444	-1.427802
H	-0.843308	5.597668	-0.691761
C	-3.113706	-0.403138	-0.340648
C	-3.884594	-1.015811	0.691938
C	-4.684507	-2.126789	0.355634
H	-5.280134	-2.620475	1.139969
C	-4.731386	-2.617490	-0.956323
H	-5.357296	-3.491581	-1.197161
C	-3.988170	-1.986868	-1.962368
H	-4.043511	-2.367777	-2.994556
C	-3.177403	-0.865697	-1.685477
C	-3.897442	-0.490089	2.130156
H	-3.092156	0.270706	2.207648
C	-3.591968	-1.583691	3.175074
H	-3.543961	-1.140979	4.192276
H	-2.624829	-2.084296	2.972853
H	-4.381298	-2.364653	3.196113
C	-5.243728	0.197791	2.456993
H	-5.221793	0.646726	3.472675
H	-6.079965	-0.532988	2.431484
H	-5.492955	1.001606	1.733012
C	-2.455925	-0.165206	-2.837472
H	-1.778051	0.593443	-2.395813
C	-1.571594	-1.134179	-3.646756
H	-1.006661	-0.583237	-4.427953
H	-2.172250	-1.913177	-4.162418
H	-0.840350	-1.637247	-2.981794
C	-3.462648	0.568416	-3.752958
H	-2.930228	1.125739	-4.552747
H	-4.085586	1.292967	-3.187548
H	-4.155200	-0.146118	-4.247010
C	1.433694	0.446922	-1.812008
H	2.010683	1.275375	-1.365504
H	0.787983	0.754567	-2.654870
C	1.960060	-0.889874	-1.764210
H	1.603773	-1.584522	-2.553120
Si	3.627591	-1.350978	-1.017965
O	3.460635	-2.697862	-0.012000
Si	2.185594	-3.445507	0.806088
C	0.510150	-2.754509	0.275702
H	0.063695	-3.321603	-0.568487
C	-0.436283	-2.077504	1.121872
H	-0.160781	-1.830203	2.163606
H	-1.515025	-2.250553	0.972440
C	4.370576	0.077463	-0.024795
H	5.298673	-0.256589	0.485408
H	3.665491	0.445671	0.748871
H	4.633730	0.935142	-0.679632
C	4.830800	-1.870063	-2.386854
H	5.798382	-2.206789	-1.957871
H	5.036878	-1.028103	-3.081621
H	4.416486	-2.710558	-2.982665
C	2.253344	-5.281640	0.341897
H	3.248310	-5.713669	0.580204
H	2.076530	-5.424300	-0.745221
H	1.484170	-5.865748	0.890945
C	2.492588	-3.264216	2.665193
H	3.492230	-3.673721	2.922746
H	1.733089	-3.820515	3.254668
H	2.470522	-2.204555	2.990662

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PtIPrICySMe2cis SCF Done: -2676.92880555 A.U.

N	-0.780343	0.556713	1.514656
C	-2.198382	0.711051	1.256372
N	1.351724	0.113266	1.340403
C	-2.655407	1.866114	0.563232
C	-4.046285	1.986154	0.354826
H	-4.430251	2.865338	-0.184742
C	-4.944370	1.020544	0.829585
H	-6.025678	1.141314	0.656046
C	-4.468285	-0.093314	1.534621
H	-5.182808	-0.839774	1.915205
C	-3.088878	-0.277367	1.767452
C	-1.722848	2.993723	0.122701
H	-0.685507	2.603743	0.111461
C	-2.009835	3.485932	-1.308232
H	-1.951356	2.651118	-2.035505
H	-1.246707	4.232829	-1.606615
H	-3.004946	3.972499	-1.397552
C	-1.781469	4.154815	1.142656
H	-2.796928	4.604296	1.187827
H	-1.068573	4.955712	0.854853
H	-1.518532	3.818680	2.167688
C	-2.620825	-1.480208	2.593851
H	-1.520577	-1.567131	2.473146
C	-3.235279	-2.813672	2.121328
H	-4.334936	-2.842682	2.272557
H	-2.805692	-3.658152	2.699950
H	-3.025383	-2.991532	1.047754
C	-2.915256	-1.259834	4.096226
H	-2.453112	-0.328898	4.482823
H	-2.527870	-2.107254	4.700161
H	-4.008270	-1.185843	4.279327
C	0.184117	0.169660	0.602450
C	-0.220013	0.757202	2.777057
H	-0.819519	1.089605	3.628912
C	1.111180	0.469978	2.668683
H	1.912072	0.481932	3.412821
C	2.672955	-0.289299	0.887672
C	3.696267	0.693271	0.793348
C	4.983559	0.253810	0.418027
H	5.794634	0.992318	0.326937
C	5.245753	-1.093159	0.145768
H	6.256994	-1.408430	-0.156826
C	4.221325	-2.042747	0.260361
H	4.442965	-3.100061	0.054151
C	2.917693	-1.670032	0.644186
C	3.477695	2.174325	1.113159
H	2.383648	2.358153	1.105046
C	4.032062	2.528769	2.512980
H	3.582941	1.914823	3.320536
H	3.834071	3.595157	2.751489
H	5.131268	2.373051	2.555860
C	4.094258	3.106840	0.050347
H	5.204657	3.078334	0.066318
H	3.793236	4.156869	0.247909
H	3.746382	2.833620	-0.964675
C	1.843695	-2.738930	0.862957
H	0.866255	-2.282043	0.598905
C	2.019002	-3.976041	-0.036577
H	2.127128	-3.693599	-1.103965
H	1.140437	-4.647311	0.062352

H	2.909382	-4.576699	0.245936
C	1.785879	-3.158671	2.350586
H	2.747858	-3.615038	2.667681
H	0.982629	-3.907558	2.517421
H	1.587481	-2.295750	3.018484
Pt	-0.067915	-0.055811	-1.355129
Cl	1.340579	1.808308	-1.653435
Cl	-0.358739	-0.184818	-3.733848
S	-1.562703	-1.836416	-1.120650
C	-1.041466	-3.135618	-2.303629
H	-0.862750	-2.657501	-3.287742
H	-0.103097	-3.569083	-1.912731
H	-1.833958	-3.909273	-2.342507
C	-3.088772	-1.276217	-1.966603
H	-3.512415	-0.457885	-1.354564
H	-2.806901	-0.906092	-2.972592
H	-3.797030	-2.127501	-2.012985

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PtIPrICySMe2trans SCF Done: -2676.93610480 A.U.

N	-1.037095	1.102779	1.151164
C	-2.443624	0.947603	0.818040
N	1.141098	0.947646	1.208662
C	-2.995483	1.760880	-0.210088
C	-4.371096	1.612288	-0.483342
H	-4.828159	2.220255	-1.278482
C	-5.165264	0.713061	0.240643
H	-6.237730	0.614842	0.007470
C	-4.599058	-0.055336	1.265675
H	-5.233529	-0.751988	1.834454
C	-3.228269	0.042103	1.584116
C	-2.174114	2.814761	-0.953279
H	-1.112629	2.492937	-0.933836
C	-2.554253	2.946573	-2.439292
H	-2.510105	1.966311	-2.953592
H	-1.838370	3.621984	-2.950737
H	-3.569050	3.377294	-2.579263
C	-2.280065	4.182613	-0.238910
H	-3.328401	4.551473	-0.236176
H	-1.654192	4.940668	-0.755545
H	-1.941494	4.129639	0.816341
C	-2.661568	-0.766096	2.753664
H	-1.561022	-0.818016	2.620937
C	-3.174772	-2.218715	2.785617
H	-4.259943	-2.273685	3.016835
H	-2.645210	-2.788952	3.577088
H	-2.986859	-2.725420	1.819044
C	-2.956955	-0.061681	4.098722
H	-2.545898	0.967669	4.134816
H	-2.514200	-0.631214	4.943081
H	-4.051351	0.011104	4.276182
C	0.031274	0.493401	0.530896
C	-0.596540	1.923968	2.190318
H	-1.294557	2.503936	2.800366
C	0.766535	1.822358	2.229958
H	1.505311	2.287251	2.888620
C	2.527138	0.592058	0.951755
C	3.331014	1.484625	0.191081
C	4.682216	1.129695	-0.005373
H	5.329977	1.794176	-0.597102
C	5.212065	-0.049377	0.533250
H	6.269484	-0.306712	0.360641
C	4.400941	-0.898429	1.298111
H	4.830724	-1.815665	1.727960
C	3.043633	-0.598302	1.534958
C	2.808464	2.814304	-0.356900
H	1.702081	2.743698	-0.403190
C	3.185912	3.979752	0.587490
H	2.798033	3.832538	1.616090
H	2.775058	4.938616	0.206599
H	4.289140	4.089655	0.661230
C	3.293948	3.106075	-1.789912
H	4.387991	3.294947	-1.830787
H	2.792712	4.016502	-2.179587
H	3.047416	2.266783	-2.469007
C	2.206773	-1.494372	2.449246
H	1.142192	-1.370225	2.162949
C	2.523128	-2.992561	2.290365
H	2.445390	-3.309177	1.231602
H	1.795398	-3.594000	2.872700
H	3.536620	-3.251883	2.664835
C	2.365419	-1.057938	3.924756
H	3.419127	-1.165766	4.260902
H	1.731224	-1.684589	4.586947
H	2.071228	0.000300	4.080361
Pt	-0.021795	-0.750769	-1.013056
Cl	0.540934	0.996887	-2.503779
Cl	-0.582854	-2.595157	0.375169
S	-0.070220	-2.186056	-2.959217
C	-1.682358	-3.048892	-2.882768
H	-1.831819	-3.458088	-1.864039
H	-2.456774	-2.289233	-3.100965
H	-1.706099	-3.842544	-3.655566
C	1.043835	-3.579568	-2.551750
H	2.070009	-3.165924	-2.531850
H	0.778598	-3.982588	-1.554431
H	0.964532	-4.351472	-3.342706

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PtIPrICytrans SCF Done: -2199.02270877 A.U.

N	1.098473	-0.048872	1.160182
C	2.494515	-0.110221	0.758317
N	-1.098459	0.048933	1.160199
C	3.077058	-1.384964	0.519264
C	4.442754	-1.412722	0.169747
H	4.925614	-2.380837	-0.030948
C	5.194167	-0.233882	0.074223
H	6.258955	-0.282127	-0.204409
C	4.595782	1.005421	0.335208
H	5.197435	1.923995	0.262241
C	3.233350	1.101974	0.686630
C	2.301553	-2.691730	0.693777
H	1.222928	-2.463488	0.567920
C	2.650813	-3.751108	-0.368015
H	2.524841	-3.350205	-1.392860
H	1.974256	-4.624223	-0.264651
H	3.689699	-4.128603	-0.257343
C	2.509564	-3.255818	2.119058
H	3.578263	-3.502441	2.296392
H	1.918474	-4.185100	2.260881
H	2.199008	-2.535340	2.903598
C	2.627517	2.464890	1.027794
H	1.524894	2.374070	0.938133
C	3.062742	3.577829	0.055159
H	4.145311	3.809721	0.144140
H	2.510663	4.513592	0.281488
H	2.841013	3.299693	-0.993643
C	2.959543	2.857076	2.486793
H	2.601579	2.102612	3.217057
H	2.488885	3.828676	2.746638
H	4.056262	2.962879	2.628917
C	-0.000001	0.000011	0.331493
C	0.683175	-0.031964	2.493135
H	1.403636	-0.067889	3.314996

C	-0.683139	0.032080	2.493145
H	-1.403585	0.068035	3.315018
C	-2.494507	0.110248	0.758347
C	-3.233312	-1.101967	0.686669
C	-4.595742	-1.005452	0.335235
H	-5.197372	-1.924041	0.262273
C	-5.194154	0.233835	0.074229
H	-6.258941	0.282050	-0.204413
C	-4.442770	1.412694	0.169744
H	-4.925652	2.380794	-0.030971
C	-3.077076	1.384973	0.519269
C	-2.627445	-2.464860	1.027861
H	-1.524825	-2.374018	0.938182
C	-2.959444	-2.857012	2.486875
H	-2.601485	-2.102524	3.217116
H	-2.488765	-3.828598	2.746740
H	-4.056160	-2.962833	2.629013
C	-3.062660	-3.577838	0.055268
H	-4.145224	-3.809744	0.144267
H	-2.510565	-4.513584	0.281627
H	-2.840945	-3.299741	-0.993548
C	-2.301592	2.691756	0.693750
H	-1.222963	2.463521	0.567919
C	-2.650843	3.751090	-0.368088
H	-2.524854	3.350147	-1.392916
H	-1.974292	4.624212	-0.264750
H	-3.689732	4.128585	-0.257446
C	-2.509637	3.255897	2.119006
H	-3.578342	3.502512	2.296309
H	-1.918563	4.185192	2.260802
H	-2.199086	2.535456	2.903579
Pt	-0.000019	-0.000022	-1.569626
Cl	-0.324313	-2.270039	-1.919219
Cl	0.324297	2.270007	-1.919165

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PtIPrIDDCl2SMe2cis SCF Done: -2684.15070333 A.U.

Cl	-0.053328	-1.353705	-2.001250
N	-1.066183	-1.502554	1.503773
N	1.111379	-1.368351	1.619841
C	0.018339	-0.848412	0.968119
C	-0.652017	-2.416911	2.467330
C	0.711714	-2.327705	2.546044
C	-2.458225	-1.403423	0.995605
C	-3.460260	-1.177023	2.150048
C	-3.590595	0.277200	2.644945
C	-4.328289	1.211065	1.662785
C	-5.835179	0.929379	1.501290
C	-6.479946	1.595035	0.266334
C	-5.993366	1.044364	-1.091189
C	-6.418717	-0.410304	-1.389354
C	-5.486675	-1.160085	-2.365683
C	-4.087747	-1.480186	-1.798409
C	-4.088826	-2.542803	-0.681684
C	-2.779486	-2.644492	0.125211
C	2.527872	-1.015367	1.356895
C	3.323265	-2.262749	0.904003
C	3.106198	-2.685245	-0.563029
C	3.783233	-1.752191	-1.587100
C	5.322547	-1.845029	-1.616686
C	6.034485	-0.634753	-2.257818
C	5.895533	0.685311	-1.470291
C	6.603758	0.697689	-0.099050
C	6.062263	1.751661	0.889830
C	4.639179	1.458719	1.412056
C	4.548326	0.274006	2.394335
C	3.133477	-0.306218	2.595515
H	-2.428636	-0.511987	0.332204
H	-4.454345	-1.533515	1.808969
H	-3.197465	-1.843416	2.999999
H	-4.124840	0.278433	3.621347
H	-2.576287	0.684317	2.855911
H	-4.196791	2.265888	1.992793
H	-3.831542	1.146287	0.668804
H	-6.008169	-0.168803	1.447337
H	-6.366574	1.261760	2.420902
H	-7.585600	1.480773	0.332817
H	-6.288388	2.691527	0.304459
H	-6.360398	1.706056	-1.906153
H	-4.884838	1.126270	-1.138245
H	-6.479399	-0.986751	-0.438744
H	-7.456282	-0.412760	-1.790780
H	-5.978247	-2.107773	-2.683201
H	-5.369616	-0.555729	-3.292942
H	-3.416586	-1.816745	-2.616670
H	-3.620296	-0.539111	-1.433929
H	-4.940341	-2.362813	0.013112
H	-4.295636	-3.539133	-1.131757
H	-1.925663	-2.786016	-0.571703
H	-2.821163	-3.541482	0.784607
H	2.463940	-0.294026	0.513397
H	4.402005	-2.057882	1.068966
H	3.084298	-3.106731	1.587982
H	3.495385	-3.720004	-0.693638
H	2.017782	-2.727409	-0.783816
H	3.377195	-1.970088	-2.597863
H	3.461006	-0.706215	-1.385493
H	5.713551	-1.982716	-0.582305
H	5.619683	-2.771349	-2.157133
H	7.115191	-0.873401	-2.383690
H	5.635713	-0.482514	-3.285687
H	6.285467	1.524650	-2.087563
H	4.812983	0.906039	-1.339181
H	6.528134	-0.307872	0.372389
H	7.693654	0.861340	-0.250634
H	6.756627	1.839131	1.756067
H	6.067686	2.749394	0.396248
H	4.234802	2.367668	1.910687
H	3.974506	1.275579	0.538684
H	5.231511	-0.538371	2.063551
H	4.941037	0.593328	3.384757
H	2.436130	0.504801	2.903668
H	3.159609	-1.027499	3.443358
S	0.036951	2.311984	0.944117
Cl	-0.031394	2.006379	-2.373267
Pt	-0.000748	0.483904	-0.515973
C	-1.364028	3.382423	0.440472
H	-1.307496	3.529137	-0.656986
H	-2.294486	2.850771	0.708831
H	-1.292778	4.336194	1.000330
C	1.401212	3.393605	0.369475
H	1.294301	3.530307	-0.725582
H	1.344378	4.351120	0.924592
H	2.348430	2.874493	0.601266
H	-1.349863	-3.057401	3.014387
H	1.419463	-2.866505	3.182826

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PtIPrIDDCl2SMe2trans SCF Done: -2684.15909078 A.U.

Cl	0.188319	-0.006588	-2.456825
N	1.094080	2.250240	0.338839
N	-1.081441	2.215615	0.513520
C	0.005888	1.423978	0.260725
C	0.689705	3.548651	0.634107

C	-0.676108	3.526022	0.748623
C	2.493039	1.832952	0.083338
C	3.385318	2.133397	1.307706
C	3.233835	1.142957	2.480777
C	3.815481	-0.257992	2.202133
C	5.353085	-0.313423	2.099085
C	5.906134	-1.571997	1.396289
C	5.582020	-1.661002	-0.110454
C	6.291097	-0.608354	-0.988627
C	5.598041	-0.329909	-2.339940
C	4.234493	0.384013	-2.226986
C	4.323161	1.850091	-1.756362
C	2.997430	2.448464	-1.244225
C	-2.483042	1.737349	0.566931
C	-3.353478	2.480404	-0.470725
C	-3.177669	2.003660	-1.927559
C	-3.766483	0.606307	-2.208252
C	-5.306369	0.532910	-2.170781
C	-5.879675	-0.890579	-2.001549
C	-5.591393	-1.540171	-0.631280
C	-6.312411	-0.880745	0.563297
C	-5.651050	-1.142146	1.933651
C	-4.281015	-0.457277	2.125057
C	-4.351981	1.078667	2.245385
C	-3.014074	1.811229	2.018990
H	2.408732	0.733581	-0.052580
H	4.441627	2.142090	0.965213
H	3.188066	3.171465	1.655811
H	3.728432	1.576101	3.379110
H	2.157497	1.037505	2.738705
H	3.473932	-0.954551	2.998283
H	3.353854	-0.651640	1.269438
H	5.729208	0.587373	1.563296
H	5.789110	-0.241850	3.120494
H	7.010565	-1.610585	1.534547
H	5.506744	-2.476959	1.907910
H	5.838555	-2.677407	-0.483486
H	4.480662	-1.572450	-0.243370
H	6.378797	0.348619	-0.427019
H	7.340299	-0.931404	-1.169829
H	6.277784	0.278092	-2.979366
H	5.457412	-1.292526	-2.881519
H	3.711287	0.350421	-3.206452
H	3.575396	-0.195874	-1.544416
H	5.099311	1.947834	-0.964618
H	4.691423	2.479387	-2.596542
H	2.203187	2.293715	-2.006139
H	3.115881	3.548386	-1.114185
H	-2.397104	0.667746	0.278655
H	-4.416132	2.364056	-0.169775
H	-3.151726	3.572069	-0.397576
H	-3.654025	2.747697	-2.604890
H	-2.096694	1.992522	-2.187065
H	-3.403078	0.254627	-3.197864
H	-3.328693	-0.113761	-1.481470
H	-5.696590	1.174456	-1.348178
H	-5.714835	0.983681	-3.102684
H	-6.980677	-0.862381	-2.167313
H	-5.469888	-1.543362	-2.805150
H	-5.863737	-2.618381	-0.669685
H	-4.492575	-1.523842	-0.455839
H	-6.376376	0.218452	0.400522
H	-7.368911	-1.228690	0.589535
H	-6.341692	-0.810147	2.741931
H	-5.529593	-2.239990	2.074993
H	-3.779599	-0.866744	3.028322
H	-3.612053	-0.741555	1.283484
H	-5.111967	1.478640	1.537747
H	-4.733055	1.346331	3.255641
H	-2.236522	1.375854	2.683284
H	-3.128026	2.879999	2.311204
S	0.006360	-2.868030	-0.743029
Cl	-0.180838	-1.038470	2.162678
Pt	0.003112	-0.519392	-0.151778
C	-1.445167	-3.582819	0.112298
H	-1.445716	-3.254018	1.170553
H	-2.342670	-3.194509	-0.405281
H	-1.411542	-4.686791	0.023659
C	1.337536	-3.609698	0.270999
H	1.224672	-3.281445	1.323253
H	1.293401	-4.712953	0.177658
H	2.295141	-3.238895	-0.140865
H	1.395542	4.378168	0.736796
H	-1.381264	4.330299	0.978337

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PtIPrIDDCl2trans SCF Done: -2206.24578551 A.U.

