Electronic Supplementary Information

Cationic Palladium(II)-Indenyl complexes bearing phosphines as ancillary ligands: synthesis, study of indenyl amination and anticancer activity

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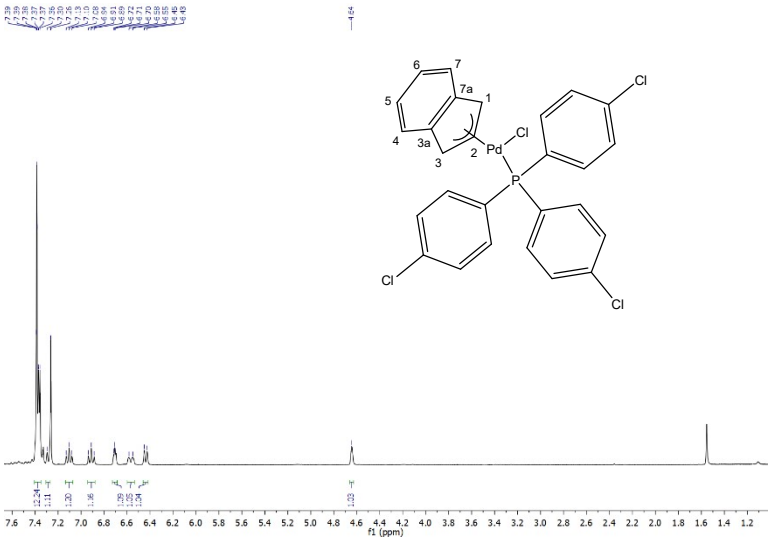
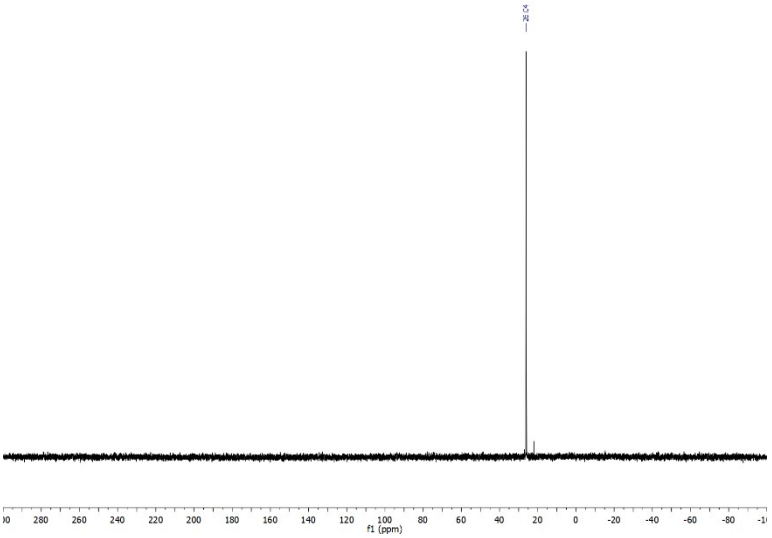
NMR spectra

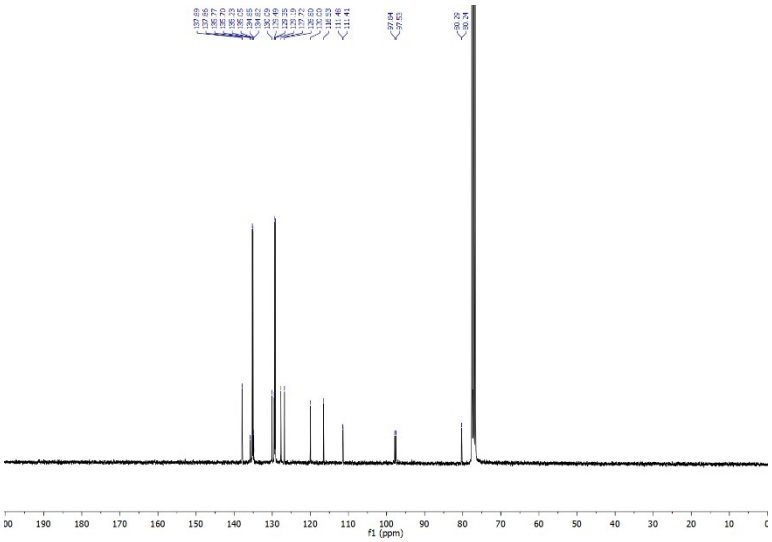
1D-NMR and 2D-NMR spectra were recorded on Bruker 300 or 400 Advance spectrometers. Chemical shifts values (ppm) are given relative to TMS (^{1}H and ^{13}C), H_3PO_4 (^{31}P) and CCl_3F (^{19}F).



