Supporting Information

Mechanistic Studies of Wacker-type Intramolecular Aerobic Oxidative Amination of Alkenes Catalyzed by $Pd(OAc)_2$/Pyridine

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General Considerations.

All commercially available compounds were purchased and used as received. ^{1}H and ^{13}C NMR spectra were recorded on AC-300 MHz spectrometers. ^{2}H NMR spectra were recorded on 500 MHz spectrometers. The chemical shifts (δ) are given in part per million relative to TMS (0 ppm for ^{1}H, and 0 ppm for ^{13}C). Flash chromatography was performed on silica gel 60 (particle size 0.040-0.063 mm, 230-400 mesh ASRM) with hexanes/ethyl acetate.

Representative procedure for deuterium crossover experiments.

$Pd(OAc)_2$ (0.4 mg, 2 μmol) was added to 13x100 mm disposable culture tubes. The reaction tubes were placed into a custom 48-well parallel reactor mounted on a large capacity mixer and the headspace was purged with molecular oxygen for ca. 15 min. Solutions of pyridine (8 μmol in 0.5 mL toluene) and a 1:1 mixture of **1** and **6-*d*$_3$-1** (0.1 mmol in 0.5 mL toluene) were added to tubes. The reactions were carried out for 24 h under an oxygen atmosphere (1 atm) at 80 °C. Following removal of the solvent under vacuum, the crude oxidative amination product was purified via column chromatography with hexanes/ethyl acetate. The purified product was dissolved in CH_2Cl_2 and analyzed by ^{1}H NMR spectroscopy and mass spectrometry (ESI-MS).

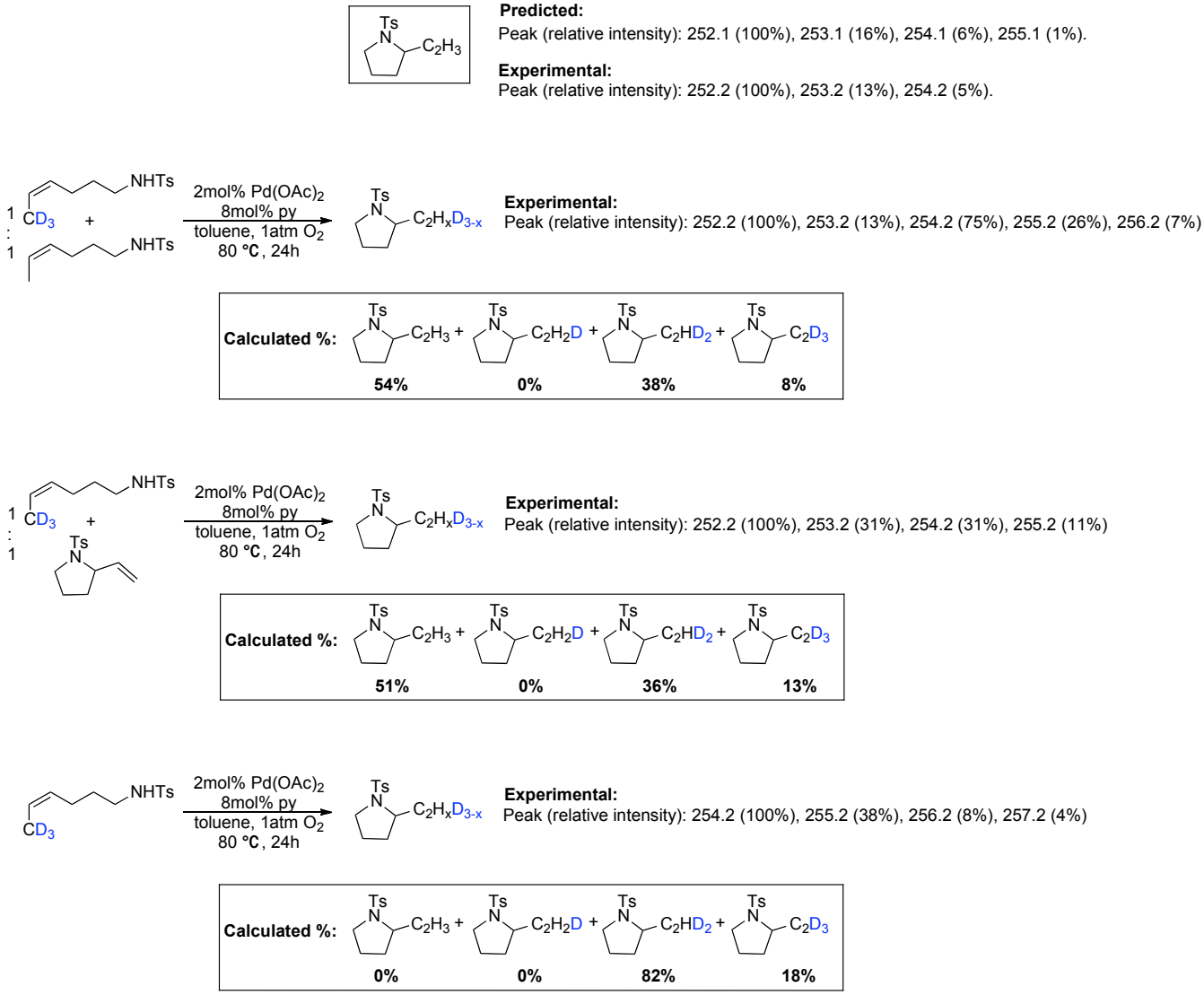


Figure S1. Results from crossover experiments.

Catalytic reaction monitored by ^{1}H NMR spectroscopy.

A freshly prepared solution of $Pd(OAc)_2$, pyridine and (*Z*)-4-hexenyltosylamide (5.0 mM palladium, 11.0 mM pyridine, 32.2 mM tosylamide, 3.0 mM 1,3,5-tri-tert-butylbenzene, in toluene-d_8, 0.7 mL) was added to a medium-wall NMR tube fused to a 14/20 ground glass joint. The NMR tube was attached to a gas/vacuum manifold containing a mercury manometer, and the solution was frozen in liquid nitrogen. The solution was degassed three times (freeze-pump-thaw cycles) and then a calibrated volume of oxygen (0.354 mmol) was condensed into the tube to achieve a final pressure of 3.5 atm in the headspace above the solution. The solution was kept cold in a bath of dry ice/acetone until it was inserted into the spectrometer probe, preheated to 40 °C.

NMR Spectral timecourse for the oxidative amination of (*Z*)-4-hexenyltosylamide.

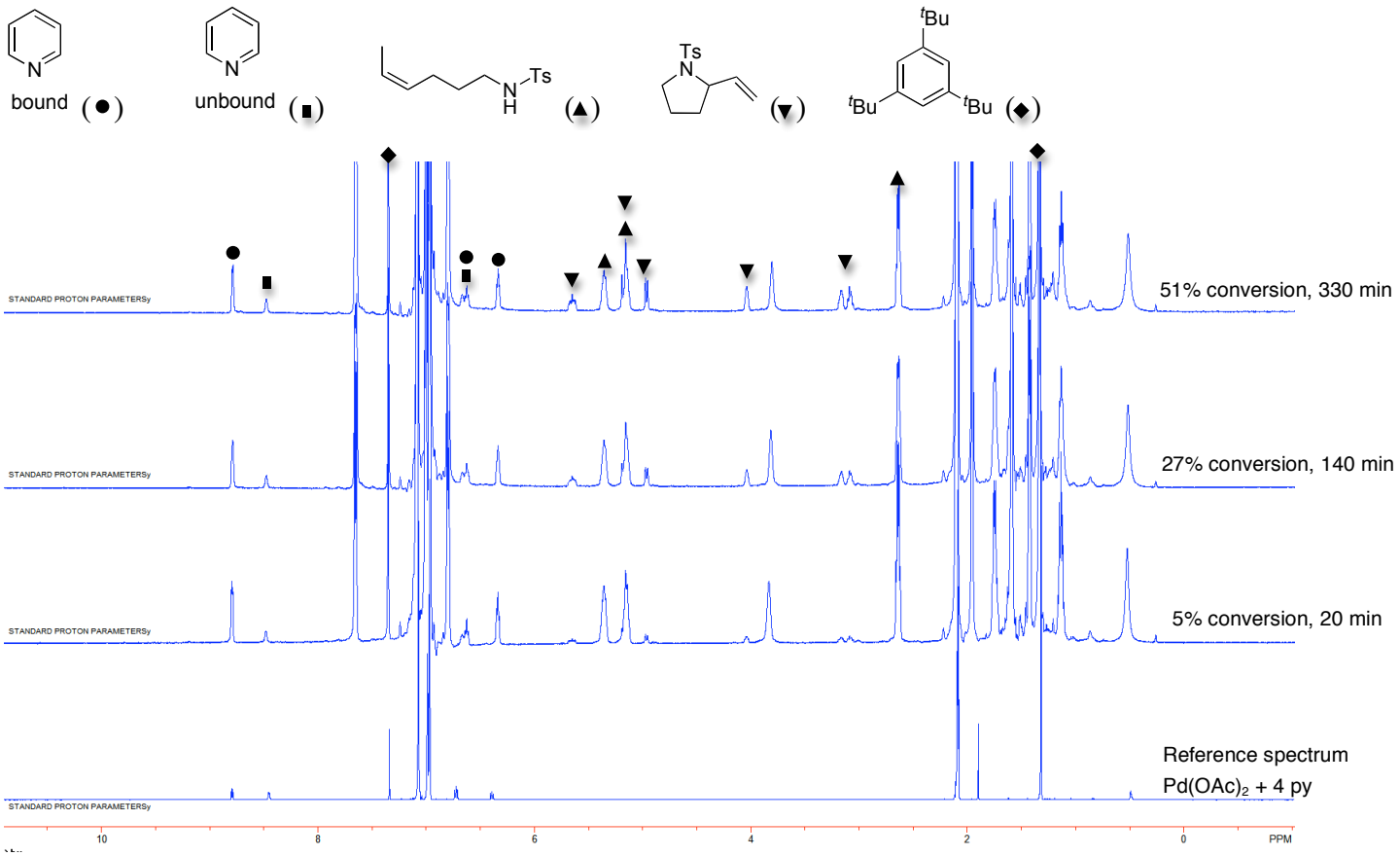
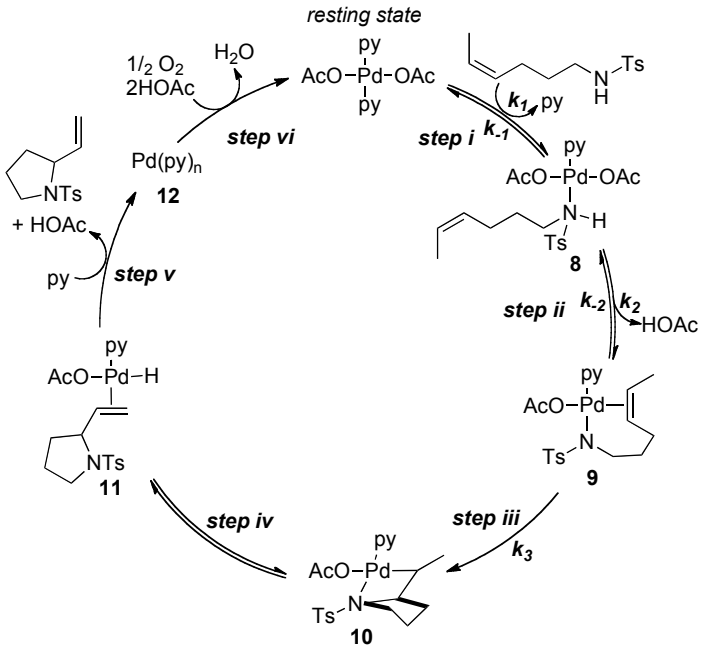


Figure S2. The full ^{1}H NMR spectral timecourse of catalytic aerobic oxidative heterocyclization of (*Z*)-4-hexenyltosylamide. Conditions: [$Pd(OAc)_2$] = 5.0 mM, [pyridine] = 11.0 mM, toluene, initial pO_2 = 3.5 atm, 40 ºC.

Mathematical derivation of the rate law based on mechanism in Scheme 5.

The following mechanism (Scheme 5) accounts for the experimental observations.



I. Derivation of the rate law based on steady-state approximation on intermediates **8** and **9**.

The rate of product formation is described by the following rate law.

$$\frac{d[\text{prod}]}{dt} = k_3 \cdot [9] \tag{S1}$$

The total palladium concentration has contribution from $Pd(OAc)_2(py)_2$, **8** and **9**.

$$[Pd]_T = [Pd(OAc)_2(py)_2] + [8] + [9] \tag{S2}$$

Applying steady-state approximation on **8** and **9**.

$$\frac{d[8]}{dt} = k_1[Pd(OAc)_2(py)_2][\text{Amide}] + k_{-2}[\text{HOAc}][9] - k_{-1}[\text{py}][8] - k_2[8] = 0 \tag{S3}$$

$$\frac{d[9]}{dt} = k_2[8] - k_{-2}[\text{HOAc}][9] - k_3[9] = 0 \tag{S4}$$

Steady-state concentrations of [**8**] and $[Pd(OAc)_2(py)_2]$ can be described as

$$[8] = \frac{\left(k_{-2}[\text{HOAc}] + k_3\right)}{k_2} \bullet [9] \tag{S5}$$

$$[Pd(OAc)_2(py)_2] = \frac{k_2k_3 + (k_{-1}k_3 + k_{-1}k_{-2}[\text{HOAc}])[\text{py}]}{k_1k_2[\text{Amide}]} \bullet [9] \tag{S6}$$

By substituting eq S5 and eq S6 into eq S2, one obtains

$$[9] = \frac{k_1 k_2 [\mathrm{Pd}]_\mathrm{T} [\mathrm{Amide}]}{k_2 k_3 + (k_{-1} k_3 + k_{-1} k_{-2} [\mathrm{HOAc}])[\mathrm{py}] + (k_1 k_2 + k_1 k_3 + k_1 k_{-2} [\mathrm{HOAc}])[\mathrm{Amide}]} \quad \text{(S7)}$$

Substitution of eq S7 into eq S1 yields the rate law.

$$\frac{d[\mathrm{prod}]}{dt} = \frac{k_1 k_2 k_3 [\mathrm{Pd}]_\mathrm{T} [\mathrm{Amide}]}{k_2 k_3 + (k_{-1} k_3 + k_{-1} k_{-2} [\mathrm{HOAc}])[\mathrm{py}] + (k_1 k_2 + k_1 k_3 + k_1 k_{-2} [\mathrm{HOAc}])[\mathrm{Amide}]} \quad \text{(S8)}$$

II. Derivation of the rate law based on pre-equilibrium approximation on intermediate **8**, and steady-state approximation on intermediate **9**.

Applying pre-equilibrium approximation on intermediate **8**

$$K_1 = \frac{k_1}{k_{-1}} = \frac{[\mathrm{py}][8]}{[\mathrm{Pd(OAc)_2(py)_2}][\mathrm{Amide}]} \quad \text{(S9)}$$

Steady-state concentrations of $[\mathrm{Pd(OAc)_2(py)_2}]$ can be described in terms of [**8**], and by applying eq S5, steady-state concentrations of $[\mathrm{Pd(OAc)_2(py)_2}]$ can be described in terms of [**9**]

$$[\mathrm{Pd(OAc)_2(py)_2}] = \frac{[\mathrm{py}]}{K_1 [\mathrm{Amide}]} \bullet [8] = \frac{\left(k_{-2} [\mathrm{HOAc}] + k_3\right)[\mathrm{py}]}{k_2 K_1 [\mathrm{Amide}]} \bullet [9] \quad \text{(S10)}$$

By substituting eq S5 and eq S10 into eq S2, one obtains

$$[9] = \frac{K_1 k_2 [\mathrm{Pd}]_\mathrm{T} [\mathrm{Amide}]}{(k_{-2} [\mathrm{HOAc}] + k_3)[\mathrm{py}] + \left(k_1 k_3 + K_1 k_2 + K_1 k_{-2} [\mathrm{HOAc}]\right)[\mathrm{Amide}]} \quad \text{(S11)}$$

Substitution of eq S11 into eq S1 yields the rate law.

$$\frac{d[\mathrm{prod}]}{dt} = \frac{K_1 k_2 k_3 [\mathrm{Pd}]_\mathrm{T} [\mathrm{Amide}]}{(k_{-2} [\mathrm{HOAc}] + k_3)[\mathrm{py}] + \left(k_1 k_3 + K_1 k_2 + K_1 k_{-2} [\mathrm{HOAc}]\right)[\mathrm{Amide}]} \quad \text{(S12)}$$

III. Derivation of the rate law in the presence of a large excess of pyridine. (Based on steady-state approximations on intermediates **8** and **9**.

The following derivation reveals the origin of the half-order [palladium] dependence when the reaction is conducted in the presence of an excess of pyridine. If no acetic acid is added to the reaction, then the steady state concentration of acetic acid can be qeuated to the concentration of **9** according to the equilibrium between **8** and **9**.

$$[9] = [\mathrm{HOAc}] \tag{S13}$$

Equation S2 can be rewritten to substitute for the steady-state concentration of acetic acid.

$$\frac{k_1k_{-2} + k_{-1}k_{-2}[\mathrm{py}]}{k_1k_2} \cdot [9]^2 + \frac{k_2k_3 + k_{-1}k_3[\mathrm{py}] + \left(k_1k_3 + k_1k_2\right)[\mathrm{Amide}]}{k_1k_2[\mathrm{Amide}]} \cdot [9] - [\mathrm{Pd}]_\mathrm{T} = 0 \tag{S14}$$

Application of the quadratic formula allows one to solve equation S14 for [**9**].

$$[9] = \sqrt{\frac{k_1k_2[\mathrm{Pd}]_\mathrm{T}}{k_1k_{-2} + k_{-1}k_{-2}[\mathrm{py}]} + \left(\frac{k_2k_3 + k_{-1}k_3[\mathrm{py}] + \left(k_1k_3 + k_1k_2\right)[\mathrm{Amide}]}{2(k_1k_{-2} + k_{-1}k_{-2}[\mathrm{py}])[\mathrm{Amide}]}\right)^2} - \frac{k_2k_3 + k_{-1}k_3[\mathrm{py}] + \left(k_1k_3 + k_1k_2\right)[\mathrm{Amide}]}{2(k_1k_{-2} + k_{-1}k_{-2}[\mathrm{py}])[\mathrm{Amide}]} \tag{S15}$$

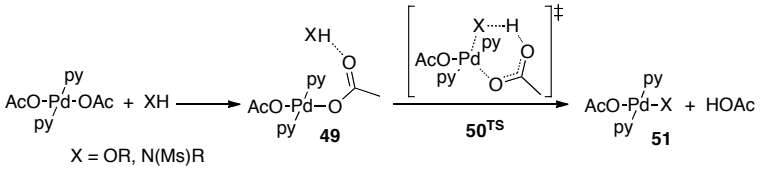
The rate law can now be solved with the $[\mathrm{Pd}]_\mathrm{T}$ term under the square root.

$$\frac{d[\mathrm{prod}]}{dt} = k_3 \cdot \sqrt{\frac{k_1k_2[\mathrm{Pd}]_\mathrm{T}}{k_1k_{-2} + k_{-1}k_{-2}[\mathrm{py}]} + \left(\frac{k_2k_3 + k_{-1}k_3[\mathrm{py}] + \left(k_1k_3 + k_1k_2\right)[\mathrm{Amide}]}{2(k_1k_{-2} + k_{-1}k_{-2}[\mathrm{py}])[\mathrm{Amide}]}\right)^2} - k_3 \cdot \frac{k_2k_3 + k_{-1}k_3[\mathrm{py}] + \left(k_1k_3 + k_1k_2\right)[\mathrm{Amide}]}{2(k_1k_{-2} + k_{-1}k_{-2}[\mathrm{py}])[\mathrm{Amide}]} \tag{S16}$$

Computational studies of Pd-amidate formation.

Previous experimental and computational studies of $Pd(OAc)_2$/pyridine-catalyzed alcohol oxidation implicate formation of a Pd-alkoxide intermediate via a proton-coupled ligand substitution pathway (Scheme S1).[1] ^1H NMR spectroscopic data support a pre-equilibrium hydrogen bonding interaction between the alcohol substrate and an acetate ligand of the $(py)_2Pd(OAc)_2$ catalyst resting state. No experimental evidence was obtained for a similar substrate-catalyst interaction in the case of the sulfonamide substrates considered in the present study, and DFT computational studies suggest that a similar pathway for formation of a Pd-NMsR intermediate, proceeding at the coordinatively saturated *trans*-$(py)_2Pd(OAc)_2$, is energetically disfavored ($\Delta G^{\ddagger} > 35$ kcal/mol). Subsequent evaluation of other possible ligand substitution transition states, involving coordination of amine or alkene to the Pd center, were also energetically disfavored.[2]

Scheme S1. Proton-Coupled Ligand Substitution Pathways Leading to Formation of Alkoxide and Amidate Palladium Species.



These computational results prompted us to evaluate a pathway involving a mono-ligated Pd species resulting from pyridine dissociation from *trans*-$(py)_2Pd(OAc)_2$ (Figure S3). Intramolecular displacement of pyridine by the carbonyl group of an acetate ligand proceeds with a barrier similar to that expected for the highest barrier during catalytic turnover (21.8 kcal/mol, **[52/py]**^{TS}). A pathway was found for reaction of (py)Pd(OAc)(κ^2-OAc) (**κ^2-53**) with the substrate to form the Pd-sulfonamide

adduct **8M** via intermediate **54** and transition-state **55**^{TS}; however, the barrier for this pathway would suggest that formation of this species is rate-limiting, a result inconsistent with the experimental data (see manuscript). Alternatively, a dissociative pathway affords a more viable intermediate **κ^1-53** that, in the presence of substrate **1M**, can be trapped to form amine adduct **8M** (Figure S3). The calculated energies of the species in Figure S3 are consistent with the inability to observe interactions between *trans*-(py)$_2$Pd(OAc)$_2$ and substrate by ^{1}H NMR spectroscopy.

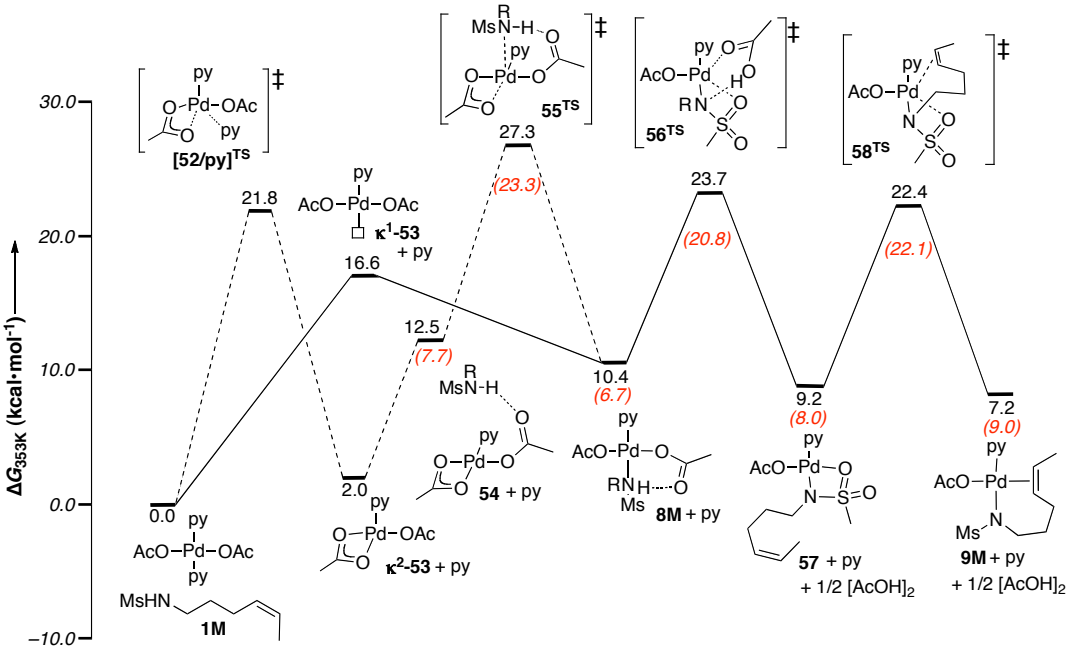


Figure S3. Lowest free energy pathway for formation of an alkene-coordinated Pd-amidate intermediate necessary for *cis*-aminopalladation. Free energies calculated without inclusion of solvation are italized in red.

Amine-adduct **8M** features a stabilizing intramolecular hydrogen bond between the amine N-H and carbonyl oxygen of acetate. Pd-amidate formation then occurs by inner-sphere proton transfer, and acetic acid will be formed and subsequently liberated from the palladium complex. Such a step is necessitated, *prior to the turnover-limiting step*, to rationalize the catalyst dependences in the presence of excess pyridine or acetic acid (Figure S3). We have identified a number of transition states that lead to formation of Pd-amidate species; however, only one transition state, **56**^{TS}, was found to have a barrier

sufficiently low in energy to be considered viable. After formation of κ^2-amidate species **57**, a transition state (**58**^{TS}), defining concomitant intramolecular alkene ligand substitution and κ^2-to-κ^1 amidate isomerization, was identified. This final transformation yields intermediate **9M** ligated by both an amidate and alkene that was expected to be critical for subsequent insertion of alkene into the palladium-amidate bond.