Cl	0.124674	2.308400	-1.017927
N	1.095139	0.092799	1.952836
N	-1.095145	-0.094298	1.952866
C	-0.000037	-0.000509	1.137847
C	0.682791	0.059830	3.281858
C	-0.682690	-0.062207	3.281874
C	2.496548	0.260930	1.490824
C	3.392310	-0.868833	2.042473
C	3.237875	-2.230398	1.333398
C	3.785984	-2.260546	-0.107980
C	5.320644	-2.158764	-0.219689
C	5.834959	-1.732175	-1.611631
C	5.496626	-0.277783	-2.002812
C	6.229495	0.799236	-1.175325
C	5.546277	2.183610	-1.174166
C	4.195658	2.233184	-0.429026
C	4.308758	2.071906	1.100958
C	2.994532	1.690491	1.812299
C	-2.496611	-0.261920	1.490833
C	-3.392101	0.867744	2.043104
C	-3.237313	2.229642	1.334715
C	-3.785298	2.260661	-0.106687
C	-5.319989	2.159282	-0.218592
C	-5.834253	1.733467	-1.610786
C	-5.496150	0.279209	-2.002675
C	-6.229379	-0.798104	-1.175895
C	-5.546456	-2.182624	-1.175430
C	-4.195944	-2.232871	-0.430141
C	-4.309146	-2.072309	1.099906
C	-2.994856	-1.691574	1.811506
H	2.414810	0.160203	0.387553
H	4.446371	-0.529331	1.962316
H	3.209136	-0.980697	3.134273
H	3.755219	-3.005476	1.942220
H	2.164220	-2.519053	1.315959
H	3.441169	-3.193228	-0.604048
H	3.303470	-1.444825	-0.690766
H	5.710436	-1.442377	0.538897
H	5.771156	-3.138683	0.054724
H	6.938995	-1.873548	-1.650015
H	5.414996	-2.420999	-2.378786
H	5.723971	-0.124505	-3.080903
H	4.396875	-0.131911	-1.919167
H	6.339729	0.452640	-0.123013
H	7.271382	0.902809	-1.551856
H	6.238955	2.932117	-0.726271

H	5.387660	2.511687	-2.225965
H	3.679731	3.191292	-0.653804
H	3.523084	1.452925	-0.847852
H	5.088397	1.316800	1.346190
H	4.682661	3.022324	1.541389
H	2.194362	2.402862	1.515784
H	3.126239	1.791629	2.913698
H	-2.414900	-0.160600	0.387615
H	-4.446248	0.528551	1.962775
H	-3.208901	0.979013	3.134960
H	-3.754511	3.004541	1.943898
H	-2.163581	2.518033	1.317513
H	-3.440241	3.193521	-0.602243
H	-3.302922	1.445152	-0.689878
H	-5.710012	1.442630	0.539619
H	-5.770291	3.139178	0.056238
H	-6.938259	1.875060	-1.649210
H	-5.414095	2.422603	-2.377559
H	-5.723329	0.126555	-3.080891
H	-4.396444	0.133057	-1.918903
H	-6.339629	-0.452070	-0.123401
H	-7.271254	-0.901215	-1.552577
H	-6.239348	-2.931261	-0.728087
H	-5.387728	-2.510121	-2.227395
H	-3.680195	-3.190978	-0.655334
H	-3.523157	-1.452552	-0.848520
H	-5.088580	-1.317089	1.345418
H	-4.683358	-3.022822	1.539857
H	-2.194819	-2.403918	1.514560
H	-3.126571	-1.793341	2.912844
Cl	-0.125078	-2.307967	-1.019379
Pt	-0.000145	0.000128	-0.772599
H	1.388099	0.127353	4.115267
H	-1.387931	-0.130261	4.115297

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PtIPrSTARCl2SMe2cis SCF Done: -4288.29344948 A.U.

Pt	-0.139990	0.194224	-2.130649
Cl	2.108787	-0.479374	-2.335362
Cl	-0.289594	0.295192	-4.530481
N	-0.710158	-0.757446	0.693106
N	0.936558	0.686718	0.689211
C	0.035847	0.050976	-0.148517
C	-0.275942	-0.626684	2.015173
C	0.732370	0.289935	2.013699
C	-1.800250	-1.638209	0.319478
C	-1.527293	-2.823095	-0.425523
C	-2.610608	-3.660078	-0.754926
C	-3.933015	-3.381262	-0.357105
C	-4.158713	-2.226800	0.412547
C	-3.118626	-1.346816	0.778408
C	-0.099071	-3.238624	-0.807641
C	0.680611	-3.836344	0.370796
C	0.056755	-4.452571	1.475874
C	0.822123	-5.055219	2.492628
C	2.224729	-5.053548	2.418431
C	2.858809	-4.435330	1.323460
C	2.093760	-3.829565	0.313945
C	-0.060579	-4.158896	-2.039279
C	-0.094948	-3.585250	-3.330054
C	-0.088850	-4.398499	-4.475689
C	-0.048548	-5.799033	-4.352633
C	-0.006976	-6.379616	-3.073398
C	-0.009387	-5.565394	-1.926097
C	-5.066699	-4.300141	-0.752577
C	-3.435436	-0.160803	1.708245
C	-3.195205	-0.491544	3.191635
C	-3.336314	-1.794953	3.713355
C	-3.146978	-2.046223	5.085992
C	-2.812947	-0.997546	5.958465
C	-2.669692	0.306242	5.448183
C	-2.859961	0.555313	4.080036
C	-4.853897	0.406931	1.501060
C	-5.099522	1.308920	0.441862
C	-6.381182	1.840457	0.222325
C	-7.450688	1.477337	1.060125
C	-7.221079	0.583038	2.118686
C	-5.934902	0.057448	2.339727
C	2.010525	1.602180	0.338023
C	1.703221	2.894814	-0.163153
C	2.764944	3.773248	-0.451351
C	4.110689	3.415722	-0.255346
C	4.378596	2.138411	0.267840
C	3.360705	1.217585	0.583006
C	0.256850	3.372487	-0.340835
C	-0.397776	3.793661	0.978859
C	0.342516	4.318845	2.059524
C	-0.300589	4.744562	3.236475
C	-1.697856	4.654369	3.354754
C	-2.448929	4.129905	2.286321
C	-1.801721	3.702501	1.114950
C	0.131865	4.436461	-1.444405
C	-0.223082	5.775857	-1.182091
C	-0.309460	6.714550	-2.228521
C	-0.043520	6.327350	-3.551967
C	0.310477	4.992257	-3.824735
C	0.398200	4.056639	-2.781943
C	5.231489	4.358623	-0.628312
C	3.754499	-0.127479	1.217760
C	3.753170	-0.082789	2.755179
C	3.502942	-1.272834	3.476147
C	3.527233	-1.285927	4.879630
C	3.804569	-0.106578	5.595883
C	4.056079	1.082478	4.891954
C	4.030305	1.093730	3.483969
C	5.097271	-0.664353	0.679692
C	6.285873	-0.631584	1.440542
C	7.494940	-1.120428	0.910926
C	7.535337	-1.656042	-0.386610
C	6.355706	-1.696974	-1.152222
C	5.150770	-1.205785	-0.624685
H	-0.721083	-1.201774	2.829694
H	1.330309	0.695515	2.832675
H	-2.404358	-4.567053	-1.344018
H	-5.182976	-1.991716	0.741186
H	0.443548	-2.319033	-1.113735
H	-1.042787	-4.469453	1.541450
H	0.314657	-5.534714	3.345398
H	2.823918	-5.532682	3.209179
H	3.958190	-4.424163	1.252651
H	2.592985	-3.351328	-0.544305
H	-0.110435	-2.488068	-3.441457
H	-0.103840	-3.926837	-5.471199
H	-0.038368	-6.436150	-5.251684
H	0.036312	-7.475487	-2.964121
H	0.041505	-6.030710	-0.928768
H	-5.244536	-4.265405	-1.849174
H	-6.014317	-4.024731	-0.248985
H	-4.836308	-5.356997	-0.502608
H	-2.731260	0.658779	1.449895
H	-3.589834	-2.627947	3.038843
H	-3.259619	-3.072017	5.472261
H	-2.659981	-1.194408	7.031448

H	-2.400533	1.136362	6.120742
H	-2.735402	1.577850	3.687644
H	-4.266578	1.582387	-0.224965
H	-6.544874	2.547998	-0.606619
H	-8.456097	1.895001	0.892071
H	-8.047864	0.294999	2.787726
H	-5.768415	-0.625920	3.186674
H	2.524822	4.770622	-0.851079
H	5.424142	1.830432	0.425782
H	-0.313862	2.494670	-0.718547
H	1.438001	4.396615	1.977238
H	0.298153	5.152384	4.066857
H	-2.201436	4.991953	4.274620
H	-3.545362	4.052634	2.363000
H	-2.399078	3.299807	0.280367
H	-0.436017	6.091931	-0.149148
H	-0.587775	7.756622	-2.002294
H	-0.112184	7.062091	-4.370171
H	0.518869	4.671262	-4.857821
H	0.677576	3.012089	-3.004855
H	4.925658	5.419829	-0.528947
H	5.535573	4.204603	-1.687119
H	6.132643	4.193797	-0.003775
H	2.985611	-0.870293	0.915603
H	3.276720	-2.199704	2.924552
H	3.322611	-2.224960	5.418643
H	3.821384	-0.115355	6.697438
H	4.273976	2.013597	5.439725
H	4.223310	2.034536	2.945088
H	6.269322	-0.226674	2.464062
H	8.410280	-1.084644	1.523719
H	8.480835	-2.042532	-0.799812
H	6.370401	-2.115066	-2.171597
H	4.232566	-1.225593	-1.233254
S	-2.400952	0.771368	-2.016174
C	-2.667521	2.200267	-3.131710
H	-2.199721	1.970996	-4.109756
H	-3.759441	2.370543	-3.214228
H	-2.172677	3.077207	-2.673787
C	-3.276822	-0.511766	-2.983639
H	-4.345409	-0.226678	-3.049890
H	-2.795918	-0.582338	-3.979264
H	-3.167287	-1.462980	-2.430348

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PtIPrSTARCl2SMe2trans SCF Done: -4288.29533517 A.U.

Pt	-0.022931	0.057101	-2.126570
Cl	-2.169530	1.047244	-2.115279
Cl	2.094242	-0.998930	-2.257969
N	0.701339	0.764718	0.712953
N	-0.839296	-0.792675	0.687692
C	-0.050876	-0.020057	-0.138122
C	0.373916	0.488065	2.042928
C	-0.570877	-0.496189	2.027800
C	1.757052	1.689591	0.332766
C	1.430088	2.948889	-0.246148
C	2.491790	3.784886	-0.643898
C	3.842590	3.435192	-0.461095
C	4.124422	2.220651	0.187187
C	3.109909	1.337613	0.606105
C	-0.020357	3.444248	-0.361648
C	-0.621707	3.862672	0.988689
C	0.161444	4.229763	2.102846
C	-0.442457	4.686130	3.290410
C	-1.840163	4.788246	3.380668
C	-2.632664	4.419930	2.276339
C	-2.028939	3.957081	1.096334
C	-0.189368	4.570497	-1.395356
C	-0.484990	4.251430	-2.738879
C	-0.618142	5.261319	-3.707722
C	-0.456168	6.611718	-3.351696
C	-0.172357	6.943070	-2.015374
C	-0.045955	5.931960	-1.046445
C	4.952764	4.335064	-0.954251
C	3.500405	0.094199	1.422880
C	3.402536	0.351034	2.936787
C	3.647792	1.618527	3.507534
C	3.588739	1.806859	4.901599
C	3.281658	0.730043	5.749768
C	3.036182	-0.538238	5.191864
C	3.097452	-0.724320	3.801553
C	4.884659	-0.466516	1.037502
C	5.040740	-1.120216	-0.206076
C	6.284608	-1.642722	-0.594672
C	7.402417	-1.521032	0.251186
C	7.260213	-0.872177	1.488239
C	6.011812	-0.351937	1.879131
C	-1.838472	-1.775611	0.300155
C	-1.423606	-3.040158	-0.202609
C	-2.418108	-3.984088	-0.526133
C	-3.790072	-3.725286	-0.356791
C	-4.161120	-2.479310	0.177666
C	-3.216692	-1.492399	0.523179
C	0.055911	-3.431369	-0.330282
C	0.697378	-3.812922	1.009615
C	-0.048148	-4.277387	2.113320
C	0.595123	-4.694805	3.294135
C	1.996233	-4.660003	3.388289
C	2.751213	-4.193275	2.295157
C	2.106615	-3.769131	1.121797
C	0.270693	-4.522531	-1.393423
C	0.542449	-5.867345	-1.066240
C	0.702299	-6.836425	-2.074789
C	0.595816	-6.475676	-3.427713
C	0.327710	-5.135966	-3.765278
C	0.167630	-4.171781	-2.758150
C	-4.831389	-4.744942	-0.758322
C	-3.709767	-0.199134	1.193999
C	-3.624670	-0.279310	2.726398
C	-3.335476	0.887223	3.468553
C	-3.285451	0.857732	4.871742
C	-3.525516	-0.342801	5.564798
C	-3.817002	-1.510191	4.838832
C	-3.866383	-1.477760	3.432571
C	-5.122533	0.211904	0.724065
C	-6.223894	0.285164	1.603112
C	-7.495706	0.671363	1.138089
C	-7.688499	0.994066	-0.214168
C	-6.597108	0.924522	-1.099919
C	-5.330246	0.537015	-0.636842
H	0.844650	1.017706	2.873859
H	-1.078549	-1.015712	2.843191
H	2.248739	4.750900	-1.111256
H	5.172154	1.936405	0.372141
H	-0.636239	2.599260	-0.736411
H	1.259307	4.164143	2.041623
H	0.188659	4.969740	4.148158
H	-2.312592	5.155445	4.305795
H	-3.730497	4.495697	2.333588
H	-2.652772	3.674609	0.232616
H	-0.645819	3.196864	-3.012863
H	-0.863860	4.989331	-4.747084
H	-0.563858	7.404037	-4.109792

H	-0.056489	7.998592	-1.720347
H	0.157673	6.205657	0.001111
H	5.202004	4.107519	-2.014295
H	5.882761	4.200852	-0.365853
H	4.663065	5.404693	-0.912142
H	2.767457	-0.706535	1.185347
H	3.885419	2.472720	2.854241
H	3.783472	2.805596	5.324722
H	3.230556	0.877756	6.840324
H	2.788595	-1.391073	5.844152
H	2.896089	-1.719930	3.374683
H	4.171697	-1.203505	-0.878430
H	6.379421	-2.151204	-1.567792
H	8.378368	-1.932567	-0.052531
H	8.125841	-0.770851	2.162780
H	5.916037	0.143701	2.857144
H	-2.101297	-4.960059	-0.924514
H	-5.228262	-2.253096	0.328333
H	0.608956	-2.544579	-0.708534
H	-1.146748	-4.320458	2.046974
H	-0.006694	-5.056234	4.143676
H	2.500378	-4.995701	4.308626
H	3.850785	-4.158410	2.354752
H	2.703155	-3.412384	0.266383
H	0.635571	-6.162921	-0.009772
H	0.915049	-7.881289	-1.796451
H	0.724949	-7.233088	-4.217399
H	0.248382	-4.840794	-4.824271
H	-0.038654	-3.121833	-3.018098
H	-4.451703	-5.781585	-0.654556
H	-5.123171	-4.609993	-1.823283
H	-5.755680	-4.648285	-0.153659
H	-3.028076	0.617505	0.870378
H	-3.132424	1.830652	2.936985
H	-3.048772	1.780037	5.426075
H	-3.482358	-0.368484	6.665392
H	-4.007016	-2.457562	5.368824
H	-4.091429	-2.401131	2.876059
H	-6.091711	0.041944	2.667969
H	-8.339625	0.720968	1.845182
H	-8.682845	1.299389	-0.577791
H	-6.731055	1.176986	-2.164269
H	-4.481541	0.479727	-1.336851
S	-0.024345	0.378813	-4.531832
C	0.316350	-1.240839	-5.310495
H	-0.596787	-1.852479	-5.181980
H	0.510049	-1.086339	-6.390390
H	1.178357	-1.722540	-4.808077
C	1.568925	1.214859	-4.867897
H	1.704745	1.303510	-5.963904
H	1.500484	2.221532	-4.413616
H	2.391496	0.644541	-4.393294

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PtIPrSTARCl2trans SCF Done: -3810.38399847 A.U.

Pt	-0.000165	0.000333	-2.247366
Cl	-2.179190	0.707792	-2.607681
Cl	2.178910	-0.706930	-2.607944
N	0.801410	0.758159	0.493818
N	-0.801533	-0.758144	0.493711
C	-0.000072	0.000080	-0.334303
C	0.487166	0.477164	1.826727
C	-0.487277	-0.477357	1.826659
C	1.863357	1.677201	0.117935
C	1.540008	2.916900	-0.499435
C	2.597545	3.786201	-0.826151
C	3.943260	3.474259	-0.556234
C	4.220196	2.253990	0.084400
C	3.208016	1.341598	0.442160
C	0.089423	3.345501	-0.763036
C	-0.639453	3.814360	0.501494
C	0.033529	4.362347	1.613880
C	-0.684260	4.844709	2.724746
C	-2.087977	4.789585	2.739677
C	-2.770705	4.240349	1.637509
C	-2.052021	3.754629	0.532919
C	-0.018034	4.365745	-1.908371
C	0.120071	3.913704	-3.240243
C	0.051997	4.811197	-4.317100
C	-0.155413	6.183096	-4.082266
C	-0.295780	6.644331	-2.763028
C	-0.229445	5.742250	-1.684563
C	5.054813	4.410608	-0.970931
C	3.592775	0.068140	1.214124
C	3.500168	0.252664	2.738105
C	3.721233	1.495759	3.368701
C	3.661837	1.614803	4.770542
C	3.379691	0.491833	5.565699
C	3.158103	-0.752927	4.947572
C	3.218706	-0.869906	3.549910
C	4.970789	-0.482841	0.795015
C	5.106635	-1.109355	-0.464670
C	6.345339	-1.618937	-0.885686
C	7.476648	-1.510810	-0.056175
C	7.354023	-0.889403	1.197078
C	6.111004	-0.382171	1.620404
C	-1.863353	-1.677240	0.117621
C	-1.539846	-2.916822	-0.499895
C	-2.597307	-3.786136	-0.826843
C	-3.943065	-3.474344	-0.556996
C	-4.220156	-2.254205	0.083831
C	-3.208074	-1.341801	0.441798
C	-0.089200	-3.345290	-0.763385
C	0.639598	-3.814181	0.501183
C	-0.033423	-4.361931	1.613647
C	0.684333	-4.844310	2.724534
C	2.088056	-4.789432	2.739408
C	2.770831	-4.240411	1.637153
C	2.052183	-3.754682	0.532547
C	0.018479	-4.365490	-1.908741
C	0.229162	-5.742109	-1.684796
C	0.295694	-6.644223	-2.763199
C	0.156270	-6.182929	-4.082537
C	-0.050396	-4.810958	-4.317490
C	-0.118682	-3.913407	-3.240665
C	-5.054505	-4.410713	-0.971946
C	-3.592961	-0.068464	1.213932
C	-3.500241	-0.253086	2.737882
C	-3.219077	0.869462	3.549796
C	-3.158423	0.752349	4.947452
C	-3.379666	-0.492529	5.565445
C	-3.661517	-1.615499	4.770169
C	-3.720961	-1.496322	3.368351
C	-4.971087	0.482354	0.795000
C	-6.111304	0.381075	1.620324
C	-7.354444	0.888126	1.197154
C	-7.477210	1.509968	-0.055877
C	-6.345913	1.618709	-0.885311
C	-5.107080	1.109300	-0.464448
H	0.994968	0.984085	2.650231
H	-0.995167	-0.984304	2.650092
H	2.353921	4.741154	-1.316596
H	5.264984	1.986133	0.306977

H	-0.453823	2.447828	-1.129266
H	1.133672	4.418565	1.609564
H	-0.139212	5.271901	3.582040
H	-2.650264	5.174387	3.605475
H	-3.871267	4.189915	1.635167
H	-2.591638	3.333572	-0.331147
H	0.280851	2.838717	-3.426431
H	0.155724	4.435253	-5.347580
H	-0.212722	6.888536	-4.926649
H	-0.463655	7.715691	-2.566900
H	-0.351443	6.114559	-0.655385
H	5.333823	4.239467	-2.033939
H	5.969372	4.258326	-0.363533
H	4.749123	5.473167	-0.884311
H	2.856369	-0.719587	0.945535
H	3.937722	2.385558	2.756976
H	3.836551	2.595680	5.241377
H	3.329212	0.585215	6.662223
H	2.930307	-1.640971	5.558747
H	3.035704	-1.847406	3.074642
H	4.228489	-1.182670	-1.126238
H	6.425446	-2.104948	-1.871363
H	8.448576	-1.911774	-0.385565
H	8.230921	-0.799938	1.858525
H	6.029257	0.091219	2.610823
H	-2.353597	-4.741012	-1.317391
H	-5.264978	-1.986471	0.306383
H	0.454009	-2.447540	-1.129475
H	-1.133578	-4.417978	1.609392
H	0.139229	-5.271315	3.581885
H	2.650310	-5.174244	3.605221
H	3.871399	-4.190126	1.634759
H	2.591874	-3.333793	-0.331554
H	0.350436	-6.114434	-0.655539
H	0.462997	-7.715658	-2.566991
H	0.213745	-6.888417	-4.926868
H	-0.153371	-4.434944	-5.348020
H	-0.278868	-2.838365	-3.427010
H	-4.748567	-5.473250	-0.885968
H	-5.333790	-4.239046	-2.034797
H	-5.968967	-4.258949	-0.364272
H	-2.856680	0.719375	0.945336
H	-3.036338	1.847067	3.074640
H	-2.930854	1.640391	5.558714
H	-3.329153	-0.586015	6.661959
H	-3.835963	-2.596468	5.240914
H	-3.937205	-2.386107	2.756519
H	-6.029462	-0.092639	2.610581
H	-8.231330	0.798197	1.858553
H	-8.449241	1.910793	-0.385131
H	-6.426108	2.105060	-1.870813
H	-4.228941	1.183092	-1.125973

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PtIPrSTAROMeCl2SMe2cisDOWN SCF Done: -4438.60341322 A.U.

