

Pd-Catalyzed Stereoselective Enol Ether Coupling toward C2-Branched Carbohydrates: Experimental and Computational Insights into Glycal-Controlled Diastereoselectivity

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1. General Consideration

Unless otherwise noted, all reactions were performed under an N₂ atmosphere in a dry solvent, and all glassware was oven-dried before use. All commercially available reagents were purchased from commercial sources and were used without further purification. All reactions were monitored using thin-layer chromatography over silica gel-coated TLC plates. The products were purified by column chromatography on silica gel (100-200 mesh) using petroleum ether–ethyl acetate as the eluent to obtain the pure products. ¹H and ¹³C NMR spectra were recorded using 500 and 600 to 126 and 151 MHz spectrometers with TMS as internal standards. All products exact masses were derived using HRMS having a QTOF analyzer. Data is reported in ppm using CDCl₃ as the solvent unless otherwise specified. Data is reported as: Chemical shifts (δ), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiple, br = broad), coupling constants (Hz), integrated intensity. Structural assignments were made with additional information from COSY, HMBC, HSQC, and NOESY experiments. Commercially available grades of organic solvents of adequate purity are used in all reactions.

2. Experimental procedures for all products

1) General procedure 1 for the products (4a-4l, 7).

In an oven-dried round bottom flask, 2-iodo glucal **2a** (0.13 mmol, 1.0 equiv.), PdCl₂(0.013 mmol, 10 mol %), AgOAc (0.26 mmol, 2.0 equiv.) was dissolved in 2 mL of dry DMF and the reaction mixture was stirred at 90 °C for 4 hours. After the starting material was converted as confirmed through TLC, the organic layer was extracted with EtOAc (10 × 3 ml). The organic layer was dried over sodium sulfate, and the remaining residue was purified by column chromatography over silica gel (100-200 mesh) using hexane/ethyl acetate as eluent.

2) General procedure 2 for the products (8).

In an oven-dried round bottom flask prepared compound **4e** (0.14 mmol, 1.0 equiv.), was dissolved in CH₃CN/EtOAc/H₂O (3:3:1 ratio) at 0 °C, and RuCl₃ (0.0070 mmol, 5 mol%) was added at 0 °C. After that, NaIO₄ (0.21 mmol, 1.5 equiv.) was added at the same temperature and the reaction mixture was stirred for 2 h. After the starting material was converted as confirmed through TLC, the organic layer was extracted with EtOAc (10 × 3 mL). The combined organic layers were dried (Na₂SO₄), evaporated, and the residue left was purified by column chromatography over silica gel (100–200 mesh) using hexane/ethyl acetate as eluent.

3) General procedure 3 for the products (9, 10).

In an oven-dried round bottom flask prepared compound **4e** (0.14 mmol, 1.0 equiv.), was dissolved in 2 mL of dry DCM under N₂ atmosphere and respective TMSN₃ (0.16 mmol, 1.2 equiv.) was added. To this solution BF₃·OEt₂ (0.14 mmol, 1.0 equiv.) was added slowly and the reaction mixture was stirred at the room temperature for 2 hours. After the starting material was converted as confirmed through TLC, the mixture was quenched with a saturated sodium bicarbonate solution (10 mL), and the organic layer was extracted with DCM (10 × 3 ml). The organic layer was dried over sodium sulfate, and the remaining residue was purified by column chromatography over silica gel (100-200 mesh) using hexane/ethyl acetate as eluent.

3. 2D - NMR Analysis of Compound 4e

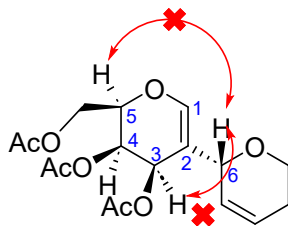


Fig1.: NOESY correlation analysis of **4e**

Table S1: NOESY Correlations of 4e

	¹ H	¹ H
H-1	6.53 (s, 1H)	-
H-3	4.25 (dd, <i>J</i> = 7.8, 3.3 Hz, 1H)	5.37 – 5.31 (m, 1H), 4.30 (dd, <i>J</i> = 11.3, 8.1 Hz, 1H)
H-4	5.37 – 5.31 (m, 1H)	4.25 (dd, <i>J</i> = 7.8, 3.3 Hz, 1H), 4.30 (dd, <i>J</i> = 11.3, 8.1 Hz, 1H)
H-5	4.30 (dd, <i>J</i> = 11.3, 8.1 Hz, 1H)	5.37 – 5.31 (m, 1H), 4.25 (dd, <i>J</i> = 7.8, 3.3 Hz, 1H)
H-6	5.63 d, <i>J</i> = 4.5 Hz, 1H)	-

4. Computational details

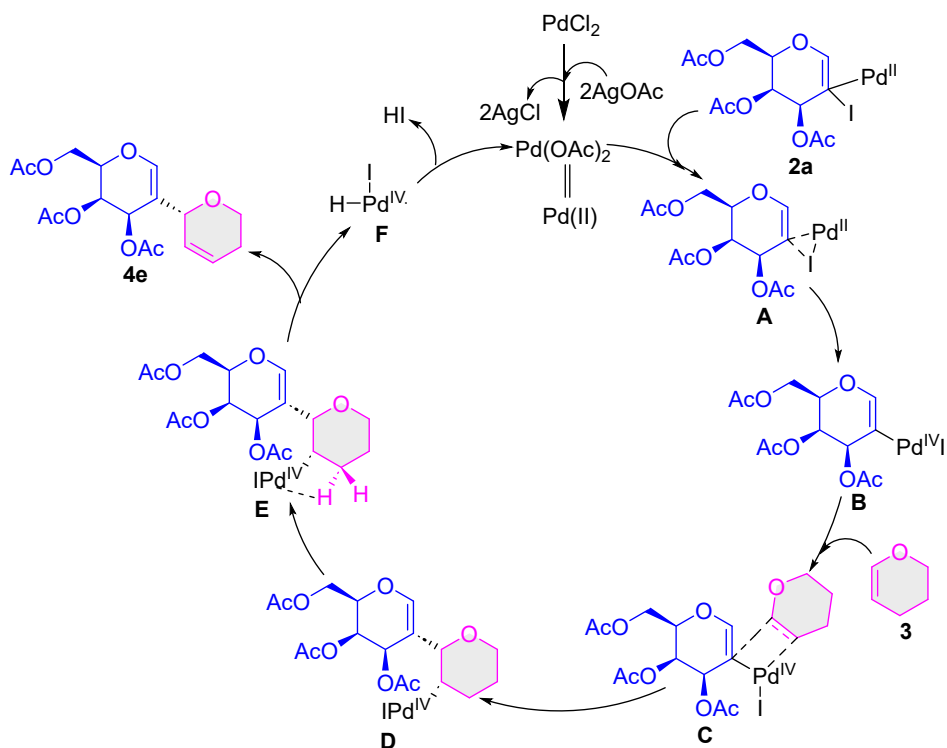
Geometry optimizations were performed using the hybrid B3LYP density functional augmented with Grimme's D3 dispersion correction (B3LYP-D3), as implemented in the Gaussian 09 program.¹⁻⁵ Solvation effects were treated using the SMD continuum solvation model.⁶ The 6-31G** basis set was employed for C, H, and O atoms,⁷ while the SDD⁸ effective core potential and corresponding basis set were used for Pd and I atoms. Harmonic vibrational frequency analyses were carried out at the same level of theory to characterize all stationary points as either minima (no imaginary frequencies) or transition states (one imaginary frequency). The Gibbs free energy of solutes in the liquid phase is calculated as:

$$G_{\text{liq}} = E_{\text{sp}} + G_{\text{ther}} + \Delta G_{\text{sol}}$$

Single-point energy refinements were subsequently performed at the PBE0-D3(BJ)/def2-TZVPD level using the Gaussian 16 package.^{9,10} For thermodynamic calculations, all positive vibrational frequencies below 100 cm⁻¹ were set to 100 cm⁻¹.¹¹ Total Gibbs free energies were obtained by combining electronic energies with thermal corrections to Gibbs free energy at the experimental temperature. Solvation free energies (ΔG_{sol}) were calculated at the M05-2X/6-31G* level of theory.¹²

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5. Computational study on Pd(OAc)₂ as an active catalyst.

Scheme S1. Proposed mechanism for the C–C coupling leading to the formation of **4e** via a Pd(II) catalyst.

Based on the control experiments and relevant literature precedents, a plausible reaction mechanism is proposed, as shown in Scheme S1. The transformation follows a classical Pd(II)/Pd(IV) catalytic method. Initial activation of PdCl₂ by AgOAc generates the catalytically active Pd(OAc)₂ species through removal of chloride as AgCl. The catalytic cycle is initiated by oxidative addition of the glucal iodide substrate to Pd(II), furnishing complex **B**. Coordination of the alkene partner to the resulting Pd(IV) center affords a π -complex **C**, which subsequently undergoes migratory insertion of the olefin into the Pd-glucal bond to generate the corresponding intermediate **D**. This intermediate undergoes β -hydride elimination to generate the functionalized product scaffold while forming a Pd-H species **E**. Finally, the Pd–I species reacts with hydride to form H–PdI (**F**), which is subsequently converted back into the active Pd(OAc)₂ species in the presence of AgOAc, thereby completing the catalytic cycle and delivering the desired product **4e**.

Based on the experimental observations, DFT calculations were performed to elucidate the origin of the stereoselective C–C bond formation using 2-iodoglucal (**1a** and **2a**) and dihydropyran (DHP, **3a**) as model substrates in DMF. Initially, PdCl₂ reacts with Ag(OAc)₂ to generate the active catalyst Pd(OAc)₂ *in situ* along with AgCl, with a calculated thermodynamic stabilization of –85.1 kcal/mol (Figure Sa). However, this species was taken as the reference point for constructing the potential energy surface of the C–C coupling reaction. Upon approach of 2-iodogalactal (**2a**) to Pd(OAc)₂, intermediate **A**_{2a} is formed; however, this step is substantially endergonic ($\Delta G = 14.7$ kcal/mol) with an associated activation barrier of 13.8 kcal/mol. The coordination and oxidative addition steps are associated with a high energy barrier (28.5 kcal/mol) from the active catalyst, indicating that these steps are likely sluggish at 90 °C. Intermediate **A** then undergoes oxidative addition of substrate **2a** to generate species **B**_{2a} with an energy barrier of 20.9 kcal/mol. We now turn to understanding the origin of the stereoselectivity in the C–C coupling product arising from

the approach of DHP to species **B_{2a}**. Species **B_{2a}** then reacts with DHP (**3a**), which can approach

from either the top (*re*) or bottom (*si*) face, leading to the formation of intermediates C_{2a} and C_{2a}' ,

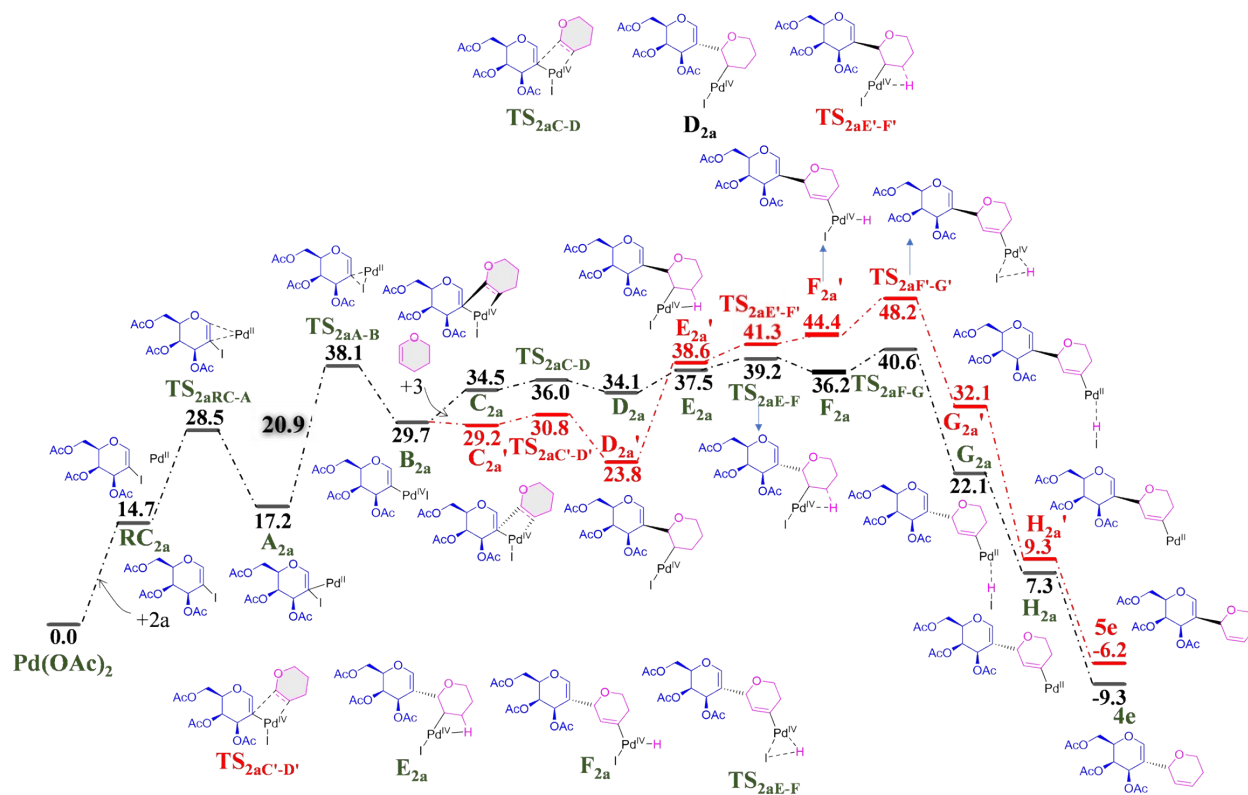
respectively. Both pathways are thermodynamically feasible; however, approach from the bottom

face is slightly more favorable than from the top face. The C–C coupling transition states (**TS_{2aC-D}**)

and $\text{TS}_{2\text{aC}'\text{-D}}$) are nearly isoenergetic ($\Delta G^\ddagger = 1.5$ and 1.6 kcal/mol for the top- and bottom-face

approaches, respectively), leading to formation of species \mathbf{D}_{2a} and \mathbf{D}_{2a}' with relative free energies

of 34.1 and 23.8 kcal/mol, respectively. In the next step, formation of a vacant coordination site on palladium leads to intermediates E_{2a} and E_{2a}' , which feature a three-atom, two-electron agostic interaction, with relative energies of 3.4 and 14.8 kcal/mol. The higher energy required to reorient E_{2a}' toward β -hydride elimination, relative to E_{2a} , indicates a less favorable pathway from E_{2a}' . The subsequent C–H activation proceeds *via* CMD transition states (TS_{2aE-F} and $TS_{2aE'-F'}$) exhibit overall activation barriers of 1.7 and 2.7 kcal/mol, leading to the formation of species F_{2a} and F_{2a}'



with relative free energies of 36.2 and 44.4 kcal/mol, respectively. In the final step, removal of HI from species F_{2a} and F_{2a}' (not formed during course of the reaction) proceeds *via* the corresponding transition states, leading to formation of the final product. The corresponding activation barriers for TS_{2aF-G} and $TS_{2aF'-G'}$ are calculated to be 4.4 and 3.8 kcal/mol, affording the final products with relative free energies of -9.3 (**4e**) and -6.2 (**5e**) kcal/mol, respectively. Overall thermodynamic and kinetic considerations support preferential formation of product **4e** rather than **5e** (Figure Sa). Overall, the reaction pathway is both thermodynamically and kinetically energy demanding, with only the product-forming step being exergonic from the active species. This observation suggests that $Pd(OAc)_2$ is unlikely to be the true active catalyst for the C–C coupling reaction.

Figure Sa. Free energy profiles for the Pd-catalyzed C-C coupling of 2-iodogalactal (**2a**) and DHP (**3a**). The relative free energies are given in kcal/mol.

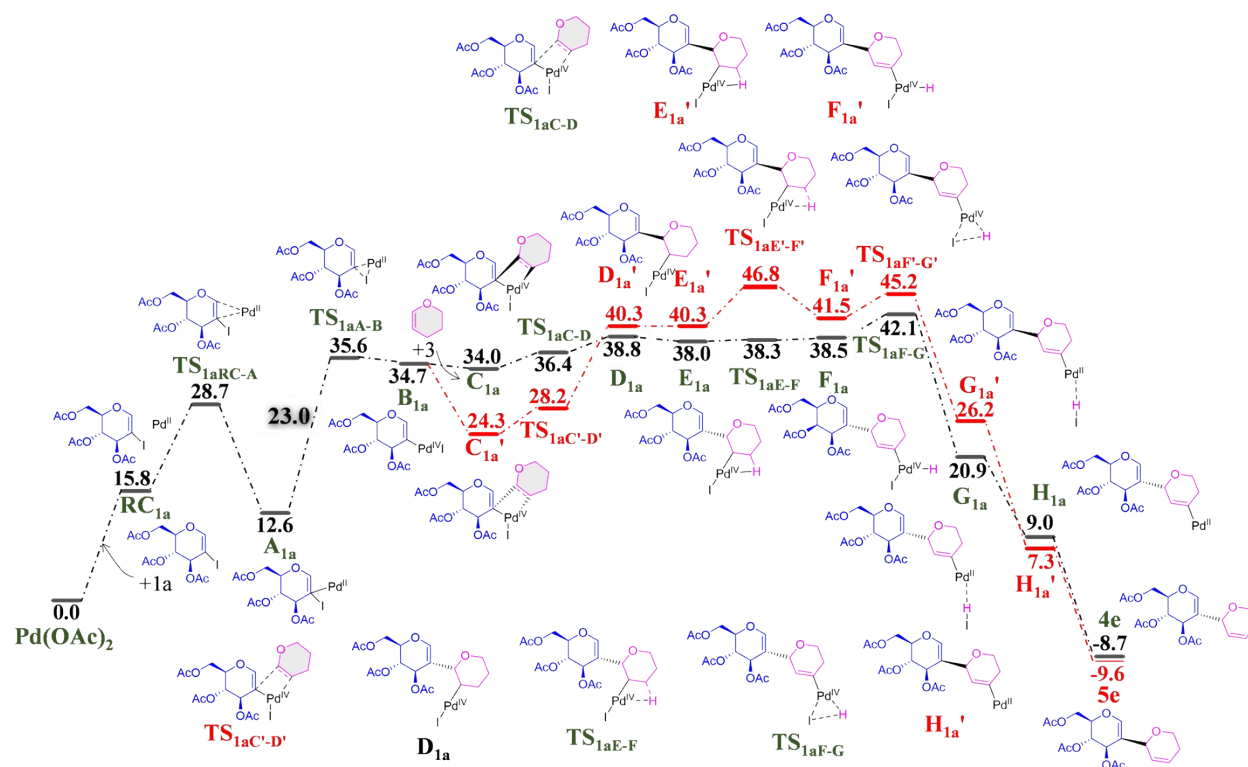
Similarly, the potential energy surface (PES) for the stereoselective C–C bond formation was

computed using 2-iodoglucal (**1a**) and dihydropyran (DHP, **3a**) as model substrates in DMF, with

the active catalyst Pd(OAc)₂ generated *in situ* from PdCl₂ and AgOAc. DFT calculations reveal

that the transformation from \mathbf{RC}_{1a} to \mathbf{B}_{1a} proceeds *via* substrate coordination and subsequent

oxidative addition, with associated activation barriers of 15.8 and 28.7 kcal/mol, respectively (Figure Sb). The oxidative addition step is associated with a high energy barrier (23.0 kcal/mol) from the active catalyst, indicating that this step is likely to be sluggish at 90 °C. Species **B**_{1a} reacts with DHP (**3a**) *via* top (*re*)- or bottom (*si*)-face approach to form intermediates **C**_{1a} and **C**_{1a'}, respectively. The corresponding C–C coupling transition states are nearly isoenergetic ($\Delta G^\ddagger = 2.4$ and 3.9 kcal/mol), leading to species **D**_{1a} and **D**_{1a'} with relative free energies of 38.8 and 40.3 kcal/mol; however, these pathways are thermodynamically unfavorable relative to the corresponding C–C coupling transition states (Figure Sb). The computed activation barriers for β -hydride elimination from species **E**_{1a} and **E**_{1a'} to afford species **F**_{1a} and **F**_{1a'} are 0.3 and 6.5 kcal/mol. Finally, removal of HI from the corresponding species proceeds *via* the associated transition states to afford the final products, with activation barriers of 3.6 and 3.7 kcal/mol, respectively. The product energies are calculated to be -8.7 and -9.6 kcal/mol, indicating that the formation of both products from Pd(OAc)₂ is thermodynamically favorable. Overall, the process is both thermodynamically and kinetically highly energy demanding for product formation.



Notably, only the product-forming step from the active catalyst is exergonic relative to all other steps, suggesting that Pd(OAc)₂ is unlikely to be the actual active catalyst for the C–C coupling reaction.

Figure Sb. Free energy profiles for the Pd-catalyzed C-C coupling of 2-iodoglucal (**1a**) and DHP (**3a**). The relative free energies are given in kcal/mol.

In conclusion, both catalytic pathways involve oxidative addition and other steps with very high energy barriers, while only the product-forming step is exergonic relative to the others from the active catalytic species (Figure Sa and Sb). Moreover, the intermediates formed after β -hydride elimination are thermodynamically unfavorable. Consequently, Pd(OAc)₂ is unlikely to be the true active catalyst for the C–C coupling reaction; however, it behaves as a pre-catalyst and is further reduced in the presence of DMF to generate Pd(0), which serves as the true active catalytic species, as illustrated in the catalytic cycle described below.¹³

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6. Computational details

Geometry optimizations were performed using the hybrid B3LYP density functional augmented with Grimme's D3 dispersion correction (B3LYP-D3), as implemented in the Gaussian 09 program.¹⁴⁻¹⁸ Solvation effects were treated using the SMD continuum solvation model.¹⁹ The 6-31G** basis set was employed for C, H, and O atoms,²⁰ while the SDD²¹ effective core potential and corresponding basis set were used for Pd and I atoms. Harmonic vibrational frequency analyses were carried out at the same level of theory to characterize all stationary points as either minima (no imaginary frequencies) or transition states (one imaginary frequency), as expected for the bond-forming event. Intrinsic reaction coordinate (IRC) calculations were performed to confirm that each transition state connects the corresponding reactant and product along the reaction pathway.^{22,23} Single-point energy refinements were subsequently performed at the B3LYP-D3/def2-TZVP level using the Gaussian 09 package.^{24,25} Thus, the single-point energies are at the SMD(DMF)/B3LYP-D3/def2-TZVP//B3LYP-D3/6-31G**,SDD level of theory. Zero-point vibrational energies well as thermal and entropic corrections, obtained from solvent-phase computations at 298 K and 1 atm, were applied to the single-point energies calculated in the solvent phase. The discussion in this manuscript is based on Gibbs free

energies in the solvent phase. Non-covalent interaction (NCI) analyses are executed with the help of VMD 1.9.3 and Multiwfn 3.8 software.^{26,27}

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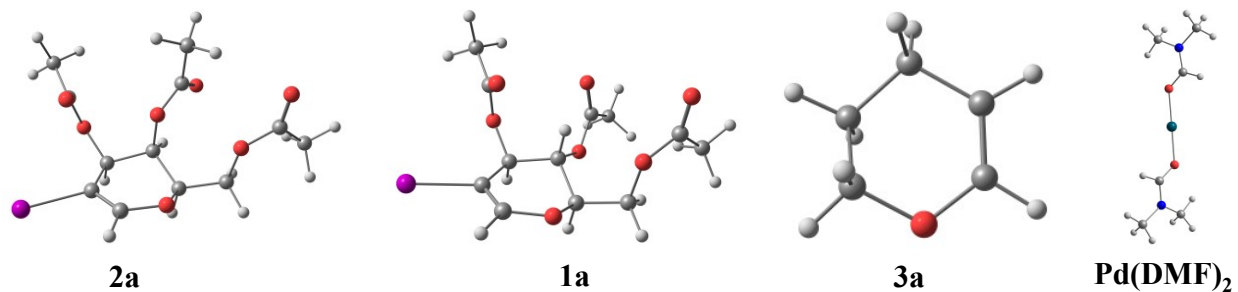
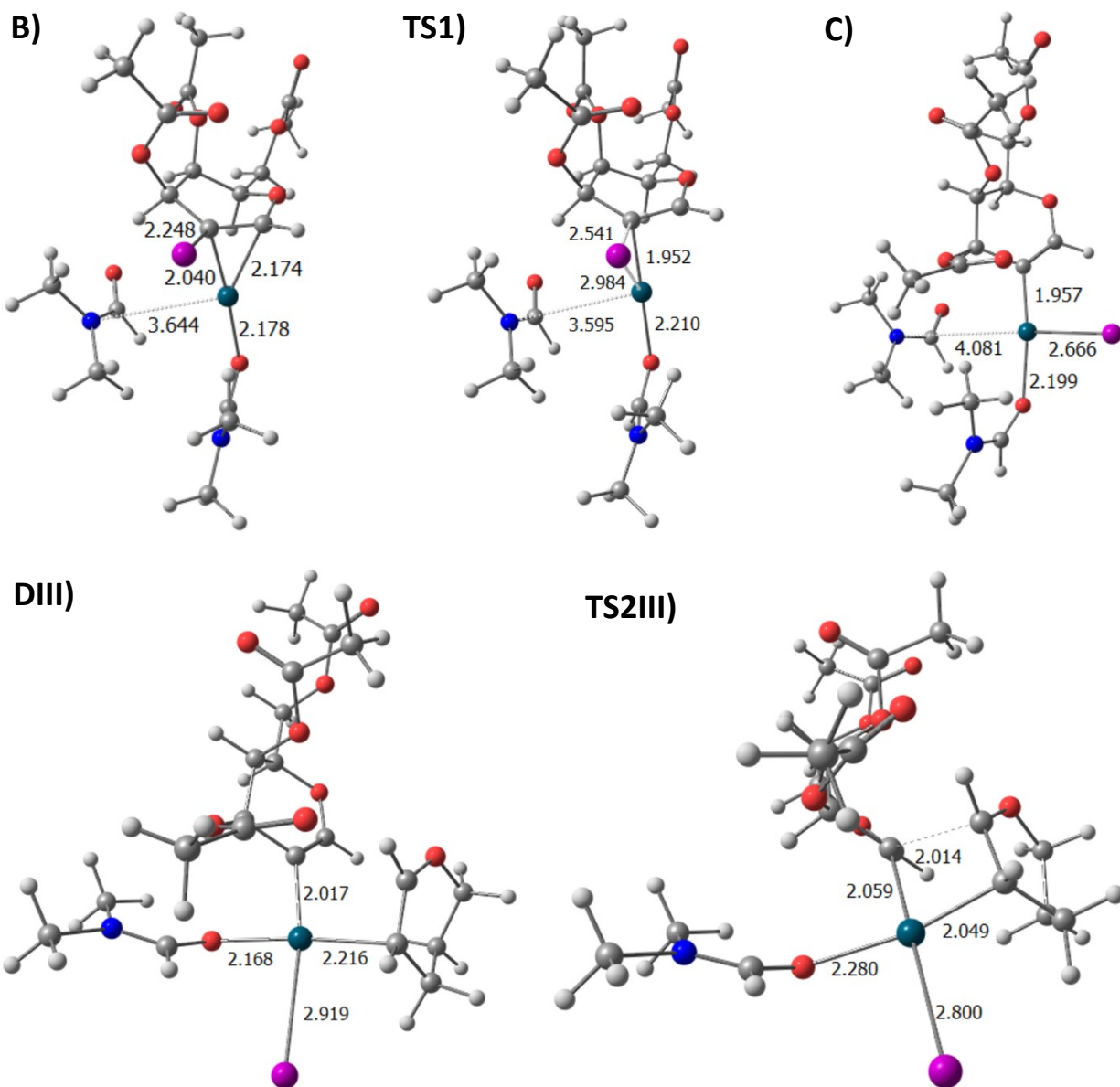


Fig. S1. The optimized structures of **2a** (2-iodogalactal), **1a** (2-iodoglucal), **3a** (Dihydropyran) and [Pd(DMF)₂].



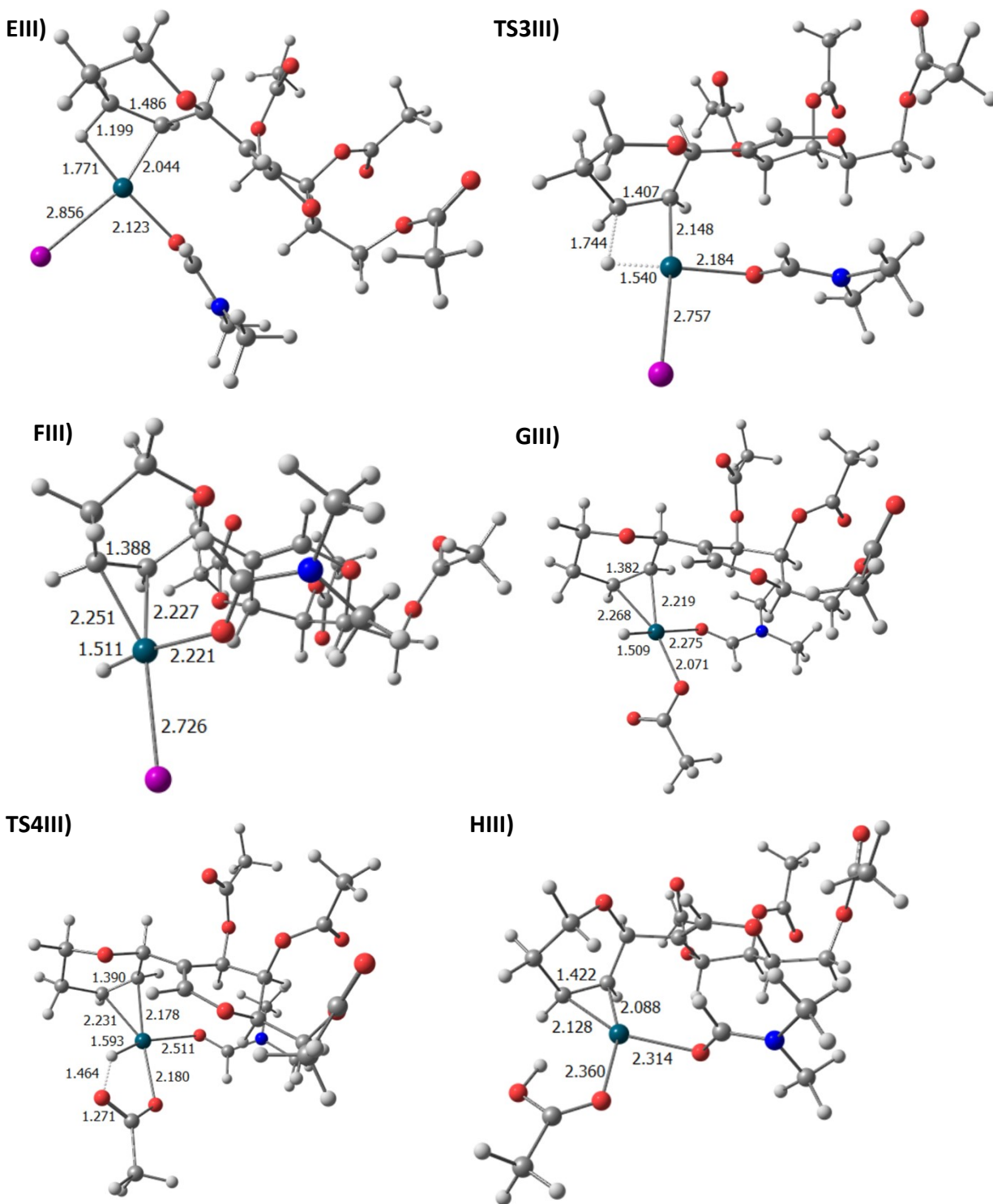
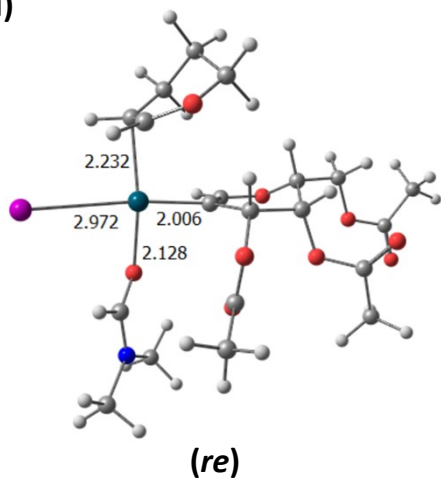
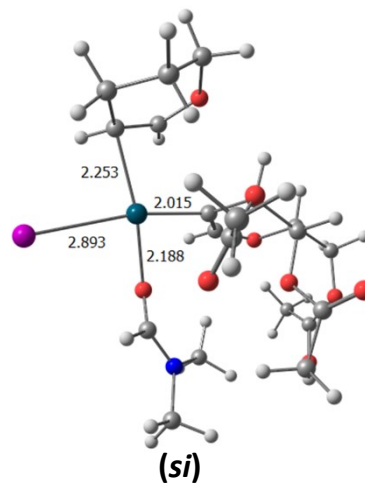


Fig. S2. The optimized structures for selected species (reaction with **2a**) together with selected bond distances shown in Fig. 1.

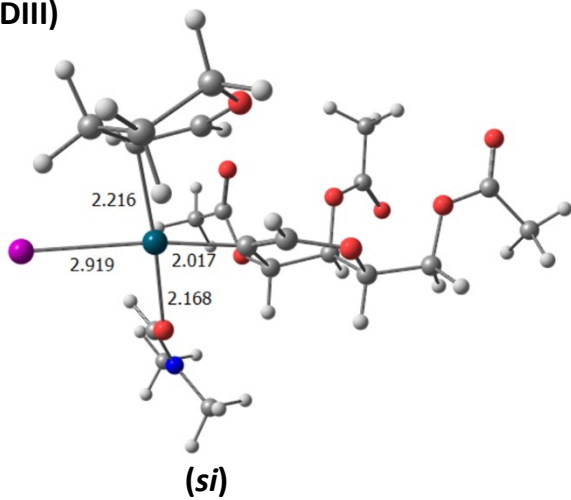
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D III)



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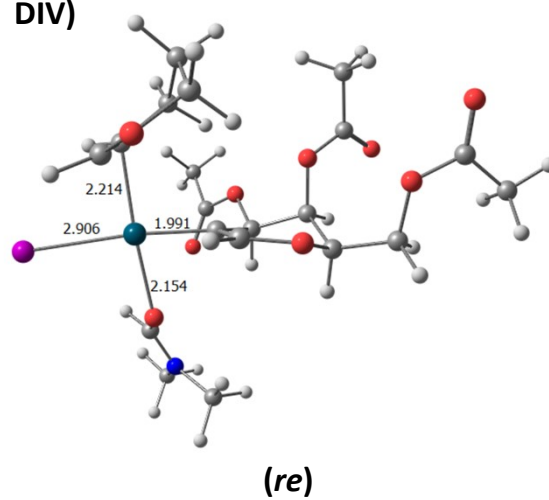
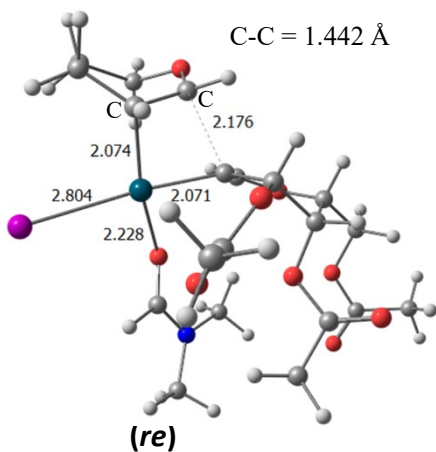
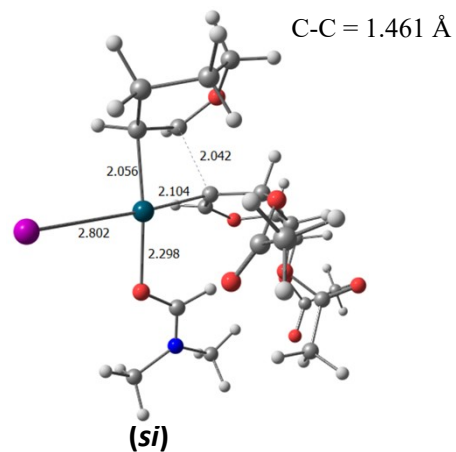


Fig. S3. Optimized structures of intermediate **D** with four distinct orientations of **2a** coordinated to the Pd center, along with selected bond distances, are shown in Fig. 1.

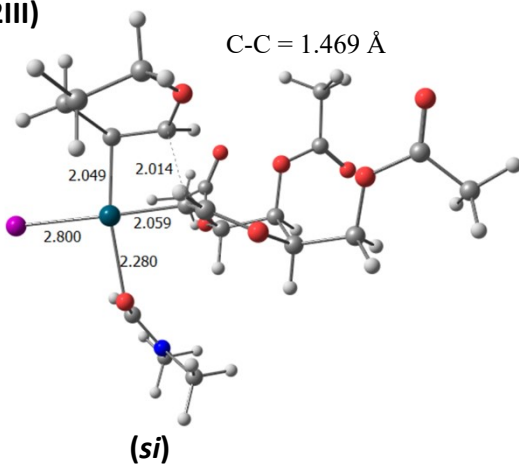
TS2I)



TS2II)



TS2III)



TS2IV)

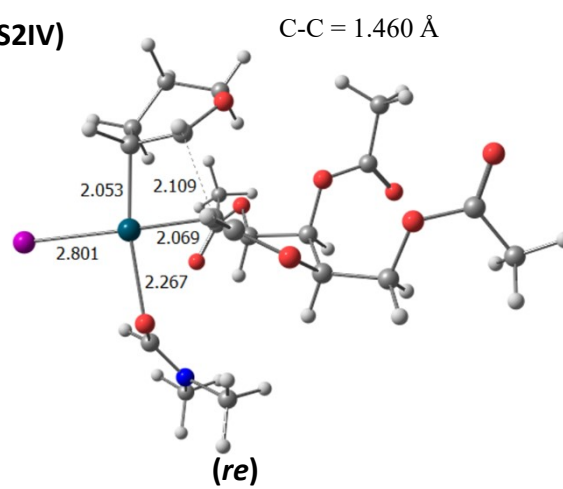


Fig. S4. Optimized structures of species TS2_{2a} with four distinct orientations, along with selected bond distances, are shown in Fig. 1.

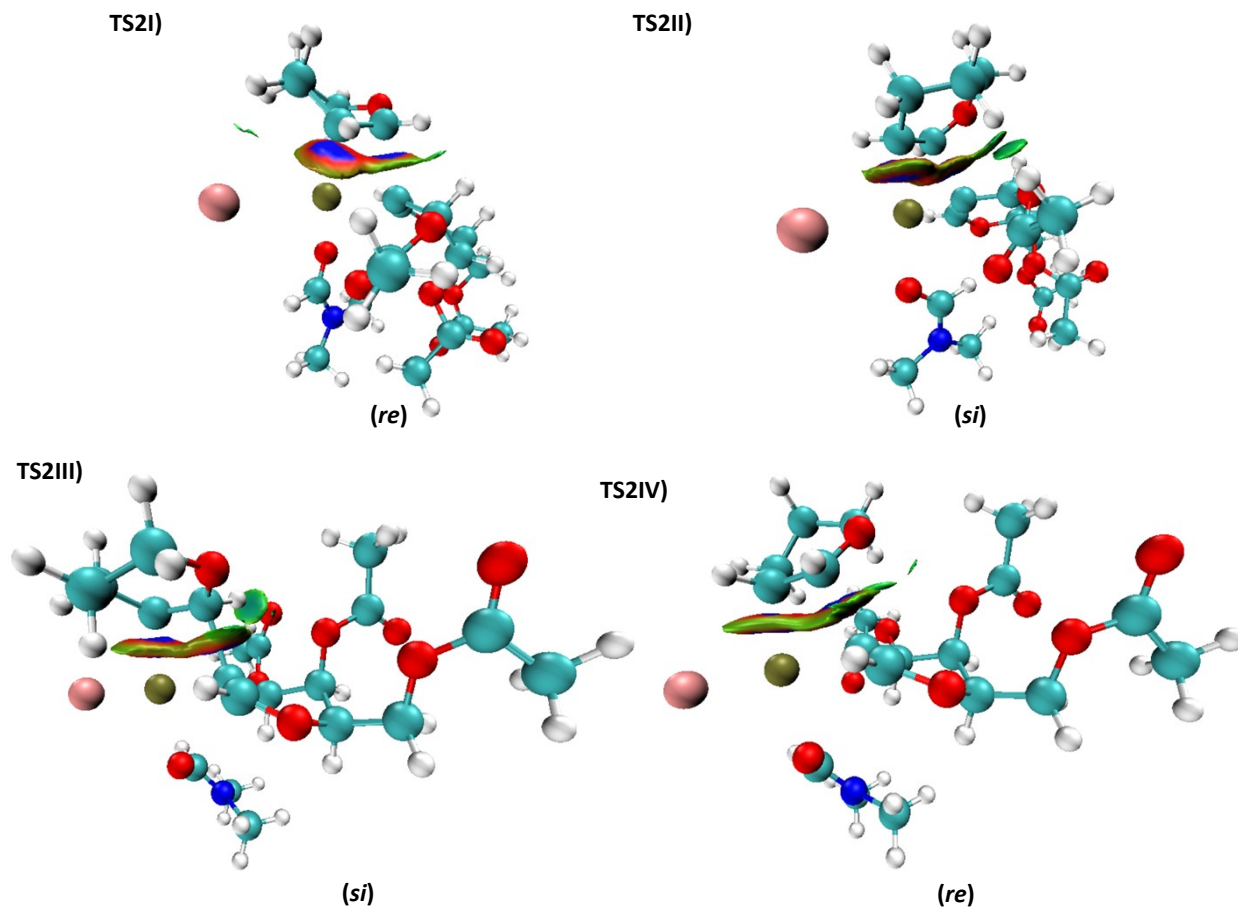


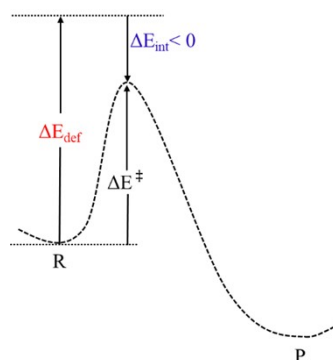
Fig. S5. Non-covalent interaction (IGMH) analysis of TS2_{2a} species with four distinct orientations.

Activation Strain Analysis

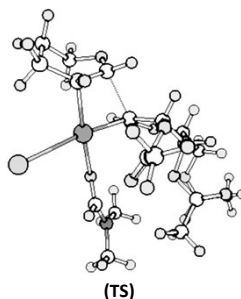
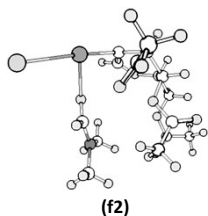
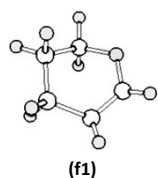
Table S1. Relative distortion energies of individual fragments with respect to the pre-reacting complex, along with total distortion ($\Delta\Delta E_{\ddagger,d}$) and interaction energies ($\Delta\Delta E_{\ddagger,i}$) for the regio- and stereocontrolling transition states at the SMD(DMF)/B3LYP-D3/def2-TZVP level. Energies are given in kcal/mol.

$$\Delta E_{\text{act}} = \Delta E_{\text{distortion}} + \Delta E_{\text{interaction}}$$

$$\Delta E_{\text{distortion}} = [\{E_{f1(\text{TS})} + E_{f2(\text{TS})}\} - \{E_{f1} + E_{f2}\}]$$



$$\Delta E_{\text{interaction}} = [E_{\text{(TS)}} - \{E_{\text{f1}} + E_{\text{f2}}\}]$$



TSs	Distortion Energy ($E_{\text{distortion}}$)		Total Distortion Energy	Interaction Energy ($E_{\text{interaction}}$)	Activation Strain Energy (E_{act})	Barrier Height
	$\Delta\Delta E_{\text{d}}^{\ddagger}$ (f1)	$\Delta\Delta E_{\text{d}}^{\ddagger}$ (f2)				
2a (2-iodogalactal)						
TS2I_{2a}	18.9	6.2	25.1	-35.5	10.4	9.7
TSII_{2a}	19.9	11.4	31.3	-40.4	9.1	8.8
TSIII_{2a}	20.6	13.9	34.5	-47.1	12.6	8.2
TSIV_{2a}	20.9	10.9	31.8	-43.1	11.3	12.1
1a (2-iodoglucal)						
TSI_{1a}	14.1	9.6	23.7	-36.1	12.4	5.5
TSII_{1a}	17.9	9.3	27.2	-36.6	9.4	9.5
TSIII_{1a}	16.4	12.8	29.2	-41.1	11.9	8.8
TSIII_{1a}	20.7	9.8	30.5	-42.0	11.5	12.6

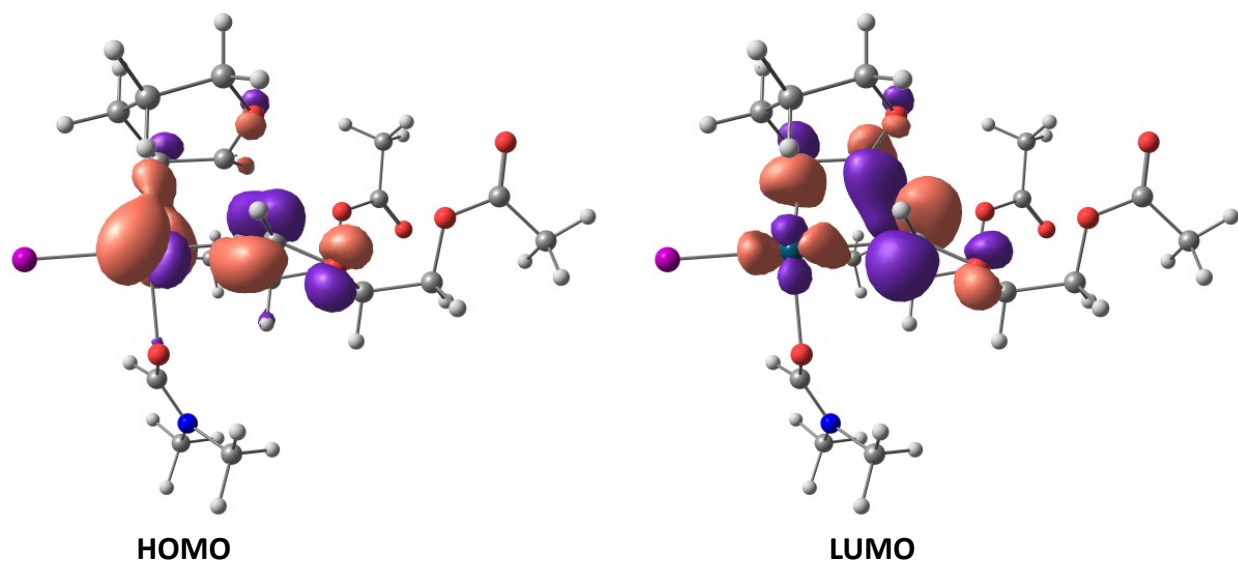


Fig. S6. HOMO of the Pd complex, showing filled Pd *d*-orbital character, and LUMO of the alkene, corresponding to the π^* antibonding orbital of the C=C bond in **TS2III_{2a}**.

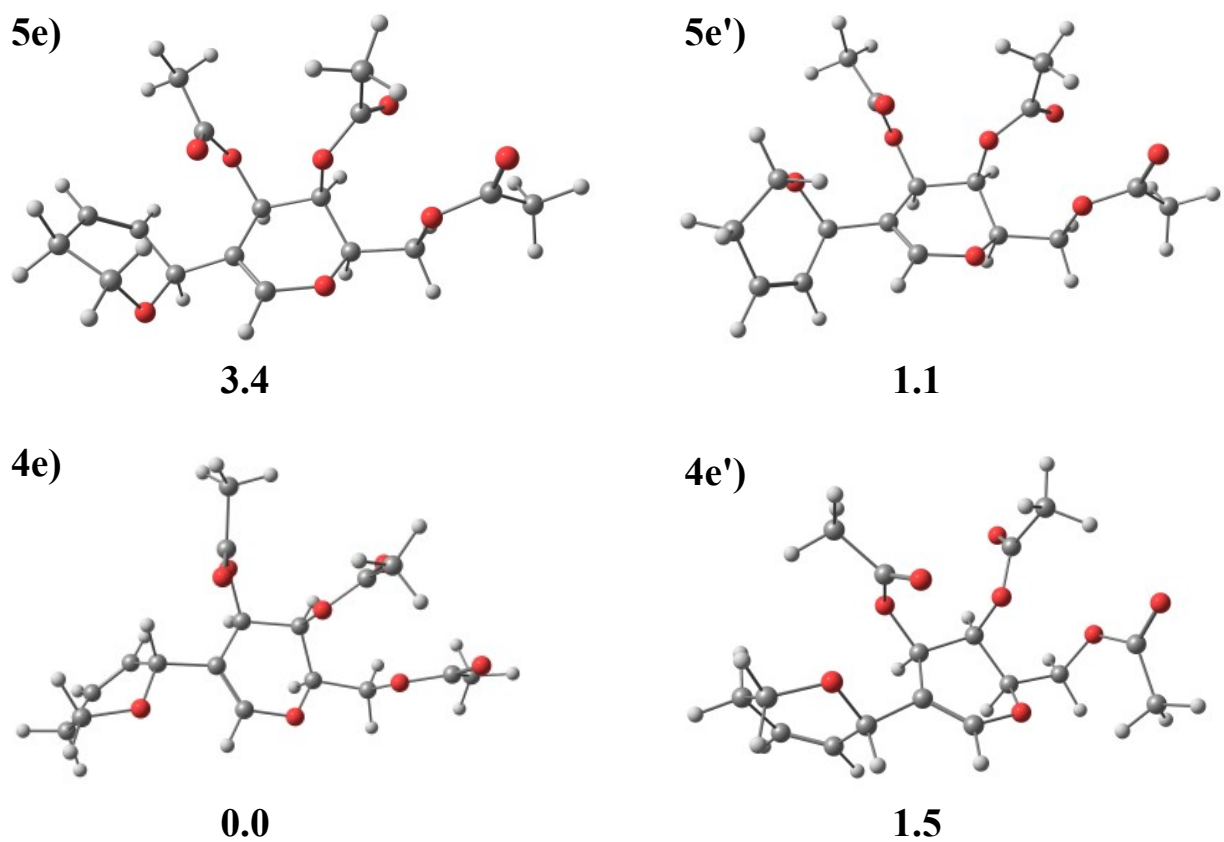


Fig. S7. Optimized structures of species of products of **5e/5e'** and **4e/4e'**. The relative free energies are given in kcal/mol.

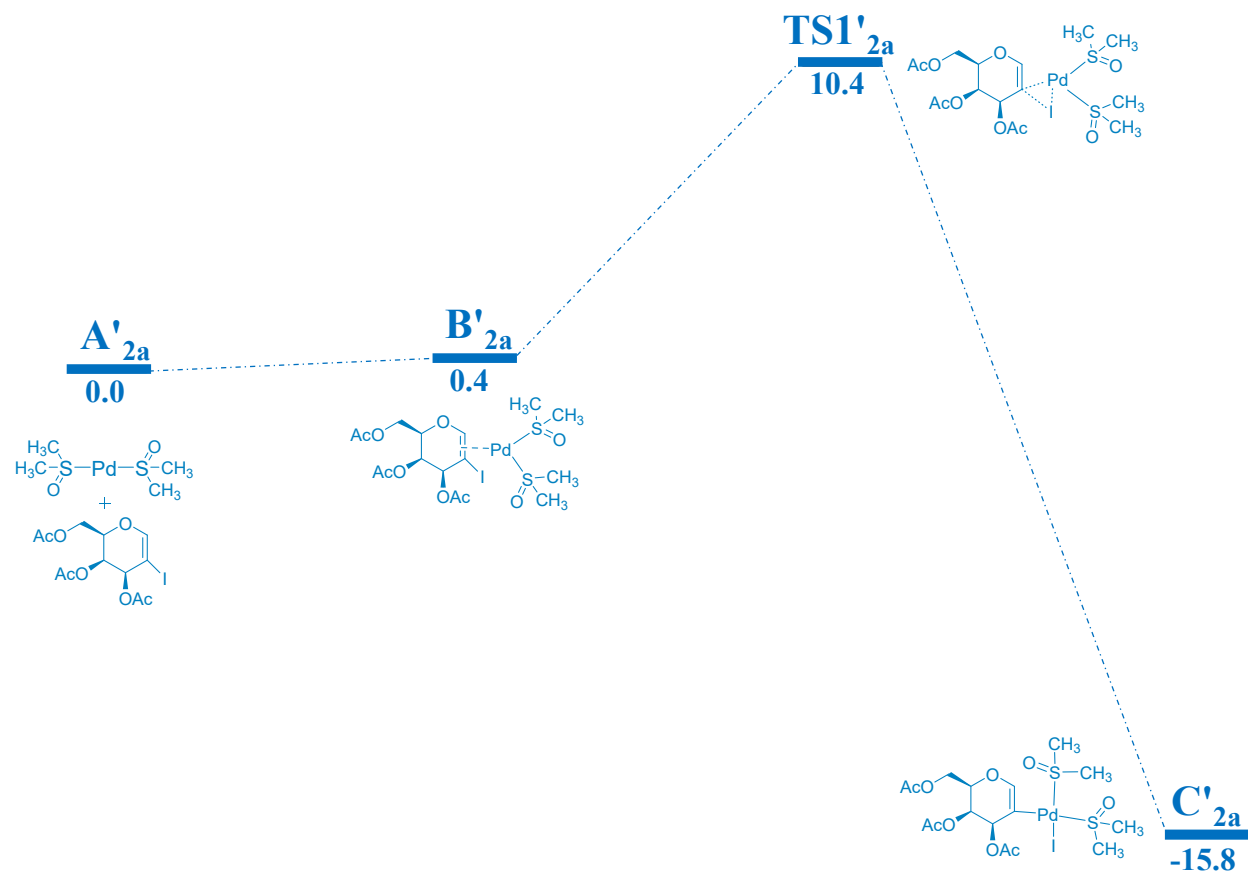


Fig. S8. Free energy profiles for oxidative addition of 2-iodogalactal (**2a**) with $\text{Pd}(\text{DMSO})_2$. Relative free energies are reported in kcal/mol.