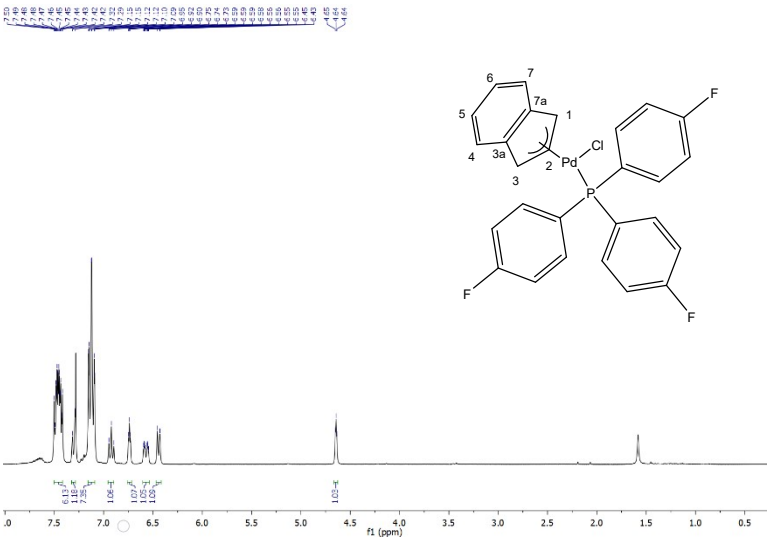
***S** 1. ^{1}H NMR spectra of **2b** in $CDCl_3$ at 298K*



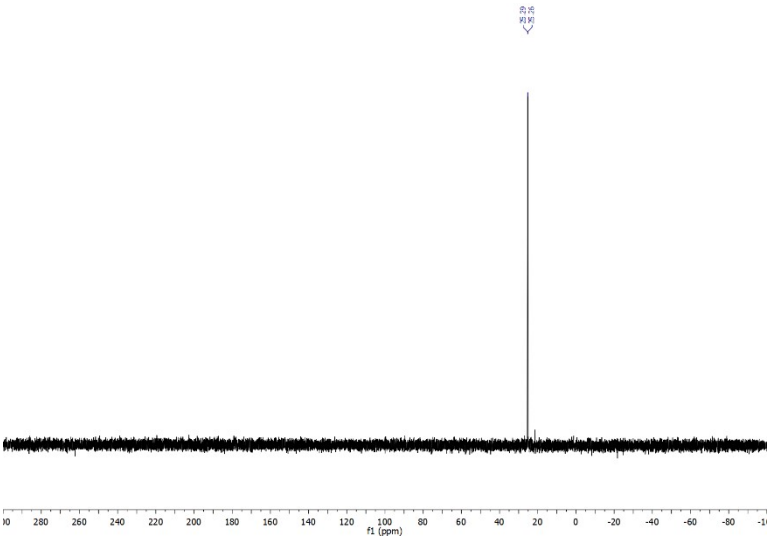
***S** 2. $^{31}P\{^{1}H\}$ NMR spectra of **2b** in $CDCl_3$ at 298K*



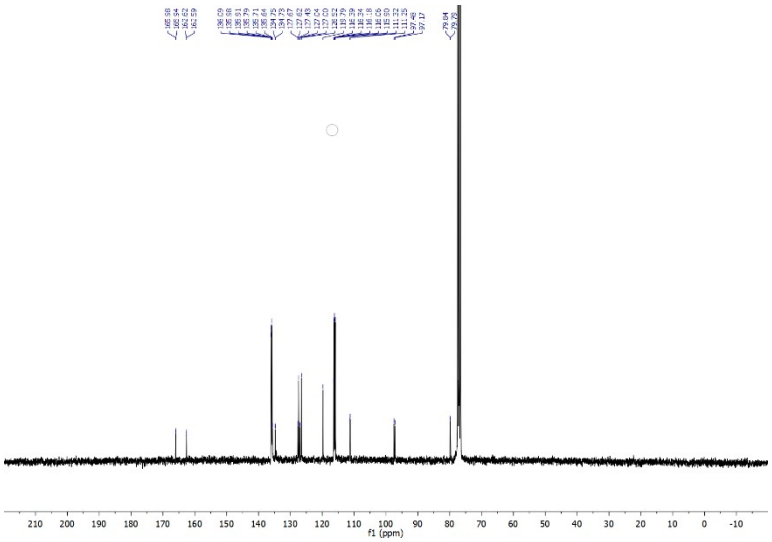
***S** 3. $^{13}C\{^1H\}$ NMR spectra of **2b** in $CDCl_3$ at 298K*