Pt	0.128356	-0.176328	-2.108810
Cl	-1.812355	1.147875	-2.305763
Cl	0.291275	-0.232845	-4.510374
N	0.902996	0.471196	0.750065
N	-1.090436	-0.437498	0.684487
C	-0.032249	-0.057996	-0.123878
C	0.429587	0.423695	2.064358
C	-0.798993	-0.164865	2.024156
C	2.203693	1.014563	0.413159
C	2.296176	2.252521	-0.281828
C	3.574447	2.765682	-0.586429
C	4.742920	2.088381	-0.190811
C	4.633889	0.884737	0.534890
C	3.383301	0.337694	0.859915
C	1.054313	3.078034	-0.652023
C	0.465345	3.834523	0.545697
C	1.221833	4.190880	1.681810
C	0.650361	4.953128	2.718685
C	-0.686940	5.374140	2.633858
C	-1.454041	5.018203	1.507772
C	-0.884132	4.252415	0.478127
C	1.301260	4.012963	-1.847689
C	1.189788	3.500151	-3.159662
C	1.438237	4.320628	-4.272767
C	1.803205	5.667547	-4.095860
C	1.910324	6.189608	-2.795317
C	1.657699	5.369259	-1.680379
C	3.331796	-0.925830	1.739086
C	3.171603	-0.599425	3.234371
C	3.671704	0.586629	3.812383
C	3.539250	0.826550	5.193674
C	2.904176	-0.116115	6.018620
C	2.402158	-1.302558	5.451995
C	2.535871	-1.540804	4.075272
C	4.531214	-1.866934	1.514977
C	4.506776	-2.793349	0.448943
C	5.587422	-3.659877	0.214500
C	6.722338	-3.615342	1.043518
C	6.760020	-2.700311	2.108662
C	5.673276	-1.838991	2.344980
C	-2.375645	-0.989020	0.290722
C	-2.449539	-2.301792	-0.256807
C	-3.704455	-2.824408	-0.598381
C	-4.884452	-2.079574	-0.405750
C	-4.802969	-0.795568	0.161509
C	-3.560486	-0.237025	0.525422
C	-1.201254	-3.175150	-0.433389
C	-0.731029	-3.810961	0.878957
C	-1.620083	-4.135494	1.925791
C	-1.159185	-4.770024	3.094081
C	0.200547	-5.094220	3.237182
C	1.099231	-4.774317	2.202452
C	0.634885	-4.136577	1.039968
C	-1.366344	-4.193861	-1.573534
C	-1.422611	-5.585947	-1.356075
C	-1.589902	-6.475521	-2.435054
C	-1.702356	-5.986081	-3.746436
C	-1.646977	-4.597907	-3.974438
C	-1.481599	-3.710824	-2.899267
C	-3.560221	1.143331	1.206188
C	-3.597756	1.048190	2.740717
C	-3.030750	2.092136	3.506897
C	-3.073629	2.063929	4.909721
C	-3.687415	0.989198	5.579765
C	-4.255806	-0.053990	4.830448
C	-4.211116	-0.024187	3.423252
C	-4.681882	2.062941	0.680829
C	-5.845506	2.341555	1.430418
C	-6.855857	3.173531	0.911952
C	-6.717592	3.746300	-0.362833
C	-5.560136	3.478457	-1.116740
C	-4.554565	2.645410	-0.600654
H	1.009961	0.816676	2.901669
H	-1.498871	-0.413388	2.824774
H	3.629844	3.711861	-1.140535
H	5.559649	0.375038	0.837968
H	0.273606	2.365753	-0.994291
H	2.274606	3.875015	1.756214

H	1.259980	5.223594	3.596106
H	-1.131955	5.978191	3.440680
H	-2.505047	5.338994	1.428565
H	-1.485689	3.979490	-0.404007
H	0.889565	2.450112	-3.313363
H	1.332262	3.900519	-5.285683
H	1.991838	6.311924	-4.969693
H	2.182558	7.246909	-2.643994
H	1.725014	5.793737	-0.665878
H	2.426562	-1.496431	1.441081
H	4.165535	1.337193	3.175279
H	3.935067	1.760375	5.624356
H	2.796276	0.073183	7.098443
H	1.895471	-2.046956	6.086845
H	2.130139	-2.468123	3.638843
H	3.625705	-2.818281	-0.211604
H	5.540678	-4.378767	-0.619498
H	7.570157	-4.295260	0.863378
H	7.640019	-2.658764	2.770446
H	5.710323	-1.143146	3.197380
H	-3.787430	-3.827409	-1.040233
H	-5.705380	-0.188831	0.314293
H	-0.391074	-2.489805	-0.769162
H	-2.688755	-3.890235	1.822604
H	-1.872259	-5.015068	3.897721
H	0.560169	-5.595413	4.149981
H	2.168416	-5.022743	2.298317
H	1.345021	-3.897210	0.231374
H	-1.334429	-5.982711	-0.332894
H	-1.632632	-7.559983	-2.243685
H	-1.833080	-6.682722	-4.590012
H	-1.731602	-4.197681	-4.997350
H	-1.441409	-2.623607	-3.087035
H	-2.604065	1.639821	0.935558
H	-2.540345	2.933907	2.991704
H	-2.618342	2.886358	5.484605
H	-3.718863	0.964741	6.680759
H	-4.738382	-0.902589	5.341855
H	-4.654691	-0.851721	2.847652
H	-5.963101	1.912286	2.437336
H	-7.754558	3.378225	1.516256
H	-7.505884	4.401631	-0.766905
H	-5.435726	3.921503	-2.117939
H	-3.657152	2.424838	-1.200603
S	2.114468	-1.398709	-1.993209
C	3.347079	-0.399786	-2.905298
H	3.501228	0.528787	-2.325318
H	4.290162	-0.978490	-2.961426
H	2.931150	-0.168530	-3.905822
C	1.975291	-2.805802	-3.158521
H	2.971056	-3.286268	-3.234113
H	1.234653	-3.513312	-2.740919
H	1.618194	-2.417432	-4.132973
O	-6.043621	-2.681744	-0.790110
C	-7.259128	-1.955705	-0.667480
H	-7.488479	-1.705174	0.393282
H	-7.240086	-1.014616	-1.261235
H	-8.055361	-2.615766	-1.060586
O	6.007700	2.516375	-0.453426
C	6.179705	3.726230	-1.182854
H	5.721138	3.668060	-2.195101
H	5.747076	4.598922	-0.644264
H	7.271422	3.871251	-1.287087

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PtIPrSTAROMeCl2SMe2cisPLANE SCF Done: -4438.60341317 A.U.

Pt	-0.128350	0.176468	-2.108703
Cl	1.812407	-1.147682	-2.305646
Cl	-0.291316	0.232934	-4.510263
N	-0.902976	-0.471356	0.750104
N	1.090381	0.437503	0.684634
C	0.032228	0.057999	-0.123771
C	-0.429608	-0.423900	2.064414
C	0.798937	0.164734	2.024281
C	-2.203623	-1.014804	0.413130
C	-2.296005	-2.252705	-0.281964
C	-3.574238	-2.765925	-0.586629
C	-4.742764	-2.088725	-0.190968
C	-4.633824	-0.885135	0.534836
C	-3.383267	-0.338049	0.859924
C	-1.054062	-3.078062	-0.652228
C	-0.465054	-3.834642	0.545414
C	-1.221566	-4.191318	1.681410
C	-0.650020	-4.953573	2.718238
C	0.687389	-5.374259	2.633486
C	1.454522	-5.017981	1.507530
C	0.884533	-4.252195	0.477928
C	-1.300862	-4.012840	-1.848036
C	-1.189412	-3.499801	-3.159924
C	-1.437716	-4.320134	-4.273169
C	-1.802495	-5.667136	-4.096487
C	-1.909562	-6.189422	-2.796032
C	-1.657083	-5.369217	-1.680952
C	-3.331812	0.925401	1.739200
C	-3.171555	0.598867	3.234444
C	-3.671373	-0.587385	3.812302
C	-3.538881	-0.827445	5.193562
C	-2.904044	0.115271	6.018636
C	-2.402301	1.301902	5.452163
C	-2.536049	1.540285	4.075465
C	-4.531280	1.866457	1.515175
C	-4.506953	2.792823	0.449089
C	-5.587637	3.659308	0.214694
C	-6.722485	3.614788	1.043816
C	-6.760053	2.699815	2.109009
C	-5.673262	1.838532	2.345281
C	2.375522	0.989220	0.290935
C	2.449242	2.302007	-0.256583
C	3.704080	2.824784	-0.598185
C	4.884178	2.080110	-0.405552
C	4.802871	0.796083	0.161694
C	3.560458	0.237374	0.525610
C	1.200849	3.175178	-0.433241
C	0.730429	3.810943	0.879060
C	1.619329	4.135641	1.925973
C	1.158216	4.770122	3.094203
C	-0.201581	5.094114	3.237168
C	-1.100112	4.774055	2.202356
C	-0.635550	4.136366	1.039928
C	1.365888	4.193892	-1.573390
C	1.422012	5.585983	-1.355943
C	1.589277	6.475558	-2.434925
C	1.701853	5.986111	-3.746295
C	1.646633	4.597927	-3.974280
C	1.481285	3.710843	-2.899104
C	3.560362	-1.143077	1.206203
C	3.597838	-1.048155	2.740745
C	3.031224	-2.092447	3.506749
C	3.074080	-2.064451	4.909579
C	3.687451	-0.989595	5.579803
C	4.255461	0.053925	4.830662
C	4.210798	0.024334	3.423459
C	4.682176	-2.062441	0.680760

C	5.845896	-2.340842	1.430287
C	6.856403	-3.172564	0.911731
C	6.718206	-3.745298	-0.363082
C	5.560656	-3.477679	-1.116918
C	4.554923	-2.644878	-0.600738
H	-1.009984	-0.816984	2.901675
H	1.498760	0.413292	2.824935
H	-3.629577	-3.712035	-1.140853
H	-5.559608	-0.375508	0.837963
H	-0.273412	-2.365660	-0.994369
H	-2.274417	-3.875694	1.755759
H	-1.259662	-5.224295	3.595565
H	1.132468	-5.978306	3.440277
H	2.505613	-5.338511	1.428386
H	1.486114	-3.978980	-0.404100
H	-0.889351	-2.449690	-3.313453
H	-1.331778	-3.899841	-5.286013
H	-1.991010	-6.311402	-4.970427
H	-2.181630	-7.246792	-2.644886
H	-1.724346	-5.793872	-0.666520
H	-2.426616	1.496077	1.441218
H	-4.165004	-1.337994	3.175096
H	-3.934479	-1.761420	5.624123
H	-2.796109	-0.074136	7.098437
H	-1.895787	2.046338	6.087106
H	-2.130524	2.467753	3.639159
H	-3.625940	2.817719	-0.211543
H	-5.540995	4.378160	-0.619342
H	-7.570331	4.294680	0.863706
H	-7.639985	2.658283	2.770882
H	-5.710222	1.142741	3.197727
H	3.786909	3.827782	-1.040077
H	5.705348	0.189436	0.314427
H	0.390786	2.489725	-0.769066
H	2.688049	3.890551	1.822892
H	1.871172	5.015292	3.897910
H	-0.561362	5.595277	4.149921
H	-2.169345	5.022319	2.298103
H	-1.345576	3.896888	0.231269
H	1.333737	5.982755	-0.332772
H	1.631895	7.560026	-2.243566
H	1.832557	6.682751	-4.589874
H	1.731363	4.197694	-4.997180
H	1.441227	2.623617	-3.086858
H	2.604287	-1.639669	0.935475
H	2.541146	-2.934325	2.991417
H	2.619097	-2.887145	5.484325
H	3.718881	-0.965303	6.680802
H	4.737715	0.902621	5.342211
H	4.654066	0.852129	2.847996
H	5.963428	-1.911611	2.437229
H	7.755175	-3.377098	1.515984
H	7.506627	-4.400428	-0.767227
H	5.436289	-3.920709	-2.118129
H	3.657427	-2.424493	-1.200629
S	-2.114530	1.398727	-1.993138
C	-3.347010	0.399704	-2.905290
H	-3.501095	-0.528894	-2.325334
H	-4.290142	0.978325	-2.961448
H	-2.931011	0.168496	-3.905796
C	-1.975432	2.805875	-3.158400
H	-2.971238	3.286258	-3.233981
H	-1.234858	3.513426	-2.740756
H	-1.618297	2.417558	-4.132857
O	6.043251	2.682440	-0.789945
C	7.258876	1.956588	-0.667366
H	7.488275	1.706026	0.393380
H	7.239973	1.015525	-1.261171
H	8.055004	2.616790	-1.060446
O	-6.007502	-2.516764	-0.453646
C	-6.179455	-3.726548	-1.183208
H	-5.720862	-3.668258	-2.195438
H	-5.746816	-4.599280	-0.644691
H	-7.271166	-3.871581	-1.287485

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PtIPrSTAROMeCl2SMe2cis SCF Done: -4438.60341317 A.U.

Pt	0.128330	-0.176372	-2.108775
Cl	-1.812501	1.147636	-2.305755
Cl	0.291380	-0.232743	-4.510328
N	0.902873	0.471321	0.750060
N	-1.090500	-0.437482	0.684525
C	-0.032329	-0.057979	-0.123849
C	0.429445	0.423918	2.064348
C	-0.799150	-0.164609	2.024168
C	2.203571	1.014671	0.413144
C	2.296085	2.252602	-0.281863
C	3.574372	2.765733	-0.586487
C	4.742822	2.088422	-0.190830
C	4.633748	0.884791	0.534912
C	3.383153	0.337778	0.859931
C	1.054220	3.078124	-0.652049
C	0.465330	3.834710	0.545662
C	1.221903	4.191258	1.681653
C	0.650450	4.953508	2.718541
C	-0.686918	5.374324	2.633849
C	-1.454107	5.018190	1.507884
C	-0.884215	4.252412	0.478227
C	1.301093	4.012975	-1.847783
C	1.189414	3.500141	-3.159728
C	1.437776	4.320578	-4.272886
C	1.802865	5.667473	-4.096057
C	1.910191	6.189558	-2.795539
C	1.657639	5.369256	-1.680552
C	3.331553	-0.925687	1.739189
C	3.171150	-0.599187	3.234423
C	3.671113	0.586953	3.812394
C	3.538466	0.826993	5.193643
C	2.903317	-0.115627	6.018587
C	2.401419	-1.302134	5.451997
C	2.535323	-1.540503	4.075311
C	4.530980	-1.866828	1.515268
C	4.506743	-2.793124	0.449125
C	5.587412	-3.659660	0.214817
C	6.722149	-3.615265	1.044089
C	6.759629	-2.700353	2.109342
C	5.672861	-1.839021	2.345522
C	-2.375620	-0.989232	0.290814
C	-2.449319	-2.302020	-0.256689
C	-3.704168	-2.824832	-0.598196
C	-4.884284	-2.080208	-0.405465
C	-4.802973	-0.796169	0.161734
C	-3.560547	-0.237416	0.525542
C	-1.200837	-3.175047	-0.433470
C	-0.730078	-3.810645	0.878777
C	-1.618706	-4.135291	1.925930
C	-1.157279	-4.769618	3.094124
C	0.202573	-5.093482	3.236814
C	1.100846	-4.773461	2.201758
C	0.635971	-4.135942	1.039369
C	-1.365933	-4.193885	-1.573496
C	-1.422332	-5.585929	-1.355816
C	-1.589713	-6.475658	-2.434651

C	-1.702113	-5.986409	-3.746109
C	-1.646623	-4.598275	-3.974329
C	-1.481173	-3.711037	-2.899297
C	-3.560413	1.143030	1.206141
C	-3.598125	1.048109	2.740675
C	-3.031406	2.092280	3.506762
C	-3.074427	2.064260	4.909586
C	-3.688072	0.989504	5.579719
C	-4.256177	-0.053904	4.830496
C	-4.211346	-0.024293	3.423297
C	-4.682057	2.062480	0.680533
C	-5.846103	2.340553	1.429673
C	-6.856443	3.172383	0.910977
C	-6.717755	3.745540	-0.363598
C	-5.559881	3.478235	-1.117048
C	-4.554304	2.645337	-0.600722
H	1.009793	0.817010	2.901625
H	-1.499064	-0.413047	2.824784
H	3.629782	3.711893	-1.140617
H	5.559489	0.375091	0.838053
H	0.273494	2.365808	-0.994201
H	2.274730	3.875550	1.755961
H	1.260141	5.224119	3.595868
H	-1.131920	5.978368	3.440684
H	-2.505169	5.338825	1.428780
H	-1.485854	3.979327	-0.403800
H	0.889120	2.450116	-3.313368
H	1.331636	3.900454	-5.285779
H	1.991424	6.311815	-4.969932
H	2.182519	7.246844	-2.644278
H	1.725095	5.793752	-0.666067
H	2.426344	-1.496298	1.441110
H	4.164990	1.337482	3.175287
H	3.934188	1.760873	5.624298
H	2.795255	0.073761	7.098379
H	1.894665	-2.046489	6.086845
H	2.129680	-2.467874	3.638909
H	3.625822	-2.817924	-0.211629
H	5.540827	-4.378441	-0.619284
H	7.569982	-4.295195	0.864063
H	7.639479	-2.658921	2.771332
H	5.709758	-1.143263	3.197999
H	-3.786994	-3.827831	-1.040080
H	-5.705456	-0.189527	0.314488
H	-0.390971	-2.489446	-0.769493
H	-2.687467	-3.890281	1.823070
H	-1.870035	-5.014761	3.898018
H	0.562605	-5.594520	4.149537
H	2.170125	-5.021604	2.297306
H	1.345793	-3.896495	0.230522
H	-1.334160	-5.982531	-0.332569
H	-1.632537	-7.560086	-2.243118
H	-1.832901	-6.683167	-4.589579
H	-1.731226	-4.198212	-4.997307
H	-1.440952	-2.623848	-3.087208
H	-2.604268	1.639559	0.935550
H	-2.541111	2.934075	2.991502
H	-2.619358	2.886856	5.484405
H	-3.719627	0.965201	6.680714
H	-4.738634	-0.902527	5.341974
H	-4.654685	-0.852002	2.847770
H	-5.964015	1.910982	2.436430
H	-7.755473	3.376670	1.514929
H	-7.506054	4.400746	-0.767858
H	-5.435133	3.921588	-2.118068
H	-3.656540	2.425210	-1.200316
S	2.114635	-1.398441	-1.993209
C	3.347113	-0.399278	-2.905210
H	3.501131	0.529275	-2.325164
H	4.290285	-0.977842	-2.961363
H	2.931192	-0.168006	-3.905730
C	1.975631	-2.805489	-3.158588
H	2.971441	-3.285845	-3.234229
H	1.235074	-3.513096	-2.741007
H	1.618451	-2.417106	-4.133008
O	-6.043395	-2.682595	-0.789737
C	-7.259055	-1.956812	-0.667038
H	-7.488386	-1.706331	0.393739
H	-7.240278	-1.015708	-1.260768
H	-8.055155	-2.617059	-1.060078
O	6.007611	2.516353	-0.453456
C	6.179694	3.726209	-1.182874
H	5.721704	3.667774	-2.195367
H	5.746520	4.598823	-0.644623
H	7.271426	3.871477	-1.286527

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PtIPrSTAROMeCl2SMe2transDOWN SCF Done: -4438.60496914 A.U.