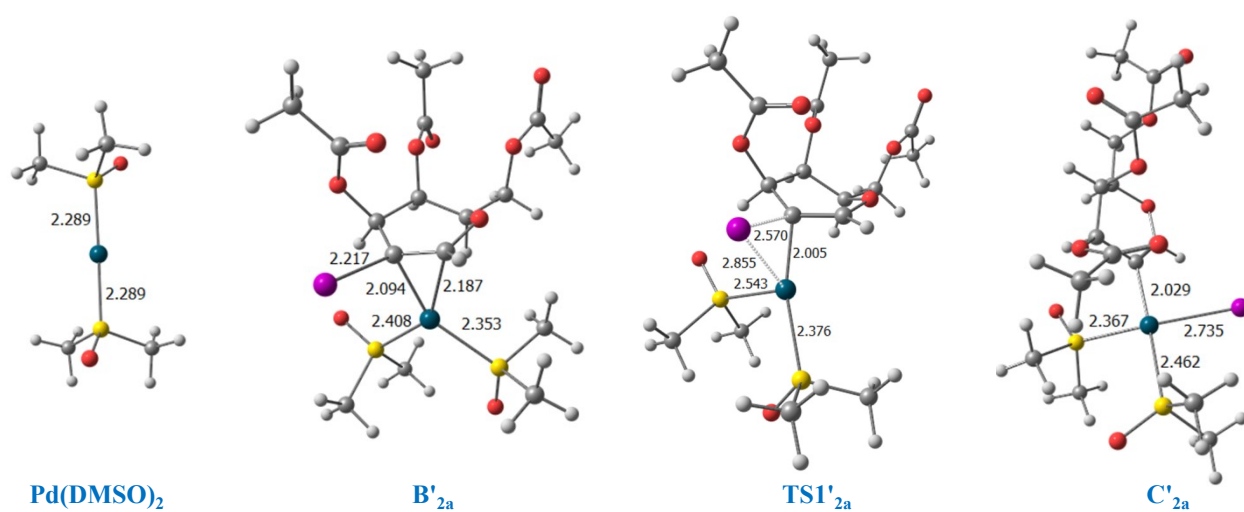
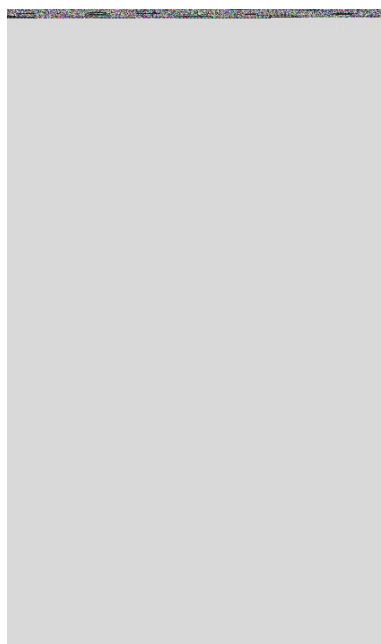
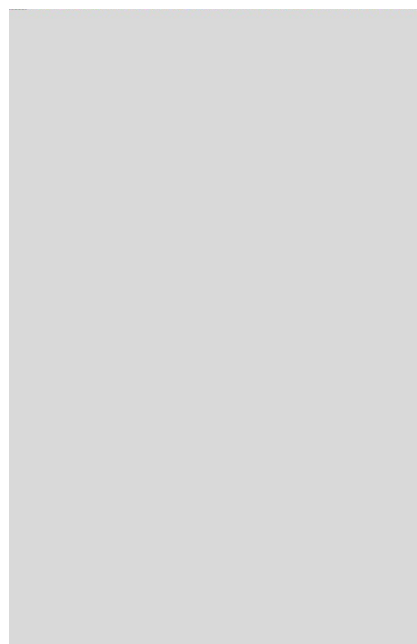


Fig. S9. The optimized structures of the species involved in the reaction of **2a** with $\text{Pd}(\text{DMSO})_2$, along with selected bond distances.

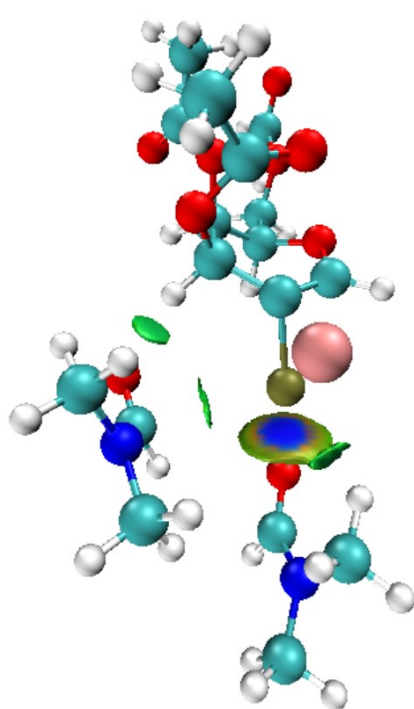


TS1_{2a}

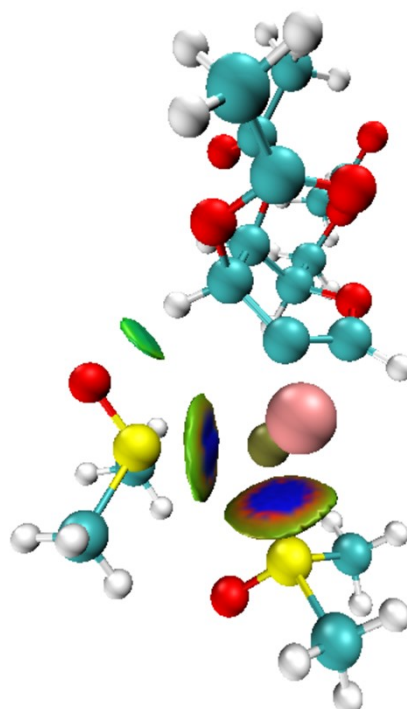


TS1'_{2a}

Fig. S10. The optimized structures of oxidative addition transition states with DMF (TS1_{2a}) and DMSO (TS1'_{2a}) as ligands, along with selected bond distances.



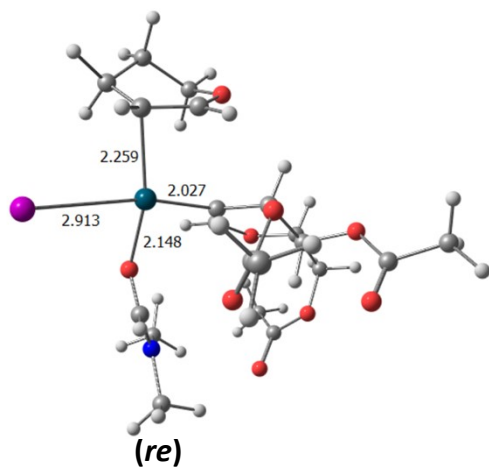
TS1_{2a}



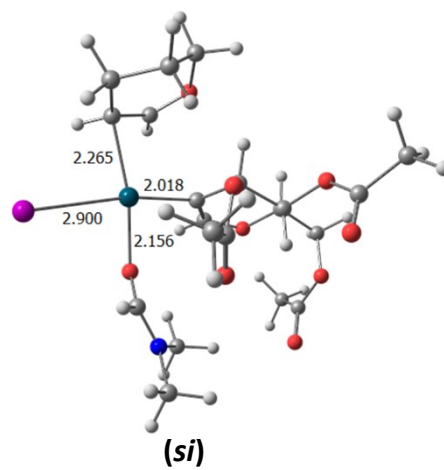
TS1'_{2a}

Fig. S11. Non-covalent interaction (IGMH) analysis of the oxidative addition transition states with DMF (TS1_{2a}) and DMSO (TS1'_{2a}) as ligands.

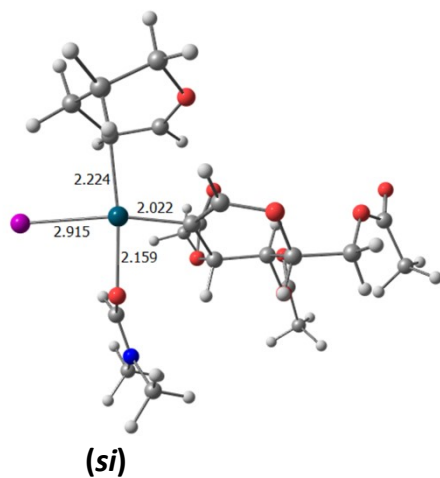
D I)



D II)



D III)



D IV)

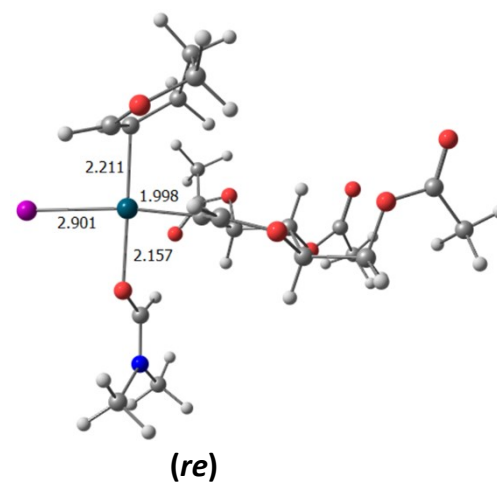


Fig. S12. Optimized structures of species **D** with four distinct orientations of **1a** coordinated to the Pd center, along with selected bond distances, are shown in Fig. 2.

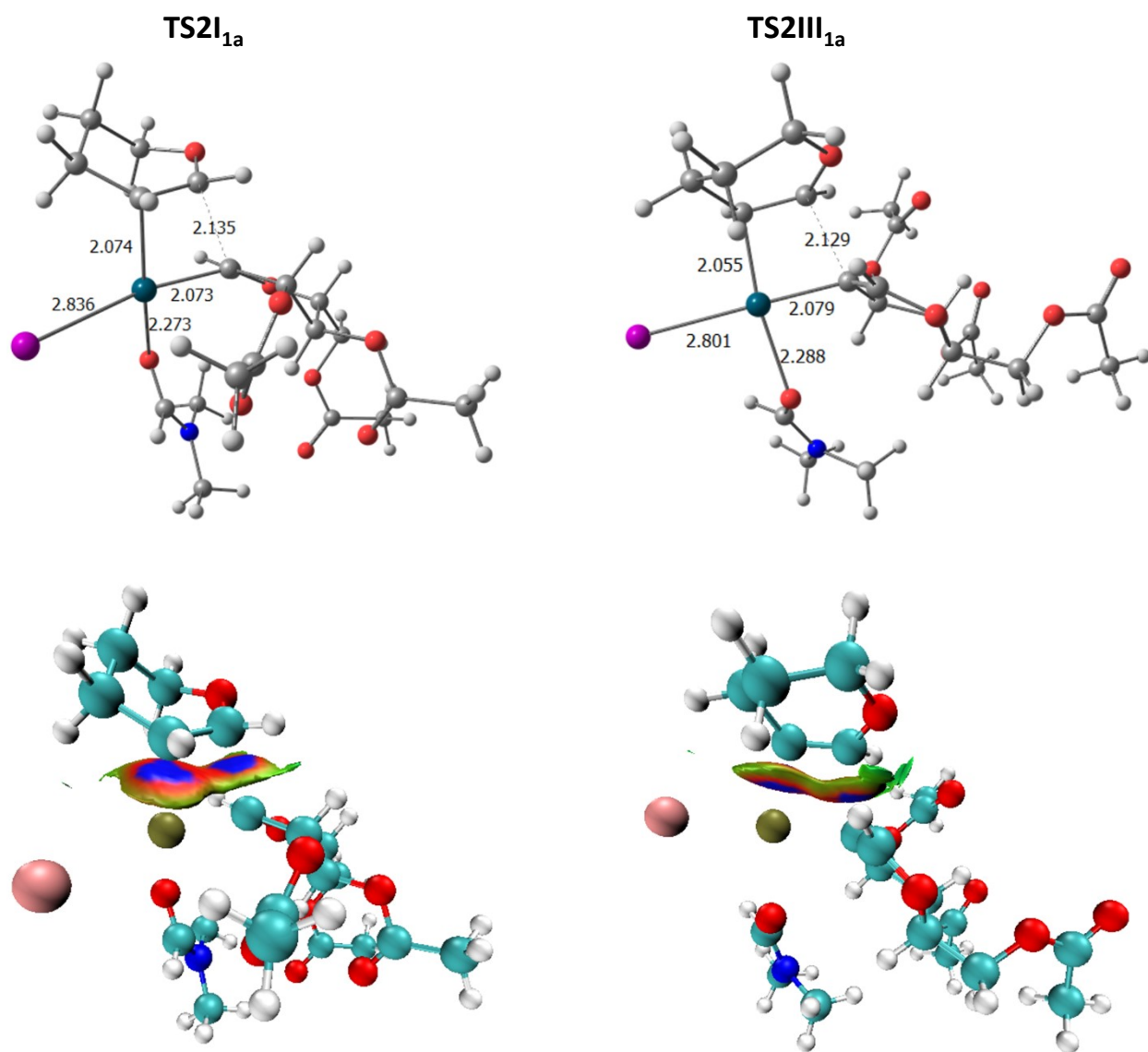


Fig. S13. Optimized structures of species **TS2I_{1a}** and **TS2III_{1a}**, along with selected bond distances and corresponding non-covalent interaction (IGMH) analysis.

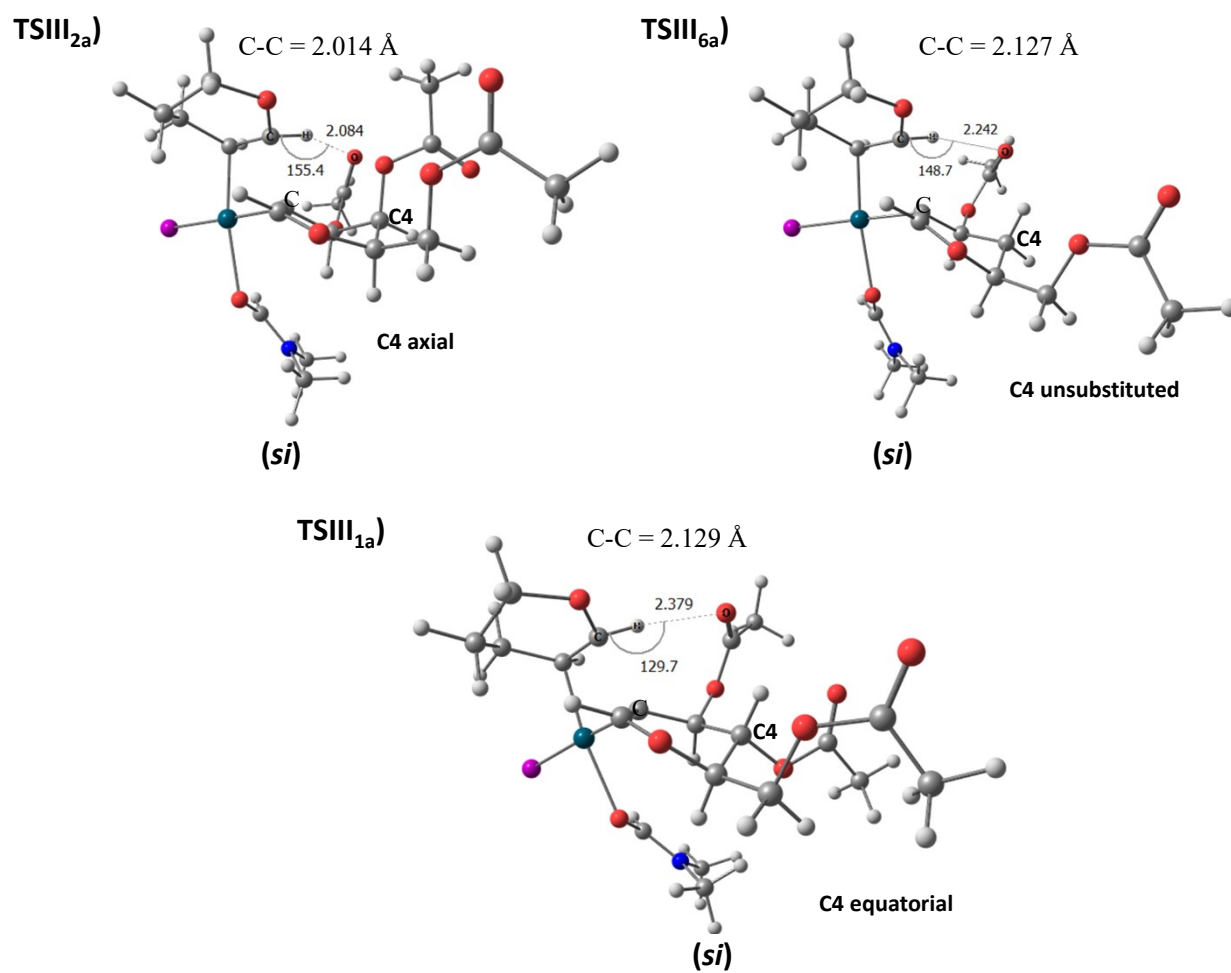


Fig. S14. Optimized structures of **TSIII** with different substrates (**1a**, **2a** and **6a**), along with selected bond distances (Å) and angle (°).

Table S2. Cartesian coordinates (Å) of the optimized structures of all reactants, intermediates, transition states and products at B3LYP-D3/6-31G**,SDD in SMD(DMF)level of theory.

(1) Computational investigation of the Pd-catalyzed C–C coupling of between 2a and 3a

[Pd(DMF)₂]

Pd	-0.000260000	0.062223000	-0.192157000
N	-4.256466000	0.004877000	0.185157000
N	4.254094000	-0.105996000	0.195581000
C	2.947466000	-0.343327000	0.322385000
H	2.698842000	-1.257926000	0.871211000
O	2.056785000	0.410949000	-0.139858000
C	-2.966647000	0.335875000	0.262769000
H	-2.754358000	1.206753000	0.891665000
O	-2.051940000	-0.286492000	-0.331088000
C	4.762865000	1.059883000	-0.518308000
H	5.369363000	1.672262000	0.157219000
H	3.929810000	1.650772000	-0.895888000
H	5.389846000	0.734401000	-1.355120000
C	5.246794000	-1.017058000	0.753622000
H	5.882556000	-0.484130000	1.468661000
H	5.878453000	-1.417620000	-0.046371000
H	4.752401000	-1.844565000	1.265867000
C	-5.276427000	0.764974000	0.898540000
H	-6.005465000	1.170080000	0.188751000
H	-4.816306000	1.590223000	1.445157000
H	-5.800002000	0.114940000	1.607562000
C	-4.717295000	-1.136235000	-0.598011000
H	-5.440535000	-0.800075000	-1.348181000
H	-5.205464000	-1.863473000	0.059520000
H	-3.869888000	-1.606401000	-1.094423000

2a

C	-5.446395000	-1.324199000	0.629466000
C	-4.572325000	-0.780016000	-0.471322000
O	-4.988491000	-0.121555000	-1.403414000
O	-3.240885000	-1.030155000	-0.422271000
H	-6.489221000	-1.164769000	0.356465000
H	-5.266138000	-2.389274000	0.801470000
H	-5.240784000	-0.794655000	1.566444000
C	1.510921000	3.654777000	0.382162000
C	1.330551000	2.213972000	-0.021171000
O	1.327088000	1.798932000	-1.156574000
O	1.190267000	1.452494000	1.101625000
H	1.705875000	4.262356000	-0.501705000
H	0.602331000	4.008369000	0.880683000
H	2.336686000	3.751699000	1.093261000
C	-1.152465000	-1.475485000	0.715181000
C	0.757162000	-1.743392000	-0.648827000
C	-0.745060000	-0.023173000	0.961169000
C	0.794245000	0.066548000	1.066739000

C	1.439346000	-0.816716000	0.035337000
O	-0.575612000	-1.980702000	-0.503600000
C	-2.646939000	-1.739178000	0.679413000
H	1.208727000	-2.401487000	-1.383864000
H	1.076069000	-0.284469000	2.064019000
H	-0.754511000	-2.065426000	1.554202000
H	-3.066577000	-1.419044000	1.636361000
H	-2.820133000	-2.813234000	0.557014000
O	-1.169918000	0.805768000	-0.125077000
C	-2.238079000	1.617944000	0.071564000
H	-1.192153000	0.333290000	1.891374000
C	-2.599205000	2.321360000	-1.203569000
H	-3.207541000	1.628656000	-1.796630000
H	-3.190358000	3.210827000	-0.981705000
H	-1.706225000	2.581202000	-1.775988000
O	-2.826660000	1.719480000	1.129331000
I	3.579002000	-0.744015000	-0.152800000

3a

C	0.529097000	-1.228143000	0.289874000
C	0.907326000	1.072239000	-0.081154000
C	-0.855184000	-1.044518000	-0.324345000
C	-1.451505000	0.297477000	0.129006000
C	-0.391537000	1.368564000	0.059833000
O	1.439994000	-0.184700000	-0.110517000
H	1.681081000	1.827984000	-0.193800000
H	-1.851298000	0.210188000	1.149837000
H	0.461120000	-1.226605000	1.387511000
H	-1.493738000	-1.886392000	-0.036861000
H	-2.304678000	0.567865000	-0.506068000
H	-0.758414000	-1.060509000	-1.416606000
H	-0.679112000	2.415664000	0.087834000
H	0.995909000	-2.164312000	-0.026992000

B_{2a}

Pd	1.355605000	-1.099846000	-0.459097000
C	3.943739000	-2.901057000	-0.045992000
O	2.707665000	-2.790479000	-0.219038000
C	-5.509622000	-3.551780000	0.075789000
C	-5.373874000	-2.237881000	-0.651496000
O	-6.307001000	-1.644417000	-1.155211000
O	-4.143832000	-1.677536000	-0.747289000
H	-6.533421000	-3.907590000	-0.036909000
H	-4.812545000	-4.299865000	-0.313511000
H	-5.292995000	-3.419477000	1.141177000
C	-2.248414000	4.240497000	0.158922000
C	-1.796677000	2.872214000	-0.282324000
O	-1.945092000	2.408914000	-1.390388000
O	-1.166241000	2.249619000	0.749830000
H	-2.800323000	4.722725000	-0.648256000
H	-2.878733000	4.159654000	1.049334000
H	-1.378352000	4.850034000	0.424841000
C	-1.824511000	-1.325211000	-0.116193000
C	-0.315415000	-0.285604000	-1.586595000
C	-1.972033000	-0.088026000	0.772671000
C	-0.730845000	0.876017000	0.653696000
C	0.147466000	0.541179000	-0.549282000
O	-1.496704000	-0.983480000	-1.466703000
C	-2.998322000	-2.285803000	-0.120512000

H	-0.036912000	-0.160025000	-2.627584000
H	-0.145719000	0.755804000	1.562774000
H	-0.972200000	-1.893088000	0.300079000
H	-3.216615000	-2.553281000	0.916491000
H	-2.715505000	-3.186420000	-0.674454000
I	1.567678000	2.188623000	-1.116953000
H	4.326251000	-3.771134000	0.502486000
C	6.306072000	-2.364913000	-0.209624000
H	6.836975000	-2.497248000	-1.158174000
H	6.766314000	-1.537754000	0.339619000
H	6.396687000	-3.278938000	0.379991000
C	4.632915000	-0.882140000	-1.273081000
H	4.877468000	-1.082708000	-2.322286000
H	3.578606000	-0.596045000	-1.201954000
H	5.252401000	-0.056672000	-0.914046000
N	4.898170000	-2.066758000	-0.463600000
O	0.829493000	-0.677970000	3.189381000
C	1.961497000	-0.609684000	2.701190000
N	2.674777000	0.526272000	2.523528000
C	2.162256000	1.816514000	2.959002000
H	2.866883000	2.280933000	3.658749000
H	2.029368000	2.484288000	2.101060000
H	1.204147000	1.669406000	3.457494000
C	3.996997000	0.512708000	1.918243000
H	4.005907000	1.129942000	1.013613000
H	4.742855000	0.907658000	2.618612000
H	4.273268000	-0.508729000	1.648916000
H	2.509839000	-1.506988000	2.365458000
O	-3.159432000	0.646355000	0.444865000
C	-4.280732000	0.410104000	1.164380000
C	-5.431604000	1.200487000	0.610536000
H	-5.111561000	2.196037000	0.293758000
H	-5.809086000	0.665049000	-0.268240000
H	-6.226453000	1.269198000	1.354141000
O	-4.338778000	-0.363365000	2.100691000
H	-2.045933000	-0.422330000	1.809181000

TS1_{2a}

Pd	1.469241000	-1.011575000	-0.497466000
C	4.170683000	-2.681456000	0.011929000
O	2.948664000	-2.634331000	-0.252505000
C	-6.123093000	-3.087186000	0.043472000
C	-5.830586000	-1.785034000	-0.657759000
O	-6.690535000	-1.033753000	-1.072387000
O	-4.536993000	-1.417515000	-0.829774000
H	-7.188817000	-3.296419000	-0.046115000
H	-5.545383000	-3.915872000	-0.375783000
H	-5.865736000	-3.002832000	1.104998000
C	-1.698183000	4.207311000	0.209123000
C	-1.597200000	2.766916000	-0.221867000
O	-1.909827000	2.336626000	-1.308837000
O	-1.075764000	2.028760000	0.793194000
H	-2.197704000	4.788171000	-0.566637000
H	-2.250192000	4.285287000	1.150400000
H	-0.692707000	4.606766000	0.378485000
C	-2.186137000	-1.380363000	-0.244650000
C	-0.623184000	-0.389101000	-1.668123000
C	-2.180578000	-0.206751000	0.741836000
C	-0.833449000	0.613749000	0.651408000
C	-0.046668000	0.215147000	-0.579183000

O	-1.841743000	-0.987434000	-1.584146000
C	-3.458479000	-2.205812000	-0.293970000
H	-0.232349000	-0.357027000	-2.678687000
H	-0.255748000	0.381744000	1.544203000
H	-1.392782000	-2.060601000	0.109617000
H	-3.678434000	-2.539164000	0.722513000
H	-3.294034000	-3.078408000	-0.934011000
I	1.783389000	1.883131000	-1.151369000
H	4.553018000	-3.502895000	0.631854000
C	6.498524000	-1.984577000	0.052494000
H	7.156315000	-2.140499000	-0.808712000
H	6.818196000	-1.079885000	0.580263000
H	6.582574000	-2.837386000	0.728618000
C	4.851348000	-0.708506000	-1.284711000
H	5.553132000	-0.744180000	-2.124185000
H	3.831926000	-0.760308000	-1.666380000
H	4.986061000	0.236138000	-0.749716000
N	5.116947000	-1.832260000	-0.394219000
O	0.909748000	-1.020162000	2.959729000
C	2.079685000	-0.800324000	2.627072000
N	2.667151000	0.416056000	2.576257000
C	1.940788000	1.619531000	2.953186000
H	2.533978000	2.199968000	3.668370000
H	1.741120000	2.242785000	2.074990000
H	0.996035000	1.335256000	3.416535000
C	4.043915000	0.581785000	2.136707000
H	4.087105000	1.242029000	1.263802000
H	4.651026000	1.021812000	2.936812000
H	4.467421000	-0.386804000	1.863448000
H	2.769794000	-1.613712000	2.348147000
O	-3.278215000	0.689133000	0.535808000
C	-4.407495000	0.493011000	1.255050000
C	-5.457554000	1.490983000	0.860171000
H	-5.019804000	2.478290000	0.694795000
H	-5.903506000	1.147748000	-0.080061000
H	-6.232600000	1.534648000	1.626124000
O	-4.546073000	-0.395661000	2.073621000
H	-2.259408000	-0.625964000	1.747300000

C_{2a}

Pd	-1.652070000	-0.556726000	-0.792893000
C	-4.784624000	0.122997000	-0.487469000
O	-3.824999000	-0.406544000	-1.097578000
C	7.201102000	0.427021000	-1.056248000
C	6.308107000	-0.465958000	-0.233040000
O	6.697517000	-1.127893000	0.708497000
O	4.994810000	-0.538817000	-0.555026000
H	8.236154000	0.241065000	-0.770173000
H	7.074997000	0.248508000	-2.128029000
H	6.961592000	1.478279000	-0.861844000
C	-0.485706000	1.750790000	3.087234000
C	-0.002767000	0.806326000	2.013896000
O	0.111394000	-0.392267000	2.136091000
O	0.265248000	1.515638000	0.888040000
H	-0.768255000	1.186164000	3.976026000
H	0.310410000	2.459439000	3.337101000
H	-1.340490000	2.328542000	2.724474000
C	2.918645000	0.272111000	-1.487727000
C	1.128109000	-1.285801000	-1.367385000
C	2.359210000	0.928670000	-0.221724000

C	0.825876000	0.940366000	-0.318906000
C	0.299027000	-0.409694000	-0.775803000
O	2.460068000	-1.076828000	-1.633542000
C	4.433046000	0.269594000	-1.604930000
H	0.822426000	-2.271478000	-1.699558000
H	0.563151000	1.692834000	-1.067411000
H	2.546959000	0.865350000	-2.337894000
H	4.783311000	1.303070000	-1.542325000
H	4.717554000	-0.146625000	-2.576869000
I	-1.707598000	-3.061707000	0.116866000
H	-5.747015000	0.221940000	-1.003274000
C	-5.988137000	1.163633000	1.348297000
H	-6.270051000	0.592138000	2.238009000
H	-5.807670000	2.203880000	1.636266000
H	-6.807520000	1.128749000	0.628384000
C	-3.588900000	0.527738000	1.606413000
H	-3.723259000	1.203608000	2.450863000
H	-3.432106000	-0.489433000	1.976352000
H	-2.704143000	0.840339000	1.045033000
N	-4.776570000	0.597794000	0.755971000
O	-0.911152000	2.645709000	-2.701428000
C	-1.854889000	2.756264000	-1.910929000
N	-1.860553000	3.518760000	-0.795641000
C	-0.704212000	4.321480000	-0.425947000
H	-0.997314000	5.371695000	-0.315880000
H	-0.284407000	3.965184000	0.519731000
H	0.049925000	4.237884000	-1.208655000
C	-3.028441000	3.609144000	0.065810000
H	-2.766726000	3.329578000	1.091589000
H	-3.419267000	4.633715000	0.076969000
H	-3.810472000	2.936916000	-0.292867000
H	-2.808153000	2.218022000	-2.059534000
O	2.738056000	0.190532000	0.946848000
C	3.755783000	0.671996000	1.699791000
C	4.110595000	-0.297188000	2.789792000
H	3.223559000	-0.802563000	3.176820000
H	4.779097000	-1.046955000	2.350886000
H	4.640456000	0.222449000	3.589306000
O	4.318337000	1.728184000	1.485663000
H	2.729874000	1.953051000	-0.143891000

DI_{2a}

Pd	1.762961000	-0.503443000	-0.315807000
C	2.126588000	2.474186000	-0.414062000
O	1.688601000	1.487835000	-1.063362000
C	-7.183073000	-1.290798000	-0.854823000
C	-6.312153000	-0.079538000	-1.073240000
O	-6.747899000	1.036079000	-1.279924000
O	-4.967562000	-0.236146000	-1.039001000
H	-8.219026000	-1.014138000	-1.049440000
H	-6.892631000	-2.118883000	-1.508210000
H	-7.096546000	-1.638286000	0.180425000
C	-0.057796000	3.016624000	2.222352000
C	-0.572052000	2.041101000	1.191943000
O	-0.884582000	2.333767000	0.060978000
O	-0.595060000	0.789857000	1.722772000
H	-0.147494000	4.032461000	1.836935000
H	-0.614543000	2.918926000	3.158610000
H	0.993779000	2.799965000	2.438790000
C	-2.889037000	-1.321712000	-0.422227000

C	-0.893236000	-0.737115000	-1.512109000
C	-2.533296000	-0.466614000	0.798558000
C	-0.980624000	-0.373913000	0.938711000
C	-0.242466000	-0.536278000	-0.363134000
O	-2.264399000	-0.853780000	-1.621473000
C	-4.373126000	-1.501185000	-0.692149000
H	-0.410697000	-0.841090000	-2.480073000
H	-0.685200000	-1.177467000	1.614903000
H	-2.505596000	-2.331282000	-0.206618000
H	-4.836451000	-1.919804000	0.205079000
H	-4.499096000	-2.203310000	-1.522452000
O	-3.088165000	0.847829000	0.696098000
C	-4.249550000	1.104974000	1.338942000
H	-2.942385000	-0.947361000	1.690251000
C	-4.711033000	2.502173000	1.037693000
H	-5.237648000	2.472514000	0.076699000
H	-5.403742000	2.840449000	1.809526000
H	-3.863517000	3.185310000	0.949126000
O	-4.841963000	0.298450000	2.030420000
I	4.702309000	-0.160866000	-0.042727000
C	-0.085205000	-3.790457000	1.247472000
C	1.911404000	-2.463880000	1.038058000
C	0.466787000	-4.607463000	0.092397000
C	1.043605000	-3.676124000	-0.983944000
C	2.018231000	-2.721005000	-0.323440000
O	0.911357000	-2.885992000	1.822657000
H	2.730873000	-2.049930000	1.618596000
H	0.232719000	-3.137229000	-1.481112000
H	-0.934618000	-3.185185000	0.923708000
H	-0.343956000	-5.223727000	-0.308346000
H	1.570883000	-4.249604000	-1.751790000
H	1.248084000	-5.282525000	0.460984000
H	3.014469000	-2.636406000	-0.746674000
H	-0.401122000	-4.414990000	2.085239000
H	2.770495000	2.341068000	0.459776000
N	1.855867000	3.733215000	-0.731199000
C	2.448767000	4.842918000	0.007125000
H	3.049502000	5.460620000	-0.668438000
H	1.658711000	5.462338000	0.443119000
H	3.089141000	4.463360000	0.805222000
C	0.972842000	4.070870000	-1.842672000
H	0.250294000	4.819375000	-1.507280000
H	1.556069000	4.485184000	-2.672311000
H	0.443567000	3.177603000	-2.166215000

DII_{2a}

Pd	-1.548900000	-0.037555000	-0.685478000
C	0.074928000	-2.566457000	0.017795000
O	-0.276008000	-1.802567000	-0.912787000
C	5.076567000	-0.439696000	-2.546398000
C	5.123516000	-0.441210000	-1.039216000
O	5.376273000	-1.433459000	-0.381764000
O	4.950009000	0.724232000	-0.371156000
H	5.289906000	-1.449885000	-2.895183000
H	4.097320000	-0.121219000	-2.907382000
H	5.826438000	0.249010000	-2.950685000
C	-0.822453000	0.947035000	3.648728000
C	-0.161109000	0.621711000	2.333972000
O	0.052487000	-0.506878000	1.939664000
O	0.112046000	1.761551000	1.664268000

H	-0.718914000	0.099791000	4.327836000
H	-0.402126000	1.850004000	4.096204000
H	-1.889164000	1.123014000	3.466772000
C	2.858073000	1.942930000	-0.929006000
C	1.027276000	0.645755000	-1.766589000
C	2.243351000	1.715880000	0.452302000
C	0.713862000	1.852323000	0.343197000
C	0.208962000	0.944265000	-0.750746000
O	2.358202000	1.002015000	-1.886711000
C	4.382618000	1.901496000	-0.972614000
H	0.737081000	0.031084000	-2.610858000
H	0.494801000	2.892408000	0.090561000
H	2.572869000	2.956108000	-1.250125000
H	4.767138000	2.735978000	-0.381646000
H	4.720230000	2.031386000	-2.004264000
O	2.562668000	0.387509000	0.882267000
C	3.046090000	0.209840000	2.133028000
H	2.635080000	2.444216000	1.165370000
C	3.340185000	-1.243035000	2.362712000
H	4.116423000	-1.559121000	1.658628000
H	3.670036000	-1.400592000	3.389952000
H	2.434327000	-1.818730000	2.160525000
O	3.205157000	1.108955000	2.935214000
I	-3.778656000	-1.800596000	-0.146058000
C	-2.227957000	4.096597000	0.027083000
C	-2.032770000	2.364550000	-1.616854000
C	-2.870855000	3.080714000	0.956440000
C	-3.778107000	2.132051000	0.168397000
C	-3.047697000	1.604219000	-1.048741000
O	-1.524275000	3.476500000	-1.103767000
H	-1.616178000	2.134883000	-2.592327000
H	-4.675547000	2.666410000	-0.172895000
H	-2.975468000	4.765614000	-0.412406000
H	-3.436213000	3.628194000	1.717383000
H	-4.120311000	1.306334000	0.797002000
H	-2.089216000	2.515996000	1.467283000
H	-3.596967000	0.975808000	-1.745842000
H	-1.466860000	4.695971000	0.528743000
H	-0.593137000	-2.799432000	0.851289000
N	1.264967000	-3.163949000	0.051755000
C	1.542938000	-4.239053000	0.997624000
H	1.607240000	-5.198511000	0.471881000
H	2.494220000	-4.054259000	1.504525000
H	0.746234000	-4.294679000	1.742462000
C	2.282121000	-2.872181000	-0.955777000
H	3.265592000	-2.868198000	-0.482290000
H	2.269007000	-3.629680000	-1.748557000
H	2.089901000	-1.890416000	-1.385007000

DIII_{2a}

Pd	-1.637742000	-0.435726000	-0.325218000
C	-2.096543000	2.466074000	-0.612212000
O	-1.814703000	1.473361000	-1.337359000
C	7.233289000	0.341806000	-1.192539000
C	6.302392000	-0.537262000	-0.396108000
O	6.665427000	-1.252634000	0.516661000
O	4.985634000	-0.534448000	-0.710719000
H	8.259572000	0.102654000	-0.914440000
H	7.098312000	0.200853000	-2.268926000
H	7.040538000	1.396385000	-0.966966000

C	-0.619446000	2.328398000	2.881695000
C	0.112924000	1.320069000	2.032125000
O	0.368566000	0.187353000	2.386569000
O	0.389893000	1.861416000	0.827122000
H	-0.455245000	2.109203000	3.937825000
H	-0.316409000	3.350966000	2.649380000
H	-1.691040000	2.233509000	2.669927000
C	2.946134000	0.447173000	-1.567010000
C	1.082408000	-1.040510000	-1.392915000
C	2.457427000	1.067936000	-0.251894000
C	0.930907000	1.148077000	-0.317693000
C	0.335776000	-0.199586000	-0.665753000
O	2.390607000	-0.852723000	-1.788649000
C	4.454579000	0.347824000	-1.716414000
H	0.737662000	-2.006593000	-1.739738000
H	0.688788000	1.850478000	-1.118601000
H	2.610162000	1.119578000	-2.371384000
H	4.873962000	1.352956000	-1.625578000
H	4.690546000	-0.049014000	-2.709407000
I	-4.509651000	-0.287723000	0.174788000
C	-0.062601000	-4.416415000	-0.437634000
C	-0.256677000	-2.450153000	0.934437000
C	-1.391040000	-4.028996000	-1.063715000
C	-2.334987000	-3.479227000	0.009533000
C	-1.638893000	-2.362528000	0.768441000
O	0.529163000	-3.333949000	0.363096000
H	0.284795000	-1.765875000	1.578230000
H	-2.600809000	-4.279149000	0.714848000
H	-0.174926000	-5.265408000	0.244139000
H	-1.809352000	-4.918118000	-1.545955000
H	-3.266218000	-3.124058000	-0.435130000
H	-1.233162000	-3.274534000	-1.842525000
H	-2.154211000	-1.913476000	1.616662000
H	0.700539000	-4.656240000	-1.179207000
H	2.886086000	2.065963000	-0.137556000
O	2.824053000	0.252009000	0.868541000
C	3.865369000	0.650173000	1.632771000
O	4.477108000	1.687650000	1.462617000
C	4.177451000	-0.383865000	2.675442000
H	3.263763000	-0.841471000	3.060300000
H	4.785353000	-1.158564000	2.194175000
H	4.754768000	0.066919000	3.483770000
H	-2.622021000	2.341015000	0.338285000
N	-1.804419000	3.720219000	-0.932707000
C	-1.081562000	4.062562000	-2.153378000
H	-1.688381000	4.739990000	-2.762518000
H	-0.143773000	4.564783000	-1.894641000
H	-0.868979000	3.157215000	-2.719899000
C	-2.159448000	4.823080000	-0.045610000
H	-1.252049000	5.343587000	0.278023000
H	-2.805379000	5.532787000	-0.572020000
H	-2.685069000	4.442775000	0.831700000

DIV_{2a}

Pd	-1.610959000	-0.379295000	-0.423463000
C	-2.613211000	2.449207000	-0.208521000
O	-1.978639000	1.672057000	-0.969285000
C	7.023841000	1.608595000	-0.672394000
C	6.247868000	0.322586000	-0.804973000
O	6.741659000	-0.779605000	-0.672868000

O	4.924101000	0.390006000	-1.083524000
H	8.083423000	1.367005000	-0.591320000
H	6.859913000	2.270997000	-1.527480000
H	6.710915000	2.143650000	0.230606000
C	-0.716826000	-0.113005000	3.787578000
C	-0.526777000	0.728386000	2.555928000
O	-1.288923000	1.600623000	2.180270000
O	0.595152000	0.369149000	1.899017000
H	-1.128240000	-1.081888000	3.481393000
H	0.234400000	-0.297796000	4.291816000
H	-1.420803000	0.373633000	4.463426000
C	2.755318000	1.452880000	-0.942668000
C	0.981342000	0.053848000	-1.679299000
C	2.396680000	1.018045000	0.482135000
C	0.870887000	0.972192000	0.609412000
C	0.295937000	0.182278000	-0.539100000
O	2.247720000	0.541187000	-1.923182000
C	4.238427000	1.649693000	-1.204609000
H	0.613997000	-0.491658000	-2.542403000
H	0.474589000	1.991614000	0.622835000
H	2.285454000	2.437471000	-1.094232000
H	4.615238000	2.385512000	-0.490543000
H	4.377667000	2.034752000	-2.220021000
I	-4.471287000	-0.856447000	-0.227942000
C	1.166252000	-3.183740000	-1.122130000
C	-1.163599000	-2.593075000	-1.056935000
C	0.944047000	-3.751101000	0.268456000
C	0.113590000	-2.764717000	1.103055000
C	-1.144998000	-2.409512000	0.326465000
O	-0.098766000	-2.897490000	-1.804277000
H	-2.089105000	-2.679387000	-1.620262000
H	0.710191000	-1.880469000	1.328519000
H	1.738200000	-2.254807000	-1.074251000
H	1.922156000	-3.931724000	0.724955000
H	-0.175641000	-3.212153000	2.058800000
H	0.428159000	-4.715979000	0.194471000
H	-2.100372000	-2.535738000	0.827389000
H	1.674634000	-3.887191000	-1.784355000
H	2.825916000	1.715103000	1.203869000
O	2.886675000	-0.311154000	0.741170000
C	4.008305000	-0.438268000	1.489132000
O	4.593294000	0.498193000	1.997828000
C	4.442486000	-1.873383000	1.553548000
H	4.986165000	-2.090946000	0.627440000
H	5.115321000	-2.018470000	2.399536000
H	3.585725000	-2.546948000	1.622219000
H	-3.326512000	2.070558000	0.526627000
N	-2.486830000	3.770732000	-0.251577000
C	-1.547466000	4.427494000	-1.154662000
H	-2.093167000	5.026680000	-1.891143000
H	-0.893171000	5.088534000	-0.577605000
H	-0.948134000	3.677110000	-1.668170000
C	-3.286525000	4.635629000	0.608715000
H	-2.628314000	5.242506000	1.239029000
H	-3.903785000	5.303097000	-0.001653000
H	-3.936374000	4.033149000	1.245796000

TS2I_{2a}

Pd	1.666834000	-0.178235000	-0.148926000
C	-0.187018000	2.238252000	-0.856598000

O	0.295390000	1.166083000	-1.278605000
C	-6.690274000	-0.711396000	-0.508417000
C	-5.494041000	0.050677000	-1.017871000
O	-5.535693000	1.218382000	-1.356663000
O	-4.300361000	-0.582981000	-1.090111000
H	-7.577977000	-0.095731000	-0.650901000
H	-6.815876000	-1.667157000	-1.025336000
H	-6.565317000	-0.916091000	0.560118000
C	0.575212000	0.214128000	4.104336000
C	0.050998000	0.076198000	2.697208000
O	-0.047060000	0.993625000	1.909670000
O	-0.243474000	-1.224702000	2.454643000
H	0.566026000	1.264319000	4.397532000
H	-0.012078000	-0.382739000	4.806180000
H	1.607275000	-0.154411000	4.131631000
C	-2.683434000	-2.193155000	-0.289216000
C	-0.547480000	-1.656002000	-1.236261000
C	-2.218980000	-1.466583000	0.978942000
C	-0.731141000	-1.770500000	1.202309000
C	0.075963000	-1.500361000	-0.049201000
O	-1.869614000	-1.904078000	-1.441864000
C	-4.134056000	-1.951204000	-0.675781000
H	-0.033865000	-1.570154000	-2.187697000
H	-0.689671000	-2.842920000	1.425918000
H	-2.598335000	-3.267890000	-0.077911000
H	-4.757583000	-2.193875000	0.186586000
H	-4.401553000	-2.607881000	-1.509616000
O	-2.395921000	-0.049384000	0.885138000
C	-3.479522000	0.489264000	1.485219000
H	-2.804056000	-1.847791000	1.819215000
C	-3.481719000	1.982547000	1.345690000
H	-3.919631000	2.225882000	0.372495000
H	-4.101566000	2.422180000	2.128382000
H	-2.465063000	2.374812000	1.379918000
O	-4.345915000	-0.167432000	2.034687000
I	3.654998000	1.797907000	-0.072490000
C	2.951252000	-2.581662000	-1.966784000
C	1.847994000	-2.754801000	0.098984000
C	4.305550000	-2.222477000	-1.351447000
C	4.190559000	-1.934108000	0.163929000
C	2.746352000	-1.764337000	0.639106000
O	2.115646000	-3.353040000	-1.063087000
H	1.243262000	-3.389379000	0.739498000
H	4.784332000	-1.062984000	0.442580000
H	2.386976000	-1.667925000	-2.203538000
H	4.678385000	-1.342516000	-1.886214000
H	4.599213000	-2.788944000	0.720644000
H	5.019088000	-3.034067000	-1.520607000
H	2.639520000	-1.656139000	1.720535000
H	3.044689000	-3.193524000	-2.864530000
H	0.348416000	2.867439000	-0.137119000
N	-1.373221000	2.708580000	-1.250157000
C	-1.781571000	4.073878000	-0.947324000
H	-1.756806000	4.689644000	-1.854175000
H	-2.799000000	4.083622000	-0.547881000
H	-1.104892000	4.508842000	-0.208414000
C	-2.212038000	1.924315000	-2.152952000
H	-3.262771000	2.140518000	-1.953149000
H	-1.985947000	2.163171000	-3.199951000
H	-2.041495000	0.863560000	-1.974216000

TS2H_{2a}

Pd	1.755341000	0.170679000	-0.487062000
C	-0.663395000	2.179426000	-0.318784000
O	0.582287000	2.144571000	-0.400498000
C	-6.796009000	-0.510473000	-0.683666000
C	-5.642082000	0.454780000	-0.611484000
O	-5.747655000	1.617119000	-0.272939000
O	-4.403231000	0.007152000	-0.934961000
H	-7.722229000	0.044161000	-0.535958000
H	-6.825302000	-1.033265000	-1.644114000
H	-6.702718000	-1.264551000	0.105330000
C	0.878342000	-1.211781000	3.603666000
C	0.236572000	-0.787303000	2.307835000
O	0.072350000	0.363423000	1.965457000
O	-0.076456000	-1.889567000	1.579519000
H	0.844655000	-0.388123000	4.317681000
H	0.394179000	-2.098436000	4.019125000
H	1.926459000	-1.462686000	3.402322000
C	-2.681037000	-1.667813000	-1.157603000
C	-0.641806000	-0.666462000	-1.890006000
C	-2.124672000	-1.635655000	0.264800000
C	-0.609076000	-1.899882000	0.232459000
C	0.110487000	-1.094591000	-0.836989000
O	-1.976406000	-0.770266000	-2.046001000
C	-4.164143000	-1.368091000	-1.287018000
H	-0.200706000	-0.175953000	-2.753473000
H	-0.503124000	-2.956846000	-0.027572000
H	-2.533605000	-2.688733000	-1.533818000
H	-4.704940000	-2.050683000	-0.627781000
H	-4.480567000	-1.537258000	-2.320668000
O	-2.358414000	-0.371235000	0.893796000
C	-3.394120000	-0.263865000	1.761789000
H	-2.617325000	-2.419549000	0.844301000
C	-3.466161000	1.116434000	2.347841000
H	-4.223464000	1.677355000	1.790287000
H	-3.788800000	1.049354000	3.388990000
H	-2.509290000	1.633452000	2.271297000
O	-4.167252000	-1.170810000	1.999874000
I	4.073804000	1.635826000	0.087528000
C	2.027071000	-4.197176000	-0.324017000
C	1.631307000	-2.191044000	-1.646769000
C	2.721435000	-3.306301000	0.691185000
C	3.590643000	-2.271527000	-0.022992000
C	2.788183000	-1.508300000	-1.071405000
O	1.288729000	-3.462524000	-1.350565000
H	1.404400000	-1.973060000	-2.684550000
H	4.415287000	-2.788182000	-0.536708000
H	2.756776000	-4.815774000	-0.859583000
H	3.327957000	-3.946821000	1.340269000
H	4.050391000	-1.586449000	0.693886000
H	1.978737000	-2.812152000	1.319038000
H	3.400793000	-1.058209000	-1.857209000
H	1.289014000	-4.854428000	0.141499000
H	-1.253722000	1.267579000	-0.212992000
N	-1.389139000	3.303655000	-0.338069000
C	-2.846341000	3.250620000	-0.395794000
H	-3.282362000	3.760279000	0.469413000
H	-3.198266000	3.749724000	-1.305927000
H	-3.191697000	2.217819000	-0.414129000
C	-0.765836000	4.617583000	-0.426976000
H	-0.901736000	5.041034000	-1.429180000
H	-1.229506000	5.289771000	0.301803000
H	0.299600000	4.530643000	-0.215096000

TS2III_{2a}

Pd	-1.763279000	-0.393477000	-0.371708000
C	-2.258795000	2.629678000	-0.590725000
O	-1.918758000	1.672493000	-1.323915000
C	6.994115000	0.838696000	-1.107739000
C	6.056245000	-0.321272000	-0.892787000
O	6.416709000	-1.427545000	-0.545093000
O	4.728447000	-0.124971000	-1.087342000
H	8.018184000	0.468857000	-1.061590000
H	6.820697000	1.331269000	-2.068913000
H	6.851234000	1.584324000	-0.317881000
C	-0.875100000	1.356497000	3.657078000
C	0.141730000	0.784541000	2.705920000
O	0.897896000	-0.130034000	2.963788000
O	0.067455000	1.430270000	1.521236000
H	-0.683213000	0.993531000	4.666951000
H	-0.861972000	2.449185000	3.635692000
H	-1.870826000	1.029240000	3.335518000
C	2.707214000	1.202632000	-1.157313000
C	0.990654000	-0.470044000	-1.538461000
C	2.291043000	1.097476000	0.320500000
C	0.763098000	1.070740000	0.304163000
C	0.284745000	-0.186792000	-0.409316000
O	2.090463000	0.172732000	-1.979330000
C	4.201926000	1.167406000	-1.429754000
H	0.765588000	-1.311949000	-2.184124000
H	0.465263000	1.910807000	-0.327062000
H	2.357386000	2.174326000	-1.524278000
H	4.665471000	1.962390000	-0.840164000
H	4.376744000	1.362382000	-2.492791000
I	-4.532607000	-0.597713000	-0.012051000
C	0.563214000	-3.804528000	-1.009499000
C	0.207005000	-1.954997000	0.551149000
C	-0.906195000	-3.654131000	-1.379519000
C	-1.736209000	-3.411847000	-0.116773000
C	-1.249994000	-2.141332000	0.566791000
O	1.029683000	-2.868581000	0.005963000
H	0.686028000	-1.509496000	1.415938000
H	-1.608722000	-4.262123000	0.571159000
H	0.754371000	-4.796734000	-0.587884000
H	-1.218273000	-4.564724000	-1.900763000
H	-2.801700000	-3.345132000	-0.347898000
H	-1.043127000	-2.815249000	-2.072149000
H	-1.658547000	-1.965282000	1.567303000
H	1.219378000	-3.669248000	-1.874941000
H	2.684117000	1.962740000	0.858543000
O	2.782621000	-0.117570000	0.897081000
C	3.902532000	-0.062310000	1.650379000
O	4.515612000	0.963870000	1.875151000
C	4.289177000	-1.435361000	2.116028000
H	3.413489000	-1.988810000	2.462010000
H	4.723063000	-1.968892000	1.263113000
H	5.034764000	-1.361768000	2.908423000
H	-2.975434000	2.494246000	0.228972000
N	-1.798054000	3.874808000	-0.725356000
C	-0.815528000	4.222354000	-1.746194000
H	-1.244978000	4.944176000	-2.449325000
H	0.062094000	4.673851000	-1.272145000
H	-0.518921000	3.324036000	-2.286066000

C	-2.258287000	4.953658000	0.140119000
H	-1.408181000	5.393676000	0.672048000
H	-2.741036000	5.734950000	-0.456602000
H	-2.974108000	4.568776000	0.869102000

TS2IV_{2a}

Pd	-1.783064000	-0.117048000	-0.775280000
C	-1.991649000	2.730092000	0.308645000
O	-1.661069000	2.146370000	-0.749773000
C	6.948695000	1.581271000	-0.543089000
C	6.155004000	0.407840000	-1.058267000
O	6.647671000	-0.660726000	-1.359005000
O	4.812548000	0.543190000	-1.192948000
H	8.009307000	1.349495000	-0.637134000
H	6.720015000	2.498632000	-1.093477000
H	6.716805000	1.756887000	0.512986000
C	-0.566962000	-1.132381000	3.739683000
C	-0.473336000	-0.160607000	2.595114000
O	-1.153753000	0.837586000	2.461168000
O	0.499530000	-0.535969000	1.727877000
H	-0.673506000	-2.155767000	3.369694000
H	0.357753000	-1.089982000	4.324615000
H	-1.414960000	-0.874524000	4.374100000
C	2.661193000	1.453038000	-0.574685000
C	0.985404000	0.250827000	-1.803441000
C	2.332187000	0.504751000	0.581859000
C	0.815309000	0.348000000	0.633010000
C	0.284417000	-0.134864000	-0.704465000
O	2.119201000	0.982393000	-1.831337000
C	4.135079000	1.745859000	-0.790319000
H	0.703311000	-0.034984000	-2.813001000
H	0.382422000	1.325282000	0.859285000
H	2.185976000	2.414431000	-0.340572000
H	4.535482000	2.141734000	0.145889000
H	4.244025000	2.503035000	-1.573692000
I	-4.580755000	-0.166300000	-0.638044000
C	0.500498000	-3.517057000	0.759451000
C	-0.099833000	-2.162977000	-1.135822000
C	-0.937382000	-4.011608000	0.794623000
C	-1.902442000	-2.848406000	0.516316000
C	-1.518517000	-2.152533000	-0.789665000
O	0.824911000	-2.901304000	-0.518114000
H	0.140117000	-2.070601000	-2.189306000
H	-1.867504000	-2.152122000	1.359091000
H	0.698938000	-2.781822000	1.541140000
H	-1.128577000	-4.455770000	1.777496000
H	-2.936650000	-3.197060000	0.449146000
H	-1.067677000	-4.799628000	0.042762000
H	-2.112327000	-2.459235000	-1.656252000
H	1.217308000	-4.335690000	0.850511000
H	2.714393000	0.931116000	1.511741000
O	2.888823000	-0.801254000	0.374434000
C	4.048115000	-1.111545000	0.998138000
O	4.635371000	-0.358853000	1.751414000
C	4.513569000	-2.478707000	0.589168000
H	5.085758000	-2.361065000	-0.338397000
H	5.169653000	-2.893204000	1.355887000
H	3.668830000	-3.142856000	0.396016000
H	-2.862901000	2.407294000	0.889112000
N	-1.341052000	3.779633000	0.813369000

C	-0.124076000	4.293410000	0.195766000
H	-0.278295000	5.323694000	-0.142668000
H	0.689748000	4.284210000	0.928590000
H	0.142181000	3.667747000	-0.655229000
C	-1.779667000	4.422713000	2.044945000
H	-0.999535000	4.338253000	2.809314000
H	-1.981501000	5.483917000	1.864628000
H	-2.689757000	3.945126000	2.411854000