We were initially concerned by the apparent experimental/computational discrepancy that resulted from a comparison of the barriers for **56**^{TS} and **58**^{TS}. Namely, the latter transition state is more stable, which is inconsistent with the fact that steady-state formation of a Pd-amidate intermediate is necessesitated by the catalyst dependence data (Figure S3). However, we noted that many of the species leading to the Pd-amidate **57** featured substantial hydrogen-bonding that could be problematic for the solvation model to account for properly. Indeed, comparison of the gas-phase barrier heights demonstrate the experimentally expected outcome: **56**^{TS} is more stable than **58**^{TS} by 1.3 kcal/mol (Figure S3).

Analysis of natural charges (NC) of alkene insertion transition state.

Table S1. Calculated Natural Charges (NC) of Alkene-bound Palladium-Amidate Complexs (**9M** and ***κ*²-16M**) and the Corresponding Alkene Insertion Transition States (**13**$^{AP\text{-}TS}$ and **17**$^{AP\text{-}TS}$).

	9M	***13*$^{AP\text{-}TS}$**		***k*²-16M**	***17*$^{AP\text{-}TS}$**
Pd	0.55	0.51	**Pd**	0.57	0.53
Substrate	–0.21	–0.12	**Substrate**	–0.13	–0.03
(py)Pd(κ¹-OAc)	0.21	0.12	**Pd(κ²-OAc)**	0.13	0.03
NMs	–0.45	–0.37	**NMs**	–0.38	–0.34
Alkene(C1-C2)	0.20	0.20	**Alkene(C1-C2)**	0.22	0.27
Pd	0.55	0.51	**Pd**	0.57	0.53
C1---Pd	–0.16	–0.38	**C1---Pd**	–0.16	–0.32
C2---N	–0.17	0.07	**C2---N**	–0.19	0.06
N	–0.88	–0.86	**N**	–0.83	–0.86

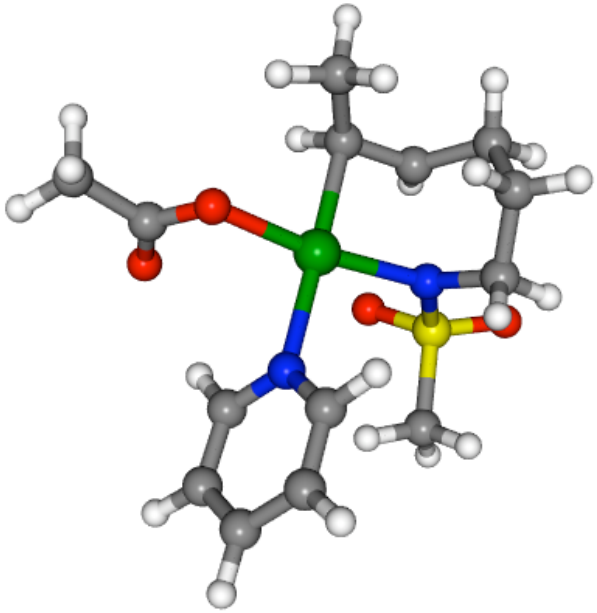
Solvation-corrected total energies (E_{sol}) and thermochemical corrections at 353K (kcal/mol) and three lowest frequencies from normal-mode analysis.

Description	*Label*	E_{sol}	*ZPE*	$G_{corr}^{(298K)}$	$G_{corr}^{(353K)}$	$E_{pcm}^{(353K)}$	freq
pyridine	**py**	-155807.97	55.78	38.99	35.19	-155837.62	384.3, 418.5, 613.3
acetic acid	**HOAc**	-143760.01	38.76	21.68	17.81	-143798.97	69.8, 422.4, 548.6
acetic acid dimer	**$[HOAc]_2$**	-287536.34	79.09	55.70	49.94	-287613.67	41.7, 50.4, 68.3
cis-alkenyl$NHSO_2CH_3$	**1M**	-551647.70	139.12	112.26	105.34	-551730.13	21.5, 30.3, 60.6
R-vinylpyrrolidine	**Vpyr**	-550882.18	125.74	101.46	95.26	-550962.84	27.4, 66.3, 85.6
trans-$(py)_2Pd(\kappa^1\text{-}OAc)_2$	**$(py)_2Pd(Oac)_2$**	-678697.49	179.10	143.62	133.96	-930896.10	30.4, 32.3, 40.5
trans(py)(NMs)Pd(alkene)(OAc) cis-AP TS	**(trans-py-amidate)13AP-TS**	-930741.55	222.38	187.43	177.59	-930896.10	–252.4, 30.4, 36.5
cis(py)(NMs)Pd(alkene)(OAc) cis-AP TS	**(cis-py-amidate)13AP-TS**	-930737.98	222.27	186.78	176.83	-930892.98	–270.7, 24.6, 31.4
(NMs)Pd(alkene)(κ^2-OAc) cis-AP TS	**17AP-TS**	-774926.00	165.15	134.64	126.39	-775047.36	–254.2, 25.2, 30.8
cis(alkene)(py)Pd(NMs-)(Oac)	**9M**	-930754.32	222.68	186.88	176.79	-930910.00	28.1, 32.1, 32.8
(NMs)(alkene)Pd(κ^2- κ^1-OAc)(py) py add trans to NMs	**[15/py]TS**	-930741.12	222.03	186.83	176.91	-930894.19	–84.4, 29.9, 37.0
(κ^2-OAc)Pd(NMs-)(η^2-alkene)	**κ2-16M**	-774936.21	165.72	135.21	126.90	-775058.29	27.9, 38.6, 43.5
(py)(κ^1-OAc)Pd(κ^2-alkyl-Npyrrolidine) cis py alkyl	**10M**	-930756.9101	223.60	187.99	178.01	-930911.08	26.3, 33.8, 38.7

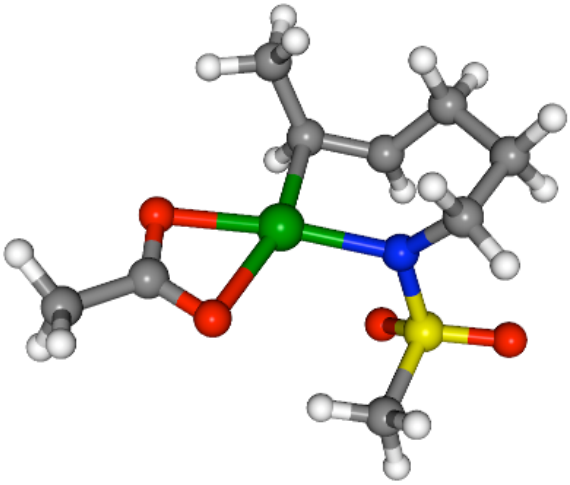
(κ^2-alkyl-Npyrrolidine)Pd(II)(κ^1-OAc)	**14**	-774920.98	166.01	135.05	126.67	-775043.49	25.5, 41.7, 53.5
Pd(κ^2-N-alkyl)(κ^2-OAc)	**18M**	-774940.49	166.60	135.94	127.66	-775060.80	26.6, 28.5, 47.3
(py)Pd(AcO)(H--vinylN) BHE TS trans to py	**trans-19 BHE-TS**	-930731.60	220.51	182.95	172.60	-930888.43	–41.2, 8.8, 22.0
(py)Pd(AcO)(H--vinylN) BHE TS cis to py	**cis-19 1°-BHE-TS**	-930737.70	220.73	184.13	173.72	-930894.47	–450.2, 16.2, 24.7
(py)Pd(OAc)(2°-BHE vinylN)	**cis-20 2°-BHE-TS**	-930734.05	220.47	183.25	172.97	-930890.56	–620.4, 15.0, 20.8
trans(py)(vinylpyrrolidine)Pd(H)Oac	**11M**	-930743.63	221.69	184.78	174.52	-930898.74	20.4, 23.9, 27.8
(py)Pd(κ^2-N-alkyl)(OAc) - 1° alkyl #2	**21**	-930761.24	224.40	190.50	181.02	-930916.27	–37.1, 29.8, 35.7
(py)Pd(OAc)(H)….trans-to-py-open	**22**	-379836.54	94.23	68.30	61.81	-379907.72	25.3, 54.3, 58.8
(py)Pd(H)(κ^2-OAc)	**23**	-379858.24	94.47	69.04	62.68	-379927.46	31.1, 39.3, 62.4
cis(py)(H)Pd(OAc) - RE TS	**24TS**	-379846.06	93.16	67.27	60.85	-379918.00	-29.1, 12.2, 37.5
cis(py)(H)Pd(OAc) - isom TS	**26TS**	-379845.25	93.24	67.76	61.39	-379916.85	-23.8, 34.7, 41.6
cis(py)(H)Pd(OAc)	**25**	-379846.03	93.25	65.47	58.58	-379918.18	5.4, 22.1, 28.6
trans-(py)Pd^0(HOAc)	**27**	-379855.84	95.93	69.27	62.64	-379926.71	11.3, 32.2, 49.5
Pd(H--vinylN)(κ^2-OAc) BHE TS	**28 1°-BHE-TS**	-774922.00	163.88	132.85	124.52	-775044.89	–522.4, 22.5, 35.1
Pd(κ^2-OAc)(2°-BHE vinylN)	**30 2°-BHE-TS**	-774919.60	163.79	132.48	124.11	-775044.14	–527.0, 22.2, 27.9
(κ^2-OAc)Pd(η^2-VP)(H)	**29M**	-774926.46	164.67	133.21	124.76	-775047.89	27.5, 32.3, 35.1
Pd(κ^2-OAc)(H)….trans-to-OAc-open	**31**	-224013.07	36.79	16.71	12.07	-224050.40	36.0, 124.5, 219.3

Pd(κ^2-N-alkyl)(κ^2-OAc) - 1° alkyl #2	**32**	-774944.78	167.31	137.31	129.22	-775065.36	20.5, 36.8, 51.4
(κ^2-κ^1-OAc)Pd(η^2-alkene to κ^2 alkene OMs)(H) isomTS	**33TS**	-774921.44	164.20	134.42	126.36	-775045.31	–102.0, 34.5, 47.8
(κ^2-alkene,O-vinylpyrrolidine)Pd(H)OAc H - alkene cis	**34**	-774923.40	164.50	133.41	125.03	-775049.44	23.2, 40.1, 44.1
(κ^2-alkene,O-vinylpyrrolidine)Pd(H)OAc RE TS H - alkene cis	**35TS**	-774922.41	163.19	131.97	123.63	-775047.65	–244.2, 19.8, 22.1
(κ^2-alkene.OMs)Pd^0(HOAc)	**36**	-774931.35	165.78	133.33	124.66	-775056.07	14.4, 25.2, 36.8
trans-$(py)_2$Pd(OAc)(OAc--HNRMs)	**49**	-1230324.99	318.50	269.83	255.75	-1230547.639	–99.9, 16.4, 19.3
trans-$(py)_2$Pd(OAc)(OAc--HNRMs) NH for OAc ligand substitution ts	**50TS**	-1230292.78	319.72	343.51	NC	-1230564.92[a]	–97.1,16.5,17.9
trans-$(py)_2$Pd(OAc)(NRMs)	**51**	-1086571.47	279.05	235.76	223.40	-1086756.18	15.2, 19.5, 24.3
(py)Pd(κ^2-OAc)(κ^1-OAc)--py trans--ts	**[52/py]TS**	-678676.22	178.19	142.52	132.86	-678812.18	–78.4, 22.1, 25.0
trans-(py)Pd(κ^1-OAc)$_2$	**κ1-53**	-522856.89	121.68	91.28	83.31	-522963.05	37.3, 37.6, 46.8
(py)Pd(k^1-OAc)(κ^2-OAc)	**κ2-53**	-522873.34	121.94	91.41	83.45	-522977.83	19.1, 34.8, 36.9
(py)Pd(κ^2-OAc)OAc--HNRMs	**54**	-1074526.51	261.78	214.94	201.87	-1074712.99	4.9, 11.0, 15.9
(py)Pd(OAc--HNRMs)(κ^1-OAc) amine add TS	**55TS**	-1074517.18	261.83	219.03	210.59	-1074706.80	-91.8, 16.1, 17.8

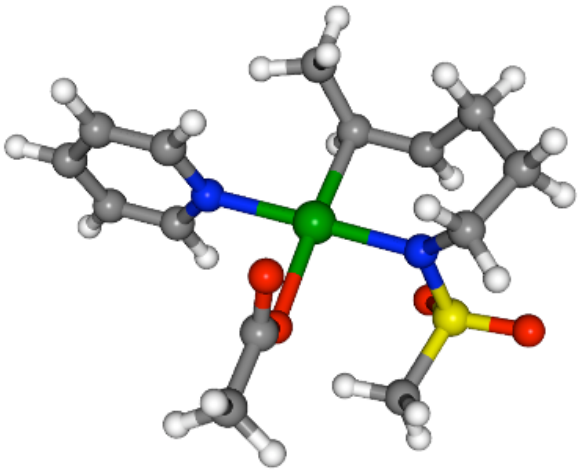
Ball-and-stick models of various [4,5]- and [6,5]-transition states for cis-aminopalladation.



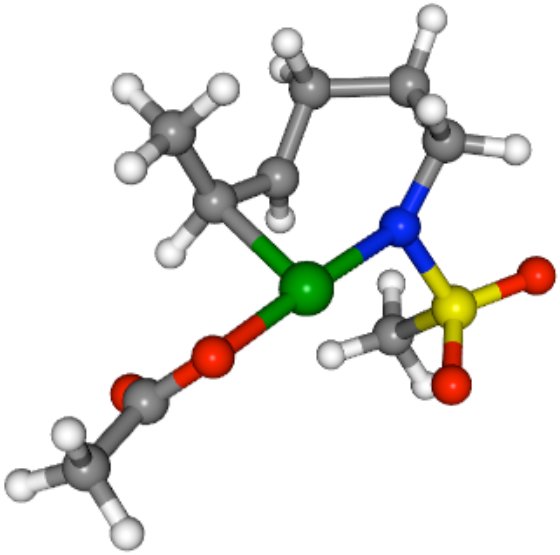
cis-**13**$^{\text{AP-TS}}$ $\Delta G^{\ddagger}_{353\text{K}}$ **= 24.3 kcal/mol**



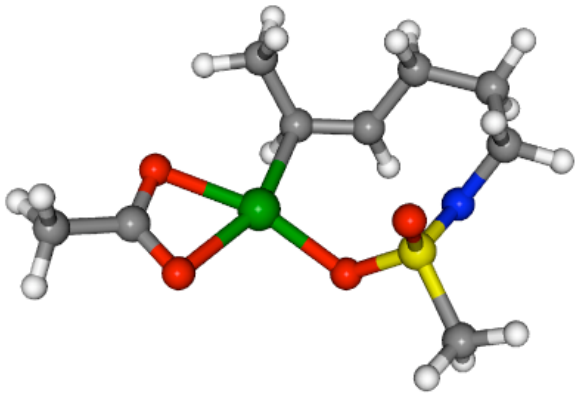
κ^2-**17**$^{\text{AP-TS}}$ $\Delta G^{\ddagger}_{353\text{K}}$ **= 14.7 kcal/mol**



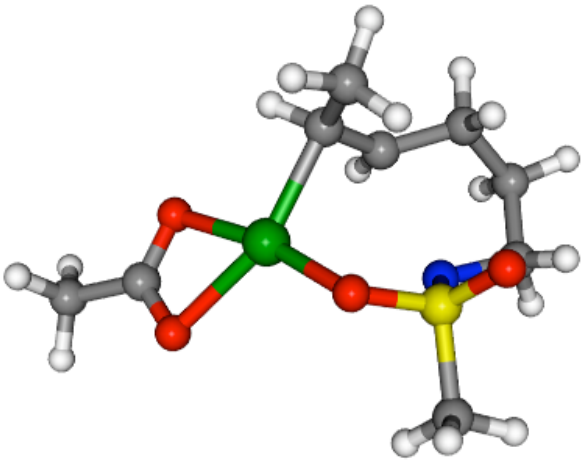
trans-**13**$^{\text{AP-TS}}$ $\Delta G^{\ddagger}_{353\text{K}}$ **= 22.0 kcal/mol**



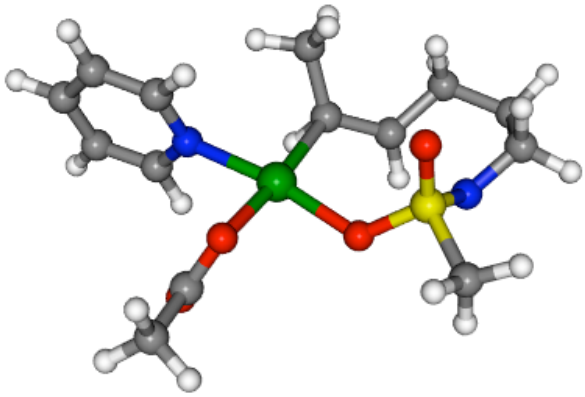
κ^1-**17**$^{\text{AP-TS}}$ $\Delta G^{\ddagger}_{353\text{K}}$ **= 28.6 kcal/mol**



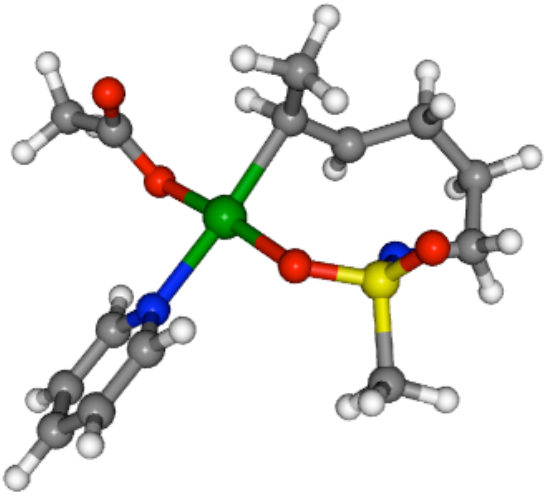
***cis*-[6,5]-A** $\Delta G^{\ddagger}_{353K}$ **= 34.6 kcal/mol**



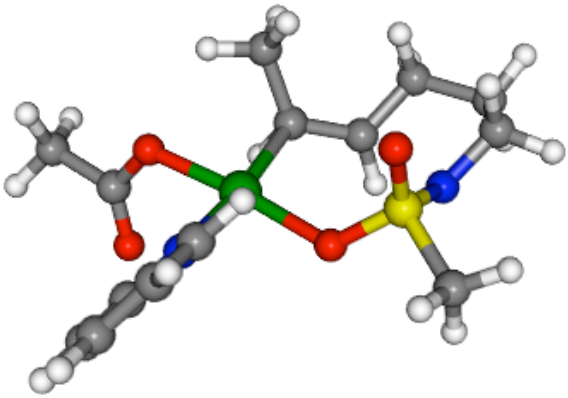
***cis*-[6,5]-D** $\Delta G^{\ddagger}_{353K}$ **= 33.4 kcal/mol**



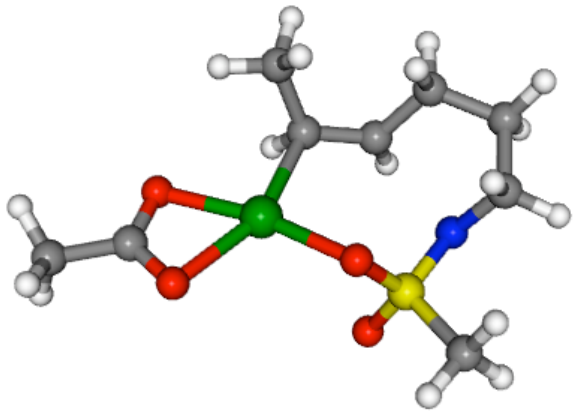
***cis*-[6,5]-B** $\Delta G^{\ddagger}_{353K}$ **= 41.7 kcal/mol**



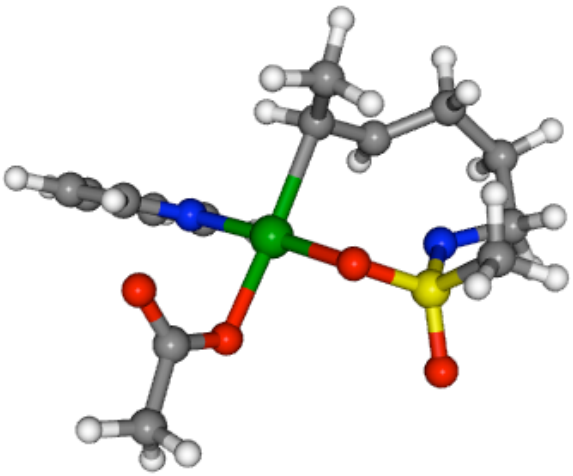
***cis*-[6,5]-F** $\Delta G^{\ddagger}_{353K}$ **= 34.3 kcal/mol**



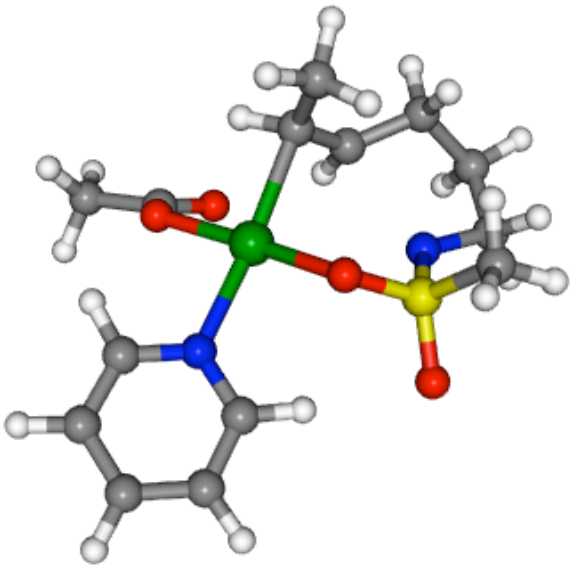
***cis*-[6,5]-C** $\Delta G^{\ddagger}_{353K}$ **= 35.8 kcal/mol**



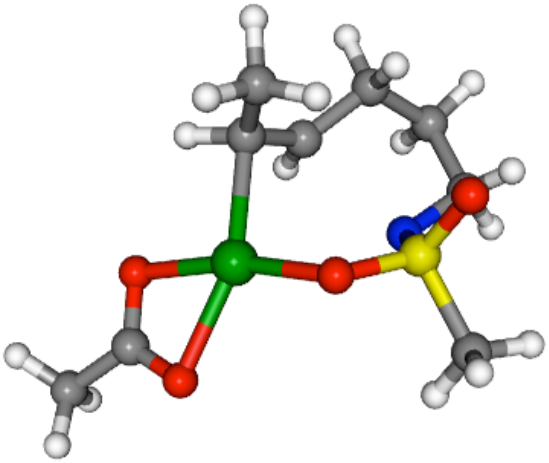
***cis*-[6,5]-G** $\Delta G^{\ddagger}_{353K}$ **= 38.4 kcal/mol**



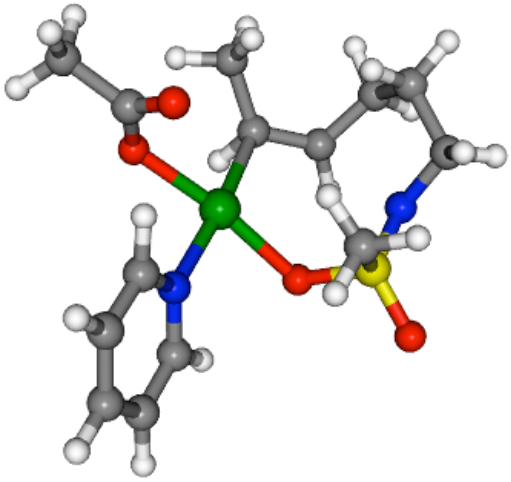
cis-[6,5]-I $\Delta G^{\ddagger}_{353K}$ **= 44.6 kcal/mol**



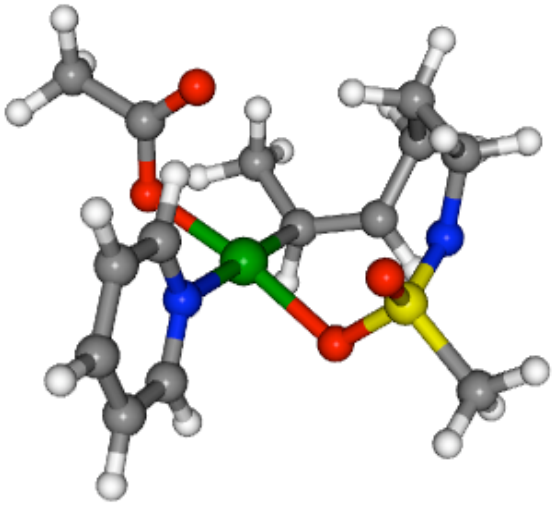
***cis*-[6,5]-H** $\Delta G^{\ddagger}_{353K}$ **= 35.3 kcal/mol**