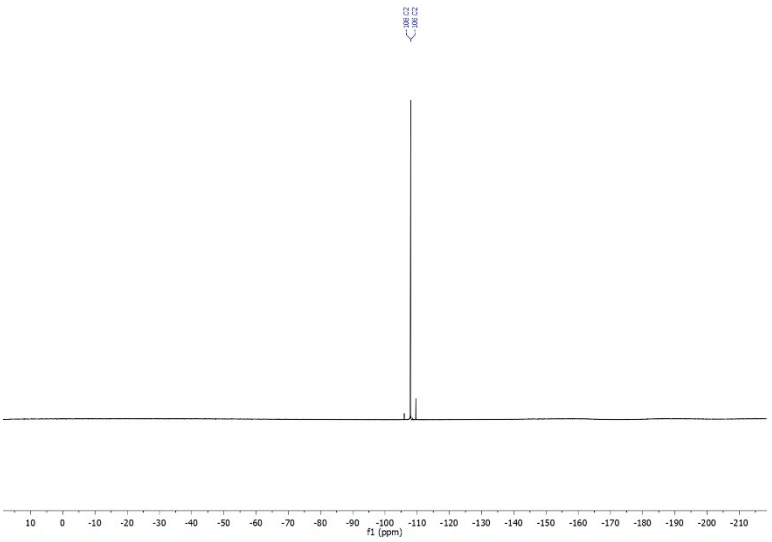
***S** 4. ^1H NMR spectra of **2c** in $CDCl_3$ at 298K*



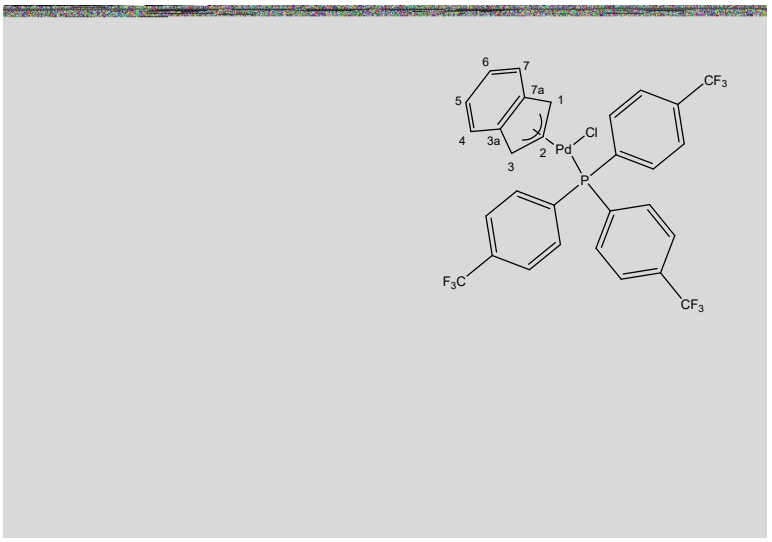
***S** 5. $^{31}P\{^1H\}$ NMR spectra of **2c** in $CDCl_3$ at 298K*