El_{2a}

Pd	2.788335000	0.117911000	-0.293987000
O	1.412659000	-1.456754000	-0.573917000
C	0.305444000	-1.292181000	-1.164022000
C	-6.589847000	-2.147942000	1.557823000
C	-5.472672000	-2.221588000	0.550413000
O	-5.563311000	-2.770096000	-0.529366000
O	-4.286399000	-1.641756000	0.860489000
H	-7.404629000	-2.787851000	1.219815000
H	-6.258186000	-2.462803000	2.551577000
H	-6.955107000	-1.118190000	1.634221000
C	-2.101266000	3.614857000	-2.591973000
C	-1.649940000	2.572245000	-1.603868000
O	-1.078828000	1.541945000	-1.900195000
O	-1.963436000	2.962716000	-0.346953000
H	-3.196169000	3.618582000	-2.628802000
H	-1.777386000	4.610853000	-2.277891000
H	-1.704148000	3.381188000	-3.579977000
C	-2.933750000	0.075562000	1.879129000
C	-0.634803000	0.011074000	1.347375000
C	-3.142988000	1.195316000	0.859237000
C	-1.874939000	2.073558000	0.800788000
C	-0.595960000	1.291264000	0.955708000
O	-1.766606000	-0.710257000	1.588830000
C	-4.101633000	-0.876118000	2.065096000
H	0.260558000	-0.570782000	1.531195000
H	-1.940060000	2.784954000	1.631053000
H	-2.781469000	0.572162000	2.849492000
H	-4.988856000	-0.287539000	2.306916000
H	-3.883723000	-1.557852000	2.892972000
I	5.069456000	-1.590416000	-0.108365000
C	2.703841000	2.378590000	2.314803000
C	0.713937000	2.051562000	0.919589000
C	3.165168000	3.208952000	1.122797000
C	2.958860000	2.431443000	-0.176525000
C	1.620622000	1.797615000	-0.279301000
O	1.385441000	1.812492000	2.165277000
H	0.451932000	3.124990000	0.849062000
H	3.795262000	1.572535000	-0.142336000
H	3.403031000	1.543032000	2.459891000
H	4.214085000	3.485389000	1.262259000
H	3.273323000	2.964925000	-1.076711000
H	2.586212000	4.137787000	1.053808000
H	1.104235000	1.875509000	-1.233641000
H	2.707869000	2.985823000	3.228166000
H	-3.993102000	1.803733000	1.174428000
O	-3.402227000	0.686766000	-0.457292000
C	-4.693077000	0.620322000	-0.866275000
C	-4.786084000	0.089188000	-2.267536000
H	-3.936905000	0.411809000	-2.872519000
H	-4.785196000	-1.005252000	-2.212776000

H	-5.725771000	0.413873000	-2.716763000
O	-5.638783000	0.924624000	-0.165663000
H	0.120375000	-0.427733000	-1.802598000
N	-0.709293000	-2.135912000	-1.053789000
C	-0.669620000	-3.298663000	-0.173709000
H	-1.428158000	-3.178876000	0.605284000
H	-0.885076000	-4.203326000	-0.750666000
H	0.315567000	-3.383613000	0.281950000
C	-1.970322000	-1.880922000	-1.746580000
H	-2.160743000	-2.672860000	-2.478740000
H	-2.779147000	-1.857912000	-1.014982000
H	-1.922075000	-0.915263000	-2.247914000

Et₂a

Pd	-2.508575000	-0.058877000	-0.758845000
C	-0.070510000	-1.783409000	-0.465903000
O	-0.856191000	-1.282194000	-1.312791000
C	6.798552000	-0.640954000	-0.384192000
C	5.458755000	-1.324341000	-0.290994000
O	5.283529000	-2.387342000	0.273498000
O	4.382140000	-0.734134000	-0.862693000
H	7.557787000	-1.319576000	0.004042000
H	7.040361000	-0.365550000	-1.414914000
H	6.794533000	0.271197000	0.221122000
C	-0.178523000	1.883472000	3.433859000
C	0.118066000	1.549838000	1.993511000
O	-0.349124000	0.598585000	1.399033000
O	0.950449000	2.471108000	1.474657000
H	-0.745711000	1.071625000	3.889790000
H	0.749365000	2.050566000	3.988070000
H	-0.762802000	2.808614000	3.479096000
C	3.135937000	1.292094000	-1.332481000
C	0.857593000	1.046788000	-1.879320000
C	2.738183000	1.647936000	0.094017000
C	1.401158000	2.423778000	0.095248000
C	0.435675000	1.920401000	-0.955744000
O	2.118088000	0.527741000	-1.985318000
C	4.458513000	0.562617000	-1.484235000
H	0.217947000	0.654548000	-2.658952000
H	1.631027000	3.475275000	-0.105024000
H	3.251527000	2.248695000	-1.866839000
H	5.236976000	1.181762000	-1.036033000
H	4.678397000	0.426705000	-2.547758000
I	-3.801210000	-2.093015000	0.762988000
C	-3.435786000	1.987726000	-1.366909000
C	-0.935690000	2.588504000	-1.098753000
C	-3.654924000	3.133212000	-0.379664000
C	-2.568305000	3.072580000	0.680351000
H	-0.821437000	3.398950000	-1.842345000
H	-2.621071000	2.106678000	1.208608000
H	-3.884156000	1.039146000	-0.774062000
H	-4.645113000	3.069599000	0.081458000
H	-2.685988000	3.870697000	1.418790000
H	-3.591169000	4.084313000	-0.920802000
H	-4.099621000	1.999352000	-2.234312000
H	3.517822000	2.268520000	0.539039000
O	2.562899000	0.474032000	0.906119000
C	3.525060000	0.195416000	1.813442000
C	3.135535000	-0.954742000	2.698034000
H	3.499118000	-0.763017000	3.709864000

H	2.057393000	-1.114850000	2.702602000
H	3.633170000	-1.854619000	2.323574000
O	4.583421000	0.792410000	1.884743000
H	-0.271443000	-1.718839000	0.605139000
N	1.041922000	-2.427079000	-0.798255000
C	1.870266000	-3.081018000	0.208221000
H	1.889269000	-4.161127000	0.021989000
H	2.891189000	-2.694948000	0.160014000
H	1.456946000	-2.904224000	1.201652000
C	1.491075000	-2.546204000	-2.180363000
H	1.508908000	-3.601773000	-2.473289000
H	0.814670000	-1.998064000	-2.833284000
H	2.496255000	-2.126093000	-2.262498000
C	-2.021226000	1.693388000	-1.693501000
H	-1.820212000	1.457588000	-2.738837000
O	-1.270865000	3.260298000	0.120585000

EIII_{2a}

Pd	2.616224000	-0.567223000	-0.208972000
O	1.446325000	1.088551000	-0.837404000
C	1.075473000	1.926355000	0.029340000
C	-4.432835000	3.108735000	2.121965000
C	-5.118791000	2.053870000	1.288933000
O	-6.035147000	1.368985000	1.697258000
O	-4.751447000	1.900580000	-0.009058000
H	-4.929009000	3.152839000	3.091289000
H	-3.376240000	2.871002000	2.262218000
H	-4.499771000	4.087345000	1.635020000
C	-2.704539000	-4.134972000	-1.923046000
C	-2.321141000	-3.117712000	-0.880755000
O	-2.617235000	-3.174296000	0.292424000
O	-1.572808000	-2.138345000	-1.460046000
H	-1.823413000	-4.463744000	-2.481483000
H	-3.188081000	-4.987623000	-1.446039000
H	-3.394104000	-3.671320000	-2.636742000
C	-2.371063000	1.378165000	-0.368916000
C	-1.298532000	0.172695000	1.391276000
C	-2.581899000	0.038334000	-1.065876000
C	-1.339057000	-0.839202000	-0.852803000
C	-0.889846000	-0.816661000	0.587823000
O	-2.126949000	1.205290000	1.036974000
C	-3.501288000	2.386869000	-0.521930000
H	-0.992757000	0.251755000	2.427039000
H	-0.536146000	-0.435261000	-1.478065000
H	-1.487729000	1.838671000	-0.824040000
H	-3.666105000	2.570742000	-1.585901000
H	-3.211619000	3.330109000	-0.053332000
I	5.062194000	0.890943000	-0.422931000
C	1.286405000	-2.673686000	2.906983000
C	0.087104000	-1.866804000	1.062892000
C	2.647291000	-2.742405000	2.217871000
C	2.505593000	-2.682855000	0.679589000
C	1.270774000	-2.068562000	0.127232000
O	0.506378000	-1.589653000	2.392333000
H	-0.450231000	-2.831889000	1.069796000
H	2.772075000	-3.612427000	0.166357000
H	0.734218000	-3.617702000	2.778448000
H	3.163971000	-3.662659000	2.507221000
H	3.445198000	-2.052390000	0.284273000
H	3.258145000	-1.904377000	2.564200000
H	1.405024000	-2.492399000	3.978381000

H	0.963631000	-2.449128000	-0.849211000
H	-2.746601000	0.196704000	-2.133097000
O	-3.711905000	-0.631350000	-0.494719000
C	-4.828075000	-0.780608000	-1.252561000
C	-5.926029000	-1.382978000	-0.425488000
H	-6.761754000	-1.670613000	-1.064025000
H	-5.549866000	-2.247932000	0.127492000
H	-6.249143000	-0.628826000	0.301529000
O	-4.904197000	-0.454738000	-2.419399000
H	1.146274000	1.711238000	1.098607000
N	0.564848000	3.115722000	-0.271696000
C	0.434266000	3.582805000	-1.649860000
H	-0.619171000	3.782653000	-1.872729000
H	1.002433000	4.509805000	-1.773562000
H	0.814724000	2.825187000	-2.333174000
C	0.080980000	4.013739000	0.773242000
H	0.223390000	3.558100000	1.754113000
H	0.628006000	4.960370000	0.731075000
H	-0.984737000	4.213048000	0.621911000

EIV_{2a}

Pd	-2.556800000	-0.028368000	0.508305000
O	-1.289967000	-1.652741000	-0.037353000
C	-0.721198000	-2.348471000	0.847014000
C	4.563231000	-3.045120000	1.479086000
C	5.127604000	-1.975468000	0.575451000
O	6.140248000	-1.353339000	0.827622000
O	4.520091000	-1.730261000	-0.612668000
H	5.232654000	-3.157730000	2.331632000
H	3.565568000	-2.772922000	1.829914000
H	4.490041000	-3.999733000	0.948026000
C	1.962036000	4.683013000	-1.167662000
C	1.931936000	3.380778000	-0.406465000
O	2.397375000	3.215993000	0.699913000
O	1.294071000	2.444395000	-1.147233000
H	2.587098000	5.402787000	-0.638362000
H	2.341510000	4.529777000	-2.181874000
H	0.943138000	5.075550000	-1.251060000
C	2.126918000	-1.151931000	-0.487813000
C	1.341042000	-0.085712000	1.479077000
C	2.246309000	0.230463000	-1.113368000
C	1.056228000	1.100303000	-0.665608000
C	0.774770000	0.925780000	0.809504000
O	2.148244000	-1.056668000	0.946922000
C	3.182309000	-2.166445000	-0.901824000
H	1.180494000	-0.252114000	2.540327000
H	0.176290000	0.791433000	-1.239878000
H	1.157977000	-1.558899000	-0.802983000
H	3.138485000	-2.293925000	-1.985730000
H	2.964940000	-3.129647000	-0.434850000
I	-4.608873000	-0.772811000	-1.331512000
C	-2.813145000	1.716050000	1.999164000
C	-0.260466000	1.778583000	1.531280000
C	-2.867135000	3.194772000	1.545388000
C	-1.467324000	3.789434000	1.452275000
H	0.193759000	2.136456000	2.473789000
H	-1.053105000	3.984784000	2.453969000
H	-3.350684000	1.519958000	2.930583000
H	-3.475641000	3.771183000	2.249011000
H	-1.479086000	4.732968000	0.900182000

H	-3.346841000	3.265130000	0.565530000
H	-3.586955000	1.162640000	1.256289000
H	2.257987000	0.155287000	-2.201821000
O	3.456386000	0.848538000	-0.658509000
C	4.420630000	1.129975000	-1.568011000
C	5.644381000	1.646351000	-0.867273000
H	6.346975000	2.057933000	-1.592601000
H	5.366977000	2.402966000	-0.128589000
H	6.104256000	0.805805000	-0.334420000
O	4.300261000	0.961408000	-2.764467000
H	-0.696951000	-2.031284000	1.892643000
N	-0.104686000	-3.497104000	0.593275000
C	-0.084421000	-4.093073000	-0.740455000
H	0.943198000	-4.136922000	-1.114078000
H	-0.482617000	-5.110758000	-0.685792000
H	-0.694476000	-3.497836000	-1.417870000
C	0.633889000	-4.200523000	1.637921000
H	0.544088000	-3.666351000	2.585387000
H	0.238312000	-5.213878000	1.755612000
H	1.691047000	-4.260752000	1.362611000
C	-1.514176000	0.999451000	1.939365000
H	-1.316219000	0.301266000	2.755568000
O	-0.600064000	2.907826000	0.739741000

TS3I_{2a}

Pd	2.910825000	0.186450000	-0.275949000
O	1.444238000	-1.354627000	-0.719783000
C	0.343843000	-1.179434000	-1.306844000
C	-6.423362000	-2.359989000	1.555846000
C	-5.320098000	-2.354327000	0.530201000
O	-5.411349000	-2.857144000	-0.571736000
O	-4.148516000	-1.748460000	0.846519000
H	-7.220864000	-3.014233000	1.204466000
H	-6.066713000	-2.700884000	2.532084000
H	-6.822688000	-1.347351000	1.676983000
C	-2.409365000	3.669801000	-2.423795000
C	-1.805214000	2.649375000	-1.496458000
O	-1.163078000	1.682565000	-1.854833000
O	-2.074217000	2.982059000	-0.212038000
H	-3.501088000	3.602412000	-2.364553000
H	-2.124512000	4.681160000	-2.120150000
H	-2.085427000	3.477627000	-3.446654000
C	-2.840909000	-0.030549000	1.921864000
C	-0.560972000	0.020515000	1.299527000
C	-3.127700000	1.125090000	0.962789000
C	-1.898126000	2.055598000	0.894919000
C	-0.587577000	1.315183000	0.958119000
O	-1.650244000	-0.752428000	1.569653000
C	-3.963886000	-1.039023000	2.085395000
H	0.361635000	-0.536893000	1.407762000
H	-1.954595000	2.730462000	1.755705000
H	-2.685899000	0.426082000	2.911210000
H	-4.866860000	-0.500286000	2.378935000
H	-3.698342000	-1.753570000	2.870528000
I	4.917644000	-1.701152000	-0.050587000
C	2.688049000	2.609166000	2.192696000
C	0.688989000	2.121928000	0.861882000
C	3.170510000	3.282041000	0.905424000
C	2.841236000	2.464091000	-0.321371000
C	1.563343000	1.877788000	-0.362464000

O	1.430369000	1.915413000	2.074089000
H	0.391214000	3.185165000	0.794939000
H	4.014074000	1.201273000	0.055536000
H	3.423831000	1.857097000	2.501494000
H	4.239481000	3.496030000	0.985772000
H	3.340146000	2.733065000	-1.249571000
H	2.657221000	4.244127000	0.766500000
H	1.049975000	1.752905000	-1.309921000
H	2.605779000	3.355170000	2.993887000
H	-3.988507000	1.682954000	1.336368000
O	-3.415069000	0.668259000	-0.367181000
C	-4.714972000	0.594751000	-0.745462000
C	-4.835109000	0.135124000	-2.170035000
H	-4.003447000	0.497424000	-2.776805000
H	-4.823110000	-0.960493000	-2.172300000
H	-5.788252000	0.471776000	-2.580497000
O	-5.647453000	0.840538000	-0.005369000
H	0.157410000	-0.302594000	-1.930933000
N	-0.678379000	-2.022078000	-1.221501000
C	-0.641984000	-3.211244000	-0.378148000
H	-1.403382000	-3.117628000	0.401524000
H	-0.853071000	-4.098656000	-0.983455000
H	0.341795000	-3.308177000	0.078461000
C	-1.938115000	-1.745703000	-1.906223000
H	-2.122625000	-2.504032000	-2.675128000
H	-2.748252000	-1.764446000	-1.176083000
H	-1.898304000	-0.757076000	-2.362534000

TS3II_{2a}

Pd	-2.622788000	-0.045214000	-0.687695000
C	-0.121902000	-1.757759000	-0.511493000
O	-0.945264000	-1.274332000	-1.328336000
C	6.825810000	-0.653494000	-0.379180000
C	5.489363000	-1.340088000	-0.265434000
O	5.321574000	-2.399129000	0.308181000
O	4.404646000	-0.755279000	-0.827488000
H	7.591860000	-1.325607000	0.006952000
H	7.055745000	-0.386522000	-1.414855000
H	6.824672000	0.264630000	0.217137000
C	-0.135637000	1.942619000	3.424101000
C	0.128052000	1.590860000	1.981617000
O	-0.356052000	0.636209000	1.406227000
O	0.948667000	2.505699000	1.433511000
H	-0.720088000	1.151745000	3.894688000
H	0.807108000	2.082478000	3.960763000
H	-0.688808000	2.886336000	3.473526000
C	3.144050000	1.251742000	-1.333358000
C	0.870287000	0.990272000	-1.879716000
C	2.743348000	1.639146000	0.084502000
C	1.408744000	2.417583000	0.059142000
C	0.447980000	1.890597000	-0.982493000
O	2.129299000	0.462130000	-1.961749000
C	4.472657000	0.530566000	-1.470706000
H	0.234460000	0.586287000	-2.656902000
H	1.642436000	3.462454000	-0.168983000
H	3.249703000	2.195198000	-1.892469000
H	5.245431000	1.163500000	-1.031629000
H	4.695328000	0.378611000	-2.531567000
I	-3.724768000	-2.108904000	0.793816000
C	-3.357469000	2.003313000	-1.401799000

C	-0.895732000	2.597977000	-1.181751000
C	-3.634375000	3.077710000	-0.373099000
C	-2.486723000	3.124487000	0.624114000
H	-0.730832000	3.355225000	-1.968306000
H	-2.454547000	2.181664000	1.188756000
H	-3.905261000	0.742205000	-0.373813000
H	-4.586147000	2.912171000	0.140211000
H	-2.610877000	3.947944000	1.332418000
H	-3.702681000	4.036130000	-0.905001000
H	-4.134864000	1.799692000	-2.134723000
H	3.521613000	2.267268000	0.521182000
O	2.563034000	0.479687000	0.916418000
C	3.537264000	0.198211000	1.810654000
C	3.165193000	-0.964639000	2.685512000
H	3.580512000	-0.807372000	3.683032000
H	2.085127000	-1.103734000	2.737099000
H	3.624398000	-1.864192000	2.263074000
O	4.593448000	0.799675000	1.874261000
H	-0.265293000	-1.658650000	0.566814000
N	0.970712000	-2.422652000	-0.874585000
C	1.863916000	-3.010901000	0.115820000
H	1.913617000	-4.095948000	-0.031381000
H	2.867368000	-2.591564000	0.014283000
H	1.486388000	-2.810896000	1.118968000
C	1.347224000	-2.594530000	-2.271777000
H	1.380336000	-3.661331000	-2.518811000
H	0.618400000	-2.096591000	-2.909048000
H	2.333445000	-2.152422000	-2.434080000
C	-2.017796000	1.735044000	-1.748876000
H	-1.819672000	1.342297000	-2.743497000
O	-1.239160000	3.369971000	-0.025359000

TS3III_{2a}

Pd	-2.798372000	0.672427000	-0.250932000
O	-1.576752000	-0.920582000	-1.110252000
C	-1.180582000	-1.862557000	-0.380579000
C	4.216237000	-3.262296000	2.175732000
C	5.014147000	-2.203450000	1.455636000
O	5.912283000	-1.571930000	1.975551000
O	4.773224000	-1.981201000	0.138387000
H	4.596265000	-3.342473000	3.193917000
H	3.155299000	-3.005562000	2.199637000
H	4.320128000	-4.229606000	1.672596000
C	2.956780000	4.214006000	-1.602733000
C	2.466708000	3.124249000	-0.685121000
O	2.629518000	3.099006000	0.515149000
O	1.808163000	2.181271000	-1.412691000
H	2.176879000	4.512477000	-2.308086000
H	3.285528000	5.071441000	-1.015018000
H	3.800735000	3.827628000	-2.185209000
C	2.444346000	-1.399421000	-0.433609000
C	1.170513000	-0.280174000	1.245172000
C	2.753248000	-0.026254000	-1.020402000
C	1.499229000	0.852813000	-0.913382000
C	0.870214000	0.757927000	0.454932000
O	2.036294000	-1.297713000	0.940962000
C	3.571995000	-2.419150000	-0.516150000
H	0.733040000	-0.416402000	2.226058000
H	0.781662000	0.490546000	-1.657479000
H	1.612670000	-1.813980000	-1.015391000

H	3.839178000	-2.556649000	-1.566376000
H	3.225111000	-3.378759000	-0.125477000
I	-4.982898000	-0.994392000	-0.024745000
C	-1.779332000	2.266745000	2.607187000
C	-0.156679000	1.790905000	0.857099000
C	-2.291394000	3.330643000	1.627810000
C	-2.297305000	2.852601000	0.193730000
C	-1.188320000	2.093784000	-0.223756000
O	-0.798379000	1.367030000	2.058569000
H	0.377302000	2.737269000	1.047955000
H	-2.823164000	3.470214000	-0.530480000
H	-1.362231000	2.754332000	3.498108000
H	-1.623394000	4.203158000	1.638335000
H	-3.687258000	1.804934000	0.295463000
H	-3.276750000	3.676702000	1.950171000
H	-2.613381000	1.631305000	2.923396000
H	-0.849536000	2.162712000	-1.254319000
H	3.048269000	-0.125430000	-2.066392000
O	3.808676000	0.591723000	-0.274930000
C	4.998737000	0.802070000	-0.892582000
C	5.992034000	1.348235000	0.090957000
H	6.891448000	1.678115000	-0.429736000
H	5.549086000	2.175218000	0.652730000
H	6.238491000	0.549066000	0.799352000
O	5.205892000	0.566635000	-2.065303000
H	-1.309553000	-1.840462000	0.705581000
N	-0.576444000	-2.956370000	-0.842788000
C	-0.377098000	-3.185725000	-2.270798000
H	-0.633294000	-2.284492000	-2.825959000
H	0.669554000	-3.445569000	-2.457070000
H	-1.009828000	-4.014659000	-2.605266000
C	-0.122809000	-4.006852000	0.063190000
H	-0.318262000	-3.718081000	1.097038000
H	-0.647730000	-4.942277000	-0.155904000
H	0.952170000	-4.167502000	-0.065873000

TS3IV_{2a}

Pd	2.584489000	-0.082335000	-0.486583000
O	1.275927000	-1.827413000	-0.253642000
C	0.655804000	-2.413692000	-1.174308000
C	-4.805952000	-2.751772000	-1.326726000
C	-5.173517000	-1.680390000	-0.328452000
O	-6.153954000	-0.971759000	-0.440236000
O	-4.417868000	-1.535160000	0.788806000
H	-5.571526000	-2.770434000	-2.102177000
H	-3.832681000	-2.547957000	-1.777641000
H	-4.757637000	-3.732165000	-0.841309000
C	-1.475698000	4.675021000	1.125376000
C	-1.604217000	3.384389000	0.354852000
O	-2.228974000	3.250835000	-0.673681000
O	-0.906370000	2.414036000	0.994811000
H	-2.127846000	5.431449000	0.687910000
H	-1.732919000	4.520757000	2.177233000
H	-0.437016000	5.019210000	1.085165000
C	-2.017222000	-1.120969000	0.389824000
C	-1.378553000	-0.060612000	-1.636007000
C	-1.976485000	0.249533000	1.049487000
C	-0.797532000	1.065147000	0.480838000
C	-0.683895000	0.902583000	-1.017007000
O	-2.182250000	-0.991124000	-1.034429000

C	-3.089878000	-2.072373000	0.899322000
H	-1.337168000	-0.218246000	-2.710221000
H	0.123631000	0.704636000	0.952378000
H	-1.051468000	-1.600343000	0.593205000
H	-2.925393000	-2.241593000	1.965861000
H	-3.001442000	-3.030817000	0.383683000
I	4.058323000	-0.835990000	1.732980000
C	2.876202000	1.484245000	-2.129964000
C	0.346349000	1.673122000	-1.829485000
C	3.008394000	2.990844000	-1.879092000
C	1.629349000	3.645809000	-1.923469000
H	-0.109486000	1.912722000	-2.807902000
H	1.280544000	3.740930000	-2.963707000
H	3.655652000	1.037583000	-2.743772000
H	3.648467000	3.411495000	-2.662198000
H	1.652492000	4.644446000	-1.480000000
H	3.491533000	3.202763000	-0.922481000
H	3.598400000	1.056386000	-0.689510000
H	-1.862612000	0.144829000	2.129710000
O	-3.194133000	0.945182000	0.757791000
C	-4.003534000	1.292912000	1.786314000
C	-5.255529000	1.930457000	1.255584000
H	-5.820136000	2.382681000	2.071528000
H	-5.004445000	2.679709000	0.500018000
H	-5.852842000	1.148906000	0.771727000
O	-3.744482000	1.094721000	2.956137000
H	0.616317000	-2.008784000	-2.190185000
N	-0.010981000	-3.553231000	-1.004617000
C	-0.027695000	-4.256483000	0.274837000
H	-1.042591000	-4.267541000	0.683863000
H	0.301684000	-5.289066000	0.123716000
H	0.641473000	-3.758517000	0.974734000
C	-0.817273000	-4.122201000	-2.078846000
H	-0.710735000	-3.521562000	-2.983723000
H	-0.494156000	-5.146995000	-2.286240000
H	-1.871496000	-4.135567000	-1.783279000
C	1.605985000	0.862290000	-2.153612000
H	1.451457000	0.027985000	-2.835945000
O	0.688424000	2.883611000	-1.169310000

Fl_{2a}

Pd	-2.804084000	0.198488000	0.241563000
O	-1.939747000	-0.445265000	2.280769000
C	-0.694325000	-0.445804000	2.449709000
C	5.679060000	-3.146518000	-1.533185000
C	4.726047000	-2.789520000	-0.422410000
O	4.867923000	-3.136788000	0.732753000
O	3.646673000	-2.023717000	-0.719955000
H	6.386256000	-3.886815000	-1.159878000
H	5.153855000	-3.540310000	-2.408041000
H	6.231799000	-2.254508000	-1.847831000
C	2.989113000	3.909765000	1.772947000
C	2.096739000	2.924711000	1.066087000
O	1.326762000	2.166047000	1.618136000
O	2.271867000	3.028695000	-0.276649000
H	2.904448000	4.902503000	1.322363000
H	2.729948000	3.950733000	2.831018000
H	4.029347000	3.583693000	1.662625000
C	2.452348000	-0.336715000	-1.961147000
C	0.284767000	0.086368000	-1.095649000

C	2.959965000	0.906582000	-1.229350000
C	1.858100000	1.985222000	-1.200160000
C	0.482737000	1.406163000	-0.981084000
O	1.232042000	-0.843917000	-1.395591000
C	3.435204000	-1.491770000	-2.041142000
H	-0.691168000	-0.373330000	-0.963587000
H	1.880572000	2.509010000	-2.161186000
H	2.247892000	-0.025260000	-2.996204000
H	4.364566000	-1.119035000	-2.476966000
H	3.022799000	-2.275726000	-2.683799000
I	-4.126521000	-2.118913000	-0.293740000
C	-2.424557000	3.541036000	-1.790278000
C	-0.660683000	2.368200000	-0.749412000
C	-3.490864000	3.190222000	-0.736902000
C	-2.885940000	2.431273000	0.430841000
C	-1.553741000	2.048446000	0.430541000
O	-1.435353000	2.515662000	-1.946735000
H	-0.211014000	3.348629000	-0.512980000
H	-3.226973000	0.523375000	-1.158685000
H	-2.878217000	3.681600000	-2.774357000
H	-4.319611000	2.630100000	-1.178498000
H	-3.426440000	2.471981000	1.375324000
H	-3.921617000	4.120393000	-0.345590000
H	-1.035745000	1.865165000	1.362952000
H	-1.923878000	4.481267000	-1.510940000
H	3.839272000	1.287537000	-1.752140000
O	3.314596000	0.614035000	0.130389000
C	4.622367000	0.395800000	0.416917000
C	4.799827000	0.075212000	1.872587000
H	5.834897000	0.257422000	2.164172000
H	4.115761000	0.655875000	2.494209000
H	4.578526000	-0.989592000	2.007063000
O	5.508522000	0.426152000	-0.413901000
H	-0.210933000	0.338876000	3.047444000
N	0.159735000	-1.342807000	1.962996000
C	-0.274329000	-2.509024000	1.203137000
H	0.013165000	-3.419337000	1.741130000
H	-1.354144000	-2.487728000	1.074685000
H	0.215289000	-2.510939000	0.225513000
C	1.597879000	-1.217473000	2.189442000
H	1.945080000	-2.013436000	2.857782000
H	2.118537000	-1.298022000	1.234000000
H	1.818519000	-0.242866000	2.623101000

FIII_{2a}

Pd	2.648633000	-0.606049000	0.095479000
O	2.030397000	1.527321000	0.131738000
C	1.846018000	2.405980000	1.000976000
C	-4.667706000	3.317154000	-0.473485000
C	-5.128730000	1.904148000	-0.734501000
O	-6.135240000	1.428923000	-0.247530000
O	-4.427565000	1.133255000	-1.604098000
H	-5.403115000	3.801756000	0.168284000
H	-3.692991000	3.321863000	0.018833000
H	-4.577788000	3.876505000	-1.410348000
C	-2.095123000	-4.459929000	1.013371000
C	-1.831532000	-2.994637000	1.242713000
O	-2.241197000	-2.350704000	2.183614000
O	-1.046521000	-2.512680000	0.241025000
H	-1.156938000	-4.997637000	0.848287000

H	-2.621529000	-4.878529000	1.871248000
H	-2.705359000	-4.576360000	0.111442000
C	-2.026311000	0.862209000	-1.097378000
C	-1.294619000	1.028700000	1.150990000
C	-2.079066000	-0.651375000	-0.915875000
C	-0.896715000	-1.093906000	-0.041398000
C	-0.694383000	-0.167540000	1.132752000
O	-2.115220000	1.526033000	0.173943000
C	-3.087679000	1.450396000	-2.016204000
H	-1.161128000	1.739959000	1.956259000
H	0.005433000	-1.080793000	-0.663095000
H	-1.053266000	1.104258000	-1.549025000
H	-2.971060000	1.007795000	-3.008142000
H	-2.936344000	2.528483000	-2.103750000
C	1.702128000	0.379384000	3.892573000
C	0.269827000	-0.553681000	2.237097000
C	3.009145000	-0.092010000	3.249329000
C	2.718379000	-1.205227000	2.264439000
C	1.435681000	-1.415917000	1.778769000
O	0.703813000	0.629549000	2.900879000
H	-0.274514000	-1.186190000	2.961258000
H	3.438198000	-2.017847000	2.212500000
H	1.339898000	-0.376681000	4.605474000
H	3.686835000	-0.469516000	4.023053000
H	3.038969000	-2.046503000	-0.140922000
H	3.527017000	0.744475000	2.768128000
H	1.838616000	1.320094000	4.431975000
H	1.162109000	-2.392921000	1.390748000
H	-2.032549000	-1.150283000	-1.885060000
O	-3.293584000	-1.011176000	-0.243827000
C	-4.194247000	-1.782948000	-0.904320000
C	-5.424444000	-1.961595000	-0.062833000
H	-6.064824000	-2.730611000	-0.495868000
H	-5.148925000	-2.223824000	0.962262000
H	-5.954584000	-1.002658000	-0.037409000
O	-4.015508000	-2.236798000	-2.015512000
H	2.349424000	2.374155000	1.970615000
N	1.056168000	3.466202000	0.825222000
C	0.319945000	3.679886000	-0.415590000
H	0.565052000	2.888096000	-1.121495000
H	-0.755470000	3.668595000	-0.216892000
H	0.595800000	4.649606000	-0.842649000
C	0.868218000	4.454771000	1.879102000
H	1.446986000	4.178478000	2.762551000
H	1.192055000	5.442582000	1.534249000
H	-0.190983000	4.509643000	2.152765000
I	3.530509000	-0.303851000	-2.465828000

GI_{2a}

Pd	-3.083324000	-0.205199000	0.416195000
O	-1.992477000	-0.597164000	2.417787000
C	-0.746417000	-0.671169000	2.533383000
C	5.666926000	-2.723497000	-1.461678000
C	4.685098000	-2.431633000	-0.356782000
O	4.874722000	-2.704236000	0.811606000
O	3.515708000	-1.825252000	-0.676788000
H	6.468557000	-3.341444000	-1.057889000
H	5.190446000	-3.235979000	-2.302582000
H	6.094493000	-1.787524000	-1.837174000
C	2.292527000	4.249695000	1.463958000

C	1.499551000	3.114632000	0.871453000
O	0.814724000	2.341305000	1.506979000
O	1.658017000	3.104010000	-0.477345000
H	3.357638000	3.996450000	1.413777000
H	2.143652000	5.169517000	0.892228000
H	2.004989000	4.399266000	2.504889000
C	2.130637000	-0.326537000	-1.957637000
C	-0.047285000	-0.077967000	-1.048874000
C	2.519189000	0.984345000	-1.274911000
C	1.323751000	1.954634000	-1.300092000
C	0.020507000	1.258887000	-0.994474000
O	0.974298000	-0.926359000	-1.350615000
C	3.220439000	-1.383303000	-2.013864000
H	-0.968477000	-0.620268000	-0.859175000
H	1.275296000	2.396932000	-2.300516000
H	1.882915000	-0.073523000	-2.999075000
H	4.097311000	-0.947300000	-2.497447000
H	2.869119000	-2.235144000	-2.604482000
C	-3.103955000	3.051539000	-1.801651000
C	-1.208459000	2.108308000	-0.762909000
C	-4.109763000	2.626317000	-0.718450000
C	-3.403814000	1.996102000	0.471439000
C	-2.039517000	1.750652000	0.453188000
O	-2.016870000	2.130639000	-1.946611000
H	-0.855422000	3.137384000	-0.575008000
H	-3.648800000	-0.074579000	-0.964131000
H	-3.585357000	3.116167000	-2.780712000
H	-4.870037000	1.953207000	-1.124213000
H	-3.921338000	2.047435000	1.428509000
H	-4.643012000	3.517638000	-0.364577000
H	-1.484119000	1.669182000	1.379568000
H	-2.700043000	4.046955000	-1.557295000
H	3.368025000	1.424193000	-1.801445000
O	2.873657000	0.777700000	0.101042000
C	4.191099000	0.744294000	0.420979000
C	4.375214000	0.519092000	1.893608000
H	3.585483000	1.003453000	2.470550000
H	4.330602000	-0.561182000	2.071308000
H	5.357025000	0.883689000	2.198823000
O	5.086125000	0.851105000	-0.393962000
H	-0.203334000	0.060756000	3.146917000
N	0.046294000	-1.588648000	1.979062000
C	-0.463044000	-2.699780000	1.181702000
H	0.024755000	-2.697229000	0.202827000
H	-0.224082000	-3.643220000	1.686329000
H	-1.541425000	-2.616584000	1.056042000
C	1.495570000	-1.544542000	2.159622000
H	1.839863000	-2.479971000	2.613950000
H	1.985354000	-1.416731000	1.192722000
H	1.764207000	-0.712696000	2.811344000
O	-3.683662000	-2.177071000	0.380728000
C	-3.955088000	-2.792722000	-0.738268000
O	-3.942566000	-2.296462000	-1.868330000
C	-4.290416000	-4.265940000	-0.532073000
H	-3.410942000	-4.788763000	-0.140508000
H	-5.089010000	-4.375336000	0.208286000
H	-4.595367000	-4.729235000	-1.472183000

GIII_{2a}

Pd	-2.831774000	0.153119000	0.182814000
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O	-2.134802000	-0.410508000	-1.908663000
C	-1.502214000	-1.494598000	-1.975171000
C	3.194394000	-2.639440000	3.330782000
C	4.058686000	-2.069077000	2.234129000
O	5.130557000	-1.534209000	2.436537000
O	3.662045000	-2.208080000	0.943653000
H	3.720692000	-2.517617000	4.277250000
H	2.233981000	-2.121191000	3.376143000
H	2.998559000	-3.702615000	3.157132000
C	3.032315000	3.592608000	-2.015548000
C	2.263653000	2.888495000	-0.928072000
O	2.342544000	3.136179000	0.254722000
O	1.459314000	1.939683000	-1.480668000
H	2.371044000	3.878667000	-2.837976000
H	3.530552000	4.472069000	-1.606954000
H	3.781779000	2.902626000	-2.419524000
C	1.424089000	-1.314208000	0.404957000
C	0.469817000	0.425815000	1.692298000
C	1.925818000	-0.271667000	-0.590007000
C	0.886158000	0.854205000	-0.706050000
C	0.278374000	1.213039000	0.626114000
O	1.211574000	-0.725692000	1.698715000
C	2.313647000	-2.537944000	0.572462000
H	0.033236000	0.631232000	2.662115000
H	0.097037000	0.496479000	-1.368722000
H	0.457429000	-1.680360000	0.028878000
H	2.390838000	-3.041884000	-0.393837000
H	1.854633000	-3.230460000	1.282085000
C	-2.170523000	3.601341000	2.018669000
C	-0.699421000	2.367617000	0.650383000
C	-3.471185000	3.135002000	1.351613000
C	-3.164857000	2.393185000	0.062203000
C	-1.863084000	2.092397000	-0.289306000
O	-1.149932000	2.597969000	1.976181000
H	-0.189104000	3.274045000	0.280877000
H	-3.933306000	2.398135000	-0.709112000
H	-1.802841000	4.511811000	1.520155000
H	-4.076624000	4.015493000	1.102858000
H	-3.149360000	0.430560000	1.631213000
H	-4.071193000	2.525829000	2.032325000
H	-2.328314000	3.833657000	3.074562000
H	-1.613032000	1.921383000	-1.332313000
H	2.081528000	-0.731525000	-1.567102000
O	3.156688000	0.292407000	-0.122061000
C	4.270983000	0.118220000	-0.878513000
C	5.460219000	0.700131000	-0.171598000
H	6.316897000	0.733813000	-0.845201000
H	5.226240000	1.700971000	0.201454000
H	5.682516000	0.060576000	0.690409000
O	4.280279000	-0.442204000	-1.955139000
H	-1.707333000	-2.305733000	-1.267456000
N	-0.541599000	-1.747576000	-2.863175000
C	-0.135540000	-0.771995000	-3.870237000
H	-0.741785000	0.127204000	-3.772670000
H	0.920990000	-0.518871000	-3.732952000
H	-0.269123000	-1.197226000	-4.870049000
C	0.175984000	-3.017866000	-2.856044000
H	-0.195457000	-3.652219000	-2.049385000
H	0.037972000	-3.533703000	-3.811871000
H	1.245368000	-2.835941000	-2.706513000
O	-3.054045000	-1.863622000	0.597883000
C	-4.255457000	-2.348977000	0.451109000

C	-4.323667000	-3.856582000	0.662938000
H	-5.359125000	-4.201424000	0.641892000
H	-3.759961000	-4.364231000	-0.127726000
H	-3.862547000	-4.128912000	1.617373000
O	-5.264036000	-1.696833000	0.160435000

TS4I_{2a}

Pd	-3.046619000	-0.259863000	0.566807000
O	-1.727560000	-0.602806000	2.658227000
C	-0.483316000	-0.662863000	2.650825000
C	5.765825000	-2.560691000	-1.609749000
C	4.809082000	-2.359638000	-0.463511000
O	5.067609000	-2.622147000	0.693840000
O	3.581247000	-1.850642000	-0.730877000
H	6.635887000	-3.105185000	-1.243567000
H	5.301763000	-3.112185000	-2.432691000
H	6.091222000	-1.588438000	-1.994867000
C	2.294424000	4.221964000	1.416088000
C	1.492084000	3.077851000	0.853246000
O	0.819138000	2.313310000	1.511525000
O	1.625839000	3.050053000	-0.497804000
H	3.359907000	3.980831000	1.329420000
H	2.116213000	5.138567000	0.847219000
H	2.040025000	4.372173000	2.465513000
C	2.083673000	-0.394776000	-1.939074000
C	-0.053867000	-0.156598000	-0.948166000
C	2.489148000	0.935388000	-1.305514000
C	1.279289000	1.887990000	-1.297676000
C	-0.004727000	1.181799000	-0.942087000
O	0.976690000	-0.997506000	-1.249611000
C	3.186659000	-1.432745000	-2.049293000
H	-0.962517000	-0.705944000	-0.716363000
H	1.189844000	2.319064000	-2.300379000
H	1.767918000	-0.164908000	-2.967927000
H	4.018157000	-0.988369000	-2.599972000
H	2.814109000	-2.301486000	-2.601086000
C	-3.140515000	2.873927000	-1.874275000
C	-1.244387000	2.025606000	-0.750633000
C	-4.171695000	2.408581000	-0.838012000
C	-3.480060000	1.902763000	0.420811000
C	-2.101987000	1.709717000	0.462019000
O	-2.019040000	1.990082000	-1.958990000
H	-0.902577000	3.065108000	-0.601014000
H	-3.747177000	-0.459833000	-0.842898000
H	-3.577447000	2.917668000	-2.875754000
H	-4.830184000	1.645746000	-1.264019000
H	-4.020789000	2.035392000	1.357451000
H	-4.813670000	3.258047000	-0.572144000
H	-1.570330000	1.730626000	1.408367000
H	-2.786084000	3.885365000	-1.616298000
H	3.305787000	1.373924000	-1.881586000
O	2.913127000	0.765085000	0.056362000
C	4.244715000	0.757860000	0.309326000
C	4.509175000	0.579395000	1.776213000
H	3.739487000	1.062107000	2.380916000
H	4.500087000	-0.495961000	1.985383000
H	5.496654000	0.974153000	2.019289000
O	5.096127000	0.849731000	-0.553518000
H	0.123356000	0.100332000	3.160356000
N	0.256296000	-1.607653000	2.053697000

C	-0.341492000	-2.728179000	1.340075000
H	0.127977000	-2.822881000	0.356785000
H	-0.176639000	-3.658463000	1.897620000
H	-1.412312000	-2.569200000	1.217926000
C	1.712520000	-1.594036000	2.137563000
H	2.068250000	-2.515505000	2.613546000
H	2.147150000	-1.517765000	1.140105000
H	2.038227000	-0.742333000	2.735825000
O	-3.773466000	-2.318525000	0.391822000
C	-4.307564000	-2.466958000	-0.756615000
O	-4.391109000	-1.536220000	-1.618027000
C	-4.876285000	-3.826413000	-1.092840000
H	-4.102954000	-4.588712000	-0.957966000
H	-5.688975000	-4.057433000	-0.396532000
H	-5.252961000	-3.860202000	-2.115596000

TS4III_{2a}

Pd	-2.846408000	0.011639000	0.398128000
O	-1.763965000	-0.090033000	2.661397000
C	-1.002559000	0.874367000	2.871272000
C	2.809637000	3.417813000	-2.604765000
C	3.758945000	2.494406000	-1.882108000
O	4.752637000	2.020690000	-2.396119000
O	3.540161000	2.222315000	-0.570835000
H	3.195988000	3.584765000	-3.609976000
H	1.810440000	2.981208000	-2.664453000
H	2.730885000	4.376988000	-2.082531000
C	2.774545000	-4.229287000	0.608260000
C	1.980248000	-3.176348000	-0.121318000
O	1.928926000	-3.051458000	-1.324970000
O	1.321672000	-2.400304000	0.780069000
H	2.155758000	-4.733345000	1.355710000
H	3.170962000	-4.953155000	-0.104127000
H	3.602213000	-3.745005000	1.138250000
C	1.327226000	1.272814000	-0.031792000
C	0.119480000	0.048787000	-1.651052000
C	1.863053000	-0.045177000	0.520008000
C	0.756264000	-1.106751000	0.438836000
C	-0.016649000	-1.017994000	-0.852283000
O	0.934963000	1.122738000	-1.404901000
C	2.275909000	2.458127000	0.071384000
H	-0.435502000	0.165240000	-2.573108000
H	0.073668000	-0.932397000	1.272629000
H	0.434287000	1.532993000	0.556066000
H	2.508244000	2.625193000	1.125490000
H	1.786346000	3.354848000	-0.315435000
C	-2.830324000	-2.635562000	-2.596452000
C	-1.088822000	-2.057577000	-1.100528000
C	-3.989747000	-2.175529000	-1.710797000
C	-3.498456000	-2.011165000	-0.280350000
C	-2.138310000	-2.010163000	0.006692000
O	-1.661524000	-1.841727000	-2.383526000
H	-0.628760000	-3.060771000	-1.079234000
H	-4.199063000	-2.265346000	0.513862000
H	-2.599991000	-3.693516000	-2.392317000
H	-4.781583000	-2.934546000	-1.733668000
H	-3.226591000	0.588059000	-1.036962000
H	-4.425744000	-1.251887000	-2.103173000
H	-3.075452000	-2.541265000	-3.657768000
H	-1.791998000	-2.309529000	0.994357000

H	2.182321000	0.081016000	1.554438000
O	2.973677000	-0.480422000	-0.274441000
C	4.186679000	-0.588575000	0.323796000
C	5.227581000	-0.949143000	-0.695795000
H	6.150879000	-1.247837000	-0.198474000
H	4.864213000	-1.750246000	-1.345025000
H	5.404985000	-0.063759000	-1.317575000
O	4.381187000	-0.397666000	1.507073000
H	-1.244082000	1.881810000	2.503336000
N	0.166513000	0.799999000	3.525641000
C	0.644399000	-0.452730000	4.098683000
H	-0.032360000	-1.259168000	3.819109000
H	1.650354000	-0.672916000	3.727571000
H	0.684177000	-0.374042000	5.190907000
C	0.998855000	1.977277000	3.735113000
H	0.550174000	2.845353000	3.248103000
H	1.101535000	2.184142000	4.806263000
H	1.996403000	1.808904000	3.316070000
O	-3.131044000	2.167911000	0.540722000
C	-3.391217000	2.622587000	-0.621831000
C	-3.618978000	4.109389000	-0.759076000
H	-4.576572000	4.364629000	-0.292209000
H	-2.836121000	4.655029000	-0.225253000
H	-3.639971000	4.414107000	-1.805977000
O	-3.486365000	1.889414000	-1.656174000

HI_{2a}

Pd	-2.935796000	-0.370642000	0.284105000
O	-1.415080000	-2.029263000	0.676455000
C	-0.364366000	-1.682247000	1.265150000
C	6.210206000	-1.900563000	-1.762704000
C	5.153463000	-2.003356000	-0.694581000
O	5.323980000	-2.540113000	0.382038000
O	3.932646000	-1.468951000	-0.941204000
H	7.055493000	-2.525967000	-1.476302000
H	5.829802000	-2.212515000	-2.739619000
H	6.548861000	-0.862565000	-1.848967000
C	1.545281000	3.598260000	2.692731000
C	1.165016000	2.551026000	1.677501000
O	0.660869000	1.479895000	1.943785000
O	1.462077000	2.995958000	0.432374000
H	2.635442000	3.701881000	2.711482000
H	1.126523000	4.570417000	2.417808000
H	1.189736000	3.300499000	3.679386000
C	2.461511000	0.192215000	-1.881851000
C	0.197859000	0.028304000	-1.238300000
C	2.679137000	1.323408000	-0.874924000
C	1.374207000	2.138954000	-0.739458000
C	0.123528000	1.307297000	-0.852104000
O	1.348264000	-0.643659000	-1.539241000
C	3.658628000	-0.707256000	-2.131663000
H	-0.678570000	-0.598332000	-1.360210000
H	1.373336000	2.875251000	-1.550560000
H	2.239517000	0.686390000	-2.840725000
H	4.508047000	-0.080020000	-2.408951000
H	3.430690000	-1.394919000	-2.951794000
C	-3.020402000	2.790085000	-2.052805000
C	-1.203778000	2.030335000	-0.741232000
C	-4.126287000	2.103875000	-1.251070000
C	-3.586076000	1.637509000	0.107900000

C	-2.176095000	1.560637000	0.338914000
O	-1.816405000	2.021429000	-2.043184000
H	-0.968126000	3.083414000	-0.496878000
H	-3.303135000	2.911843000	-3.103448000
H	-4.526406000	1.269067000	-1.838117000
H	-4.209081000	1.908844000	0.963753000
H	-4.954791000	2.809085000	-1.107003000
H	-1.799084000	1.760330000	1.342130000
H	-2.818609000	3.792649000	-1.638655000
H	3.475943000	1.970050000	-1.247662000
O	3.054466000	0.843925000	0.426266000
C	4.372223000	0.840229000	0.736828000
C	4.601824000	0.378279000	2.147882000
H	3.738381000	0.575294000	2.784384000
H	4.788339000	-0.701004000	2.122132000
H	5.492658000	0.868810000	2.544493000
O	5.252624000	1.146997000	-0.044796000
H	-0.342310000	-0.812000000	1.930411000
N	0.811522000	-2.300230000	1.145786000
C	1.007300000	-3.425969000	0.243348000
H	1.810849000	-3.183343000	-0.457556000
H	1.282495000	-4.322727000	0.810288000
H	0.085188000	-3.613832000	-0.305621000
C	1.975968000	-1.846205000	1.897266000
H	2.227475000	-2.567146000	2.684754000
H	2.822091000	-1.750005000	1.216991000
H	1.767793000	-0.872343000	2.340883000
O	-4.475145000	-2.144824000	0.071445000
C	-5.656913000	-1.794997000	0.101901000
O	-6.008558000	-0.522167000	0.264056000
C	-6.815228000	-2.733169000	-0.047365000
H	-7.489365000	-2.631291000	0.808346000
H	-7.382031000	-2.468918000	-0.946272000
H	-6.459498000	-3.760298000	-0.123569000
H	-5.151636000	-0.009158000	0.323216000

III_{2a}

Pd	2.723171000	-0.360008000	-0.463380000
O	1.536489000	1.505721000	-1.146112000
C	1.226687000	2.304526000	-0.237696000
C	-3.490124000	3.333460000	1.879592000
C	-4.386222000	2.308870000	1.226929000
O	-5.350558000	1.816642000	1.778540000
O	-4.153009000	1.955041000	-0.061723000
H	-3.882600000	3.542488000	2.874547000
H	-2.467264000	2.959970000	1.958625000
H	-3.471641000	4.259642000	1.295748000
C	-2.851912000	-4.494877000	-1.263748000
C	-2.253063000	-3.381535000	-0.442911000
O	-2.384085000	-3.254148000	0.754556000
O	-1.541607000	-2.554078000	-1.253375000
H	-2.109803000	-4.923392000	-1.942712000
H	-3.252238000	-5.265240000	-0.604141000
H	-3.662164000	-4.082680000	-1.875565000
C	-1.882415000	1.124164000	-0.543762000
C	-0.714975000	0.029783000	1.219865000
C	-2.307875000	-0.255584000	-1.034281000
C	-1.125631000	-1.217877000	-0.857990000
C	-0.487176000	-1.072522000	0.499659000
O	-1.512849000	1.085483000	0.844192000

C	-2.908470000	2.231959000	-0.725799000
H	-0.265598000	0.196060000	2.191683000
H	-0.385513000	-0.973251000	-1.626846000
H	-1.004466000	1.408720000	-1.137377000
H	-3.150294000	2.314250000	-1.787772000
H	-2.482177000	3.181645000	-0.397868000
C	2.248558000	-1.446531000	2.557273000
C	0.549444000	-2.102314000	0.915620000
C	3.317038000	-2.277222000	1.854175000
C	3.053198000	-2.294850000	0.357699000
C	1.709361000	-2.145791000	-0.082923000
O	0.932569000	-1.934669000	2.286597000
H	0.068155000	-3.088525000	0.883810000
H	3.728204000	-2.913318000	-0.238173000
H	2.354169000	-1.501075000	3.645488000
H	3.292833000	-3.302489000	2.252811000
H	4.307913000	-1.867612000	2.086202000
H	2.344313000	-0.390631000	2.255923000
H	1.417269000	-2.601749000	-1.030175000
H	-2.600729000	-0.210095000	-2.084461000
O	-3.407771000	-0.728880000	-0.246244000
C	-4.612273000	-0.893469000	-0.846068000
C	-5.645434000	-1.260169000	0.179731000
H	-6.559556000	-1.594369000	-0.312000000
H	-5.260528000	-2.037447000	0.845270000
H	-5.848580000	-0.367123000	0.782499000
O	-4.806965000	-0.743688000	-2.035310000
H	1.443927000	2.085348000	0.815073000
N	0.601056000	3.472700000	-0.432694000
C	0.255061000	3.945081000	-1.767688000
H	0.559525000	3.203495000	-2.504936000
H	-0.825175000	4.108168000	-1.838222000
H	0.765418000	4.892814000	-1.971374000
C	0.228561000	4.330126000	0.685214000
H	0.506199000	3.857563000	1.629262000
H	0.736722000	5.297399000	0.606802000
H	-0.852709000	4.501554000	0.681486000
O	4.467949000	1.228179000	-0.516011000
C	5.592697000	0.758216000	-0.330835000
C	6.845391000	1.575934000	-0.266878000
H	7.297534000	1.467903000	0.724538000
H	7.567745000	1.204602000	-1.000146000
H	6.621780000	2.624780000	-0.459938000
O	5.788813000	-0.546541000	-0.158629000
H	4.881708000	-0.964698000	-0.196666000

5e+[Pd(DMF)₂]

Pd	2.745796000	0.812201000	-0.317864000
O	1.768352000	-1.109000000	-1.397558000
C	1.344412000	-2.027781000	-0.666356000
C	-5.142608000	-3.448804000	1.880938000
C	-4.243733000	-3.114731000	0.719447000
O	-4.272241000	-3.684652000	-0.352518000
O	-3.348654000	-2.106870000	0.870280000
H	-5.711038000	-4.345850000	1.636770000
H	-4.568054000	-3.611566000	2.797744000
H	-5.838950000	-2.623933000	2.067649000
C	-3.335443000	3.475873000	-2.497274000
C	-2.313571000	2.787325000	-1.629328000
O	-1.352607000	2.176336000	-2.043917000

O	-2.627905000	2.970951000	-0.320762000
H	-2.971227000	3.534170000	-3.523335000
H	-4.262939000	2.892019000	-2.473468000
H	-3.563265000	4.474950000	-2.116710000
C	-2.419483000	-0.101669000	1.827036000
C	-0.283954000	0.483668000	0.978787000
C	-3.031567000	0.901954000	0.851372000
C	-2.105299000	2.121618000	0.737656000
C	-0.651016000	1.728530000	0.644056000
O	-1.115561000	-0.520021000	1.400337000
C	-3.249981000	-1.345517000	2.087954000
H	0.751290000	0.155870000	0.938871000
H	-2.253348000	2.742134000	1.627508000
H	-2.323828000	0.418337000	2.792239000
H	-4.235200000	-1.035446000	2.445602000
H	-2.763436000	-1.951252000	2.858819000
C	1.741981000	2.939727000	2.356497000
C	0.339039000	2.856325000	0.406483000
C	3.022982000	3.265021000	1.595675000
C	2.895248000	2.852057000	0.137364000
C	1.607795000	2.577418000	-0.410901000
O	0.619281000	3.496209000	1.677619000
H	-0.200843000	3.635100000	-0.140718000
H	1.623893000	1.850083000	2.474155000
H	3.881630000	2.782059000	2.079909000
H	3.660104000	3.271050000	-0.521088000
H	3.194812000	4.350559000	1.655543000
H	1.443901000	2.767241000	-1.472307000
H	1.748259000	3.384140000	3.357224000
H	1.993296000	-2.508458000	0.082734000
N	0.106822000	-2.530421000	-0.703114000
C	-0.917236000	-1.978099000	-1.582860000
H	-1.325052000	-2.773269000	-2.216266000
H	-1.716373000	-1.548958000	-0.978492000
H	-0.471903000	-1.205022000	-2.206919000
C	-0.319177000	-3.575438000	0.217084000
H	-1.085004000	-3.183182000	0.890482000
H	-0.738755000	-4.418391000	-0.342601000
H	0.533394000	-3.928284000	0.801522000
O	4.505026000	-0.617152000	0.106125000
C	4.689498000	-1.675239000	-0.529095000
H	4.045896000	-1.945554000	-1.374929000
N	5.651052000	-2.567766000	-0.257932000
C	6.592616000	-2.376285000	0.837320000
H	6.484122000	-3.182733000	1.571226000
H	7.618319000	-2.390054000	0.453407000
H	6.398636000	-1.419000000	1.319573000
C	5.782747000	-3.793529000	-1.034508000
H	6.776445000	-3.847129000	-1.492423000
H	5.649687000	-4.667389000	-0.386904000
H	5.027108000	-3.818479000	-1.822424000
O	-3.148086000	0.330380000	-0.461293000
H	-4.018777000	1.206093000	1.203386000
C	-4.369119000	-0.086935000	-0.878464000
C	-4.267216000	-0.748522000	-2.223083000
H	-5.225826000	-0.682567000	-2.739948000
H	-3.471437000	-0.305842000	-2.825066000
H	-4.031968000	-1.805075000	-2.049914000
O	-5.385954000	0.033556000	-0.225385000