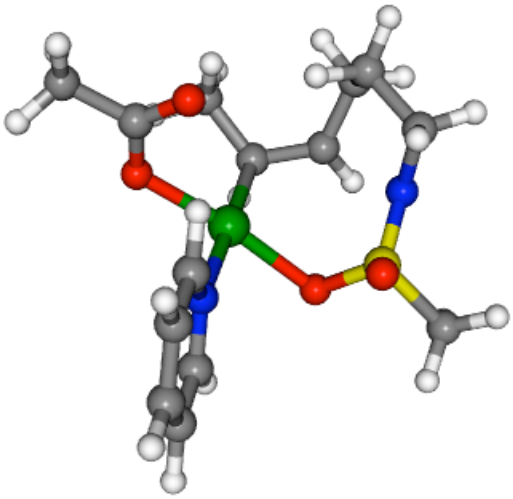
***cis*-[6,5]-J** $\Delta G^{\ddagger}_{353K}$ **= 33.2 kcal/mol**



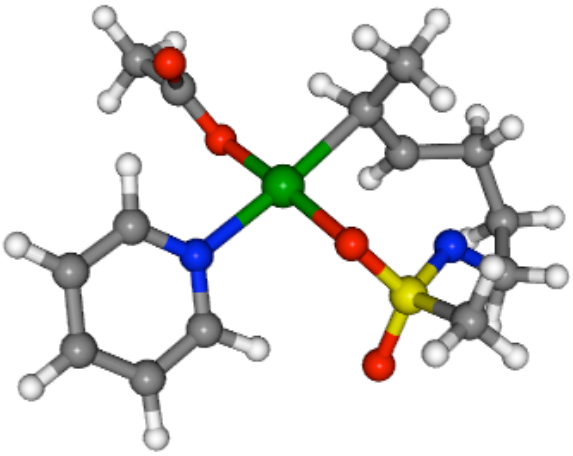
***cis*-[6,5]-K** $\Delta G^{\ddagger}_{298K}$ **= 41.2 kcal/mol**



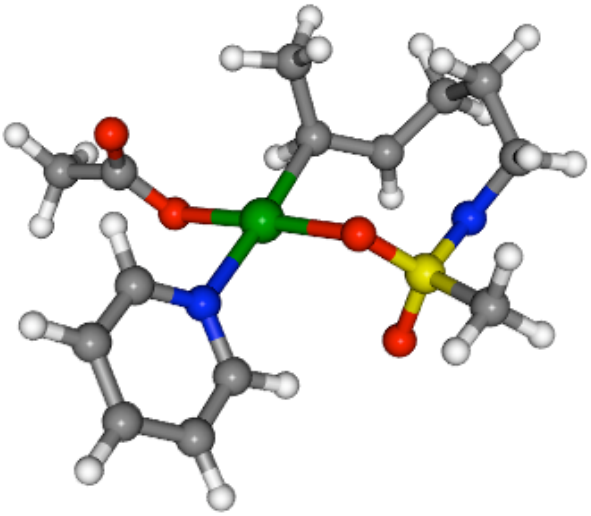
***cis*-[6,5]-N** $\Delta G^{\ddagger}_{298K}$ **= 41.7 kcal/mol**



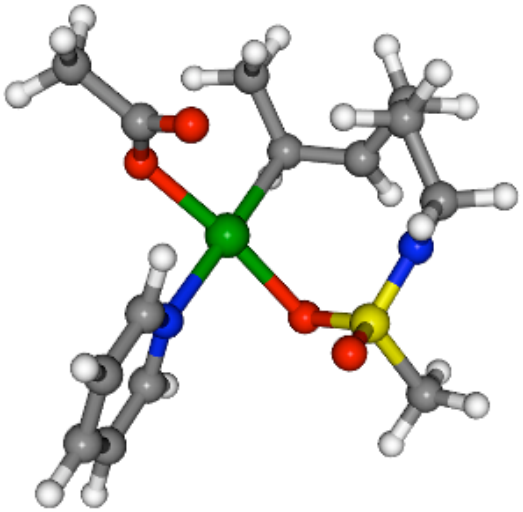
cis-[6,5]-L $\Delta G^{\ddagger}_{298K}$ **= 41.2 kcal/mol**



***cis*-[6,5]-O** $\Delta G^{\ddagger}_{298K}$ **= 39.0 kcal/mol**



***cis*-[6,5]-M** $\Delta G^{\ddagger}_{298K}$ **= 41.7 kcal/mol**



***cis*-[6,5]-P** $\Delta G^{\ddagger}_{298K}$ **= 41.6 kcal/mol**

Cartesian Coordinates for Optimized Complexes.

Py

N	0.013626	0.000000	0.007873
C	0.045790	0.000000	1.347809
C	1.227556	0.000000	2.094507
C	2.445542	0.000000	1.411944
C	2.427702	0.000000	0.015826
C	1.190137	0.000000	-0.634246
H	-0.921617	0.000000	1.847427
H	1.188716	0.000000	3.180378
H	3.387116	0.000000	1.955566
H	3.348682	0.000000	-0.560733
H	1.139078	0.000000	-1.721850

HOAc

C	1.267274	0.000000	-0.601072
C	-0.039216	0.000000	0.148978
O	-1.103693	0.000000	-0.698365
O	-0.172045	0.000000	1.354154
H	2.095470	0.000000	0.108363
H	1.327608	0.882663	-1.246945
H	1.327608	-0.882663	-1.246945
H	-1.908802	0.000000	-0.146471

$[AcOH]_2$

C	1.568066	0.005396	2.931707
C	1.339487	0.009255	1.444316
O	0.099391	-0.321251	1.104818
O	2.216910	0.291268	0.627407
O	1.953162	0.340298	-2.066356
C	0.713077	0.009749	-2.405856
C	0.484467	0.013724	-3.893242
O	-0.164358	-0.272219	-1.588946
H	-0.004184	-0.304760	0.107715
H	0.879392	0.707880	3.413563
H	1.353026	-0.989570	3.336356
H	2.599496	0.283208	3.151251
H	2.056736	0.323810	-1.069253
H	1.173104	-0.688759	-4.375150
H	-0.546978	-0.264034	-4.112784
H	0.699538	1.008705	-4.297838

1M

C	-4.973637	-7.853715	-2.794513
C	-3.775940	-7.108109	-2.271907
C	-3.286726	-5.929661	-2.686352
C	-3.815744	-5.037848	-3.779761
C	-4.235249	-3.651129	-3.252055
C	-4.704766	-2.723333	-4.375037
N	-5.076794	-1.410412	-3.810742
S	-5.600008	-0.196424	-4.873589
O	-6.553934	0.617256	-4.107177
O	-5.966036	-0.774322	-6.174795
C	-4.098236	0.769702	-5.119286
H	-5.538267	-3.174156	-4.929663
H	-3.890527	-2.562382	-5.090394
H	-3.396599	-3.180679	-2.722376
H	-5.041409	-3.778257	-2.515386
H	-4.663202	-5.504668	-4.294428
H	-3.030203	-4.900639	-4.539376
H	-5.768857	-1.472063	-3.064055
H	-2.399391	-5.548463	-2.177144
H	-3.248796	-7.604887	-1.455895
H	-4.679426	-8.839941	-3.179253
H	-5.698202	-8.035794	-1.989067
H	-5.492800	-7.323906	-3.598316
H	-4.351479	1.573082	-5.815238
H	-3.782289	1.171621	-4.155689
H	-3.329177	0.125293	-5.550484

VPyr

N	0.500901	0.665188	0.784136
C	0.926869	-0.741380	0.552340
C	2.197685	-0.602883	-0.296385
C	2.766647	0.750166	0.148021
C	1.519830	1.650246	0.318613
C	1.751570	2.781425	1.283362
C	1.921613	4.053347	0.917675
S	-1.129919	1.025167	0.780797
O	-1.282692	2.399398	1.264629
O	-1.804763	-0.102797	1.434226
H	0.140706	-1.321867	0.060714
H	1.128705	-1.219684	1.517621
H	1.942774	-0.575759	-1.363695
H	2.892818	-1.434080	-0.139807
H	3.277268	0.651576	1.114346
H	3.474707	1.190894	-0.559963
H	1.238934	2.064869	-0.662932
C	-1.665696	1.020006	-0.953697
H	1.817622	2.491066	2.331571
H	2.137137	4.830509	1.645495
H	1.833478	4.368825	-0.120830
H	-2.735526	1.242643	-0.950689
H	-1.124192	1.794847	-1.500725
H	-1.490183	0.031590	-1.384421

$(py)_2Pd(OAc)_2$

C	-2.469541	0.340104	1.103933
N	-1.794562	-0.043733	0.002594
C	-2.470985	-0.430708	-1.096763
C	-3.863613	-0.441771	-1.130141
C	-4.572732	-0.050180	0.006671
C	-3.862104	0.344705	1.141397
Pd	0.263075	-0.039029	-0.000470
O	0.264957	-2.057660	-0.334611
C	0.274283	-2.489580	-1.563752
O	0.276339	-1.767796	-2.572296
N	2.320985	-0.034321	-0.003523
C	2.997444	0.342028	1.099589
C	4.390111	0.352708	1.132972
C	5.099245	-0.027837	-0.007581
C	4.388565	-0.411698	-1.146058
C	2.995965	-0.407517	-1.108608
O	0.256900	1.979591	0.333673
C	0.267510	2.411570	1.562786
O	0.275505	1.689817	2.571322
C	0.287717	3.932071	1.670467
C	0.301205	-4.009974	-1.671532
H	-1.865443	-0.733148	-1.945429
H	-1.862913	0.645357	1.950816
H	-4.372746	-0.755062	-2.036086
H	-4.370022	0.655632	2.048837
H	-5.659401	-0.052704	0.008267
H	2.391683	0.637092	1.950802
H	2.389095	-0.705413	-1.958044
H	4.899251	0.657209	2.041915
H	4.896462	-0.713824	-2.056488
H	6.185918	-0.025300	-0.009170
H	-0.462486	4.376084	1.008077
H	0.109475	4.238961	2.703610
H	1.266714	4.307460	1.348390
H	0.120376	-4.317690	-2.703983
H	1.283280	-4.380677	-1.353407
H	-0.444222	-4.457570	-1.006181

$13^{AP\text{-}TS}$ (*trans* py-amidate)

C	-1.731725	1.262066	1.756535
S	-1.409658	0.583443	0.112186
O	-1.028308	-0.831265	0.284720
O	-2.559176	0.926710	-0.743324
N	-0.083771	1.440477	-0.457362
C	1.244455	0.818748	-0.341305
C	1.523524	-0.001823	-1.604899
C	1.198649	0.902735	-2.808798
C	-0.121706	1.597322	-2.638591
C	-0.339114	2.984644	-2.880010
C	0.686549	3.889048	-3.546841
Pd	-0.392282	3.447011	-0.816703
O	-0.506234	3.822435	1.377468
C	0.547772	4.101322	2.029839
C	0.501383	4.404101	3.503126
N	-0.703496	5.497422	-1.146795
H	1.979633	1.622411	-0.219793
H	1.291445	0.186666	0.551858
H	-2.630095	0.763932	2.130352
H	-1.880548	2.339936	1.672445

H	-0.875467	1.038489	2.396569
H	-1.372881	3.222016	-3.147095
H	0.397730	4.935992	-3.414578
H	1.695849	3.772398	-3.140618
H	0.733749	3.690171	-4.628241
H	-1.004618	0.964745	-2.632683
H	2.001374	1.630538	-2.961616
H	1.128001	0.298020	-3.725504
H	0.878693	-0.886845	-1.602952
H	2.565770	-0.341301	-1.647794
H	1.502315	4.638205	3.874552
H	-0.186579	5.229755	3.703308
H	0.135703	3.518268	4.037228
O	1.622215	4.163630	1.455303
C	0.387476	6.341271	-1.386999
C	0.180000	7.708211	-1.607060
C	-1.118449	8.231303	-1.586918
C	-2.209421	7.387454	-1.346714
C	-2.001945	6.020514	-1.126653
H	1.397484	5.934380	-1.402667
H	1.028621	8.364605	-1.793905
H	-1.279836	9.294588	-1.758094
H	-3.219429	7.794345	-1.331047
H	-2.850566	5.364120	-0.939809

Iso-13$^{AP\text{-}TS}$ (*cis* py-amidate)

Pd	-0.035190	-0.379120	0.011282
O	-1.292246	-1.775499	-0.809223
C	-2.244929	-2.293416	-0.083029
O	-2.518193	-1.970824	1.079646
C	-3.019829	-3.397926	-0.795771
H	-2.475964	-4.344344	-0.681850
H	-4.007484	-3.514847	-0.342600
H	-3.111334	-3.193023	-1.866566
N	1.483064	0.911831	0.690369
S	1.468809	1.463720	2.274071
C	2.344844	1.638544	-0.255962
C	2.438734	-1.009283	0.701105
H	2.516026	-0.994839	1.783859
C	1.459400	-1.889065	0.151631
H	0.982522	-2.520256	0.906554
C	1.665397	-2.591917	-1.183358
H	2.049491	-1.931732	-1.966995
H	2.377096	-3.424830	-1.073092
H	0.715280	-3.002093	-1.535024
N	-1.592468	1.131550	-0.144614
C	-1.524354	2.127994	-1.046945
C	-2.525738	3.086474	-1.185895
C	-3.645422	3.012427	-0.353935
C	-3.719729	1.976379	0.577309
C	-2.678163	1.050049	0.651342
H	-2.701362	0.199655	1.326282
H	-4.573319	1.870579	1.239645
H	-4.444349	3.744623	-0.435291
H	-2.425100	3.867766	-1.933088
H	-0.638865	2.146173	-1.674203
H	3.033884	2.281304	0.302752
C	3.154144	0.613441	-1.064066
H	1.746446	2.272273	-0.925309
C	3.614093	-0.474295	-0.074721
H	4.345156	-0.048230	0.620551

H	4.097006	-1.299410	-0.615340
H	2.531731	0.173415	-1.850460
H	4.010950	1.094442	-1.550841
O	2.808294	1.980092	2.622352
C	0.354535	2.889986	2.310571
O	0.865228	0.404920	3.095667
H	0.381241	3.273331	3.333996
H	0.722535	3.647460	1.614658
H	-0.651346	2.563012	2.047893

$17^{AP\text{-}TS}$ (κ^2-OAc)

C	-1.731725	1.262066	1.756535
S	-1.409658	0.583443	0.112186
O	-2.559176	0.926710	-0.743324
N	-0.083771	1.440477	-0.457362
Pd	-0.392282	3.447011	-0.816703
O	-0.674594	5.516603	-0.857903
C	-0.743229	5.598405	0.423421
O	-0.613128	4.539582	1.113538
C	1.244455	0.818748	-0.341305
C	1.523524	-0.001823	-1.604899
C	1.198649	0.902735	-2.808798
C	-0.121706	1.597322	-2.638591
C	-0.339114	2.984644	-2.880010
C	0.686549	3.889048	-3.546841
O	-1.028308	-0.831265	0.284720
C	-1.002042	6.931050	1.072632
H	1.979633	1.622411	-0.219793
H	1.291445	0.186666	0.551858
H	-2.630095	0.763932	2.130352
H	-1.880548	2.339936	1.672445
H	-0.875467	1.038489	2.396569
H	-1.372881	3.222016	-3.147095
H	0.397730	4.935992	-3.414578
H	1.695849	3.772398	-3.140618
H	0.733749	3.690171	-4.628241
H	-1.004618	0.964745	-2.632683
H	2.001374	1.630538	-2.961616
H	1.128001	0.298020	-3.725504
H	0.878693	-0.886845	-1.602952
H	2.565770	-0.341301	-1.647794
H	-0.564800	6.957104	2.074015
H	-0.602910	7.741376	0.456893
H	-2.085358	7.076444	1.167366

Iso-17$^{AP\text{-}TS}$ (κ^1-OAc)

N	0.837731	2.340479	0.504328
C	0.461023	1.771427	-1.549105
C	-0.675553	0.901491	-1.433014
C	-2.076055	1.335414	-1.828753
H	-2.797397	0.579877	-1.507289
H	-2.377687	2.290590	-1.387129
H	-2.156639	1.427682	-2.922737
H	-0.453000	-0.149275	-1.639342
H	1.425730	1.283843	-1.651926
C	0.384688	3.190555	-2.046617
H	0.880355	3.218627	-3.027838
H	-0.658615	3.480336	-2.200527
C	1.055992	4.177951	-1.073936
C	0.588355	3.780446	0.325057
H	2.148688	4.099829	-1.128771
H	0.783884	5.210539	-1.322567
H	-0.486780	3.955992	0.444598
H	1.110059	4.345230	1.101938
S	2.201919	1.883884	1.397674
O	1.717560	0.936698	2.424026
O	2.952158	3.085067	1.799116
C	3.260088	0.922660	0.290682
H	2.707113	0.055985	-0.077781
H	3.616461	1.560313	-0.520998
H	4.100222	0.590466	0.905968
Pd	-0.464350	0.752548	0.650220
O	-0.603791	-2.142303	-0.526197
C	-1.488616	-1.943659	0.312592
O	-1.734858	-0.792681	0.891748
C	-2.406433	-3.061831	0.788373
H	-2.358716	-3.905185	0.095710
H	-2.075443	-3.398218	1.778567
H	-3.436717	-2.707439	0.890295

9M

Pd	-0.000936	-0.320019	-1.041649
N	-0.699005	-1.212380	-2.711553
S	-2.169034	-1.936078	-2.601397
O	-2.314405	-2.373658	-1.196698
O	-2.290186	-2.930498	-3.688738
C	-3.470750	-0.710107	-2.896208
H	-3.380285	0.064786	-2.133733
H	-4.425052	-1.238213	-2.824357
H	-3.346744	-0.295784	-3.900142
C	-0.229530	-0.750773	-4.020810
H	-0.776475	0.137954	-4.377297
H	-0.396170	-1.560003	-4.743558
C	1.272547	-0.420317	-3.961580
H	1.416882	0.582854	-3.540798
H	1.660650	-0.396017	-4.987649
C	2.064368	-1.453149	-3.130763
H	1.742447	-2.464548	-3.397055
H	3.130505	-1.376307	-3.388216
C	1.964516	-1.227007	-1.636315
H	2.600807	-0.423163	-1.262371
C	1.421543	-2.087616	-0.691884
C	0.826640	-3.446793	-0.939090
H	-0.067241	-3.602270	-0.327629

H	0.539771	-3.601320	-1.979237
H	1.566450	-4.210782	-0.655950
H	1.684898	-1.889947	0.347284
N	0.682359	0.575054	0.749578
C	1.458450	1.676793	0.739489
C	1.857133	2.307106	1.917398
C	1.429888	1.792672	3.141864
C	0.610871	0.661339	3.146738
C	0.259945	0.081402	1.930881
H	-0.380667	-0.793767	1.882826
H	0.243085	0.230536	4.072563
H	1.722091	2.267470	4.074448
H	2.481702	3.193036	1.862321
H	1.715575	2.064367	-0.239764
O	-1.525022	1.098673	-1.097142
C	-1.143150	2.279911	-1.496777
O	0.015638	2.582175	-1.817099
C	-2.272468	3.302830	-1.552254
H	-2.977106	3.030597	-2.347247
H	-2.832107	3.309471	-0.610919
H	-1.869997	4.297256	-1.757534

[15/py]^{TS}

Pd	-0.148586	-0.373777	-1.057920
C	1.368914	-1.966525	-0.587398
C	1.873403	-1.112094	-1.565891
C	2.056209	-1.419202	-3.035988
C	1.250665	-0.469245	-3.944245
C	-0.240458	-0.847708	-4.015705
N	-0.706083	-1.376819	-2.724994
S	-2.234152	-2.016397	-2.683245
O	-2.460306	-2.484917	-1.300606
O	-2.357881	-2.974220	-3.799466
C	-3.447450	-0.706156	-2.995530
H	-3.317905	0.077439	-2.247522
H	-3.293477	-0.314799	-4.003905
H	-4.433034	-1.172981	-2.922182
H	-0.820120	0.028162	-4.349125
H	-0.377733	-1.643073	-4.759340
H	1.660466	-0.486303	-4.961950
H	1.358580	0.559056	-3.575675
H	1.798461	-2.458628	-3.259846
H	3.127061	-1.298362	-3.254597
H	2.414890	-0.229248	-1.219935
H	1.572877	-1.691624	0.446577
C	0.917556	-3.388364	-0.783881
H	0.102360	-3.635453	-0.096950
H	1.755952	-4.065114	-0.559275
H	0.569366	-3.583991	-1.798432
O	-1.538485	1.184633	-1.240825
C	-0.898150	2.082794	-0.561988
O	0.236220	1.837928	-0.082943
C	-1.581638	3.412799	-0.347021
H	-0.847378	4.176684	-0.079511
H	-2.302056	3.316057	0.474854
H	-2.135575	3.713039	-1.241479
N	-0.744344	-0.604905	1.451763
C	-1.704707	-1.502523	1.735592
C	-2.134204	-1.757344	3.040701
C	-1.543478	-1.056273	4.093150

C	-0.549381	-0.119771	3.800317
H	0.565352	0.808346	2.185706
C	-0.185673	0.075033	2.466475
H	-0.065095	0.454339	4.585088
H	-1.852829	-1.232927	5.120262
H	-2.915544	-2.490771	3.217747
H	-2.137075	-2.019661	0.882829

κ^2-16M

C	4.129037	-0.547926	-1.719795
S	4.654728	-2.250847	-1.438997
O	6.103971	-2.327297	-1.711520
O	4.163270	-2.633563	-0.095638
N	3.829470	-3.076958	-2.648674
Pd	1.871696	-3.429092	-2.276021
O	1.079540	-1.590203	-3.153016
C	-0.096125	-1.996925	-2.889476
O	-0.228069	-3.142601	-2.323265
C	4.603242	-4.067579	-3.409136
C	4.881691	-5.394147	-2.688832
C	3.593962	-6.110522	-2.252549
C	2.768023	-5.291803	-1.294704
C	1.390082	-5.327021	-1.163436
C	0.429121	-6.191417	-1.934211
C	-1.305458	-1.162312	-3.201263
H	4.038970	-4.250314	-4.333000
H	5.555907	-3.606994	-3.694116
H	4.570968	0.052496	-0.920677
H	3.039149	-0.502775	-1.688358
H	4.497901	-0.232208	-2.697006
H	-1.077874	-0.442827	-3.991491
H	-1.600434	-0.610117	-2.300429
H	-2.143491	-1.801469	-3.493304
H	0.973495	-4.868453	-0.265982
H	-0.502274	-5.652157	-2.130761
H	0.837592	-6.549010	-2.882830
H	0.179459	-7.070424	-1.321377
H	3.324074	-4.809419	-0.491617
H	3.007679	-6.404536	-3.131344
H	3.866821	-7.042721	-1.732544
H	5.518597	-5.204457	-1.815844
H	5.450695	-6.048964	-3.362363

10M

C	3.406738	-1.203315	2.372223
C	3.109091	-0.880508	0.901498
C	2.044755	0.213138	1.007352
N	2.444435	1.016323	2.228177
C	3.451239	0.167308	3.066042
Pd	1.080638	1.019281	3.853975
O	-0.607506	1.946193	2.834737
C	-1.490837	1.157233	2.313668
C	-2.623242	1.861251	1.567278
S	3.126420	2.597593	1.817626
O	3.646798	3.156424	3.068860
C	2.888157	0.295860	4.487924
C	2.924106	-0.948731	5.367406
C	1.674229	3.527234	1.292421
O	4.031283	2.424862	0.670212
H	1.047269	-0.191414	1.195585
H	2.003418	0.856960	0.126466
H	1.991430	4.573545	1.296204
H	0.849269	3.344099	1.986808
H	1.408668	3.215455	0.280875
H	-3.232627	1.137374	1.020819
H	-2.224525	2.612215	0.875945
H	-3.257932	2.392984	2.287132
H	3.378914	1.135900	4.994110
H	2.520187	-0.727801	6.361632
H	2.340484	-1.781067	4.959407
H	3.956000	-1.309048	5.513194
H	4.453565	0.599979	2.954896
H	2.599181	-1.817035	2.784915
H	4.348208	-1.744401	2.511821
H	4.000980	-0.489211	0.398948
H	2.747671	-1.748172	0.339838
O	-1.476368	-0.086450	2.402216
N	0.006918	0.763565	5.609369
C	-1.131461	0.038810	5.569759
C	-1.919441	-0.152552	6.703961
C	-1.532234	0.429950	7.911137
C	-0.359363	1.187222	7.943469
C	0.384375	1.326042	6.774573
H	-1.396105	-0.366584	4.596171
H	-2.824406	-0.747099	6.626845
H	-2.131773	0.299624	8.808009
H	-0.017411	1.665088	8.856242
H	1.305723	1.897801	6.752708