Pt	-0.054422	-0.045095	-2.111489
Cl	1.608955	-1.723393	-2.182274
Cl	-1.672465	1.685235	-2.179944
N	-0.926417	-0.459051	0.743060
N	1.075864	0.431426	0.685908
C	0.046290	-0.000826	-0.123339
C	-0.498322	-0.321778	2.066094
C	0.738260	0.253897	2.031334
C	-2.247135	-0.942529	0.380599
C	-2.400439	-2.233439	-0.211183
C	-3.685025	-2.633659	-0.606497
C	-4.810357	-1.809784	-0.403823
C	-4.656081	-0.578600	0.256363
C	-3.381950	-0.134592	0.666565
C	-1.221322	-3.210058	-0.348257
C	-0.774557	-3.802778	0.996363
C	-1.622301	-3.888982	2.120384
C	-1.190529	-4.520122	3.302747
C	0.095087	-5.080545	3.377931
C	0.952069	-4.996130	2.263709
C	0.522563	-4.358672	1.088687
C	-1.482209	-4.331802	-1.366766
C	-1.086716	-4.164345	-2.712023
C	-1.336805	-5.165500	-3.666901
C	-1.989711	-6.353509	-3.294639
C	-2.378836	-6.536402	-1.956194
C	-2.122098	-5.537056	-1.001203
C	-3.292146	1.162117	1.490656
C	-3.266623	0.880454	3.003038
C	-3.921372	-0.229239	3.579289
C	-3.910487	-0.430806	4.972787
C	-3.242577	0.474010	5.814400
C	-2.586366	1.583897	5.250683
C	-2.600165	1.784155	3.861187
C	-4.393149	2.181029	1.134074
C	-4.298797	2.906158	-0.075384
C	-5.285862	3.837132	-0.437085
C	-6.392610	4.061977	0.402042
C	-6.498668	3.346574	1.605877
C	-5.506373	2.416796	1.969963
C	2.360675	0.963468	0.266973
C	2.439382	2.282097	-0.272535
C	3.692922	2.768791	-0.670386
C	4.861035	1.993113	-0.532260

C	4.777437	0.717219	0.051869
C	3.537415	0.190405	0.469006
C	1.212567	3.202282	-0.360593
C	0.794707	3.777340	0.998528
C	1.691339	3.925653	2.077382
C	1.281372	4.537843	3.277074
C	-0.031454	5.018158	3.415188
C	-0.936754	4.872596	2.346627
C	-0.527814	4.253203	1.154360
C	1.393287	4.312350	-1.408765
C	1.724320	5.639696	-1.064641
C	1.909369	6.617182	-2.060198
C	1.762269	6.283906	-3.416586
C	1.428868	4.963471	-3.770591
C	1.247086	3.989733	-2.776105
C	3.532072	-1.164159	1.199687
C	3.536122	-0.994705	2.727891
C	2.905755	-1.969545	3.533123
C	2.920693	-1.869642	4.933539
C	3.570019	-0.790541	5.561074
C	4.202388	0.184954	4.772136
C	4.185121	0.083160	3.368077
C	4.672982	-2.095711	0.739097
C	5.785581	-2.392967	1.555741
C	6.813163	-3.238997	1.096851
C	6.744348	-3.807025	-0.185340
C	5.638954	-3.519088	-1.007068
C	4.616518	-2.672404	-0.550399
H	-1.114854	-0.647500	2.906468
H	1.411542	0.555789	2.836208
H	-3.839917	-3.610326	-1.085165
H	-5.519368	0.069724	0.456542
H	-0.357605	-2.637039	-0.747400
H	-2.636705	-3.462498	2.069604
H	-1.869916	-4.578498	4.168498
H	0.429418	-5.583877	4.299221
H	1.962662	-5.433216	2.308319
H	1.194329	-4.299360	0.216820
H	-0.544677	-3.249049	-2.998096
H	-1.006889	-5.018770	-4.708197
H	-2.183890	-7.139608	-4.041934
H	-2.880263	-7.468396	-1.648842
H	-2.415059	-5.700443	0.048184
H	-2.326132	1.649011	1.237684
H	-4.444072	-0.949207	2.930096
H	-4.427683	-1.304877	5.400528
H	-3.229561	0.314299	6.904381
H	-2.052598	2.298284	5.897843
H	-2.075050	2.651189	3.429259
H	-3.442913	2.719621	-0.743681
H	-5.186574	4.393125	-1.383395
H	-7.165799	4.794643	0.120052
H	-7.357210	3.515272	2.276035
H	-5.597303	1.875715	2.924263
H	3.785776	3.773873	-1.104814
H	5.673352	0.096860	0.186261
H	0.359659	2.590107	-0.725209
H	2.727058	3.564882	1.975394
H	1.998783	4.645387	4.106696
H	-0.349558	5.506370	4.350268
H	-1.969291	5.245692	2.439798
H	-1.237801	4.149194	0.317700
H	1.834026	5.916343	-0.004516
H	2.167497	7.648284	-1.769276
H	1.902815	7.049983	-4.195910
H	1.304786	4.692897	-4.831833
H	0.981855	2.956117	-3.047400
H	2.583819	-1.677250	0.930587
H	2.382369	-2.811607	3.052555
H	2.413657	-2.638254	5.538634
H	3.579188	-0.709171	6.659747
H	4.713593	1.036174	5.250275
H	4.679653	0.857502	2.760672
H	5.850089	-1.966718	2.568395
H	7.670309	-3.458030	1.754148
H	7.545556	-4.473822	-0.542632
H	5.568362	-3.959381	-2.014833
H	3.759010	-2.439757	-1.201424
S	-0.243396	-0.328554	-4.514811
C	-0.071655	1.315945	-5.297093
H	0.995411	1.597090	-5.214856
H	-0.352193	1.235452	-6.365925
H	-0.707434	2.050776	-4.764784
C	-2.034739	-0.600269	-4.775754
H	-2.238625	-0.638710	-5.864127
H	-2.278781	-1.574650	-4.311408
H	-2.605935	0.206501	-4.275905
O	6.015925	2.565241	-0.973880
C	7.221451	1.818493	-0.882791
H	7.484873	1.581579	0.173068
H	7.163622	0.867437	-1.458084
H	8.014997	2.456228	-1.316235
O	-5.998960	-2.298746	-0.857067
C	-7.167107	-1.508266	-0.685566
H	-7.395466	-1.332150	0.390143
H	-7.079766	-0.523512	-1.197125
H	-7.998380	-2.080037	-1.139850

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PtIPrSTAROMeCl2SMe2transPLANE SCF Done: -4438.60489401 A.U.

Pt	-0.047871	-0.120397	-2.099416
Cl	1.362290	-2.019084	-2.047732
Cl	-1.427141	1.797606	-2.268560
N	-0.979826	-0.304983	0.762511
N	1.110934	0.349814	0.680549
C	0.039714	0.003471	-0.115349
C	-0.540493	-0.161413	2.081580
C	0.754163	0.266803	2.030456
C	-2.349973	-0.636072	0.411255
C	-2.665203	-1.916247	-0.119453
C	-3.996041	-2.176708	-0.507804
C	-5.002536	-1.206759	-0.349812
C	-4.687228	0.026658	0.251932
C	-3.377871	0.326895	0.653168
C	-1.623884	-3.044384	-0.203784
C	-1.275372	-3.644523	1.166337
C	-2.123432	-3.550210	2.289283
C	-1.792284	-4.190230	3.499153
C	-0.609273	-4.939903	3.603583
C	0.247618	-5.037312	2.490335
C	-0.080454	-4.391574	1.287549
C	-2.021828	-4.154241	-1.191002
C	-1.646053	-4.053404	-2.548693
C	-2.021983	-5.040232	-3.476503
C	-2.784272	-6.147805	-3.064905
C	-3.156569	-6.264810	-1.714434
C	-2.774219	-5.279651	-0.786363
C	-3.125464	1.631028	1.428644
C	-3.151977	1.403559	2.950671
C	-3.953194	0.411798	3.556211
C	-3.982593	0.261991	4.955969
C	-3.209170	1.101023	5.774976

C	-2.406994	2.093586	5.182022
C	-2.380718	2.242662	3.786306
C	-4.078944	2.770557	1.019179
C	-3.855998	3.453890	-0.197472
C	-4.706730	4.493357	-0.606782
C	-5.802215	4.870553	0.191172
C	-6.035170	4.197651	1.401563
C	-5.179197	3.159097	1.813413
C	2.444152	0.731981	0.247464
C	2.665426	2.032137	-0.298547
C	3.965300	2.379881	-0.693664
C	5.044347	1.486769	-0.543143
C	4.822112	0.228750	0.043206
C	3.530419	-0.163013	0.452796
C	1.547737	3.081622	-0.396306
C	1.210129	3.726311	0.954659
C	2.114124	3.760815	2.036861
C	1.789857	4.440348	3.226657
C	0.557481	5.102567	3.351416
C	-0.355193	5.071646	2.279584
C	-0.032831	4.385613	1.097492
C	1.846788	4.147742	-1.463903
C	2.345114	5.427772	-1.141351
C	2.638140	6.362634	-2.151575
C	2.433603	6.034281	-3.501812
C	1.933497	4.761932	-3.834226
C	1.644336	3.829880	-2.825025
C	3.375885	-1.511326	1.178486
C	3.365852	-1.339313	2.705448
C	2.586205	-2.209913	3.498610
C	2.581683	-2.102929	4.898922
C	3.360658	-1.120942	5.537758
C	4.143378	-0.250134	4.760629
C	4.145631	-0.359344	3.357405
C	4.425062	-2.553440	0.733560
C	5.400430	-3.071076	1.612606
C	6.339398	-4.023511	1.171746
C	6.318286	-4.478104	-0.156043
C	5.350094	-3.968985	-1.041654
C	4.416117	-3.017606	-0.602827
H	-1.192362	-0.375976	2.931082
H	1.456765	0.523289	2.826015
H	-4.228325	-3.160626	-0.934322
H	-5.493354	0.760266	0.396237
H	-0.686754	-2.605766	-0.607984
H	-3.058404	-2.972319	2.217310
H	-2.470035	-4.104423	4.363864
H	-0.354853	-5.449114	4.546913
H	1.178598	-5.622935	2.558589
H	0.590685	-4.474065	0.417049
H	-1.021590	-3.203451	-2.865862
H	-1.704022	-4.948224	-4.527729
H	-3.075184	-6.924004	-3.790867
H	-3.741255	-7.135546	-1.375770
H	-3.054645	-5.392709	0.273076
H	-2.101580	1.978161	1.173413
H	-4.562276	-0.254776	2.925661
H	-4.616235	-0.519038	5.406492
H	-3.228338	0.981490	6.870025
H	-1.790497	2.755591	5.811157
H	-1.742793	3.017715	3.332197
H	-3.010322	3.148524	-0.834267
H	-4.509867	5.013018	-1.558436
H	-6.469236	5.687150	-0.128732
H	-6.887895	4.483576	2.038453
H	-5.368098	2.651198	2.771576
H	4.166509	3.366883	-1.132845
H	5.646366	-0.482726	0.183839
H	0.628464	2.563073	-0.745127
H	3.089361	3.257148	1.945563
H	2.512356	4.456716	4.058667
H	0.307640	5.643024	4.278425
H	-1.325765	5.586453	2.362345
H	-0.747946	4.373579	0.258906
H	2.501816	5.701486	-0.086368
H	3.026378	7.356814	-1.877165
H	2.658507	6.767642	-4.292751
H	1.762286	4.496373	-4.890168
H	1.246360	2.836039	-3.080807
H	2.385920	-1.925343	0.887547
H	1.960898	-2.974043	3.009821
H	1.956795	-2.788208	5.493755
H	3.354506	-1.032946	6.635952
H	4.757962	0.524054	5.247915
H	4.759214	0.332763	2.759325
H	5.428020	-2.733127	2.659366
H	7.089596	-4.413244	1.878857
H	7.049851	-5.226773	-0.500345
H	5.317612	-4.318109	-2.086472
H	3.664490	-2.618934	-1.302691
S	-0.214877	-0.467294	-4.494849
C	0.234346	1.106478	-5.311628
H	1.323437	1.239496	-5.168082
H	0.008066	1.028003	-6.393393
H	-0.321305	1.941148	-4.840395
C	-2.016434	-0.469702	-4.819111
H	-2.186624	-0.505857	-5.913321
H	-2.422764	-1.382352	-4.343327
H	-2.473795	0.427703	-4.357831
O	6.256161	1.932316	-0.977355
C	7.376661	1.065020	-0.869417
H	7.604240	0.809913	0.190546
H	7.225871	0.120729	-1.439055
H	8.236100	1.613816	-1.298927
O	-6.302515	-1.379138	-0.719673
C	-6.678979	-2.606995	-1.327216
H	-6.119181	-2.791499	-2.271599
H	-6.521756	-3.473554	-0.645779
H	-7.757896	-2.521286	-1.557240

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PtIPrSTAROMeCl2SMe2trans SCF Done: -4438.60476821 A.U.

Pt	-0.029590	-0.061565	-2.091778
Cl	1.138943	-2.116805	-2.092983
Cl	-1.140691	2.028499	-2.209867
N	-1.010784	-0.231205	0.753141
N	1.145716	0.161642	0.714939
C	0.050877	-0.018648	-0.103427
C	-0.574819	-0.193978	2.080438
C	0.763227	0.072118	2.057341
C	-2.406963	-0.381401	0.380484
C	-2.869876	-1.597317	-0.191732
C	-4.220030	-1.684193	-0.590995
C	-5.104786	-0.606972	-0.402819
C	-4.647459	0.560957	0.237187
C	-3.313546	0.690351	0.649062
C	-1.971150	-2.839467	-0.309633
C	-1.714618	-3.525004	1.040783
C	-2.554774	-3.361639	2.161807
C	-2.319145	-4.078958	3.350547
C	-1.242019	-4.976149	3.435055
C	-0.393338	-5.143684	2.323834
C	-0.625000	-4.421156	1.142519

C	-2.488867	-3.857435	-1.339379
C	-2.084689	-3.757848	-2.688958
C	-2.566937	-4.658294	-3.654705
C	-3.465805	-5.676148	-3.289794
C	-3.867855	-5.792349	-1.947771
C	-3.379392	-4.894477	-0.981771
C	-2.911328	1.933185	1.461406
C	-2.966047	1.666872	2.976010
C	-3.890473	0.771204	3.555301
C	-3.938236	0.584050	4.949972
C	-3.060433	1.288855	5.790138
C	-2.135196	2.184956	5.223535
C	-2.090645	2.371639	3.832739
C	-3.724539	3.187474	1.084642
C	-3.446946	3.849365	-0.132852
C	-4.169321	4.991695	-0.513287
C	-5.188522	5.496373	0.314910
C	-5.474924	4.846143	1.526084
C	-4.747322	3.703647	1.908968
C	2.524372	0.389587	0.316946
C	2.913762	1.660135	-0.184045
C	4.264760	1.870469	-0.531124
C	5.220779	0.851767	-0.372062
C	4.825239	-0.389618	0.162529
C	3.493208	-0.641112	0.522196
C	1.931934	2.836734	-0.295225
C	1.646762	3.513203	1.051392
C	2.534949	3.451013	2.145442
C	2.267109	4.158474	3.332904
C	1.108353	4.944846	3.443557
C	0.211229	5.010329	2.360295
C	0.476460	4.296833	1.180135
C	2.375119	3.855937	-1.358759
C	2.941210	5.106072	-1.031736
C	3.360654	5.993861	-2.040788
C	3.218288	5.646888	-3.394099
C	2.652446	4.403062	-3.731460
C	2.236178	3.519091	-2.723933
C	3.155049	-1.983616	1.192444
C	3.139664	-1.868806	2.724829
C	2.234592	-2.654879	3.471867
C	2.218332	-2.601892	4.875143
C	3.110594	-1.759620	5.563366
C	4.018416	-0.974515	4.832413
C	4.032597	-1.029634	3.426073
C	4.070917	-3.132783	0.718373
C	4.949083	-3.812295	1.589046
C	5.765238	-4.859517	1.120065
C	5.715490	-5.248257	-0.227595
C	4.843160	-4.577647	-1.104933
C	4.032034	-3.531971	-0.638026
H	-1.259008	-0.360235	2.915158
H	1.482153	0.206411	2.868245
H	-4.565505	-2.619210	-1.049628
H	-5.360866	1.380926	0.403156
H	-0.983151	-2.504013	-0.690982
H	-3.408591	-2.668008	2.104824
H	-2.988975	-3.937077	4.214063
H	-1.063416	-5.545312	4.361357
H	0.455699	-5.844075	2.376894
H	0.039444	-4.558554	0.273856
H	-1.355037	-2.982093	-2.969765
H	-2.225461	-4.570760	-4.698902
H	-3.840466	-6.385139	-4.045500
H	-4.559845	-6.595244	-1.645709
H	-3.685316	-5.008090	0.070527
H	-1.853340	2.164887	1.214088
H	-4.582173	0.209602	2.907920
H	-4.668580	-0.120379	5.379897
H	-3.094115	1.139394	6.881148
H	-1.436468	2.740657	5.869360
H	-1.356638	3.069547	3.399103
H	-2.662076	3.446363	-0.792883
H	-3.931901	5.491556	-1.466314
H	-5.754889	6.393520	0.017504
H	-6.269164	5.230612	2.186308
H	-4.976604	3.213609	2.867506
H	4.549916	2.852205	-0.930428
H	5.587605	-1.172545	0.283039
H	0.963652	2.433789	-0.663337
H	3.452100	2.846212	2.066261
H	2.975375	4.097112	4.175005
H	0.903177	5.505842	4.369326
H	-0.702820	5.621098	2.432968
H	-0.225640	4.358044	0.332688
H	3.050253	5.394599	0.025211
H	3.797701	6.966560	-1.762563
H	3.541264	6.343656	-4.184176
H	2.529384	4.123784	-4.790583
H	1.789223	2.546806	-2.983310
H	2.125546	-2.256382	0.873086
H	1.521491	-3.308338	2.944359
H	1.496049	-3.218837	5.433406
H	3.096079	-1.713705	6.664067
H	4.723562	-0.310826	5.358556
H	4.747249	-0.407091	2.865031
H	4.998108	-3.526529	2.650412
H	6.443040	-5.374068	1.820380
H	6.352089	-6.069488	-0.594352
H	4.791098	-4.871559	-2.165784
H	3.356405	-3.006759	-1.331663
S	-0.230944	-0.318721	-4.496284
C	0.433177	1.196607	-5.276428
H	1.532164	1.161623	-5.152023
H	0.181612	1.185367	-6.355402
H	0.014861	2.089688	-4.771496
C	-2.014277	-0.065814	-4.822556
H	-2.182364	-0.054988	-5.917652
H	-2.544308	-0.924121	-4.367903
H	-2.346678	0.875818	-4.342962
O	6.539468	0.975203	-0.690550
C	6.991647	2.201552	-1.247750
H	6.472869	2.438632	-2.203665
H	6.851510	3.054168	-0.545165
H	8.072702	2.072452	-1.445137
O	-6.414436	-0.611693	-0.778602
C	-6.932736	-1.767614	-1.421881
H	-6.396803	-1.989390	-2.372078
H	-6.881159	-2.666453	-0.766611
H	-7.993284	-1.547460	-1.647897

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PtIPrSTAROMeCl2transDOWN SCF Done: -3960.67945402 A.U.

Pt	0.012373	0.008090	-2.165465
Cl	2.055873	-1.031473	-2.524444
Cl	-1.986663	1.155058	-2.491338
N	-1.022699	-0.428173	0.577735
N	0.993233	0.452629	0.580659
C	-0.015589	0.017459	-0.251406
C	-0.642673	-0.248367	1.913068
C	0.597183	0.317532	1.913680
C	-2.325733	-0.959520	0.223642
C	-2.425261	-2.251840	-0.353883

C	-3.708445	-2.754948	-0.647355
C	-4.863610	-1.995413	-0.388619
C	-4.744888	-0.725099	0.196729
C	-3.484815	-0.189836	0.530437
C	-1.198631	-3.140882	-0.597685
C	-0.744552	-3.890917	0.659561
C	-1.622601	-4.251250	1.704526
C	-1.158525	-4.974361	2.818894
C	0.191419	-5.354852	2.908452
C	1.077370	-5.004935	1.872697
C	0.610723	-4.280567	0.763235
C	-1.398889	-4.047164	-1.823273
C	-1.505396	-3.431734	-3.094052
C	-1.688142	-4.196159	-4.253250
C	-1.770789	-5.601075	-4.166078
C	-1.667973	-6.221248	-2.912551
C	-1.481517	-5.449085	-1.747094
C	-3.414464	1.182374	1.220323
C	-3.351186	1.079037	2.753990
C	-3.888191	-0.012017	3.469817
C	-3.840995	-0.044674	4.877047
C	-3.253279	1.012037	5.591210
C	-2.709759	2.102688	4.886833
C	-2.758505	2.134177	3.484553
C	-4.544108	2.123544	0.762637
C	-4.455391	2.742725	-0.503582
C	-5.474415	3.594218	-0.962719
C	-6.605266	3.840372	-0.164691
C	-6.704993	3.230262	1.097500
C	-5.682182	2.382452	1.558747
C	2.301447	0.943437	0.187301
C	2.412661	2.221405	-0.430825
C	3.690443	2.658610	-0.820542
C	4.828127	1.855183	-0.611000
C	4.701685	0.615082	0.031299
C	3.444887	0.141099	0.458838
C	1.196812	3.138887	-0.622039
C	0.782795	3.872253	0.661061
C	1.658814	4.057216	1.752276
C	1.259463	4.800248	2.879223
C	-0.021651	5.374645	2.931626
C	-0.905920	5.192828	1.851894
C	-0.507173	4.446424	0.731242
C	1.390458	4.109225	-1.797322
C	1.796447	5.448944	-1.615814
C	2.000456	6.294284	-2.721680
C	1.799862	5.814552	-4.027191
C	1.391769	4.482136	-4.219736
C	1.190876	3.639198	-3.114622
C	3.345160	-1.195102	1.216386
C	3.407542	-1.013125	2.743525
C	2.809572	-1.991742	3.572854
C	2.872143	-1.884680	4.969555
C	3.537563	-0.797308	5.569746
C	4.136992	0.177266	4.757320
C	4.071892	0.069686	3.353235
C	4.380460	-2.237570	0.757251
C	5.666718	-2.315090	1.339738
C	6.602521	-3.265565	0.897537
C	6.264693	-4.169030	-0.125551
C	4.984098	-4.113708	-0.700726
C	4.052458	-3.154958	-0.263820
H	-1.301645	-0.529632	2.737891
H	1.237713	0.638760	2.737847
H	-3.800003	-3.761126	-1.080952
H	-5.657515	-0.141290	0.379713
H	-0.355919	-2.471831	-0.881754
H	-2.685061	-3.968639	1.645060
H	-1.862103	-5.244888	3.622657
H	0.551805	-5.924019	3.780240
H	2.138431	-5.298471	1.921857
H	1.309512	-4.018750	-0.047214
H	-1.456040	-2.329227	-3.155835
H	-1.762759	-3.696819	-5.232543
H	-1.912036	-6.205529	-5.076245
H	-1.729817	-7.318472	-2.831137
H	-1.400081	-5.948591	-0.769447
H	-2.468867	1.664424	0.894429
H	-4.344542	-0.852337	2.923387
H	-4.266846	-0.906810	5.415183
H	-3.213821	0.985578	6.691810
H	-2.238684	2.934881	5.434116
H	-2.323334	2.989107	2.941991
H	-3.581826	2.534965	-1.143156
H	-5.381820	4.066951	-1.953703
H	-7.405154	4.507440	-0.524022
H	-7.584494	3.418273	1.734203
H	-5.765281	1.927888	2.558047
H	3.798542	3.648987	-1.285705
H	5.605172	0.011489	0.189998
H	0.343958	2.490575	-0.918368
H	2.668439	3.618774	1.717663
H	1.959175	4.935294	3.719742
H	-0.330896	5.964716	3.809045
H	-1.912966	5.639181	1.878897
H	-1.200360	4.314916	-0.115404
H	1.945429	5.839540	-0.596766
H	2.314531	7.338040	-2.559469
H	1.954263	6.479163	-4.892352
H	1.221359	4.096832	-5.237782
H	0.863676	2.596682	-3.264910
H	2.349684	-1.626510	0.980835
H	2.280161	-2.840775	3.110575
H	2.393479	-2.652736	5.598060
H	3.585641	-0.713039	6.667088
H	4.662447	1.031831	5.213305
H	4.544104	0.841740	2.724355
H	5.931386	-1.634994	2.164538
H	7.601197	-3.305648	1.361412
H	6.995988	-4.918939	-0.467443
H	4.703434	-4.821712	-1.496895
H	3.059810	-3.099433	-0.738609
O	6.088489	2.277084	-0.959922
C	6.186314	2.972912	-2.203977
H	5.912227	2.304009	-3.051075
H	5.532647	3.874220	-2.241430
H	7.239833	3.294892	-2.321573
O	-6.123017	-2.485902	-0.637340
C	-6.299124	-3.112333	-1.908448
H	-6.154149	-2.378910	-2.734305
H	-5.594327	-3.961131	-2.064244
H	-7.336002	-3.500944	-1.947421

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PtIPrSTAROMeCl2transPLANE SCF Done: -3960.69365502 A.U.