4e+[Pd(DMF)₂]

Pd	2.684467000	-1.161789000	-0.331895000
C	-3.984329000	2.793567000	2.803979000
C	-4.691932000	2.127456000	1.650040000
O	-5.758240000	1.555482000	1.759930000
O	-4.154704000	2.218811000	0.407386000
H	-4.603044000	2.680515000	3.693924000
H	-3.006910000	2.338217000	2.976326000
H	-3.832376000	3.858808000	2.600703000
C	-2.752180000	-3.599967000	-2.459591000
C	-2.289521000	-2.857067000	-1.232085000
O	-2.634708000	-3.106558000	-0.097642000
O	-1.424798000	-1.876201000	-1.597694000
H	-3.385053000	-2.935760000	-3.058447000
H	-1.900307000	-3.890572000	-3.080921000
H	-3.322152000	-4.481498000	-2.165176000
C	-1.830297000	1.410137000	0.191766000
C	-1.066309000	-0.271069000	1.683969000
C	-2.134633000	0.302392000	-0.812282000
C	-1.043069000	-0.776969000	-0.725421000
C	-0.690929000	-1.105907000	0.705827000
O	-1.779050000	0.891618000	1.527602000
C	-2.786915000	2.595021000	0.176422000
H	-0.822702000	-0.444532000	2.724920000
H	-0.149344000	-0.390292000	-1.223523000
H	-0.842652000	1.814595000	-0.063385000
H	-2.769462000	3.042828000	-0.819749000
H	-2.448048000	3.346154000	0.893413000
C	1.509593000	-3.306771000	2.681111000
C	0.155181000	-2.327806000	1.013495000
C	2.804097000	-3.358855000	1.868794000
C	2.504418000	-3.124866000	0.384230000
C	1.232719000	-2.623258000	-0.027423000
O	0.715731000	-2.175908000	2.321281000
H	-0.524243000	-3.198334000	1.042272000
H	3.022123000	-3.800672000	-0.299860000
H	0.927920000	-4.230070000	2.521908000
H	3.271573000	-4.342201000	2.011243000
H	3.511558000	-2.619186000	2.263092000
H	1.709088000	-3.215262000	3.753410000
H	0.823894000	-2.957117000	-0.982078000
O	4.772060000	-0.040578000	-0.367475000
C	4.681982000	0.927242000	0.414047000
H	4.525465000	0.779660000	1.493749000
N	4.755165000	2.217130000	0.055155000
C	4.919826000	2.615305000	-1.336300000
H	4.985328000	1.725053000	-1.959357000
H	4.062840000	3.219989000	-1.652207000
H	5.831611000	3.212025000	-1.447767000
C	4.625204000	3.288015000	1.033713000
H	4.467097000	2.867384000	2.028966000
H	5.530853000	3.904272000	1.047228000
H	3.771569000	3.924921000	0.778313000
O	1.984946000	0.888271000	-1.200549000
C	1.714354000	1.841596000	-0.444790000
H	1.819865000	1.761023000	0.645116000
N	1.280025000	3.041081000	-0.860702000
C	1.043630000	3.313995000	-2.272791000
H	1.497080000	2.527859000	-2.874947000
H	-0.033285000	3.350217000	-2.476024000
H	1.483279000	4.279924000	-2.537887000
C	0.889662000	4.077642000	0.086471000
H	1.084610000	3.743876000	1.107424000

H	1.455375000	4.995215000	-0.104336000
H	-0.179609000	4.297103000	-0.015686000
O	-3.395645000	-0.300239000	-0.489927000
H	-2.172142000	0.710291000	-1.823725000
C	-4.419679000	-0.165016000	-1.368617000
O	-4.322877000	0.383118000	-2.447696000
C	-5.666049000	-0.775369000	-0.796012000
H	-6.008537000	-0.132059000	0.022723000
H	-6.436422000	-0.843443000	-1.564698000
H	-5.447332000	-1.763319000	-0.381987000

5e

C	5.548878000	-0.935956000	-0.319513000
C	4.512661000	-0.535881000	0.700398000
O	4.766883000	0.085261000	1.713433000
O	3.222578000	-0.883898000	0.481960000
H	6.535728000	-0.698731000	0.077105000
H	5.490594000	-2.002953000	-0.554622000
H	5.397413000	-0.380855000	-1.251620000
C	-2.085833000	3.271258000	-0.341918000
C	-1.611571000	1.863192000	-0.084089000
O	-1.576766000	1.333521000	1.003510000
O	-1.265303000	1.286828000	-1.264182000
H	-2.255304000	3.780065000	0.607416000
H	-1.352055000	3.820733000	-0.938433000
H	-3.021167000	3.240039000	-0.910490000
C	1.316015000	-1.430537000	-0.904735000
C	-0.693543000	-1.998331000	0.173389000
C	0.789795000	-0.012327000	-1.112451000
C	-0.734916000	-0.063018000	-1.356448000
C	-1.423529000	-1.120439000	-0.528548000
O	0.671274000	-2.059731000	0.211407000
C	2.817995000	-1.556171000	-0.724480000
H	-1.150708000	-2.776939000	0.774525000
H	-0.882227000	-0.287761000	-2.418745000
H	1.067763000	-1.995953000	-1.816968000
H	3.303173000	-1.125525000	-1.604226000
H	3.083615000	-2.616113000	-0.655707000
O	1.038838000	0.781267000	0.054012000
C	2.038986000	1.690317000	0.011310000
H	1.284872000	0.444713000	-1.971139000
C	2.195184000	2.351576000	1.350562000
H	2.819843000	1.695222000	1.967781000
H	2.698762000	3.312426000	1.235185000
H	1.227322000	2.475477000	1.840963000
O	2.725409000	1.905522000	-0.968909000
C	-2.937705000	-1.356875000	-0.650017000
C	-3.774753000	-0.134349000	-0.956057000
C	-4.683335000	0.337123000	-0.099184000
C	-3.709465000	-1.202646000	1.592767000
C	-4.871772000	-0.265784000	1.268092000
H	-3.941877000	-1.856191000	2.438589000
H	-2.813037000	-0.618939000	1.833129000
H	-4.930629000	0.524178000	2.028209000
H	-5.827806000	-0.807414000	1.310084000
O	-3.441033000	-2.071689000	0.480976000
H	-3.628879000	0.321935000	-1.930958000
H	-5.315978000	1.177733000	-0.378566000
H	-3.083021000	-2.048709000	-1.493639000

5e'

C	5.414590000	-1.237084000	-0.288708000
C	4.397353000	-0.877892000	0.764783000
O	4.683352000	-0.374922000	1.833137000
O	3.088318000	-1.116940000	0.511352000
H	6.410324000	-1.125843000	0.140079000
H	5.280449000	-2.258900000	-0.655270000
H	5.318761000	-0.558552000	-1.143357000
C	-2.076055000	3.539199000	-0.428889000
C	-1.465639000	2.189896000	-0.143633000
O	-1.290145000	1.730631000	0.961315000
O	-1.156394000	1.586096000	-1.322865000
H	-2.169486000	4.104228000	0.499168000
H	-1.473770000	4.097452000	-1.150865000
H	-3.069279000	3.391158000	-0.865504000
C	1.178029000	-1.366441000	-0.955051000
C	-0.906246000	-1.751270000	0.076891000
C	0.817718000	0.109725000	-1.129869000
C	-0.697217000	0.214580000	-1.401573000
C	-1.518376000	-0.778929000	-0.615866000
O	0.438940000	-1.964744000	0.123551000
C	2.651875000	-1.665614000	-0.745494000
H	-1.446834000	-2.495282000	0.653389000
H	-0.832048000	-0.000946000	-2.467897000
H	0.893448000	-1.872481000	-1.890551000
H	3.204093000	-1.238451000	-1.585847000
H	2.803044000	-2.749887000	-0.733911000
O	1.145590000	0.852599000	0.048976000
C	2.291094000	1.568252000	0.054148000
H	1.372026000	0.519628000	-1.976829000
C	2.494942000	2.214702000	1.393949000
H	2.919691000	1.457349000	2.062431000
H	3.200284000	3.041891000	1.304072000
H	1.544857000	2.554347000	1.811500000
O	3.056768000	1.639372000	-0.889023000
C	-3.030142000	-0.738461000	-0.794780000
C	-3.849631000	0.146816000	1.255443000
C	-4.575642000	-2.131926000	0.582523000
C	-4.886847000	-0.953952000	1.468628000
H	-5.081550000	-3.074199000	0.785646000
H	-4.894682000	-1.258323000	2.523389000
H	-5.896160000	-0.577844000	1.247552000
H	-2.895294000	-0.124364000	1.725187000
H	-3.211363000	-0.547903000	-1.862933000
O	-3.653470000	0.379758000	-0.142068000
C	-3.712366000	-2.038219000	-0.432932000
H	-4.172819000	1.100339000	1.681356000
H	-3.472000000	-2.898507000	-1.053207000

4e

C	5.224469000	-1.840088000	-0.656358000
C	4.408044000	-1.262647000	0.472393000
O	4.891401000	-0.725043000	1.448935000
O	3.057649000	-1.341585000	0.400619000
H	6.276715000	-1.809801000	-0.374641000
H	4.931236000	-2.870039000	-0.881020000
H	5.083093000	-1.247367000	-1.566718000
C	-0.705804000	4.010730000	-0.386700000
C	-0.949144000	2.575070000	0.003892000

O	-1.130522000	2.185287000	1.135957000
O	-0.945435000	1.795518000	-1.110372000
H	-0.952496000	4.667751000	0.447957000
H	0.354952000	4.128698000	-0.637019000
H	-1.286695000	4.283881000	-1.271357000
C	0.949601000	-1.443247000	-0.783355000
C	-0.989234000	-1.468421000	0.569934000
C	0.747615000	0.061020000	-0.966734000
C	-0.757042000	0.354962000	-1.075204000
C	-1.551667000	-0.426308000	-0.057256000
O	0.289283000	-1.919500000	0.396878000
C	2.395035000	-1.906269000	-0.745376000
H	-1.529324000	-2.066833000	1.293681000
H	-1.069657000	0.066166000	-2.083844000
H	0.495451000	-1.930778000	-1.659879000
H	2.872784000	-1.596394000	-1.678074000
H	2.423125000	-2.998751000	-0.677279000
O	1.256066000	0.779359000	0.166222000
C	2.440164000	1.424254000	0.037115000
H	1.259405000	0.396079000	-1.870554000
C	2.850106000	2.028234000	1.348958000
H	3.342312000	1.238844000	1.928750000
H	3.561020000	2.838108000	1.179862000
H	1.981566000	2.384017000	1.907045000
O	3.082326000	1.466718000	-0.993750000
C	-3.021047000	-0.094947000	0.127364000
C	-3.815475000	-0.430438000	-1.121662000
H	-3.108039000	0.988051000	0.313719000
C	-4.953589000	-1.128412000	-1.082177000
C	-4.924579000	-0.791675000	1.370535000
C	-5.554986000	-1.579786000	0.223508000
H	-5.163807000	-1.230556000	2.343474000
H	-5.297972000	0.244942000	1.363221000
H	-6.641725000	-1.426403000	0.220987000
H	-5.392461000	-2.656969000	0.369559000
O	-3.500292000	-0.798197000	1.271502000
H	-3.417580000	-0.064824000	-2.065644000
H	-5.480502000	-1.370462000	-2.003425000

4e'

C	-4.296349000	-2.193187000	-1.043499000
C	-4.196427000	-0.742349000	-0.641575000
O	-4.611705000	0.170486000	-1.327562000
O	-3.672234000	-0.429832000	0.569915000
H	-4.821788000	-2.247569000	-1.996689000
H	-3.303611000	-2.637005000	-1.145466000
H	-4.848971000	-2.766793000	-0.292107000
C	2.410307000	3.040444000	-0.221716000
C	1.476840000	1.869020000	-0.397404000
O	0.881521000	1.600848000	-1.414701000
O	1.419378000	1.174584000	0.770710000
H	2.354812000	3.691479000	-1.094853000
H	2.163690000	3.603222000	0.683111000
H	3.432769000	2.663858000	-0.111165000
C	-1.407262000	-1.319893000	1.026074000
C	0.089750000	-1.870311000	-0.713659000
C	-0.743559000	0.050643000	1.129333000
C	0.769252000	-0.112848000	0.884060000
C	1.068746000	-1.098067000	-0.221842000
O	-1.208873000	-1.873187000	-0.289360000

C	-2.895443000	-1.356678000	1.346667000
H	0.255627000	-2.607216000	-1.495099000
H	1.199683000	-0.497338000	1.815043000
H	-0.916440000	-1.982545000	1.754952000
H	-3.027709000	-1.047100000	2.386200000
H	-3.265186000	-2.380012000	1.247938000
C	4.399442000	-1.420936000	1.070758000
C	2.507645000	-1.410383000	-0.577432000
C	5.107846000	-0.343363000	0.292857000
C	4.560131000	-0.315551000	-1.132477000
H	2.499783000	-2.215244000	-1.335226000
H	4.902169000	-1.209501000	-1.678965000
H	4.869454000	-1.804676000	1.974355000
H	6.188890000	-0.530649000	0.273094000
H	4.901766000	0.567070000	-1.680873000
H	4.967828000	0.635557000	0.772832000
H	-0.912794000	0.482076000	2.117651000
O	-1.307491000	0.904232000	0.130789000
C	-1.874380000	2.068776000	0.518373000
C	-2.438965000	2.780882000	-0.677199000
H	-2.745324000	3.790639000	-0.401948000
H	-1.693910000	2.808168000	-1.476738000
H	-3.302590000	2.209556000	-1.035809000
O	-1.922278000	2.456650000	1.668929000
C	3.237998000	-1.927262000	0.648729000
H	2.745835000	-2.740611000	1.177828000
O	3.134505000	-0.251155000	-1.133515000

DMF

C	-0.864407000	-0.644192000	-0.000003000
O	-1.961589000	-0.089115000	-0.000004000
H	-0.760810000	-1.745543000	-0.000032000
N	0.340577000	-0.022007000	0.000042000
C	0.434810000	1.428884000	-0.000012000
H	0.973735000	1.777600000	0.889170000
H	0.973750000	1.777534000	-0.889206000
H	-0.572251000	1.846651000	-0.000002000
C	1.587378000	-0.767601000	-0.000006000
H	2.183234000	-0.525319000	-0.888585000
H	2.183135000	-0.525656000	0.888734000
H	1.381198000	-1.840847000	-0.000217000

AcOAg

Ag	1.136500000	-0.002863000	-0.000020000
O	-0.946005000	-1.100529000	0.000050000
C	-1.555425000	0.015233000	0.000237000
O	-0.963920000	1.136493000	-0.000104000
C	-3.074939000	-0.017734000	-0.000005000
H	-3.427551000	-0.562291000	0.881909000
H	-3.498972000	0.987568000	-0.000657000
H	-3.427405000	-0.563437000	-0.881261000

AcOH

H	1.726458000	-0.814063000	0.000102000
O	0.778685000	-1.042755000	0.000047000
C	0.091256000	0.122003000	-0.000054000
O	0.642838000	1.204275000	-0.000033000

C	-1.394402000	-0.111542000	-0.000004000
H	-1.680587000	-0.691833000	0.882936000
H	-1.918632000	0.843945000	-0.000597000
H	-1.680542000	-0.692972000	-0.882200000

AgCl

Ag	0.000000000	0.000000000	0.641321000
Cl	0.000000000	0.000000000	-1.773064000

(2) Computational investigation of the Pd-catalyzed C–C coupling of between 1a and 3a

1a

C	5.122435000	-0.821687000	-0.138412000
C	4.147188000	-0.991992000	1.001849000
O	4.379597000	-0.650199000	2.140959000
O	2.939250000	-1.565243000	0.752762000
H	6.059232000	-0.445988000	0.272374000
H	5.304497000	-1.767419000	-0.657376000
H	4.746967000	-0.101059000	-0.872807000
C	-1.077932000	3.362532000	1.228228000
C	-0.858814000	1.890081000	1.015902000
O	-0.668009000	1.067436000	1.885274000
O	-0.902556000	1.600980000	-0.312868000
H	-1.130488000	3.576361000	2.295783000
H	-0.245456000	3.915888000	0.781989000
H	-1.997197000	3.687040000	0.732108000
C	1.080728000	-1.592490000	-0.772280000
C	-1.050403000	-2.010019000	0.183054000
C	0.839183000	-0.109640000	-0.490477000
C	-0.622909000	0.257496000	-0.764282000
C	-1.513891000	-0.814530000	-0.199408000
O	0.255377000	-2.387919000	0.100348000
C	2.527658000	-1.994631000	-0.556746000
H	-1.673339000	-2.794866000	0.598638000
H	-0.769267000	0.337351000	-1.845505000
H	0.810778000	-1.826451000	-1.811665000
H	3.126731000	-1.545226000	-1.348439000
H	2.622814000	-3.082951000	-0.617307000
I	-3.620539000	-0.412655000	-0.105122000
H	1.092085000	0.107706000	0.544997000
O	1.684509000	0.643468000	-1.376601000
C	2.328965000	1.730474000	-0.865884000
C	3.171607000	2.382023000	-1.925577000
H	3.735902000	3.206310000	-1.489937000
H	3.854670000	1.651571000	-2.369242000
H	2.526183000	2.758491000	-2.725806000
O	2.219530000	2.100011000	0.283609000

B_{1a}

Pd	1.472078000	-1.079032000	-0.502524000
C	4.151637000	-2.671494000	0.146134000
O	2.927618000	-2.652455000	-0.120800000
C	-5.787779000	-2.696766000	0.044026000
C	-5.372484000	-1.747783000	-1.055186000
O	-6.150471000	-1.041781000	-1.660142000

O	-4.059867000	-1.676151000	-1.398336000
H	-6.875549000	-2.685206000	0.107797000
H	-5.444864000	-3.716791000	-0.153225000
H	-5.375705000	-2.383969000	1.009462000
C	-2.417694000	3.994830000	0.383551000
C	-2.005758000	2.673792000	-0.205638000
O	-2.253302000	2.293915000	-1.331497000
O	-1.303293000	1.955994000	0.706863000
H	-2.942517000	4.585243000	-0.367659000
H	-3.071692000	3.819870000	1.243135000
H	-1.537594000	4.538996000	0.739426000
C	-1.808166000	-1.582997000	-0.545777000
C	-0.139247000	-0.453495000	-1.791530000
C	-2.135514000	-0.276733000	0.174888000
C	-0.891758000	0.597914000	0.418266000
C	0.116981000	0.426943000	-0.722020000
O	-1.254366000	-1.266261000	-1.828314000
C	-3.034882000	-2.451482000	-0.748551000
H	0.243793000	-0.289393000	-2.793444000
H	-0.437212000	0.289021000	1.360362000
H	-1.066295000	-2.163597000	0.025974000
H	-3.354567000	-2.819058000	0.226513000
H	-2.784929000	-3.305923000	-1.384927000
I	1.340586000	2.241742000	-1.215434000
H	4.552041000	-3.504685000	0.737234000
C	6.474555000	-1.969509000	0.155948000
H	7.087374000	-2.087116000	-0.743923000
H	6.831561000	-1.098372000	0.713927000
H	6.579001000	-2.859882000	0.778598000
C	4.789949000	-0.624304000	-1.061484000
H	5.174320000	-0.798601000	-2.072680000
H	3.711467000	-0.446268000	-1.115779000
H	5.278304000	0.259097000	-0.642361000
N	5.074274000	-1.777870000	-0.215231000
H	-2.858006000	0.266653000	-0.427635000
O	-2.721501000	-0.607038000	1.449312000
C	-3.803418000	0.112397000	1.852316000
C	-4.278054000	-0.365043000	3.196604000
H	-4.440148000	-1.446713000	3.183003000
H	-3.508762000	-0.156812000	3.947710000
H	-5.200531000	0.149545000	3.465578000
O	-4.296111000	1.013512000	1.206123000
O	0.755609000	-0.906977000	3.037141000
C	1.890982000	-0.620384000	2.646694000
N	2.378142000	0.632688000	2.492608000
C	1.581917000	1.798232000	2.847250000
H	2.120977000	2.408002000	3.581731000
H	1.379131000	2.411282000	1.963648000
H	0.638654000	1.464803000	3.279067000
C	3.726720000	0.872403000	2.003210000
H	3.696942000	1.465967000	1.083428000
H	4.315418000	1.415944000	2.752070000
H	4.220053000	-0.078874000	1.791467000
H	2.633297000	-1.394958000	2.388973000

TS1_{1a}

Pd	1.515881000	-1.008851000	-0.589115000
C	4.293026000	-2.506273000	0.093891000
O	3.102771000	-2.526630000	-0.290708000
C	-6.232166000	-2.277352000	0.099246000

C	-5.789769000	-1.316849000	-0.978636000
O	-6.529726000	-0.518906000	-1.511955000
O	-4.491883000	-1.339035000	-1.383118000
H	-7.307951000	-2.166743000	0.232454000
H	-6.001767000	-3.313883000	-0.165219000
H	-5.735289000	-2.055090000	1.049741000
C	-1.704780000	4.086554000	0.348013000
C	-1.669441000	2.690427000	-0.210702000
O	-2.033035000	2.363034000	-1.321378000
O	-1.156329000	1.836530000	0.709340000
H	-2.159712000	4.762842000	-0.375868000
H	-2.271515000	4.102778000	1.283641000
H	-0.683925000	4.413259000	0.570905000
C	-2.203449000	-1.526042000	-0.659908000
C	-0.479177000	-0.523561000	-1.902471000
C	-2.353529000	-0.228903000	0.133543000
C	-0.986526000	0.435342000	0.390703000
C	-0.060413000	0.138641000	-0.773608000
O	-1.662663000	-1.202403000	-1.954435000
C	-3.519473000	-2.253596000	-0.846288000
H	0.012502000	-0.471215000	-2.867035000
H	-0.573582000	0.026063000	1.313971000
H	-1.499163000	-2.207915000	-0.156941000
H	-3.820085000	-2.654959000	0.121478000
H	-3.390471000	-3.084119000	-1.546981000
I	1.699357000	1.908437000	-1.155115000
H	4.674187000	-3.338097000	0.700736000
C	6.544771000	-1.649132000	0.417000000
H	7.295014000	-1.659295000	-0.380260000
H	6.726949000	-0.781313000	1.059695000
H	6.642060000	-2.559071000	1.011939000
C	4.941063000	-0.409325000	-1.006667000
H	5.716341000	-0.344519000	-1.776840000
H	3.967341000	-0.508726000	-1.485092000
H	4.955248000	0.507319000	-0.409806000
N	5.206239000	-1.566401000	-0.159936000
H	-2.994086000	0.444235000	-0.430273000
O	-2.965220000	-0.539306000	1.397845000
C	-3.950183000	0.292038000	1.840652000
C	-4.462184000	-0.168820000	3.176602000
H	-4.664460000	-1.243125000	3.164934000
H	-3.694000000	0.014323000	3.936115000
H	-5.365107000	0.384381000	3.435562000
O	-4.331998000	1.269314000	1.233322000
O	0.659222000	-1.310393000	2.749804000
C	1.819460000	-0.942567000	2.534953000
N	2.265460000	0.332175000	2.605236000
C	1.378599000	1.419555000	2.991709000
H	1.842251000	2.004721000	3.793592000
H	1.178718000	2.080461000	2.142160000
H	0.437335000	1.001461000	3.347833000
C	3.644185000	0.679053000	2.297960000
H	3.678485000	1.396802000	1.471414000
H	4.130249000	1.128972000	3.171924000
H	4.198658000	-0.216008000	2.008562000
H	2.618261000	-1.656735000	2.275273000

C_{1a}

Pd	1.761781000	0.576708000	-0.876020000
C	4.573969000	-0.949494000	-0.715270000

O	3.818999000	-0.091232000	-1.234291000
C	-6.650950000	0.180017000	-0.110471000
C	-5.755294000	1.242258000	0.481766000
O	-5.924649000	1.725051000	1.580726000
O	-4.711235000	1.706249000	-0.254088000
H	-7.464395000	-0.004950000	0.590449000
H	-7.063345000	0.501610000	-1.071958000
H	-6.107270000	-0.755331000	-0.275336000
C	0.018256000	-1.077577000	3.106417000
C	-0.519914000	-0.240582000	1.976192000
O	-0.921684000	0.899112000	2.080459000
O	-0.468437000	-0.931347000	0.810168000
H	-0.300492000	-0.650223000	4.057936000
H	-0.320094000	-2.112650000	3.023998000
H	1.112673000	-1.074807000	3.067599000
C	-2.858794000	0.853178000	-1.538907000
C	-0.790339000	1.996513000	-1.306125000
C	-2.447014000	-0.021091000	-0.352422000
C	-0.948128000	-0.321567000	-0.421016000
C	-0.166416000	0.905021000	-0.840235000
O	-2.145686000	2.096627000	-1.510786000
C	-4.345405000	1.165096000	-1.536792000
H	-0.285585000	2.920943000	-1.564939000
H	-0.804253000	-1.125790000	-1.146153000
H	-2.619767000	0.332009000	-2.478253000
H	-4.893839000	0.254810000	-1.775772000
H	-4.564122000	1.917719000	-2.299834000
I	2.332688000	2.767534000	0.509307000
H	5.405369000	-1.347232000	-1.309210000
C	5.490524000	-2.402383000	0.999731000
H	6.030258000	-1.972366000	1.849359000
H	4.998234000	-3.325019000	1.321462000
H	6.201724000	-2.634521000	0.205527000
C	3.487540000	-0.999679000	1.478168000
H	3.765028000	-0.029492000	1.900889000
H	2.509098000	-0.903065000	1.000093000
H	3.416855000	-1.738113000	2.276972000
N	4.489694000	-1.452071000	0.514222000
H	-2.697385000	0.480007000	0.579649000
O	-3.186286000	-1.255820000	-0.470952000
C	-3.574902000	-1.879258000	0.673695000
C	-4.276962000	-3.170293000	0.354409000
H	-4.997211000	-3.032942000	-0.456236000
H	-3.535832000	-3.903754000	0.018239000
H	-4.776524000	-3.546957000	1.247077000
O	-3.362507000	-1.444726000	1.785926000
O	0.463776000	-2.556043000	-2.643272000
C	1.194433000	-2.867165000	-1.696007000
N	0.799354000	-3.507756000	-0.575135000
C	-0.588631000	-3.895470000	-0.370761000
H	-0.658388000	-4.978509000	-0.217420000
H	-0.992022000	-3.386361000	0.509540000
H	-1.168871000	-3.616880000	-1.249807000
C	1.729162000	-3.797476000	0.503810000
H	1.438953000	-3.257781000	1.411570000
H	1.735747000	-4.871642000	0.722458000
H	2.737039000	-3.492100000	0.215291000
H	2.275561000	-2.638922000	-1.691365000

DI_{1a}

Pd	1.601644000	-0.064916000	-0.241602000
C	0.251252000	2.545997000	0.406524000
O	0.884492000	1.942910000	-0.501979000
C	-4.312504000	2.278773000	-2.565417000
C	-4.295582000	2.062307000	-1.073379000
O	-4.127155000	2.956529000	-0.267363000
O	-4.539035000	0.820416000	-0.583070000
H	-4.201110000	3.345315000	-2.758608000
H	-3.499289000	1.730246000	-3.044679000
H	-5.256728000	1.930261000	-2.996684000
C	-0.008912000	-1.181704000	3.659112000
C	-0.555456000	-0.735968000	2.330864000
O	-0.843650000	0.408521000	2.041683000
O	-0.653242000	-1.784807000	1.483032000
H	-0.117453000	-0.380091000	4.390101000
H	-0.521975000	-2.082443000	4.004933000
H	1.053624000	-1.423830000	3.542544000
C	-3.062074000	-0.955864000	-1.345824000
C	-0.881921000	0.013445000	-1.724324000
C	-2.583521000	-1.171843000	0.095884000
C	-1.111627000	-1.583555000	0.118366000
C	-0.289939000	-0.623726000	-0.708915000
O	-2.217426000	-0.057981000	-2.072533000
C	-4.469043000	-0.370902000	-1.388847000
H	-0.374128000	0.705653000	-2.384645000
H	-1.041569000	-2.594299000	-0.291638000
H	-3.077837000	-1.926949000	-1.860044000
H	-5.170609000	-1.076238000	-0.939462000
H	-4.772007000	-0.189371000	-2.421871000
I	4.032087000	1.130226000	0.831464000
C	1.627125000	-2.739791000	-2.811999000
C	1.672306000	-2.709205000	-0.455697000
C	3.146818000	-2.786083000	-2.788360000
C	3.689307000	-1.848157000	-1.699123000
C	2.828984000	-1.950892000	-0.443120000
O	1.076662000	-3.188306000	-1.539669000
H	1.193103000	-3.031552000	0.463106000
H	3.726084000	-0.818694000	-2.067254000
H	1.255998000	-1.719449000	-2.971989000
H	3.526309000	-2.506261000	-3.775568000
H	4.717613000	-2.118824000	-1.436820000
H	3.459377000	-3.818598000	-2.593140000
H	3.315348000	-1.889973000	0.525577000
H	1.192668000	-3.407084000	-3.557152000
H	0.427175000	2.335100000	1.461936000
N	-0.663872000	3.473066000	0.155598000
C	-1.322799000	4.202156000	1.236607000
H	-1.130439000	5.275118000	1.132457000
H	-2.400104000	4.022172000	1.187054000
H	-0.941019000	3.866150000	2.202230000
C	-1.033504000	3.843026000	-1.209108000
H	-0.766361000	3.038364000	-1.892479000
H	-2.111008000	4.011328000	-1.242641000
H	-0.513569000	4.760555000	-1.507056000
H	-2.732432000	-0.276364000	0.695263000
O	-3.394945000	-2.252648000	0.603234000
C	-3.795715000	-2.210581000	1.900935000
C	-4.636736000	-3.415703000	2.221554000
H	-4.043645000	-4.325614000	2.084193000
H	-4.988479000	-3.357328000	3.251538000
H	-5.488515000	-3.471877000	1.536978000
O	-3.509064000	-1.320023000	2.672460000

DII_{1a}

Pd	1.625407000	0.074716000	-0.695587000
C	0.676294000	2.662342000	0.553816000
O	0.934397000	2.111481000	-0.548309000
C	-4.812759000	2.290885000	-2.256174000
C	-4.679872000	1.947881000	-0.793153000
O	-4.547492000	2.778993000	0.082318000
O	-4.780297000	0.646323000	-0.411426000
H	-4.830629000	3.376571000	-2.350220000
H	-3.972305000	1.888813000	-2.825309000
H	-5.735954000	1.872944000	-2.670646000
C	0.360318000	-0.569053000	3.355589000
C	-0.405739000	-0.289717000	2.091695000
O	-0.901725000	0.778781000	1.795525000
O	-0.436291000	-1.390081000	1.306471000
H	0.202788000	0.240270000	4.069044000
H	0.056855000	-1.524556000	3.790635000
H	1.426906000	-0.633660000	3.110686000
C	-3.089309000	-0.819525000	-1.363549000
C	-1.036217000	0.311546000	-1.863896000
C	-2.519203000	-1.057522000	0.038283000
C	-1.013749000	-1.330449000	-0.029342000
C	-0.326503000	-0.366702000	-0.957716000
O	-2.409112000	0.256871000	-2.017212000
C	-4.566025000	-0.446800000	-1.323172000
H	-0.609752000	1.018436000	-2.566599000
H	-0.877950000	-2.356428000	-0.375761000
H	-2.975513000	-1.734730000	-1.962709000
H	-5.142408000	-1.284584000	-0.927131000
H	-4.925801000	-0.222596000	-2.329404000
I	4.187224000	0.988793000	0.309321000
C	1.129560000	-4.177494000	-0.871735000
C	1.568268000	-2.162597000	-2.087464000
C	1.881149000	-3.582717000	0.307853000
C	3.084018000	-2.770576000	-0.182708000
C	2.668468000	-1.841122000	-1.303896000
O	0.733957000	-3.168168000	-1.865415000
H	1.338241000	-1.632339000	-3.006565000
H	3.862231000	-3.445104000	-0.566058000
H	1.743408000	-4.907578000	-1.409853000
H	2.201345000	-4.407191000	0.953058000
H	3.532357000	-2.203169000	0.636460000
H	1.211284000	-2.947161000	0.891628000
H	3.440579000	-1.265110000	-1.808279000
H	0.193199000	-4.652392000	-0.575234000
H	1.233079000	2.408648000	1.459712000
N	-0.251162000	3.600558000	0.699313000
C	-0.518622000	4.196578000	2.002056000
H	-0.436173000	5.286269000	1.938325000
H	-1.531587000	3.936979000	2.327046000
H	0.197495000	3.827401000	2.737986000
C	-1.144249000	3.978941000	-0.391746000
H	-2.169029000	3.671897000	-0.154056000
H	-1.120746000	5.064994000	-0.525461000
H	-0.824734000	3.491022000	-1.310948000
O	-3.187935000	-2.228613000	0.552152000
H	-2.720151000	-0.199550000	0.675233000
C	-3.485048000	-2.269925000	1.878140000
C	-4.123614000	-3.586332000	2.226123000

H	-3.390479000	-4.389450000	2.094742000
H	-4.464041000	-3.569192000	3.261413000
O	-3.251306000	-1.369257000	2.655470000
H	-4.962529000	-3.792779000	1.555440000

DIII_{1a}

Pd	-1.739626000	-0.337941000	-0.254887000
C	-1.387031000	2.578793000	-0.727512000
O	-1.429699000	1.489894000	-1.362301000
C	6.731440000	-0.299284000	-0.357806000
C	5.835128000	-1.388084000	0.184352000
O	6.050743000	-1.975328000	1.222654000
O	4.742596000	-1.759739000	-0.533132000
H	7.562200000	-0.170518000	0.335268000
H	7.119425000	-0.570030000	-1.345088000
H	6.202558000	0.652725000	-0.458207000
C	0.476394000	1.557096000	3.231210000
C	0.803725000	0.594746000	2.122699000
O	1.031171000	-0.590650000	2.266679000
O	0.802527000	1.232529000	0.932292000
H	0.503111000	1.038320000	4.189544000
H	1.198337000	2.378897000	3.231631000
H	-0.517869000	1.985462000	3.067920000
C	2.871274000	-0.665916000	-1.609400000
C	0.730229000	-1.678802000	-1.317850000
C	2.592020000	0.092036000	-0.309214000
C	1.125646000	0.513896000	-0.290096000
C	0.222741000	-0.651861000	-0.627052000
O	2.052611000	-1.836898000	-1.687744000
C	4.324718000	-1.091700000	-1.737817000
H	0.154667000	-2.536901000	-1.641552000
H	1.002034000	1.298600000	-1.038611000
H	2.638043000	-0.012887000	-2.464247000
H	4.930256000	-0.212766000	-1.955322000
H	4.424771000	-1.797691000	-2.567380000
I	-4.423578000	0.647830000	0.311765000
C	-1.334384000	-4.556830000	-0.349486000
C	-0.998024000	-2.627483000	1.046086000
C	-2.505178000	-3.816679000	-0.973174000
C	-3.271027000	-3.043245000	0.104469000
C	-2.301669000	-2.167476000	0.878117000
O	-0.474953000	-3.684406000	0.465798000
H	-0.294063000	-2.133177000	1.707122000
H	-3.748033000	-3.747617000	0.800407000
H	-1.675603000	-5.351128000	0.322018000
H	-3.146145000	-4.553583000	-1.467150000
H	-4.068383000	-2.443298000	-0.337904000
H	-2.143620000	-3.123788000	-1.741605000
H	-2.677002000	-1.589846000	1.721019000
H	-0.661720000	-4.986240000	-1.093423000
H	-1.869521000	2.688430000	0.247461000
N	-0.773688000	3.664457000	-1.183171000
C	-0.067689000	3.677195000	-2.461083000
H	-0.514687000	4.428381000	-3.119996000
H	0.983533000	3.932832000	-2.294423000
H	-0.136337000	2.696157000	-2.928264000
C	-0.762306000	4.906177000	-0.415572000
H	0.270814000	5.189896000	-0.190255000
H	-1.231146000	5.707334000	-0.995519000
H	-1.308681000	4.773401000	0.519679000

H	2.834652000	-0.523791000	0.554707000
O	3.421843000	1.273801000	-0.327353000
C	3.921681000	1.721541000	0.855110000
C	4.632594000	3.032477000	0.664217000
H	3.879958000	3.828159000	0.613694000
H	5.290588000	3.221151000	1.512976000
H	5.197035000	3.047857000	-0.270808000
O	3.784084000	1.141441000	1.911678000

DIV_{1a}

Pd	-1.723432000	-0.361232000	-0.286821000
C	-1.625630000	2.699638000	-0.418964000
O	-1.886571000	1.647283000	-1.057310000
C	6.936924000	0.352535000	-0.778427000
C	6.026104000	-0.840157000	-0.945565000
O	6.366472000	-1.981259000	-0.718625000
O	4.758492000	-0.636867000	-1.387436000
H	7.923071000	-0.010837000	-0.490113000
H	7.017315000	0.926343000	-1.707077000
H	6.567312000	1.026462000	0.000829000
C	-0.153784000	-0.452145000	3.837334000
C	-0.085834000	0.360096000	2.575676000
O	-0.853379000	1.264392000	2.292521000
O	0.911363000	-0.059809000	1.774680000
H	-0.792050000	-1.322209000	3.643982000
H	0.831784000	-0.812106000	4.138024000
H	-0.607586000	0.140691000	4.632754000
C	2.783457000	0.726141000	-1.350516000
C	0.786072000	-0.485901000	-1.772848000
C	2.540709000	0.440706000	0.134868000
C	1.053783000	0.542670000	0.456748000
C	0.242948000	-0.176450000	-0.590597000
O	2.083133000	-0.226692000	-2.158757000
C	4.252853000	0.666587000	-1.723445000
H	0.250610000	-1.004580000	-2.561954000
H	0.769522000	1.595816000	0.538859000
H	2.415126000	1.735927000	-1.586762000
H	4.775927000	1.464026000	-1.193860000
H	4.367779000	0.826170000	-2.800143000
I	-4.582105000	-0.256166000	0.196292000
C	0.322664000	-3.714699000	-1.144613000
C	-1.803423000	-2.625671000	-0.861710000
C	0.144113000	-4.182311000	0.288736000
C	-0.361015000	-3.021108000	1.157968000
C	-1.596226000	-2.421388000	0.504600000
O	-0.914954000	-3.162872000	-1.701462000
H	-2.782732000	-2.525974000	-1.322371000
H	0.430114000	-2.280530000	1.280817000
H	1.090017000	-2.940465000	-1.211009000
H	1.107377000	-4.556684000	0.649471000
H	-0.626352000	-3.374812000	2.158515000
H	-0.569670000	-5.014198000	0.317047000
H	-2.495398000	-2.343475000	1.108726000
H	0.580315000	-4.531870000	-1.821247000
H	-1.354511000	2.662112000	0.639287000
N	-1.652823000	3.911154000	-0.966093000
C	-1.998076000	4.122190000	-2.368425000
H	-2.917102000	4.713513000	-2.437960000
H	-1.189625000	4.667623000	-2.865500000
H	-2.145878000	3.161434000	-2.859282000

C	-1.352131000	5.101319000	-0.177678000
H	-0.498443000	5.629377000	-0.614784000
H	-2.216300000	5.773590000	-0.170752000
H	-1.110381000	4.819913000	0.848705000
H	2.914492000	-0.552760000	0.385201000
O	3.234012000	1.436680000	0.910199000
C	4.228325000	1.035049000	1.748573000
C	4.794450000	2.217218000	2.484596000
H	3.998369000	2.737213000	3.025942000
H	5.563990000	1.884323000	3.180873000
H	5.223705000	2.926537000	1.769777000
O	4.596516000	-0.114745000	1.863577000

TS2I_{1a}

Pd	1.756976000	-0.097064000	-0.270203000
C	-0.296553000	2.157743000	-1.083356000
O	0.456951000	1.267902000	-1.540819000
C	-6.385272000	-0.076761000	-0.766719000
C	-5.115820000	0.548161000	-1.288022000
O	-5.048529000	1.701426000	-1.666285000
O	-3.995473000	-0.208943000	-1.356367000
H	-7.197807000	0.636882000	-0.900864000
H	-6.623898000	-1.006703000	-1.291598000
H	-6.284115000	-0.303505000	0.299196000
C	0.777965000	0.750034000	3.600437000
C	-0.055688000	0.403662000	2.397481000
O	-0.596086000	1.215290000	1.671482000
O	-0.104777000	-0.935158000	2.225202000
H	0.528112000	1.754558000	3.943850000
H	0.643940000	0.023677000	4.404871000
H	1.830914000	0.733609000	3.295059000
C	-2.595249000	-1.953332000	-0.475970000
C	-0.389071000	-1.679348000	-1.385641000
C	-2.095966000	-1.083431000	0.690389000
C	-0.682901000	-1.547120000	1.047666000
C	0.191248000	-1.453455000	-0.187247000
O	-1.713638000	-1.877940000	-1.616896000
C	-3.988907000	-1.585021000	-0.944679000
H	0.165977000	-1.717389000	-2.317147000
H	-0.759299000	-2.591411000	1.370727000
H	-2.629950000	-2.999474000	-0.144286000
H	-4.684922000	-1.773705000	-0.125581000
H	-4.270132000	-2.217653000	-1.792600000
I	3.554133000	2.003344000	0.362276000
C	2.950847000	-3.197585000	-1.881750000
C	1.903003000	-2.679337000	0.169554000
C	4.311018000	-2.966525000	-1.246869000
C	4.245266000	-1.749181000	-0.312504000
C	2.905416000	-1.669289000	0.443689000
O	1.993838000	-3.539410000	-0.847260000
H	1.345937000	-3.106854000	0.997926000
H	4.403903000	-0.839615000	-0.897481000
H	2.588748000	-2.300274000	-2.403598000
H	5.061837000	-2.817857000	-2.028938000
H	5.055324000	-1.785116000	0.423868000
H	4.583937000	-3.872124000	-0.692423000
H	2.983680000	-1.463475000	1.512366000
H	2.937580000	-4.043199000	-2.570498000
H	-0.047346000	2.707114000	-0.171169000
N	-1.449603000	2.500864000	-1.657002000

C	-2.245890000	3.619359000	-1.164482000
H	-2.256416000	4.430587000	-1.901853000
H	-3.271697000	3.284613000	-0.991206000
H	-1.821090000	3.996032000	-0.231664000
C	-1.899023000	1.834951000	-2.878259000
H	-1.486353000	2.334570000	-3.763327000
H	-1.572546000	0.795367000	-2.864054000
H	-2.987725000	1.865008000	-2.906909000
H	-2.128160000	-0.029246000	0.428821000
O	-2.931863000	-1.341062000	1.835310000
C	-3.842841000	-0.402133000	2.206164000
C	-4.529381000	-0.818032000	3.477236000
H	-3.789751000	-0.977457000	4.267586000
H	-5.239540000	-0.048355000	3.778989000
H	-5.054179000	-1.765843000	3.320125000
O	-4.065536000	0.612744000	1.580240000

TS2II_{1a}

Pd	1.791997000	0.082185000	-0.621699000
C	0.253783000	2.728513000	0.167813000
O	0.581757000	1.993170000	-0.788689000
C	-6.373481000	0.682210000	-0.434721000
C	-5.068135000	1.417021000	-0.608130000
O	-4.895936000	2.567429000	-0.258722000
O	-4.032081000	0.776302000	-1.202704000
H	-7.115612000	1.387365000	-0.061002000
H	-6.720426000	0.250608000	-1.378438000
H	-6.256306000	-0.128421000	0.290558000
C	0.746441000	-0.616874000	3.257995000
C	-0.115828000	-0.429602000	2.039076000
O	-0.649782000	0.614568000	1.722073000
O	-0.196156000	-1.585162000	1.339548000
H	0.543704000	0.176447000	3.978347000
H	0.590400000	-1.597408000	3.713189000
H	1.794849000	-0.551740000	2.943527000
C	-2.739956000	-1.220726000	-1.483731000
C	-0.543296000	-0.580512000	-2.190822000
C	-2.198604000	-1.145108000	-0.051743000
C	-0.760658000	-1.664337000	0.005809000
C	0.087543000	-1.026559000	-1.074436000
O	-1.871854000	-0.549949000	-2.422673000
C	-4.116062000	-0.595764000	-1.621143000
H	-0.002983000	-0.188670000	-3.047716000
H	-0.792260000	-2.745932000	-0.152235000
H	-2.811444000	-2.273297000	-1.787341000
H	-4.821362000	-1.171131000	-1.019764000
H	-4.436772000	-0.634701000	-2.666716000
I	4.028934000	1.451300000	0.341258000
C	1.708682000	-4.217454000	-0.101990000
C	1.601141000	-2.349498000	-1.666414000
C	2.478937000	-3.302300000	0.835175000
C	3.467604000	-2.447030000	0.043654000
C	2.755925000	-1.688845000	-1.069922000
O	1.132925000	-3.541385000	-1.267916000
H	1.427070000	-2.203972000	-2.726301000
H	4.223685000	-3.100634000	-0.417006000
H	2.361958000	-4.996653000	-0.510403000
H	2.998867000	-3.935193000	1.562267000
H	4.003419000	-1.758252000	0.700861000
H	1.784857000	-2.664822000	1.384199000
H	3.423120000	-1.300468000	-1.845565000

H	0.862675000	-4.698862000	0.393787000
H	0.832917000	2.749801000	1.096673000
N	-0.795087000	3.553027000	0.146186000
C	-1.147210000	4.361821000	1.304281000
H	-1.186025000	5.421128000	1.028058000
H	-2.130335000	4.063309000	1.685258000
H	-0.405147000	4.229461000	2.094310000
C	-1.695047000	3.617297000	-1.000935000
H	-2.707565000	3.329590000	-0.700286000
H	-1.713383000	4.638318000	-1.398753000
H	-1.341706000	2.933535000	-1.771777000
H	-2.264320000	-0.128801000	0.325748000
O	-2.993441000	-2.034585000	0.762110000
C	-3.876770000	-1.503664000	1.647440000
C	-4.515753000	-2.594317000	2.461196000
H	-5.264611000	-2.166157000	3.127311000
H	-4.979209000	-3.332063000	1.799245000
H	-3.749358000	-3.112696000	3.046285000
O	-4.105929000	-0.316126000	1.748369000

TS2III_{1a}

Pd	-1.941287000	-0.149623000	-0.177412000
C	-1.143138000	2.822936000	-0.366796000
O	-1.112127000	1.785958000	-1.071993000
C	6.441613000	0.377457000	-1.439031000
C	5.728088000	-0.941046000	-1.260068000
O	6.251046000	-1.928579000	-0.791274000
O	4.428104000	-1.043333000	-1.645648000
H	7.486422000	0.234941000	-1.164534000
H	6.380053000	0.731797000	-2.472453000
H	6.010971000	1.149880000	-0.792681000
C	1.757739000	-1.174884000	4.024434000
C	1.601006000	-1.288987000	2.533509000
O	1.943853000	-2.238999000	1.858745000
O	1.012226000	-0.175061000	2.031494000
H	2.056425000	-2.138651000	4.437347000
H	2.532546000	-0.431283000	4.237350000
H	0.827877000	-0.834992000	4.488559000
C	2.300383000	0.070466000	-1.536083000
C	0.405710000	-1.343100000	-1.379382000
C	2.368442000	0.056714000	-0.009146000
C	0.959688000	0.045038000	0.592002000
C	0.013797000	-0.858050000	-0.178746000
O	1.578298000	-1.084937000	-2.006550000
C	3.675208000	0.061236000	-2.177316000
H	-0.188067000	-2.041666000	-1.959134000
H	0.592503000	1.070729000	0.547157000
H	1.768048000	0.965427000	-1.879663000
H	4.150998000	1.022221000	-1.980787000
H	3.579128000	-0.069130000	-3.259459000
I	-4.512899000	0.941304000	0.029471000
C	-1.529604000	-4.223978000	-0.878945000
C	-1.026442000	-2.470035000	0.745156000
C	-2.750835000	-3.406464000	-1.268728000
C	-3.396682000	-2.812440000	-0.015531000
C	-2.382403000	-1.946164000	0.718165000
O	-0.667330000	-3.590320000	0.119328000
H	-0.422843000	-2.319452000	1.628745000
H	-3.713501000	-3.629008000	0.651352000
H	-1.829982000	-5.175554000	-0.428648000

H	-3.440272000	-4.070210000	-1.800353000
H	-4.290116000	-2.236594000	-0.264210000
H	-2.472846000	-2.600849000	-1.957490000
H	-2.692253000	-1.593415000	1.706322000
H	-0.882278000	-4.436176000	-1.733646000
H	-1.933410000	2.978777000	0.377611000
N	-0.248373000	3.808191000	-0.448752000
C	0.882761000	3.733567000	-1.369301000
H	1.057315000	4.721340000	-1.803862000
H	1.784986000	3.411698000	-0.837355000
H	0.660482000	3.022690000	-2.164420000
C	-0.296642000	4.958584000	0.447240000
H	0.617185000	4.998330000	1.049914000
H	-0.375318000	5.883495000	-0.133093000
H	-1.157318000	4.881522000	1.114075000
H	2.946349000	-0.801974000	0.323353000
O	3.030447000	1.280666000	0.376641000
C	3.918872000	1.234976000	1.406764000
C	4.485729000	2.601926000	1.666767000
H	3.684506000	3.270386000	1.999197000
H	5.255997000	2.541872000	2.435490000
H	4.903022000	3.021046000	0.746516000
O	4.191118000	0.222412000	2.016668000

TS2IV_{1a}

Pd	-1.810485000	-0.199883000	-0.667535000
C	-1.766596000	2.763015000	0.306846000
O	-2.053772000	2.045445000	-0.679510000
C	6.720933000	0.404983000	-0.743632000
C	5.705657000	-0.384477000	-1.533175000
O	5.889331000	-1.515881000	-1.925498000
O	4.518430000	0.202191000	-1.845223000
H	7.637064000	-0.182505000	-0.687482000
H	6.933769000	1.369730000	-1.214050000
H	6.361479000	0.594111000	0.272375000
C	0.132481000	-1.371926000	3.595541000
C	-0.021306000	-0.356997000	2.497888000
O	-0.759591000	0.608081000	2.532718000
O	0.803312000	-0.641837000	1.461651000
H	-0.666630000	-1.249847000	4.326787000
H	0.127045000	-2.389165000	3.196655000
H	1.100763000	-1.214402000	4.084026000
C	2.697964000	1.482409000	-0.961880000
C	0.781192000	0.469677000	-2.017374000
C	2.451252000	0.449585000	0.142648000
C	0.959878000	0.335399000	0.412482000
C	0.243326000	-0.029319000	-0.871225000
O	1.902642000	1.206018000	-2.139423000
C	4.152029000	1.517682000	-1.399213000
H	0.351391000	0.280577000	-2.997033000
H	0.587076000	1.292322000	0.787981000
H	2.421471000	2.477907000	-0.594523000
H	4.755899000	1.860758000	-0.557957000
H	4.276465000	2.219683000	-2.229044000
I	-4.532940000	-0.622152000	-0.152618000
C	0.986412000	-3.484426000	0.298962000
C	0.005772000	-2.022843000	-1.364487000
C	-0.392038000	-4.105897000	0.457852000
C	-1.470915000	-3.012154000	0.445572000
C	-1.345648000	-2.192911000	-0.835933000

O	1.088418000	-2.671066000	-0.908636000
H	0.084818000	-1.872972000	-2.435536000
H	-1.352252000	-2.383110000	1.331697000
H	1.244982000	-2.851275000	1.148964000
H	-0.409115000	-4.668956000	1.397205000
H	-2.474890000	-3.440606000	0.503110000
H	-0.568828000	-4.817179000	-0.358463000
H	-2.016641000	-2.516515000	-1.637799000
H	1.764018000	-4.240988000	0.172786000
H	-1.511358000	2.318356000	1.274432000
N	-1.734849000	4.097619000	0.278662000
C	-2.039836000	4.853921000	-0.929512000
H	-2.902933000	5.504676000	-0.753188000
H	-1.181364000	5.476648000	-1.203052000
H	-2.264398000	4.165571000	-1.743232000
C	-1.404794000	4.867203000	1.472225000
H	-0.529558000	5.497546000	1.281757000
H	-2.246148000	5.510979000	1.750389000
H	-1.183714000	4.192520000	2.301607000
H	2.858196000	-0.523454000	-0.134860000
O	3.103490000	0.936563000	1.327532000
C	4.026184000	0.132415000	1.926064000
C	4.500553000	0.752064000	3.209782000
H	3.663338000	0.821887000	3.912127000
H	5.293855000	0.142459000	3.641838000
H	4.863856000	1.767383000	3.025872000
O	4.397665000	-0.927164000	1.466982000

El_{1a}

Pd	-2.726126000	0.202209000	0.281516000
O	-1.411743000	-1.452421000	0.269617000
C	-0.440771000	-1.532093000	1.075428000
C	6.287812000	-2.172605000	-0.824620000
C	4.956327000	-2.460879000	-0.177198000
O	4.837311000	-3.030955000	0.887337000
O	3.817001000	-2.078453000	-0.811770000
H	7.063357000	-2.659863000	-0.234388000
H	6.322008000	-2.542284000	-1.853665000
H	6.487980000	-1.095988000	-0.844947000
C	2.126384000	2.823890000	2.934665000
C	1.805781000	1.909545000	1.785961000
O	1.368766000	0.779043000	1.886708000
O	2.066044000	2.518451000	0.608206000
H	1.799376000	2.369043000	3.869775000
H	3.207965000	2.989852000	2.964027000
H	1.642794000	3.795099000	2.796566000
C	2.797010000	-0.205076000	-1.930113000
C	0.467016000	0.065607000	-1.581335000
C	3.000247000	0.644950000	-0.675745000
C	1.977909000	1.775949000	-0.644055000
C	0.603640000	1.257627000	-0.985920000
O	1.481125000	-0.781670000	-1.917481000
C	3.809517000	-1.329600000	-2.042705000
H	-0.496943000	-0.339387000	-1.861428000
H	2.279634000	2.541264000	-1.366716000
H	2.891554000	0.424465000	-2.826261000
H	4.784268000	-0.897086000	-2.264973000
H	3.526181000	-2.003133000	-2.856356000
I	-5.104035000	-1.347824000	0.014446000
C	-2.629553000	2.864505000	-1.930206000

C	-0.595170000	2.152775000	-0.758212000
C	-2.948860000	3.515358000	-0.589869000
C	-2.737872000	2.516675000	0.547411000
C	-1.449369000	1.785956000	0.451414000
O	-1.356127000	2.189437000	-1.972381000
H	-0.206372000	3.165424000	-0.540326000
H	-3.636327000	1.731664000	0.425185000
H	-3.403115000	2.117078000	-2.157441000
H	-3.975994000	3.890644000	-0.609183000
H	-2.958873000	2.910042000	1.542381000
H	-2.287028000	4.371189000	-0.410476000
H	-0.874301000	1.668793000	1.368527000
H	-2.637785000	3.614982000	-2.729863000
H	-0.358982000	-0.867573000	1.935800000
N	0.541160000	-2.412653000	0.951987000
C	0.599157000	-3.368377000	-0.150395000
H	1.561639000	-3.266385000	-0.655728000
H	0.497881000	-4.386606000	0.240482000
H	-0.207884000	-3.166628000	-0.852275000
C	1.580648000	-2.522125000	1.974370000
H	1.428342000	-3.433755000	2.563555000
H	2.561213000	-2.573609000	1.495193000
H	1.547269000	-1.652242000	2.630969000
H	2.900155000	0.017692000	0.207731000
O	4.328974000	1.196161000	-0.747016000
C	5.064558000	1.233927000	0.396452000
C	6.409590000	1.851233000	0.134144000
H	7.067008000	1.673939000	0.985375000
H	6.851989000	1.449546000	-0.780947000
H	6.282112000	2.930569000	-0.005646000
O	4.664200000	0.835583000	1.470400000