14

C	3.200885	-1.233802	2.091899
C	2.626651	-0.674409	0.780699
C	1.664976	0.414145	1.259294
N	2.348604	0.999542	2.481258
C	3.444765	0.012729	2.956708
Pd	1.307455	0.849332	4.309960
O	-0.649285	1.595377	4.441483
C	-1.412329	1.833482	3.419317
C	-2.868601	2.120480	3.763297
S	3.022665	2.632707	2.182371
O	3.947535	2.893786	3.289380
C	3.135849	-0.028425	4.455531
C	3.064148	-1.362259	5.177564
C	1.569223	3.684886	2.309638
O	3.519369	2.645445	0.799833
H	0.692548	0.035114	1.573221
H	1.489739	1.197881	0.521695
H	1.828440	4.603350	1.776547
H	1.383690	3.874734	3.367384
H	0.706825	3.177673	1.864688
H	-3.438183	2.356723	2.861684
H	-2.929814	2.954803	4.471269
H	-3.310869	1.247486	4.257627
H	3.758643	0.696294	4.992727
H	2.799056	-1.215925	6.231226
H	2.332210	-2.052046	4.741948
H	4.041109	-1.874158	5.163904
H	4.431586	0.432306	2.731236
H	2.468808	-1.899009	2.562017
H	4.126618	-1.800473	1.950328
H	3.419056	-0.233031	0.165475
H	2.113891	-1.435698	0.183801
O	-1.021718	1.842536	2.237708

18M

C	2.866074	-0.565514	0.698938
C	1.872723	0.533207	1.080574
N	2.409458	1.096113	2.378760
C	3.401917	0.051135	2.985500
C	3.240625	-1.165462	2.061734
Pd	1.181787	0.966036	4.098693
C	2.912825	-0.030568	4.433660
C	2.755340	-1.386651	5.101197
S	3.166119	2.692725	2.167996
C	1.738852	3.792109	2.214118
O	-0.865150	2.006421	4.204650
C	-0.969784	1.467466	5.345334
C	-2.205775	1.646265	6.192623
O	-0.015592	0.730015	5.794713
O	3.762911	2.748540	0.825597
O	4.001500	2.917124	3.349153
H	0.876289	0.132489	1.282236
H	1.790932	1.322106	0.330677
H	2.139820	4.794933	2.043473
H	1.258110	3.713205	3.190138
H	1.047875	3.517235	1.414994
H	-2.781385	2.509427	5.850410
H	-1.933239	1.761305	7.245890
H	-2.831906	0.749568	6.107458
H	3.494632	0.650594	5.064551
H	2.331054	-1.258543	6.102290
H	2.096130	-2.066954	4.552338
H	3.730906	-1.887375	5.216806
H	4.419675	0.448715	2.901706
H	2.431912	-1.814166	2.414284
H	4.159613	-1.759476	2.032827
H	3.741101	-0.122916	0.209529
H	2.424302	-1.298852	0.016242

$19^{BHE\text{-}TS}$ (trans py-H)

Pd	-0.018037	-0.028422	0.173257
H	-0.253513	-0.111018	1.716066
C	1.488579	0.092585	1.800416
C	2.109252	-0.065749	0.545831
N	0.054778	0.110978	-2.001266
O	-2.101617	-0.075578	-0.053842
C	-2.629331	1.080285	-0.331597
O	-1.995775	2.134408	-0.496982
C	-4.152832	1.057134	-0.427236
H	-4.574172	1.030890	0.585456
H	-4.515361	1.955051	-0.933770
H	-4.499474	0.158985	-0.948429
C	0.136399	1.323271	-2.581206
C	0.001738	1.501425	-3.957837
C	-0.241056	0.388628	-4.763370
C	-0.345236	-0.866419	-4.159584
C	-0.193031	-0.959696	-2.778039
H	-0.280727	-1.911984	-2.264447
H	-0.547947	-1.760384	-4.741257
H	-0.357281	0.497125	-5.838373
H	0.070532	2.500161	-4.377275
H	0.278393	2.163002	-1.911333
H	1.413283	1.084248	2.239237
H	1.506561	-0.727605	2.511875
H	2.507044	0.830665	0.067865
C	2.816930	-1.361774	0.160012
H	2.175631	-2.209173	0.421477
C	3.252099	-1.400964	-1.320369
H	2.548766	-0.874938	-1.968489
H	3.313084	-2.442258	-1.662869
C	4.655286	-0.771322	-1.312326
H	5.238852	-1.013246	-2.206133
H	4.587979	0.320995	-1.245065
N	4.133432	-1.489302	0.877200
S	4.297370	-2.496045	2.197755
O	3.089707	-2.344886	3.020410
O	5.635792	-2.253470	2.747056
C	5.291174	-1.344331	-0.040273
C	4.283243	-4.201754	1.578450
H	4.399275	-4.849558	2.450961
H	5.120031	-4.347455	0.891901
H	3.326744	-4.400245	1.089612
H	5.760065	-2.317446	-0.248791
H	6.047437	-0.696003	0.407652

$19^{1°\text{-BHE-TS}}$ (cis py-H)

Pd	-3.244590	0.242324	-0.549640
H	-1.708255	0.312266	-0.192527
C	-2.117367	1.735572	0.664433
C	-3.399889	2.195305	0.294139
O	-5.300690	0.214472	-1.090354
C	-6.109244	-0.403553	-0.283471
C	-7.580888	-0.315636	-0.682813
O	-5.765858	-1.020163	0.739016
H	-8.182954	-0.994017	-0.073756
H	-7.706103	-0.550945	-1.745236
H	-7.941572	0.709807	-0.532910
C	-4.984685	3.394113	-1.341803
C	-3.573291	3.315045	-0.726594
C	-5.757642	4.298369	-0.367674
C	-4.734564	5.378853	0.007683
N	-3.442612	4.647482	-0.042458
S	-2.030956	5.523933	-0.139852
O	-0.914384	4.572932	-0.033698
O	-2.162583	6.654241	0.786186
C	-1.949662	6.222837	-1.812977
H	-2.805981	6.881346	-1.973493
H	-1.021392	6.797052	-1.866763
H	-1.932250	5.409958	-2.542661
H	-4.754493	6.200692	-0.723418
H	-4.884216	5.807603	1.001094
H	-6.661215	4.729874	-0.809887
H	-6.061537	3.736198	0.523383
H	-4.922989	3.877514	-2.326155
H	-2.800071	3.216565	-1.495454
H	-4.201660	2.104458	1.026326
H	-1.240040	2.205504	0.229486
H	-1.967307	1.303612	1.650677
H	-5.424622	2.402180	-1.469775
N	-2.982075	-1.733102	-1.367495
C	-3.668866	-2.761504	-0.829750
C	-3.553034	-4.062967	-1.319028
C	-2.708958	-4.311670	-2.401133
C	-2.002940	-3.243454	-2.958735
C	-2.163688	-1.973747	-2.409741
H	-4.330434	-2.505293	-0.006818
H	-4.125265	-4.858998	-0.852822
H	-2.602742	-5.315527	-2.803612
H	-1.334608	-3.384097	-3.802639
H	-1.628515	-1.117065	-2.805624

11M

Pd	1.081183	-0.800305	-0.692457
N	2.869633	-0.051189	0.187497
C	2.861752	1.177396	0.744845
C	4.017335	-0.758036	0.181531
C	4.005928	1.734047	1.315678
H	1.910458	1.702323	0.716971
C	5.201156	-0.261260	0.720170
H	3.970085	-1.743300	-0.268311
C	5.197051	1.008550	1.301385
H	3.951221	2.724441	1.756628
H	6.102042	-0.865780	0.684125
H	6.104086	1.421824	1.734196
O	0.803975	0.946121	-1.912664
C	0.243399	1.963586	-1.346690
O	-0.087118	2.011289	-0.143022
C	0.003558	3.157436	-2.266239
H	-0.627329	2.858913	-3.111479
H	-0.474823	3.974314	-1.720881
H	0.956433	3.501618	-2.685078
N	-3.152915	-2.161342	-0.195890
S	-3.617751	-3.691505	-0.663209
C	-4.106654	-1.305499	0.551903
O	-5.002767	-3.590183	-1.136356
O	-2.550343	-4.232121	-1.514177
C	-3.213357	-0.165553	1.054690
H	-4.914176	-0.980798	-0.107695
H	-4.553658	-1.851656	1.396842
C	-1.860001	-0.851022	1.305990
H	-3.108527	0.609456	0.287615
H	-3.621615	0.309569	1.952085
H	-1.029412	-0.140920	1.324730
H	-1.879306	-1.393492	2.259933
C	-1.727246	-1.862727	0.144897
C	-1.040631	-1.285068	-1.079955
H	-1.204931	-2.773520	0.454082
H	-1.426846	-0.322553	-1.408103
C	-0.242507	-2.007548	-1.948856
H	-0.024236	-1.616991	-2.939828
H	-0.060443	-3.065060	-1.787250
C	-3.651160	-4.710233	0.838249
H	-3.962872	-5.711055	0.529167
H	-2.649527	-4.746129	1.272808
H	-4.375143	-4.293995	1.542134
H	1.286521	-2.103731	0.125814

$20^{2°\text{-BHE-TS}}$ (cis py-H)

O	4.134654	-0.097309	-0.667735
Pd	2.411318	-0.672818	0.409720
H	1.201565	-1.188848	1.314262
C	3.525664	-1.080263	2.128701
H	4.116414	-0.198004	2.356686
H	4.092462	-1.993361	1.956715
C	2.194468	-1.167382	2.612095
H	1.812219	-2.156458	2.864291
C	1.595540	-0.030945	3.450746
C	0.060815	0.125877	3.368234
H	-0.329915	-0.110337	2.375787
C	2.754826	2.084949	5.915424
H	3.583464	2.504818	6.491180
H	2.718863	2.543487	4.924655
H	-0.204401	1.167685	3.588341
C	-0.470479	-0.793020	4.479388
C	0.528449	-0.565203	5.618550
H	-0.450916	-1.841806	4.158905
H	0.625225	-1.410986	6.302036
H	0.245726	0.318792	6.209726
H	-1.495805	-0.555382	4.779473
S	3.093850	0.311622	5.745652
O	3.030998	-0.272044	7.090415
O	4.289604	0.186988	4.907885
H	2.104359	0.896785	3.169763
C	4.399943	1.170133	-0.634933
O	3.670302	2.040181	-0.121812
C	5.728085	1.552431	-1.282531
H	6.548787	1.273945	-0.609652
H	5.771245	2.629705	-1.460897
H	5.875231	1.004883	-2.219117
H	1.815634	2.224155	6.455378
N	1.171800	-0.263858	-1.311897
N	1.807230	-0.344186	4.896567
C	1.167892	0.987627	-1.814714
C	0.430236	1.326420	-2.949285
C	-0.320644	0.342418	-3.592575
C	-0.309602	-0.954070	-3.073765
C	0.445230	-1.212875	-1.931803
H	1.788814	1.707171	-1.287177
H	0.457740	2.347549	-3.316974
H	-0.900315	0.578172	-4.481095
H	-0.873098	-1.756348	-3.540195
H	0.480754	-2.204694	-1.492877

21

C	4.645251	-2.512360	-4.718140
C	5.301000	-2.249243	-3.340836
C	6.222910	-1.011792	-3.511159
N	5.850406	-0.476324	-4.905134
C	5.490818	-1.702519	-5.700250
C	6.031356	0.102129	-2.486876
C	4.656990	0.763597	-2.651897
Pd	4.190425	0.866233	-4.633728
O	3.724348	0.894396	-6.770739
C	2.727581	0.186192	-7.199722
C	2.462589	0.298164	-8.701061
S	7.276572	0.360235	-5.630698
O	7.449343	1.620488	-4.903535
N	2.619616	2.156400	-4.213341
C	6.737638	0.704169	-7.313594
O	8.381741	-0.611603	-5.669914
H	2.396586	1.350598	-8.998755
H	3.297434	-0.142639	-9.260867
H	1.541331	-0.224480	-8.969150
H	4.641831	1.756932	-2.186619
H	3.853279	0.169446	-2.193799
H	7.267965	-1.340048	-3.551864
H	7.440633	1.458997	-7.676406
H	5.707369	1.075578	-7.302043
H	6.826193	-0.212551	-7.898672
H	6.410955	-2.236836	-5.969607
H	4.948173	-1.407171	-6.597836
H	4.638310	-3.573117	-4.988901
H	3.613697	-2.149352	-4.746882
H	5.901133	-3.103788	-3.011315
H	4.543707	-2.067499	-2.572720
H	6.821218	0.847384	-2.618795
H	6.159709	-0.324227	-1.478551
O	2.016155	-0.549489	-6.490614
C	1.353440	1.774506	-4.484770
C	0.266980	2.618581	-4.259006
C	0.489658	3.897941	-3.749045
C	1.801762	4.291454	-3.479717
C	2.837263	3.392084	-3.719854
H	1.242873	0.783346	-4.915576
H	-0.733723	2.267607	-4.490874
H	-0.339994	4.576088	-3.568343
H	2.029823	5.278050	-3.088532
H	3.870648	3.653325	-3.522381

22

Pd	1.062625	-1.556275	-1.301228
H	2.251694	-1.361684	-0.334880
O	-0.849561	-1.913793	-1.993953
C	-1.561846	-1.601744	-3.036052
O	-1.097857	-1.116413	-4.078771
C	-3.048569	-1.896437	-2.898085
H	-3.199714	-2.970365	-2.738314
H	-3.585117	-1.580332	-3.795444
H	-3.454050	-1.378666	-2.021431
N	2.449460	-1.246152	-2.764258
C	1.961100	-1.017311	-4.003931
C	2.810567	-0.803606	-5.089689
C	4.190744	-0.831494	-4.900656
C	4.684016	-1.073092	-3.616266
C	3.788737	-1.272696	-2.571808
H	4.126545	-1.458498	-1.561600
H	5.749875	-1.106655	-3.413779
H	4.870104	-0.669681	-5.733033
H	2.372465	-0.621648	-6.065801
H	0.872586	-1.013126	-4.106724
C	3.141310	0.812713	3.412774
H	2.777030	-0.054277	3.948791
H	5.186451	0.592427	4.019959
H	5.934074	2.625260	2.739448
H	4.204592	3.916238	1.440943
H	1.833258	3.123816	1.482382
H	0.442735	-0.142968	3.494774
O	-0.730213	2.641005	1.266043
C	-1.819241	2.017400	1.463067
O	-1.826094	0.972127	2.209908
C	-3.104573	2.462281	0.812679
H	-3.081237	3.538667	0.624057
H	-3.213753	1.946743	-0.149662
H	-3.962507	2.199361	1.437192

23

Pd	0.223391	1.076890	2.583224
N	2.218359	1.508125	2.715177
C	2.614865	2.601146	2.025691
C	3.938342	3.031810	2.010943
C	4.893522	2.313154	2.732136
C	4.482871	1.184982	3.443688

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C	2.318998	-1.092639	0.353995
N	1.602574	-0.024317	-0.057541
C	2.255230	1.137874	-0.275309
C	3.630748	1.268487	-0.100271
C	4.368873	0.160585	0.319339
C	3.696855	-1.040808	0.550246
Pd	-0.451654	-0.166892	-0.351179
O	-2.454404	-0.292218	-0.597375
C	-3.198180	0.166724	0.366796
C	-4.692908	0.041274	0.102995
O	-2.777552	0.670175	1.421042
H	-0.860774	0.456117	0.985019
H	1.755658	-2.002060	0.531951
H	4.223685	-1.929675	0.882704
H	5.442737	0.232895	0.467181
H	4.105068	2.226479	-0.288469
H	1.641373	1.973683	-0.591652
H	-5.262403	0.420876	0.953276
H	-4.957430	0.603708	-0.799482
H	-4.951912	-1.007427	-0.079580
C	-4.601253	0.198760	-0.403189
Pd	-0.565010	-0.687974	0.835978
O	1.349761	-1.234266	0.909688
C	2.087497	-1.195550	-0.182645
C	3.500038	-1.719755	0.053078
O	1.718724	-0.782178	-1.279450
H	-0.230461	0.763828	0.546322
H	-2.640964	-0.215002	-1.235360
H	-5.083606	0.289739	-1.371171
H	-6.377890	0.588618	0.766640
H	-5.143187	0.365584	2.948060
H	-2.699703	-0.140169	2.897298
H	4.040528	-1.777206	-0.894144
H	4.031953	-1.046933	0.736140
H	3.469348	-2.706321	0.528195

24^{TS}

C	-3.239473	-0.085475	-0.340266
N	-2.581679	-0.212141	0.832511
C	-3.271459	-0.044082	1.980697
C	-4.634321	0.240813	1.997502
C	-5.315095	0.364333	0.784960

26^{TS}

Pd	-0.494601	-0.415491	0.754225
H	-0.097715	0.775590	1.646337
O	1.651738	1.143061	2.144502
C	2.172464	0.201160	1.514874
O	1.524037	-0.665022	0.801146
N	-2.549121	-0.096634	0.755262
C	-3.271158	-0.240112	1.887884
C	-4.649815	-0.046931	1.926776
C	-5.318430	0.310488	0.754731
C	-4.575318	0.463124	-0.416901
C	-3.198888	0.254449	-0.375441
H	-2.582954	0.373903	-1.260261
H	-5.045847	0.744962	-1.353590
H	-6.393028	0.470154	0.755236
H	-5.180842	-0.174151	2.864875
H	-2.710348	-0.511542	2.774934
C	3.679124	-0.007550	1.543976
H	4.161554	0.768425	2.140878
H	3.906110	-0.992973	1.965935
H	4.075341	0.008431	0.522805
C	-0.149733	3.103145	2.738024
H	-0.216748	3.815314	3.555897
C	0.059351	1.745117	2.985125
H	0.159866	1.363303	3.996688
C	0.141975	0.863336	1.909630
H	0.306459	-0.197128	2.061191
H	2.030634	-0.346925	-1.899660
O	2.363402	-0.929081	-2.661790
C	1.307451	-1.632036	-3.053660
O	0.201056	-1.506752	-2.517354
C	1.568596	-2.579952	-4.187758
H	1.937838	-2.026057	-5.057753
H	2.347170	-3.295459	-3.901315
H	0.651882	-3.111408	-4.446278

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Pd	0.064331	-0.101499	-0.915824
N	0.027570	1.261170	0.621326
C	-0.175294	2.578988	0.390030
H	-0.261104	2.866227	-0.651423
C	-0.269055	3.521672	1.411495
H	-0.432195	4.565498	1.160456

29M

Pd	-4.753518	0.814807	0.596934
H	-3.692121	0.067287	1.409828
C	-6.180275	-0.069561	1.954216
C	-6.042642	-0.927912	0.869732
H	-7.013924	0.627031	2.002380
H	-5.675220	-0.278359	2.892828
H	-5.398619	-1.800769	0.969408
C	-7.026990	-0.980083	-0.290450
H	-7.534840	-0.013587	-0.368650
C	-6.378395	-1.383345	-1.634489
H	-5.347109	-1.028067	-1.713760
H	-6.946431	-0.936439	-2.459259
C	-6.505163	-2.915425	-1.670255
H	-5.734005	-3.384840	-1.047656
H	-6.414529	-3.327721	-2.680013
C	-7.893207	-3.164179	-1.069779
H	-8.671003	-3.071865	-1.843441
H	-8.003023	-4.139518	-0.591343
N	-8.007015	-2.084870	-0.059052
S	-9.488921	-1.781764	0.650806
O	-10.108485	-3.087648	0.899219
O	-9.261096	-0.819595	1.735368
C	-10.501934	-0.938783	-0.594119
H	-11.472140	-0.745568	-0.129297
H	-10.023040	0.003728	-0.869479
H	-10.625996	-1.591351	-1.461194
O	-3.642996	2.313234	-0.419932
C	-4.694812	2.779495	-0.993855
O	-5.819609	2.221884	-0.792638
H	-3.626885	3.988267	-2.414080
C	-4.574887	4.000248	-1.868908
H	-4.584207	4.894034	-1.232698
H	-5.417859	4.059102	-2.561786

28$^{1°\text{-BHE-TS}}$

H	3.157830	-0.179246	1.007288
Pd	1.716343	-0.127548	0.397226
C	3.704333	0.069311	-0.562080
C	2.651088	-0.003215	-1.503578
H	4.387018	-0.769192	-0.443744
H	4.135826	1.038131	-0.321742
C	2.448463	-1.193867	-2.428045
H	2.281275	0.932883	-1.919271
H	2.995196	-0.954231	-3.352563
C	2.918542	-2.567692	-1.905539
C	2.030779	-3.572976	-2.652846
C	0.667297	-2.871757	-2.667380
N	1.010787	-1.431083	-2.753524
S	0.287970	-0.495720	-3.953659
O	1.134360	0.699921	-4.105227
O	-0.037788	-1.315855	-5.132957
C	-1.268639	-0.008247	-3.192065
H	-1.060154	0.458911	-2.228449
H	-1.881479	-0.902239	-3.056921
H	-1.753685	0.681662	-3.887628
H	0.045505	-3.168668	-3.515530
H	0.112928	-3.054473	-1.737669
H	2.389279	-3.712612	-3.679892
H	3.987120	-2.723771	-2.085839
H	2.739122	-2.640563	-0.825562
O	-0.452733	-0.077602	0.083270
C	-0.624216	-0.143322	1.347561
O	0.394549	-0.227988	2.108620
C	-2.012174	-0.094731	1.933510
H	-2.718712	-0.620771	1.285257
H	-2.020425	-0.525509	2.937521
H	-2.333685	0.951888	2.001937
H	1.995646	-4.553346	-2.166692

$30^{2°\text{-BHE-TS}}$

H	3.982039	-0.287176	-0.689934
Pd	2.811290	-0.642228	0.291232
C	4.267711	-1.674442	1.381160
C	4.963743	-1.314468	0.202970
C	5.307392	-2.347394	-0.877104
C	5.500794	-1.777248	-2.299231
C	6.982781	-1.370823	-2.338144
C	7.675621	-2.507717	-1.577215
N	6.656463	-2.907050	-0.573067
S	6.833475	-4.373903	0.212381
C	6.422681	-5.666407	-0.991951
O	5.809189	-4.433226	1.260548
O	8.261217	-4.508481	0.516990
H	6.545875	-6.621457	-0.475073
H	5.385341	-5.545237	-1.312212
H	7.110961	-5.608733	-1.837933
H	7.911021	-3.340284	-2.255990
H	8.598972	-2.208843	-1.076830
H	7.370242	-1.263862	-3.355851
H	7.137296	-0.415356	-1.822819
H	5.312667	-2.572752	-3.031162
H	4.814550	-0.956429	-2.522456
H	4.546166	-3.133516	-0.856644
H	5.682093	-0.498384	0.277482
H	3.938431	-2.701521	1.516943
H	4.446320	-1.116056	2.298472
O	0.943706	-0.815008	1.381967
C	0.363222	-0.105290	0.494146
O	1.038822	0.321053	-0.501687
C	-1.094641	0.249520	0.634910
H	-1.182442	1.155170	1.247861
H	-1.635263	-0.554634	1.141149
H	-1.535651	0.453525	-0.343999

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Pd	-4.771864	0.837448	0.589059
H	-3.806581	0.018279	1.453486
O	-6.535648	0.307829	1.504155
C	-7.260896	1.022466	0.701573
O	-6.689379	1.705945	-0.191712
C	-8.756496	0.969235	0.846008
H	-9.042413	0.918861	1.900320
H	-9.128534	0.063691	0.351674
H	-9.206147	1.841760	0.366490

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C	5.537213	-2.441528	-3.327226
C	6.278740	-1.084576	-3.471244
N	5.819311	-0.551265	-4.851166
C	5.368743	-1.758918	-5.631970
C	4.652472	-2.601356	-4.580455
C	5.941409	-0.031826	-2.418323
C	4.506095	0.461421	-2.600682
Pd	4.194446	0.803279	-4.559904
O	2.555661	2.098188	-4.489355
C	2.488431	2.244300	-5.763402
C	1.438084	3.163467	-6.336154
S	7.206091	0.263040	-5.662815
C	6.466874	0.912506	-7.172209
O	3.312171	1.636838	-6.514109
O	8.180833	-0.777275	-6.024642
O	7.609776	1.367390	-4.791969
H	0.528099	3.131296	-5.730687
H	1.816995	4.192965	-6.318971
H	1.219767	2.893050	-7.372205
H	4.307777	1.397528	-2.068083
H	3.752001	-0.281323	-2.304605
H	7.358779	-1.259705	-3.517676
H	7.257977	1.516889	-7.624837
H	5.591248	1.519175	-6.932374
H	6.206941	0.079924	-7.827612
H	6.246785	-2.285606	-6.025188
H	4.727504	-1.441175	-6.457352
H	4.556518	-3.643273	-4.902343
H	3.647565	-2.204089	-4.405385
H	6.269611	-3.253479	-3.268051
H	4.945034	-2.467973	-2.407425
H	6.639673	0.804524	-2.517409
H	6.099404	-0.466719	-1.417733

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N	-1.120431	-0.936766	1.021492
C	-0.969549	0.313771	0.231161
C	-2.445336	0.690675	-0.074692
C	-3.193546	-0.651296	-0.036912
C	-2.528089	-1.389572	1.129540
C	-0.144954	0.122643	-1.034776
C	0.175330	-1.105777	-1.599192
Pd	1.931633	-0.348310	-0.572442
O	1.324835	-1.053964	1.590868
S	0.000205	-1.405461	2.147436
C	-0.204260	-0.370207	3.615965
O	3.866843	-0.134275	0.033204
C	4.751836	0.356202	-0.796589
C	6.150512	0.438844	-0.194017
O	4.532654	0.726027	-1.954882
O	-0.315888	-2.782389	2.530944
H	2.454557	0.210259	-1.887074
H	6.129100	1.050819	0.714589
H	6.850551	0.867525	-0.913802
H	6.486050	-0.562572	0.098092
H	-0.046884	0.675575	3.343055
H	0.555747	-0.689891	4.333219
H	-1.203677	-0.532290	4.026001
H	-0.109869	-2.032638	-1.107213
H	0.443173	-1.179900	-2.648918
H	-0.096532	1.019332	-1.652243
H	-0.501909	1.101165	0.836089
H	-2.821878	1.356214	0.711870
H	-2.543346	1.214011	-1.030305
H	-3.036510	-1.204617	-0.969483
H	-4.271192	-0.534387	0.112063
H	-2.578810	-2.477377	1.052957
H	-2.972375	-1.088179	2.090402