Pt	-0.033471	-0.029219	-2.216320
Cl	1.755015	-1.465386	-2.564861
Cl	-1.834899	1.383639	-2.584253
N	-1.021549	-0.396871	0.544500
N	1.007259	0.473651	0.502389
C	-0.015570	0.017991	-0.303471
C	-0.615281	-0.208863	1.869110
C	0.627807	0.352594	1.842581

C	-2.338019	-0.897861	0.191301
C	-2.474153	-2.184182	-0.393406
C	-3.765154	-2.648215	-0.715785
C	-4.903008	-1.862010	-0.456312
C	-4.750300	-0.601942	0.155673
C	-3.485212	-0.103634	0.496762
C	-1.266498	-3.101848	-0.636056
C	-0.746880	-3.763497	0.645502
C	-1.562409	-3.991545	1.773895
C	-1.058792	-4.664847	2.903002
C	0.268774	-5.124103	2.920583
C	1.094047	-4.897784	1.802477
C	0.590988	-4.220561	0.679595
C	-1.525999	-4.124324	-1.754371
C	-1.499427	-3.687735	-3.098361
C	-1.754318	-4.579873	-4.151478
C	-2.043213	-5.930346	-3.880401
C	-2.071600	-6.376637	-2.548828
C	-1.813221	-5.480827	-1.494091
C	-3.395552	1.242328	1.236080
C	-3.359767	1.071388	2.764203
C	-3.999572	0.001159	3.425310
C	-3.973711	-0.098513	4.829699
C	-3.306728	0.870791	5.596832
C	-2.666070	1.942801	4.948042
C	-2.693710	2.041106	3.547934
C	-4.498037	2.229781	0.805767
C	-4.394159	2.874659	-0.447522
C	-5.381932	3.774808	-0.878133
C	-6.497004	4.047561	-0.064755
C	-6.611628	3.411646	1.181994
C	-5.619051	2.512522	1.614948
C	2.315106	0.956469	0.095402
C	2.436449	2.223100	-0.549388
C	3.714389	2.660951	-0.921450
C	4.862538	1.884585	-0.663092
C	4.730586	0.654449	0.006038
C	3.464045	0.178013	0.402241
C	1.222453	3.129875	-0.797502
C	0.733204	3.838716	0.470975
C	1.577125	4.114588	1.567341
C	1.100682	4.831776	2.681192
C	-0.227579	5.287929	2.715007
C	-1.080760	5.014870	1.628690
C	-0.604658	4.294097	0.521359
C	1.454046	4.112498	-1.956690
C	1.781881	5.468581	-1.748298
C	2.013413	6.327941	-2.838456
C	1.916830	5.845173	-4.153983
C	1.586876	4.495021	-4.373141
C	1.358827	3.638857	-3.284529
C	3.393453	-1.133637	1.203936
C	3.388546	-0.894188	2.723098
C	2.750926	-1.834301	3.564357
C	2.751626	-1.672060	4.958798
C	3.392706	-0.564304	5.543950
C	4.031104	0.376557	4.719179
C	4.028654	0.212632	3.320628
C	4.489819	-2.138018	0.796777
C	5.618805	-2.395097	1.604084
C	6.606488	-3.309788	1.192205
C	6.479276	-3.987132	-0.031380
C	5.356146	-3.740563	-0.842355
C	4.373264	-2.825207	-0.432889
H	-1.258344	-0.489650	2.706114
H	1.286562	0.676227	2.651322
H	-3.857147	-3.636632	-1.184177
H	-5.651438	-0.001243	0.345668
H	-0.444332	-2.460657	-1.020592
H	-2.607198	-3.642484	1.767914
H	-1.713489	-4.834890	3.773035
H	0.660719	-5.657986	3.801028
H	2.137484	-5.251455	1.802199
H	1.238935	-4.052992	-0.196281
H	-1.271595	-2.630248	-3.312364
H	-1.720467	-4.218874	-5.191925
H	-2.238926	-6.632966	-4.706238
H	-2.290363	-7.433222	-2.324477
H	-1.826413	-5.844951	-0.454823
H	-2.432858	1.715822	0.947320
H	-4.522747	-0.767753	2.835408
H	-4.479625	-0.943151	5.324691
H	-3.283130	0.791242	6.695381
H	-2.134707	2.707628	5.536904
H	-2.181760	2.879839	3.048737
H	-3.532745	2.651489	-1.097442
H	-5.277975	4.266348	-1.858818
H	-7.271867	4.754610	-0.401793
H	-7.478524	3.617374	1.830518
H	-5.717319	2.032115	2.600512
H	3.841755	3.623013	-1.437345
H	5.607878	0.029178	0.218608
H	0.392240	2.474151	-1.137302
H	2.623420	3.770681	1.546803
H	1.777641	5.039717	3.525601
H	-0.598300	5.856410	3.582903
H	-2.124875	5.366262	1.640914
H	-1.274370	4.091275	-0.330306
H	1.850190	5.861236	-0.721680
H	2.267088	7.384454	-2.654507
H	2.093227	6.519270	-5.007456
H	1.500896	4.105622	-5.400244
H	1.097917	2.581777	-3.458425
H	2.426085	-1.620724	0.956095
H	2.238138	-2.700414	3.115263
H	2.241519	-2.414446	5.593364
H	3.390746	-0.434347	6.637904
H	4.535372	1.249558	5.164086
H	4.527119	0.960947	2.684605
H	5.725978	-1.883051	2.572708
H	7.478359	-3.496374	1.839962
H	7.249398	-4.707213	-0.351341
H	5.241411	-4.265769	-1.804232
H	3.504947	-2.623820	-1.080799
O	6.044788	2.407355	-1.087657
C	7.233140	1.652705	-0.890371
H	7.444658	1.486588	0.190332
H	7.185251	0.665528	-1.401975
H	8.055046	2.248851	-1.329747
O	-6.178467	-2.233941	-0.749560
C	-6.391933	-3.479503	-1.401442
H	-5.872761	-3.525129	-2.384670
H	-6.053861	-4.337568	-0.777550
H	-7.483303	-3.560614	-1.563645

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PtIPrSTAROMeCl2trans SCF Done: -3960.69390659 A.U.

Pt	0.000308	-0.000413	-2.206192
Cl	1.638332	-1.603476	-2.563463
Cl	-1.637833	1.602864	-2.562418
N	-1.050719	-0.339388	0.534287
N	1.050459	0.339691	0.534327
C	-0.000066	0.000006	-0.292637

C	-0.645258	-0.221399	1.867230
C	0.644819	0.222159	1.867254
C	-2.403566	-0.707270	0.155314
C	-2.651628	-1.961449	-0.461859
C	-3.976334	-2.295310	-0.807770
C	-5.039516	-1.413520	-0.538983
C	-4.777778	-0.188092	0.105438
C	-3.475779	0.182583	0.469556
C	-1.531927	-2.982366	-0.714349
C	-1.089073	-3.714709	0.557598
C	-1.936162	-3.894606	1.671356
C	-1.508416	-4.634480	2.790048
C	-0.226684	-5.209300	2.811533
C	0.629748	-5.032201	1.708079
C	0.202668	-4.288938	0.595549
C	-1.873819	-3.954428	-1.855177
C	-1.789898	-3.498249	-3.190299
C	-2.115867	-4.343022	-4.262738
C	-2.534330	-5.664730	-4.020504
C	-2.620198	-6.130399	-2.698083
C	-2.290910	-5.282201	-1.623946
C	-3.270289	1.496871	1.241983
C	-3.266399	1.288495	2.765802
C	-4.004408	0.263446	3.395352
C	-4.002362	0.129136	4.797067
C	-3.261556	1.018155	5.593125
C	-2.523136	2.045047	4.975993
C	-2.527182	2.178039	3.578485
C	-4.273013	2.590881	0.825360
C	-4.107053	3.238972	-0.419591
C	-5.003973	4.234822	-0.838030
C	-6.088594	4.602344	-0.020708
C	-6.264460	3.964149	1.217666
C	-5.362647	2.968716	1.638500
C	2.403351	0.707379	0.155351
C	2.651553	1.961392	-0.462102
C	3.976306	2.295037	-0.808055
C	5.039383	1.413181	-0.539067
C	4.777499	0.187932	0.105648
C	3.475446	-0.182514	0.469816
C	1.532002	2.982444	-0.714711
C	1.089482	3.715175	0.557144
C	1.936810	3.895342	1.670680
C	1.509312	4.635495	2.789280
C	0.227601	5.210356	2.810895
C	-0.629057	5.033019	1.707659
C	-0.202224	4.289474	0.595221
C	1.873980	3.954138	-1.855841
C	2.290858	5.282053	-1.625049
C	2.620182	6.129896	-2.699458
C	2.534559	5.663723	-4.021717
C	2.116305	4.341867	-4.263510
C	1.790297	3.497453	-3.190804
C	3.269806	-1.496547	1.242619
C	3.265981	-1.287658	2.766367
C	2.526572	-2.176765	3.579362
C	2.522568	-2.043305	4.976827
C	3.261233	-1.016379	5.593606
C	4.002246	-0.127807	4.797240
C	4.004248	-0.262585	3.395572
C	4.272337	-2.590831	0.826252
C	5.361432	-2.969267	1.639823
C	6.263017	-3.965015	1.219224
C	6.087447	-4.602913	-0.019341
C	5.003362	-4.234773	-0.837101
C	4.106671	-3.238620	-0.418901
H	-1.322113	-0.460791	2.690306
H	1.321568	0.461777	2.690351
H	-4.154141	-3.259566	-1.301108
H	-5.621685	0.488565	0.302708
H	-0.649652	-2.413348	-1.078586
H	-2.946071	-3.454741	1.661965
H	-2.186784	-4.765323	3.648660
H	0.105479	-5.794711	3.683769
H	1.638118	-5.475976	1.711078
H	0.874142	-4.159948	-0.269025
H	-1.459490	-2.463917	-3.382308
H	-2.035516	-3.968245	-5.295744
H	-2.785643	-6.330623	-4.861584
H	-2.939994	-7.165536	-2.496146
H	-2.350274	-5.662369	-0.592071
H	-2.264850	1.885524	0.972333
H	-4.586359	-0.442760	2.782595
H	-4.585302	-0.679315	5.267113
H	-3.256501	0.911093	6.689564
H	-1.933543	2.746546	5.587828
H	-1.939583	2.980813	3.104135
H	-3.270399	2.942671	-1.072628
H	-4.852944	4.726645	-1.812449
H	-6.792264	5.384285	-0.348352
H	-7.108498	4.242998	1.869020
H	-5.507665	2.486598	2.617425
H	4.154220	3.259175	-1.301584
H	5.621325	-0.488761	0.303145
H	0.649525	2.413589	-1.078670
H	2.946701	3.455445	1.661197
H	2.187856	4.766522	3.647725
H	-0.104362	5.795989	3.683058
H	-1.637403	5.476850	1.710748
H	-0.873887	4.160278	-0.269174
H	2.350045	5.662616	-0.593311
H	2.939816	7.165148	-2.497854
H	2.785894	6.329327	-4.863018
H	2.036159	3.966692	-5.296388
H	1.460050	2.463007	-3.382472
H	2.264294	-1.885153	0.973147
H	1.938794	-2.979570	3.105284
H	1.932821	-2.744470	5.588897
H	3.256220	-0.908940	6.690009
H	4.585382	0.680663	5.267009
H	4.586372	0.443271	2.782575
H	5.506228	-2.487365	2.618885
H	7.106643	-4.244326	1.870912
H	6.790934	-5.385096	-0.346802
H	4.852568	-4.726356	-1.811678
H	3.270450	-2.941866	-1.072294
O	6.340404	1.658063	-0.852811
C	6.661155	2.863434	-1.535673
H	6.137703	2.934956	-2.515072
H	6.410887	3.763017	-0.929114
H	7.753495	2.839137	-1.709366
O	-6.340514	-1.658630	-0.852670
C	-6.661123	-2.864213	-1.535226
H	-6.137691	-2.935907	-2.514623
H	-6.410718	-3.763615	-0.928454
H	-7.753472	-2.840103	-1.708893

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PtIPrSTARPh2Cl2SMe2cis SCF Done: -5211.81295015 A.U.

Pt	-0.035812	-0.280880	-1.757122
Cl	-1.214168	1.749760	-1.973811
Cl	-0.000757	-0.471886	-4.156350
N	1.052778	0.016382	1.058032

N	-1.135142	0.106546	1.070113
C	-0.050651	-0.050168	0.223923
C	0.657185	0.213407	2.384345
C	-0.705191	0.245341	2.392582
C	2.448929	-0.076823	0.674491
C	3.057218	0.997028	-0.037558
C	4.429459	0.897692	-0.344756
C	5.203340	-0.218660	0.020272
C	4.576772	-1.250970	0.741572
C	3.216362	-1.199801	1.106744
C	2.289812	2.274162	-0.408110
C	2.144853	3.245303	0.770860
C	3.039494	3.274690	1.861245
C	2.902594	4.237313	2.879740
C	1.870069	5.187825	2.822419
C	0.967891	5.164876	1.741403
C	1.102916	4.200646	0.729787
C	2.871276	2.966961	-1.652631
C	2.505685	2.497764	-2.934602
C	3.035303	3.091317	-4.092801
C	3.940106	4.163681	-3.990961
C	4.305667	4.641038	-2.720821
C	3.772887	4.049176	-1.560919
C	6.690693	-0.334148	-0.338395
C	2.640115	-2.301805	2.015353
C	2.680563	-1.919230	3.505658
C	3.661663	-1.060707	4.045434
C	3.685819	-0.769792	5.423098
C	2.728390	-1.332819	6.282634
C	1.745122	-2.189939	5.754238
C	1.723255	-2.479856	4.381160
C	3.297797	-3.678279	1.794220
C	2.836250	-4.519697	0.757864
C	3.419180	-5.777286	0.528841
C	4.483033	-6.220959	1.333949
C	4.950472	-5.396539	2.370925
C	4.360069	-4.140905	2.601888
C	-2.542534	0.203561	0.719669
C	-3.224003	-0.930083	0.203881
C	-4.592378	-0.808573	-0.107196
C	-5.294963	0.393940	0.077482
C	-4.600413	1.486807	0.624203
C	-3.236215	1.423933	0.966097
C	-2.526509	-2.285130	0.030614
C	-2.372837	-3.046447	1.351254
C	-3.305647	-2.931983	2.404254
C	-3.163140	-3.691447	3.580131
C	-2.085793	-4.581933	3.724697
C	-1.146772	-4.704674	2.683733
C	-1.290291	-3.940463	1.513498
C	-3.169362	-3.130695	-1.082283
C	-3.849715	-4.339852	-0.830750
C	-4.426876	-5.072516	-1.885887
C	-4.332074	-4.607415	-3.207509
C	-3.655127	-3.401141	-3.469646
C	-3.080144	-2.670403	-2.418029
C	-6.759737	0.559388	-0.338692
C	-2.582816	2.650699	1.624831
C	-2.633015	2.596037	3.161064
C	-1.635159	3.267268	3.904445
C	-1.661632	3.273435	5.307912
C	-2.689918	2.608175	6.001460
C	-3.688170	1.938598	5.275052
C	-3.659376	1.932792	3.867082
C	-3.156202	3.981992	1.096373
C	-4.021742	4.791777	1.862843
C	-4.532170	5.995726	1.341934
C	-4.181696	6.413305	0.047852
C	-3.317685	5.614905	-0.723708
C	-2.811665	4.412357	-0.205004
H	1.381941	0.318171	3.194304
H	-1.412176	0.359577	3.217205
H	4.904565	1.738719	-0.872047
H	5.166566	-2.131033	1.042238
H	1.261763	1.970353	-0.698697
H	3.861937	2.543772	1.912769
H	3.615492	4.246032	3.720132
H	1.767880	5.946302	3.614994
H	0.151843	5.902664	1.682848
H	0.399289	4.190832	-0.118266
H	1.781927	1.670890	-3.029195
H	2.722888	2.717176	-5.080837
H	4.350330	4.633194	-4.899601
H	5.006152	5.486639	-2.627568
H	4.055339	4.442260	-0.571530
H	7.115266	-1.074621	0.372698
H	1.568372	-2.420948	1.749055
H	4.411860	-0.603850	3.380883
H	4.458809	-0.094329	5.823566
H	2.743823	-1.101735	7.359562
H	0.983241	-2.631610	6.416264
H	0.942304	-3.143214	3.975058
H	2.011996	-4.168234	0.117332
H	3.035927	-6.417853	-0.281844
H	4.940205	-7.207620	1.157998
H	5.777666	-5.734929	3.015424
H	4.722784	-3.517585	3.433857
H	-5.116960	-1.686541	-0.511777
H	-5.130033	2.441317	0.771619
H	-1.499099	-2.059782	-0.333256
H	-4.158329	-2.242770	2.300311
H	-3.905105	-3.587303	4.388146
H	-1.977831	-5.180226	4.643454
H	-0.298157	-5.400907	2.780321
H	-0.553849	-4.048588	0.700023
H	-3.931749	-4.716247	0.200444
H	-4.954955	-6.014709	-1.667309
H	-4.783121	-5.181771	-4.032574
H	-3.568530	-3.023451	-4.500906
H	-2.548496	-1.727264	-2.633765
H	-7.175760	1.355360	0.318597
H	-1.509452	2.645836	1.337698
H	-0.822306	3.785377	3.370186
H	-0.869140	3.798754	5.864860
H	-2.710053	2.610306	7.102987
H	-4.498816	1.412794	5.805003
H	-4.444871	1.398398	3.310196
H	-4.297430	4.485132	2.883485
H	-5.206770	6.611596	1.958537
H	-4.578983	7.357047	-0.358910
H	-3.034171	5.928080	-1.741312
H	-2.149469	3.781287	-0.819382
S	1.185199	-2.268472	-1.626825
C	2.714066	-1.969155	-2.584391
H	3.303810	-1.220309	-2.025177
H	3.276995	-2.920749	-2.649841
H	2.429209	-1.578764	-3.581084
C	0.386445	-3.486450	-2.737625
H	1.051296	-4.370219	-2.807733
H	-0.583380	-3.765472	-2.284932
H	0.218980	-3.004209	-3.720997
C	-7.590097	-0.699974	-0.062280

C	-8.146709	-0.901165	1.220161
C	-7.790636	-1.694210	-1.043954
C	-8.880325	-2.061831	1.517267
C	-8.519990	-2.859476	-0.748074
C	-9.068024	-3.047990	0.532343
H	-8.004615	-0.130951	1.997127
H	-7.378654	-1.548178	-2.054936
H	-9.312777	-2.194325	2.522239
H	-8.663412	-3.623970	-1.528359
H	-9.645185	-3.958142	0.761142
C	-6.918689	1.077985	-1.779356
C	-5.841065	1.180113	-2.682548
C	-8.201894	1.485748	-2.213301
C	-6.042271	1.667484	-3.988409
C	-8.403347	1.973002	-3.513297
C	-7.321266	2.063742	-4.409297
H	-4.826049	0.892465	-2.368496
H	-9.055934	1.413628	-1.519308
H	-5.183263	1.740002	-4.674307
H	-9.411398	2.286942	-3.829347
H	-7.476868	2.447472	-5.430310
C	7.447772	0.979238	-0.077313
C	7.821288	1.869171	-1.104853
C	7.771378	1.320173	1.256050
C	8.490162	3.071015	-0.806783
C	8.441164	2.516677	1.555816
C	8.802201	3.400231	0.522140
H	7.597952	1.618477	-2.153110
H	7.494104	0.631748	2.072290
H	8.772735	3.751795	-1.625597
H	8.687830	2.759074	2.602097
H	9.329798	4.339205	0.753353
C	6.929503	-0.917055	-1.737187
C	6.179314	-0.522272	-2.866865
C	7.959884	-1.866059	-1.918083
C	6.455447	-1.058076	-4.137950
C	8.235995	-2.405316	-3.185511
C	7.483540	-2.002058	-4.302510
H	5.365474	0.212035	-2.760867
H	8.556951	-2.186490	-1.047937
H	5.858265	-0.732882	-5.004789
H	9.042825	-3.146962	-3.299896
H	7.696363	-2.423753	-5.297695

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PtIPrSTARPh2Cl2SMe2trans SCF Done: -5211.81368523 A.U.