EH_{1a}

Pd	2.826475000	-0.043272000	-0.737381000
C	0.663276000	1.673758000	0.324589000
O	1.450276000	1.565443000	-0.658966000
C	-6.395568000	2.106946000	-0.247354000
C	-4.959064000	2.398886000	0.107942000
O	-4.625761000	3.073790000	1.059838000
O	-3.972408000	1.895977000	-0.677891000
H	-7.034245000	2.702218000	0.404791000
H	-6.608507000	2.350192000	-1.292428000
H	-6.626406000	1.047209000	-0.093113000
C	-1.050664000	-2.578292000	2.997531000
C	-1.278366000	-1.707881000	1.792845000
O	-1.058138000	-0.514717000	1.737683000
O	-1.772558000	-2.443003000	0.771728000
H	-0.767631000	-1.961843000	3.851144000
H	-1.952181000	-3.151907000	3.231475000
H	-0.249814000	-3.289871000	2.773337000
C	-3.143875000	-0.041067000	-1.817993000
C	-0.763352000	-0.108312000	-1.842910000
C	-3.059605000	-0.800633000	-0.496525000
C	-1.937619000	-1.834595000	-0.535080000
C	-0.679162000	-1.241354000	-1.130077000
O	-1.893412000	0.607053000	-2.095065000
C	-4.222655000	1.026140000	-1.799217000
H	0.090954000	0.370248000	-2.300788000
H	-2.267321000	-2.686728000	-1.139420000
H	-3.366492000	-0.739892000	-2.636609000

H	-5.194541000	0.536494000	-1.731640000
H	-4.182946000	1.617024000	-2.718848000
I	4.782061000	1.242600000	0.874043000
C	3.061483000	-2.197051000	-1.555676000
C	0.598569000	-2.044996000	-1.059539000
C	2.896483000	-3.459607000	-0.706159000
C	2.016633000	-3.211525000	0.526354000
H	0.370804000	-3.035339000	-1.502381000
H	2.622321000	-2.811234000	1.346348000
H	3.813187000	-1.491829000	-0.933599000
H	3.864845000	-3.855935000	-0.388658000
H	1.571387000	-4.159161000	0.860398000
H	2.434724000	-4.212345000	-1.354933000
H	3.665377000	-2.351993000	-2.452634000
H	0.779001000	1.061203000	1.219812000
N	-0.354700000	2.522693000	0.353153000
C	-1.182657000	2.667360000	1.549410000
H	-0.984121000	3.636242000	2.021988000
H	-2.238939000	2.624663000	1.270893000
H	-0.962757000	1.863431000	2.250815000
C	-0.689551000	3.380691000	-0.779523000
H	-0.005396000	3.185179000	-1.603482000
H	-1.714088000	3.166908000	-1.093324000
H	-0.611109000	4.431387000	-0.480903000
C	1.793492000	-1.471281000	-1.803114000
H	1.608243000	-1.149329000	-2.827691000
O	0.977027000	-2.240215000	0.313987000
O	-4.317302000	-1.480143000	-0.317773000
H	-2.891112000	-0.101007000	0.318515000
C	-4.935357000	-1.373153000	0.889518000
C	-6.219224000	-2.155247000	0.886996000
H	-6.781414000	-1.943913000	1.796625000
H	-6.817621000	-1.909582000	0.005360000
H	-5.987999000	-3.225025000	0.841426000
O	-4.492683000	-0.740973000	1.825031000

EIII_{1a}

Pd	2.610222000	0.560549000	0.337115000
O	1.424416000	-0.999824000	1.150957000
C	1.023574000	-1.948798000	0.426105000
C	-4.273966000	-2.917041000	-2.894762000
C	-4.985366000	-1.753498000	-2.247832000
O	-5.716991000	-0.995474000	-2.847206000
O	-4.850161000	-1.563602000	-0.905681000
H	-4.540928000	-2.931470000	-3.951266000
H	-3.190880000	-2.821999000	-2.792751000
H	-4.577773000	-3.862235000	-2.432567000
C	-2.851189000	4.338736000	0.881713000
C	-2.594899000	3.027464000	0.192917000
O	-2.977574000	2.719236000	-0.916077000
O	-1.855505000	2.216630000	0.994920000
H	-1.913373000	4.769827000	1.243717000
H	-3.340930000	5.028278000	0.193961000
H	-3.495665000	4.161017000	1.748102000
C	-2.596219000	-1.365680000	-0.011370000
C	-1.078175000	-0.304825000	-1.529623000
C	-2.883070000	0.032384000	0.541119000
C	-1.592812000	0.847918000	0.586121000
C	-0.829879000	0.720583000	-0.708748000
O	-2.010831000	-1.285793000	-1.320075000

C	-3.842647000	-2.227876000	-0.126255000
H	-0.554047000	-0.452235000	-2.465047000
H	-0.979899000	0.475171000	1.413434000
H	-1.892905000	-1.871879000	0.658597000
H	-4.270801000	-2.372020000	0.867677000
H	-3.582356000	-3.207144000	-0.532094000
I	4.983748000	-0.981752000	0.136547000
C	1.915119000	2.284101000	-2.687585000
C	0.220728000	1.760769000	-1.021537000
C	2.321552000	3.359151000	-1.678704000
C	2.389023000	2.801069000	-0.255454000
C	1.195628000	2.008564000	0.122443000
O	0.913741000	1.367722000	-2.202292000
H	-0.303198000	2.718270000	-1.205377000
H	2.691823000	3.537585000	0.491670000
H	1.550868000	2.755691000	-3.609676000
H	1.582093000	4.168073000	-1.665298000
H	3.346697000	2.075512000	-0.253322000
H	3.276851000	3.794492000	-1.984105000
H	2.784218000	1.666127000	-2.941062000
H	0.730039000	2.236071000	1.081128000
H	1.242333000	-1.986131000	-0.644192000
N	0.311242000	-2.970125000	0.891953000
C	-0.030034000	-3.090363000	2.307348000
H	0.206487000	-2.160809000	2.822870000
H	-1.098917000	-3.302099000	2.405555000
H	0.535570000	-3.913577000	2.756090000
C	-0.109208000	-4.060011000	0.015697000
H	0.199533000	-3.854453000	-1.010333000
H	0.343540000	-4.999507000	0.347910000
H	-1.198474000	-4.161259000	0.049605000
H	-3.634240000	0.534849000	-0.065391000
O	-3.371161000	-0.158049000	1.883579000
C	-4.333883000	0.686873000	2.340199000
C	-4.711921000	0.331530000	3.750757000
H	-5.473334000	1.021953000	4.113315000
H	-5.091121000	-0.694629000	3.787030000
H	-3.828481000	0.379399000	4.394966000
O	-4.808989000	1.589317000	1.683575000

EIV_{1a}

Pd	2.712053000	0.333664000	-0.439841000
O	1.694464000	-1.308246000	0.432289000
C	1.242464000	-2.313031000	-0.174747000
C	-3.468717000	-3.776672000	-1.889154000
C	-4.496229000	-2.718695000	-1.566706000
O	-5.345580000	-2.347142000	-2.347621000
O	-4.512653000	-2.173725000	-0.318861000
H	-3.653429000	-4.127649000	-2.904296000
H	-2.456804000	-3.372305000	-1.819006000
H	-3.547221000	-4.620304000	-1.195665000
C	-3.838488000	4.221178000	-0.623393000
C	-3.191595000	2.867326000	-0.736087000
O	-3.219902000	2.150864000	-1.716442000
O	-2.571166000	2.550790000	0.423975000
H	-3.127104000	4.957210000	-0.238661000
H	-4.215417000	4.533461000	-1.597595000
H	-4.668021000	4.152836000	0.087761000
C	-2.443183000	-1.224169000	0.544681000
C	-0.895066000	-0.312230000	-0.995391000

C	-3.081686000	0.162859000	0.616704000
C	-1.989025000	1.231320000	0.593798000
C	-0.915689000	0.891336000	-0.414222000
O	-1.750780000	-1.339785000	-0.709761000
C	-3.446749000	-2.360332000	0.626506000
H	-0.188660000	-0.599704000	-1.763734000
H	-1.551418000	1.302458000	1.592634000
H	-1.716180000	-1.346903000	1.358979000
H	-3.912593000	-2.351175000	1.613483000
H	-2.938542000	-3.317334000	0.495073000
I	5.238181000	-0.545126000	0.585349000
C	2.530254000	2.401113000	-1.400413000
C	0.079819000	1.970960000	-0.756578000
C	2.524218000	3.563636000	-0.379410000
C	1.109431000	3.892603000	0.096264000
H	-0.417395000	2.671122000	-1.458062000
H	0.556142000	4.448261000	-0.677284000
H	2.876184000	2.682434000	-2.400425000
H	2.979605000	4.451494000	-0.828872000
H	1.139699000	4.508135000	0.999004000
H	3.132785000	3.291774000	0.487122000
H	3.497333000	1.732883000	-1.143846000
H	1.345190000	-2.419827000	-1.258641000
N	0.612019000	-3.313313000	0.430956000
C	0.387312000	-3.328239000	1.873194000
H	-0.682538000	-3.443894000	2.072678000
H	0.922795000	-4.171242000	2.321936000
H	0.742908000	-2.396681000	2.310275000
C	0.088045000	-4.446234000	-0.324393000
H	0.300924000	-4.322490000	-1.387633000
H	0.550420000	-5.373853000	0.027691000
H	-0.994660000	-4.513982000	-0.182160000
C	1.347088000	1.505521000	-1.449505000
H	1.160510000	1.049392000	-2.423948000
O	0.389142000	2.703722000	0.429807000
H	-3.760723000	0.289678000	-0.224625000
O	-3.810675000	0.248669000	1.854971000
C	-4.980426000	0.942028000	1.851970000
C	-5.602373000	0.918113000	3.220227000
H	-6.528494000	1.492746000	3.215284000
H	-5.808477000	-0.115669000	3.515293000
H	-4.906016000	1.338227000	3.952560000
O	-5.441521000	1.489460000	0.872528000

TS3I_{1a}

Pd	-2.853295000	0.288039000	0.296555000
O	-1.449496000	-1.369416000	0.427813000
C	-0.466162000	-1.408681000	1.212717000
C	6.193659000	-2.346085000	-0.855638000
C	4.878435000	-2.536299000	-0.142681000
O	4.775999000	-3.051416000	0.951199000
O	3.733942000	-2.126900000	-0.749977000
H	6.968483000	-2.846479000	-0.275442000
H	6.164867000	-2.761198000	-1.867234000
H	6.445283000	-1.282737000	-0.932408000
C	2.301061000	2.984075000	2.790491000
C	1.900541000	2.028567000	1.701956000
O	1.432226000	0.919712000	1.877124000
O	2.135970000	2.567186000	0.485516000
H	1.924546000	2.629610000	3.750234000

H	3.394716000	3.031733000	2.824624000
H	1.927392000	3.989822000	2.581284000
C	2.724412000	-0.293711000	-1.934863000
C	0.412078000	0.040651000	-1.522735000
C	2.981088000	0.607396000	-0.726421000
C	1.987298000	1.762771000	-0.722187000
C	0.591902000	1.254798000	-0.986244000
O	1.396885000	-0.838449000	-1.862144000
C	3.710028000	-1.444115000	-2.018472000
H	-0.568924000	-0.360717000	-1.741800000
H	2.279745000	2.481684000	-1.494537000
H	2.808714000	0.291843000	-2.861263000
H	4.686672000	-1.041944000	-2.286280000
H	3.392470000	-2.151624000	-2.789643000
I	-4.963705000	-1.455824000	-0.071818000
C	-2.603488000	2.985554000	-1.850860000
C	-0.578944000	2.177619000	-0.735048000
C	-2.956605000	3.522129000	-0.460692000
C	-2.620802000	2.537456000	0.634182000
C	-1.392616000	1.863047000	0.516307000
O	-1.411718000	2.176915000	-1.901762000
H	-0.168728000	3.191847000	-0.576068000
H	-3.905331000	1.408166000	0.219789000
H	-3.419231000	2.344958000	-2.205772000
H	-4.008773000	3.817737000	-0.443183000
H	-3.041271000	2.722255000	1.619997000
H	-2.363872000	4.421359000	-0.240710000
H	-0.841268000	1.574772000	1.406183000
H	-2.493990000	3.821252000	-2.554247000
H	-0.360014000	-0.693893000	2.031274000
N	0.514725000	-2.299977000	1.125232000
C	0.540133000	-3.325887000	0.087542000
H	1.501881000	-3.284837000	-0.427679000
H	0.412143000	-4.315237000	0.540987000
H	-0.264901000	-3.145958000	-0.622613000
C	1.574319000	-2.353651000	2.130552000
H	1.422521000	-3.216954000	2.789191000
H	2.543390000	-2.457134000	1.636373000
H	1.570379000	-1.437915000	2.722292000
H	2.887740000	0.024269000	0.187635000
O	4.319451000	1.122257000	-0.855823000
C	5.093878000	1.172229000	0.261026000
C	6.445044000	1.744654000	-0.063267000
H	7.121274000	1.588070000	0.777177000
H	6.851943000	1.291413000	-0.970895000
H	6.340263000	2.819522000	-0.248700000
O	4.719888000	0.815099000	1.358759000

TS3II_{1a}

Pd	-2.958016000	0.170084000	-0.704080000
C	-0.710961000	-1.598453000	0.265030000
O	-1.459317000	-1.403715000	-0.728920000
C	6.332058000	-2.139217000	-0.236847000
C	4.881705000	-2.428519000	0.059601000
O	4.510964000	-3.150134000	0.961944000
O	3.927245000	-1.874938000	-0.731536000
H	6.943643000	-2.762641000	0.415029000
H	6.576659000	-2.350116000	-1.282264000
H	6.566551000	-1.088528000	-0.039371000
C	0.987657000	2.513203000	3.061352000

C	1.273065000	1.674553000	1.846429000
O	1.098563000	0.475159000	1.765076000
O	1.764970000	2.446318000	0.850265000
H	0.758056000	1.868484000	3.910203000
H	1.839861000	3.157087000	3.296213000
H	0.129120000	3.157936000	2.847571000
C	3.161603000	0.124495000	-1.806331000
C	0.779453000	0.206391000	-1.850295000
C	3.072307000	0.848667000	-0.464126000
C	1.950217000	1.882606000	-0.475010000
C	0.695162000	1.313043000	-1.097967000
O	1.908449000	-0.499246000	-2.125510000
C	4.223233000	-0.960417000	-1.803889000
H	-0.075136000	-0.256849000	-2.322550000
H	2.283878000	2.756762000	-1.044692000
H	3.407318000	0.844944000	-2.599084000
H	5.201436000	-0.491543000	-1.691301000
H	4.199884000	-1.509085000	-2.749949000
I	-4.648024000	-1.379341000	0.827302000
C	-2.980787000	2.292278000	-1.532662000
C	-0.577212000	2.115396000	-0.986298000
C	-2.960962000	3.426343000	-0.531648000
C	-1.997897000	3.182100000	0.648880000
H	-0.336339000	3.142499000	-1.325405000
H	-2.550263000	2.803352000	1.513327000
H	-4.092466000	1.200537000	-0.696471000
H	-3.963134000	3.650971000	-0.158105000
H	-1.518063000	4.128439000	0.935525000
H	-2.631403000	4.303789000	-1.104363000
H	-3.734767000	2.349962000	-2.314084000
H	-0.845083000	-1.047330000	1.198295000
N	0.292775000	-2.469008000	0.273078000
C	1.070286000	-2.712995000	1.485691000
H	0.818347000	-3.697847000	1.896477000
H	2.137435000	-2.696184000	1.247295000
H	0.855684000	-1.940948000	2.224046000
C	0.636987000	-3.271991000	-0.895966000
H	-0.023648000	-3.016131000	-1.722712000
H	1.673062000	-3.066934000	-1.175805000
H	0.527059000	-4.335610000	-0.657917000
C	-1.767488000	1.637680000	-1.805774000
H	-1.599728000	1.223605000	-2.796387000
O	-0.992726000	2.191302000	0.389530000
O	4.320265000	1.540921000	-0.260080000
H	2.908589000	0.127155000	0.331975000
C	5.054730000	1.229602000	0.840630000
C	6.301297000	2.067814000	0.889424000
H	6.875023000	1.824399000	1.783486000
H	6.906157000	1.878905000	-0.003173000
H	6.038339000	3.129993000	0.890160000
O	4.739309000	0.381798000	1.649455000

TS3III_{1a}

Pd	2.728167000	0.638838000	0.254908000
O	1.429806000	-0.892974000	1.112371000
C	1.046971000	-1.864829000	0.415762000
C	-4.336790000	-2.878414000	-2.918031000
C	-5.040406000	-1.733522000	-2.230723000
O	-5.794014000	-0.971255000	-2.796578000
O	-4.871438000	-1.566262000	-0.889595000

H	-4.631750000	-2.874412000	-3.967198000
H	-3.252099000	-2.776156000	-2.842243000
H	-4.621094000	-3.834992000	-2.466973000
C	-2.838535000	4.313874000	0.960286000
C	-2.595856000	3.015040000	0.243859000
O	-2.996651000	2.727304000	-0.864240000
O	-1.845862000	2.188358000	1.019363000
H	-1.896420000	4.728367000	1.330186000
H	-3.323514000	5.022407000	0.288636000
H	-3.483575000	4.123530000	1.823717000
C	-2.599781000	-1.374635000	-0.039772000
C	-1.107199000	-0.286497000	-1.562488000
C	-2.882064000	0.013423000	0.539009000
C	-1.590992000	0.827163000	0.581343000
C	-0.846393000	0.723463000	-0.726359000
O	-2.035248000	-1.272156000	-1.356324000
C	-3.843697000	-2.240682000	-0.146106000
H	-0.597303000	-0.416318000	-2.508492000
H	-0.965824000	0.437109000	1.391584000
H	-1.883636000	-1.886717000	0.611336000
H	-4.249710000	-2.406872000	0.853580000
H	-3.587092000	-3.210099000	-0.577022000
I	4.883668000	-1.076439000	0.171599000
C	1.920989000	2.278406000	-2.680651000
C	0.191973000	1.774339000	-1.042202000
C	2.381055000	3.321612000	-1.653895000
C	2.287922000	2.824867000	-0.228991000
C	1.145850000	2.074549000	0.108136000
O	0.913153000	1.368786000	-2.201795000
H	-0.340277000	2.720159000	-1.258837000
H	2.771709000	3.428421000	0.535245000
H	1.550435000	2.784304000	-3.581718000
H	1.724740000	4.201991000	-1.693672000
H	3.652307000	1.750381000	-0.280419000
H	3.388838000	3.660679000	-1.906326000
H	2.768736000	1.647062000	-2.966547000
H	0.733112000	2.144618000	1.110915000
H	1.267370000	-1.925238000	-0.654294000
N	0.349663000	-2.891837000	0.899547000
C	0.008963000	-2.991553000	2.315696000
H	0.285062000	-2.069118000	2.824088000
H	-1.066858000	-3.161071000	2.423276000
H	0.544535000	-3.833644000	2.766495000
C	-0.052514000	-4.003602000	0.043335000
H	0.249209000	-3.809155000	-0.987121000
H	0.418116000	-4.929670000	0.388673000
H	-1.139743000	-4.126060000	0.080266000
H	-3.640943000	0.525557000	-0.049481000
O	-3.352960000	-0.199948000	1.884146000
C	-4.312045000	0.634798000	2.366240000
C	-4.670609000	0.255194000	3.775547000
H	-5.445856000	0.922551000	4.151654000
H	-5.022523000	-0.780687000	3.804809000
H	-3.783091000	0.320181000	4.412769000
O	-4.796990000	1.547211000	1.730873000

TS3IV_{1a}

Pd	-2.645110000	0.049891000	0.501758000
O	-1.330204000	-1.648315000	0.048328000
C	-0.757344000	-2.332007000	0.931469000

C	4.527959000	-3.062230000	1.459002000
C	5.090849000	-1.988483000	0.559210000
O	6.102585000	-1.365871000	0.813831000
O	4.482806000	-1.739979000	-0.628052000
H	5.199594000	-3.179748000	2.309153000
H	3.531811000	-2.790056000	1.813991000
H	4.451831000	-4.014235000	0.923697000
C	2.079479000	4.631368000	-1.220637000
C	1.925223000	3.370440000	-0.406695000
O	2.319845000	3.227743000	0.730239000
O	1.282053000	2.438597000	-1.146773000
H	1.096266000	4.998638000	-1.530680000
H	2.589192000	5.391392000	-0.627922000
H	2.655309000	4.420319000	-2.127406000
C	2.091202000	-1.160828000	-0.494058000
C	1.318156000	-0.094527000	1.475027000
C	2.214331000	0.223478000	-1.115226000
C	1.028241000	1.097001000	-0.665868000
C	0.752647000	0.919227000	0.808947000
O	2.120045000	-1.068020000	0.940270000
C	3.144101000	-2.174660000	-0.915992000
H	1.161460000	-0.261315000	2.536727000
H	0.145069000	0.796886000	-1.239499000
H	1.118507000	-1.564638000	-0.803429000
H	3.097289000	-2.297373000	-2.000333000
H	2.927896000	-3.139674000	-0.452625000
I	-4.431975000	-0.805292000	-1.429718000
C	-2.727196000	1.674496000	2.118302000
C	-0.260036000	1.787655000	1.540298000
C	-2.866462000	3.155894000	1.760206000
C	-1.503547000	3.773667000	1.428493000
H	0.237014000	2.208273000	2.432725000
H	-0.985153000	4.076397000	2.351074000
H	-3.451892000	1.291701000	2.833788000
H	-3.300534000	3.667990000	2.626397000
H	-1.617684000	4.658266000	0.797333000
H	-3.562146000	3.296482000	0.929781000
H	-3.685271000	1.125668000	0.829169000
H	2.231143000	0.153640000	-2.203867000
O	3.422559000	0.839332000	-0.650027000
C	4.386573000	1.140157000	-1.553739000
C	5.604157000	1.657512000	-0.842902000
H	6.305749000	2.083675000	-1.560656000
H	5.318550000	2.402645000	-0.095573000
H	6.068951000	0.813980000	-0.319163000
O	4.270192000	0.985949000	-2.752374000
H	-0.722664000	-2.003870000	1.974843000
N	-0.145037000	-3.489857000	0.691833000
C	-0.140064000	-4.103678000	-0.632784000
H	0.881324000	-4.144055000	-1.024215000
H	-0.528990000	-5.124083000	-0.560461000
H	-0.765802000	-3.521565000	-1.307478000
C	0.597358000	-4.182780000	1.739225000
H	0.538375000	-3.622746000	2.674275000
H	0.183738000	-5.184668000	1.891846000
H	1.648122000	-4.274513000	1.446914000
C	-1.479680000	1.019103000	2.044799000
H	-1.275104000	0.205432000	2.738985000
O	-0.677708000	2.860665000	0.705992000

FI_{1a}

Pd	-2.633343000	0.316351000	0.205242000
O	-2.071659000	-0.306164000	2.294850000
C	-1.039378000	-0.731650000	2.866698000
C	5.127461000	-3.115832000	-0.746434000
C	3.723718000	-2.960650000	-0.215138000
O	3.355468000	-3.395790000	0.855631000
O	2.799748000	-2.319427000	-0.976927000
H	5.672355000	-3.778934000	-0.074811000
H	5.128545000	-3.533323000	-1.757518000
H	5.645795000	-2.151529000	-0.780989000
C	2.604177000	2.859154000	2.633066000
C	2.020912000	2.013734000	1.536215000
O	1.402403000	0.980010000	1.698092000
O	2.285425000	2.557102000	0.324759000
H	2.227916000	2.519719000	3.598405000
H	3.694070000	2.755297000	2.609659000
H	2.364493000	3.914785000	2.479894000
C	2.388713000	-0.294645000	-2.189869000
C	0.146035000	0.414233000	-1.753349000
C	2.777303000	0.535606000	-0.964741000
C	1.970244000	1.827299000	-0.895760000
C	0.505918000	1.536709000	-1.116051000
O	0.975550000	-0.559524000	-2.215207000
C	3.104514000	-1.636239000	-2.207016000
H	-0.890001000	0.174933000	-1.963120000
H	2.339565000	2.517239000	-1.661591000
H	2.657221000	0.251929000	-3.104108000
H	4.173798000	-1.463595000	-2.332691000
H	2.742217000	-2.242958000	-3.041691000
I	-3.815926000	-2.000625000	-0.569304000
C	-2.326701000	3.904787000	-1.375491000
C	-0.528104000	2.548776000	-0.669923000
C	-3.338253000	3.402329000	-0.334481000
C	-2.665720000	2.499696000	0.682780000
C	-1.344449000	2.105594000	0.533375000
O	-1.381184000	2.899258000	-1.761520000
H	0.016716000	3.452983000	-0.342870000
H	-2.988374000	0.769206000	-1.183539000
H	-2.829953000	4.219127000	-2.293057000
H	-4.179646000	2.891671000	-0.811887000
H	-3.137964000	2.419520000	1.660484000
H	-3.760181000	4.264441000	0.196820000
H	-0.775038000	1.758258000	1.388018000
H	-1.782158000	4.773184000	-0.972436000
H	-0.882691000	-0.487569000	3.925407000
N	-0.079447000	-1.487711000	2.343378000
C	-0.093886000	-1.932361000	0.953055000
H	0.931040000	-2.075655000	0.610826000
H	-0.638792000	-2.878488000	0.861351000
H	-0.581737000	-1.190686000	0.321746000
C	1.093136000	-1.852779000	3.132309000
H	1.234586000	-2.936980000	3.110731000
H	1.979815000	-1.368433000	2.715297000
H	0.962238000	-1.529822000	4.167177000
H	2.620377000	-0.045199000	-0.058383000
O	4.174197000	0.855260000	-1.114230000
C	4.971934000	0.756491000	-0.017554000
C	6.381856000	1.147686000	-0.359435000
H	7.040478000	0.920896000	0.478912000
H	6.717050000	0.624944000	-1.259349000
H	6.415041000	2.222262000	-0.569582000
O	4.577627000	0.409284000	1.076767000

FIII_{1a}

Pd	-2.492798000	-0.408595000	0.135697000
O	-2.258196000	1.762885000	0.727602000
C	-1.958946000	2.698355000	-0.053793000
C	4.405897000	-3.011873000	-2.611043000
C	4.927205000	-1.911350000	-1.719827000
O	5.895984000	-2.029875000	-1.001015000
O	4.317762000	-0.693857000	-1.752125000
H	5.045114000	-3.884697000	-2.479627000
H	3.375948000	-3.270347000	-2.355900000
H	4.428040000	-2.702856000	-3.661389000
C	2.313760000	1.203184000	4.117707000
C	2.165066000	0.280139000	2.941021000
O	2.816040000	-0.721050000	2.731570000
O	1.179258000	0.728424000	2.118925000
H	2.687243000	2.167319000	3.759103000
H	1.344883000	1.375310000	4.595154000
H	3.017119000	0.779390000	4.834741000
C	1.917427000	-0.608469000	-1.350772000
C	0.995694000	-2.274484000	0.073736000
C	2.142519000	0.246045000	-0.099716000
C	0.956366000	0.072982000	0.843067000
C	0.550420000	-1.376993000	0.958957000
O	1.824685000	-1.993274000	-0.978193000
C	3.037606000	-0.479224000	-2.369692000
H	0.728738000	-3.323546000	0.105428000
H	0.125237000	0.656709000	0.438173000
H	0.975630000	-0.310278000	-1.833800000
H	3.054515000	0.542866000	-2.751794000
H	2.861184000	-1.156189000	-3.207562000
I	-2.636673000	-0.069666000	-2.542588000
C	-1.971806000	-3.423667000	2.712090000
C	-0.436416000	-1.749730000	2.046782000
C	-3.242699000	-2.626724000	2.403177000
C	-2.896322000	-1.157785000	2.237571000
C	-1.577822000	-0.751959000	2.122758000
O	-0.901734000	-3.073161000	1.827359000
H	0.077786000	-1.707456000	3.026512000
H	-3.648203000	-0.428534000	2.533446000
H	-1.661025000	-3.244488000	3.753071000
H	-3.943580000	-2.727029000	3.240452000
H	-2.471364000	-1.869750000	-0.216470000
H	-3.747855000	-3.025611000	1.519117000
H	-2.133579000	-4.496606000	2.584705000
H	-1.301918000	0.267417000	2.372315000
H	-2.399975000	2.767349000	-1.054913000
N	-1.094652000	3.666657000	0.241284000
C	-0.381497000	3.696125000	1.514689000
H	-0.430895000	2.718135000	1.988946000
H	0.664994000	3.953876000	1.331733000
H	-0.820436000	4.450025000	2.177981000
C	-0.903482000	4.804837000	-0.652178000
H	-1.460303000	4.649005000	-1.578064000
H	-1.258869000	5.722248000	-0.170564000
H	0.158443000	4.920038000	-0.886087000
H	3.076017000	-0.035835000	0.384459000
O	2.207028000	1.616152000	-0.544399000
C	3.015022000	2.469430000	0.136763000
C	3.046778000	3.823272000	-0.517944000

H	3.988369000	3.911630000	-1.071858000
H	2.218178000	3.961137000	-1.212389000
H	3.036594000	4.598544000	0.250970000
O	3.651711000	2.157582000	1.121539000

GI_{1a}

Pd	2.717276000	-0.276044000	-0.006298000
O	2.478481000	0.180537000	2.182453000
C	1.538923000	0.587520000	2.905661000
C	-1.450073000	4.051015000	-1.434667000
C	-2.367295000	3.461644000	-0.392951000
O	-2.369857000	3.802542000	0.771905000
O	-3.278738000	2.524423000	-0.767410000
H	-0.843167000	4.819262000	-0.956291000
H	-0.802731000	3.283188000	-1.864592000
H	-2.025970000	4.502214000	-2.249327000
C	-2.389816000	-2.754927000	2.661201000
C	-1.930578000	-1.851029000	1.552883000
O	-1.308085000	-0.816433000	1.699226000
O	-2.294139000	-2.350437000	0.349195000
H	-3.483575000	-2.744147000	2.697299000
H	-2.070754000	-3.783583000	2.470342000
H	-1.987358000	-2.404847000	3.611902000
C	-2.522136000	0.586041000	-2.047950000
C	-0.261636000	-0.102998000	-1.689149000
C	-2.885117000	-0.294219000	-0.850048000
C	-2.055957000	-1.576042000	-0.860814000
C	-0.602103000	-1.273446000	-1.136416000
O	-1.119086000	0.904074000	-2.024722000
C	-3.290808000	1.898956000	-2.062774000
H	0.763346000	0.158643000	-1.923207000
H	-2.454353000	-2.244448000	-1.631140000
H	-2.741272000	0.050648000	-2.982180000
H	-4.340291000	1.693591000	-2.281124000
H	-2.898304000	2.552181000	-2.844586000
C	2.100370000	-3.730465000	-1.733512000
C	0.432938000	-2.333481000	-0.823455000
C	3.213636000	-3.322745000	-0.756349000
C	2.667068000	-2.447939000	0.357764000
C	1.360781000	-1.979853000	0.327497000
O	1.175429000	-2.667810000	-1.997040000
H	-0.115707000	-3.231827000	-0.487674000
H	2.877824000	-0.623161000	-1.465370000
H	2.514584000	-4.023312000	-2.701426000
H	4.032081000	-2.817990000	-1.278452000
H	3.204700000	-2.458796000	1.304433000
H	3.641481000	-4.228550000	-0.309081000
H	0.868371000	-1.661738000	1.239905000
H	1.548971000	-4.592506000	-1.325663000
H	1.498936000	0.267055000	3.955349000
N	0.554944000	1.414559000	2.560463000
C	0.420370000	1.964013000	1.213797000
H	-0.219139000	1.313710000	0.610536000
H	-0.048740000	2.946888000	1.285536000
H	1.399115000	2.061361000	0.745290000
C	-0.546445000	1.683002000	3.480157000
H	-0.648367000	2.761339000	3.636380000
H	-1.475228000	1.286897000	3.060747000
H	-0.358772000	1.198491000	4.440381000
O	3.331189000	1.665760000	-0.460849000

C	4.617813000	1.842765000	-0.528236000
O	5.474290000	0.960376000	-0.387379000
C	5.016629000	3.287733000	-0.806779000
H	4.582799000	3.949824000	-0.050274000
H	6.102859000	3.396392000	-0.806765000
H	4.621469000	3.603070000	-1.778543000
H	-2.719311000	0.255101000	0.074744000
O	-4.280368000	-0.621510000	-0.986141000
C	-5.034487000	-0.678405000	0.143977000
O	-4.600068000	-0.476534000	1.258428000
C	-6.458000000	-1.020126000	-0.196301000
H	-6.492255000	-1.964427000	-0.748308000
H	-7.045558000	-1.101186000	0.718067000
H	-6.881840000	-0.245219000	-0.842961000

GIII_{1a}

Pd	-2.781381000	0.139963000	0.121431000
O	-1.981841000	-0.868454000	-1.739690000
C	-1.305138000	-1.907075000	-1.531475000
C	3.238515000	-1.235539000	4.270954000
C	4.086606000	-0.832815000	3.089878000
O	5.047390000	-0.098216000	3.168883000
O	3.802369000	-1.359939000	1.865636000
H	3.659529000	-0.774139000	5.164024000
H	2.205276000	-0.905746000	4.142120000
H	3.234767000	-2.323770000	4.393158000
C	2.967840000	3.465448000	-2.325075000
C	2.430514000	2.687927000	-1.155590000
O	2.724511000	2.862203000	0.007915000
O	1.557707000	1.739071000	-1.585054000
H	2.154819000	3.794266000	-2.978137000
H	3.536413000	4.323924000	-1.966970000
H	3.621787000	2.808936000	-2.908005000
C	1.547644000	-1.020863000	1.009551000
C	0.338467000	0.890557000	1.735763000
C	2.122656000	-0.145094000	-0.106179000
C	1.029101000	0.777483000	-0.635428000
C	0.246317000	1.391918000	0.499352000
O	1.116217000	-0.178613000	2.091743000
C	2.557607000	-2.011860000	1.564296000
H	-0.208198000	1.292228000	2.579618000
H	0.362762000	0.184002000	-1.265482000
H	0.681298000	-1.583202000	0.631852000
H	2.786608000	-2.752272000	0.796126000
H	2.136620000	-2.531329000	2.427425000
C	-2.336882000	3.974778000	1.029563000
C	-0.740497000	2.482679000	0.146163000
C	-3.573692000	3.286080000	0.441154000
C	-3.155742000	2.252658000	-0.591351000
C	-1.823349000	1.929106000	-0.766944000
O	-1.290702000	3.042020000	1.327344000
H	-0.215441000	3.274300000	-0.419740000
H	-3.863825000	2.028432000	-1.387307000
H	-1.957480000	4.728953000	0.322598000
H	-4.194588000	4.039171000	-0.059570000
H	-3.169006000	0.757899000	1.443577000
H	-4.190701000	2.843203000	1.227127000
H	-2.572676000	4.479516000	1.969481000
H	-1.486551000	1.504790000	-1.708422000
H	-1.478866000	-2.517139000	-0.637969000

N	-0.342927000	-2.342919000	-2.341853000
C	0.022845000	-1.619533000	-3.556093000
H	-0.744908000	-0.882272000	-3.787121000
H	0.981530000	-1.111547000	-3.412143000
H	0.115177000	-2.326297000	-4.385530000
C	0.451010000	-3.521286000	-2.009216000
H	0.090375000	-3.963141000	-1.078611000
H	0.375456000	-4.262717000	-2.810804000
H	1.498158000	-3.233180000	-1.884135000
O	-2.965101000	-1.725535000	1.003587000
C	-4.111992000	-2.323104000	0.836041000
C	-4.119032000	-3.759913000	1.343729000
H	-5.126753000	-4.177632000	1.304743000
H	-3.454693000	-4.370197000	0.721521000
H	-3.739185000	-3.806464000	2.368808000
O	-5.113662000	-1.822767000	0.313189000
O	2.567340000	-1.027505000	-1.154703000
H	2.963019000	0.431446000	0.275975000
C	3.693776000	-0.685738000	-1.840882000
C	4.055023000	-1.763374000	-2.824060000
H	4.899605000	-1.437478000	-3.431259000
H	4.325466000	-2.674404000	-2.280013000
H	3.201665000	-2.001561000	-3.465113000
O	4.309144000	0.341600000	-1.653795000

TS4I_{1a}

Pd	3.036839000	0.113195000	0.519519000
O	1.943078000	0.746752000	2.664308000
C	0.715891000	0.923767000	2.786382000
C	-5.661826000	2.319322000	-0.971853000
C	-4.428195000	2.479627000	-0.117163000
O	-4.454794000	2.824125000	1.045205000
O	-3.208596000	2.246293000	-0.671616000
H	-6.522022000	2.649992000	-0.390616000
H	-5.590770000	2.908926000	-1.890725000
H	-5.813144000	1.273057000	-1.256627000
C	-2.127908000	-3.330676000	2.291422000
C	-1.604026000	-2.246417000	1.392501000
O	-1.132396000	-1.190144000	1.764301000
O	-1.740187000	-2.600787000	0.093087000
H	-3.220267000	-3.343246000	2.216596000
H	-1.757538000	-4.309973000	1.977408000
H	-1.837816000	-3.125566000	3.322133000
C	-2.048709000	0.571829000	-1.956061000
C	0.201669000	0.160707000	-1.308346000
C	-2.442274000	-0.483556000	-0.921505000
C	-1.448980000	-1.639306000	-0.960619000
C	-0.032557000	-1.115046000	-0.972152000
O	-0.740265000	1.086982000	-1.653319000
C	-3.020799000	1.736617000	-2.004061000
H	1.201980000	0.579843000	-1.345469000
H	-1.638911000	-2.236392000	-1.858702000
H	-2.017461000	0.117281000	-2.956258000
H	-3.952203000	1.392832000	-2.452161000
H	-2.606211000	2.537282000	-2.623093000
C	2.958047000	-3.181476000	-1.619212000
C	1.096022000	-2.080622000	-0.679184000
C	3.970032000	-2.756423000	-0.546145000
C	3.268181000	-2.075358000	0.619565000
C	1.913795000	-1.755283000	0.561862000

O	1.937011000	-2.202310000	-1.832034000
H	0.633203000	-3.064967000	-0.485249000
H	3.673247000	0.120307000	-0.944519000
H	3.446488000	-3.331793000	-2.585814000
H	4.742480000	-2.109584000	-0.973527000
H	3.748012000	-2.163798000	1.593985000
H	4.486254000	-3.651374000	-0.175452000
H	1.334867000	-1.633679000	1.473599000
H	2.487828000	-4.134311000	-1.326177000
H	0.129178000	0.327957000	3.498795000
N	-0.024998000	1.810796000	2.109070000
C	0.554438000	2.739326000	1.148230000
H	0.051164000	2.630151000	0.182928000
H	0.420650000	3.770272000	1.498677000
H	1.618490000	2.538504000	1.028702000
C	-1.452255000	1.953990000	2.371383000
H	-1.647658000	2.856486000	2.964475000
H	-1.995618000	2.044403000	1.430016000
H	-1.822469000	1.079180000	2.907251000
O	3.918892000	2.081079000	0.098636000
C	4.400962000	2.059184000	-1.079987000
O	4.354086000	1.037686000	-1.838523000
C	5.098500000	3.299756000	-1.586043000
H	6.130144000	3.292001000	-1.215850000
H	5.123831000	3.320885000	-2.676700000
H	4.609850000	4.197475000	-1.200890000
O	-3.754509000	-0.957899000	-1.280047000
H	-2.463085000	-0.038505000	0.071922000
C	-4.626576000	-1.234661000	-0.273130000
C	-5.917289000	-1.768390000	-0.827978000
H	-5.765988000	-2.814100000	-1.119454000
H	-6.693265000	-1.720859000	-0.063700000
H	-6.221521000	-1.216611000	-1.720414000
O	-4.370847000	-1.082535000	0.903266000

TS4III_{1a}

Pd	-2.801590000	-0.121598000	0.589432000
O	-1.430379000	-0.251629000	2.645032000
C	-0.661551000	0.712917000	2.827748000
C	2.632747000	3.682587000	-2.879098000
C	3.609725000	2.604498000	-2.477968000
O	4.429256000	2.125384000	-3.231737000
O	3.617120000	2.169901000	-1.187401000
H	2.817604000	3.935308000	-3.922931000
H	1.602016000	3.340179000	-2.762734000
H	2.765517000	4.577453000	-2.262131000
C	2.761174000	-4.243812000	-0.655893000
C	2.163202000	-2.904139000	-0.987133000
O	2.243120000	-2.336966000	-2.055988000
O	1.513772000	-2.399568000	0.093917000
H	3.121318000	-4.722652000	-1.566814000
H	3.598865000	-4.088818000	0.031758000
H	2.029201000	-4.883104000	-0.155046000
C	1.525152000	1.373283000	-0.230006000
C	-0.043215000	0.364498000	-1.700465000
C	2.126366000	-0.021903000	-0.042982000
C	0.995853000	-1.043925000	0.045129000
C	-0.021251000	-0.801019000	-1.044038000
O	0.811607000	1.411944000	-1.476105000
C	2.567399000	2.477817000	-0.255710000

H	-0.755782000	0.587156000	-2.484411000
H	0.520364000	-0.950709000	1.025024000
H	0.820638000	1.585430000	0.586027000
H	3.043095000	2.542810000	0.724383000
H	2.088570000	3.435683000	-0.467670000
C	-2.923902000	-2.433961000	-2.619631000
C	-1.069233000	-1.866605000	-1.274416000
C	-3.994743000	-2.249676000	-1.541488000
C	-3.339193000	-2.148272000	-0.172261000
C	-1.959616000	-2.022482000	-0.046372000
O	-1.824207000	-1.539542000	-2.432512000
H	-0.562556000	-2.835108000	-1.440528000
H	-3.908571000	-2.531777000	0.673205000
H	-2.555613000	-3.472308000	-2.608844000
H	-4.664114000	-3.119216000	-1.552894000
H	-3.465044000	0.464984000	-0.731327000
H	-4.613976000	-1.374805000	-1.760842000
H	-3.321305000	-2.226436000	-3.616621000
H	-1.458967000	-2.357643000	0.860055000
H	-0.911142000	1.722287000	2.469662000
N	0.517727000	0.634296000	3.458885000
C	0.998269000	-0.636807000	3.989184000
H	0.155133000	-1.312169000	4.133281000
H	1.709967000	-1.094171000	3.295052000
H	1.496048000	-0.463071000	4.947077000
C	1.402579000	1.786567000	3.575273000
H	0.954526000	2.650285000	3.079581000
H	1.573967000	2.028516000	4.629736000
H	2.362309000	1.564536000	3.100593000
O	-3.395132000	1.955676000	0.928151000
C	-3.901722000	2.415521000	-0.147530000
C	-4.422909000	3.833503000	-0.133144000
H	-3.792001000	4.466771000	0.494606000
H	-4.483800000	4.241969000	-1.143032000
H	-5.429910000	3.827099000	0.299800000
O	-4.022121000	1.734051000	-1.214254000
O	2.873572000	-0.008404000	1.188026000
H	2.787994000	-0.250708000	-0.876627000
C	4.031370000	-0.723738000	1.241674000
C	4.699699000	-0.540752000	2.575322000
H	5.646319000	-1.080891000	2.585959000
H	4.873089000	0.522772000	2.765403000
H	4.052491000	-0.918099000	3.372933000
O	4.445345000	-1.403688000	0.327258000

III_{1a}

Pd	2.886633000	0.267365000	0.218859000
O	1.422769000	2.026935000	0.370143000
C	0.443301000	1.878366000	1.136112000
C	-5.953984000	2.523484000	-1.455314000
C	-4.877521000	2.433070000	-0.404982000
O	-4.927432000	2.990696000	0.671787000
O	-3.785552000	1.668975000	-0.668414000
H	-6.697942000	3.249546000	-1.128951000
H	-5.543900000	2.824243000	-2.423975000
H	-6.438070000	1.549538000	-1.586961000
C	-1.199039000	-3.018651000	2.997792000
C	-1.133790000	-2.040997000	1.856021000
O	-0.869313000	-0.859368000	1.957913000
O	-1.401864000	-2.666581000	0.688292000

H	-2.217021000	-3.411505000	3.081558000
H	-0.529545000	-3.863042000	2.807973000
H	-0.918560000	-2.520185000	3.925871000
C	-2.492682000	-0.010351000	-1.786010000
C	-0.151423000	-0.031177000	-1.476611000
C	-2.596910000	-0.894325000	-0.542323000
C	-1.459425000	-1.912289000	-0.557808000
C	-0.155699000	-1.259693000	-0.944011000
O	-1.258869000	0.722250000	-1.747049000
C	-3.635603000	0.974076000	-1.920832000
H	0.758855000	0.484681000	-1.756723000
H	-1.711821000	-2.701691000	-1.274090000
H	-2.494120000	-0.640133000	-2.687750000
H	-4.543142000	0.420932000	-2.171288000
H	-3.413153000	1.684530000	-2.722789000
C	2.962317000	-2.895730000	-2.030079000
C	1.119070000	-2.066980000	-0.807252000
C	4.060348000	-2.276567000	-1.163632000
C	3.473586000	-1.766391000	0.158999000
C	2.059088000	-1.636366000	0.318389000
O	1.794686000	-2.073344000	-2.074257000
H	0.815562000	-3.107311000	-0.585272000
H	3.293376000	-3.019842000	-3.066005000
H	4.553071000	-1.473704000	-1.724503000
H	4.046134000	-2.037168000	1.049493000
H	4.828337000	-3.036020000	-0.968345000
H	1.630430000	-1.796133000	1.308779000
H	2.691555000	-3.891906000	-1.640667000
H	0.462041000	1.149784000	1.952098000
N	-0.701911000	2.561100000	1.051907000
C	-0.933426000	3.554717000	0.013146000
H	-1.834090000	3.289170000	-0.545649000
H	-1.067516000	4.545302000	0.463373000
H	-0.078519000	3.576230000	-0.661138000
C	-1.750885000	2.389712000	2.052350000
H	-1.784975000	3.258905000	2.721343000
H	-2.720627000	2.295912000	1.558057000
H	-1.557738000	1.490027000	2.638422000
O	4.516050000	1.964413000	-0.009122000
C	5.674279000	1.578578000	0.160461000
O	5.955153000	0.317258000	0.478898000
C	6.881519000	2.455938000	0.029128000
H	7.434616000	2.464303000	0.973643000
H	7.547660000	2.049141000	-0.738231000
H	6.583543000	3.469935000	-0.236074000
H	5.075622000	-0.158456000	0.504848000
O	-3.866413000	-1.572875000	-0.605755000
H	-2.547711000	-0.275553000	0.350860000
C	-4.545398000	-1.757750000	0.556851000
C	-5.873484000	-2.408332000	0.285877000
H	-5.727858000	-3.350603000	-0.250832000
H	-6.393524000	-2.591700000	1.226057000
H	-6.479494000	-1.756312000	-0.351712000
O	-4.126545000	-1.427292000	1.646323000

III_{1a}

Pd	2.596519000	-0.376120000	-0.453703000
O	1.292841000	1.387563000	-1.203045000
C	1.089895000	2.306373000	-0.383103000
C	-3.491245000	3.345494000	2.345671000

C	-4.344134000	2.175889000	1.914651000
O	-5.157446000	1.637379000	2.634644000
O	-4.244080000	1.725038000	0.634182000
H	-3.751329000	3.591674000	3.375082000
H	-2.428728000	3.099984000	2.284495000
H	-3.677661000	4.216500000	1.708544000
C	-2.721384000	-4.617128000	-0.380543000
C	-2.357505000	-3.265443000	0.169918000
O	-2.719496000	-2.815090000	1.236324000
O	-1.559191000	-2.601807000	-0.704743000
H	-1.833502000	-5.137867000	-0.749189000
H	-3.214314000	-5.208861000	0.391132000
H	-3.403704000	-4.475107000	-1.224747000
C	-2.029932000	1.114181000	-0.168594000
C	-0.641477000	0.148677000	1.521375000
C	-2.446178000	-0.315842000	-0.517992000
C	-1.214262000	-1.214250000	-0.444849000
C	-0.463155000	-0.985896000	0.842457000
O	-1.488332000	1.170691000	1.159224000
C	-3.169645000	2.115514000	-0.235953000
H	-0.120059000	0.373342000	2.443916000
H	-0.566014000	-0.978149000	-1.294697000
H	-1.262838000	1.426602000	-0.884720000
H	-3.581621000	2.122090000	-1.246579000
H	-2.798272000	3.116446000	-0.010484000
C	2.386444000	-1.238808000	2.693773000
C	0.580451000	-2.014986000	1.239123000
C	3.421617000	-2.088799000	1.965128000
C	3.037547000	-2.228860000	0.501034000
C	1.660141000	-2.139278000	0.159369000
O	1.070636000	-1.784523000	2.564024000
H	0.079104000	-2.992071000	1.300505000
H	3.678016000	-2.879395000	-0.098533000
H	2.579538000	-1.212840000	3.770764000
H	3.466483000	-3.081248000	2.438080000
H	4.412728000	-1.633821000	2.082939000
H	2.419742000	-0.205217000	2.313559000
H	1.301139000	-2.674342000	-0.720848000
H	1.467567000	2.252697000	0.645915000
N	0.398869000	3.423933000	-0.646740000
C	-0.168136000	3.687434000	-1.963640000
H	0.110314000	2.885348000	-2.646105000
H	-1.260168000	3.745594000	-1.897235000
H	0.210585000	4.640988000	-2.346337000
C	0.133467000	4.412043000	0.390439000
H	0.588024000	4.098139000	1.331897000
H	0.545764000	5.384650000	0.101220000
H	-0.946472000	4.519611000	0.538855000
O	4.270618000	1.236581000	-0.821837000
C	5.421980000	0.827009000	-0.655806000
C	6.645699000	1.674970000	-0.817084000
H	7.193724000	1.709152000	0.129941000
H	7.308301000	1.227361000	-1.564264000
H	6.366655000	2.683366000	-1.121373000
O	5.674824000	-0.432052000	-0.308869000
H	4.781948000	-0.875122000	-0.229221000
O	-2.927421000	-0.276949000	-1.876686000
C	-3.944606000	-1.108034000	-2.222723000
C	-4.283726000	-0.936067000	-3.677306000
H	-3.418042000	-1.208222000	-4.289897000
H	-5.132247000	-1.569193000	-3.936294000
H	-4.519085000	0.111664000	-3.887261000

O	-4.489123000	-1.871363000	-1.452545000
H	-3.229322000	-0.668675000	0.150974000

5e+[Pd(DMF)₂]

Pd	2.766507000	-0.330063000	0.528628000
O	1.540370000	1.575271000	1.141822000
C	0.420045000	1.424453000	1.674184000
C	-5.631893000	2.807288000	-1.548542000
C	-4.522540000	2.835440000	-0.527130000
O	-4.635099000	3.331421000	0.574548000
O	-3.322917000	2.281120000	-0.843997000
H	-6.471809000	3.378210000	-1.153753000
H	-5.311017000	3.236886000	-2.502159000
H	-5.960885000	1.779232000	-1.735570000
C	-2.934113000	-3.109131000	2.665260000
C	-2.218244000	-2.182812000	1.720799000
O	-1.575499000	-1.205063000	2.049144000
O	-2.392441000	-2.586430000	0.442190000
H	-2.657497000	-2.874629000	3.693406000
H	-4.012707000	-2.971812000	2.536757000
H	-2.699063000	-4.152315000	2.437093000
C	-2.215458000	0.403745000	-1.860092000
C	-0.076345000	-0.171953000	-1.022130000
C	-2.777875000	-0.494212000	-0.759075000
C	-1.927314000	-1.754364000	-0.659482000
C	-0.459523000	-1.391291000	-0.615950000
O	-0.891493000	0.818661000	-1.496540000
C	-3.064287000	1.635689000	-2.105345000
H	0.958633000	0.153804000	-0.978632000
H	-2.139318000	-2.394841000	-1.521743000
H	-2.159320000	-0.156636000	-2.804854000
H	-3.984731000	1.325718000	-2.598695000
H	-2.529068000	2.334258000	-2.755234000
C	2.077950000	-2.650916000	-2.080364000
C	0.524328000	-2.492860000	-0.251233000
C	3.308812000	-2.873124000	-1.206360000
C	3.059094000	-2.377270000	0.211002000
C	1.719217000	-2.133748000	0.648317000
O	0.922229000	-3.199564000	-1.452363000
H	-0.047095000	-3.251647000	0.293565000
H	1.934182000	-1.578721000	-2.290023000
H	4.181767000	-2.384661000	-1.659032000
H	3.780982000	-2.740770000	0.946955000
H	3.526348000	-3.952006000	-1.184384000
H	1.486493000	-2.295806000	1.702725000
H	2.174840000	-3.165598000	-3.042063000
H	0.185043000	0.539830000	2.277614000
N	-0.598282000	2.286961000	1.567167000
C	-0.495215000	3.494028000	0.759524000
H	-1.336754000	3.532169000	0.063261000
H	-0.519209000	4.384802000	1.398933000
H	0.442021000	3.474837000	0.204863000
C	-1.836068000	2.094472000	2.315759000
H	-1.900362000	2.818898000	3.137814000
H	-2.693329000	2.246955000	1.655634000
H	-1.870450000	1.082924000	2.721676000
H	-2.771907000	0.042259000	0.188790000
O	-4.129148000	-0.834760000	-1.123130000
C	-5.061020000	-0.870464000	-0.134499000
C	-6.405206000	-1.239322000	-0.697214000

H	-6.376429000	-2.276186000	-1.049197000
H	-7.167900000	-1.137733000	0.074837000
H	-6.647488000	-0.606796000	-1.555886000
O	-4.819523000	-0.642994000	1.032967000
O	4.484019000	1.152415000	0.188999000
C	5.605200000	0.785165000	-0.216145000
H	5.817790000	-0.271306000	-0.429799000
N	6.645708000	1.601444000	-0.428838000
C	6.554446000	3.038290000	-0.202546000
H	7.337846000	3.353922000	0.494584000
H	6.689135000	3.576481000	-1.147540000
H	5.577653000	3.278743000	0.215180000
C	7.919370000	1.093315000	-0.921958000
H	8.170905000	1.569244000	-1.876201000
H	8.717238000	1.310128000	-0.203250000
H	7.859993000	0.013124000	-1.070649000

4e+[Pd(DMF)₂]