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C	-0.747594	-0.775633	0.675408
N	-1.168542	0.604549	0.330203
C	-2.644397	0.723299	0.159021
C	-3.150241	-0.644283	0.689660
C	-1.998949	-1.607831	0.364191
S	-0.277701	1.882136	0.922303
O	1.135216	1.504860	0.797250
C	-3.072241	0.976030	-1.282184
Pd	-2.207314	2.687610	-2.178211
O	-1.562862	4.615911	-3.093458
C	-2.066421	4.869151	-4.191109
O	-2.934103	4.050438	-4.777204
C	-2.355818	0.583951	-2.423016
O	-0.806664	3.109591	0.312816
C	-0.631955	2.000183	2.699392
C	-1.751563	6.107865	-4.980147
H	-1.083816	6.752258	-4.407274
H	-2.675769	6.641679	-5.224798
H	-1.274992	5.827622	-5.926211
H	-1.697051	2.196336	2.841691
H	-0.042029	2.837748	3.079670
H	-0.328543	1.074536	3.193344
H	-2.879809	0.352464	-3.348285
H	-1.354836	0.164462	-2.334551
H	-4.157480	1.075895	-1.368153
H	-3.029937	1.540824	0.779994
H	-3.301514	-0.588742	1.776159
H	-4.100649	-0.936122	0.232518
H	-2.019457	-1.879181	-0.696803
H	-2.031499	-2.531556	0.950741
H	0.129217	-1.059659	0.088656
H	-0.482996	-0.858557	1.740277
H	-3.043475	3.268194	-4.142595

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N	0.772699	2.705101	-0.191220
C	0.173359	1.924641	-1.309826
C	-1.331071	1.696787	-1.221423
C	-2.158370	2.056765	-0.167419
H	-1.783631	1.481129	-2.189959
H	0.667991	0.947217	-1.399747
C	0.523308	2.774646	-2.560533
H	0.601177	2.148827	-3.454938
H	-0.267025	3.515667	-2.735225
C	1.830444	3.478892	-2.180469
C	1.603836	3.828680	-0.706044
H	2.680419	2.792421	-2.285164
H	2.032989	4.362646	-2.794120
H	1.041535	4.764168	-0.597533
H	2.522646	3.931693	-0.124697
S	1.245086	1.955064	1.238627
O	0.096738	1.151713	1.687176
O	1.792282	3.015865	2.092509
C	2.586491	0.804270	0.857801
H	2.182424	-0.029526	0.279298
H	3.379138	1.343383	0.332991
H	2.954838	0.444583	1.822367
Pd	-1.713550	-0.093114	-0.060805
O	0.414541	-1.375788	-0.111344
C	-0.334686	-2.301328	0.297522
O	-1.603262	-2.119684	0.441705
C	0.215803	-3.661476	0.664555
H	-0.467315	-4.452398	0.341332
H	1.203734	-3.806647	0.220858
H	0.305863	-3.727082	1.755866
H	-3.225865	2.171508	-0.327375
H	-1.751065	2.491506	0.739424
H	-3.186163	-0.177531	-0.423211

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N	-0.986387	-0.913030	0.978826
C	-1.172496	0.423135	0.351250
C	-2.703161	0.455692	0.089112
C	-3.088516	-1.023992	-0.063489
C	-2.230621	-1.719294	0.998960
C	-0.365128	0.602640	-0.927828
C	0.214261	-0.429769	-1.659555
Pd	1.770007	0.594506	-0.569865
O	1.392813	-0.449068	1.656246
S	0.198104	-1.187151	2.109030
C	-0.321392	-0.403627	3.656611
O	3.734783	1.288693	-0.170496
C	4.174734	1.997011	-1.142682
C	5.583572	2.541231	-1.010593
O	3.513488	2.245267	-2.191528
O	0.239626	-2.632740	2.345542
H	2.224894	1.453894	-1.828430
H	5.726738	2.971289	-0.014733
H	5.788732	3.287117	-1.780605
H	6.293791	1.712527	-1.115077
H	-0.437311	0.670308	3.495200
H	0.472195	-0.590477	4.384290
H	-1.255108	-0.861244	3.991245
H	0.434915	-0.302679	-2.715749
H	0.176827	-1.454371	-1.296201
H	-0.568238	1.552097	-1.424404
H	-0.896764	1.220965	1.052615
H	-3.215160	0.892139	0.956084
H	-2.954612	1.060874	-0.786865
H	-2.821242	-1.389103	-1.061344
H	-4.156922	-1.205077	0.089196
H	-2.004844	-2.763259	0.772511
H	-2.718622	-1.678250	1.984791

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C	-4.265142	-3.356238	0.243913
C	-4.063775	-2.704881	-0.974029
C	-3.148571	-1.658657	-1.038266
N	-2.449568	-1.263550	0.042277
C	-2.646582	-1.876586	1.224468
C	-3.545750	-2.931138	1.361000
Pd	-1.227497	0.381832	-0.082378
N	0.882878	-0.863789	-0.429373
C	2.096513	-0.034422	-0.180006
C	3.404036	-0.790566	0.091299
C	4.507697	0.168544	0.586459
C	5.789069	-0.552903	0.914987
C	6.993875	-0.403267	0.343051
C	7.384240	0.531221	-0.770316
N	-0.231100	2.164945	-0.139977
C	0.072371	2.767200	1.026359
C	0.660991	4.029595	1.055666
C	0.933229	4.682547	-0.146910
C	0.606402	4.050465	-1.348649
C	0.016963	2.790370	-1.305768
O	-0.158428	-0.066226	2.258184
C	0.383450	-1.131947	2.688904
C	0.684681	-1.223167	4.184618
O	-2.870376	1.353394	-0.838878
C	-3.493224	2.195367	-0.045263
C	-4.740163	2.795742	-0.690451
O	0.707252	-2.121434	1.962203
O	-3.154103	2.481414	1.101573
S	0.878970	-1.773307	-1.881044
O	1.702953	-1.051864	-2.862790
O	-0.520398	-2.089401	-2.197664
H	-0.163253	2.203680	1.922795
H	-0.270491	2.258967	-2.206393
H	0.888455	4.487432	2.012909
H	0.796697	4.520193	-2.308355
H	1.388266	5.669324	-0.149226
H	0.064650	-0.526497	4.755340
H	0.540120	-2.247165	4.543009
H	1.738112	-0.963373	4.352440
H	-5.014784	3.718553	-0.173900
H	-4.586349	2.985327	-1.756852
H	-5.568667	2.083051	-0.594788
H	0.723241	-1.492697	0.410393
C	1.665507	-3.353454	-1.475888
H	2.217897	0.648828	-1.024189
H	1.834530	0.554925	0.702123
H	3.225294	-1.567343	0.845768
H	3.758537	-1.281719	-0.822351
H	4.676675	0.949452	-0.164468
H	4.145097	0.680231	1.491607
H	5.702118	-1.290817	1.714878
H	7.805048	-1.027445	0.721447
H	8.173322	1.221447	-0.440518
H	7.794741	-0.029573	-1.621336
H	6.547581	1.131620	-1.139104
H	-2.956570	-1.119280	-1.955936
H	-2.069375	-1.492397	2.055250
H	-4.601263	-2.997575	-1.870220
H	-3.672305	-3.399840	2.331505
H	-4.972588	-4.177489	0.321364

H	1.542103	-3.987456	-2.357752
H	2.721243	-3.194575	-1.257155
H	1.147711	-3.782410	-0.614780

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C	-4.050183	-3.592188	0.140600
C	-4.292993	-2.573649	-0.779368
C	-3.460549	-1.460261	-0.793163
N	-2.422376	-1.336611	0.055704
C	-2.171433	-2.322334	0.938156
C	-2.969740	-3.460660	1.009927
Pd	-1.249989	0.363626	-0.056573
N	0.876023	-0.876488	-0.369294
C	2.077768	-0.012068	-0.208160
C	3.393943	-0.733791	0.107104
C	4.503479	0.264139	0.498282
C	5.787899	-0.427840	0.871802
C	6.979255	-0.338936	0.267237
C	7.350552	0.486325	-0.933751
N	-0.277867	2.159110	-0.202261
C	0.040480	2.831088	0.919829
C	0.602955	4.103399	0.861850
C	0.830372	4.692963	-0.380609
C	0.487360	3.988846	-1.535626
C	-0.073048	2.722592	-1.406860
O	-0.122149	0.151548	2.223640
C	0.409717	-0.865305	2.759169
C	0.643064	-0.819882	4.268444
O	-2.904400	1.338947	-0.781432
C	-3.469284	2.219501	0.019101
C	-4.717642	2.843482	-0.602550
O	0.735221	-1.926252	2.138246
O	-3.075026	2.527969	1.137311
S	0.842755	-1.869300	-1.764441

O	1.619886	-1.189550	-2.807394
O	-0.552805	-2.243222	-2.010703
H	-0.155457	2.307014	1.848109
H	-0.372056	2.134072	-2.266839
H	0.846034	4.618634	1.785058
H	0.643991	4.407258	-2.524216
H	1.264692	5.686284	-0.449657
H	-0.321186	-0.910798	4.782995
H	1.295633	-1.634564	4.590757
H	1.071469	0.144825	4.558146
H	-5.107175	3.623534	0.054235
H	-4.487091	3.264075	-1.586803
H	-5.484495	2.074378	-0.748258
H	0.749172	-1.439527	0.518906
C	1.682180	-3.402410	-1.288267
H	2.177635	0.600648	-1.106972
H	1.820869	0.642493	0.627502
H	3.225765	-1.439863	0.930336
H	3.735402	-1.305139	-0.763886
H	4.662573	0.973325	-0.322498
H	4.152586	0.856558	1.357568
H	5.710522	-1.088247	1.737128
H	7.796227	-0.928474	0.685460
H	8.147762	1.200377	-0.685335
H	7.742814	-0.151142	-1.737723
H	6.508329	1.053515	-1.339449
H	-3.614571	-0.630297	-1.470655
H	-1.294014	-2.204367	1.564497
H	-5.115216	-2.631049	-1.484973
H	-2.731419	-4.227011	1.740126
H	-4.686779	-4.471826	0.175127
H	1.555624	-4.094107	-2.124625
H	2.738645	-3.209532	-1.104456
H	1.197943	-3.794737	-0.391446

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C	2.349687	4.228304	0.788918
C	1.848562	3.456740	1.836694
C	1.045210	2.354547	1.549453
N	0.727715	2.015389	0.282302
C	1.202243	2.765636	-0.734674
C	2.020942	3.870654	-0.519965
Pd	-0.548490	0.433939	-0.171431
N	0.281496	-0.843657	1.247228
C	1.737176	-1.065028	1.199929
C	2.144445	-1.789910	-0.087927
C	3.667793	-2.008506	-0.187962
C	4.055758	-2.813211	-1.401548
C	4.795935	-2.425673	-2.451927
C	5.444940	-1.087894	-2.686000
N	-1.886214	-1.055024	-0.690712
C	-1.583850	-1.948683	-1.650518
C	-2.480128	-2.934763	-2.051497
C	-3.732722	-2.994647	-1.435662
C	-4.039254	-2.063878	-0.444179
C	-3.092620	-1.101271	-0.094552
O	-1.203498	1.555267	-1.761513
C	-2.431103	2.018610	-1.763017
C	-2.747903	2.864439	-2.993443
O	-3.266212	1.824539	-0.879125
S	-0.382894	-0.802966	2.747804
O	-1.789706	-0.373052	2.609483
O	0.466707	-0.083576	3.733495
H	-0.600992	-1.857948	-2.099235
H	-3.278436	-0.354795	0.664672
H	-2.195151	-3.634598	-2.830732
H	-5.000825	-2.066617	0.058846
H	-4.455667	-3.752006	-1.726926
H	0.660422	1.722886	2.342311
H	0.880453	2.470417	-1.726402
H	2.069382	3.690608	2.873209
H	2.382322	4.439230	-1.371188
H	2.980906	5.090551	0.986409
H	-2.419858	2.360095	-3.908541
H	-3.819964	3.068737	-3.039685
H	-2.207522	3.817264	-2.932069
C	-0.423359	-2.528610	3.302586
H	2.293223	-0.118364	1.283384
H	2.053834	-1.670895	2.060543
H	1.622730	-2.755923	-0.132788
H	1.806253	-1.209336	-0.956918
H	4.176549	-1.037471	-0.180208
H	4.008120	-2.541057	0.714239
H	3.666630	-3.833502	-1.414057
H	4.962019	-3.159068	-3.242817
H	6.534811	-1.194279	-2.778638
H	5.092823	-0.645158	-3.628072
H	5.246363	-0.370419	-1.884418
H	-0.837757	-2.525872	4.313828
H	-1.063109	-3.092358	2.621325
H	0.589455	-2.937387	3.316194

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C	-0.252604	-1.714006	2.680215
N	-0.690538	-0.925235	1.688766
C	-2.001314	-0.636618	1.639244
C	-2.915707	-1.124873	2.577696
C	-2.452670	-1.944788	3.607873
C	-1.090001	-2.247286	3.662502
Pd	0.941787	-0.125831	-0.299181
O	-0.888890	-1.134078	-1.422010
C	-0.158039	-2.146992	-1.434244
C	-0.608922	-3.473887	-1.987654
N	3.013229	0.034174	-0.110948
C	3.612833	1.185362	0.247702
C	4.995925	1.278890	0.387622
C	5.783457	0.151266	0.152520
C	5.152874	-1.038058	-0.217393
C	3.766089	-1.060759	-0.341146
O	0.860086	1.827061	0.199102
C	-0.304460	2.438588	0.164092
O	-1.370816	1.897978	-0.116903
O	1.036783	-2.069261	-0.920969
C	-0.204989	3.920059	0.505908
H	-2.305109	0.012892	0.824114
H	0.814555	-1.928915	2.683940
H	-3.966573	-0.862020	2.495453
H	-0.681465	-2.881130	4.444784
H	-3.138020	-2.340428	4.353589
H	2.943666	2.022211	0.415459
H	3.224766	-1.954505	-0.631767
H	5.437578	2.227446	0.676977
H	5.719371	-1.943163	-0.413094
H	6.864231	0.197769	0.254354
H	-1.393741	-3.321637	-2.732803
H	0.232652	-4.019317	-2.424700
H	-1.019634	-4.080481	-1.170900
H	0.400201	4.438369	-0.247281
H	-1.204197	4.360408	0.532254
H	0.286459	4.057742	1.475653

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Pd	0.113626	-0.040401	0.000040
N	-1.935205	-0.040200	0.000088
C	-2.603682	-0.391907	-1.117466
C	-3.996312	-0.406572	-1.144220
C	-4.705857	-0.039827	0.000113
C	-3.996191	0.326737	1.144429
C	-2.603563	0.311700	1.117649
H	-1.992394	0.559075	1.980703
H	-4.502751	0.620553	2.058165
H	-5.792434	-0.039669	0.000119
H	-4.502968	-0.700214	-2.057960
H	-1.992610	-0.639335	-1.980564
O	0.333212	1.290689	-1.475273
C	0.186709	0.928904	-2.731382
O	-0.243353	-0.169594	-3.092275
C	0.578571	2.015701	-3.717574
H	1.548038	2.448444	-3.450948
H	-0.160878	2.824663	-3.681712
H	0.613625	1.603917	-4.728462
O	0.333308	-1.371266	1.475562
C	0.187447	-1.009045	2.731607
O	-0.242262	0.089640	3.092359
C	0.579736	-2.095543	3.717960
H	-0.159800	-2.904451	3.682744
H	0.615345	-1.683415	4.728689
H	1.549033	-2.528462	3.450992

κ^2-53

Pd	0.383540	0.268800	-0.030976
N	-1.526054	-0.441639	0.174205
C	-1.890940	-1.677226	-0.218743
C	-2.444400	0.382473	0.718617
C	-3.199194	-2.132445	-0.074356
H	-1.098738	-2.282000	-0.645228
C	-3.767663	-0.009671	0.896971
H	-2.090208	1.367962	1.002920
C	-4.154676	-1.289575	0.494710
H	-3.453489	-3.134588	-0.404581
H	-4.474168	0.682883	1.343073
H	-5.181092	-1.622239	0.621573
O	0.122153	2.320986	0.282547
C	1.383161	2.509818	0.108909
O	2.096467	1.491639	-0.168540
C	1.987614	3.873867	0.259451
H	2.287492	4.015969	1.305084
H	2.878899	3.963192	-0.366853
H	1.256859	4.645356	0.003021
O	1.036980	-1.584652	-0.466720
C	1.698858	-2.186770	0.504953
O	1.793932	-1.766235	1.654349
C	2.370378	-3.475944	0.049080
H	2.586907	-4.105778	0.915207
H	1.752931	-4.018175	-0.673616
H	3.315827	-3.224577	-0.447004

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C	-3.351958	0.545221	-1.274109
N	-3.167423	-0.335244	-0.270924
C	-4.165222	-0.578392	0.601899
C	-5.400906	0.051386	0.489872
C	-5.605034	0.963814	-0.547926
C	-4.561968	1.214889	-1.439388
Pd	-1.378257	-1.311540	-0.158003
O	0.441514	-2.272104	-0.569961
C	0.265100	-2.049401	-1.816050
C	1.296536	-2.420691	-2.836398
O	-1.613373	-1.453529	1.847348
C	-0.860001	-0.706120	2.605118
C	-0.994404	-1.010037	4.090025
O	-0.826415	-1.466861	-2.158453
O	-0.076368	0.165108	2.202231
N	1.297834	1.424197	-0.036407
C	2.686784	1.581659	0.430730
C	3.432746	0.249065	0.309286
C	4.875490	0.342656	0.843492
C	5.594605	-0.980264	0.786380
C	6.721604	-1.284029	0.124039
C	7.570625	-0.379929	-0.729010
S	0.439389	2.783354	-0.472983
C	0.134648	3.734612	1.039055
O	-0.873878	2.314549	-0.946727
O	1.295815	3.602360	-1.342627
H	0.729025	0.839116	0.592099
H	-0.310137	-1.829582	4.342294
H	-2.008083	-1.332346	4.343542
H	-0.712466	-0.133300	4.678172
H	-0.459922	4.607315	0.757315
H	1.092666	4.050145	1.458813
H	-0.410035	3.099397	1.741262
H	2.717388	1.928368	1.476496
H	3.165546	2.341333	-0.194217
H	2.883465	-0.527127	0.858091
H	3.444290	-0.058280	-0.743598
H	4.840443	0.682176	1.890972
H	5.423525	1.113177	0.288249
H	5.117321	-1.780602	1.355299
H	7.085338	-2.309742	0.205351
H	7.165704	0.632599	-0.815168
H	7.673489	-0.787596	-1.744225
H	8.587540	-0.299911	-0.319752
H	0.814476	-2.718069	-3.771762
H	1.934460	-3.223177	-2.458212
H	1.921452	-1.542418	-3.039461
H	-2.504202	0.716752	-1.926459
H	-4.667165	1.924638	-2.253251
H	-6.559161	1.472242	-0.656220
H	-6.182231	-0.173806	1.208816
H	-3.936236	-1.279649	1.396136

8M

N	2.440361	0.915089	-0.003929
C	2.397463	2.249966	-0.188865
C	3.548872	3.031889	-0.119212
C	4.775140	2.417852	0.137431
C	4.808084	1.035178	0.327186
C	3.618118	0.316163	0.256690
Pd	0.728084	-0.233911	-0.108714
N	-1.055333	-1.386043	-0.151867
S	-0.942524	-2.730286	-1.293617
O	0.468604	-3.114177	-1.343962
O	1.395851	-1.069119	1.654683
C	0.805447	-1.928212	2.417930
O	-0.333152	-2.412566	2.233497
O	0.290272	0.503238	-1.940676
C	-0.332871	1.640036	-2.095148
C	-0.625274	1.957448	-3.556031
C	1.626557	-2.373284	3.617800
O	-0.657491	2.407978	-1.179580
C	-2.334921	-0.617695	-0.247386
C	-2.469583	0.365960	0.917139
C	-3.732337	1.239361	0.763648
C	-3.974170	2.114227	1.968011
C	-3.780503	3.438542	2.065703
C	-3.270911	4.377628	1.005529
C	-1.845243	-4.034914	-0.425736
O	-1.683003	-2.359524	-2.500937
H	3.581725	-0.754086	0.420971
H	1.417564	2.671602	-0.389598
H	5.737217	0.512227	0.530152
H	3.471492	4.104433	-0.266351
H	5.687971	3.004899	0.190580
H	0.968025	-2.748153	4.404844
H	2.292180	-3.188507	3.307110
H	2.247331	-1.555852	3.994198
H	-2.340787	-0.099700	-1.207070
H	-3.178821	-1.320808	-0.243096
H	-2.502827	-0.184393	1.866943
H	-1.592597	1.021482	0.943262
H	-3.633501	1.842255	-0.145360
H	-4.608913	0.588818	0.618632
H	-4.334758	1.589998	2.855121
H	-4.013882	3.905686	3.024228
H	-4.050147	5.095665	0.711309
H	-2.431230	4.969618	1.394075
H	-2.917975	3.863401	0.107770
H	0.316106	2.065257	-4.107120
H	-1.175748	1.131580	-4.019006
H	-1.200992	2.882595	-3.630919
H	-1.772119	-4.922644	-1.059181
H	-1.367124	-4.202775	0.541940
H	-2.889479	-3.737327	-0.311293
H	-0.947238	-1.821635	0.804853

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Pd	0.740267	-0.367646	0.530086
N	-0.819978	1.033470	-1.042608
H	-0.561881	0.302614	-1.739010
O	-0.129111	-1.200271	-2.550644
C	0.154821	-2.154489	-1.807718
O	0.479930	-2.075605	-0.550738
C	0.164945	-3.576103	-2.352211
H	-0.167649	-4.290937	-1.594394
H	1.191223	-3.839552	-2.638294
H	-0.465957	-3.640434	-3.241776
S	0.023189	2.463902	-1.361937
O	1.451218	2.120141	-1.408877
O	-0.473661	3.485344	-0.429893
C	-0.447707	2.961587	-3.038923
H	0.099399	3.882618	-3.255330
H	-1.523424	3.145590	-3.075931
H	-0.154619	2.168942	-3.731046
C	-2.282264	1.155393	-0.821714
H	-2.763695	1.675493	-1.665045
H	-2.431790	1.757667	0.076205
C	-2.918862	-0.225636	-0.649157
H	-2.770958	-0.818103	-1.561466
H	-2.419746	-0.751669	0.170984
C	-4.426263	-0.116188	-0.340611
H	-4.909680	0.486535	-1.126160
H	-4.562180	0.430634	0.599099
C	-5.095563	-1.465408	-0.286402
H	-5.090639	-2.014431	-1.230311
C	-5.668868	-2.062250	0.769863
H	-6.096846	-3.053341	0.609269
C	-5.799769	-1.537582	2.174133
H	-5.344237	-0.552379	2.307214
H	-5.323379	-2.223252	2.888269
H	-6.856893	-1.464091	2.465925
O	1.000348	1.147496	1.832700
C	-0.183670	1.245089	2.367508
O	-1.078856	0.436492	2.045901
C	-0.406779	2.384946	3.326690
H	0.481463	2.554694	3.942549
H	-1.275716	2.182176	3.957504
H	-0.592322	3.295259	2.743514
N	2.768658	-0.746714	0.530892
C	3.264876	-1.995821	0.457453
C	4.636335	-2.236463	0.460581
C	5.514562	-1.153214	0.531646
C	4.987368	0.137126	0.599597
C	3.604880	0.306713	0.601660
H	3.138327	1.283527	0.654858
H	5.629555	1.010682	0.647924
H	6.589393	-1.312193	0.532123
H	4.999206	-3.258125	0.407587
H	2.531794	-2.790890	0.382827