Pt	0.059410	0.085838	-1.741811
Cl	-0.694100	2.326154	-1.777953
Cl	0.774981	-2.170875	-1.827012
N	1.053691	0.086071	1.110015
N	-1.133821	0.183838	1.061425
C	-0.024221	0.096318	0.247236
C	0.615856	0.177601	2.433913
C	-0.747310	0.217278	2.404805
C	2.452924	-0.093143	0.758304
C	3.180412	0.969135	0.151962
C	4.526837	0.733841	-0.195657
C	5.167544	-0.490504	0.063385
C	4.437037	-1.493126	0.724027
C	3.090591	-1.321409	1.097265
C	2.569558	2.366256	-0.039867
C	2.461083	3.157113	1.273216
C	3.259809	2.889268	2.404330
C	3.176975	3.698920	3.553555
C	2.297524	4.793250	3.587547
C	1.491680	5.067460	2.465616
C	1.569390	4.253966	1.324010
C	3.289118	3.204227	-1.109862
C	2.828155	3.183030	-2.444509
C	3.475850	3.930151	-3.443934
C	4.599763	4.712878	-3.127003
C	5.062309	4.749888	-1.800080
C	4.409468	4.007000	-0.800877
C	6.619196	-0.766200	-0.346327
C	2.408062	-2.416210	1.934456
C	2.509611	-2.133631	3.443868
C	3.600366	-1.444888	4.016551
C	3.676582	-1.241432	5.407778
C	2.661410	-1.722469	6.250883
C	1.569266	-2.410902	5.690899
C	1.496140	-2.614289	4.303762
C	2.914053	-3.832716	1.594582
C	2.522082	-4.429428	0.374824
C	2.963973	-5.716023	0.027347
C	3.810291	-6.434151	0.891820
C	4.207509	-5.851241	2.105950
C	3.761106	-4.562852	2.455663
C	-2.530294	0.249192	0.661768
C	-3.180380	-0.924217	0.190132
C	-4.549892	-0.842551	-0.135834
C	-5.281746	0.349367	-0.002295
C	-4.615310	1.482297	0.495751
C	-3.251969	1.463880	0.848346
C	-2.466558	-2.280959	0.101219
C	-2.347103	-2.988465	1.457229
C	-3.219685	-2.733858	2.535883
C	-3.120172	-3.468732	3.732709
C	-2.149268	-4.474700	3.868534
C	-1.269573	-4.735135	2.800375
C	-1.365402	-3.994977	1.610782
C	-3.100652	-3.193882	-0.962367
C	-3.926833	-4.289320	-0.636731
C	-4.503614	-5.081339	-1.647299
C	-4.261280	-4.792449	-2.999951
C	-3.437174	-3.702197	-3.335712
C	-2.864234	-2.912869	-2.326447
C	-6.758983	0.456316	-0.397561
C	-2.634141	2.719001	1.487290
C	-2.635358	2.640232	3.021969
C	-1.579090	3.232183	3.749425
C	-1.567054	3.210398	5.153602
C	-2.615070	2.595155	5.862362
C	-3.673635	2.004962	5.151081
C	-3.683087	2.028297	3.743825
C	-3.287393	4.026137	0.986115
C	-3.957933	4.918463	1.849547
C	-4.531622	6.106656	1.357794
C	-4.443479	6.425095	-0.006233
C	-3.777684	5.542382	-0.876666
C	-3.207537	4.357386	-0.386734
H	1.316611	0.204889	3.271010
H	-1.480822	0.264391	3.212329
H	5.093370	1.546824	-0.671682
H	4.924039	-2.453743	0.955173
H	1.533331	2.230643	-0.414916
H	3.962553	2.041280	2.386165
H	3.812496	3.473638	4.425229
H	2.240451	5.433500	4.482378
H	0.798109	5.923643	2.478656
H	0.940260	4.474589	0.446240
H	1.925059	2.600809	-2.686363
H	3.088416	3.910864	-4.475532
H	5.105361	5.302487	-3.908596

H	5.935162	5.367792	-1.535186
H	4.771865	4.060234	0.237918
H	7.011362	-1.488459	0.404002
H	1.326684	-2.407019	1.679655
H	4.400866	-1.057004	3.367357
H	4.537376	-0.700033	5.832423
H	2.718019	-1.559528	7.338980
H	0.762451	-2.789039	6.339077
H	0.633086	-3.148419	3.874976
H	1.873005	-3.863801	-0.312950
H	2.642931	-6.160339	-0.928562
H	4.156628	-7.444133	0.619911
H	4.868378	-6.402488	2.794364
H	4.072075	-4.125806	3.416834
H	-5.056070	-1.750167	-0.496114
H	-5.169588	2.427134	0.610173
H	-1.430532	-2.094946	-0.255321
H	-3.995049	-1.958066	2.436867
H	-3.814507	-3.255566	4.561504
H	-2.077644	-5.056381	4.801485
H	-0.502569	-5.520690	2.891870
H	-0.679577	-4.210125	0.775178
H	-4.120997	-4.531149	0.419511
H	-5.145806	-5.932747	-1.370139
H	-4.708645	-5.415452	-3.790963
H	-3.235184	-3.471044	-4.394332
H	-2.212364	-2.062979	-2.582653
H	-7.188000	1.255997	0.245334
H	-1.571634	2.760366	1.161847
H	-0.746063	3.706012	3.205879
H	-0.726666	3.671880	5.696459
H	-2.604769	2.573444	6.963824
H	-4.501022	1.519554	5.693575
H	-4.516471	1.557394	3.199106
H	-4.032982	4.689830	2.923098
H	-5.049697	6.786869	2.053158
H	-4.890755	7.355580	-0.391230
H	-3.699537	5.777456	-1.950376
H	-2.692861	3.668821	-1.075305
S	0.280256	0.260516	-4.153310
C	-0.640010	-1.132008	-4.901593
H	-1.715862	-0.903521	-4.781522
H	-0.391263	-1.187261	-5.979827
H	-0.383898	-2.073579	-4.376834
C	1.989047	-0.302200	-4.487957
H	2.140381	-0.360445	-5.583940
H	2.665918	0.458556	-4.054952
H	2.155393	-1.280107	-3.994674
C	-7.549174	-0.818790	-0.073298
C	-8.045538	-1.013499	1.234930
C	-7.777075	-1.826708	-1.034029
C	-8.746291	-2.181681	1.576708
C	-8.474479	-2.999625	-0.693522
C	-8.962060	-3.181859	0.611636
H	-7.881296	-0.232707	1.996756
H	-7.412261	-1.687472	-2.063822
H	-9.130770	-2.309738	2.601497
H	-8.640560	-3.774837	-1.458558
H	-9.513690	-4.098160	0.875916
C	-6.964300	0.928612	-1.845584
C	-5.972779	0.804919	-2.840173
C	-8.206868	1.500670	-2.202939
C	-6.218838	1.235949	-4.157529
C	-8.453670	1.932235	-3.515059
C	-7.457874	1.800113	-4.500669
H	-4.991779	0.376651	-2.582695
H	-8.993524	1.605277	-1.437071
H	-5.428405	1.134623	-4.918499
H	-9.428259	2.378980	-3.769821
H	-7.647471	2.141932	-5.530701
C	7.509637	0.478230	-0.241867
C	7.745822	1.324614	-1.346133
C	8.093418	0.815282	0.999325
C	8.538422	2.478247	-1.210978
C	8.889243	1.964608	1.136639
C	9.113839	2.802421	0.029595
H	7.311810	1.071516	-2.326260
H	7.922881	0.161853	1.871633
H	8.709955	3.125650	-2.085699
H	9.341136	2.204562	2.112626
H	9.740525	3.702578	0.133177
C	6.745357	-1.472368	-1.706559
C	5.670135	-1.597431	-2.609009
C	7.994011	-2.030180	-2.067455
C	5.840172	-2.255624	-3.842181
C	8.164764	-2.687213	-3.295054
C	7.085325	-2.801424	-4.191184
H	4.683367	-1.189281	-2.341361
H	8.846054	-1.941588	-1.373062
H	4.985098	-2.347041	-4.531070
H	9.146103	-3.116574	-3.553773
H	7.215923	-3.319376	-5.154715

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PtIPrSTARPh2Cl2trans SCF Done: -4733.90347917 A.U.

Pt	-0.000019	0.000057	-1.766696
Cl	-1.224838	1.933908	-2.135252
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N	1.102722	-0.020179	0.976699
N	-1.102737	0.020251	0.976691
C	-0.000007	0.000036	0.147801
C	0.682089	-0.000620	2.309581
C	-0.682117	0.000677	2.309577
C	2.502685	-0.110106	0.597034
C	3.137120	0.998553	-0.024708
C	4.498335	0.876086	-0.366775
C	5.232496	-0.294546	-0.107810
C	4.579146	-1.359176	0.538315
C	3.223951	-1.296128	0.913558
C	2.400309	2.321870	-0.275542
C	2.245222	3.170339	0.992337
C	3.138898	3.088177	2.081022
C	2.993653	3.933062	3.197636
C	1.953645	4.876400	3.242479
C	1.054074	4.966316	2.163123
C	1.198062	4.118744	1.052491
C	3.005841	3.120142	-1.441626
C	2.726692	2.712512	-2.765589
C	3.268809	3.401019	-3.861950
C	4.104143	4.514140	-3.654034
C	4.388823	4.928833	-2.342544
C	3.842767	4.238079	-1.244726
C	6.696020	-0.456120	-0.532950
C	2.604260	-2.470774	1.689014
C	2.674595	-2.273834	3.212727
C	3.702511	-1.536701	3.838525
C	3.749434	-1.410070	5.240263
C	2.768103	-2.018632	6.039831
C	1.738577	-2.756596	5.426436
C	1.693975	-2.882537	4.029061
C	3.189653	-3.834095	1.270415
C	2.801721	-4.400950	0.035312
C	3.318198	-5.637704	-0.383286

C	4.235919	-6.333651	0.424401
C	4.629257	-5.780047	1.653566
C	4.108357	-4.542127	2.074455
C	-2.502697	0.110146	0.597007
C	-3.137097	-0.998536	-0.024724
C	-4.498315	-0.876111	-0.366796
C	-5.232501	0.294511	-0.107853
C	-4.579178	1.359172	0.538241
C	-3.223983	1.296167	0.913488
C	-2.400254	-2.321839	-0.275543
C	-2.245178	-3.170301	0.992336
C	-3.138917	-3.088180	2.080978
C	-2.993684	-3.933048	3.197604
C	-1.953628	-4.876332	3.242505
C	-1.054001	-4.966211	2.163194
C	-1.197974	-4.118652	1.052548
C	-3.005753	-3.120102	-1.441654
C	-3.842534	-4.238153	-1.244809
C	-4.388543	-4.928893	-2.342661
C	-4.103961	-4.514069	-3.654129
C	-3.268768	-3.400829	-3.861991
C	-2.726698	-2.712340	-2.765599
C	-6.696039	0.456020	-0.533002
C	-2.604281	2.470843	1.688894
C	-2.674568	2.273959	3.212615
C	-1.693926	2.882689	4.028901
C	-1.738497	2.756793	5.426280
C	-2.768013	2.018854	6.039726
C	-3.749364	1.410266	5.240206
C	-3.702471	1.536851	3.838459
C	-3.189697	3.834149	1.270287
C	-4.108532	4.542086	2.074267
C	-4.629478	5.779983	1.653379
C	-4.236054	6.333668	0.424274
C	-3.318200	5.637824	-0.383345
C	-2.801675	4.401087	0.035256
H	1.399602	0.006039	3.133113
H	-1.399639	-0.005997	3.133101
H	4.993448	1.730266	-0.851424
H	5.135080	-2.287311	0.745317
H	1.373607	2.061201	-0.611901
H	3.964507	2.359640	2.052872
H	3.705015	3.855002	4.035665
H	1.844375	5.542487	4.113240
H	0.234714	5.702571	2.182912
H	0.496604	4.201376	0.206152
H	2.067650	1.843060	-2.929360
H	3.031569	3.069890	-4.885683
H	4.527000	5.058885	-4.513347
H	5.038975	5.800966	-2.167049
H	4.066435	4.578714	-0.221822
H	7.150675	-1.155911	0.203067
H	1.525639	-2.509607	1.424940
H	4.474822	-1.048949	3.223302
H	4.560471	-0.828459	5.707444
H	2.802132	-1.916654	7.136209
H	0.959071	-3.234529	6.041222
H	0.878949	-3.455555	3.557576
H	2.097777	-3.852874	-0.611468
H	3.000444	-6.059298	-1.350386
H	4.641085	-7.304267	0.096494
H	5.345380	-6.315499	2.297661
H	4.416461	-4.128111	3.046868
H	-4.993396	-1.730319	-0.851432
H	-5.135138	2.287300	0.745202
H	-1.373548	-2.061157	-0.611884
H	-3.964563	-2.359687	2.052780
H	-3.705091	-3.855021	4.035597
H	-1.844361	-5.542406	4.113277
H	-0.234608	-5.702428	2.183028
H	-0.496473	-4.201258	0.206242
H	-4.066128	-4.578888	-0.221922
H	-5.038581	-5.801120	-2.167209
H	-4.526784	-5.058802	-4.513467
H	-3.031603	-3.069595	-4.885708
H	-2.067765	-1.842797	-2.929329
H	-7.150678	1.155917	0.202924
H	-1.525674	2.509670	1.424767
H	-0.878905	3.455685	3.557381
H	-0.958977	3.234742	6.041035
H	-2.802013	1.916918	7.136109
H	-4.560392	0.828674	5.707422
H	-4.474795	1.049076	3.223270
H	-4.416692	4.128013	3.046639
H	-5.345700	6.315361	2.297424
H	-4.641257	7.304268	0.096367
H	-3.000375	6.059481	-1.350394
H	-2.097630	3.853087	-0.611477
C	-7.488304	-0.852682	-0.421944
C	-8.058139	-1.219727	0.817195
C	-7.642894	-1.728616	-1.517678
C	-8.760398	-2.427814	0.961267
C	-8.341205	-2.940829	-1.375292
C	-8.902878	-3.295004	-0.136648
H	-7.951564	-0.543556	1.682381
H	-7.219201	-1.453215	-2.496322
H	-9.203558	-2.691079	1.935285
H	-8.449235	-3.611155	-2.242864
H	-9.455429	-4.241873	-0.027682
C	-6.853214	1.130934	-1.906431
C	-5.785370	1.285052	-2.813568
C	-8.127620	1.619703	-2.277075
C	-5.987946	1.903560	-4.062288
C	-8.330441	2.237822	-3.519964
C	-7.258363	2.380637	-4.420967
H	-4.777818	0.933505	-2.543508
H	-8.973976	1.507119	-1.579033
H	-5.137756	2.015757	-4.753921
H	-9.331395	2.613581	-3.787002
H	-7.414782	2.867332	-5.396909
C	7.488305	0.852588	-0.422109
C	7.642830	1.728383	-1.517967
C	8.058219	1.219789	0.816942
C	8.341157	2.940610	-1.375780
C	8.760499	2.427891	0.960817
C	8.902912	3.294940	-0.137215
H	7.219081	1.452862	-2.496552
H	7.951696	0.543730	1.682223
H	8.449128	3.610825	-2.243444
H	9.203726	2.691271	1.934773
H	9.455475	4.241820	-0.028401
C	6.853163	-1.131235	-1.906289
C	5.785363	-1.285169	-2.813509
C	8.127493	-1.620312	-2.276778
C	5.987912	-1.903809	-4.062168
C	8.330283	-2.238567	-3.519605
C	7.258255	-2.381202	-4.420694
H	4.777868	-0.933379	-2.543556
H	8.973809	-1.507867	-1.578667
H	5.137763	-2.015860	-4.753874
H	9.331174	-2.614582	-3.786525
H	7.414652	-2.867996	-5.396590

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PtIPrSTARtolCl2SMe2cis SCF Done: -4602.58794742 A.U.

Pt	-0.163493	0.172235	-2.275064
Cl	2.180469	0.366416	-2.419919
Cl	-0.282631	0.252089	-4.679048
N	-0.425794	-0.967843	0.523194
N	0.583708	0.974934	0.579802
C	-0.000191	0.069529	-0.289470
C	-0.106611	-0.710191	1.859214
C	0.500277	0.509483	1.894946
C	-1.110994	-2.177790	0.110545
C	-0.405963	-3.170757	-0.631047
C	-1.101656	-4.339036	-0.997067
C	-2.445048	-4.565482	-0.638818
C	-3.096250	-3.583139	0.127424
C	-2.457558	-2.391189	0.528779
C	1.085006	-3.033395	-0.973313
C	1.997303	-3.327661	0.223692
C	1.624331	-4.156509	1.300120
C	2.534895	-4.458726	2.330763
C	3.848975	-3.949597	2.321391
C	4.215471	-3.106759	1.245138
C	3.309345	-2.799587	0.220652
C	1.486376	-3.855091	-2.209002
C	1.274346	-3.318817	-3.499245
C	1.603785	-4.055065	-4.646454
C	2.158209	-5.352200	-4.555289
C	2.371938	-5.880752	-3.265606
C	2.046475	-5.145355	-2.111391
C	-3.157201	-5.826242	-1.074376
C	-3.209683	-1.414865	1.452424
C	-2.907717	-1.662201	2.940035
C	-2.585968	-2.933398	3.455349
C	-2.358343	-3.119905	4.832478
C	-2.442939	-2.047157	5.742170
C	-2.764978	-0.772590	5.219003
C	-2.993621	-0.583494	3.849709
C	-4.730271	-1.394879	1.203208
C	-5.264893	-0.619675	0.149913
C	-6.643730	-0.587917	-0.104973
C	-7.552788	-1.331763	0.681282
C	-7.018022	-2.104111	1.732225
C	-5.636259	-2.132133	1.993563
C	1.258400	2.224795	0.268174
C	0.513893	3.325971	-0.231241
C	1.190246	4.535704	-0.479145
C	2.568115	4.688569	-0.244281
C	3.269724	3.586504	0.275573
C	2.649178	2.352745	0.551193
C	-1.002590	3.251432	-0.448882
C	-1.797356	3.406262	0.851386
C	-1.337063	4.173715	1.941001
C	-2.123287	4.339082	3.095217
C	-3.399495	3.748635	3.207443
C	-3.855339	2.970554	2.118606
C	-3.069611	2.803059	0.967954
C	-1.472210	4.204567	-1.560481
C	-2.305519	5.314930	-1.324782
C	-2.693336	6.163454	-2.380011
C	-2.265074	5.933737	-3.702348
C	-1.429632	4.815076	-3.934001
C	-1.039550	3.968450	-2.888087
C	3.277410	5.982055	-0.574040
C	3.488676	1.231255	1.187583
C	3.431304	1.249182	2.723736
C	3.600432	0.040045	3.437171
C	3.591562	0.018261	4.838427
C	3.416886	1.202716	5.592059
C	3.246826	2.405822	4.878630
C	3.253418	2.430971	3.470667
C	4.947116	1.227049	0.686820
C	6.025455	1.674704	1.476543
C	7.341297	1.667701	0.976733
C	7.630207	1.209450	-0.323775
C	6.545507	0.757654	-1.110735
C	5.233269	0.766151	-0.618729
H	-0.337889	-1.420536	2.655621
H	0.888416	1.090763	2.734110
H	-0.563153	-5.099455	-1.583642
H	-4.144626	-3.739968	0.425347
H	1.263672	-1.974386	-1.256578
H	0.608302	-4.581036	1.336777
H	2.214583	-5.112910	3.159232
H	5.232573	-2.681980	1.207403
H	3.622030	-2.145480	-0.609438
H	0.858314	-2.303278	-3.609408
H	1.434493	-3.601139	-5.637276
H	2.810066	-6.887590	-3.158814
H	2.242624	-5.582072	-1.119062
H	-3.340439	-5.822306	-2.170830
H	-4.137672	-5.939633	-0.570900
H	-2.549618	-6.729672	-0.857907
H	-2.842080	-0.392309	1.220846
H	-2.501949	-3.794703	2.773902
H	-2.105726	-4.126623	5.205314
H	-2.830826	0.092003	5.900692
H	-3.231800	0.424159	3.471101
H	-4.575830	-0.043351	-0.487730
H	-7.025843	0.033148	-0.932928
H	-7.697855	-2.694436	2.369242
H	-5.261035	-2.732501	2.836851
H	0.613142	5.384154	-0.878510
H	4.351298	3.676130	0.463234
H	-1.209855	2.228467	-0.835047
H	-0.345298	4.649829	1.888029
H	-1.732678	4.944589	3.930365
H	-4.844527	2.485509	2.171124
H	-3.457681	2.195450	0.133742
H	-2.660916	5.524984	-0.304044
H	-3.346408	7.026026	-2.164857
H	-1.076867	4.598269	-4.956226
H	-0.386675	3.104311	-3.101944
H	2.604267	6.857270	-0.470993
H	3.640597	5.972126	-1.625397
H	4.162373	6.142772	0.074363
H	3.049039	0.265472	0.858483
H	3.729456	-0.901203	2.878121
H	3.717119	-0.944072	5.362853
H	3.103587	3.348234	5.433662
H	3.109650	3.389717	2.948139
H	5.843177	2.029804	2.502581
H	8.163237	2.025221	1.619806
H	6.731293	0.390778	-2.134329
H	4.404516	0.423592	-1.259022
S	-2.480736	-0.109998	-2.217664
C	-2.811367	-1.601944	-3.224389
H	-2.375016	-2.460102	-2.680495
H	-3.908952	-1.722492	-3.315639
H	-2.316463	-1.471551	-4.207009
C	-3.220829	1.148957	-3.324046
H	-4.299037	0.917023	-3.433128
H	-3.083412	2.135877	-2.843647

H	-2.681967	1.122326	-4.291940
C	9.042826	1.190972	-0.864492
H	9.123716	1.772226	-1.808064
H	9.764602	1.618894	-0.140124
H	9.373899	0.155982	-1.098936
C	3.419616	1.169182	7.104349
H	4.414791	0.870493	7.500117
H	3.171851	2.159342	7.536459
H	2.686305	0.433048	7.497525
C	-2.195785	-2.238683	7.221881
H	-1.354271	-1.606174	7.577777
H	-3.086395	-1.951997	7.821604
H	-1.951604	-3.292336	7.463391
C	-9.040262	-1.277531	0.413180
H	-9.589771	-2.041539	0.998588
H	-9.462831	-0.284470	0.681427
H	-9.267425	-1.441854	-0.661322
C	2.532919	-6.126146	-5.800061
H	1.705731	-6.132500	-6.541118
H	3.412002	-5.671610	-6.307464
H	2.791106	-7.178817	-5.566731
C	4.844279	-4.301449	3.405228
H	5.367660	-3.400503	3.789256
H	4.355737	-4.806139	4.262905
H	5.631631	-4.986433	3.020721
C	-4.263051	3.961523	4.431322
H	-3.657291	4.239605	5.317418
H	-4.996851	4.781479	4.266107
H	-4.848513	3.053630	4.684421
C	-2.677115	6.841807	-4.839858
H	-3.223330	6.281794	-5.629269
H	-3.334932	7.663060	-4.491310
H	-1.792797	7.301861	-5.331276

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PtIPrSTARtolCl2SMe2trans SCF Done: -4602.58914896 A.U.