Pd	-2.455025000	0.558558000	-0.581776000
C	4.423536000	-1.369220000	3.864356000
C	5.091776000	-0.849028000	2.614476000
O	6.044891000	-0.099741000	2.625265000
O	4.641563000	-1.270626000	1.400973000
H	4.936985000	-0.941682000	4.725397000
H	3.367566000	-1.091932000	3.889824000
H	4.488745000	-2.461676000	3.913156000
C	2.763775000	3.517122000	-2.552486000
C	2.524621000	2.683492000	-1.323157000
O	3.057828000	2.844183000	-0.244583000
O	1.620077000	1.709873000	-1.588716000
H	3.264219000	2.898399000	-3.304130000
H	1.815283000	3.857880000	-2.977245000
H	3.393232000	4.371864000	-2.303674000
C	2.262723000	-1.071094000	0.904886000
C	1.114372000	0.765082000	1.881076000
C	2.538880000	-0.168285000	-0.299525000
C	1.319299000	0.709403000	-0.575809000
C	0.744300000	1.272023000	0.699942000
O	2.002368000	-0.266047000	2.061437000
C	3.415606000	-2.003194000	1.236217000
H	0.736812000	1.132865000	2.826902000
H	0.562931000	0.099580000	-1.076894000
H	1.379740000	-1.688813000	0.698894000
H	3.580686000	-2.679847000	0.395877000
H	3.169473000	-2.601914000	2.114887000
C	-1.871978000	3.582910000	1.870661000
C	-0.253024000	2.409532000	0.602313000
C	-3.090703000	3.161070000	1.052701000
C	-2.638274000	2.624713000	-0.309701000
C	-1.270827000	2.264136000	-0.529988000
O	-0.881253000	2.555002000	1.876852000
H	0.322356000	3.336648000	0.405168000
H	-3.184844000	3.036518000	-1.161151000
H	-1.440239000	4.510826000	1.459748000
H	-3.749688000	4.029245000	0.921746000
H	-3.662898000	2.417127000	1.620115000
H	-2.129333000	3.766670000	2.918679000
H	-0.833120000	2.455445000	-1.510580000
H	3.423344000	0.438534000	-0.113915000
O	2.762007000	-1.036809000	-1.428707000

C	3.655520000	-0.644355000	-2.374754000
C	3.724939000	-1.664095000	-3.477745000
H	4.049346000	-2.628203000	-3.073738000
H	2.732285000	-1.806280000	-3.915801000
H	4.425054000	-1.330686000	-4.243719000
O	4.297433000	0.383141000	-2.314872000
O	-4.274182000	-0.841258000	-0.391051000
C	-5.282713000	-0.560524000	0.287038000
H	-5.419233000	0.438067000	0.724837000
N	-6.283312000	-1.411103000	0.550907000
C	-6.274737000	-2.781535000	0.055423000
H	-5.388410000	-2.939011000	-0.557786000
H	-6.266915000	-3.484463000	0.895873000
H	-7.171935000	-2.965026000	-0.545407000
C	-7.423425000	-1.012151000	1.365524000
H	-7.312714000	0.027893000	1.679089000
H	-8.351738000	-1.114737000	0.792984000
H	-7.491262000	-1.645958000	2.256676000
O	-1.375924000	-1.405992000	-1.192382000
C	-1.035507000	-2.288373000	-0.381887000
H	-1.425240000	-2.308000000	0.645022000
N	-0.173080000	-3.279903000	-0.653529000
C	0.457009000	-3.410741000	-1.961915000
H	0.122012000	-2.599141000	-2.605886000
H	1.544183000	-3.361636000	-1.855772000
H	0.183566000	-4.371574000	-2.411313000
C	0.182722000	-4.273139000	0.350629000
H	-0.340431000	-4.062960000	1.285914000
H	-0.092356000	-5.276253000	0.006791000
H	1.262618000	-4.250705000	0.536101000

5e

C	5.054070000	-0.618622000	0.318412000
C	3.932646000	-0.966108000	1.268535000
O	3.972651000	-0.746753000	2.460010000
O	2.816555000	-1.564806000	0.776413000
H	5.885205000	-0.228944000	0.905580000
H	5.386200000	-1.494565000	-0.247098000
H	4.741314000	0.146887000	-0.399415000
C	-1.562840000	3.054656000	1.130308000
C	-1.176742000	1.641358000	0.787652000
O	-1.058260000	0.732349000	1.583274000
O	-0.971309000	1.527356000	-0.546518000
H	-1.777505000	3.128670000	2.196589000
H	-0.741637000	3.730098000	0.871013000
H	-2.440050000	3.355363000	0.550462000
C	1.222190000	-1.512261000	-1.027489000
C	-1.006324000	-2.098556000	-0.502940000
C	0.850158000	-0.080623000	-0.654150000
C	-0.569310000	0.249056000	-1.115014000
C	-1.508651000	-0.904111000	-0.845582000
O	0.316272000	-2.416099000	-0.377672000
C	2.638698000	-1.871780000	-0.618331000
H	-1.643067000	-2.950248000	-0.291266000
H	-0.544812000	0.478761000	-2.185743000
H	1.138650000	-1.651814000	-2.115393000
H	3.329950000	-1.319243000	-1.254382000
H	2.805548000	-2.943408000	-0.764356000
C	-3.024953000	-0.787927000	-1.074480000
C	-3.612038000	0.593942000	-0.879977000

C	-4.473523000	0.868618000	0.103021000
C	-3.903313000	-1.350787000	1.059298000
C	-4.855440000	-0.159290000	1.135625000
H	-4.296282000	-2.220177000	1.593838000
H	-2.931481000	-1.081882000	1.494163000
H	-4.818078000	0.276469000	2.142504000
H	-5.894256000	-0.482192000	0.976200000
O	-3.729526000	-1.766094000	-0.304349000
H	-3.326852000	1.348539000	-1.606593000
H	-4.927620000	1.855371000	0.171580000
H	-3.222407000	-1.069833000	-2.119370000
H	0.926389000	0.037553000	0.424665000
O	1.781932000	0.798336000	-1.314391000
C	2.281294000	1.846764000	-0.606356000
C	3.223637000	2.650201000	-1.459820000
H	2.656952000	3.147775000	-2.254238000
H	3.725767000	3.399687000	-0.848059000
H	3.958628000	1.997395000	-1.938835000
O	1.990697000	2.087280000	0.546468000

4e

C	5.006596000	-1.206026000	-0.331475000
C	4.087196000	-1.373002000	0.855031000
O	4.418798000	-1.136779000	1.996851000
O	2.818948000	-1.814968000	0.648022000
H	5.987879000	-0.912803000	0.040778000
H	5.096342000	-2.135395000	-0.902427000
H	4.641134000	-0.428801000	-1.010860000
C	-0.556974000	3.591164000	1.377838000
C	-0.544217000	2.103132000	1.157184000
O	-0.401950000	1.262529000	2.019916000
O	-0.700962000	1.823671000	-0.162210000
H	-0.675221000	3.805148000	2.440440000
H	0.397784000	4.000612000	1.030658000
H	-1.355394000	4.065837000	0.802053000
C	0.897728000	-1.556781000	-0.780467000
C	-1.214229000	-1.757308000	0.280074000
C	0.841744000	-0.067791000	-0.435658000
C	-0.580192000	0.450955000	-0.625494000
C	-1.580432000	-0.505771000	-0.021048000
O	0.029889000	-2.293020000	0.092557000
C	2.297493000	-2.129548000	-0.655970000
H	-1.897643000	-2.476164000	0.715068000
H	-0.760454000	0.562570000	-1.699336000
H	0.562961000	-1.705744000	-1.817533000
H	2.910256000	-1.719622000	-1.458312000
H	2.261671000	-3.218087000	-0.761888000
C	-2.999490000	-0.013852000	0.192720000
C	-3.654119000	0.360228000	-1.123818000
H	-2.955704000	0.894225000	0.822220000
C	-4.862833000	-0.085804000	-1.475361000
C	-5.135298000	-0.817385000	0.872082000
C	-5.683124000	-0.944255000	-0.547979000
H	-5.559837000	-1.571627000	1.540730000
H	-5.378115000	0.176569000	1.279910000
H	-6.736406000	-0.637350000	-0.568974000
H	-5.657107000	-1.994352000	-0.871200000
O	-3.721834000	-1.023196000	0.891422000
H	-3.089770000	1.023455000	-1.774771000
H	-5.286518000	0.183579000	-2.441060000

H	1.171710000	0.085714000	0.589800000
O	1.724936000	0.611512000	-1.349631000
C	2.482596000	1.632478000	-0.868098000
C	3.319066000	2.223240000	-1.968960000
H	2.663770000	2.741946000	-2.677103000
H	4.034591000	2.930970000	-1.550534000
H	3.841199000	1.436558000	-2.520478000
O	2.463901000	2.004090000	0.286725000

6a

C	-5.932296000	-0.564910000	0.171460000
C	-4.874449000	0.219673000	-0.563046000
O	-5.111733000	1.029018000	-1.435034000
O	-3.576157000	0.007154000	-0.231401000
H	-6.910516000	-0.270119000	-0.207522000
H	-5.793186000	-1.640559000	0.022385000
H	-5.886151000	-0.372501000	1.248260000
C	1.889162000	3.586486000	0.114185000
C	1.087475000	2.321760000	-0.051786000
O	0.495640000	1.993961000	-1.059465000
O	1.118363000	1.596488000	1.093093000
H	1.866387000	4.158809000	-0.813447000
H	1.474804000	4.186934000	0.930140000
H	2.923338000	3.342707000	0.375996000
C	-1.695459000	-0.944537000	0.903374000
C	0.125632000	-1.530979000	-0.502569000
C	-1.062674000	0.433553000	1.056817000
C	0.464790000	0.302014000	1.158980000
C	0.947313000	-0.685007000	0.131850000
O	-1.212831000	-1.608780000	-0.290637000
C	-3.207939000	-0.916138000	0.810164000
H	0.459307000	-2.245564000	-1.248164000
H	0.747190000	-0.041448000	2.158527000
H	-1.429964000	-1.579906000	1.760379000
H	-3.616783000	-0.594690000	1.773793000
H	-3.576677000	-1.921173000	0.582974000
I	3.063317000	-0.801061000	-0.239912000
H	-1.317939000	1.038216000	0.187851000
H	-1.451188000	0.921297000	1.955178000

[Pd(DMSO)₂]

Pd	-0.000001000	-0.048039000	0.000026000
S	-2.280754000	-0.027086000	0.187675000
S	2.280745000	-0.027094000	-0.187651000
O	2.894420000	-0.317803000	-1.542355000
O	-2.894551000	-0.317823000	1.542321000
C	-3.064015000	-1.122580000	-1.031429000
H	-4.149131000	-1.000622000	-0.968495000
H	-2.695653000	-0.859791000	-2.026605000
H	-2.777141000	-2.146781000	-0.785004000
C	-2.962146000	1.546314000	-0.411750000
H	-4.054327000	1.490837000	-0.388615000
H	-2.602203000	2.333119000	0.254027000
H	-2.597486000	1.721256000	-1.427398000

C	2.962080000	1.546370000	0.411681000
H	2.597427000	1.721347000	1.427325000
H	4.054265000	1.490973000	0.388530000
H	2.602080000	2.333123000	-0.254130000
C	3.064206000	-1.122554000	1.031363000
H	4.149309000	-1.000586000	0.968211000
H	2.696036000	-0.859713000	2.026596000
H	2.777301000	-2.146769000	0.785039000

B_{2a}

Pd	1.639669000	-0.615452000	-0.137794000
C	-4.942783000	-3.630457000	0.243938000
C	-4.929430000	-2.314109000	-0.491584000
O	-5.917041000	-1.805813000	-0.984408000
O	-3.752882000	-1.651645000	-0.607062000
H	-5.926539000	-4.084399000	0.126971000
H	-4.173670000	-4.312040000	-0.131365000
H	-4.751100000	-3.467247000	1.309865000
C	-2.510910000	4.398605000	0.047950000
C	-1.886880000	3.071163000	-0.299091000
O	-1.940950000	2.534870000	-1.382897000
O	-1.230973000	2.579859000	0.785377000
H	-3.038857000	4.793913000	-0.820091000
H	-3.206891000	4.276708000	0.883620000
H	-1.737573000	5.105759000	0.364363000
C	-1.480650000	-1.071066000	0.036326000
C	-0.011425000	0.053541000	-1.406814000
C	-1.759019000	0.160749000	0.906591000
C	-0.634733000	1.261845000	0.770877000
C	0.305691000	0.978523000	-0.390719000
O	-1.158194000	-0.724547000	-1.310112000
C	-2.557888000	-2.140028000	0.032668000
H	0.285434000	0.185245000	-2.441466000
H	-0.050842000	1.269476000	1.692241000
H	-0.593501000	-1.555633000	0.483593000
H	-2.758032000	-2.419203000	1.070136000
H	-2.184060000	-3.013435000	-0.511459000
I	1.601793000	2.682681000	-0.966177000
O	-3.018854000	0.760918000	0.574881000
C	-4.108000000	0.411790000	1.296579000
C	-5.330777000	1.092320000	0.751370000
H	-5.112535000	2.126300000	0.473501000
H	-5.638102000	0.550786000	-0.150448000
H	-6.136415000	1.052808000	1.485222000
O	-4.085876000	-0.369407000	2.228353000
H	-1.795894000	-0.166066000	1.947943000
O	2.118330000	0.817393000	2.877707000
S	2.447053000	-2.717589000	-0.820345000
O	3.555747000	-3.418937000	-0.050661000
C	2.916598000	-2.707114000	-2.576692000
H	3.784928000	-2.052604000	-2.677397000
H	3.164910000	-3.726781000	-2.883533000
H	2.081189000	-2.310121000	-3.158612000
C	1.034841000	-3.857994000	-0.936033000
H	0.261353000	-3.386527000	-1.546930000
H	1.367666000	-4.801998000	-1.376379000
H	0.664856000	-4.017615000	0.078654000
S	2.793933000	-0.156409000	1.924538000
C	4.497655000	0.412894000	1.649203000
H	5.019047000	-0.333035000	1.043223000

H	4.436979000	1.357646000	1.104844000
H	4.993083000	0.552030000	2.614091000
C	3.171104000	-1.681810000	2.838359000
H	3.803716000	-1.451700000	3.699854000
H	2.215317000	-2.098095000	3.165746000
H	3.655169000	-2.376145000	2.145616000

TS1_{2a}

Pd	1.731586267	-0.494143918	-0.229739839
C	-5.703878798	-3.451136381	-0.325603269
C	-5.498387418	-2.095056508	-0.950680062
O	-6.390565761	-1.439462857	-1.450674821
O	-4.249588463	-1.567414587	-0.956151681
H	-6.718122827	-3.783529339	-0.545428907
H	-4.983453996	-4.184136837	-0.699977176
H	-5.578620056	-3.385784362	0.760679066
C	-2.052328763	4.321334675	0.575437596
C	-1.750613803	2.941216919	0.049433423
O	-1.901483285	2.580565008	-1.095403473
O	-1.264655921	2.174083229	1.062123447
H	-2.461341156	4.937963338	-0.225142786
H	-2.769065183	4.259557247	1.400195312
H	-1.137036376	4.778555311	0.964820631
C	-1.981974028	-1.291375382	-0.153221800
C	-0.429244889	-0.111111462	-1.444699579
C	-2.192292928	-0.123006182	0.813263171
C	-0.907130018	0.787977235	0.875117361
C	-0.004914056	0.505783114	-0.300992505
O	-1.575902601	-0.848601480	-1.460615701
C	-3.153716510	-2.242768706	-0.313149938
H	0.032255255	-0.018496825	-2.420488953
H	-0.383348623	0.561956239	1.803809637
H	-1.156652125	-1.886916395	0.271260116
H	-3.437520630	-2.599064452	0.680124853
H	-2.839824087	-3.094269034	-0.925060919
I	1.760823204	2.297906700	-0.827018567
O	-3.313718538	0.679442447	0.434462598
C	-4.507231890	0.431920285	1.025955838
C	-5.573556941	1.304417939	0.429936428
H	-5.191560210	2.305484481	0.216858069
H	-5.884777141	0.843610634	-0.514539840
H	-6.431882650	1.353181903	1.101015709
O	-4.677500719	-0.409789318	1.886113490
H	-2.372585469	-0.534124617	1.809180977
O	1.192515250	-0.011634599	3.256042388
S	3.655118431	-1.726961385	-0.881541049
O	4.510063544	-2.372589924	0.201053043
C	4.727530803	-0.634958162	-1.855244412
H	5.024465260	0.189326045	-1.203774417
H	5.601929890	-1.199313162	-2.190321007
H	4.157245414	-0.249429799	-2.704050487
C	3.322839485	-2.984966997	-2.148529885
H	2.789225317	-2.511416803	-2.976708779
H	4.271595363	-3.413654810	-2.482652775
H	2.694232762	-3.750540926	-1.688731668
S	2.145861958	-0.678606204	2.272255166
C	3.834473889	-0.128521674	2.654938356
H	4.517622683	-0.694539287	2.016113502
H	3.888665264	0.936784905	2.421068873
H	4.042550712	-0.302915526	3.714442502

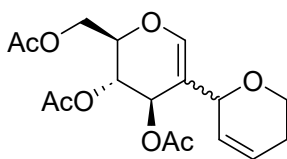
C	2.337056032	-2.422046179	2.746880919
H	2.655882435	-2.484479178	3.790929031
H	1.366066718	-2.904054955	2.611901514
H	3.078679843	-2.862105820	2.074424453

C_{2a}

Pd	-1.663664000	0.073332000	-0.419693000
C	7.250386000	0.511938000	-0.937462000
C	6.234236000	-0.543070000	-0.580293000
O	6.516475000	-1.598668000	-0.048233000
O	4.931373000	-0.307154000	-0.861424000
H	8.247518000	0.097927000	-0.789415000
H	7.138207000	0.849609000	-1.971887000
H	7.127514000	1.385167000	-0.287478000
C	-0.738063000	1.205312000	3.458882000
C	0.035794000	0.625695000	2.301239000
O	0.238336000	-0.555398000	2.127268000
O	0.428390000	1.626129000	1.470703000
H	-0.811616000	0.467933000	4.258831000
H	-0.273653000	2.122519000	3.828885000
H	-1.746066000	1.458924000	3.110529000
C	2.997708000	1.091279000	-1.259004000
C	1.023721000	-0.174169000	-1.721265000
C	2.506731000	1.183457000	0.192571000
C	0.994561000	1.418446000	0.146440000
C	0.313227000	0.399240000	-0.741892000
O	2.363505000	0.025623000	-1.976478000
C	4.499358000	0.943275000	-1.429150000
H	0.615216000	-0.891059000	-2.424054000
H	0.852280000	2.408191000	-0.292367000
H	2.734445000	2.046398000	-1.738199000
H	4.984437000	1.792382000	-0.940981000
H	4.742476000	0.958464000	-2.496586000
I	-1.313334000	-2.633251000	-0.597018000
O	2.778705000	-0.031284000	0.900835000
C	3.828803000	-0.052302000	1.751940000
C	4.042308000	-1.439329000	2.285733000
H	3.090115000	-1.948443000	2.447602000
H	4.613699000	-1.993224000	1.532044000
H	4.621486000	-1.399207000	3.209233000
O	4.515939000	0.917674000	2.010893000
H	3.001440000	2.019502000	0.691710000
O	-0.953648000	3.156390000	-1.566881000
S	-3.934301000	-0.269035000	0.468595000
O	-4.748715000	0.984941000	0.743825000
C	-3.752945000	-1.152888000	2.036994000
H	-3.135712000	-0.526715000	2.684573000
H	-4.749999000	-1.290681000	2.462817000
H	-3.258519000	-2.108262000	1.854181000
C	-4.986447000	-1.423638000	-0.443297000
H	-4.469035000	-2.379554000	-0.538281000
H	-5.923892000	-1.528181000	0.108455000
H	-5.162918000	-0.988230000	-1.429143000
S	-2.015641000	2.376520000	-0.835917000
C	-2.426315000	3.241857000	0.698170000
H	-3.243798000	2.701806000	1.180470000
H	-1.523660000	3.230570000	1.310210000
H	-2.717211000	4.264697000	0.444386000
C	-3.564378000	2.540100000	-1.758465000
H	-3.712995000	3.605216000	-1.953814000

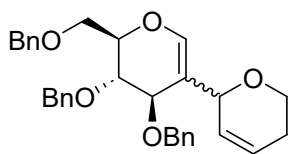
H	-3.444162000	1.986494000	-2.691617000
H	-4.376257000	2.129808000	-1.156021000

7. Characterization data of products



4a

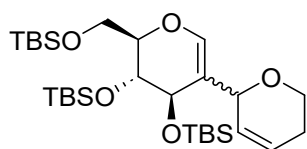
The compound was synthesized according to the general procedure (1), affording **4a**, and purified by column chromatography giving a light yellowish sticky solid (34.3 mg, 77% yield). R_f (Hexane/ EtOAc = 70/30): 0.65; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 6.53 (s, 1H), 6.45 (s, 1H), 5.94 – 5.90 (m, 1H), 5.81 – 5.77 (m, 1H), 5.58 – 5.50 (m, 4H), 5.14 – 5.11 (m, 1H), 5.04 (t, $J = 4.3$ Hz, 1H), 4.52 (s, 1H), 4.49 (s, 1H), 4.38 – 4.33 (m, 2H), 4.29 (dd, $J = 7.3, 3.7$ Hz, 1H), 4.24 (dt, $J = 9.6, 4.9$ Hz, 1H), 4.14 (d, $J = 3.4$ Hz, 0.5H), 4.11 (t, $J = 3.1$ Hz, 1H), 4.09 (d, $J = 3.6$ Hz, 0.5H), 3.88 – 3.84 (m, 1H), 3.70 (td, $J = 6.9, 3.5$ Hz, 1H), 3.59 (dq, $J = 8.5, 4.6$ Hz, 2H), 2.12 – 2.06 (m, 2H), 2.03 – 2.01 (m, 9H), 1.99 (d, $J = 2.8$ Hz, 6H), 1.94 (s, 3H) 1.87 (dd, $J = 23.3, 19.8$ Hz, 2H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 169.6, 169.5, 169.2, 168.9, 168.7, 168.6, 144.8, 144.1, 127.2, 126.4, 125.3, 124.4, 109.2, 108.9, 72.8, 72.6, 71.8, 68.8, 66.5, 66.4, 64.7, 63.8, 61.4, 60.4, 60.2, 58.9, 24.2, 23.8, 19.9, 19.9, 19.8, 19.7, 19.7. **HRMS (ESI)** m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{17}\text{H}_{23}\text{O}_8$ 355.1387; found 355.1383.



4b

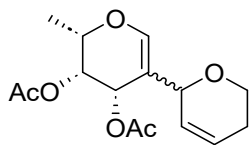
The compound was synthesized according to the general procedure (1), affording **4b**, and purified by column chromatography giving a brownish oil (31.6 mg, 69% yield). R_f (Hexane/ EtOAc = 80/20): 0.50; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.20 – 7.14 (m, 28H), 6.44 (s, 1H), 6.29 (s, 0.83H), 5.85 – 5.79 (m, 0.63H), 5.69 (ddd, $J = 9.5, 4.4, 2.3$ Hz, 1.28H), 5.62 – 5.56 (m, 2H), 4.62 – 4.50

(m, 4.81H), 4.39 (ddd, $J = 12.4, 10.3, 6.0$ Hz, 7.46H), 4.27 – 4.23 (m, 1.18H), 4.17 – 4.10 (m, 2.36H), 3.93 (d, $J = 3.0$ Hz, 1.43H), 3.89 – 3.85 (m, 1.30H), 3.81 (dd, $J = 11.1, 5.7$ Hz, 1H), 3.72 – 3.67 (m, 3H), 3.60 – 3.54 (m, 3.45H), 2.14 – 2.07 (m, 1.87H), 1.86 (ddd, $J = 13.5, 6.7, 2.5$ Hz, 1.81H). ^{13}C NMR (151 MHz, CDCl_3) δ 144.9, 143.9, 142.1, 138.6, 138.5, 138.4, 138.2, 138.2, 138.1, 138.1, 128.5, 128.5, 128.5, 128.5, 128.4, 128.4, 128.0, 127.9, 127.9, 127.9, 127.9, 127.8, 127.7, 127.6, 127.2, 126.6, 124.4, 112.3, 111.6, 76.7, 75.9, 75.8, 73.9, 73.8, 73.5, 73.3, 73.2, 73.0, 72.8, 72.7, 72.1, 71.8, 69.7, 68.4, 68.3, 68.2, 66.4, 62.9, 59.3, 25.5, 25.2. HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{32}\text{H}_{32}\text{O}_5\text{Na}^+$ 521.2298; found 521.2296.



4c

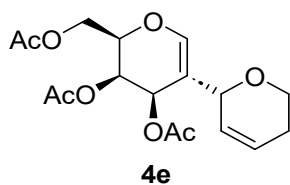
The compound was synthesized according to the general procedure (1), affording **4c**, and purified by column chromatography giving a light yellowish sticky solid (31.6 mg, 68% yield). R_f (Hexane/EtOAc = 90/10): 0.45; ^1H NMR (600 MHz, CDCl_3) δ 6.57 (s, 0.81H), 6.22 (s, 1H), 5.92 – 5.81 (m, 1.22H), 5.64 (d, $J = 9.0$ Hz, 1.65H), 4.55 (s, 1.29H), 4.10 – 4.02 (m, 3H), 3.88 (t, $J = 9.7$ Hz, 4.27H), 3.76 (d, $J = 1.8$ Hz, 1.66H), 3.68 – 3.65 (m, 3.11H), 3.54 – 3.50 (m, 1.58H), 1.93 – 1.71 (m, 3.49H), 1.22 – 1.19 (m, 8.69H), 0.83 – 0.80 (m, 31H), -0.02 – -0.04 (m, 30.33H). ^{13}C NMR (151 MHz, CDCl_3) δ 144.9, 142.3, 126.2, 125.3, 109.9, 78.9, 78.6, 73.2, 72.1, 69.6, 68.8, 68.2, 63.3, 60.6, 60.2, 59.4, 56.7, 30.4, 29.2, 27.9, 25.3, 25.2, 25.0, 24.9, 24.8, 24.7, 24.6, 17.5, 17.4, 17.3, 17.0, 16.9, 16.9, -4.1, -5.3, -5.3, -5.4, -5.6, -5.7, -5.7, -6.0, -6.1, -6.2, -6.3, -6.4. HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{29}\text{H}_{58}\text{O}_5\text{NaSi}_3^+$ 593.3484; found 593.3475.



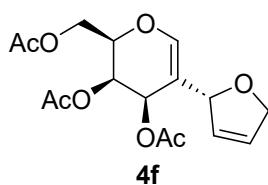
4d

The compound was synthesized according to the general procedure (1), affording **4d**, and purified by column chromatography giving a light yellowish gummy solid (30.1 mg, 69% yield). R_f (Hexane/EtOAc = 70/30): 0.50; ^1H NMR (600 MHz, CDCl_3) δ 6.54 (s, 1H), 6.48 (s, 0.56H), 6.37

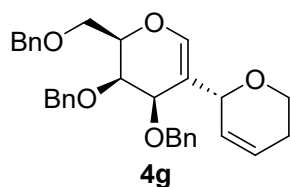
(s, 1H), 5.93 – 5.89 (m, 1H), 5.80 (d, $J = 4.9$ Hz, 1H), 5.78 – 5.72 (m, 1.90H), 5.63 (dd, $J = 19.1$, 7.2 Hz, 2H), 5.30 – 5.25 (m, 2.43H), 4.63 (s, 1H), 4.23 (d, $J = 6.5$ Hz, 1H), 4.17– 4.12 (m, 1.83H), 3.64– 3.60 (m, 3H), 2.12– 2.08 (m, 3.47H), 2.04 (s, 3.84H), 1.96 (s, 7H), 1.23– 1.20 (m, 5.07H). ^{13}C NMR (151 MHz, CDCl_3) δ 169.9, 169.1, 168.7, 168.5, 138.4, 133.4, 125.8, 125.5, 123.7, 123.5, 91.3, 71.2, 70.8, 67.9, 65.4, 63.9, 63.5, 61.8, 29.9, 19.7, 19.6, 19.6, 19.4, 15.4, 15.1. HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{15}\text{H}_{21}\text{O}_6^+$ 297.1333; found 297.1327.



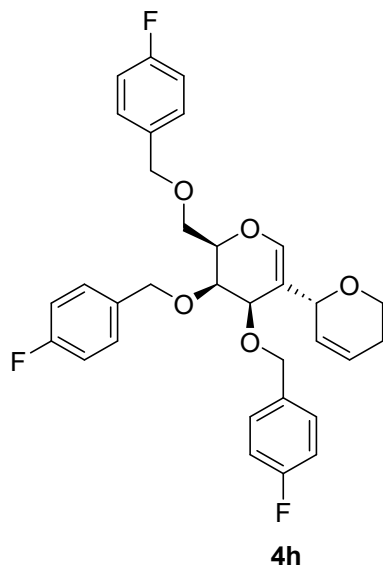
The compound was synthesized according to the general procedure (1), affording **4e**, and purified by column chromatography giving a brownish sticky solid (35.6 mg, 80% yield). R_f (Hexane/EtOAc = 70/30): 0.65; ^1H NMR (600 MHz, CDCl_3) δ 6.53 (s, 1H), 5.75 – 5.70 (m, 1H), 5.67 – 5.62 (m, 2H), 5.37 – 5.31 (m, 1H), 4.30 (dd, $J = 11.3$, 8.1 Hz, 1H), 4.25 (dd, $J = 7.8$, 3.3 Hz, 1H), 4.20 – 4.17 (m, 1H), 4.15 (s, 2H), 3.93 (dd, $J = 10.3$, 2.5 Hz, 1H), 2.10 – 2.06 (m, 1H), 2.03 (s, 3H), 2.02 (s, 3H), 1.98 (s, 3H), 1.97 – 1.94 (m, 1H). ^{13}C NMR (151 MHz, CDCl_3) δ 170.7, 170.4, 169.9, 142.5, 126.2, 123.8, 110.8, 72.5, 71.3, 66.2, 64.9, 63.3, 61.8, 30.6, 20.8, 20.8, 20.7. HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{17}\text{H}_{22}\text{O}_8\text{Na}^+$ 377.1207; found 377.1200.



The compound was synthesized according to the general procedure (1), affording **4f**, and purified by column chromatography giving a light yellowish sticky solid (33.3 mg, 78% yield). R_f (Hexane/EtOAc = 70/30): 0.60; ^1H NMR (600 MHz, CDCl_3) δ 6.46 (s, 1H), 5.82 – 5.79 (m, 1H), 5.61 (d, $J = 4.3$ Hz, 2H), 5.31 (t, $J = 4.4$ Hz, 1H), 5.13 (td, $J = 4.2$, 2.0 Hz, 1H), 4.63 – 4.58 (m, 1H), 4.52 – 4.49 (m, 1H), 4.40 (dd, $J = 12.1$, 8.9 Hz, 1H), 4.32 – 4.29 (m, 1H), 4.16 (dd, $J = 12.1$, 2.8 Hz, 1H), 2.02 (s, 3H), 2.00 (s, 3H), 1.93 (s, 3H). ^{13}C NMR (151 MHz, CDCl_3) δ 169.8, 169.1, 168.5, 142.7, 127.0, 125.9, 109.5, 83.6, 74.5, 71.6, 64.8, 60.5, 60.4, 19.8, 19.7, 16.9. HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{16}\text{H}_{20}\text{O}_8\text{Na}^+$ 363.1050; found 363.1040.

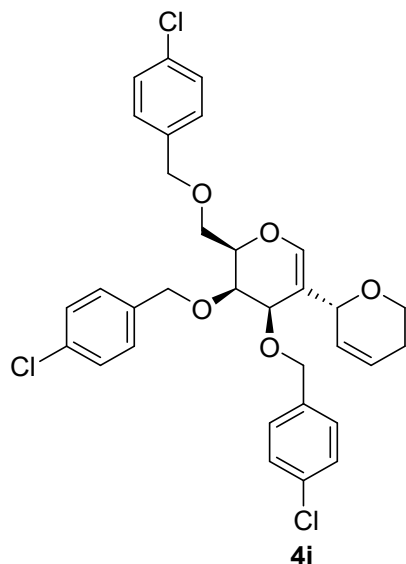


The compound was synthesized according to the general procedure (1), affording **4g**, and purified by column chromatography giving a colorless viscous solid (32.6 mg, 71% yield). R_f (Hexane/EtOAc = 80/20): 0.45; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.28 – 7.16 (m, 15H), 6.31 (s, 1H), 5.74 (s, 1H), 5.75 – 5.58 (m, 1H), 4.81 (d, $J = 12.0$ Hz, 1H), 4.60 (d, $J = 11.9$ Hz, 1H), 4.54 (dd, $J = 19.8$, 11.9 Hz, 2H), 4.40 (d, $J = 11.8$ Hz, 2H), 4.33 (d, $J = 11.8$ Hz, 2H), 3.97 (t, $J = 6.4$ Hz, 1H), 3.88 (d, $J = 1.6$ Hz, 1H), 3.81 – 3.74 (m, 1H), 3.66 – 3.60 (m, 1H), 3.51 – 3.40 (m, 2H), 2.55 – 2.46 (m, 1H), 2.27 – 2.22 (m, 1H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 138.8, 138.5, 138.1, 133.2, 129.9, 128.4, 128.4, 128.3, 128.3, 128.3, 128.3, 128.2, 128.2, 127.9, 127.8, 127.7, 127.5, 127.4, 127.3, 125.2, 125.2, 92.7, 78.6, 75.2, 73.9, 73.6, 72.0, 70.5, 69.7, 62.9, 30.8. **HRMS (ESI)** m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{32}\text{H}_{34}\text{O}_5\text{Na}^+$ 521.2298; found 521.2296.

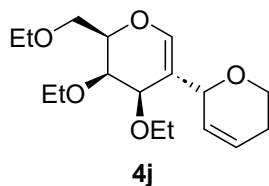


The compound was synthesized according to the general procedure (1), affording **4h**, and purified by column chromatography giving amber sticky solid (32.4 mg, 70% yield). R_f (Hexane/EtOAc = 80/20): 0.42; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.19 – 7.13 (m, 6H), 6.95 – 6.89 (m, 6H), 6.33 (s, 1H), 5.74 – 5.68 (m, 1H), 5.65 – 5.61 (m, 1H), 4.68 (d, $J = 10.9$ Hz, 1H), 4.60 (t, $J = 11.9$ Hz, 1H), 4.53 (d, $J = 11.7$ Hz, 1H), 4.46 (dd, $J = 11.4$, 5.1 Hz, 2H), 4.34 – 4.28 (m, 2H), 4.16 (s, 3H), 3.94 – 3.89 (m, 2H), 3.83 (dd, $J = 11.0$, 8.2 Hz, 1H), 3.67 (dd, $J = 11.1$, 3.0 Hz, 1H), 2.35 – 2.27 (m,

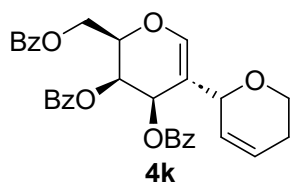
1H), 1.81 (dd, $J = 17.2, 1.8$ Hz, 1H). ^{13}C NMR (151 MHz, CDCl_3) δ 163.3, 163.0, 161.4, 141.5, 134.4, 133.9, 133.8, 129.6, 129.6, 129.5, 129.5, 129.4, 129.3, 125.9, 124.7, 115.4, 115.3, 115.3, 115.2, 115.1, 115.0, 112.7, 75.2, 74.6, 73.0, 72.9, 72.6, 71.9, 69.9, 67.7, 66.3, 31.0. HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{32}\text{H}_{31}\text{F}_3\text{O}_5\text{Na}^+$ 575.2016; found 575.2014.



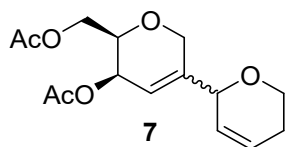
The compound was synthesized according to the general procedure (1), affording **4i**, and purified by column chromatography giving a light yellowish sticky solid (31.7 mg, 68% yield). R_f (Hexane/EtOAc = 80/20): 0.45; ^1H NMR (600 MHz, CDCl_3) δ 7.20 – 7.13 (m, 6H), 2 6.9 – 6.90 (m, 6H), 6.35 (s, 1H), 5.77 – 5.69 (m, 1H), 5.67 – 5.60 (m, 1H), 4.66 (d, $J = 10.3$ Hz, 1H), 4.61 (d, $J = 11.7$ Hz, 1H), 4.53 (d, $J = 11.7$ Hz, 1H), 4.46 (dd, $J = 11.4, 5.1$ Hz, 2H), 4.34 – 4.28 (m, 2H), 4.16 (bs, 3H), 3.93 – 3.87 (m, 2H), 3.85 – 3.80 (m, 1H), 3.67 (dd, $J = 11.1, 3.0$ Hz, 1H), 2.33 – 2.25 (m, 1H), 1.83 – 1.78 (m, 1H). ^{13}C NMR (151 MHz, CDCl_3) δ 163.2, 161.6, 161.6, 141.6, 134.1, 134.0, 133.9, 129.3, 129.5, 129.5, 129.7, 129.6, 129.3, 126.0, 124.6, 115.1, 115.3, 115.3, 115.2, 115.1, 115.0, 112.8, 75.1, 74.8, 73.1, 72.9, 72.6, 71.9, 70.0, 67.5, 66., 431.1. HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{32}\text{H}_{31}\text{Cl}_3\text{O}_5\text{Na}^+$ 623.1129; found 623.1122.



The compound was synthesized according to the general procedure (1), affording **4j**, and purified by column chromatography giving a light yellowish sticky solid (30.3 mg, 69% yield). R_f (Hexane/EtOAc = 80/20): 0.55; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 6.23 (dd, $J = 14.4, 6.3$ Hz, 1H), 6.17 (dd, $J = 11.5, 1.8$ Hz, 1H), 5.72 (s, 1H), 4.09 (s, 1H), 3.92 (t, $J = 6.5$ Hz, 1H), 3.79 (ddd, $J = 13.7, 6.2, 3.6$ Hz, 2H), 3.73 – 3.68 (m, 2H), 3.64 – 3.59 (m, 2H), 3.57 – 3.54 (m, 2H), 3.47 – 3.44 (m, 4H), 2.48 (dd, $J = 15.1, 8.0$ Hz, 1H), 2.26 – 2.21 (m, 1H), 1.17 – 1.14 (m, 6H), 1.09 (s, 3H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 132.7, 130.3, 125.3, 124.9, 92.5, 77.7, 75.9, 69.9, 69.4, 68.3, 66.9, 65.3, 62.9, 30.9, 15.3, 15.5, 15.2. **HRMS (ESI)** m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{17}\text{H}_{29}\text{O}_5^+$ 313.2010; found 313.2006.

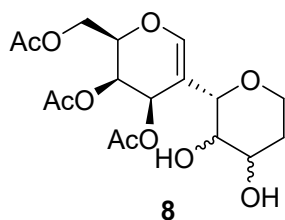


The compound was synthesized according to the general procedure (1), affording **4k**, and purified by column chromatography giving an amber sticky solid (29.6 mg, 64% yield). R_f (Hexane/EtOAc = 70/30): 0.45 $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 8.04 (d, $J = 7.1$ Hz, 2H), 7.96 – 7.95 (m, 2H), 7.89 (d, $J = 1.2$ Hz, 1H), 7.83 (s, 1H), 7.54 (s, 1H), 7.47 (dd, $J = 5.4, 1.9$ Hz, 2H), 7.40 (s, 3H), 7.34 (s, 2H), 7.28 (s, 1H), 6.71 (s, 1H), 6.08 (d, $J = 4.4$ Hz, 1H), 5.81 – 5.78 (m, 1H), 5.69 (ddd, $J = 10.0, 5.6, 2.1$ Hz, 1H), 5.61 – 5.58 (m, 1H), 4.89 – 4.86 (m, 1H), 4.66 – 4.61 (m, 1H), 4.52 – 4.49 (m, 1H), 4.13 (s, 2H), 4.04 – 4.01 (m, 1H), 2.18 – 2.13 (m, 1H), 2.09 – 2.06 (m, 1H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 166.5, 165.9, 165.3, 143.0, 133.8, 133.8, 133.7, 133.4, 133.4, 133.2, 130.2, 130.2, 130.2, 129.9, 129.8, 129.8, 128.6, 128.5, 128.5, 128.5, 128.5, 128.4, 126.1, 123.9, 111.0, 72.6, 71.5, 66.2, 66.0, 63.7, 62.5, 30.6. **HRMS (ESI)** m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{32}\text{H}_{28}\text{O}_8\text{Na}^+$ 563.1676; found 563.1676.

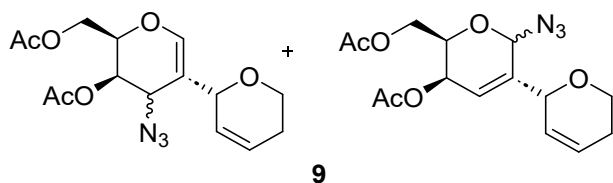


The compound was synthesized according to the general procedure (1), affording **7**, and purified by column chromatography giving a light red gummy liquid (27.0 mg, 62% yield). R_f (Hexane/

EtOAc = 70/30): 0.60; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 5.94 – 5.88 (m, 0.23H), 5.76 (dd, $J = 7.7$, 5.4 Hz, 1H), 5.69 – 5.59 (m, 2.36H), 5.21 (d, $J = 5.0$ Hz, 1.23H), 4.24 – 4.09 (m, 7.40H), 3.99 – 3.85 (m, 1.23H), 3.65 (dd, $J = 8.3$, 2.3 Hz, 1.26H), 2.22 – 2.12 (m, 1.22H), 2.04 (s, 3.67H), 2.01 (s, 3.79H), 1.99 – 1.92 (m, 1.24H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 170.9, 170.4, 142.1, 141.8, 126.3, 123.5, 118.8, 118.7, 74.1, 73.6, 73.2, 73.1, 66.2, 65.9, 65.5, 65.4, 64.9, 63.3, 29.3, 21.1, 20.9. **HRMS (ESI)** m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{15}\text{H}_{20}\text{O}_6\text{Na}^+$ 319.1152; found 319.1150.

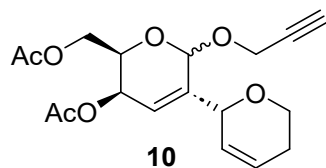


The compound was synthesized according to the general procedure (2), affording **8**, and purified by column chromatography giving a yellowish liquid (37.8 mg, 69% yield). R_f (Hexane/ EtOAc = 50/50): 0.50; $^1\text{H NMR}$ (600 MHz, CDCl_3) 5.60 (s, 0.60H), 5.59 (s, 1H), 5.57 (t, $J = 5.0$ Hz, 1.65H), 5.51 – 5.49 (m, 1.78H), 4.34 (dd, $J = 8.2$ Hz, 1.62H), 4.09 – 4.08 (m, 1.77H), 4.01 – 3.99 (m, 3.36H), 3.78 – 3.73 (m, 3.34H), 2.08 (bs, 5.62H), 2.05 (bs, 5.83H), 2.00 (s, 4.68H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 170.3, 169.8, 169.3, 159.5, 121.1, 78.8, 73.3, 69.3, 68.9, 68.7, 65.8, 62.1, 61.8, 30.5, 20.7, 20.6, 20.4. **HRMS (ESI)** m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{17}\text{H}_{24}\text{O}_{10}\text{Na}^+$ 411.1262; found 411.1250.



The compound was synthesized according to the general procedure (3), affording **9**, and purified by column chromatography giving beige sticky solid (39.1 mg, 82% yield). R_f (Hexane/ EtOAc = 70/30): 0.55; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 6.66 (s, 0.71H), 6.59 (s, 1H), 6.04 – 5.96 (m, 1.73H), 5.79 (d, $J = 4.2$ Hz, 2.85H), 5.67 (s, 1.89H), 5.06 – 5.02 (m, 2.33H), 4.96 (s, 1.76H), 4.18 (d, $J = 6.9$ Hz, 12.54H), 4.10 – 4.07 (m, 1.62H), 2.27 – 2.14 (m, 4.24H), 2.04 – 2.00 (m, 14.14H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 169.7, 169.5, 169.3, 169.3, 168.9, 168.9, 143.5, 142.7, 140.8, 140.6, 125.4, 125.3, 125.2, 125.2, 122.5, 122.4, 119.2, 118.7, 108.5, 107.9, 83.8, 83.2, 71.7, 71.6, 70.2,

69.9, 68.9, 67.7, 67.5, 65.9, 65.9, 65.4, 65.2, 64.8, 61.8, 61.5, 61.5, 61.2, 53.1, 52.4, 29.5, 27.7, 27.2, 19.8, 19.7, 19.7. **HRMS (ESI)** m/z : $[M+Na]^+$ calcd for $C_{15}H_{19}N_3O_6Na^+$ 360.1166; found 360.1160.



The compound was synthesized according to the general procedure (3), affording **10**, and purified by column chromatography giving a light yellowish gummy solid (41.5 mg, 84% yield). R_f (Hexane/ EtOAc = 70/30): 0.60; **1H NMR (600 MHz, $CDCl_3$)** δ 6.12 (d, J = 5.6 Hz, 1H), 6.01 (d, J = 5.4 Hz, 1H), 5.77 (ddd, J = 9.3, 5.2, 2.2 Hz, 2H), 5.70 – 5.64 (m, 2H), 5.35 (s, 1H), 5.24 (s, 1H), 5.06 – 5.02 (m, 2H), 4.27 – 4.22 (m, 6H), 4.19 – 4.16 (m, 8H), 4.06 – 4.00 (m, 2H), 2.40 (d, J = 2.3 Hz, 2H), 2.20 – 2.09 (m, 4H), 2.01 – 2.00 (m, 12H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.6, 169.4, 169.3, 141.4, 141.2, 125.3, 125.1, 122.9, 122.7, 119.2, 118.4, 92.0, 90.9, 78.1, 77.9, 73.9, 73.7, 71.2, 70.4, 66.0, 65.8, 65.4, 65.2, 62.0, 61.9, 61.7, 61.7, 53.8, 53.5, 27.8, 19.9, 19.8. **HRMS (ESI)** m/z : $[M+Na]^+$ calcd for $C_{18}H_{22}O_7Na^+$ 373.1258; found 373.1250.