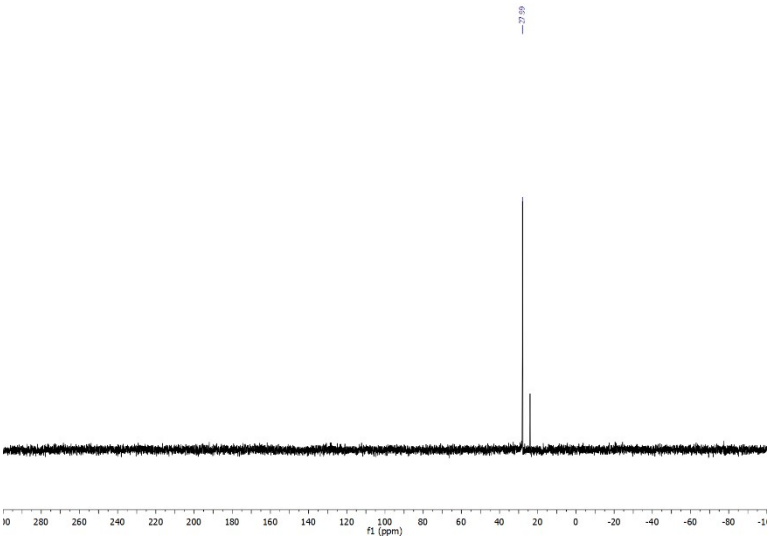
***S** 6. $^{13}C\{^1H\}$ NMR spectra of **2c** in $CDCl_3$ at 298K*



***S** 7. $^{19}F\{^1H\}$ NMR spectra of **2c** in $CDCl_3$ at 298K*



***S** 8. ^1H NMR spectra of **2d** in $CDCl_3$ at 298K*



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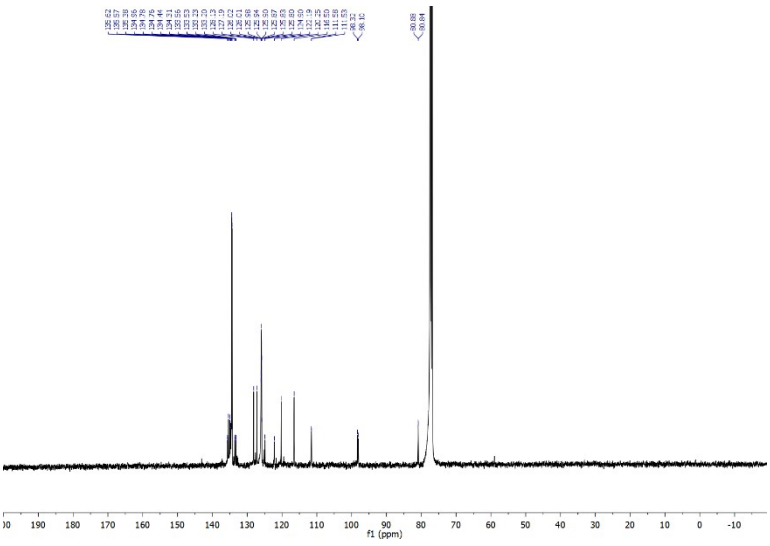

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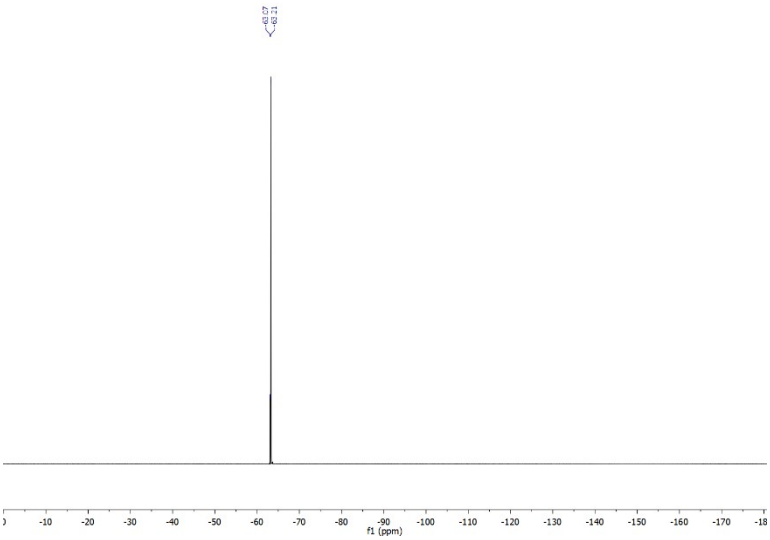