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Pd	0.795703	0.004501	0.066893
O	-0.278605	-1.747808	-0.076190
C	-0.293524	-2.514429	0.976706
C	-1.117610	-3.786237	0.806584
N	-0.759343	1.144769	0.753608
S	0.012015	1.864475	2.048027
C	-0.051273	0.752202	3.473521
O	0.296401	-2.283043	2.042481
C	-2.129608	0.641063	0.982622
C	-2.862618	0.433923	-0.346096
C	-4.289265	-0.111595	-0.134859
C	-5.066999	-0.198313	-1.422703
C	-5.599300	-1.287337	-1.998279
C	-5.563530	-2.708954	-1.505554
O	-0.625700	3.127933	2.440968
O	1.424512	1.890108	1.547383
H	-1.887751	-3.819890	1.585143
H	-1.584318	-3.844127	-0.178929
H	-0.467573	-4.655423	0.956738
H	-2.107893	-0.301433	1.547532
H	-2.672971	1.381636	1.586619
H	-2.911206	1.390744	-0.882740
H	-2.290858	-0.262005	-0.970001
H	-4.237557	-1.088404	0.360053
H	-4.825315	0.558511	0.556406
H	-5.197565	0.754907	-1.938842
H	-6.129697	-1.143165	-2.940989
H	-6.580952	-3.089487	-1.338443
H	-5.101605	-3.367305	-2.254233
H	-5.006579	-2.823315	-0.571173
H	0.627450	1.176716	4.217955
H	-1.072835	0.744113	3.860147
H	0.264893	-0.247704	3.164222
H	-0.635086	2.370840	-0.546202
O	-0.506174	3.046209	-1.285826
C	0.634607	2.816583	-1.920471
O	1.374746	1.865820	-1.669313
C	0.937925	3.846135	-2.980402
H	0.077533	3.967444	-3.646574
H	1.118790	4.814687	-2.500143
H	1.819957	3.551650	-3.551061
N	2.529887	-0.983234	-0.528182
C	3.007608	-1.993315	0.227748
C	3.207306	-0.602984	-1.629242
C	4.186775	-2.659354	-0.098155
H	2.417832	-2.252408	1.101197
C	4.389295	-1.229889	-2.017502
H	2.784241	0.228935	-2.180714
C	4.889934	-2.275967	-1.241053
H	4.537887	-3.463862	0.540308
H	4.902173	-0.893174	-2.912927
H	5.810841	-2.780805	-1.520056

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Pd	-0.245851	-0.109769	0.482130
O	1.628099	-1.072618	0.823473
S	1.029919	-2.494371	0.760765
N	-0.540862	-2.147987	0.547055
C	-1.327485	-2.890884	-0.457680
C	-1.896491	-4.204757	0.093368
C	-2.793173	-4.923142	-0.935493
C	-3.288859	-6.255174	-0.435351
C	-4.557106	-6.647996	-0.239479
C	-5.819500	-5.864146	-0.478827
H	-6.453091	-6.364938	-1.224231
H	-6.414613	-5.795257	0.442249
H	-5.631094	-4.846089	-0.831832
H	-4.712091	-7.660836	0.136012
H	-2.500899	-6.974345	-0.202308
H	-2.210875	-5.083596	-1.856463
H	-3.628824	-4.268347	-1.209283
H	-2.469318	-3.995141	1.005581
H	-1.070348	-4.871634	0.378169
H	-0.738100	-3.085031	-1.364250
H	-2.143234	-2.215654	-0.733914
O	1.659209	-3.442351	-0.167502
C	1.241928	-3.141763	2.428833
H	0.787404	-4.134273	2.465082
H	0.751211	-2.460541	3.125640
H	2.315972	-3.200952	2.622981
O	-2.140111	0.342290	-0.060158
C	-2.992658	0.796738	0.823215
O	-2.717921	1.139656	1.977203
C	-4.421771	0.857783	0.295606
H	-4.971626	1.652341	0.806676
H	-4.445236	1.009412	-0.786899
H	-4.918213	-0.095457	0.516691
N	0.403839	1.871032	0.510422
C	-0.240197	2.843853	1.187119
C	0.242421	4.151656	1.221225
C	1.417876	4.464397	0.538552
C	2.082331	3.450115	-0.154629
C	1.546465	2.165798	-0.142455
H	2.031618	1.340276	-0.652971
H	3.002708	3.641637	-0.697099
H	1.811973	5.477015	0.547966
H	-0.304679	4.904115	1.780459
H	-1.145774	2.535801	1.701478

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Pd	0.893457	0.293105	0.330870
N	2.649191	0.934514	1.243766
C	2.570440	1.942750	2.134719
C	3.679109	2.382044	2.853006
C	4.910460	1.757115	2.643250
C	4.984210	0.708697	1.724881
C	3.830659	0.320810	1.046257
N	-0.934487	-0.355291	-0.241987
S	-1.933156	0.535030	0.698272
O	-1.061479	1.636459	1.244599
O	-3.195710	0.910525	0.033854
C	-2.340258	-0.516064	2.104333
H	-2.873552	0.103923	2.829734
H	-1.406683	-0.911523	2.512001
H	-2.981228	-1.323810	1.743535
C	-1.298574	-0.734242	-1.610126
C	-1.370074	0.381886	-2.665733
C	-0.070939	1.181237	-2.874541
C	0.282890	2.095313	-1.726195
C	1.514182	2.539849	-1.387600
C	2.813568	2.218868	-2.075055
H	3.621273	2.060851	-1.350832
H	3.121988	3.061064	-2.711960
H	2.745920	1.331526	-2.711319
H	3.818012	-0.506368	0.344974
H	5.917266	0.187352	1.535411
H	5.793207	2.077550	3.189585
H	3.569027	3.194422	3.564242
H	1.587500	2.386347	2.265440
H	1.572055	3.280354	-0.589332
H	-0.559452	2.515874	-1.179369
H	-2.187959	1.066353	-2.410738
H	-2.269655	-1.247616	-1.583393
H	-1.642629	-0.093430	-3.618970
H	-0.553194	-1.482881	-1.906660
H	0.758250	0.499276	-3.104321
H	-0.204574	1.807451	-3.771282
O	1.639159	-1.640360	0.309456
C	1.310655	-2.358719	1.353475
O	0.695259	-1.950980	2.341481
C	1.748091	-3.817724	1.244506
H	2.634362	-3.931271	0.614187
H	1.932368	-4.224230	2.242386
H	0.932556	-4.391840	0.787383

***cis*-[6,5]-A**

N	2.631276	-2.010885	0.618929
C	2.806298	0.210807	-0.620515
C	3.870106	0.502322	0.388795
H	2.967207	-0.632826	-1.282649
H	3.453691	1.090792	1.215539
C	3.647288	-1.680331	1.608305
H	3.224166	-1.211693	2.508476
S	1.125019	-2.158019	1.040671
O	0.725270	-1.594866	2.349722
C	0.674632	-3.911509	1.020307
H	0.937010	-4.324195	0.045104
H	-0.399165	-3.985862	1.204307
H	1.239834	-4.401716	1.816639
O	0.269600	-1.683408	-0.160312
Pd	-0.181430	0.286250	-0.421403
C	1.785851	1.119717	-0.945717
H	1.479373	1.044630	-1.997240
C	1.805400	2.533800	-0.378789
H	1.765599	2.546982	0.715742
H	2.723613	3.058472	-0.683779
H	0.951119	3.106806	-0.743643
O	-1.200605	2.071388	-0.696907
C	-2.331966	1.520425	-0.416336
O	-2.332544	0.280752	-0.144951
C	-3.587716	2.341131	-0.386641
H	-4.456332	1.709457	-0.588942
H	-3.527530	3.157452	-1.111567
H	-3.703816	2.778243	0.612792
H	4.192494	-2.582877	1.926671
H	4.582582	1.178250	-0.119816
C	4.625714	-0.717004	0.922894
H	5.124336	-1.238434	0.095179
H	5.405077	-0.397121	1.625808

***cis*-[6,5]-B**

N	2.633929	-2.006397	0.333978
C	2.845809	0.359358	-0.425945
C	4.073745	0.347489	0.433358
H	2.875329	-0.236894	-1.332467
H	3.835190	0.713613	1.438710
C	3.843713	-2.026817	1.144724
H	3.656909	-1.765465	2.196965
S	1.224907	-2.092971	1.033213
O	1.128798	-1.576173	2.419569
C	0.665459	-3.815642	1.061004
H	0.688037	-4.201380	0.040665
H	-0.348899	-3.831796	1.465521
H	1.348064	-4.374318	1.706447
O	0.210308	-1.514629	0.037249
Pd	-0.256496	0.466968	-0.162769
C	1.847246	1.335468	-0.317896
H	1.479788	1.638701	-1.305869
C	1.995251	2.449838	0.712148
H	1.909605	2.073852	1.738501
H	2.970931	2.951690	0.627368
H	1.229257	3.216256	0.577022
O	-2.200262	-0.159890	0.060726
C	-2.904900	-0.231456	-1.036886
O	-2.535701	0.144674	-2.155344
C	-4.276263	-0.867500	-0.827530
H	-4.176803	-1.954119	-0.940871
H	-4.974338	-0.505779	-1.587159
H	-4.662194	-0.668700	0.176185
H	4.312694	-3.023351	1.123032
H	4.751177	1.101349	-0.008400
C	4.795313	-0.998155	0.521328
H	5.089180	-1.333282	-0.482311
H	5.710625	-0.901827	1.118853
N	-1.037670	2.351048	-0.448849
C	-1.506865	3.047541	0.605426
C	-1.228158	2.832501	-1.692646
C	-2.159710	4.267464	0.454469
H	-1.353042	2.599169	1.580747
C	-1.864857	4.050854	-1.919685
H	-0.888945	2.203968	-2.506237
C	-2.337873	4.783313	-0.830998
H	-2.521706	4.792585	1.332566
H	-1.997807	4.399332	-2.938740
H	-2.844748	5.732605	-0.980632

***cis*-[6,5]-C**

N	2.619033	-1.815894	0.480085
C	2.818226	0.444524	-0.442292
C	4.011452	0.543279	0.460703
H	2.919734	-0.189281	-1.317897
H	3.731029	1.016527	1.408239
C	3.760196	-1.753869	1.382485
H	3.486193	-1.398171	2.386960
S	1.176152	-2.090231	1.030033
O	0.874934	-1.689565	2.427905
C	0.817794	-3.862912	0.898428
H	0.976434	-4.169610	-0.136549
H	-0.217679	-4.029153	1.203762
H	1.502883	-4.387063	1.569685
O	0.190595	-1.547728	-0.015516
Pd	-0.272276	0.449854	-0.322322
C	1.768012	1.372723	-0.425354
H	1.427558	1.613113	-1.441512
C	1.785285	2.526820	0.569532
H	1.783416	2.171251	1.606791
H	2.680014	3.154398	0.436869
H	0.905362	3.157132	0.433995
O	-0.936345	2.344344	-0.659297
C	-1.308831	2.664341	-1.871988
O	-1.335935	1.891165	-2.835600
C	-1.701970	4.130420	-2.013210
H	-2.370995	4.254969	-2.868322
H	-0.797632	4.724706	-2.195455
H	-2.171426	4.507814	-1.100266
H	4.238599	-2.740284	1.493948
H	4.698009	1.251470	-0.037365
C	4.742051	-0.774854	0.729179
H	5.108143	-1.202994	-0.213254
H	5.611790	-0.603685	1.375569
N	-2.257878	-0.212238	-0.093763
C	-2.618941	-0.792358	1.066461
C	-3.165860	-0.068722	-1.077372
C	-3.918694	-1.240224	1.290733
H	-1.840239	-0.899008	1.814483
C	-4.482168	-0.503568	-0.925820
H	-2.808090	0.404466	-1.986561
C	-4.868450	-1.094542	0.277515
H	-4.170723	-1.694657	2.243815
H	-5.182893	-0.374718	-1.744805
H	-5.889402	-1.437102	0.423442

***cis*-[6,5]-D**

N	1.996761	-1.701437	0.098035
C	2.571232	0.477975	-0.836508
C	3.610932	0.413735	0.235960
H	2.873083	0.024139	-1.779889
H	3.207453	0.710358	1.209302
C	3.265128	-1.994493	0.772727
H	3.182051	-1.937963	1.866408
S	0.723897	-1.568147	1.053035
O	0.960698	-1.038007	2.415394
C	-0.045637	-3.195221	1.263315
H	-0.269792	-3.597897	0.274222
H	-0.957567	-3.058569	1.848848
H	0.659303	-3.836172	1.798623
O	-0.345214	-0.805085	0.261427
Pd	0.021684	-0.032612	-1.612474
C	1.483064	1.379018	-0.911524
H	1.422158	1.880721	-1.883180
C	1.068605	2.226713	0.275188
H	0.948054	1.630000	1.184012
H	1.814968	3.010295	0.476886
H	0.115687	2.726171	0.075474
O	0.047854	0.524097	-3.597319
C	-0.914389	-0.281759	-3.904622
O	-1.409257	-1.001953	-2.988400
C	-1.430329	-0.319138	-5.315043
H	-2.189451	0.463182	-5.438352
H	-1.895333	-1.286505	-5.520464
H	-0.621800	-0.122078	-6.024374
H	3.612461	-3.003252	0.507293
H	4.351542	1.183107	-0.052368
C	4.299567	-0.949700	0.304342
H	4.680448	-1.215868	-0.691100
H	5.158372	-0.926745	0.985382

***cis*-[6,5]-F**

C	-0.108170	-3.079043	1.193313
S	0.668270	-1.443540	1.068123
O	-0.360106	-0.652791	0.256584
Pd	-0.020888	0.260281	-1.593753
O	0.255064	1.004546	-3.468007
C	-0.112045	2.243791	-3.716796
C	0.010996	2.616539	-5.191576
N	1.983495	-1.567705	0.178223
C	3.206359	-1.926915	0.908912
C	4.319018	-0.965483	0.450034
C	3.710368	0.430827	0.322955
C	2.670059	0.492823	-0.752046
C	1.643100	1.452262	-0.872888
C	1.271569	2.373662	0.273896
O	0.834794	-0.967568	2.460025
N	-1.755167	-0.761376	-2.320597
H	2.944971	-0.019035	-1.673626
H	3.316293	0.786216	1.280901
H	3.085184	-1.830506	1.996260
H	-0.287699	-3.454819	0.184475
H	-1.042873	-2.968062	1.748119
H	0.575982	-3.736225	1.736091
H	1.658336	1.928769	-1.856346
H	1.020332	1.817556	1.183325
H	2.097431	3.060616	0.516154
H	0.408395	2.984121	-0.005212
H	0.095140	3.701353	-5.292403
H	-0.895725	2.292858	-5.718603
H	0.866305	2.121693	-5.661016
H	3.493732	-2.965347	0.687842
H	4.489294	1.149629	0.010458
H	4.714620	-1.281270	-0.524986
H	5.154758	-0.976161	1.159534
O	-0.530412	3.042590	-2.880548
C	-2.768954	-1.064654	-1.488193
C	-3.927014	-1.700049	-1.932422
C	-4.035728	-2.042316	-3.281376
C	-2.980408	-1.729315	-4.139588
C	-1.858759	-1.082702	-3.623456
H	-2.624449	-0.792423	-0.448673
H	-4.723323	-1.917258	-1.227241
H	-4.925715	-2.540408	-3.656413
H	-3.018802	-1.974358	-5.196516
H	-1.019612	-0.788374	-4.244775

***cis*-[6,5]-G**

N	2.550013	-1.891879	0.779915
C	2.918613	0.011313	-0.628618
C	3.474486	0.705656	0.575337
H	3.502979	-0.803162	-1.040938
H	2.729545	1.394656	0.988403
C	2.864679	-1.204931	2.027072
H	2.016791	-0.643047	2.452531
S	1.063695	-2.372018	0.500738
O	1.017174	-3.223769	-0.694737
C	0.425464	-3.292255	1.924441
H	1.063382	-4.167656	2.062885
H	-0.595490	-3.590790	1.677651
H	0.431914	-2.653862	2.810106
O	0.067906	-1.186218	0.460256
Pd	-0.054977	-0.200465	-1.349206
C	1.944847	0.620569	-1.470940
H	2.064510	0.300210	-2.511210
C	1.670607	2.122108	-1.321528
H	1.245646	2.387652	-0.347764
H	2.596619	2.704377	-1.448495
H	0.966561	2.449054	-2.090890
O	-0.667955	0.677238	-3.119846
C	-1.862295	0.202105	-3.006916
O	-2.138268	-0.482144	-1.976229
C	-2.869456	0.440521	-4.095319
H	-2.788061	-0.363434	-4.837253
H	-2.672510	1.391074	-4.598465
H	-3.881551	0.425442	-3.682882
H	3.215933	-1.918647	2.788136
H	4.299513	1.340213	0.204540
C	3.991412	-0.227850	1.673348
H	4.856674	-0.799484	1.315544
H	4.308971	0.348394	2.550729

***cis*-[6,5]-H**

N	1.899925	-1.634118	0.207040
C	2.404356	0.459836	-0.843847
C	3.570394	0.342590	0.089585
H	2.561953	0.041750	-1.837508
H	3.314632	0.662449	1.106146
C	3.200483	-2.055030	0.696926
H	3.274627	-2.003557	1.797192
S	0.562595	-2.007201	0.921937
O	0.046793	-3.390559	0.758450
C	0.630481	-1.738860	2.719572
H	1.285570	-2.491360	3.164221
H	-0.386781	-1.864152	3.095737
H	0.994615	-0.729779	2.922601
O	-0.456301	-0.939379	0.482074
Pd	-0.313334	-0.033574	-1.387537
C	1.309047	1.330532	-0.744335
H	1.113738	1.855096	-1.682205
C	1.011180	2.121097	0.514834
H	0.943586	1.473542	1.395431
H	1.787676	2.876350	0.710865
H	0.057207	2.649912	0.422695
O	-0.429885	0.946321	-3.167310
C	0.521489	0.833552	-4.066231
O	1.600566	0.263998	-3.898918
C	0.158805	1.477494	-5.400293
H	-0.440552	2.381746	-5.259034
H	-0.437265	0.766997	-5.987039
H	1.068538	1.706431	-5.960588
H	3.453764	-3.083477	0.399600
H	4.307565	1.069543	-0.297147
C	4.202845	-1.056666	0.085624
H	4.428019	-1.345351	-0.948978
H	5.147599	-1.064452	0.641937
N	-2.007032	-1.167878	-2.011747
C	-2.255915	-2.400198	-1.525985
C	-2.870800	-0.621161	-2.889417
C	-3.381742	-3.127690	-1.910467
H	-1.541442	-2.802807	-0.816775
C	-4.021174	-1.284935	-3.308509
H	-2.600982	0.360997	-3.261287
C	-4.283252	-2.563439	-2.812695
H	-3.535577	-4.120087	-1.498512
H	-4.690865	-0.801347	-4.013006
H	-5.170703	-3.107861	-3.124370

***cis*-[6,5]-I**

Pd	-0.141595	-0.153052	-1.579147
O	-0.311088	-1.091934	0.246504
S	0.709655	-2.170137	0.653798
N	2.078565	-1.707101	0.021364
C	3.346697	-2.063988	0.632512
C	4.313287	-0.915636	0.277088
C	3.547223	0.412869	0.334031
H	2.849353	0.194931	-1.714222
C	1.354493	1.325571	-0.736966
C	2.501429	0.528970	-0.736567
C	0.842344	2.012033	0.513505
H	0.733411	1.303544	1.340461
H	1.517060	2.817947	0.840593
H	-0.142344	2.455763	0.336617
H	1.214937	1.881055	-1.666037
H	4.249854	1.244718	0.144590
H	3.121008	0.585028	1.328580
H	5.173778	-0.904723	0.956583
H	3.741074	-3.023041	0.263512
H	3.287471	-2.141094	1.731382
H	4.705859	-1.059923	-0.738908
C	0.686874	-1.988675	2.466054
H	-0.353098	-2.123164	2.770401
H	1.041463	-0.994701	2.746165
H	1.305953	-2.770638	2.910555
O	0.284515	-3.560777	0.402621
O	-1.603012	-1.398624	-2.292763
C	-2.822048	-0.939797	-2.230533
O	-3.137285	0.222800	-1.940112
C	-3.876053	-1.996130	-2.540237
H	-3.539273	-2.670254	-3.333302
H	-4.038557	-2.601145	-1.640012
H	-4.818051	-1.516103	-2.817014
N	-0.105342	0.771227	-3.420020
C	-1.104967	1.606224	-3.774855
C	-1.145838	2.202250	-5.034403
C	-0.137340	1.922519	-5.956527
C	0.885204	1.045766	-5.587550
C	0.866575	0.490492	-4.311482
H	1.631044	-0.206017	-3.983885
H	1.684972	0.784985	-6.273400
H	-0.150682	2.370873	-6.946126
H	-1.969124	2.865712	-5.279225
H	-1.887517	1.742415	-3.035759

***cis*-[6,5]-J**

N	1.162349	1.653030	-0.620868
C	-0.761998	2.313732	-1.967383
C	-1.985724	2.331154	-1.257594
C	-2.411813	3.531488	-0.435197
H	-3.293409	3.290501	0.166553
H	-1.623370	3.863119	0.246674
H	-2.679146	4.377743	-1.086449
H	-2.793647	1.834729	-1.805613
H	-0.617649	1.466360	-2.636822
C	0.124626	3.482330	-2.256538
H	-0.317953	3.947518	-3.157253
H	0.081216	4.230543	-1.458760
C	1.564231	3.065306	-2.558904
C	2.182524	2.481427	-1.271284
H	1.564660	2.307936	-3.354661
H	2.156256	3.914953	-2.918752
H	2.516333	3.312777	-0.635956
H	3.060822	1.871462	-1.526627
S	0.888753	1.980712	0.917974
O	-0.482868	1.386284	1.259993
O	1.061022	3.388473	1.344220
C	2.001337	0.992769	1.952327
H	1.869720	-0.058064	1.689420
H	3.025184	1.321814	1.757951
H	1.733832	1.174188	2.995717
Pd	-1.682680	0.505725	-0.164081
O	-2.887002	-0.700618	-1.323757
C	-2.721167	-1.722403	-0.550243
O	-1.990466	-1.586295	0.474699
C	-3.370254	-3.031323	-0.900180
H	-4.353917	-2.862237	-1.347434
H	-2.748701	-3.553827	-1.637749
H	-3.456238	-3.658859	-0.009893

***cis*-[6,5]-K**

N	0.185423	-0.140892	-0.470631
C	-0.601200	0.137424	1.831866
C	0.375617	1.281499	1.768399
C	1.703212	0.938701	1.047309
C	1.410857	0.626649	-0.430117
H	2.279006	0.117945	-0.876699
H	1.279767	1.568622	-0.984025
H	2.161856	0.066984	1.530066
H	2.404277	1.777706	1.143047
H	0.606778	1.607645	2.790715
H	-0.096865	2.121740	1.246177
H	-1.475397	0.200073	1.196536
S	-0.030881	-1.530520	-1.114273
C	1.490397	-2.533478	-1.080521
H	1.879879	-2.604787	-0.061966
H	1.232273	-3.522725	-1.462556
H	2.223113	-2.069742	-1.745513
O	-0.528662	-1.611621	-2.499033
O	-1.035716	-2.263680	-0.173979
Pd	-0.476489	-2.873550	1.712266
C	-0.581008	-0.856460	2.806475
H	-1.576777	-1.257912	3.034988
C	0.384095	-0.784821	3.978450
H	1.427802	-0.907968	3.671519
H	0.301154	0.183430	4.492539
H	0.154469	-1.565598	4.703127
O	-0.101056	-3.668535	3.537495
C	1.147527	-3.966359	3.787638
O	2.077929	-3.849084	2.983822
H	2.336983	-4.983475	5.269757
H	1.379067	-3.623835	5.897366
H	0.565817	-5.144636	5.516008
C	1.372795	-4.474772	5.205600
N	-0.573208	-4.808703	0.884336
C	-1.641828	-5.116596	0.123301
C	-1.817421	-6.386147	-0.418290
C	-0.852358	-7.363824	-0.178385
C	0.259490	-7.032754	0.594463
C	0.367203	-5.745314	1.113957
H	1.214942	-5.428039	1.710812
H	1.043634	-7.754725	0.797631
H	-0.962039	-8.362259	-0.591918
H	-2.695403	-6.591231	-1.021643
H	-2.341687	-4.311624	-0.062906

***cis*-[6,5]-L**

N	0.421620	-0.235031	-0.355548
C	-0.366812	0.220305	1.756553
C	0.947805	0.930010	1.922294
H	-1.096080	0.677430	1.101483
H	1.129258	1.125065	2.985971
H	0.911469	1.893619	1.400677
C	2.113769	0.087920	1.346771
H	2.145715	-0.888564	1.842838
H	3.071055	0.591946	1.529329
C	1.862328	-0.089337	-0.160215
H	2.424025	-0.947730	-0.546576
H	2.203879	0.808519	-0.696745
S	-0.204644	-1.500585	-1.050341
O	0.723090	-2.545786	-1.528683
C	-1.156204	-0.915985	-2.471508
H	-1.838014	-0.132765	-2.137272
H	-1.709809	-1.761493	-2.885103
H	-0.448906	-0.524898	-3.205503
O	-1.357798	-2.005002	-0.154319
Pd	-0.638802	-2.724722	1.673366
C	-0.836863	-0.768257	2.663787
H	-1.931474	-0.819861	2.672631
C	-0.222454	-0.807708	4.063154
H	0.852019	-1.008684	4.044178
H	-0.376495	0.154851	4.573584
H	-0.693415	-1.587989	4.662068
O	-0.111896	-3.591157	3.432334
C	1.166239	-3.702771	3.671854
O	2.069892	-3.320977	2.920432
C	1.468940	-4.346912	5.020210
H	0.825070	-5.214759	5.191354
H	1.264233	-3.624816	5.819729
H	2.520066	-4.638950	5.068152
C	0.666299	-5.286659	0.733125
N	-0.505433	-4.626290	0.755712
C	0.799615	-6.518905	0.097838
C	-1.576430	-5.161247	0.144257
C	-0.310079	-7.083899	-0.527841
C	-1.520744	-6.391406	-0.503052
H	-2.486731	-4.573332	0.175834
H	-2.411480	-6.789143	-0.978394
H	-0.233658	-8.044555	-1.029283
H	1.763920	-7.016269	0.096988
H	1.493633	-4.798512	1.237102