8. NMR Spectra:

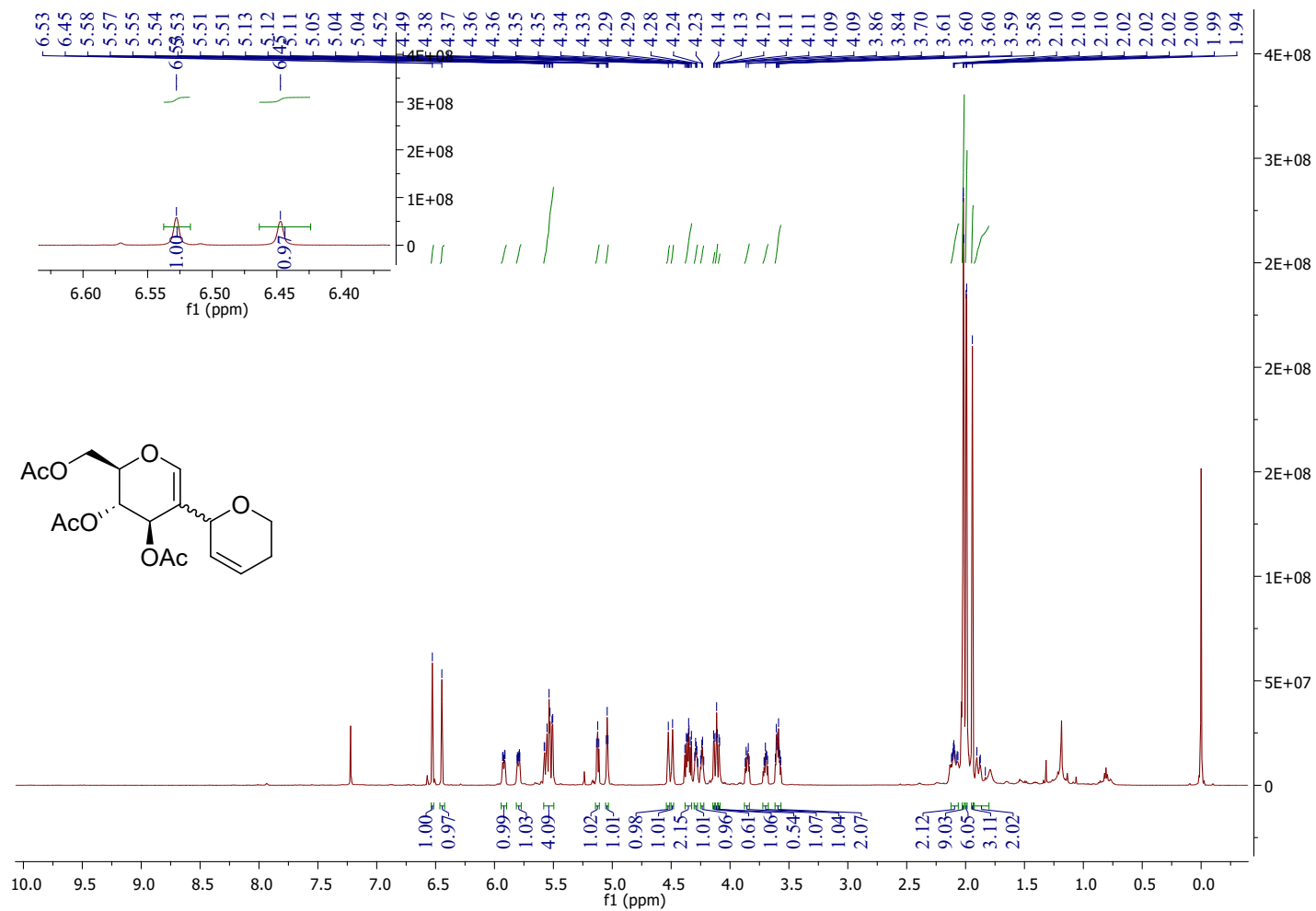


Fig.: ¹H NMR (600 MHz, CDCl₃) of compound 4a

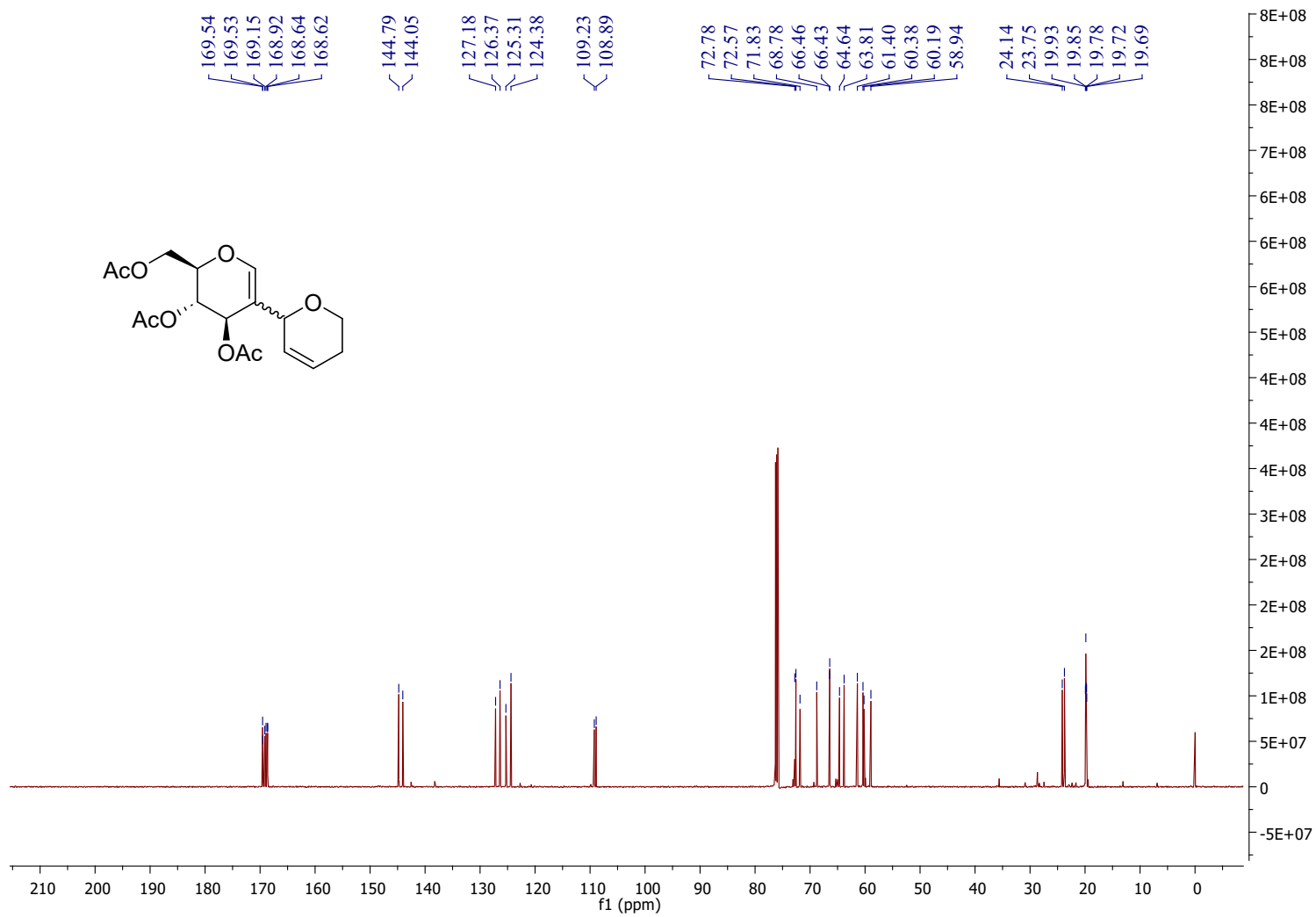


Fig.: ¹³CNMR (151 MHz, CDCl₃) of compound 4a

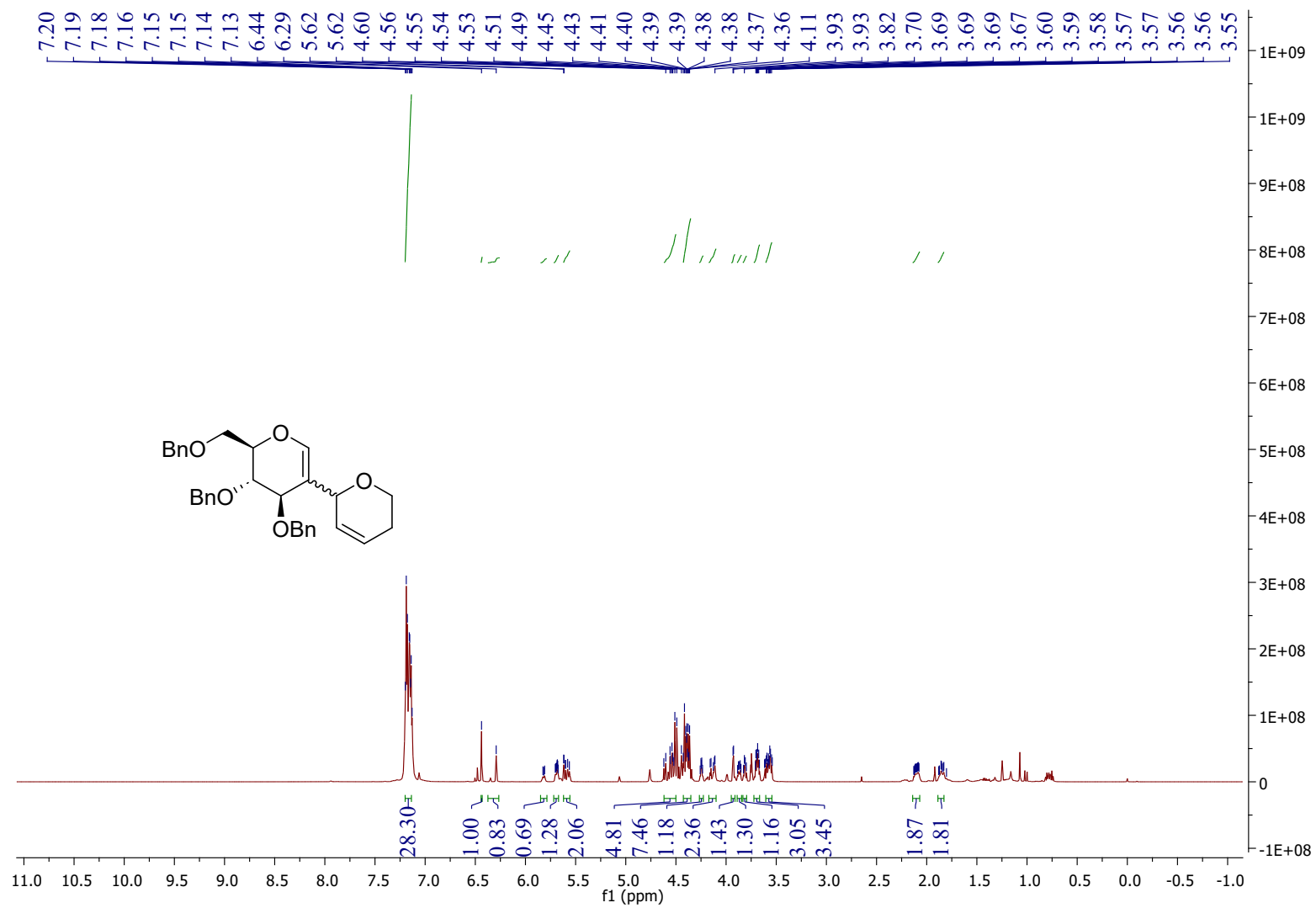


Fig.: $^1\text{H NMR}$ (600 MHz, CDCl_3) of compound **4b**

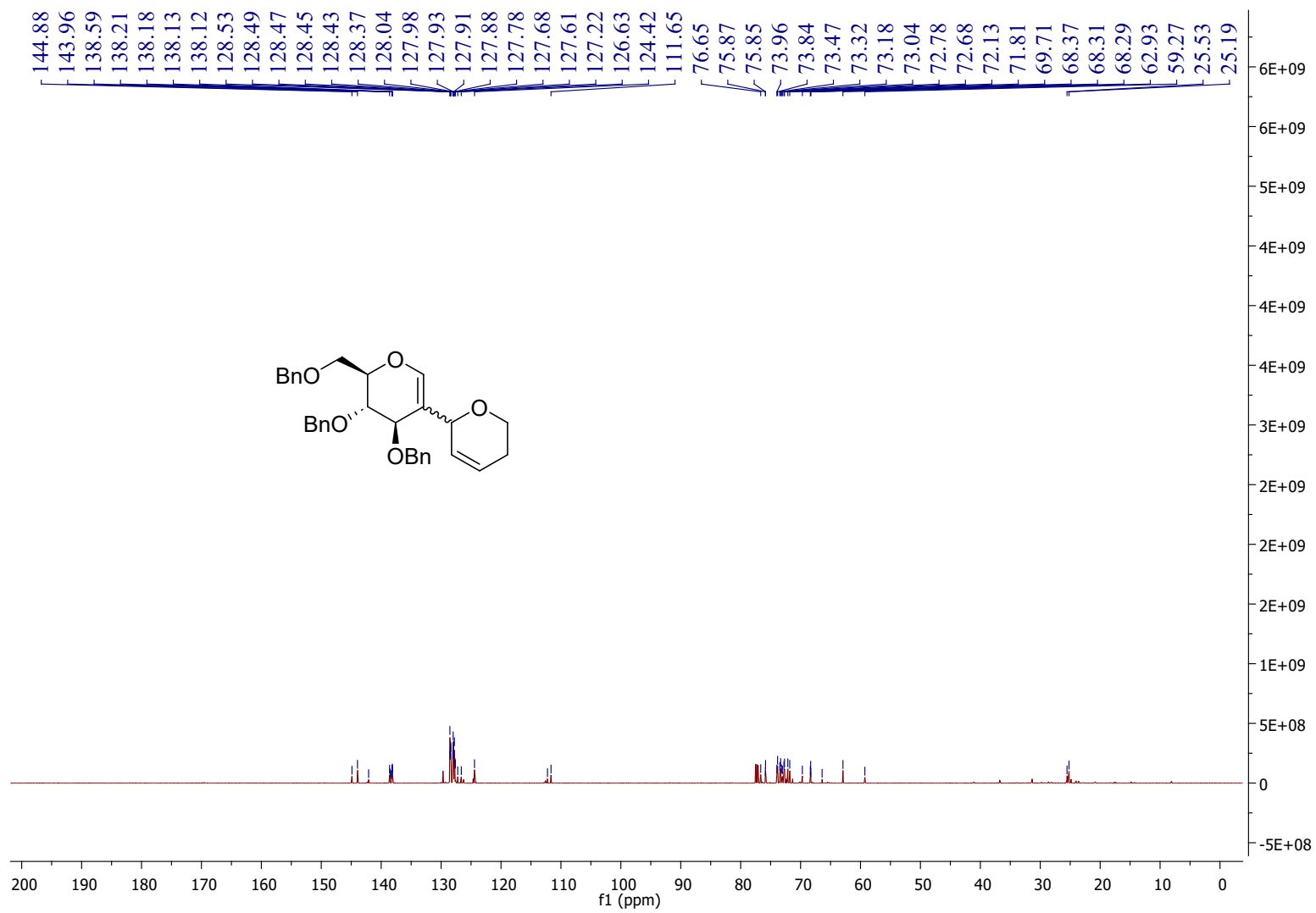


Fig.: ¹³CNMR (151 MHz, CDCl₃) of compound **4b**

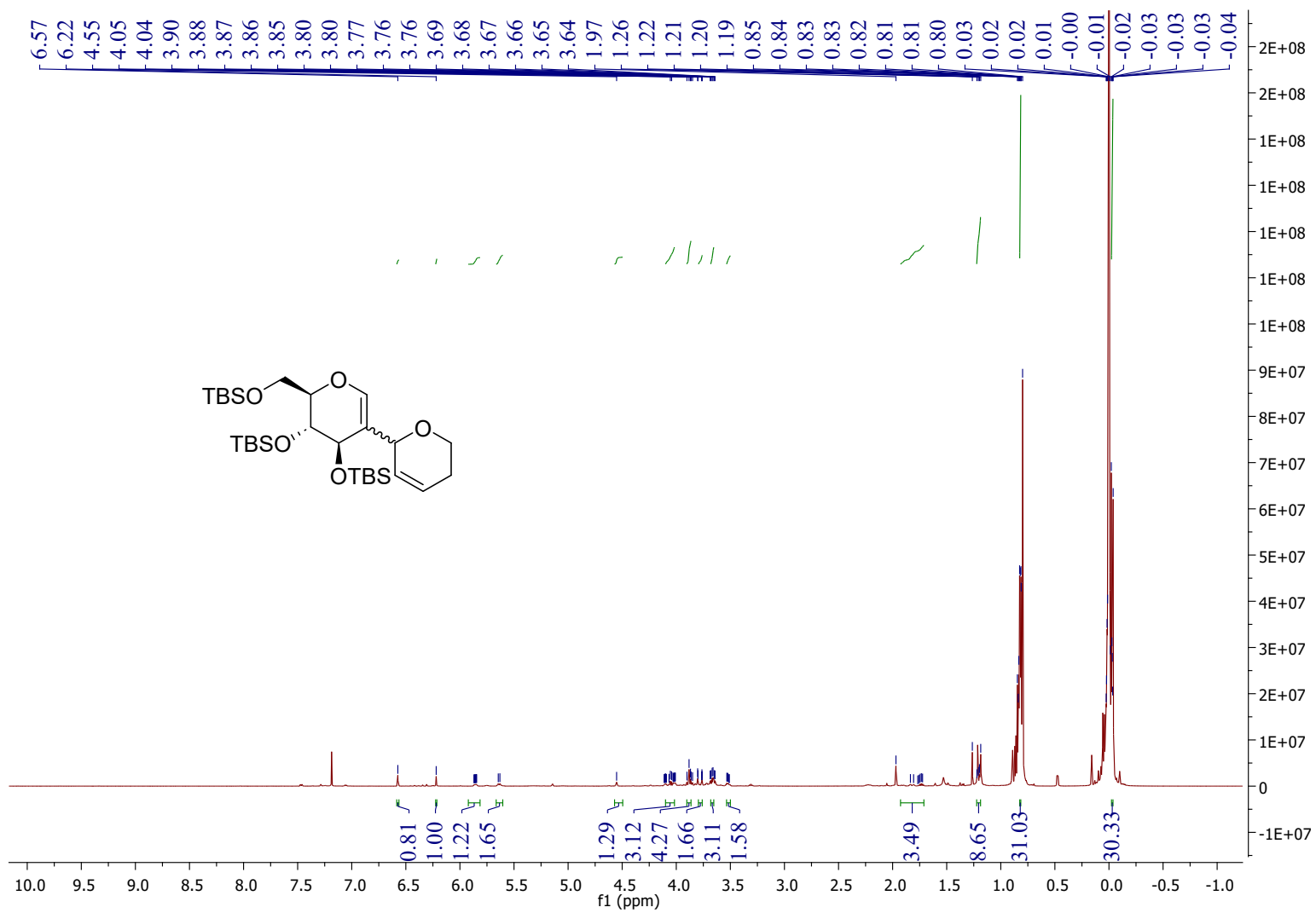


Fig.: ¹HNMR (600 MHz, CDCl₃) of compound 4c

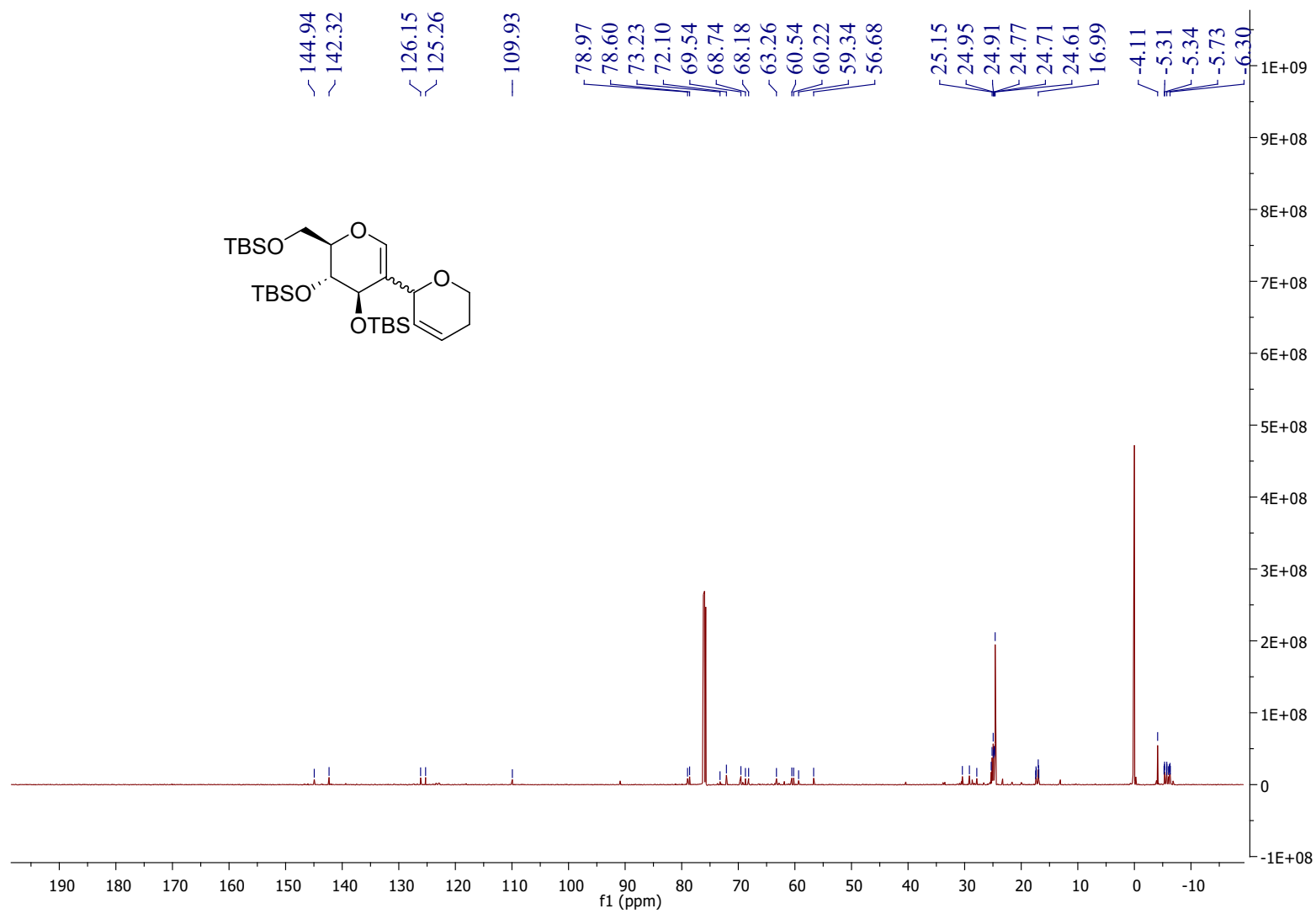


Fig.: ^{13}C NMR (151 MHz, CDCl_3) of compound 4c

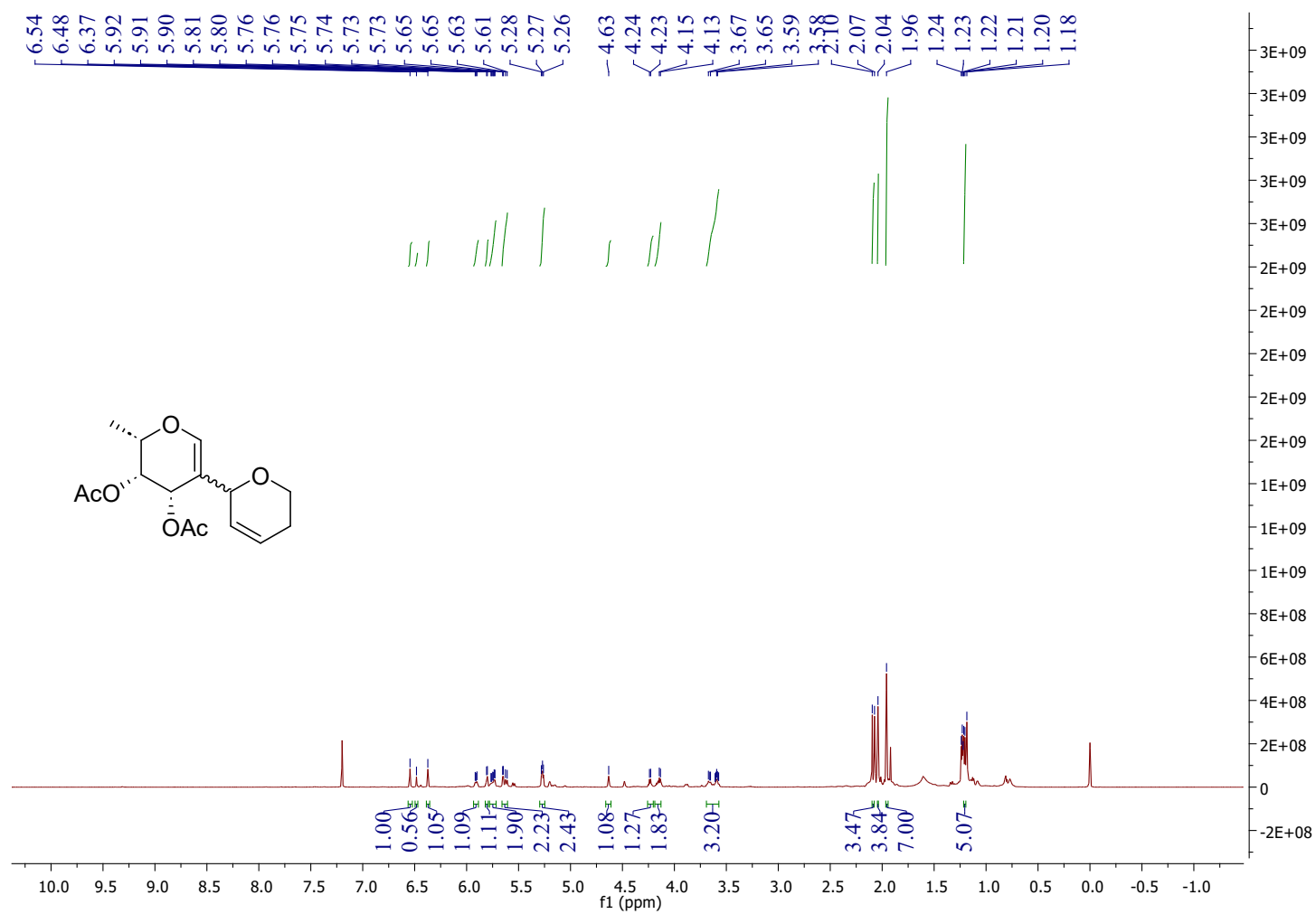


Fig.: ¹H NMR (600 MHz, CDCl₃) of compound 4d

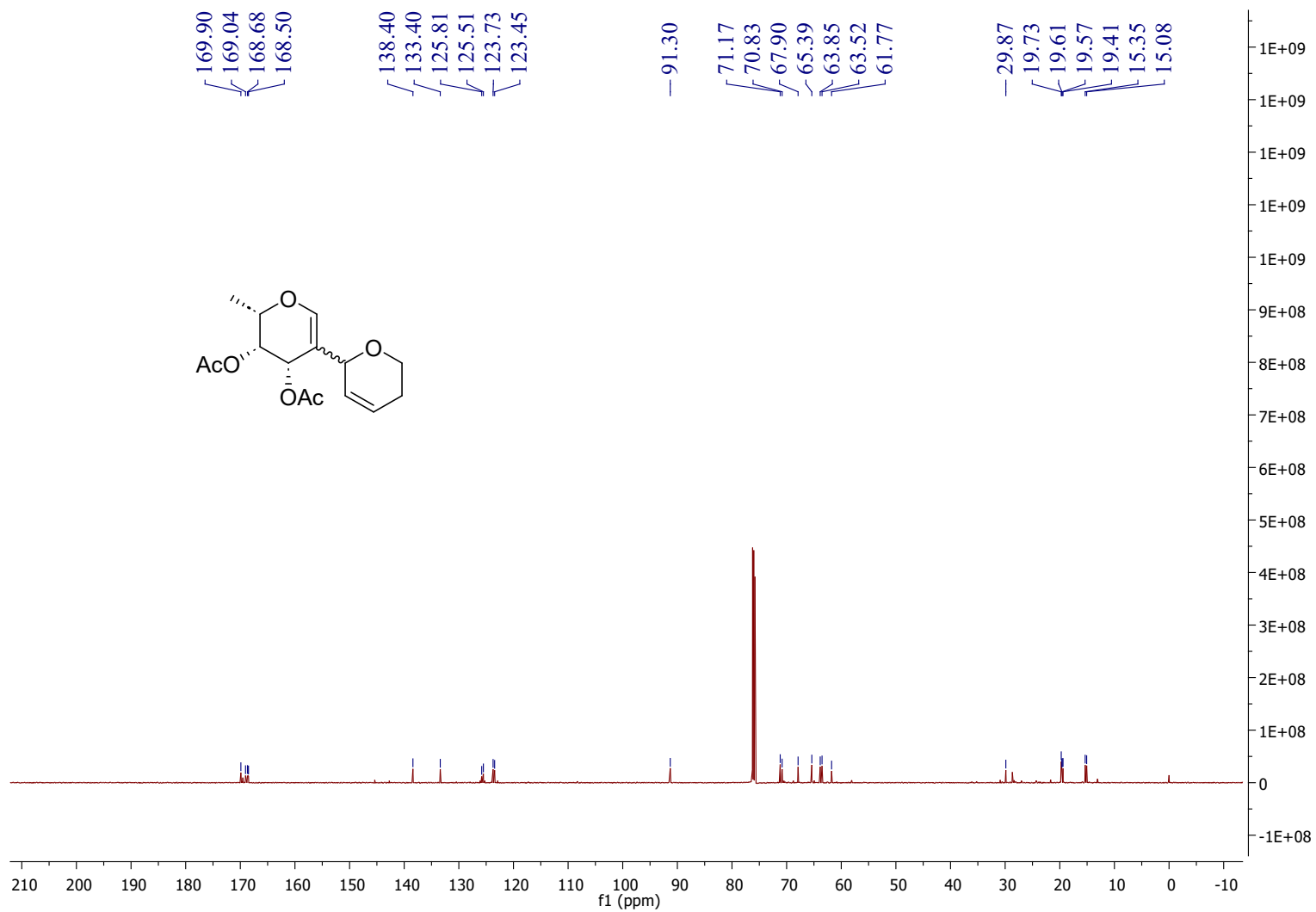


Fig.: ^{13}C NMR (151 MHz, CDCl_3) of compound **4d**

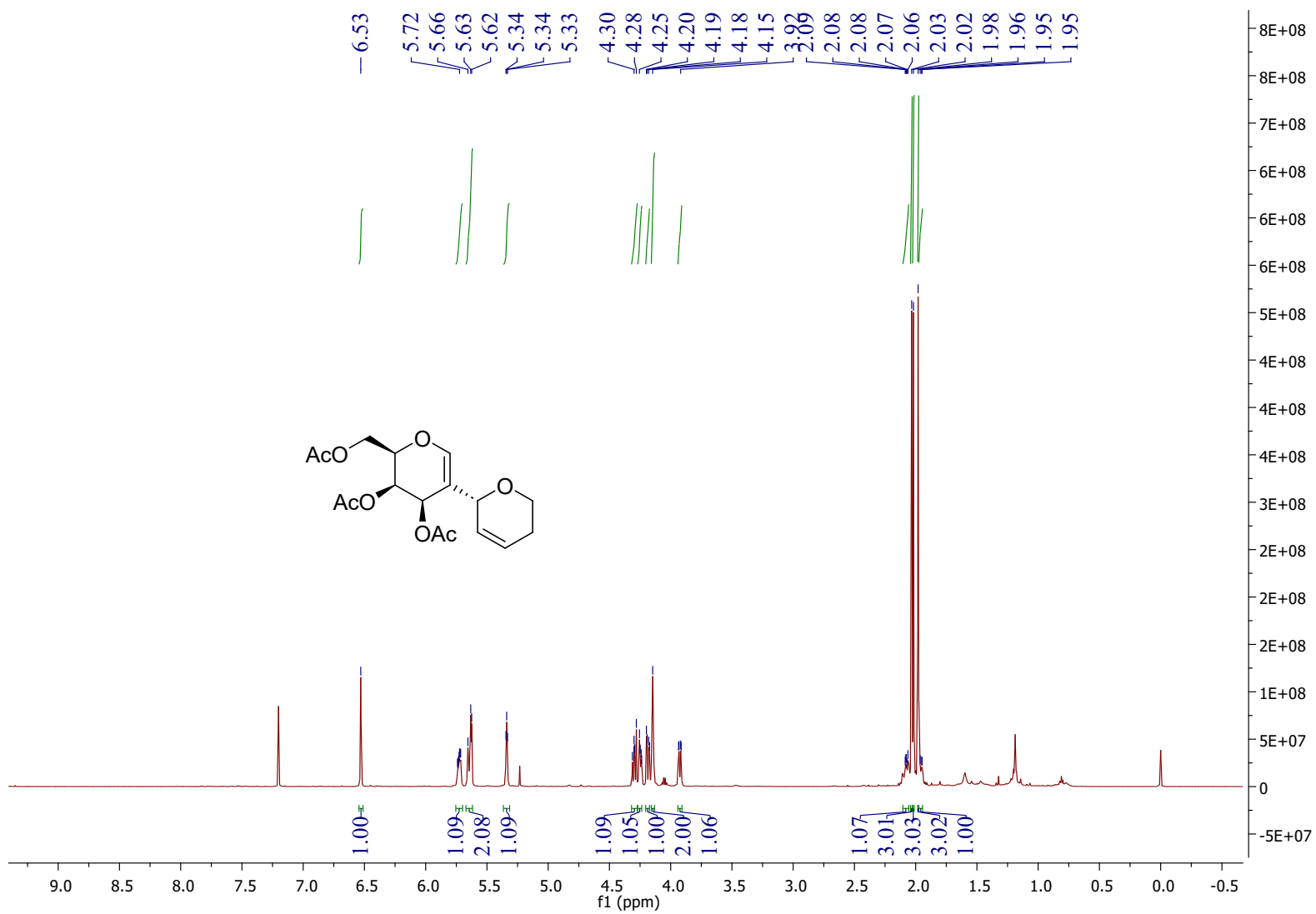


Fig.: ^1H NMR (600 MHz, CDCl_3) of compound 4e

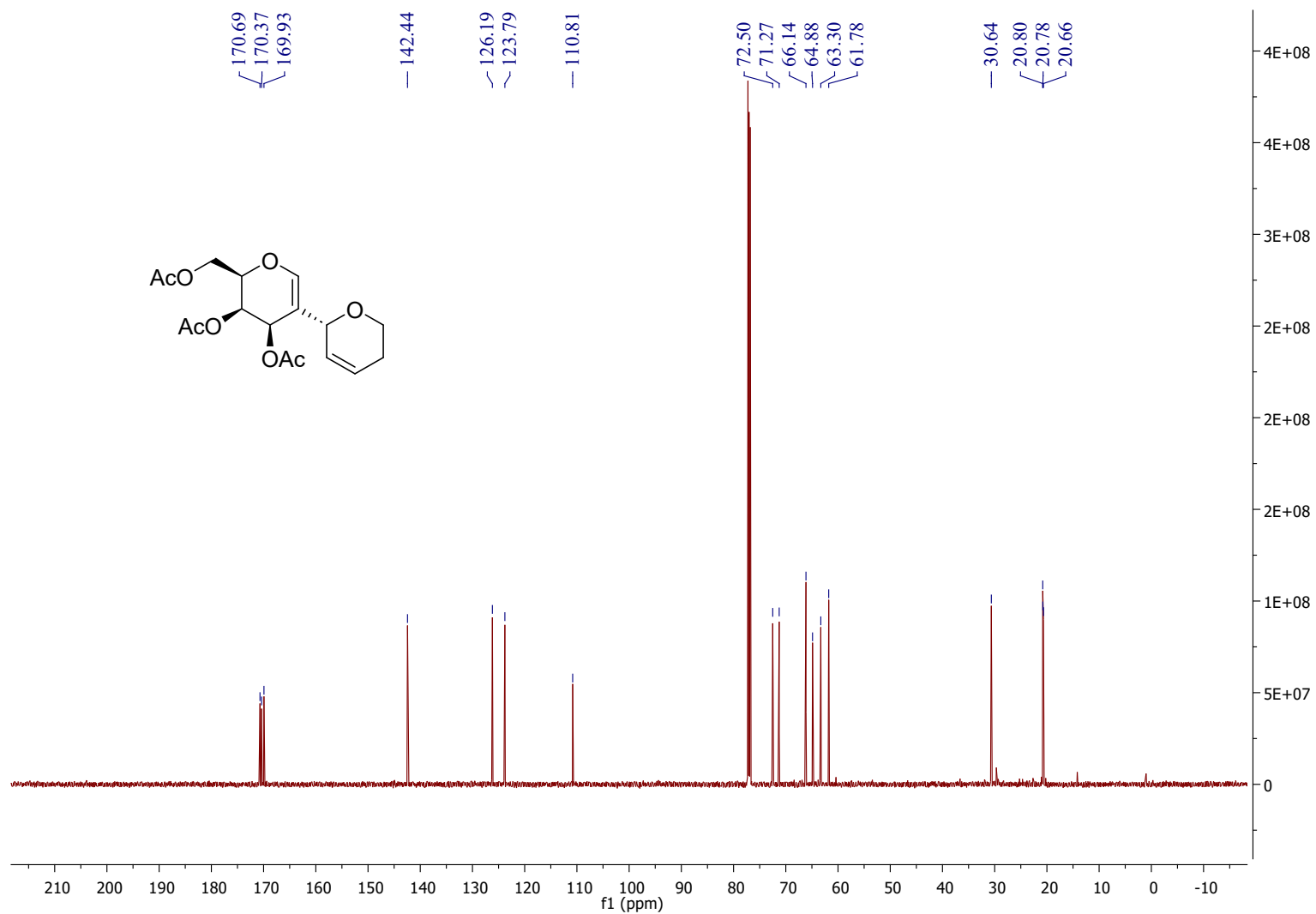


Fig.: ^{13}C NMR (151 MHz, CDCl_3) of compound 4e

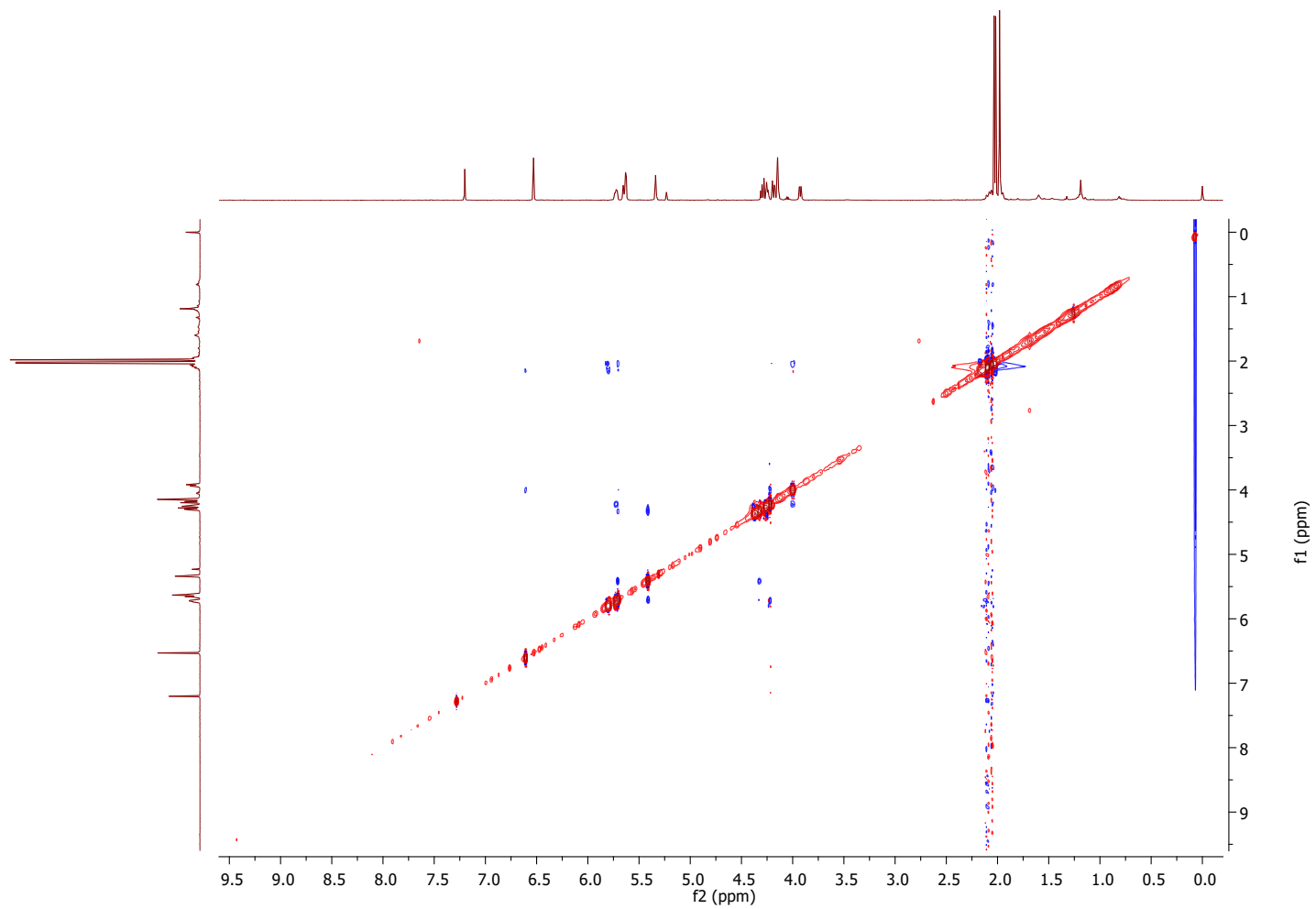


Fig.: NOESY of compound 4e

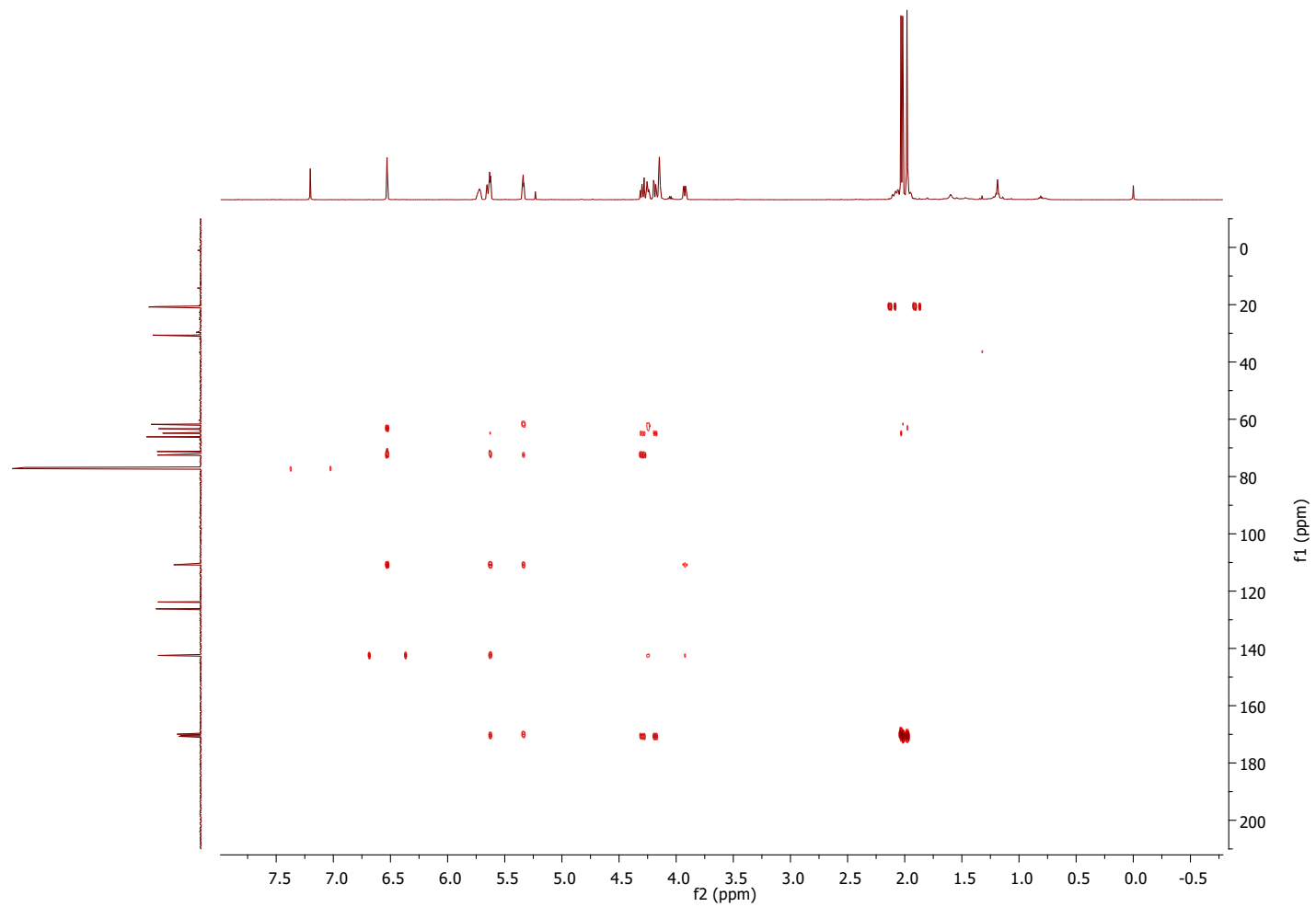


Fig.: HSQC of compound **4e**

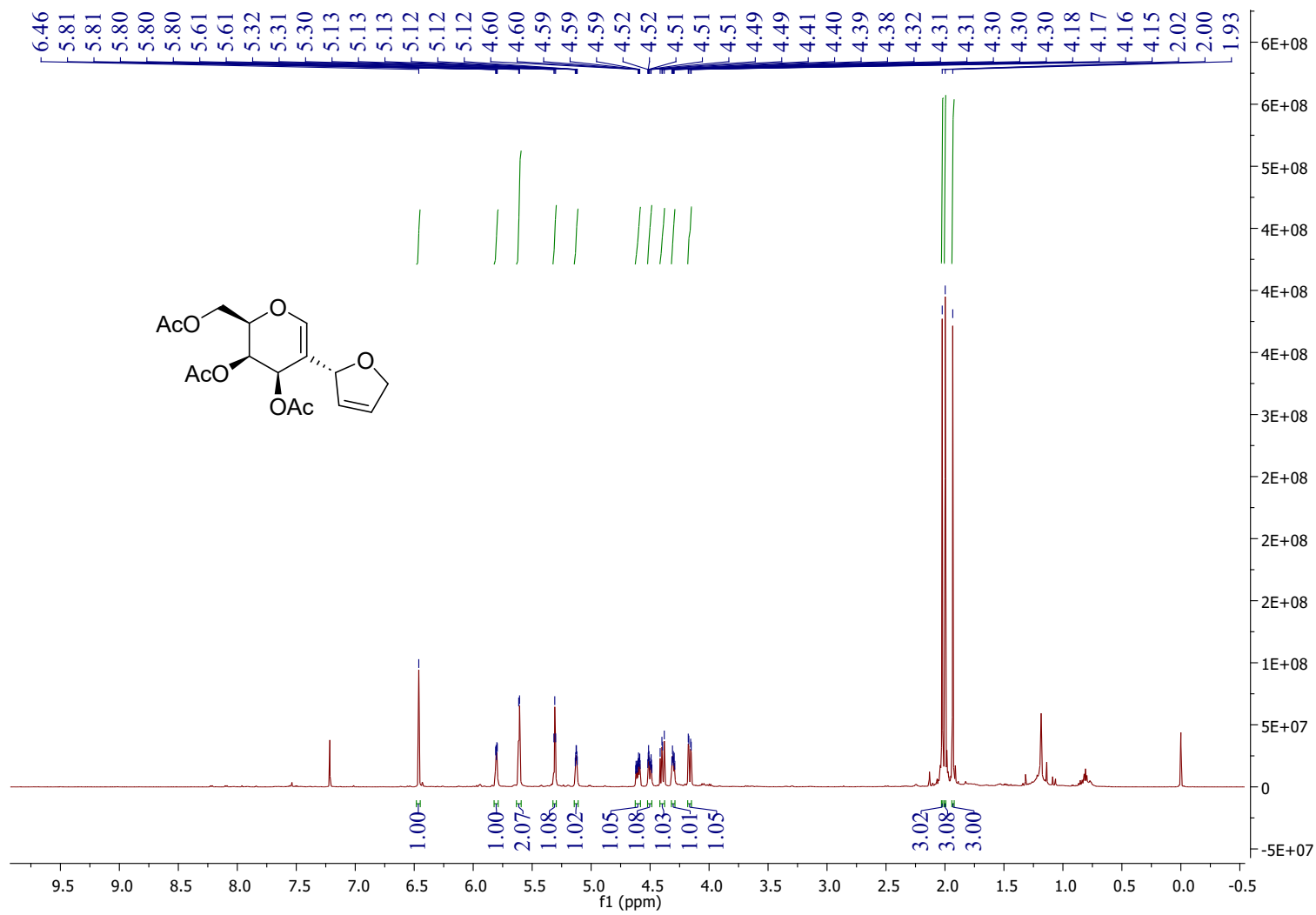


Fig.: ¹HNMR (600 MHz, CDCl₃) of compound 4f

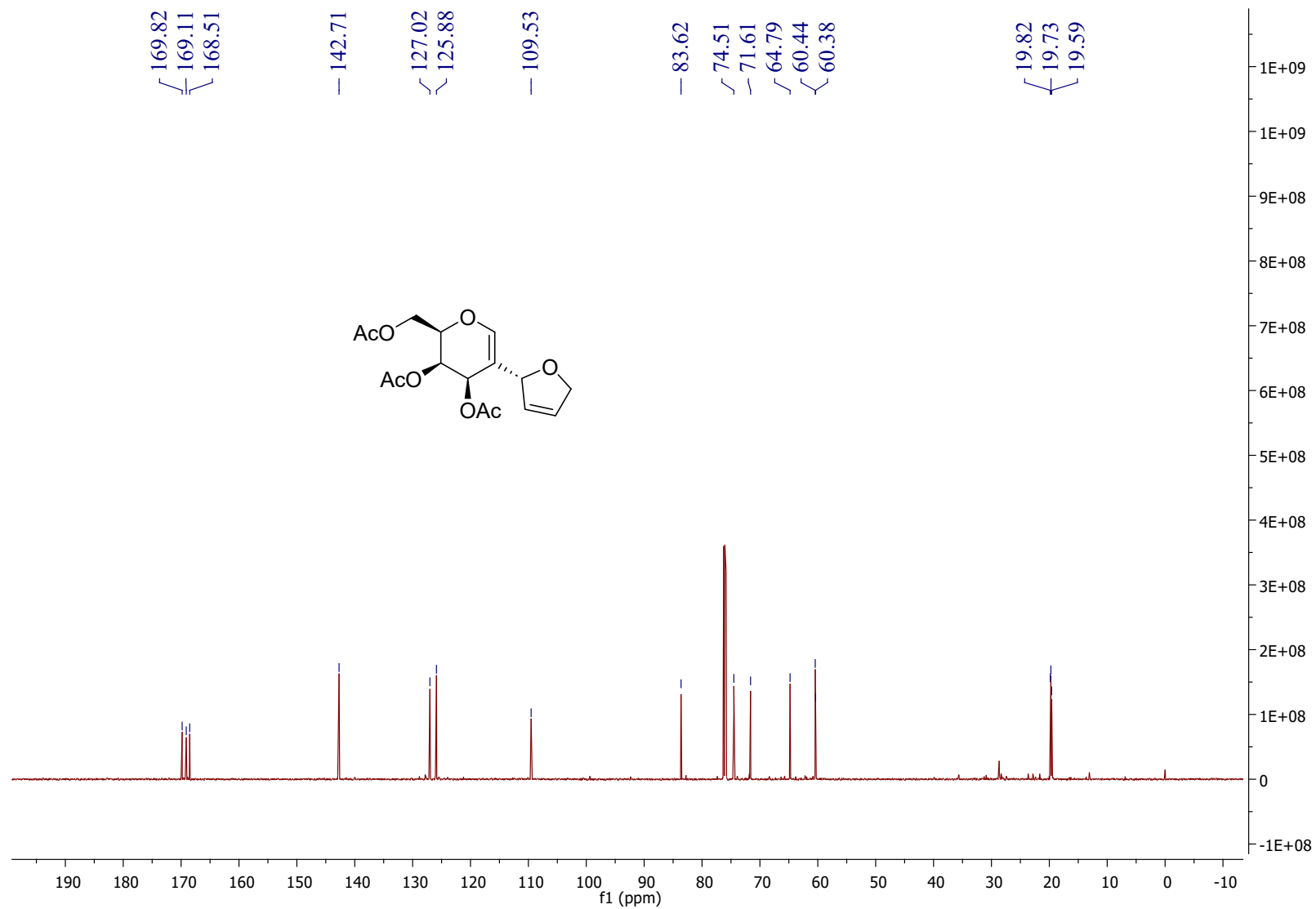


Fig.: ^{13}C NMR (151 MHz, CDCl_3) of compound 4f

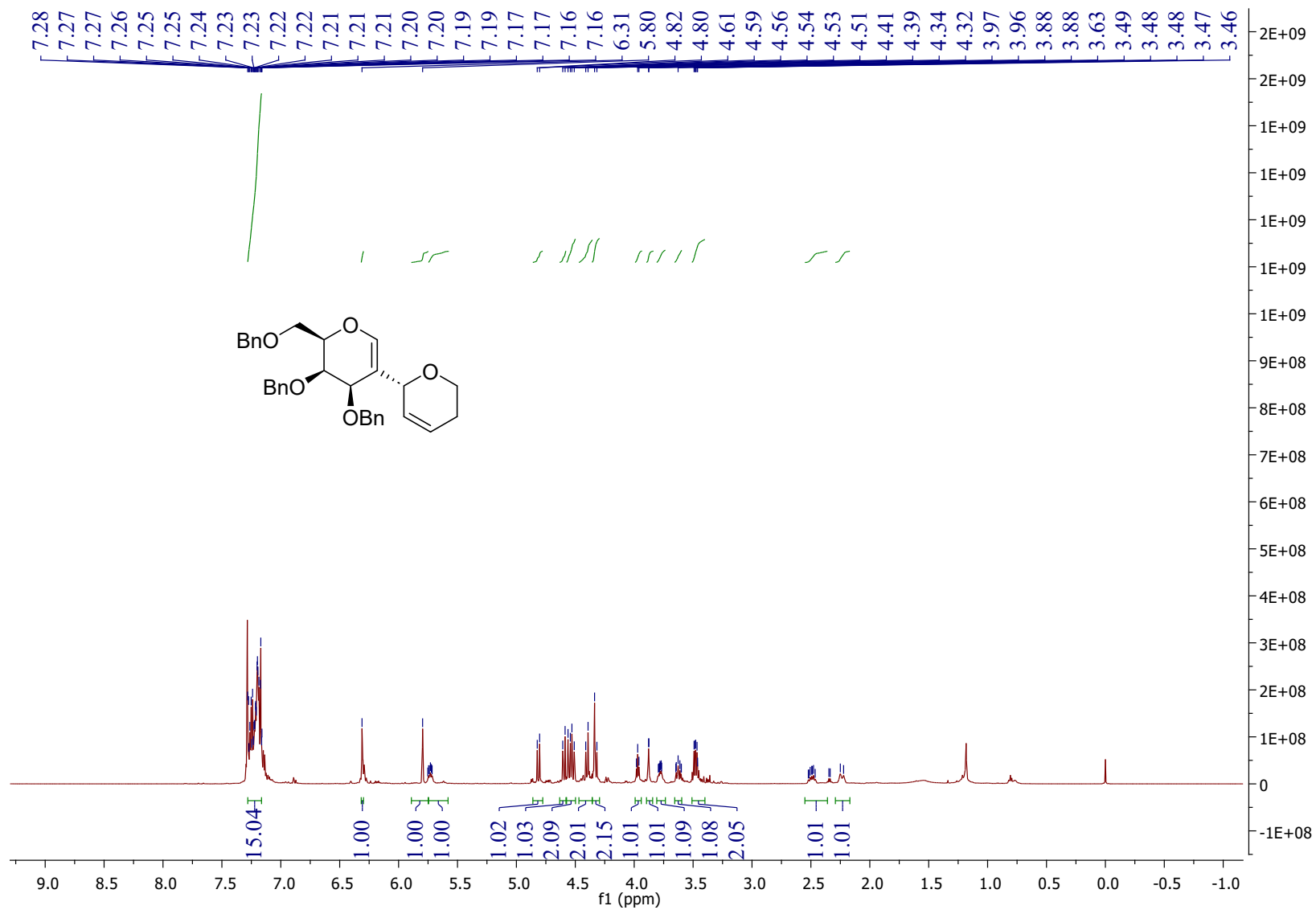


Fig.: ^1H NMR (600 MHz, CDCl_3) of compound **4g**

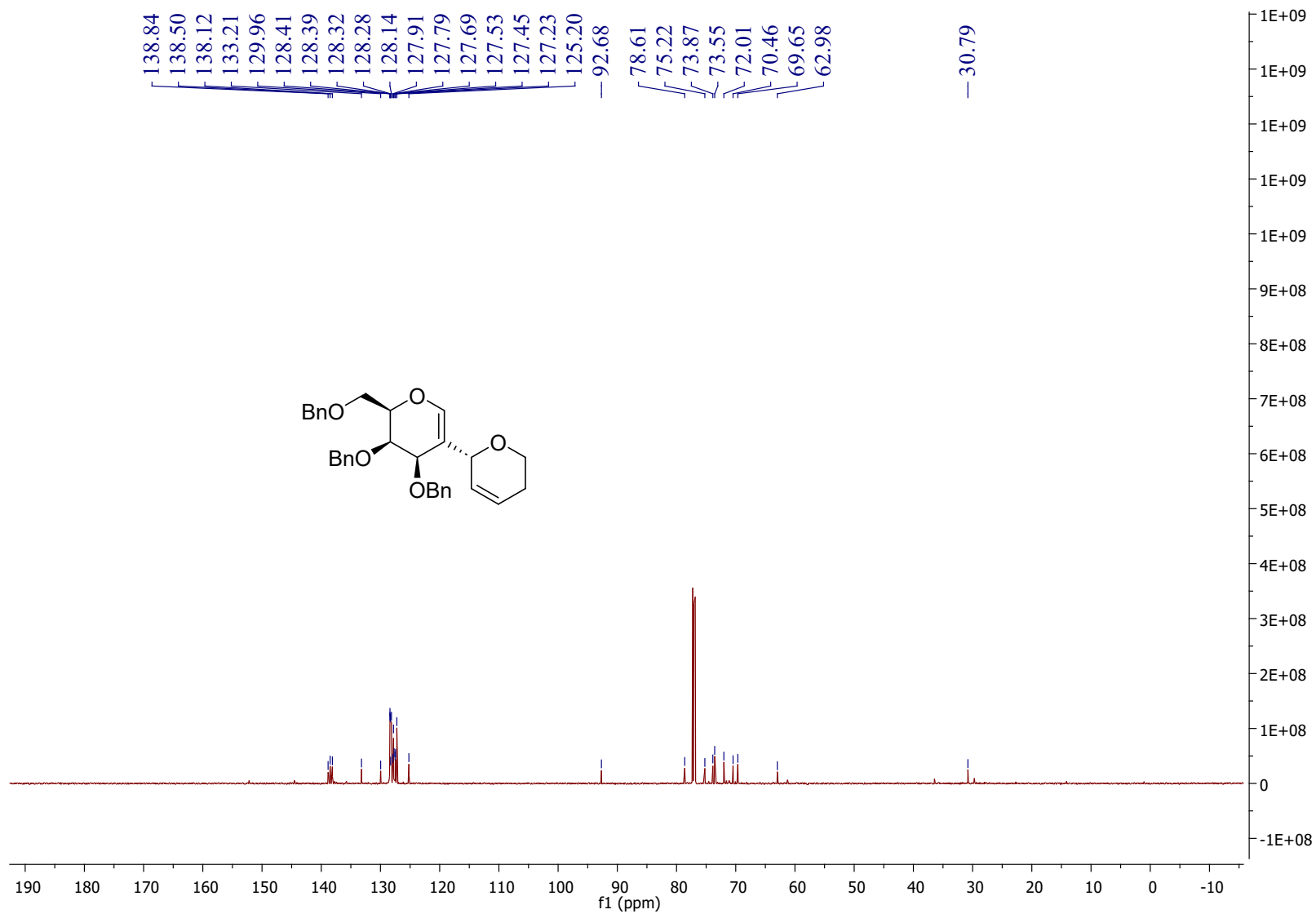


Fig.: ^{13}C NMR (151 MHz, CDCl_3) of compound 4g

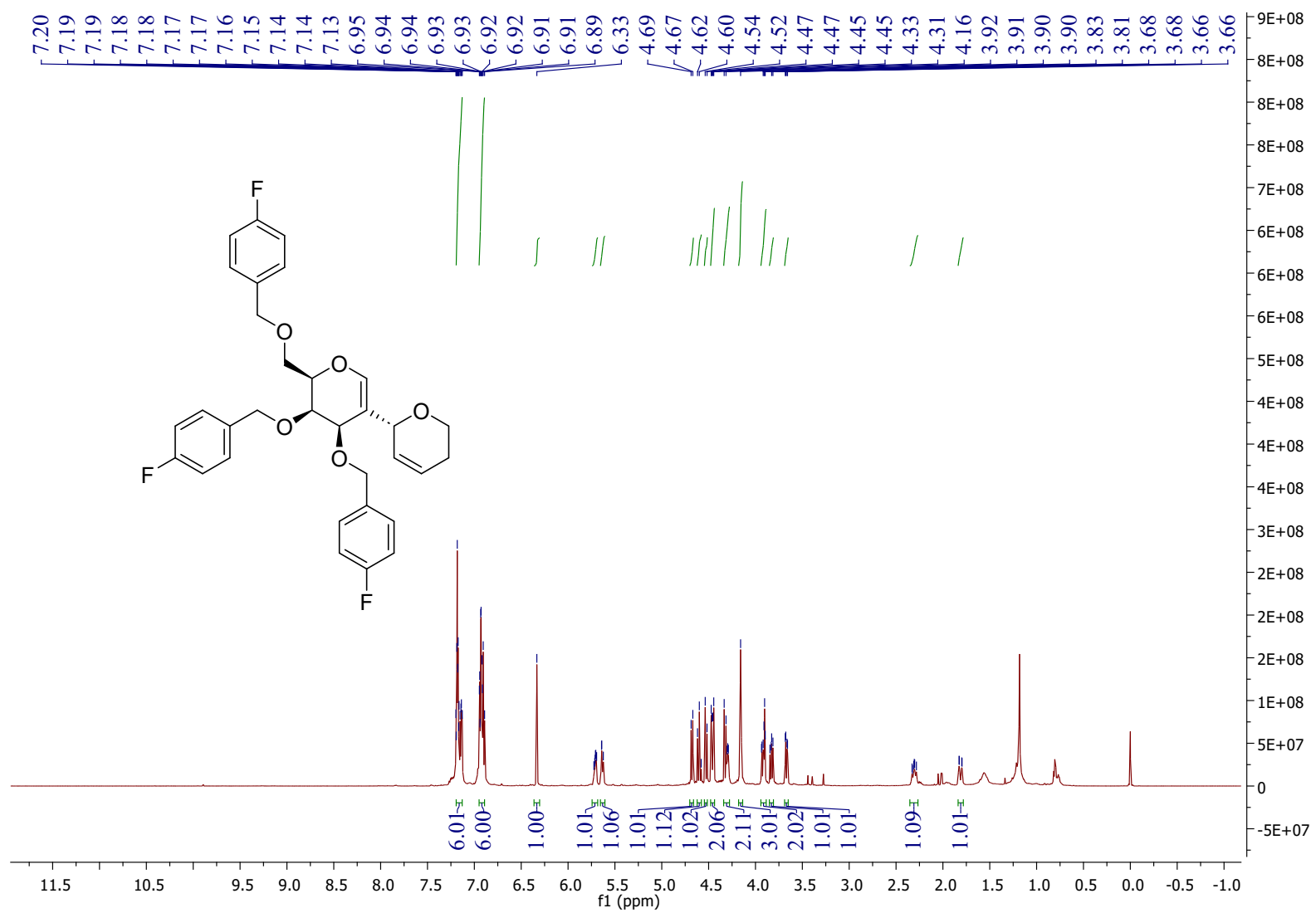


Fig.: $^1\text{H NMR}$ (600 MHz, CDCl_3) of compound **4h**

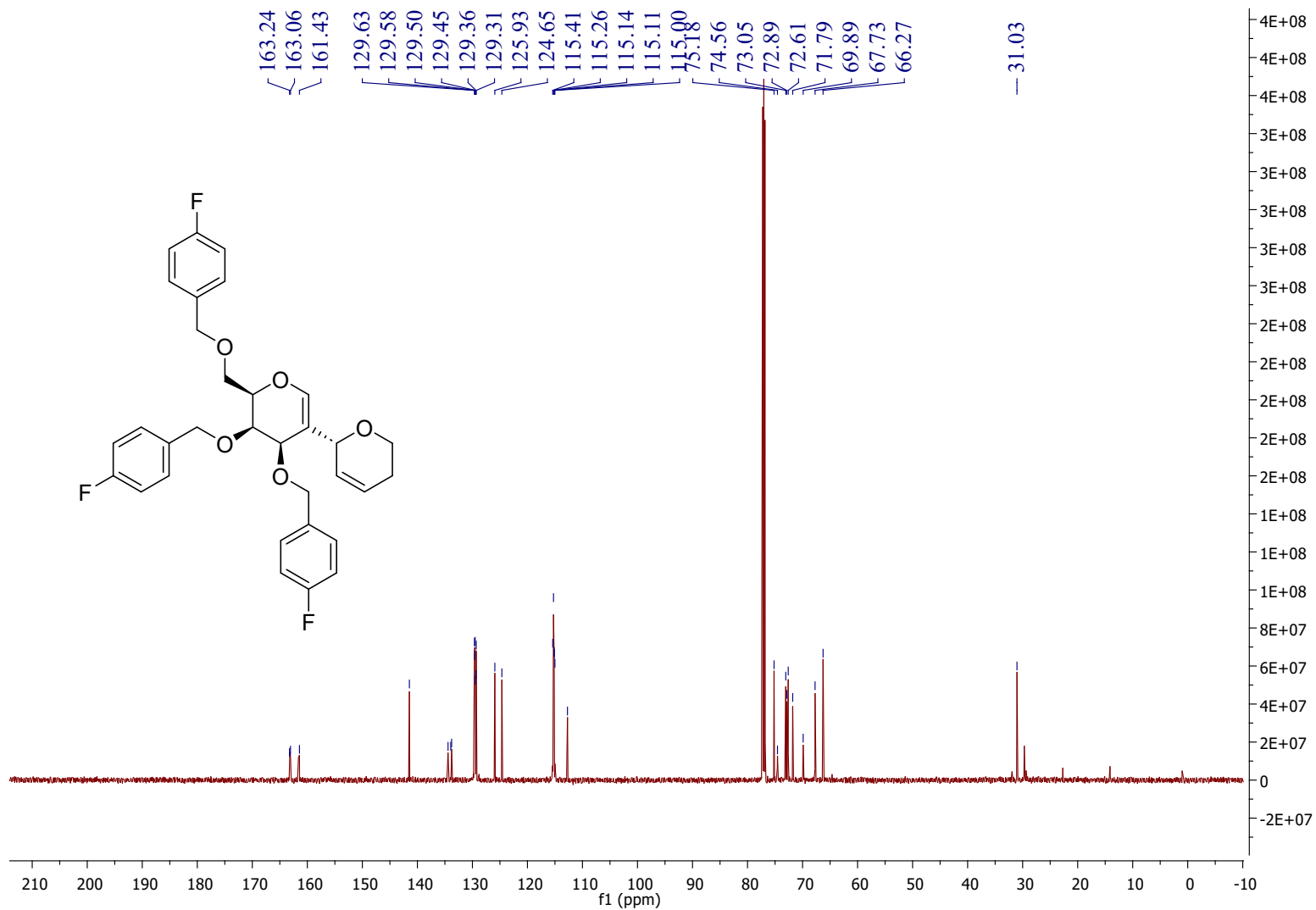
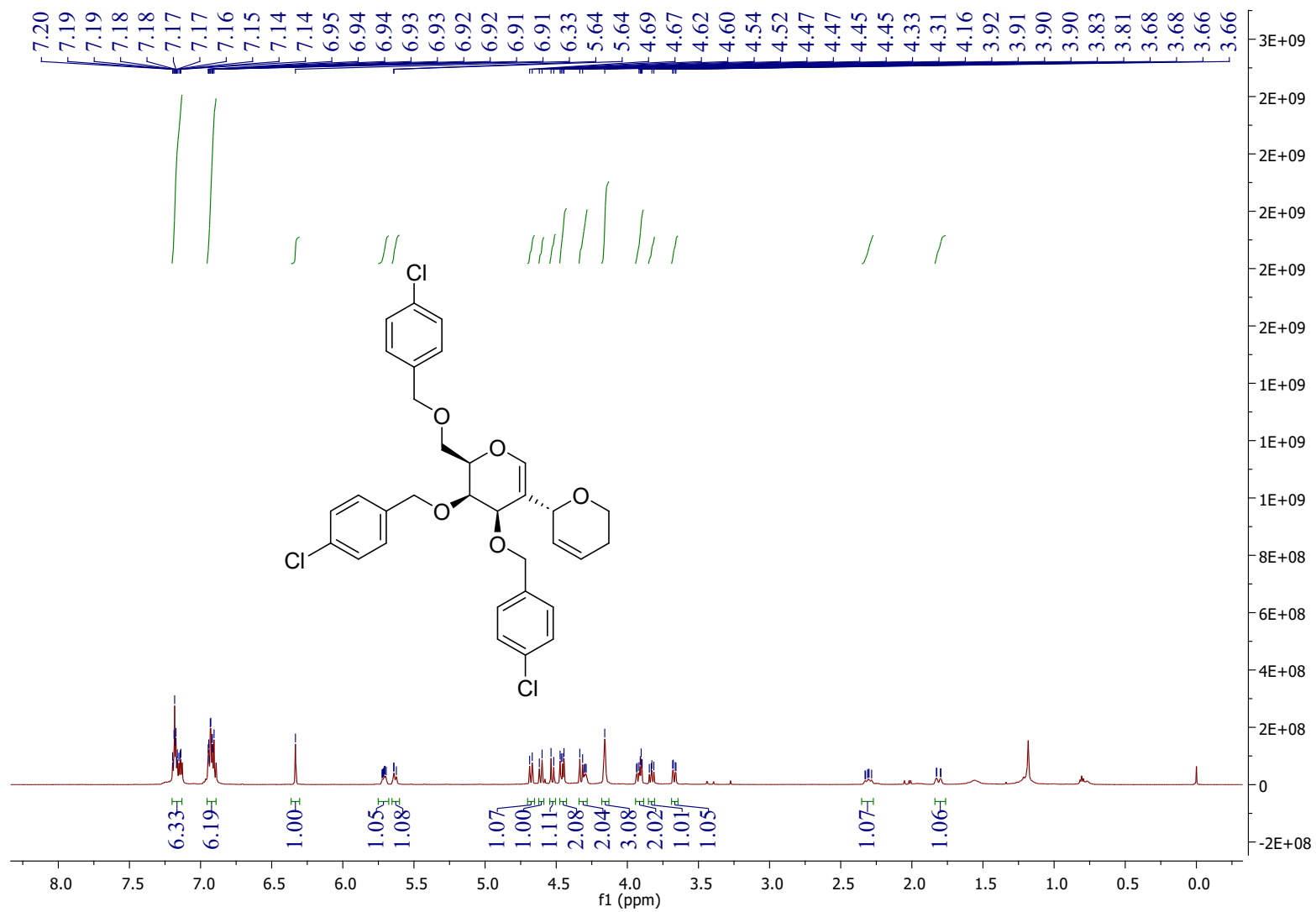