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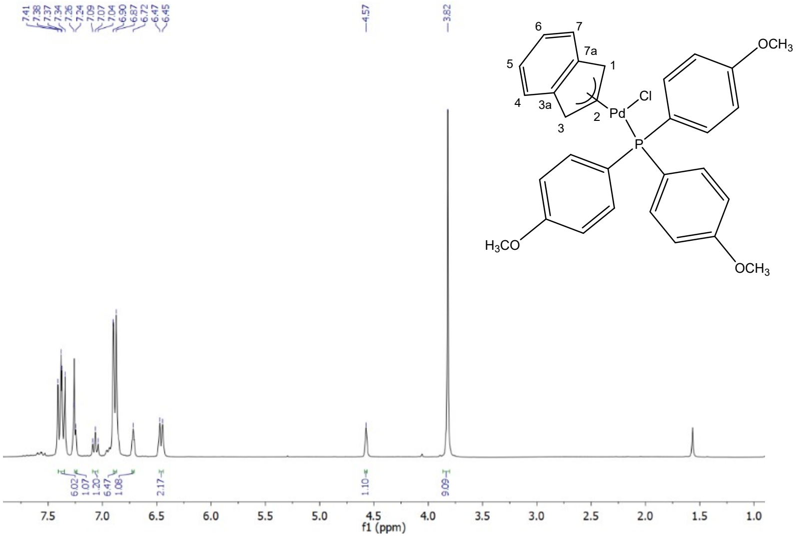

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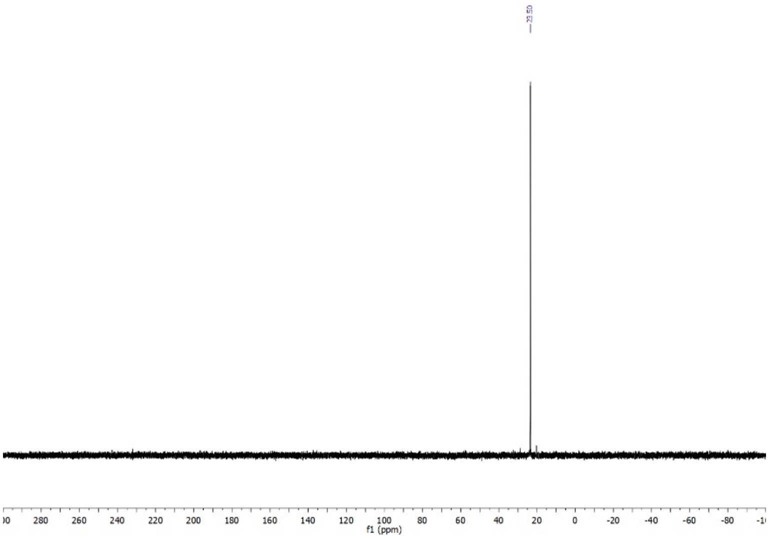
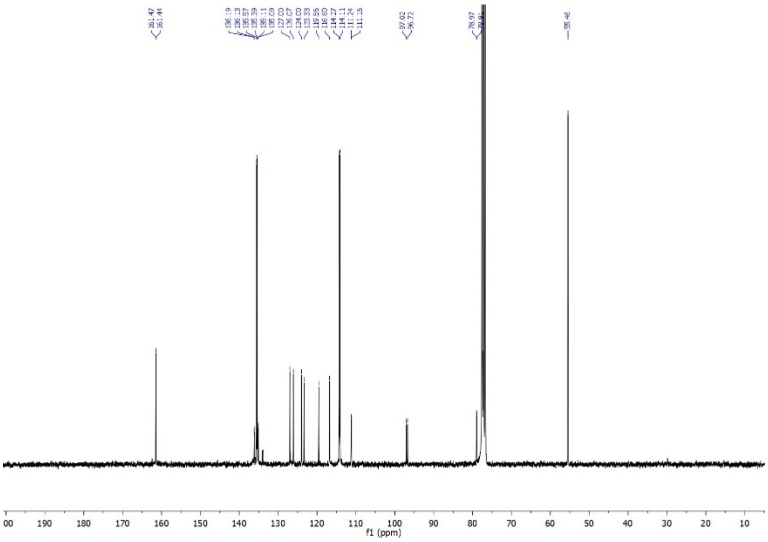