***cis*-[6,5]-M**

C	0.268297	-0.046681	-0.437662
N	-0.305386	-0.343309	1.748058
C	1.019960	-0.454240	2.364874
C	2.095127	-0.194487	1.297873
C	1.549950	-0.727973	-0.035965
S	-1.297137	0.812370	2.181908
O	-2.669853	0.505383	1.740440
C	0.228851	1.242910	-1.041662
C	1.505178	2.060092	-1.221063
C	-1.310084	0.979135	3.987547
O	-0.836523	2.221847	1.757582
Pd	-1.254300	2.628474	-0.262388
O	-1.752411	3.001009	-2.202610
C	-1.230252	4.059012	-2.764538
O	-0.470312	4.862066	-2.215116
N	-2.672253	4.059796	0.419279
C	-3.698397	3.653638	1.190111
C	-4.649525	4.546170	1.677400
C	-4.529993	5.900066	1.364258
C	-3.463488	6.313222	0.567242
C	-2.553220	5.364148	0.106918
C	-1.662889	4.232541	-4.217376
H	-0.396682	1.187218	-1.939263
H	-0.581915	-0.690008	-0.637482
H	2.293973	1.487483	-1.734331
H	1.297764	2.953622	-1.814006
H	1.917308	2.403392	-0.266196
H	1.381963	-1.807582	0.046269
H	2.291373	-0.560184	-0.829595
H	1.121962	-1.480838	2.742653
H	1.181640	0.219688	3.216885
H	3.039332	-0.687733	1.558726
H	2.293384	0.878851	1.219264
H	-2.058125	1.739500	4.219012
H	-1.595401	0.015785	4.414016
H	-0.332853	1.296781	4.353050
H	-1.715925	5.617863	-0.535561
H	-3.329776	7.355536	0.296388
H	-5.256235	6.619108	1.733151
H	-5.466134	4.176618	2.289338
H	-3.735196	2.591186	1.410681
H	-2.752542	4.330477	-4.273793
H	-1.190341	5.118850	-4.645228
H	-1.388084	3.347641	-4.801263

***cis*-[6,5]-N**

C	2.812556	0.246545	-0.819419
N	2.302101	-1.574268	0.489932
C	2.642885	-1.074198	1.819902
C	2.963826	0.424168	1.687453
C	3.693027	0.631341	0.336470
S	0.918667	-2.258563	0.182657
C	1.269183	-3.910536	-0.461596
C	1.844019	1.120734	-1.384152
C	1.988412	2.619235	-1.117837
O	-0.034176	-2.404479	1.301919
O	0.341890	-1.599490	-1.090148
Pd	-0.141020	0.407509	-0.752521
O	-0.798516	2.319632	-0.568736
C	-0.729404	2.852184	0.620832
O	-0.294473	2.289398	1.631325
N	-2.074406	-0.255521	-0.206410
C	-2.785007	-1.034962	-1.039843
C	-4.043670	-1.522791	-0.703403
C	-4.577607	-1.201749	0.544681
C	-3.831331	-0.402874	1.408965
C	-2.581316	0.055541	1.000169
C	-1.226367	4.292999	0.661828
H	1.655370	0.886996	-2.438046
H	3.123073	-0.599997	-1.416798
H	2.959583	2.979746	-1.488842
H	1.202373	3.173147	-1.632292
H	1.924005	2.864561	-0.054392
H	4.602139	0.018731	0.323441
H	3.989252	1.682639	0.239498
H	3.533559	-1.609017	2.182306
H	1.835579	-1.233120	2.544210
H	3.597036	0.765629	2.515836
H	2.039500	1.012370	1.703648
H	-1.955910	0.680587	1.628617
H	-4.201567	-0.134438	2.392897
H	-5.556058	-1.571328	0.838265
H	-4.585494	-2.143737	-1.409380
H	-2.316065	-1.270738	-1.988416
H	-1.378494	4.607364	1.696468
H	-0.477730	4.946778	0.198494
H	-2.153339	4.402371	0.091055
H	0.331690	-4.349245	-0.809540
H	1.983120	-3.821624	-1.281596
H	1.689711	-4.501869	0.354155

***cis*-[6,5]-O**

N	-0.072850	-0.272851	-0.130918
C	0.381209	0.178175	2.111331
C	2.885601	0.329643	1.670952
H	3.781527	-0.272029	1.849617
H	3.080041	1.337720	2.066181
H	2.738869	0.412692	0.589273
H	-0.402990	-0.341018	2.666268
H	1.815283	-0.667801	3.347741
C	-0.052587	1.523496	1.606821
H	-0.176817	2.142022	2.512745
H	0.723385	1.990708	0.994309
C	-1.394288	1.449806	0.863491
H	-2.140854	0.992525	1.525918
H	-1.757749	2.451584	0.610620
C	-1.215538	0.581503	-0.405126
H	-2.136998	0.022676	-0.619700
H	-1.014620	1.235669	-1.269728
S	0.158358	-1.645818	-0.839044
O	1.400343	-2.254499	-0.175485
O	-0.999501	-2.564817	-0.962936
C	0.778732	-1.381546	-2.521702
H	1.665693	-0.748913	-2.469247
H	-0.010429	-0.899372	-3.103792
H	1.021390	-2.355289	-2.951731
Pd	1.387913	-2.462568	1.903310
O	1.238376	-2.698482	3.918280
C	2.319970	-3.029749	4.579395
O	3.427075	-3.231891	4.077116
C	2.080967	-3.158179	6.080218
H	3.011602	-3.425471	6.584377
H	1.321497	-3.923445	6.274341
H	1.698897	-2.214571	6.484118
N	1.228989	-4.557135	1.582402
C	0.268802	-5.055085	0.779960
H	-0.394162	-4.334710	0.311630
C	2.106383	-5.397788	2.165136
H	2.855518	-4.933681	2.798606
C	2.047834	-6.774366	1.963354
H	2.778484	-7.414671	2.446874
C	1.049860	-7.298531	1.142963
H	0.979481	-8.369127	0.971520
C	0.146525	-6.422068	0.543623
H	-0.645715	-6.780171	-0.105746
C	1.679815	-0.309101	2.325062

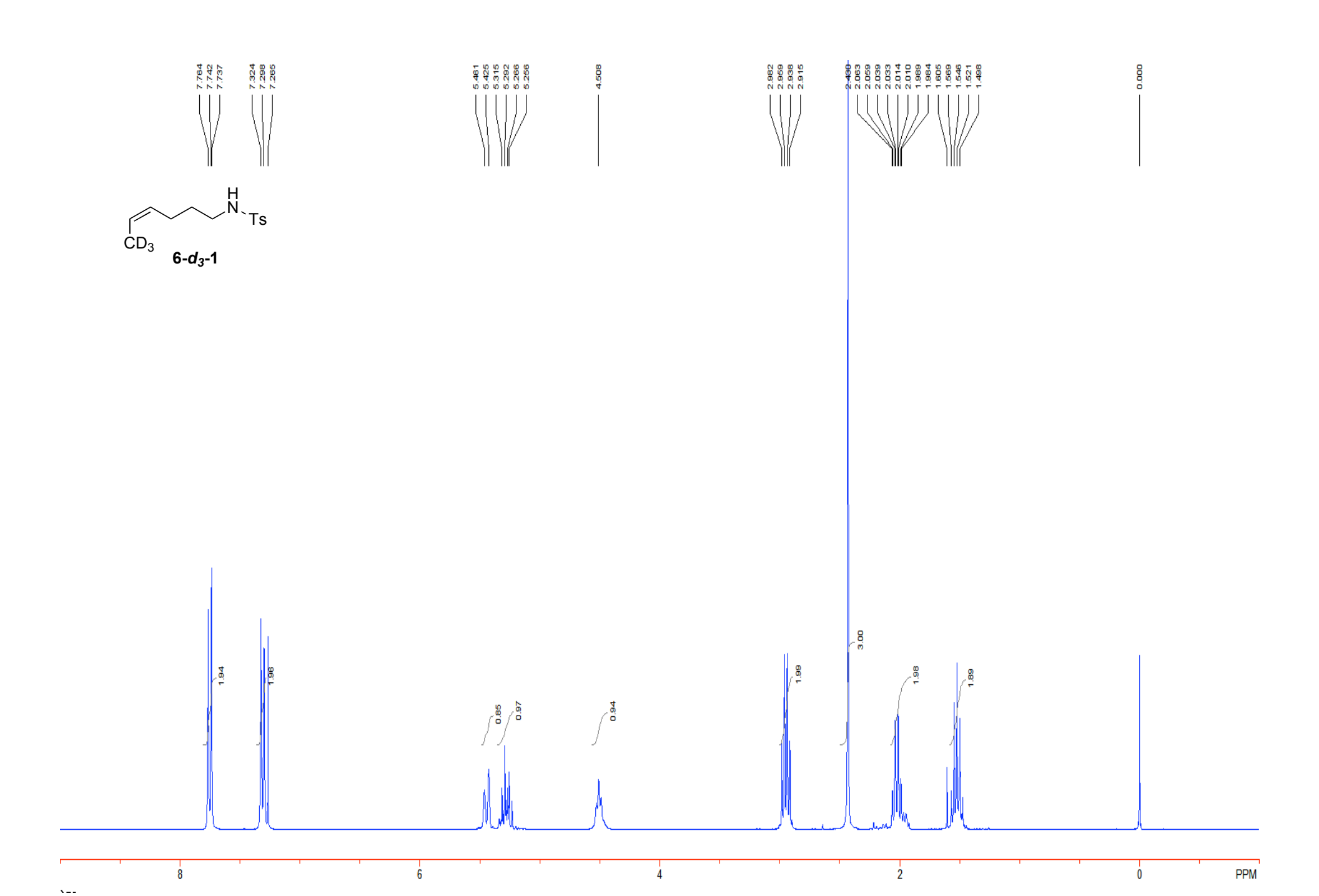
***cis*-[6,5]-P**

N	-0.595045	-0.547631	-0.181376
C	-0.766034	0.157926	2.001179
C	0.545313	-0.090377	4.149812
H	0.675250	-0.792686	4.973958
H	0.171730	0.857935	4.564456
H	1.531643	0.098394	3.717652
H	-1.789707	0.136863	1.652523
H	-1.345138	-1.072964	3.588252
C	0.095402	1.297579	1.533752
H	-0.515619	2.008650	0.965439
H	0.512268	1.823609	2.400870
C	1.250515	0.792199	0.633692
H	1.903463	1.627348	0.350936
H	1.854914	0.061078	1.182136
C	0.622541	0.137942	-0.608566
H	0.353517	0.917637	-1.336831
H	1.336274	-0.541218	-1.089136
S	-0.810954	-2.089582	-0.410032
O	-1.277499	-2.701504	0.929735
C	-2.326157	-2.281153	-1.376683
O	0.261435	-2.833822	-1.101434
Pd	0.231494	-2.602529	2.374895
O	1.618400	-2.720714	3.853007
C	2.822854	-2.310895	3.561801
O	3.178231	-1.856765	2.468888
C	3.791999	-2.418915	4.733848
H	4.819174	-2.300872	4.382526
H	3.674521	-3.376296	5.250228
H	3.571539	-1.626642	5.459281
N	0.854756	-4.510960	1.707706
C	-0.020733	-5.529530	1.651789
H	-1.029191	-5.310390	1.983868
C	2.117673	-4.701631	1.285528
H	2.772387	-3.839009	1.348765
C	2.547924	-5.933004	0.797270
H	3.573422	-6.043749	0.460600
C	1.647930	-6.995862	0.747695
H	1.958120	-7.967092	0.372673
C	0.339185	-6.789321	1.184041
H	-0.398218	-7.585130	1.162188
C	-0.446115	-0.647591	3.128110
H	-2.568094	-3.344740	-1.428383
H	-3.126330	-1.725267	-0.886045
H	-2.134850	-1.882528	-2.374917

References:

(1) Steinhoff, B. A.; Guzei, I. A.; Stahl, S. S. *J. Am. Chem. Soc.* **2004**, *126*, 11268-11278.

(2) A mechanism involving dissociation of acetate to form a cationic intermediate is unlikely given the non-polar nature of the solvent medium. Evaluation of the free energy to form a charge-separated species suggests it is disfavored by more than 30 kcal/mol.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H
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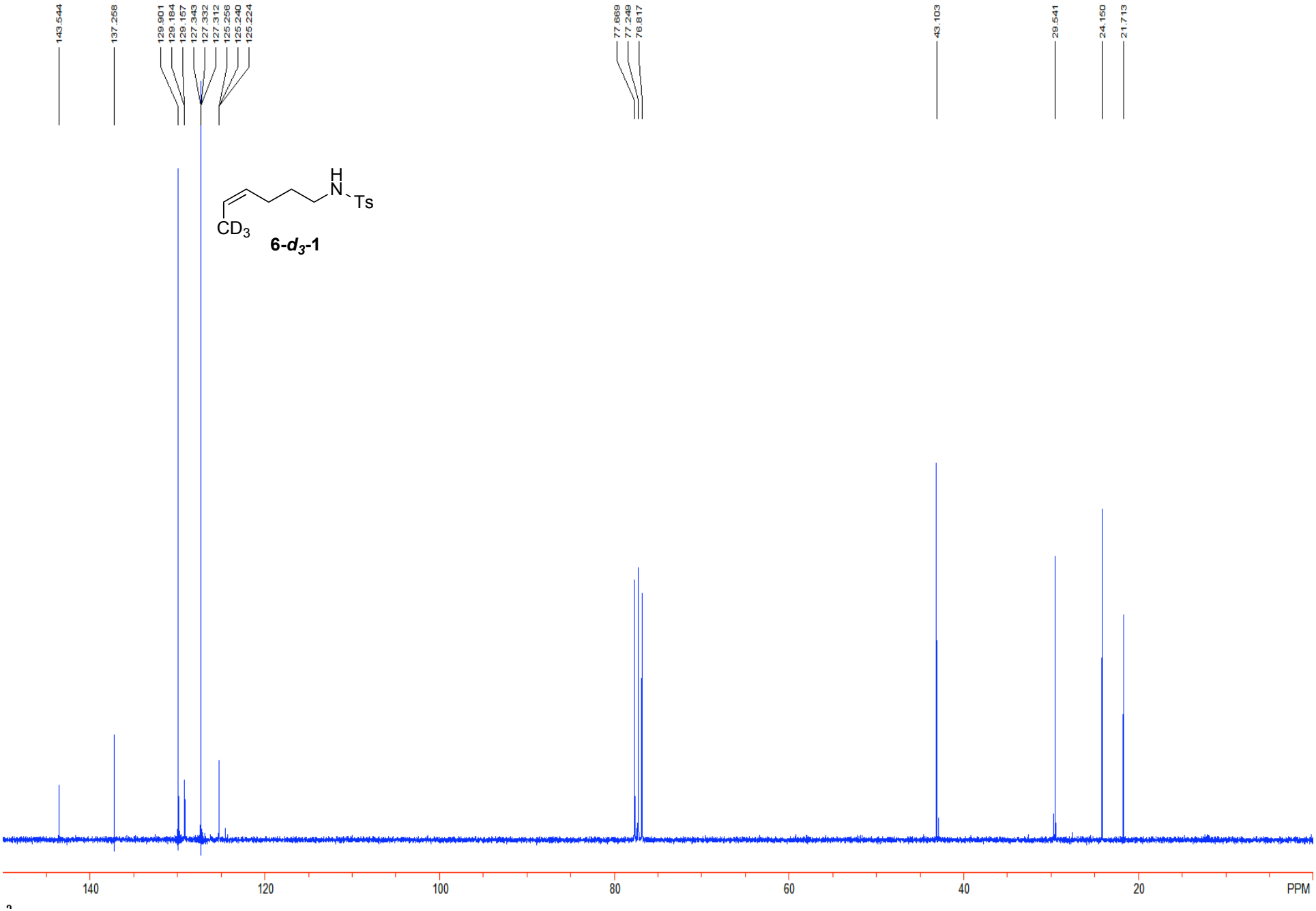
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29.541
24.150
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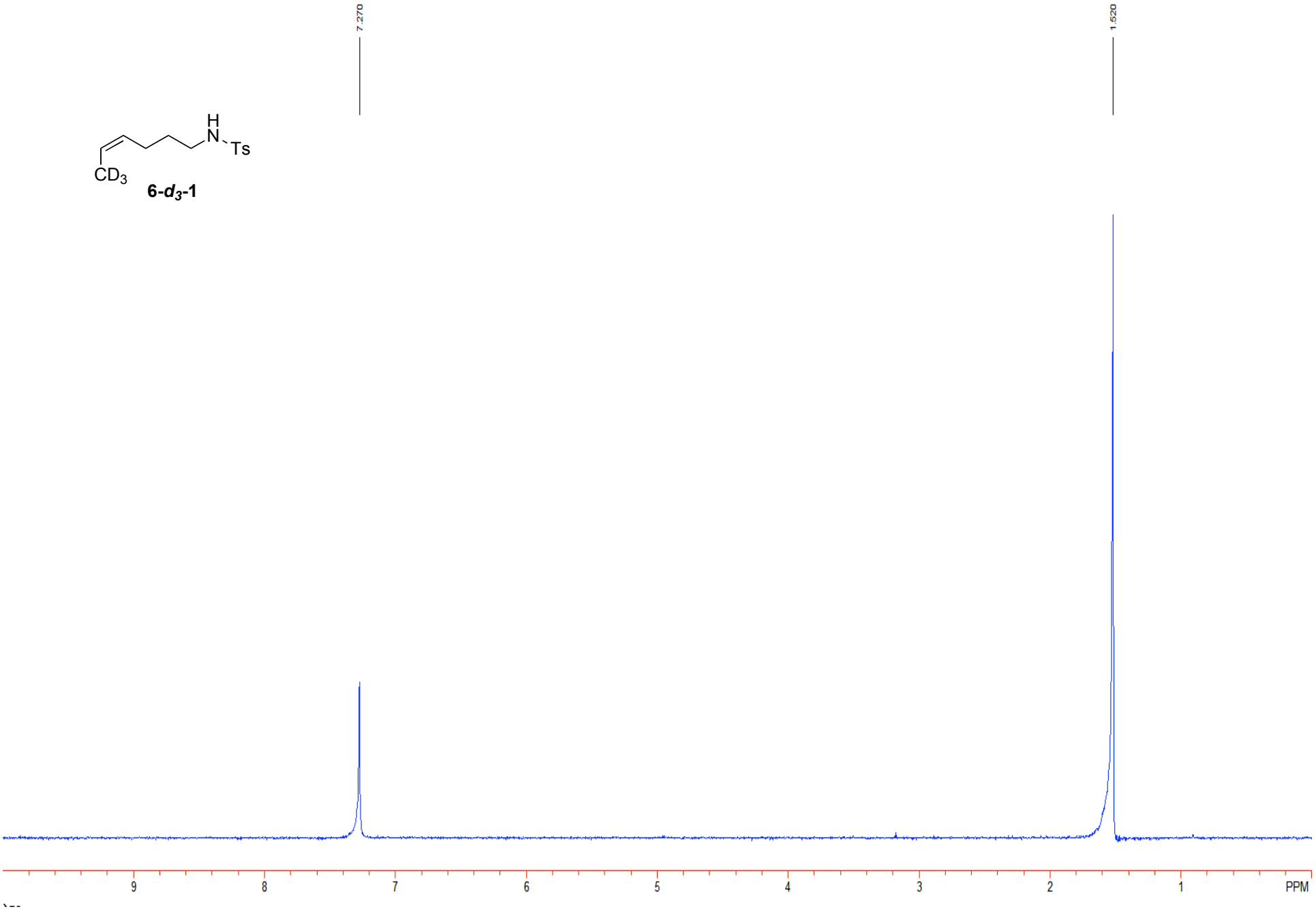
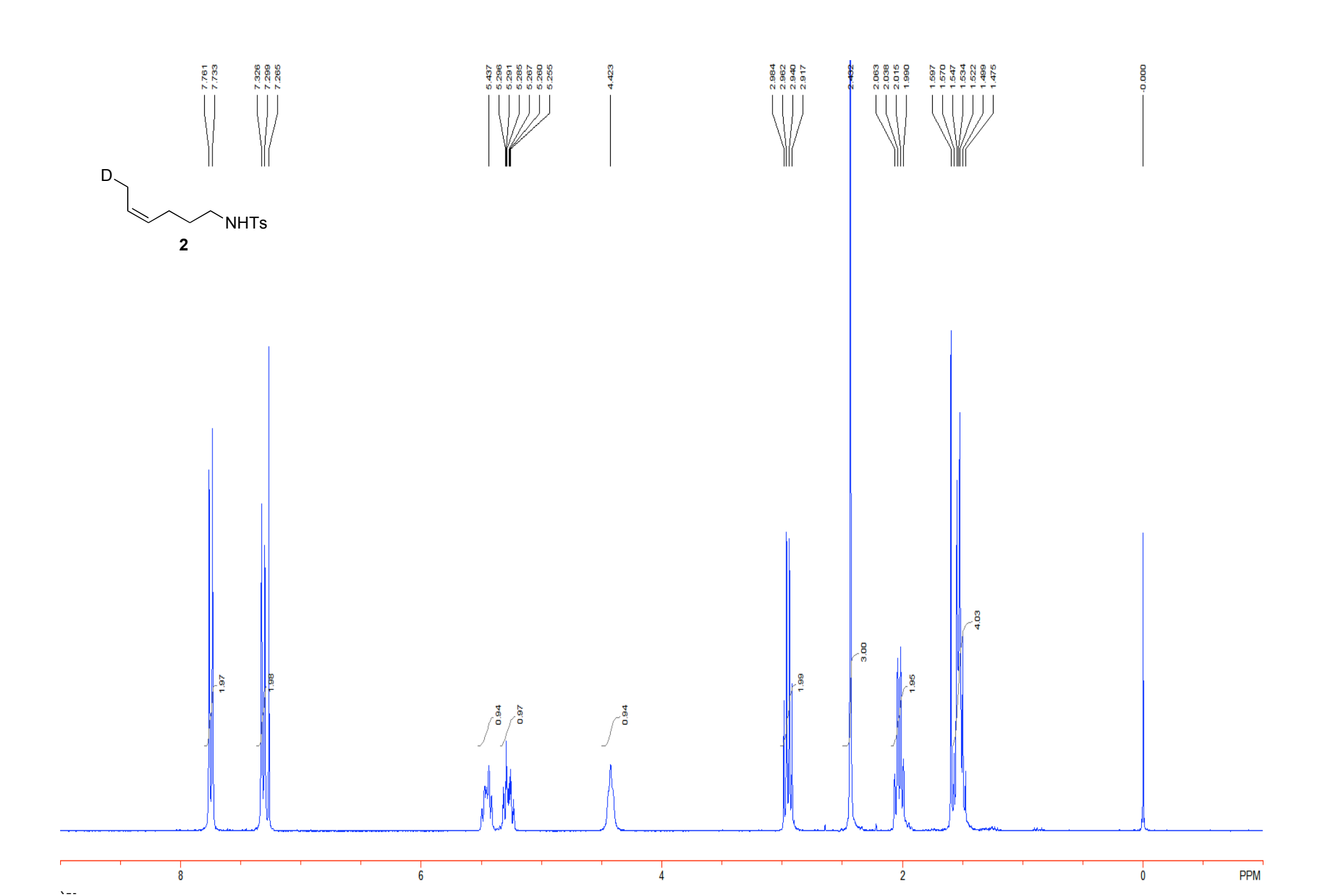
20
PPM