Fig.: ^{13}C NMR (151 MHz, CDCl_3) of compound 4h



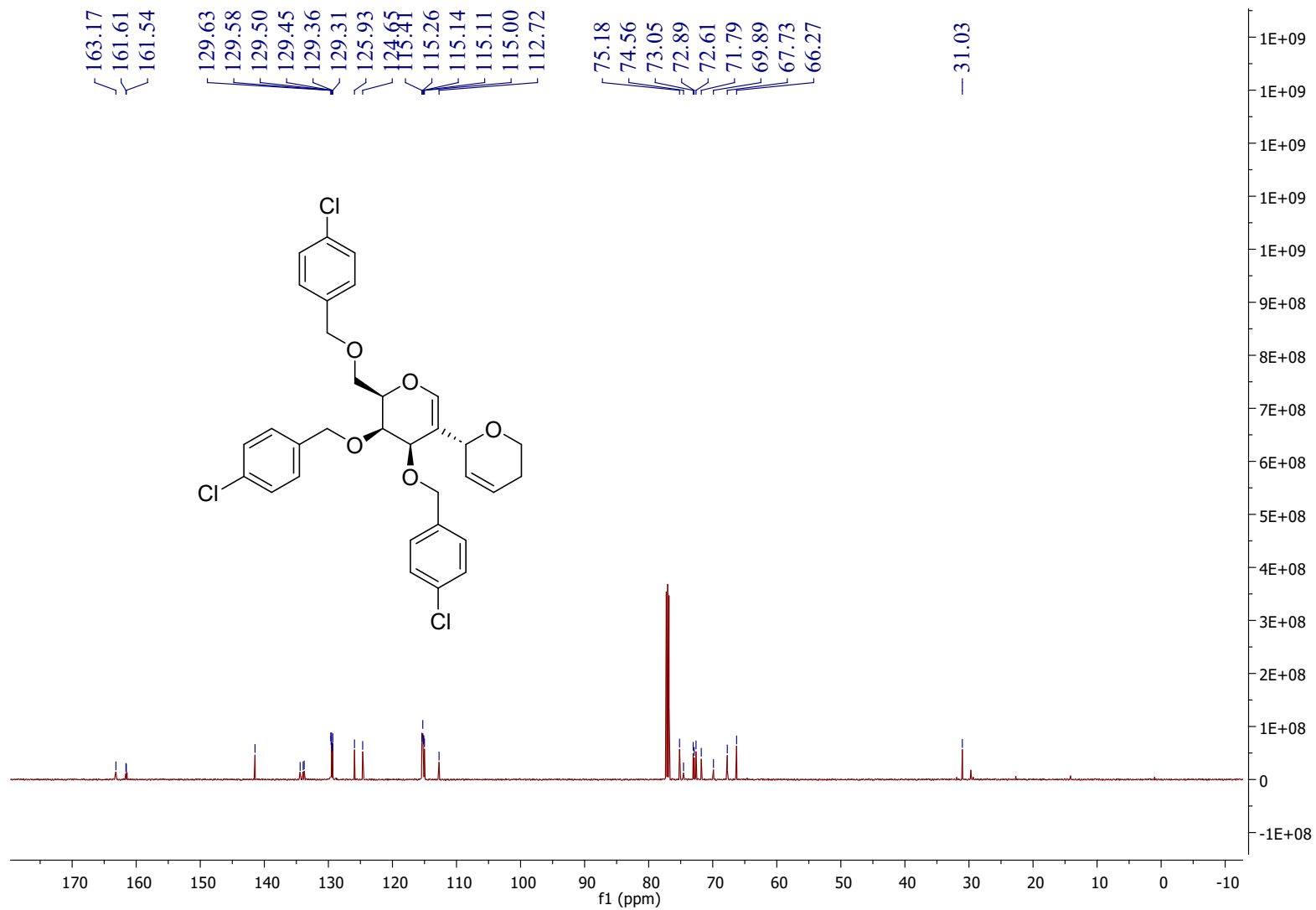


Fig.: ^{13}C NMR (151 MHz, CDCl_3) of compound 4i

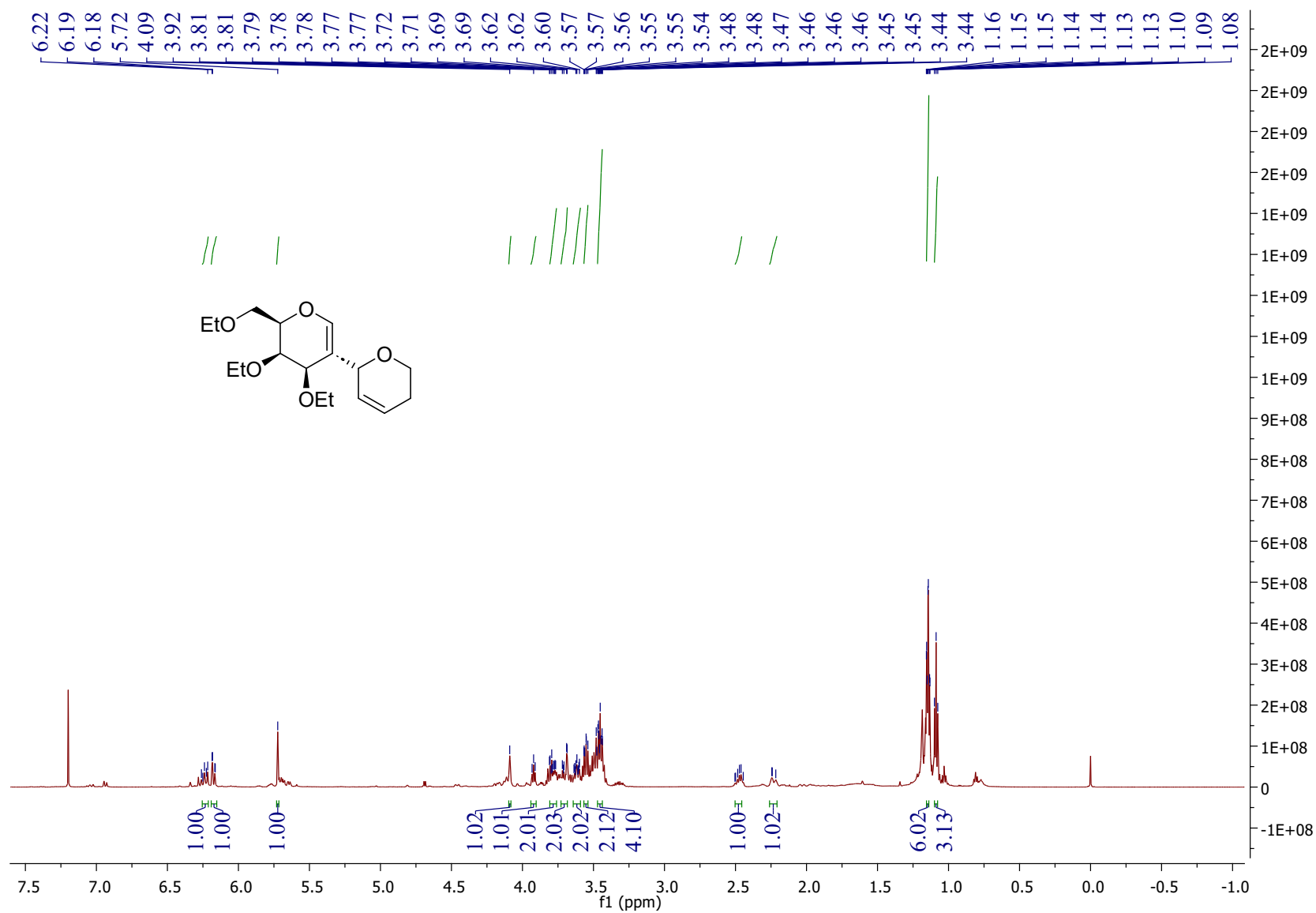


Fig.: ¹HNMR (600 MHz, CDCl₃) of compound 4j

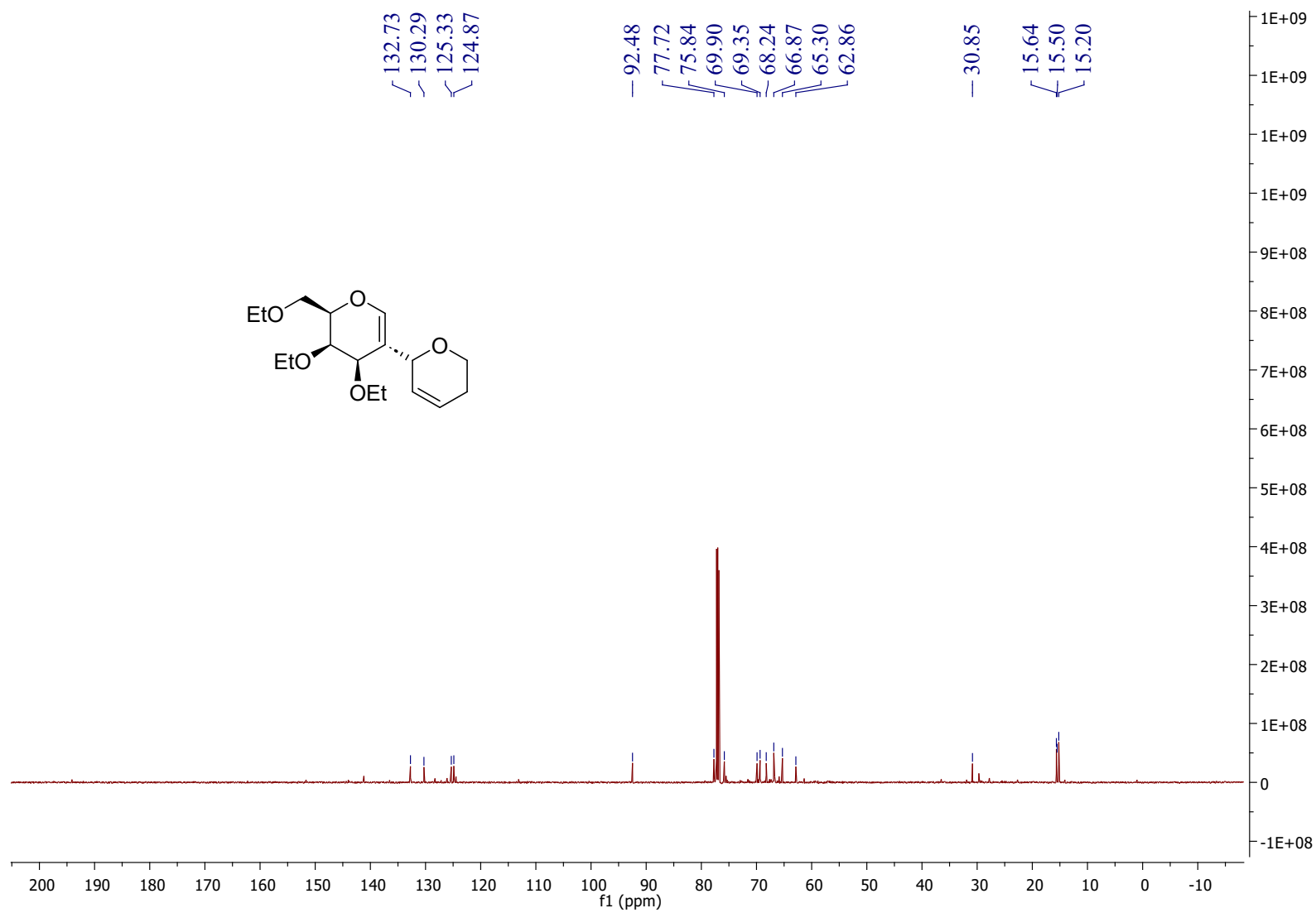


Fig.: ^{13}C NMR (151 MHz, CDCl_3) of compound 4j

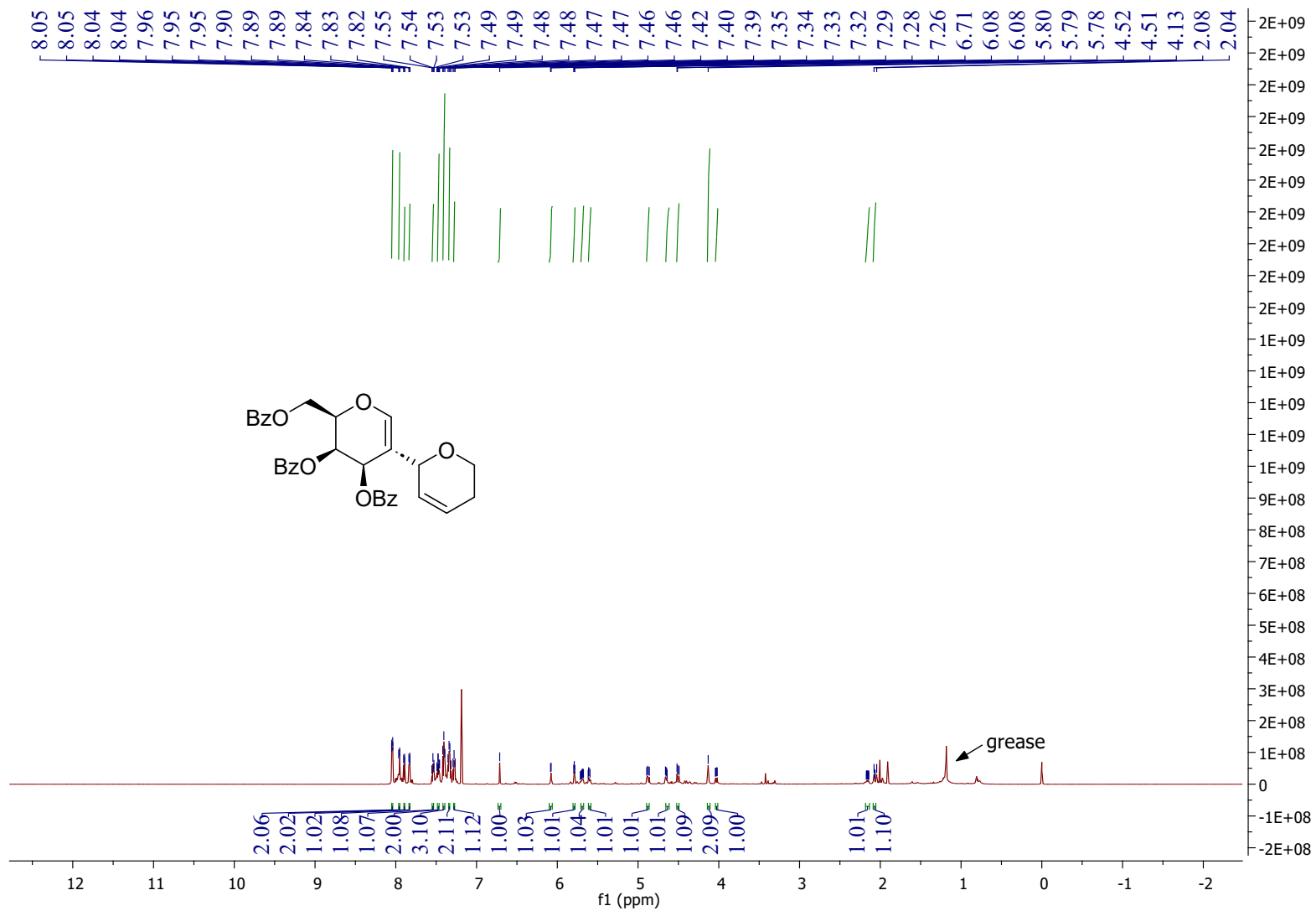


Fig.: ¹H NMR (600 MHz, CDCl₃) of compound 4k

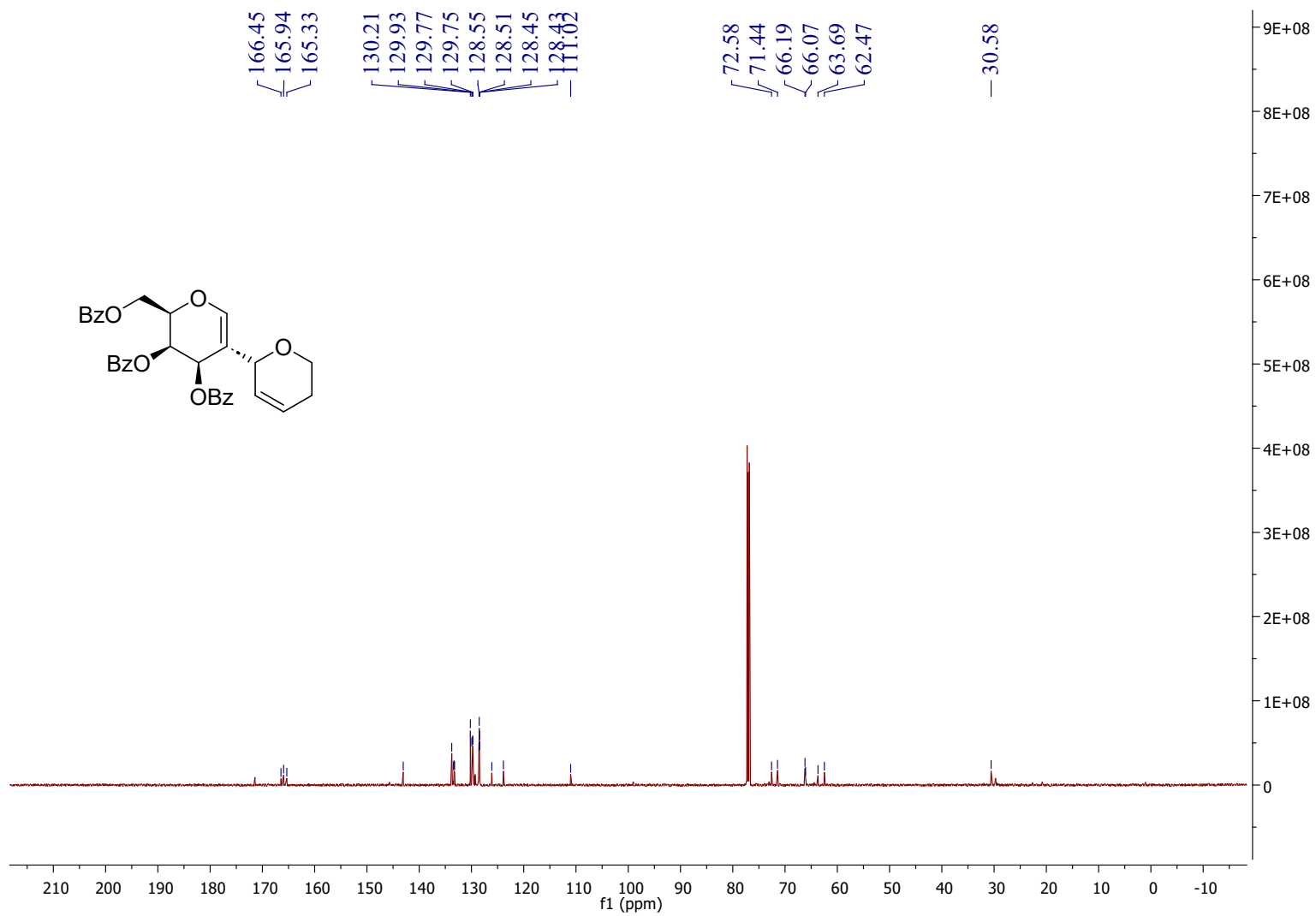


Fig : ^{13}C NMR (151 MHz, CDCl_3) of compound 4k

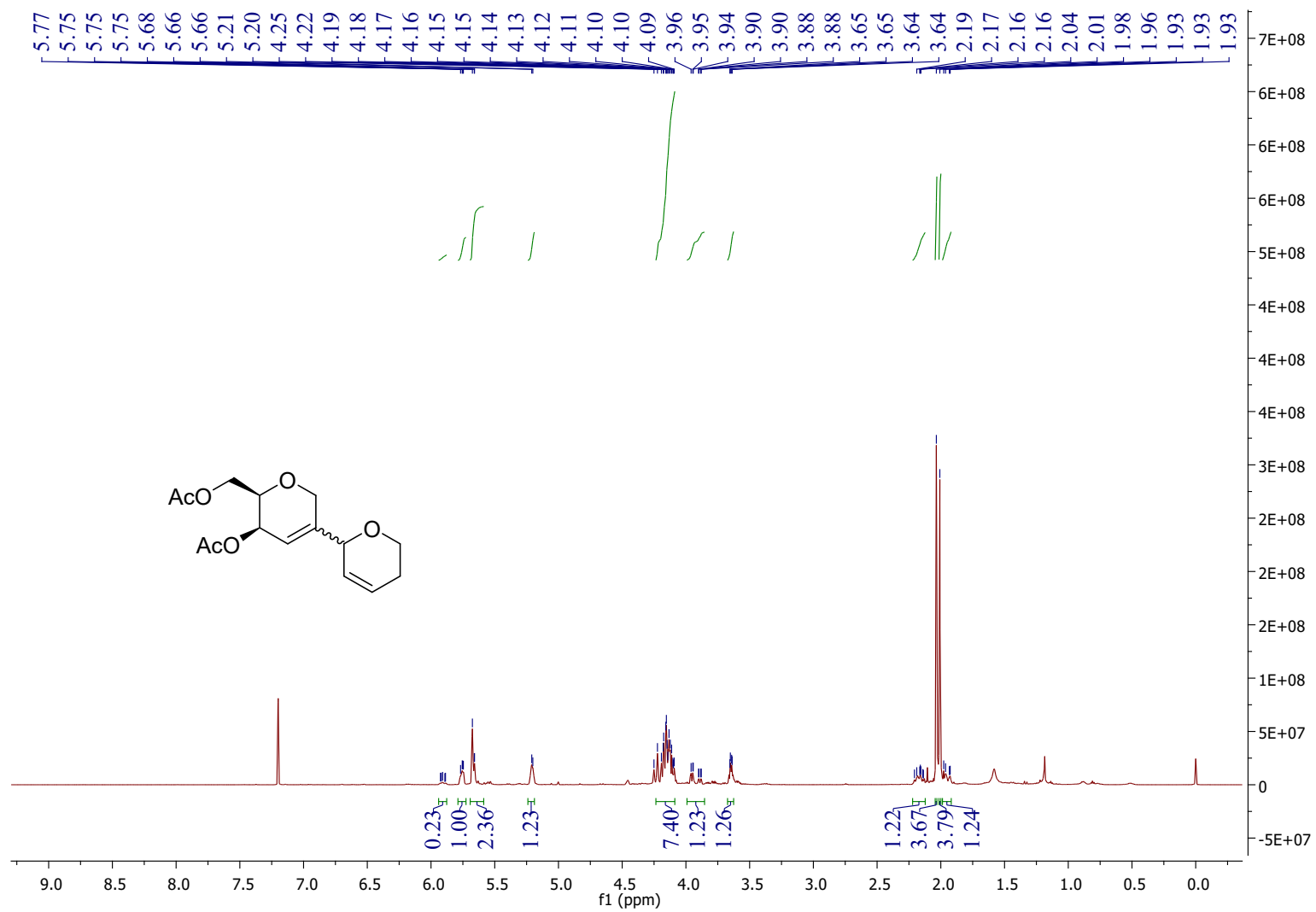


Fig.: ¹H NMR (600 MHz, CDCl₃) of compound 7

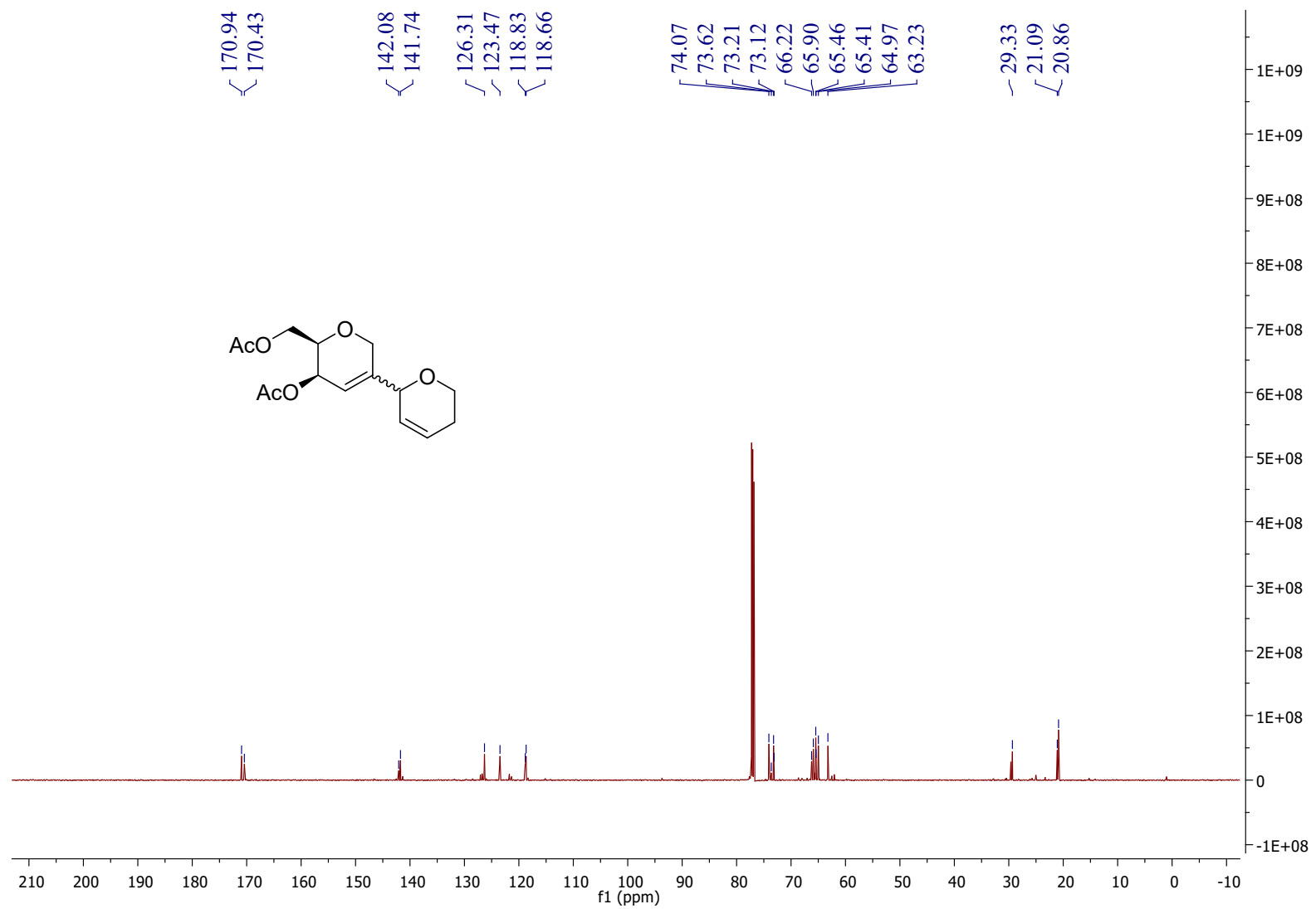


Fig.: ^{13}C NMR (151 MHz, CDCl_3) of compound 7

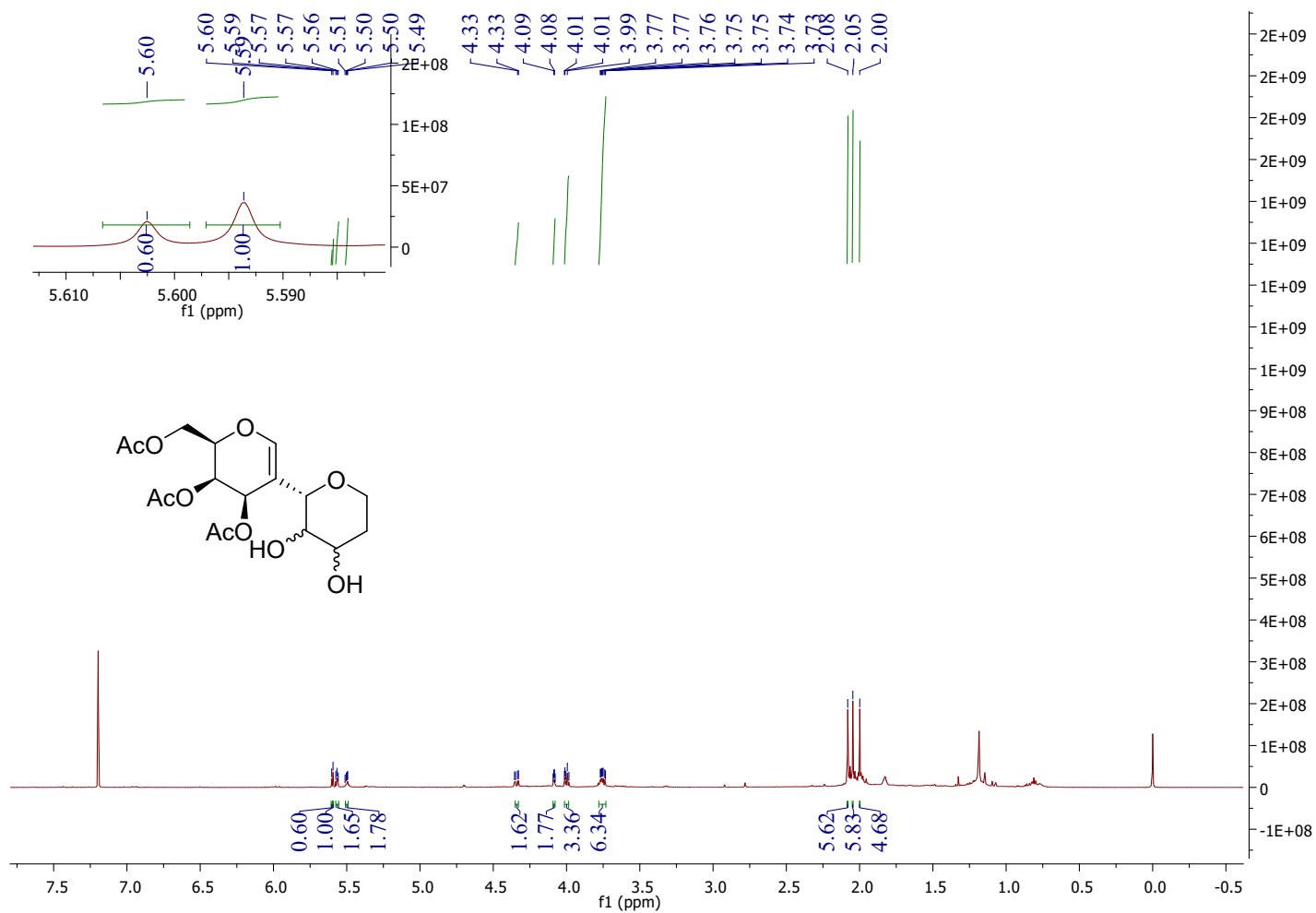


Fig.: ¹H NMR (600 MHz, CDCl₃) of compound 8

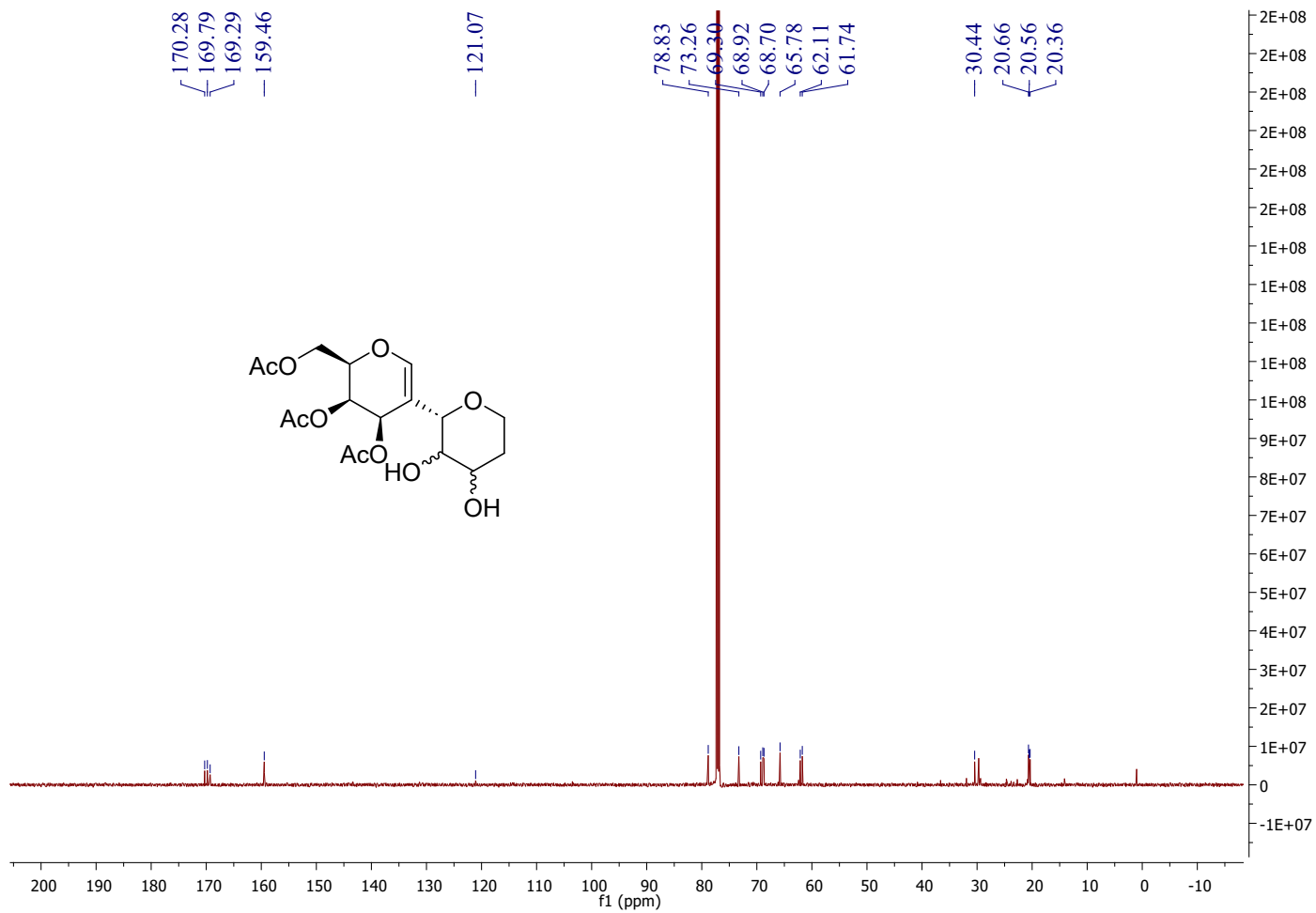


Fig.: ^{13}C NMR (151 MHz, CDCl_3) of compound **8**

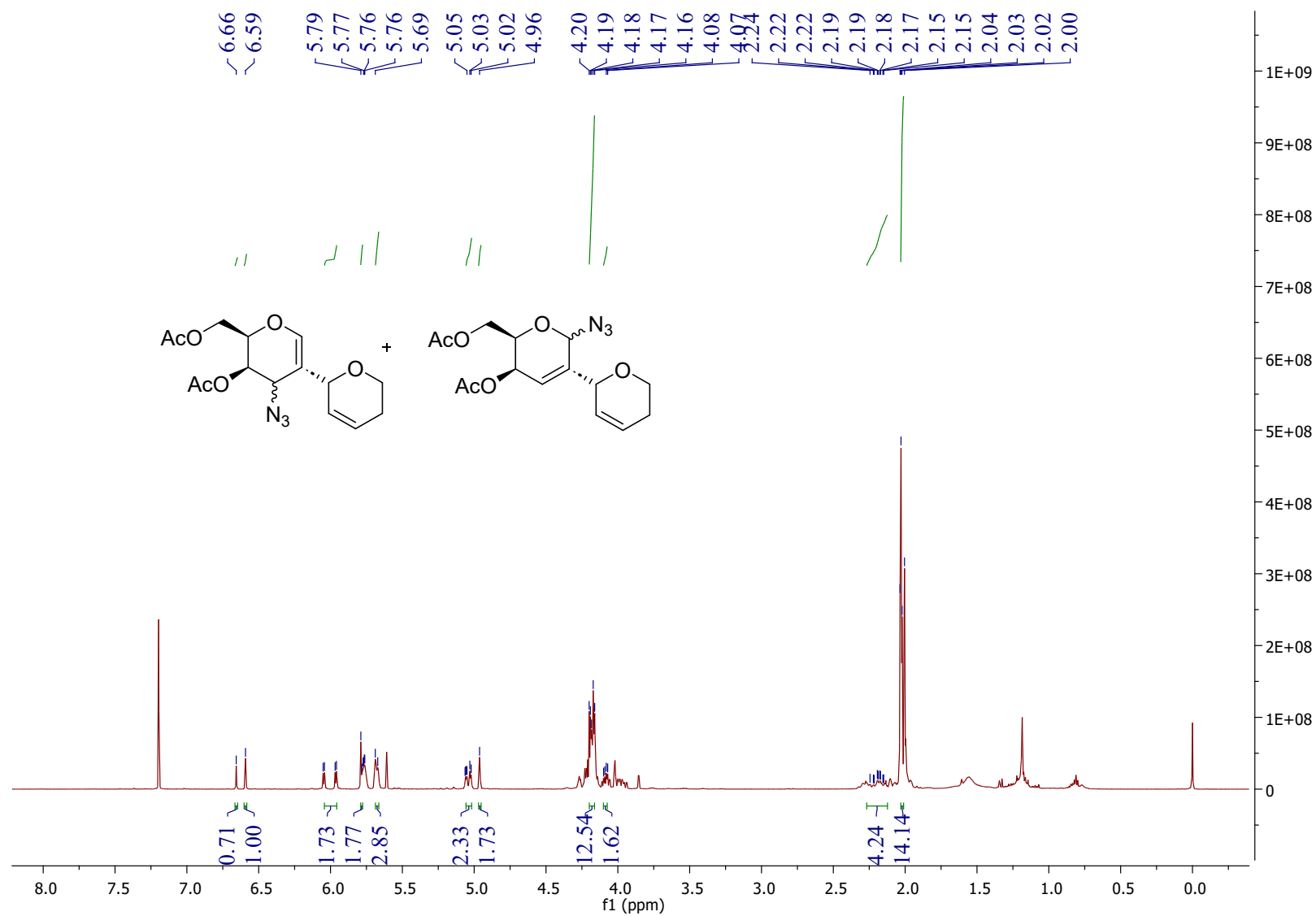


Fig.: ^1H NMR (600 MHz, CDCl_3) of compound **9**

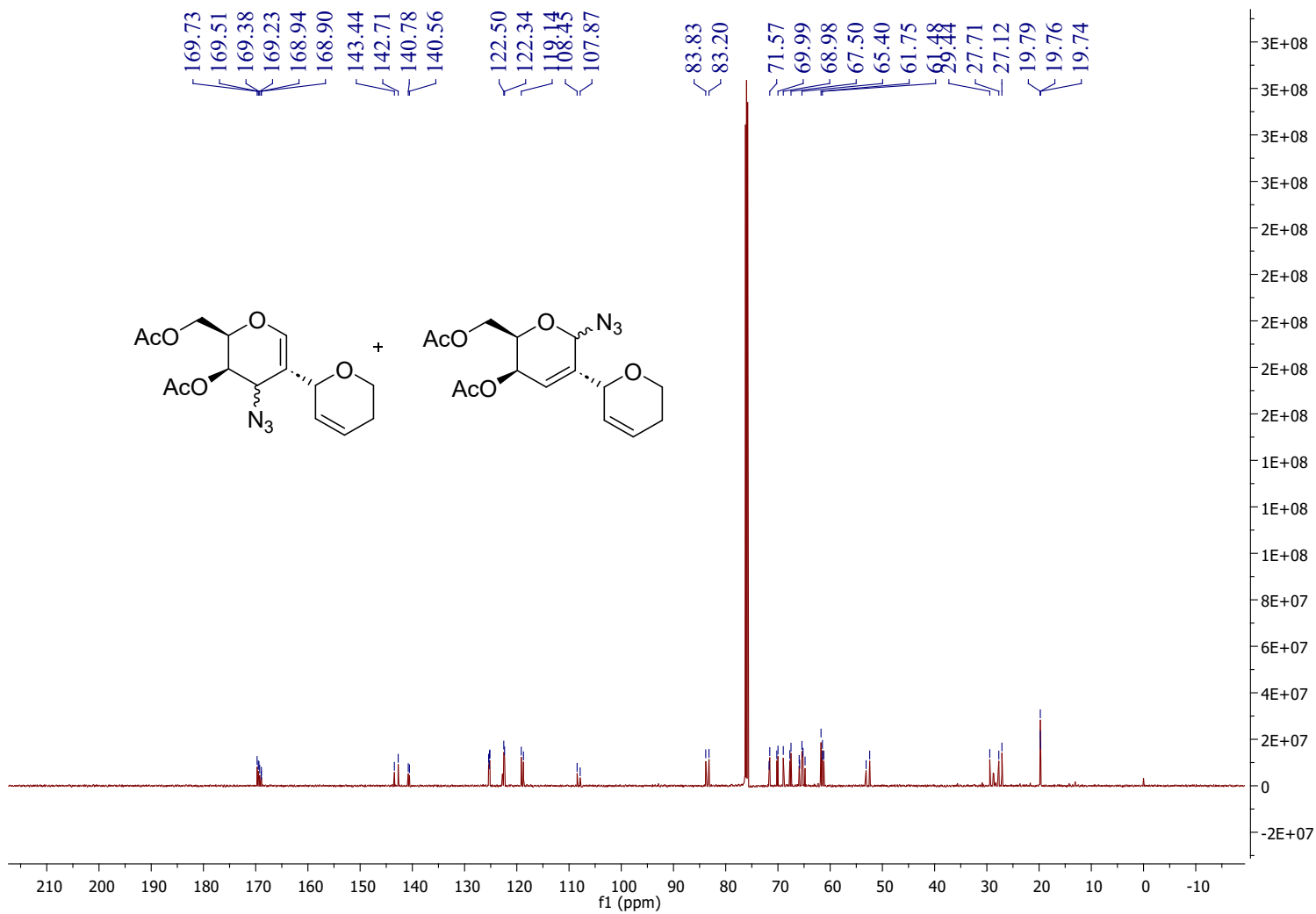


Fig.: ^{13}C NMR (151 MHz, CDCl_3) of compound **9**

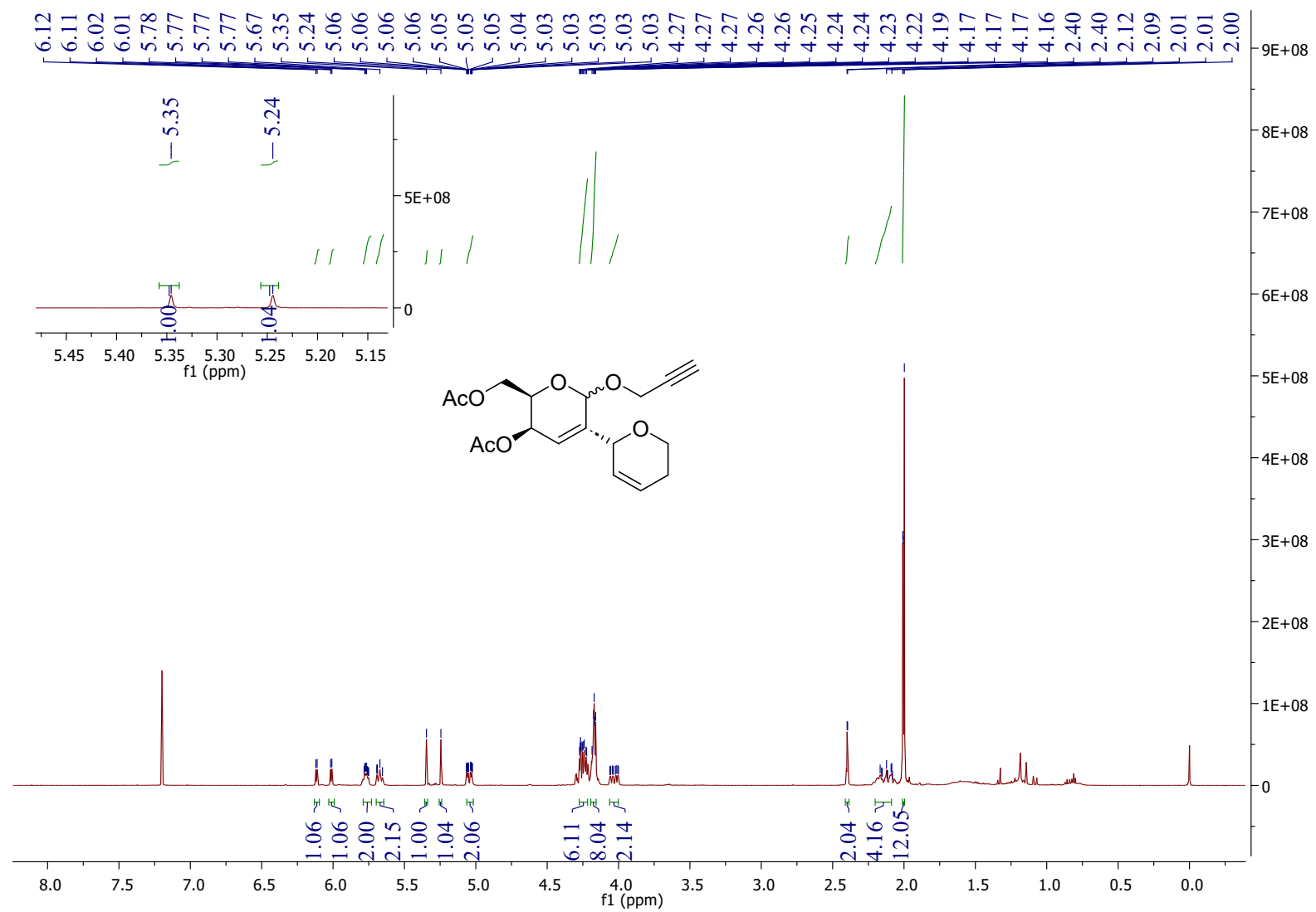


Fig.: ^1H NMR (600 MHz, CDCl_3) of compound **10**

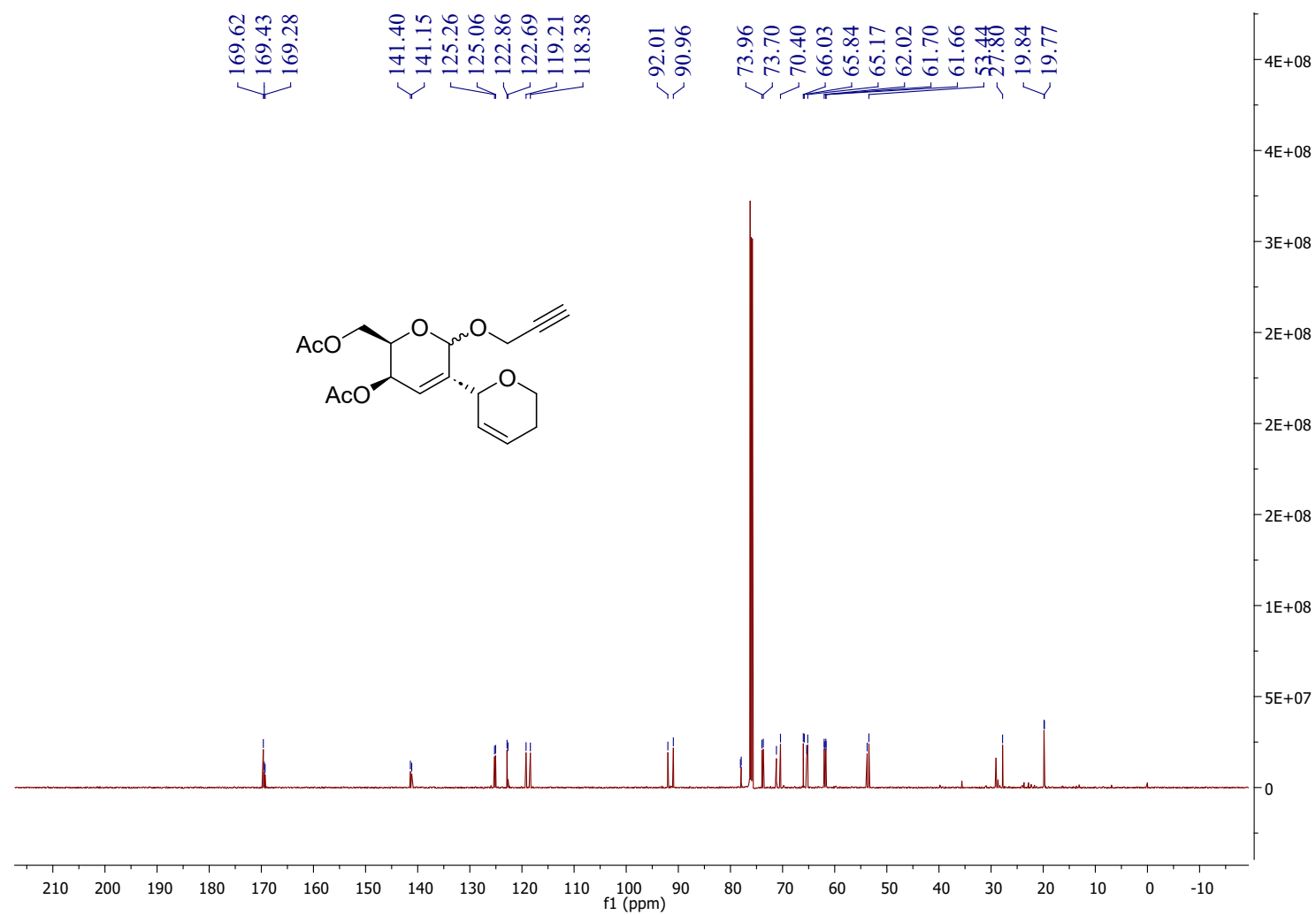


Fig.: ^{13}C NMR (151 MHz, CDCl_3) of compound 10