***S** 13. [31]P{[1]H} NMR spectra of **2e** in $CDCl_3$ at 298K*



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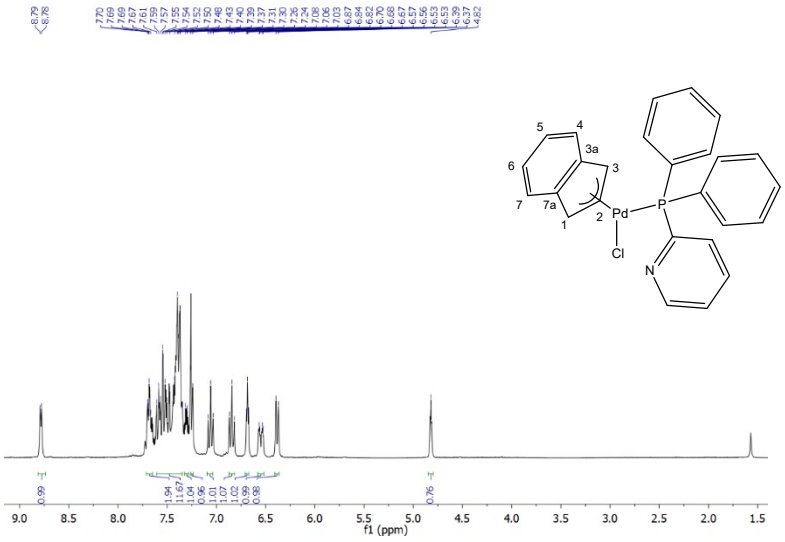

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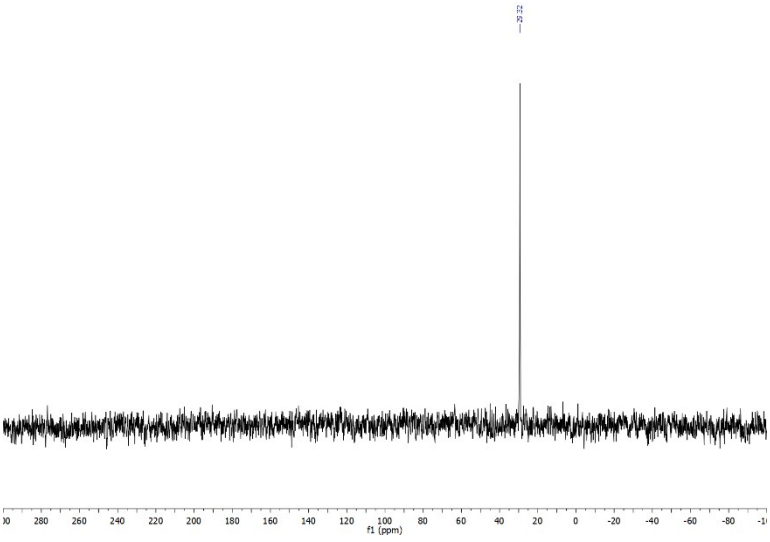

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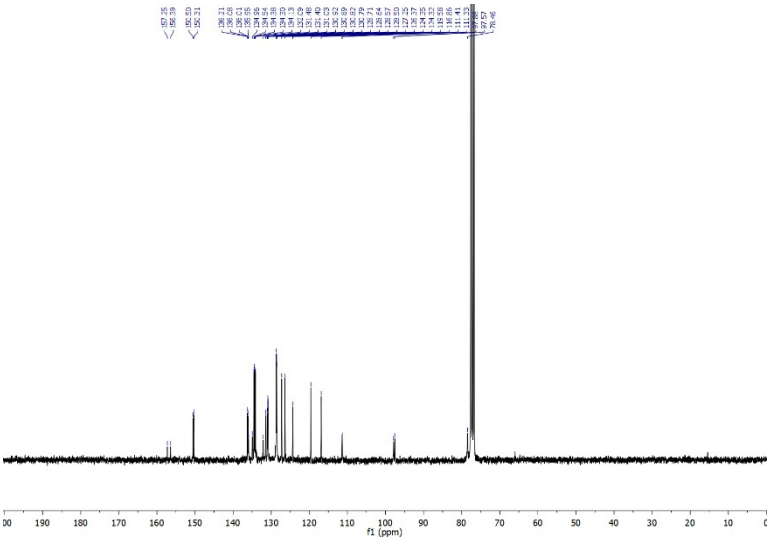