6-*d*$_3$-1

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D
NHTs
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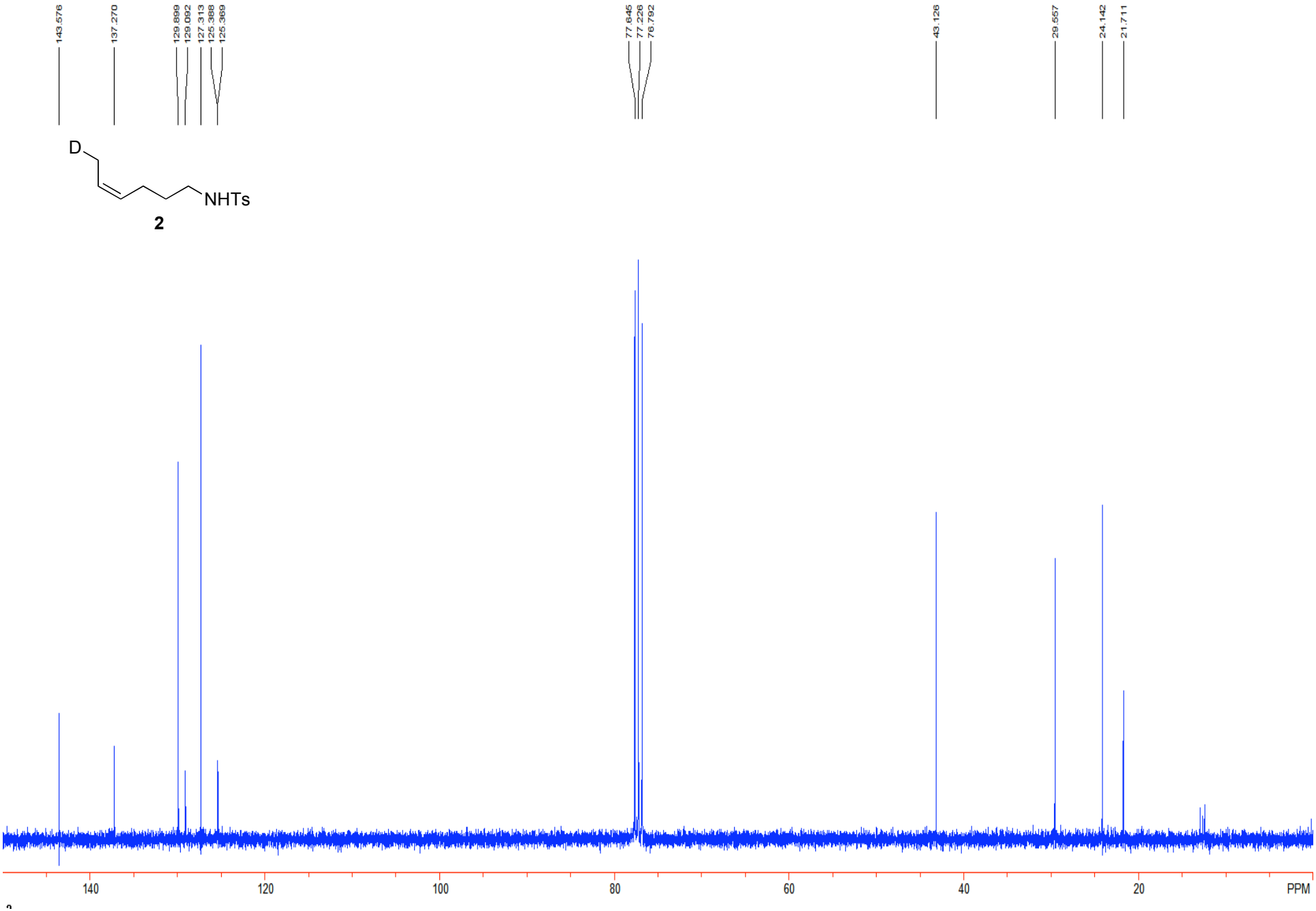
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D
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80
60
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20
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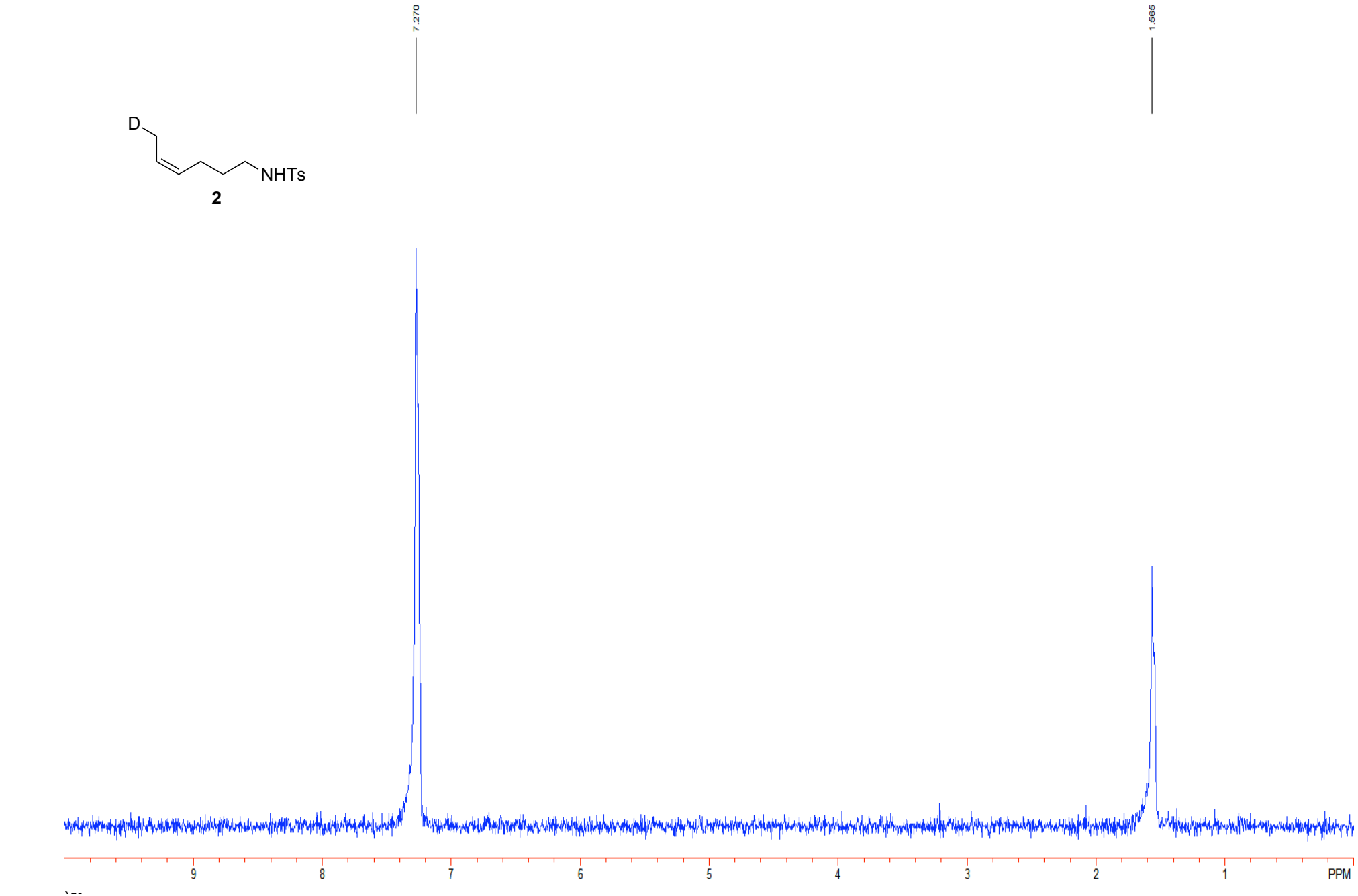
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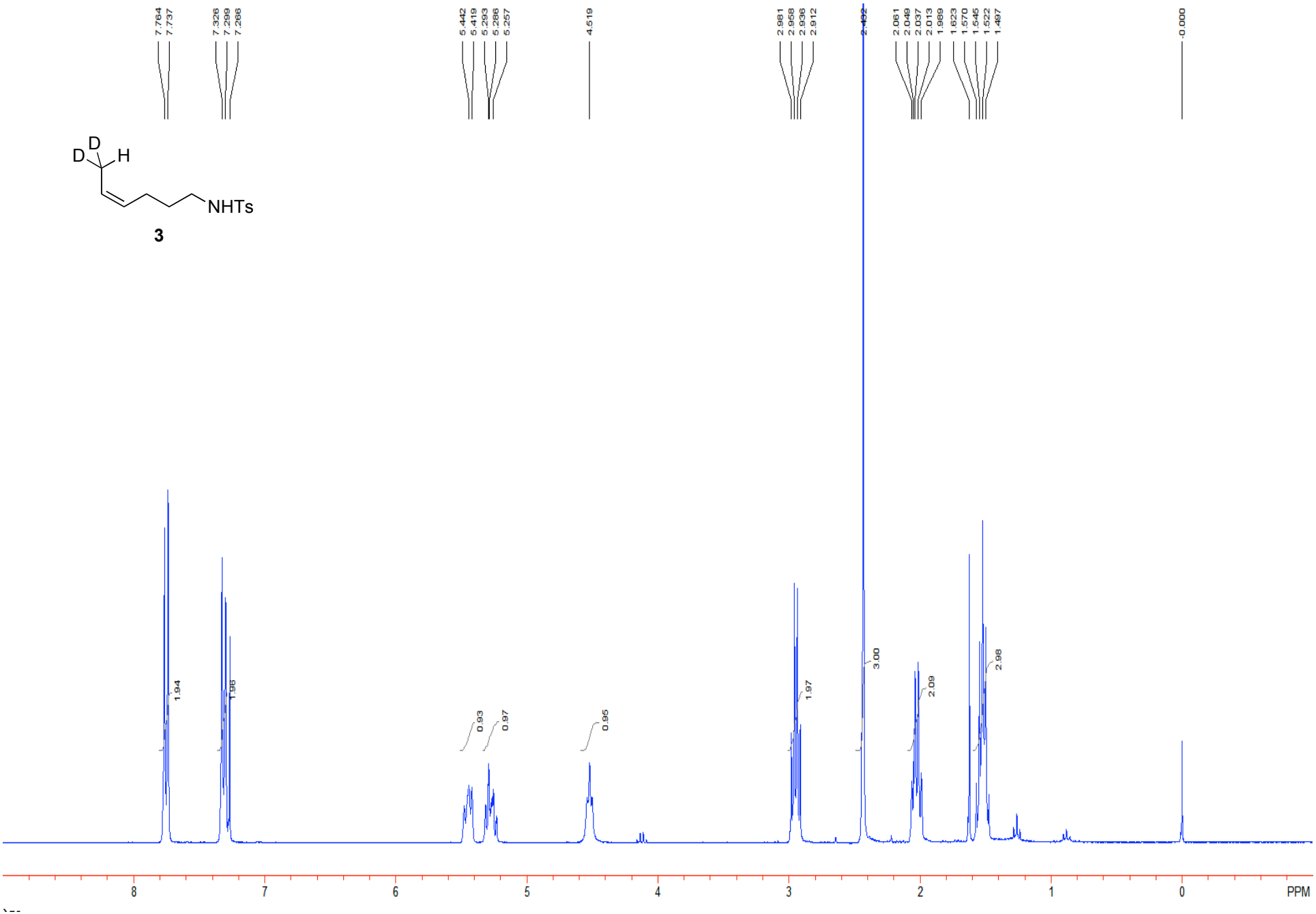
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D
D
H
NHTs
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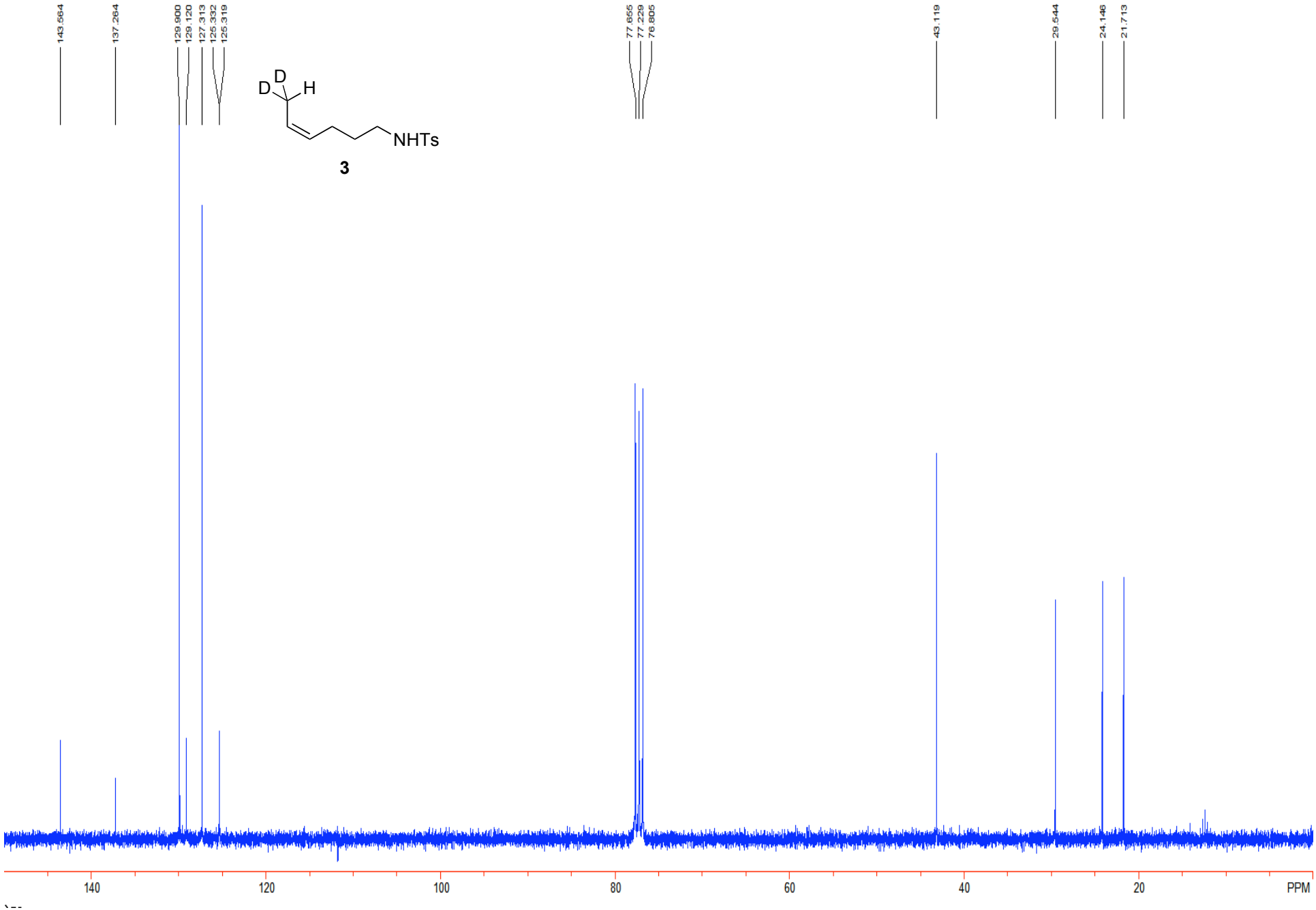
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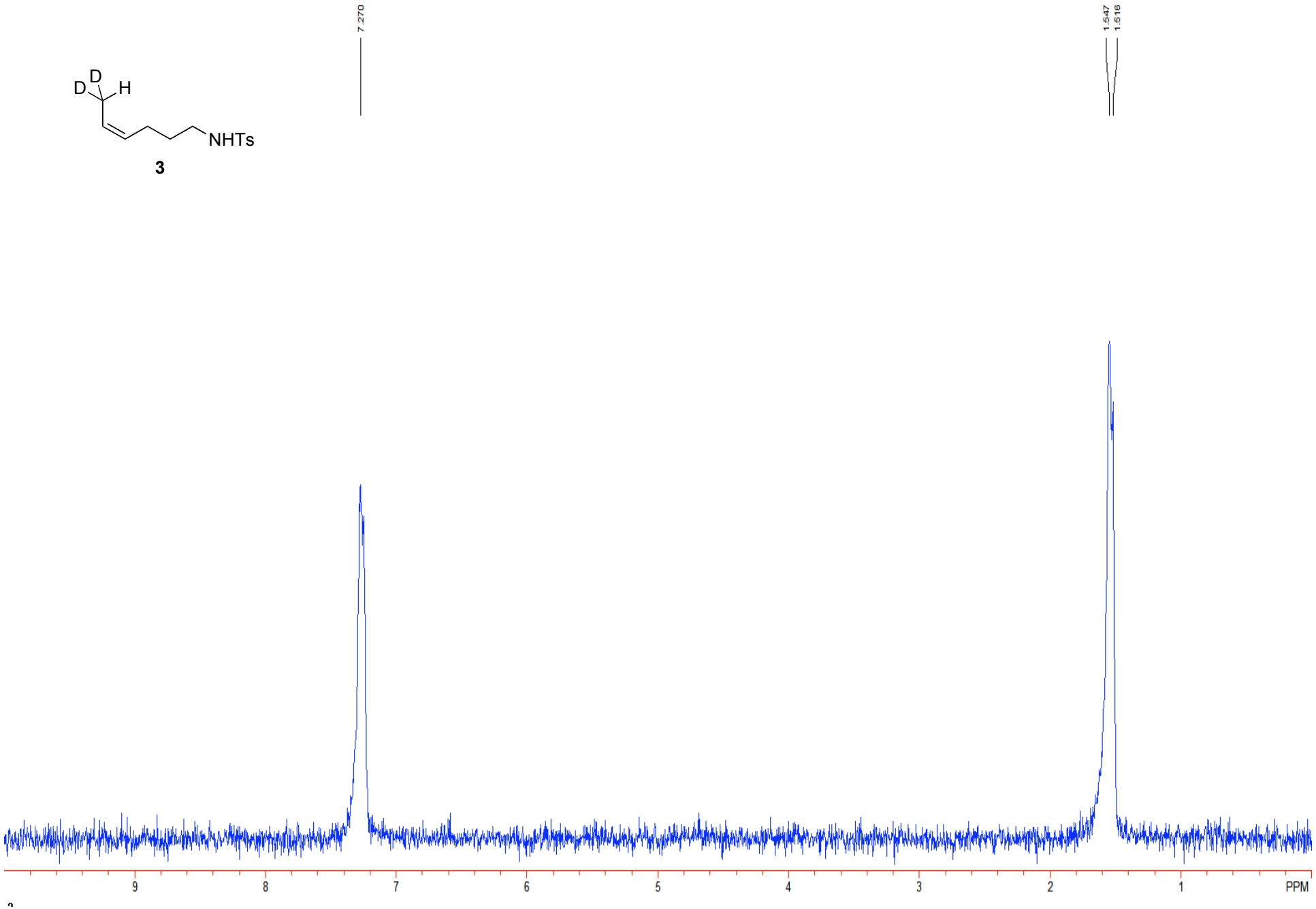
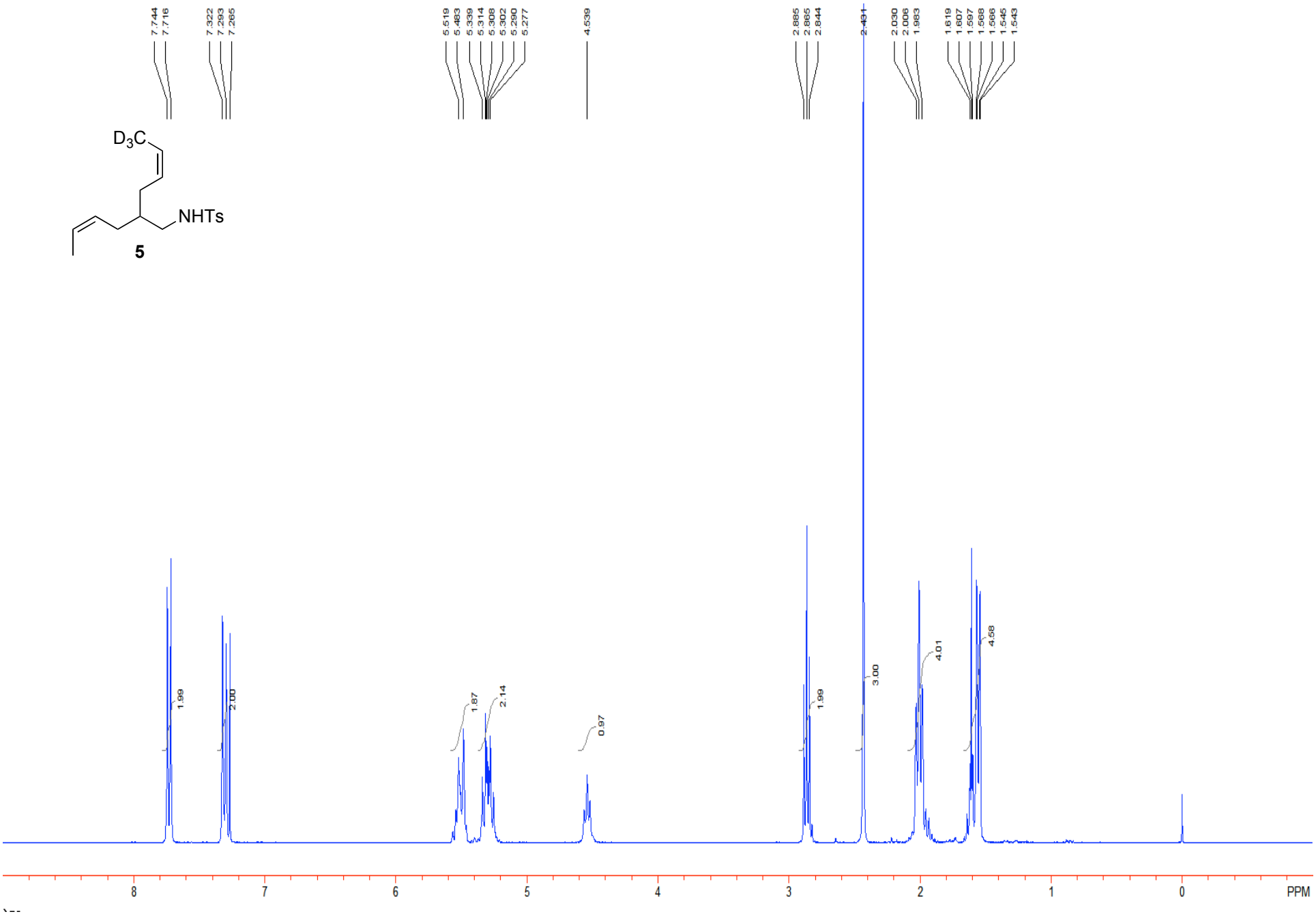
3

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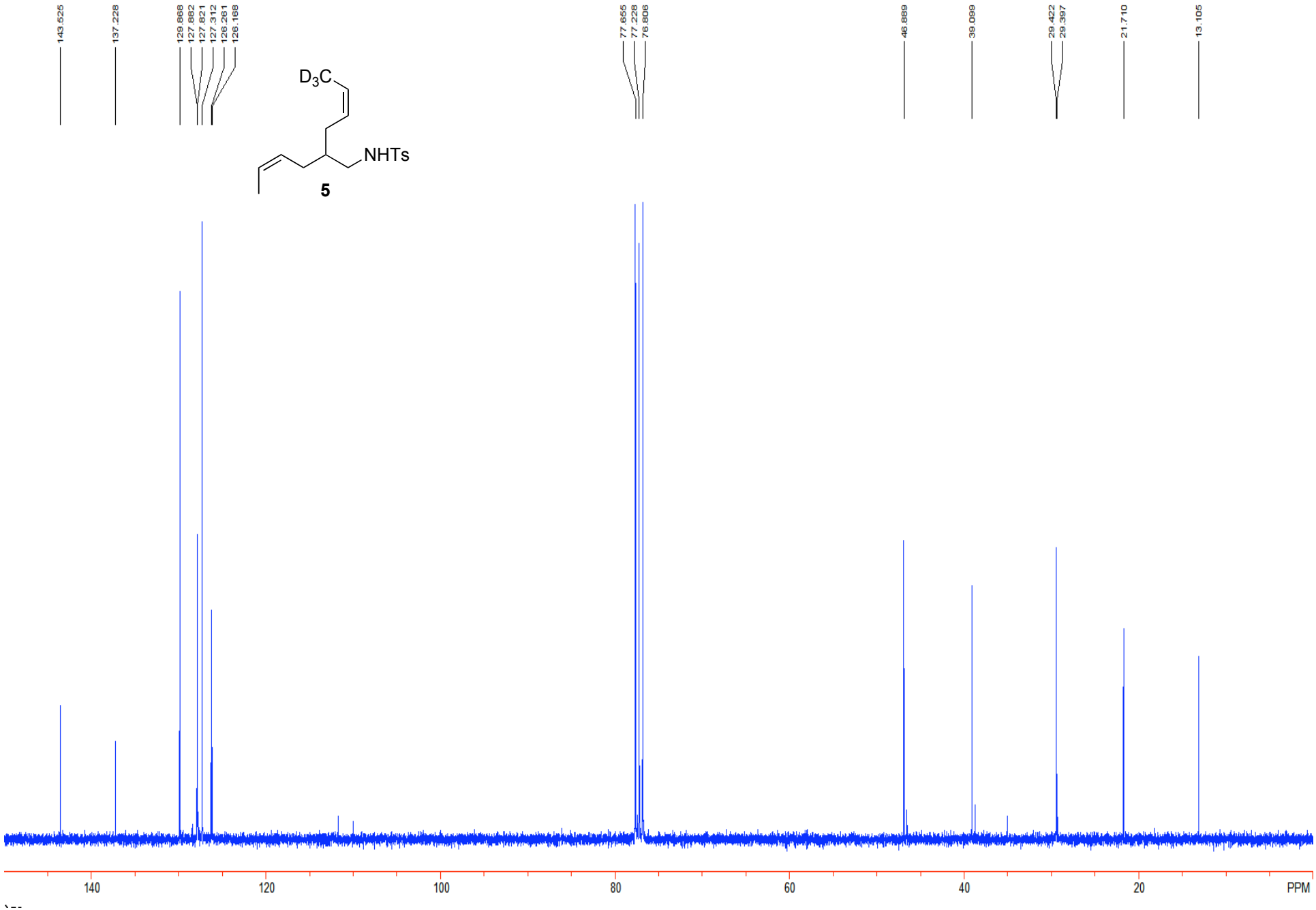
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5