Pt	0.060373	0.053780	-2.286986
Cl	2.413954	0.271789	-2.251400
Cl	-2.299964	-0.096630	-2.442758
N	-0.234463	-1.032443	0.509122
N	0.332475	1.082438	0.572702
C	0.033888	0.055514	-0.296946
C	-0.092601	-0.684878	1.854905
C	0.240513	0.637670	1.895265
C	-0.694903	-2.340719	0.073366
C	0.213016	-3.249097	-0.540979
C	-0.296334	-4.482829	-0.991574
C	-1.644126	-4.852449	-0.827044
C	-2.491317	-3.962451	-0.144782
C	-2.046405	-2.711960	0.326873
C	1.719463	-2.959238	-0.638466
C	2.442158	-3.088732	0.710209
C	1.952488	-3.857877	1.784139
C	2.702822	-4.013081	2.965341
C	3.969757	-3.414018	3.114210
C	4.452388	-2.632049	2.038245
C	3.704204	-2.469269	0.863785
C	2.427124	-3.805827	-1.708845
C	2.534107	-3.326511	-3.032586
C	3.151089	-4.094099	-4.033026
C	3.687151	-5.370900	-3.754379
C	3.585318	-5.843821	-2.428959
C	2.973793	-5.075131	-1.423647
C	-2.164554	-6.161861	-1.375346
C	-3.002457	-1.854617	1.174039
C	-2.796058	-2.090384	2.679742
C	-2.393547	-3.333287	3.208509
C	-2.256075	-3.521137	4.597126
C	-2.513224	-2.477094	5.507973
C	-2.915584	-1.231061	4.972769
C	-3.056020	-1.041436	3.591118
C	-4.481360	-2.032122	0.777479
C	-4.947228	-1.475855	-0.436043
C	-6.284034	-1.620168	-0.831559
C	-7.215749	-2.326581	-0.035973
C	-6.747430	-2.881145	1.171336
C	-5.406537	-2.735819	1.574457
C	0.713787	2.446118	0.242647
C	-0.271435	3.356330	-0.231207
C	0.124253	4.681722	-0.498141
C	1.441855	5.131760	-0.299374
C	2.379596	4.214226	0.204970
C	2.048635	2.875188	0.493314
C	-1.748641	2.965631	-0.386441
C	-2.505492	2.932219	0.946624
C	-2.106950	3.666505	2.080843
C	-2.886308	3.668266	3.253344
C	-4.093202	2.944812	3.333979
C	-4.485061	2.199821	2.196459
C	-3.706576	2.190043	1.030376
C	-2.468189	3.842562	-1.424635
C	-3.370375	4.866260	-1.074939
C	-3.980533	5.661880	-2.062780
C	-3.716344	5.462862	-3.432396
C	-2.809824	4.433768	-3.778284
C	-2.200043	3.640815	-2.797121
C	1.840473	6.549845	-0.639986
C	3.114681	1.971483	1.135712
C	2.993425	1.947067	2.666956
C	3.302350	0.765260	3.377258
C	3.236585	0.722871	4.777180
C	2.861998	1.859075	5.531097
C	2.555728	3.037157	4.819993
C	2.620045	3.082332	3.414783
C	4.547240	2.329085	0.685018
C	5.545372	2.757889	1.582332
C	6.843385	3.065947	1.131629
C	7.194295	2.955779	-0.227447
C	6.188952	2.526163	-1.125038
C	4.895730	2.220083	-0.682046
H	-0.243695	-1.412116	2.655382
H	0.420803	1.307159	2.738878
H	0.393802	-5.182514	-1.486596
H	-3.543733	-4.238761	0.025385
H	1.838882	-1.904525	-0.964791
H	0.969841	-4.348775	1.700177
H	2.292158	-4.621736	3.788555
H	5.436951	-2.141702	2.122334
H	4.106277	-1.858582	0.038826
H	2.152889	-2.320114	-3.267227
H	3.228392	-3.684812	-5.054689
H	4.000256	-6.833793	-2.174412
H	2.927972	-5.468565	-0.395510
H	-2.510670	-6.039360	-2.425538
H	-3.028561	-6.537723	-0.790864
H	-1.379309	-6.944886	-1.382002
H	-2.756944	-0.788505	0.978986
H	-2.178055	-4.171899	2.527826
H	-1.938545	-4.506023	4.978948
H	-3.116918	-0.387843	5.654861
H	-3.363039	-0.055634	3.205524
H	-4.238133	-0.934598	-1.082948
H	-6.613156	-1.170951	-1.783986

H	-7.446125	-3.438330	1.818070
H	-5.083050	-3.175524	2.530298
H	-0.633474	5.385799	-0.874857
H	3.417044	4.541362	0.376693
H	-1.783513	1.935092	-0.801310
H	-1.175014	4.252946	2.050183
H	-2.547774	4.253727	4.124793
H	-5.419407	1.614468	2.223955
H	-4.041078	1.606894	0.156839
H	-3.606089	5.047101	-0.014683
H	-4.682121	6.456375	-1.757238
H	-2.582630	4.249854	-4.842333
H	-1.498616	2.842311	-3.085497
H	0.999244	7.257963	-0.495995
H	2.150970	6.626077	-1.705517
H	2.697088	6.894572	-0.026253
H	2.925902	0.936733	0.774731
H	3.585478	-0.142986	2.820983
H	3.474131	-0.219944	5.297975
H	2.257875	3.942272	5.375649
H	2.368535	4.019796	2.894269
H	5.315217	2.853218	2.654108
H	7.600550	3.399240	1.861409
H	6.425185	2.426732	-2.198157
H	4.132380	1.892323	-1.405591
S	0.239306	-0.134236	-4.699810
C	-0.874897	1.112740	-5.441274
H	-0.398428	2.098597	-5.281452
H	-0.962799	0.915102	-6.527945
H	-1.862151	1.075048	-4.939812
C	-0.706803	-1.651813	-5.090838
H	-0.776993	-1.759449	-6.191356
H	-0.136995	-2.498989	-4.663959
H	-1.705564	-1.594400	-4.614997
C	8.589914	3.273216	-0.717085
H	8.573649	4.027251	-1.533048
H	9.229772	3.668593	0.097236
H	9.089919	2.369413	-1.128597
C	2.794743	1.802560	7.041264
H	3.787975	1.569311	7.482428
H	2.453523	2.764990	7.472265
H	2.097669	1.009795	7.388340
C	-2.366800	-2.670715	7.000984
H	-1.644504	-1.947089	7.436285
H	-3.333253	-2.511994	7.526632
H	-2.013310	-3.691519	7.248794
C	-8.658849	-2.466165	-0.467576
H	-9.231203	-3.119148	0.221463
H	-9.170141	-1.479282	-0.497158
H	-8.738401	-2.896711	-1.488706
C	4.379857	-6.179028	-4.829488
H	3.849272	-6.107284	-5.801758
H	5.416982	-5.814642	-5.001493
H	4.450187	-7.251127	-4.555289
C	4.800658	-3.618586	4.362033
H	5.295749	-2.678919	4.684684
H	4.187406	-3.992248	5.206794
H	5.609955	-4.362013	4.188133
C	-4.954101	2.972927	4.577849
H	-4.423746	3.437677	5.433181
H	-5.886573	3.555086	4.408702
H	-5.267943	1.952063	4.881893
C	-4.388355	6.298566	-4.499463
H	-5.138054	5.703797	-5.066411
H	-4.917544	7.169879	-4.063967
H	-3.655599	6.680448	-5.241623

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PtIPrSTARtolCl2trans SCF Done: -4124.67843044 A.U.

Pt	0.000030	0.000017	-2.372532
Cl	2.275243	0.264540	-2.736712
Cl	-2.275266	-0.264485	-2.736292
N	-0.419852	-1.020088	0.369214
N	0.419676	1.020145	0.369210
C	-0.000039	0.000007	-0.458874
C	-0.248542	-0.635154	1.702079
C	0.248230	0.635282	1.702071
C	-1.011717	-2.293831	-0.005909
C	-0.207853	-3.293129	-0.619986
C	-0.815452	-4.520964	-0.942735
C	-2.170609	-4.787655	-0.671834
C	-2.924906	-3.785627	-0.036797
C	-2.376397	-2.537048	0.316718
C	1.290749	-3.090400	-0.885059
C	2.148828	-3.235110	0.376299
C	1.766100	-4.018484	1.483198
C	2.623114	-4.177622	2.588455
C	3.892572	-3.565909	2.627371
C	4.268879	-2.770772	1.519055
C	3.415092	-2.606861	0.418749
C	1.801004	-3.965488	-2.040924
C	1.475487	-3.608334	-3.369288
C	1.899290	-4.388825	-4.452778
C	2.667616	-5.560110	-4.256718
C	2.989547	-5.913347	-2.930992
C	2.566812	-5.130450	-1.840418
C	-2.799276	-6.100170	-1.080476
C	-3.250614	-1.528388	1.081409
C	-3.092167	-1.651736	2.605343
C	-2.795377	-2.870356	3.247864
C	-2.694970	-2.944950	4.650418
C	-2.886577	-1.808694	5.461584
C	-3.182625	-0.587263	4.812032
C	-3.284865	-0.509714	3.416446
C	-4.732156	-1.591940	0.661608
C	-5.119544	-1.078825	-0.597613
C	-6.455936	-1.126776	-1.016961
C	-7.464330	-1.689403	-0.200335
C	-7.073920	-2.199899	1.053354
C	-5.733527	-2.151020	1.480393
C	1.011702	2.293810	-0.005924
C	0.207962	3.293169	-0.620086
C	0.815703	4.520913	-0.942866
C	2.170888	4.787469	-0.671909
C	2.925041	3.785405	-0.036782
C	2.376375	2.536890	0.316764
C	-1.290648	3.090543	-0.885190
C	-2.148754	3.235335	0.376135
C	-1.765992	4.018724	1.483024
C	-2.623007	4.177948	2.588256
C	-3.892515	3.566319	2.627166
C	-4.268845	2.771165	1.518882
C	-3.415046	2.607164	0.418588
C	-1.800809	3.965646	-2.041088
C	-2.566512	5.130683	-1.840626
C	-2.989173	5.913576	-2.931232
C	-2.667260	5.560268	-4.256943
C	-1.899061	4.388893	-4.452960
C	-1.475333	3.608406	-3.369440
C	2.799666	6.099924	-1.080577
C	3.250441	1.528212	1.081605
C	3.091891	1.651735	2.605508
C	3.284282	0.509766	3.416752

C	3.181925	0.587484	4.812325
C	2.886067	1.809040	5.461719
C	2.694745	2.945246	4.650410
C	2.795272	2.870482	3.247877
C	4.732008	1.591558	0.661846
C	5.733507	2.150155	1.480804
C	7.073924	2.198780	1.053812
C	7.464231	1.688508	-0.200003
C	6.455703	1.126390	-1.016808
C	5.119286	1.078685	-0.597506
H	-0.504746	-1.306084	2.524956
H	0.504355	1.306250	2.524943
H	-0.200505	-5.292496	-1.431230
H	-3.988338	-3.967720	0.184320
H	1.419648	-2.045374	-1.240306
H	0.783889	-4.517383	1.484007
H	2.295927	-4.798423	3.439538
H	5.251485	-2.269944	1.516295
H	3.738190	-1.988582	-0.434859
H	0.877825	-2.698704	-3.548016
H	1.632097	-4.079359	-5.477242
H	3.588779	-6.820242	-2.743299
H	2.844686	-5.431675	-0.818212
H	-3.114489	-6.068212	-2.146680
H	-3.701377	-6.329328	-0.478542
H	-2.086930	-6.944321	-0.979618
H	-2.899212	-0.510390	0.807009
H	-2.632300	-3.778864	2.647004
H	-2.459326	-3.913324	5.122901
H	-3.329717	0.325080	5.414286
H	-3.507876	0.458840	2.939455
H	-4.353122	-0.649137	-1.262688
H	-6.722925	-0.716188	-2.005418
H	-7.834375	-2.644321	1.717396
H	-5.470499	-2.550701	2.471862
H	0.200871	5.292496	-1.431425
H	3.988479	3.967392	0.184389
H	-1.419606	2.045519	-1.240426
H	-0.783741	4.517545	1.483823
H	-2.295798	4.798738	3.439341
H	-5.251476	2.270387	1.516121
H	-3.738165	1.988862	-0.434994
H	-2.844385	5.431949	-0.818431
H	-3.588348	6.820518	-2.743586
H	-1.631919	4.079338	-5.477411
H	-0.877777	2.698700	-3.548137
H	2.087689	6.944279	-0.978789
H	3.113945	6.068280	-2.147065
H	3.702345	6.328545	-0.479312
H	2.898961	0.510212	0.807300
H	3.507140	-0.458887	2.939889
H	3.328761	-0.324830	5.414686
H	2.459220	3.913711	5.122763
H	2.632412	3.778958	2.646911
H	5.470551	2.549675	2.472357
H	7.834485	2.642832	1.717980
H	6.722585	0.716009	-2.005381
H	4.352776	0.649379	-1.262730
C	8.904322	1.728702	-0.660956
H	9.004249	2.254009	-1.634949
H	9.554794	2.246936	0.071790
H	9.311545	0.704849	-0.808081
C	2.783772	1.882521	6.968996
H	3.756384	1.644835	7.452032
H	2.478005	2.891703	7.310112
H	2.045131	1.152174	7.363177
C	-2.784252	-1.881954	6.968870
H	-2.044452	-1.152622	7.362779
H	-3.756436	-1.642668	7.451960
H	-2.479923	-2.891497	7.310202
C	-8.904387	-1.729913	-0.661372
H	-9.554821	-2.248148	0.071409
H	-9.311777	-0.706159	-0.808697
H	-9.004148	-2.255415	-1.635278
C	3.139168	-6.384858	-5.433889
H	2.304578	-6.619205	-6.128259
H	3.905252	-5.839488	-6.027544
H	3.590850	-7.343264	-5.107899
C	4.833172	-3.765074	3.795567
H	5.288269	-2.806990	4.123630
H	4.316155	-4.215944	4.666398
H	5.674177	-4.440135	3.523216
C	-4.833141	3.765677	3.795308
H	-4.315970	4.215977	4.666342
H	-5.673693	4.441348	3.523054
H	-5.288877	2.807777	4.123010
C	-3.138539	6.385129	-5.434146
H	-3.903032	5.839055	-6.029185
H	-3.591995	7.342662	-5.108066
H	-2.303387	6.621192	-6.127276

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PtIPr SCF Done: -1279.91465662 A.U.

Pt	0.000051	-0.000035	-1.594928
C	-0.000015	0.000032	0.269840
N	-1.110189	-0.010678	1.078232
C	-0.769632	0.071369	2.511002
H	-1.277337	-0.734390	3.082404
H	-1.107830	1.044149	2.934698
C	0.769558	-0.071228	2.511023
H	1.277253	0.734555	3.082401
H	1.107731	-1.043992	2.934777
N	1.110149	0.010746	1.078258
C	-2.482322	0.023399	0.645140
C	-3.119281	1.279155	0.442062
C	-4.483034	1.278668	0.083738
H	-4.996018	2.238110	-0.090492
C	-4.551120	-1.147303	0.148074
H	-5.117139	-2.084221	0.024122
C	-5.195445	0.080216	-0.060914
H	-6.260817	0.102735	-0.341358
C	-3.189560	-1.203914	0.508718
C	-2.362336	2.602972	0.546430
H	-1.354869	2.378597	0.955912
C	-3.044011	3.600789	1.505178
H	-2.427350	4.517854	1.614270
H	-3.193475	3.165847	2.515782
H	-4.039461	3.919867	1.129716
C	-2.144317	3.212507	-0.855328
H	-1.556518	4.152649	-0.788411
H	-3.111891	3.449531	-1.347205
H	-1.588103	2.495611	-1.498751
C	-2.497080	-2.555801	0.676184
H	-1.513227	-2.362933	1.154547
C	-2.207034	-3.180967	-0.706274
H	-1.657358	-4.140291	-0.598202
H	-1.589898	-2.487652	-1.319761
H	-3.149996	-3.387540	-1.256537
C	-3.276895	-3.523138	1.588757
H	-2.694881	-4.454557	1.752234
H	-4.248588	-3.822835	1.141906
H	-3.490047	-3.073539	2.581265
C	2.482283	-0.023365	0.645186

C	3.189538	1.203932	0.508735
C	4.551086	1.147288	0.148053
H	5.117120	2.084193	0.024066
C	5.195388	-0.080244	-0.060940
H	6.260751	-0.102775	-0.341418
C	4.482961	-1.278682	0.083740
H	4.995917	-2.238137	-0.090504
C	3.119217	-1.279138	0.442104
C	2.497073	2.555827	0.676194
H	1.513219	2.362966	1.154560
C	2.207033	3.180995	-0.706260
H	1.657409	4.140349	-0.598191
H	1.589851	2.487704	-1.319726
H	3.149995	3.387517	-1.256543
C	3.276893	3.523154	1.588778
H	2.694891	4.454581	1.752251
H	4.248596	3.822835	1.141937
H	3.490027	3.073548	2.581286
C	2.362267	-2.602949	0.546503
H	1.354761	-2.378551	0.955867
C	2.144362	-3.212621	-0.855208
H	1.556567	-4.152763	-0.788231
H	3.111958	-3.449696	-1.347018
H	1.588172	-2.495806	-1.498733
C	3.043902	-3.600655	1.505400
H	2.427305	-4.517762	1.614501
H	3.193230	-3.165625	2.515986
H	4.039422	-3.919662	1.130064

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PtSIPrCl2DIMER SCF Done: -4400.49507690 A.U.

N	4.269801	1.136790	0.261410
C	3.920147	2.467413	-0.182966
N	4.143693	-0.971059	0.946703
C	4.555275	2.984457	-1.349776
C	4.255980	4.307453	-1.732988
H	4.727210	4.724193	-2.636832
C	3.368376	5.097625	-0.991882
H	3.144191	6.127188	-1.314190
C	2.774289	4.579175	0.165284
H	2.090712	5.211201	0.753039
C	3.041339	3.265817	0.605922
C	5.573155	2.185296	-2.166693
H	5.493607	1.125845	-1.844709
C	5.280771	2.218399	-3.680509
H	4.242917	1.893121	-3.887650
H	5.972038	1.535835	-4.218240
H	5.426765	3.233692	-4.107164
C	7.013639	2.680211	-1.893652
H	7.145573	3.726996	-2.241653
H	7.754250	2.051908	-2.432671
H	7.274330	2.664832	-0.814303
C	2.446770	2.797824	1.936161
H	2.554145	1.695417	1.994731
C	0.941473	3.100502	2.063874
H	0.739706	4.191641	2.108194
H	0.536979	2.651290	2.993362
H	0.367116	2.674305	1.218119
C	3.226325	3.413918	3.122434
H	4.311610	3.183150	3.077431
H	2.834048	3.031383	4.088348
H	3.127437	4.520518	3.132278
C	3.480282	0.025013	0.289625
C	5.499820	0.939461	1.061890
H	5.400821	1.474673	2.033232
C	5.543008	-0.583232	1.229940
H	5.848930	-0.903814	2.243877
C	3.702857	-2.323905	1.202769
C	3.713739	-3.289418	0.156019
C	3.321924	-4.606824	0.474661
H	3.312003	-5.368207	-0.320740
C	2.953714	-4.966901	1.776606
H	2.650063	-6.002520	1.998477
C	2.978199	-4.008620	2.797922
H	2.693835	-4.299808	3.821185
C	3.353604	-2.674770	2.540962
C	4.182128	-2.978434	-1.265468
H	4.237505	-1.877178	-1.380210
C	5.595673	-3.554528	-1.513010
H	6.335002	-3.178111	-0.774696
H	5.955632	-3.279569	-2.527012
H	5.597737	-4.663587	-1.443110
C	3.188506	-3.476407	-2.333503
H	3.129954	-4.585595	-2.362161
H	3.506011	-3.131371	-3.338516
H	2.172997	-3.074219	-2.147143
C	3.416695	-1.682764	3.705916
H	3.524808	-0.666117	3.271413
C	2.134956	-1.676309	4.564504
H	1.233654	-1.494716	3.947847
H	2.193550	-0.877152	5.332983
H	1.997876	-2.637208	5.104138
C	4.649267	-1.959817	4.599898
H	4.563413	-2.951549	5.092785
H	4.736650	-1.194043	5.399617
H	5.599992	-1.966020	4.026379
Pt	1.720742	-0.159293	-0.525773
Cl	2.630124	0.107626	-2.664296
Cl	0.535269	-0.475336	1.534430
N	-4.143595	-0.971100	-0.946819
C	-3.702773	-2.323979	-1.202730
N	-4.269822	1.136731	-0.261500
C	-3.353524	-2.674981	-2.540883
C	-2.978104	-4.008851	-2.797713
H	-2.693739	-4.300136	-3.820948
C	-2.953593	-4.967023	-1.776296
H	-2.649919	-6.002659	-1.998056
C	-3.321802	-4.606815	-0.474386
H	-3.311874	-5.368118	0.321092
C	-3.713644	-3.289385	-0.155875
C	-3.416613	-1.683080	-3.705931
H	-3.524708	-0.666394	-3.271512
C	-2.134864	-1.676723	-4.564513
H	-1.233565	-1.495080	-3.947868
H	-2.193435	-0.877642	-5.333073
H	-1.997798	-2.637679	-5.104051
C	-4.649174	-1.960191	-4.599893
H	-4.563347	-2.951973	-5.092686
H	-4.736526	-1.194494	-5.399690
H	-5.599912	-1.966309	-4.026392
C	-4.182084	-2.978279	1.265569
H	-4.237482	-1.877015	1.380218
C	-3.188507	-3.476140	2.333694
H	-3.129972	-4.585326	2.362491
H	-3.506042	-3.130980	3.338656
H	-2.172984	-3.073990	2.147328
C	-5.595633	-3.554373	1.513110
H	-6.334942	-3.178030	0.774738
H	-5.955624	-3.279326	2.527076
H	-5.597672	-4.663438	1.443308
C	-3.480255	0.024982	-0.289670
C	-5.542941	-0.583304	-1.229982
H	-6.218290	-1.074303	-0.493195

C	-5.499631	0.939401	-1.062308
H	-6.384268	1.345789	-0.536301
C	-3.920245	2.467366	0.182902
C	-3.041417	3.265833	-0.605893
C	-2.774457	4.579188	-0.165182
H	-2.090864	5.211265	-0.752865
C	-3.368652	5.097569	0.991957
H	-3.144541	6.127130	1.314320
C	-4.256278	4.307330	1.732970
H	-4.727591	4.724015	2.636795
C	-4.555486	2.984337	1.349683
C	-2.446719	2.797922	-1.936102
H	-2.554184	1.695531	-1.994803
C	-3.226034	3.414221	-3.122423
H	-4.311355	3.183588	-3.077592
H	-2.833676	3.031725	-4.088320
H	-3.127005	4.520809	-3.132154
C	-0.941370	3.100458	-2.063570
H	-0.739474	4.191583	-2.107653
H	-0.536811	2.651376	-2.993092
H	-0.367170	2.674034	-1.217823
C	-5.573387	2.185085	2.166476
H	-5.493694	1.125642	1.844502
C	-5.281219	2.218233	3.680327
H	-4.243352	1.893087	3.887617
H	-5.972472	1.535583	4.217966
H	-5.427394	3.233506	4.106965
C	-7.013891	2.679839	1.893218
H	-7.145974	3.726631	2.241139
H	-7.754507	2.051489	2.432173
H	-7.274432	2.664362	0.813834
Pt	-1.720719	-0.159263	0.525771
Cl	-0.535301	-0.475432	-1.534481
Cl	-2.630093	0.107862	2.664268
H	-5.400195	1.474332	-2.033765
H	-5.849053	-0.904144	-2.243775
H	6.384340	1.345577	0.535472
H	6.218464	-1.074478	0.493423

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PtSIPrCl2SMe2cis SCF Done: -2678.12543653 A.U.