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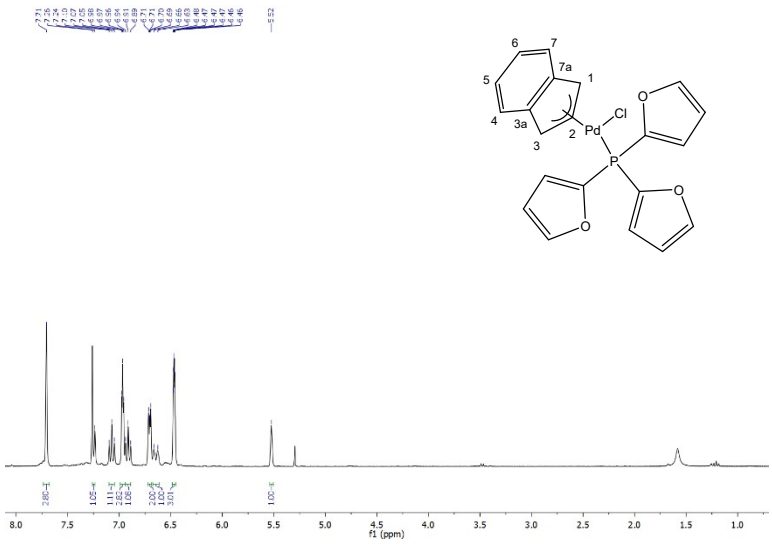
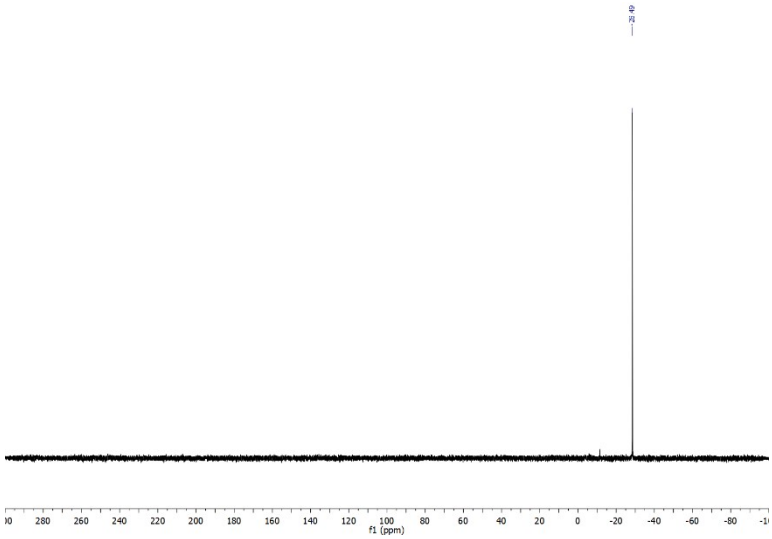
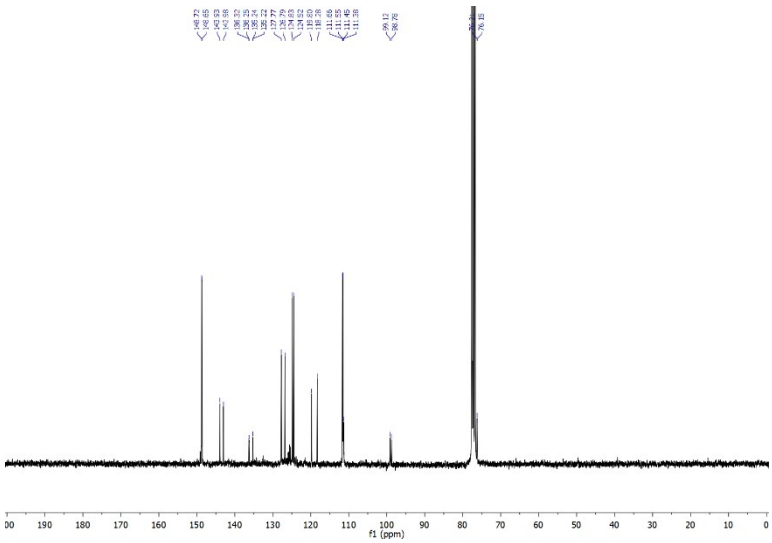