N	-0.815000	-0.994980	-1.219572
C	-2.201408	-1.133472	-0.847830
N	1.360244	-0.587588	-1.184872
C	-2.571823	-1.956626	0.257004
C	-3.948524	-2.093390	0.540580
H	-4.256451	-2.715428	1.395397
C	-4.927126	-1.473237	-0.247175
H	-5.994279	-1.601664	-0.005074
C	-4.544804	-0.700163	-1.351861
H	-5.319253	-0.228591	-1.977369
C	-3.185876	-0.516308	-1.679932
C	-1.565597	-2.750147	1.091481
H	-0.546974	-2.380338	0.858807
C	-1.759916	-2.548157	2.607211
H	-1.692877	-1.475141	2.877550
H	-0.958208	-3.074490	3.163492
H	-2.733901	-2.948855	2.961555
C	-1.624636	-4.250218	0.718551
H	-2.613682	-4.691962	0.966635
H	-0.852476	-4.817002	1.279857
H	-1.451325	-4.418709	-0.365495
C	-2.826610	0.285210	-2.935209
H	-1.728748	0.452721	-2.916423
C	-3.495832	1.674371	-2.978524
H	-4.601582	1.598782	-3.047850
H	-3.150955	2.239866	-3.869715
H	-3.243246	2.265675	-2.076157
C	-3.175562	-0.510058	-4.215845
H	-2.712655	-1.518834	-4.228039
H	-2.836079	0.033871	-5.122608
H	-4.272953	-0.657099	-4.304179
C	0.184934	-0.360690	-0.523978
C	-0.268290	-1.857707	-2.289762
H	-0.888911	-1.812088	-3.204541
C	1.130938	-1.274935	-2.476254
H	1.176067	-0.531137	-3.304861
C	2.686866	-0.083196	-0.908684
C	3.697112	-1.012690	-0.519176
C	5.007802	-0.528616	-0.340165
H	5.799263	-1.227427	-0.027202
C	5.322100	0.821556	-0.539256
H	6.352623	1.178900	-0.384608
C	4.321675	1.713885	-0.940469
H	4.578334	2.771284	-1.109522
C	2.992784	1.286249	-1.145161
C	3.430325	-2.507420	-0.322521
H	2.329030	-2.647281	-0.313708
C	4.030863	-3.338613	-1.481695
H	3.682226	-3.001692	-2.480997
H	3.768375	-4.412403	-1.372994
H	5.139227	-3.264873	-1.487985
C	3.959542	-3.034487	1.027276
H	5.069033	-3.007912	1.072824
H	3.652013	-4.091730	1.171311
H	3.557744	-2.437675	1.868380
C	1.969161	2.293135	-1.671811
H	0.961449	1.841709	-1.561757
C	1.968556	3.600499	-0.855452
H	1.798487	3.396376	0.221451
H	1.173443	4.284574	-1.221759
H	2.928284	4.150267	-0.950746
C	2.200132	2.580037	-3.173331
H	3.191263	3.052392	-3.342556
H	1.425066	3.271348	-3.567870
H	2.171292	1.651839	-3.781474
Pt	-0.065417	0.630841	1.177533
Cl	1.505255	-0.800304	2.189325
Cl	-0.338439	1.739361	3.292767
S	-1.751351	2.009023	0.309277
C	-1.397009	3.729321	0.831786
H	-1.151592	3.721311	1.912880
H	-0.528849	4.076282	0.243885
H	-2.287682	4.347536	0.602718
C	-3.196877	1.692329	1.389651
H	-4.000081	2.404366	1.113898
H	-3.523508	0.653466	1.197808
H	-2.870954	1.812116	2.442060
H	1.904481	-2.042329	-2.663724
H	-0.246381	-2.914760	-1.938444

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PtSIPrCl2SMe2trans SCF Done: -2678.13189990 A.U.

N	1.207484	1.249429	0.807615
C	2.562852	0.750462	0.738156
N	-0.996414	1.444466	0.692987
C	2.979906	-0.292946	1.615142
C	4.326787	-0.708064	1.550410
H	4.669740	-1.518143	2.212539
C	5.236989	-0.105099	0.673633
H	6.283771	-0.447688	0.641935
C	4.814849	0.941299	-0.155606
H	5.537295	1.417898	-0.836407
C	3.480391	1.395491	-0.142747

C	2.059589	-0.921388	2.662964
H	1.010324	-0.697936	2.382763
C	2.174091	-2.456957	2.715219
H	2.014030	-2.900705	1.713194
H	1.400630	-2.872798	3.392560
H	3.163673	-2.790161	3.094836
C	2.328155	-0.311479	4.058999
H	3.360910	-0.536679	4.401899
H	1.623506	-0.727355	4.810042
H	2.216776	0.793129	4.062347
C	3.092434	2.580878	-1.029937
H	1.983580	2.628701	-1.050072
C	3.562000	2.413526	-2.489253
H	4.669172	2.448693	-2.573211
H	3.161298	3.237837	-3.116019
H	3.203740	1.453986	-2.909578
C	3.635522	3.908058	-0.448039
H	3.315465	4.079230	0.601412
H	3.292465	4.772955	-1.054697
H	4.746448	3.916058	-0.451034
C	0.066319	0.663877	0.348032
C	0.906520	2.433162	1.645822
H	1.591720	3.269811	1.411763
C	-0.553306	2.727232	1.285314
H	-0.651317	3.538352	0.529025
C	-2.394153	1.244048	0.382122
C	-3.272416	0.852613	1.435711
C	-4.644310	0.721877	1.139380
H	-5.338694	0.411575	1.935802
C	-5.139082	0.974385	-0.146316
H	-6.214797	0.861173	-0.356653
C	-4.263912	1.380926	-1.160997
H	-4.661936	1.594338	-2.165214
C	-2.881557	1.537278	-0.924561
C	-2.797778	0.618343	2.871977
H	-1.690261	0.545937	2.845696
C	-3.192181	1.803558	3.785446
H	-2.825270	2.779258	3.402972
H	-2.785400	1.663744	4.809530
H	-4.296712	1.885855	3.871562
C	-3.322408	-0.704199	3.466797
H	-4.423591	-0.683196	3.611622
H	-2.866207	-0.882636	4.463307
H	-3.066662	-1.558782	2.811017
C	-1.993695	2.076131	-2.047016
H	-0.935572	1.883549	-1.777323
C	-2.231749	1.359717	-3.390372
H	-2.110278	0.263971	-3.281801
H	-1.489403	1.701569	-4.139862
H	-3.242813	1.566595	-3.802144
C	-2.182128	3.603448	-2.203466
H	-3.221135	3.851004	-2.510350
H	-1.495704	4.003695	-2.979358
H	-1.982182	4.149149	-1.257309
Pt	-0.044428	-1.025414	-0.677687
Cl	-1.061379	-2.180044	1.129990
Cl	0.986959	-0.008143	-2.545085
S	-0.172460	-3.032907	-2.038452
C	-1.911636	-3.587279	-1.909148
H	-2.520112	-2.848840	-2.464827
H	-2.010157	-4.585617	-2.379486
H	-2.215636	-3.598596	-0.843765
C	0.639808	-4.339255	-1.047641
H	0.483408	-5.319203	-1.540529
H	1.719378	-4.096731	-1.031434
H	0.231001	-4.327872	-0.017915
H	-1.174550	2.997092	2.160381
H	1.037029	2.170644	2.719825

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PtSIPrCl2trans SCF Done: -2200.22044245 A.U.

N	1.109524	-0.113483	1.150651
C	2.485278	-0.296481	0.744889
N	-1.109939	0.113249	1.150331
C	2.926817	-1.572612	0.291721
C	4.290880	-1.712838	-0.039065
H	4.656456	-2.686086	-0.401394
C	5.188273	-0.645446	0.089779
H	6.248539	-0.780966	-0.177086
C	4.736904	0.592754	0.563864
H	5.449713	1.425647	0.668092
C	3.384621	0.797570	0.904082
C	2.011663	-2.795400	0.211482
H	0.960795	-2.444915	0.264367
C	2.152230	-3.555709	-1.121853
H	1.993964	-2.880302	-1.985567
H	1.392089	-4.360954	-1.183076
H	3.150526	-4.031811	-1.225000
C	2.259778	-3.740436	1.410628
H	3.293845	-4.146371	1.393074
H	1.558569	-4.601054	1.381589
H	2.127592	-3.224431	2.385019
C	2.953909	2.154820	1.465180
H	1.843552	2.169642	1.483088
C	3.405981	3.335347	0.581846
H	4.511815	3.436873	0.565537
H	2.996224	4.288370	0.977783
H	3.049007	3.209244	-0.458671
C	3.464379	2.340868	2.913840
H	3.148272	1.515675	3.586566
H	3.090972	3.294557	3.343411
H	4.574337	2.372570	2.941862
C	-0.000104	-0.000334	0.366568
C	0.724474	-0.251041	2.573324
H	1.394180	0.346204	3.220759
C	-0.725122	0.251849	2.573033
H	-0.807204	1.319512	2.878091
C	-2.485428	0.297350	0.744139
C	-3.385884	-0.795770	0.903675
C	-4.737871	-0.589863	0.563003
H	-5.451471	-1.422057	0.667392
C	-5.187977	0.648557	0.088275
H	-6.248056	0.784952	-0.178892
C	-4.289564	1.715041	-0.040828
H	-4.654164	2.688482	-0.403612
C	-2.925678	1.573681	0.290264
C	-2.956585	-2.153120	1.465600
H	-1.846247	-2.169158	1.483275
C	-3.467052	-2.337584	2.914466
H	-3.150027	-1.512241	3.586577
H	-3.094586	-3.291346	3.344697
H	-4.577041	-2.368109	2.942654
C	-3.410193	-3.333762	0.583212
H	-4.516138	-3.434136	0.567335
H	-3.001313	-4.286943	0.979671
H	-3.053398	-3.208752	-0.457494
C	-2.009438	2.795643	0.209552
H	-0.958873	2.444263	0.262666
C	-2.149269	3.555495	-1.124122
H	-1.991570	2.879557	-1.987514
H	-1.388391	4.360018	-1.185669
H	-3.147122	4.032467	-1.227466
C	-2.256790	3.741439	1.408270

H	-3.290517	4.148230	1.390503
H	-1.554872	4.601466	1.378851
H	-2.125070	3.225774	2.382903
Pt	0.000148	-0.001206	-1.532389
Cl	-1.094961	-2.007805	-1.912690
Cl	1.095321	2.004584	-1.916352
H	-1.394880	-0.345042	3.220733
H	0.806363	-1.318501	2.879155

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PtSIPrClSMe2cis+ SCF Done: -2217.75933407 A.U.

N	-0.979264	0.373832	1.304762
C	-2.342197	0.633285	0.898694
N	1.228254	0.040740	1.265584
C	-2.651862	1.834842	0.194256
C	-4.004599	2.060781	-0.142023
H	-4.274765	2.976855	-0.689709
C	-5.012242	1.159797	0.229045
H	-6.060563	1.366066	-0.038254
C	-4.688658	0.007746	0.959785
H	-5.491609	-0.679657	1.267816
C	-3.355998	-0.281570	1.319651
C	-1.617708	2.912734	-0.136693
H	-0.607049	2.500223	0.065053
C	-1.640888	3.322812	-1.622974
H	-1.484419	2.447667	-2.286629
H	-0.828999	4.047993	-1.833148
H	-2.598381	3.807954	-1.905303
C	-1.811047	4.143549	0.780668
H	-2.793667	4.628381	0.602159
H	-1.023526	4.900168	0.584358
H	-1.767685	3.873998	1.856474
C	-3.065025	-1.508010	2.189953
H	-1.963872	-1.659969	2.197065
C	-3.699369	-2.804880	1.645843
H	-4.808153	-2.763440	1.664841
H	-3.397391	-3.670262	2.271052
H	-3.380596	-3.009673	0.604183
C	-3.529281	-1.264653	3.646768
H	-3.099601	-0.339088	4.083188
H	-3.241298	-2.116605	4.296938
H	-4.633326	-1.161890	3.698326
C	0.095754	0.082539	0.525562
C	-0.525101	0.744774	2.671418
H	-1.191614	0.307799	3.437764
C	0.899197	0.178801	2.707989
H	0.954229	-0.822033	3.190097
C	2.591257	-0.223056	0.849629
C	3.497650	0.874959	0.796229
C	4.832354	0.598125	0.438098
H	5.555740	1.425705	0.377559
C	5.256431	-0.706926	0.157147
H	6.304037	-0.896778	-0.123887
C	4.351538	-1.772640	0.245055
H	4.703356	-2.795540	0.041151
C	3.003395	-1.562192	0.600782
C	3.100891	2.308757	1.157976
H	1.992297	2.343252	1.236025
C	3.690415	2.709604	2.531899
H	3.414832	1.999931	3.340506
H	3.341415	3.720474	2.828938
H	4.799429	2.737002	2.493351
C	3.508125	3.336821	0.082002
H	4.610930	3.413909	-0.015266
H	3.136089	4.345266	0.357992
H	3.094449	3.072613	-0.910674
C	2.075531	-2.766919	0.768409
H	1.030815	-2.389526	0.814546
C	2.156712	-3.741495	-0.424318
H	2.014519	-3.213701	-1.390183
H	1.388849	-4.538265	-0.329099
H	3.139124	-4.254669	-0.473186
C	2.364871	-3.505351	2.096238
H	3.394195	-3.920957	2.102449
H	1.659252	-4.350132	2.241413
H	2.279415	-2.832450	2.974358
Pt	0.087163	-0.147280	-1.403804
Cl	1.650664	1.218515	-2.343744
S	-1.633213	-1.720477	-1.278149
C	-1.045941	-3.017535	-2.437086
H	-0.715495	-2.575916	-3.398092
H	-0.204856	-3.539832	-1.946176
H	-1.884286	-3.722997	-2.604369
C	-2.968231	-0.989133	-2.299777
H	-3.739050	-1.770861	-2.450610
H	-3.392744	-0.144219	-1.726129
H	-2.570340	-0.639121	-3.271936
H	1.626055	0.845572	3.207880
H	-0.553127	1.852095	2.774164

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PtSIPrClSMe2trans+ SCF Done: -2217.76895492 A.U.

N	-1.021127	-1.256428	-1.123962
C	-2.400116	-0.870403	-0.959182
N	1.190353	-1.179187	-0.975880
C	-3.275161	-1.723614	-0.235398
C	-4.626514	-1.330421	-0.128839
H	-5.331366	-1.971187	0.423767
C	-5.086177	-0.137433	-0.700047
H	-6.145507	0.147136	-0.603101
C	-4.199727	0.697777	-1.398215
H	-4.578344	1.630379	-1.842324
C	-2.844716	0.346344	-1.550383
C	-2.803427	-3.009747	0.443406
H	-1.707412	-3.091700	0.283997
C	-3.020836	-2.951298	1.971397
H	-2.499180	-2.081304	2.419049
H	-2.625337	-3.870721	2.450682
H	-4.098026	-2.880692	2.230027
C	-3.470386	-4.258666	-0.173998
H	-4.568031	-4.255956	-0.007737
H	-3.068475	-5.183733	0.288617
H	-3.304588	-4.322723	-1.269925
C	-1.876386	1.271250	-2.294073
H	-1.082626	0.642396	-2.752232
C	-1.188368	2.261379	-1.329497
H	-1.881919	2.703392	-0.591940
H	-0.714976	3.110359	-1.874531
H	-0.108857	1.912006	-0.912457
C	-2.537188	2.065369	-3.442074
H	-3.096561	1.389465	-4.119109
H	-1.767459	2.590687	-4.043319
H	-3.244482	2.834572	-3.069682
C	0.033632	-0.613806	-0.577516
C	-0.589863	-2.298003	-2.089188
H	-0.875029	-1.990225	-3.118865
C	0.938673	-2.343390	-1.869462
H	1.518656	-2.231006	-2.807119
C	2.538293	-0.764802	-0.642660
C	3.261318	-1.490624	0.347842
C	4.584704	-1.084547	0.617147
H	5.165896	-1.622909	1.381263
C	5.175107	-0.013473	-0.065714
H	6.210103	0.283801	0.164989

C	4.453137	0.669727	-1.052661
H	4.934681	1.495800	-1.598740
C	3.128491	0.307265	-1.372843
C	2.688664	-2.706430	1.079826
H	1.588724	-2.705921	0.922512
C	3.268903	-4.017911	0.496710
H	3.117268	-4.103343	-0.599593
H	2.800774	-4.901507	0.978526
H	4.362856	-4.079131	0.676085
C	2.922999	-2.654722	2.603562
H	3.998317	-2.755654	2.859582
H	2.392836	-3.494377	3.098507
H	2.548395	-1.707823	3.038743
C	2.420309	1.027360	-2.522459
H	1.352204	0.720186	-2.507777
C	2.463581	2.562752	-2.374133
H	2.082632	2.891373	-1.384270
H	1.858166	3.051053	-3.166433
H	3.496159	2.956311	-2.473697
C	3.001825	0.592531	-3.887840
H	4.069701	0.882068	-3.976301
H	2.452517	1.073982	-4.723926
H	2.947454	-0.506543	-4.029574
Pt	-0.207943	1.007351	0.578049
Cl	0.217310	-0.253971	2.474467
S	-0.467909	3.012599	1.937529
C	1.069706	3.130907	2.919322
H	1.888203	3.356390	2.209968
H	0.959168	3.962786	3.641539
H	1.260940	2.167303	3.429792
C	-1.679741	2.592231	3.241309
H	-1.720154	3.431444	3.962403
H	-2.662345	2.478037	2.745719
H	-1.386106	1.644074	3.731885
H	1.272131	-3.276485	-1.371354
H	-1.088180	-3.263828	-1.875016

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Py SCF Done: -248.102926303 A.U.

N	0.000001	1.428388	0.000000
C	-1.149108	0.728785	0.000682
C	1.149109	0.728784	-0.000682
C	-1.207410	-0.677262	-0.000261
C	1.207409	-0.677263	0.000261
C	-0.000001	-1.395412	0.000000
H	-2.083359	1.321304	-0.000537
H	2.083360	1.321302	0.000538
H	-2.179703	-1.194820	-0.000777
H	2.179702	-1.194823	0.000777
H	-0.000001	-2.497473	0.00000

5. Author Contributions

Benon P. Maliszewski: conducted the experimental work; wrote and edited the manuscript.

Dr. Tahani A. C. A. Bayrakdar: conducted the experimental work; edited the manuscript.

Perrine Lambert: conducted the experimental work.

Lama Hamdouna and **Dr. Xavier Trivelli**: conducted the ^{195}Pt NMR studies.

Prof. Dr. Luigi Cavallo and **Dr. Albert Poater**: conducted the DFT studies.

Marek Beliš: carried out the single-crystal X-ray studies.

Prof. Dr. Olivier Lafon: supervised and validated the ^{195}Pt NMR studies; secured funding.

Prof. Dr. Kristof Van Hecke: supervised and validated the XRD results.

Dr. Dominic Ormerod: wrote and edited the manuscript.

Prof. Dr. Catherine S. J. Cazin: supervised the work; wrote and edited the manuscript and secured funding.

Prof. Dr. Fady Nahra: supervised the experimental work; wrote and edited the manuscript.

Prof. Dr. Steven P. Nolan: concept originator; supervised project; wrote and edited the manuscript; secured funding.

All authors have given approval to the final version of the manuscript.

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