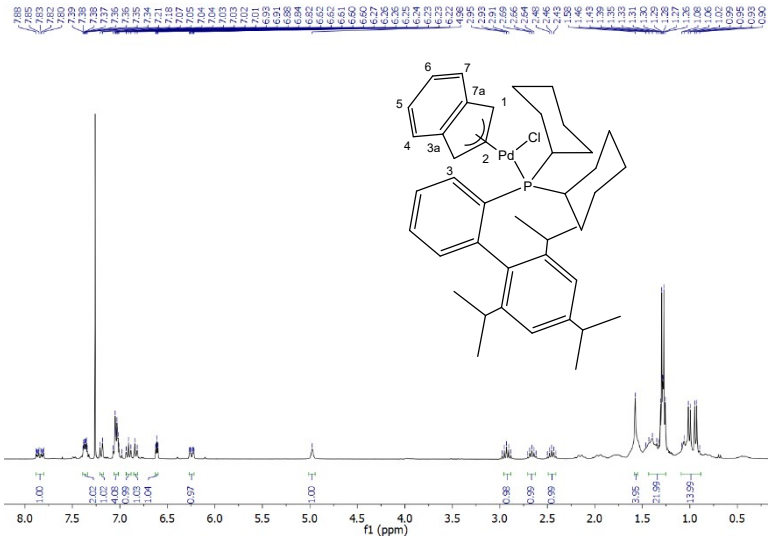
***S** 18. ^{1}H NMR spectra of **2g** in $CDCl_3$ at 298K*



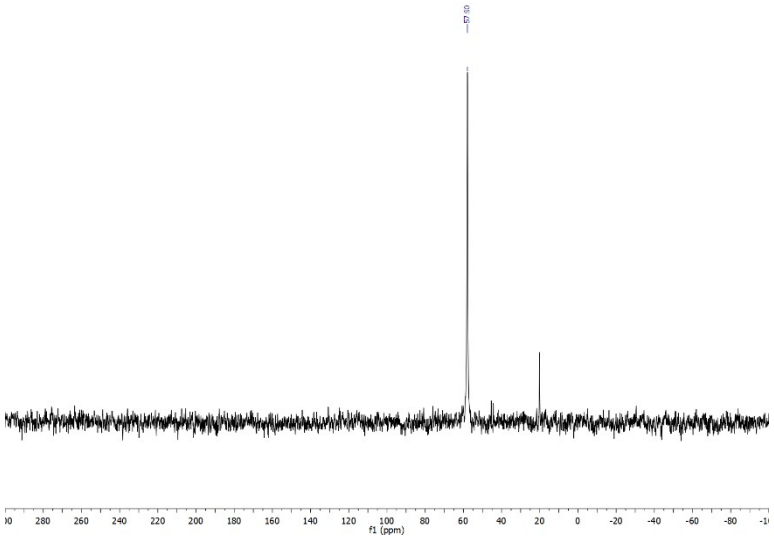
***S** 19. $^{31}P\{^{1}H\}$ NMR spectra of **2g** in $CDCl_3$ at 298K*



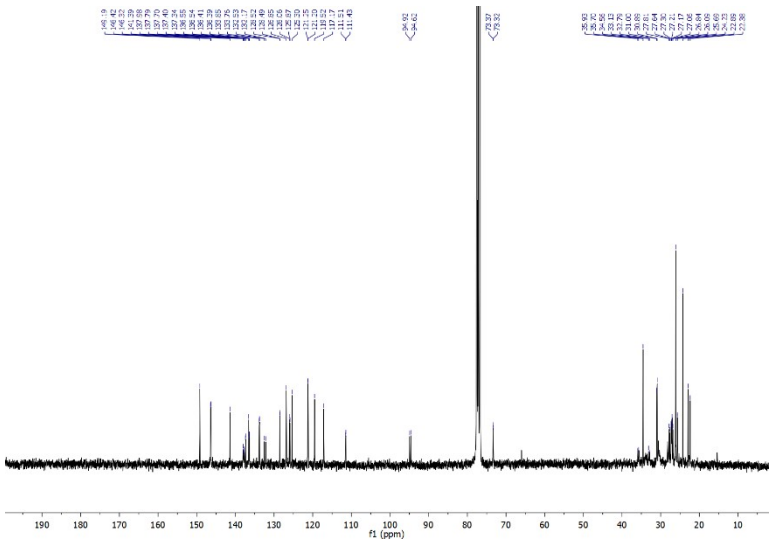
***S** 20. $^{13}C\{^{1}H\}$ NMR spectra of **2g** in $CDCl_3$ at 298K*



***S** 21. ^{1}H NMR spectra of **2h** in $CDCl_3$ at 298K*



***S** 22. $^{31}P\{^{1}H\}$ NMR spectra of **2h** in $CDCl_3$ at 298K*



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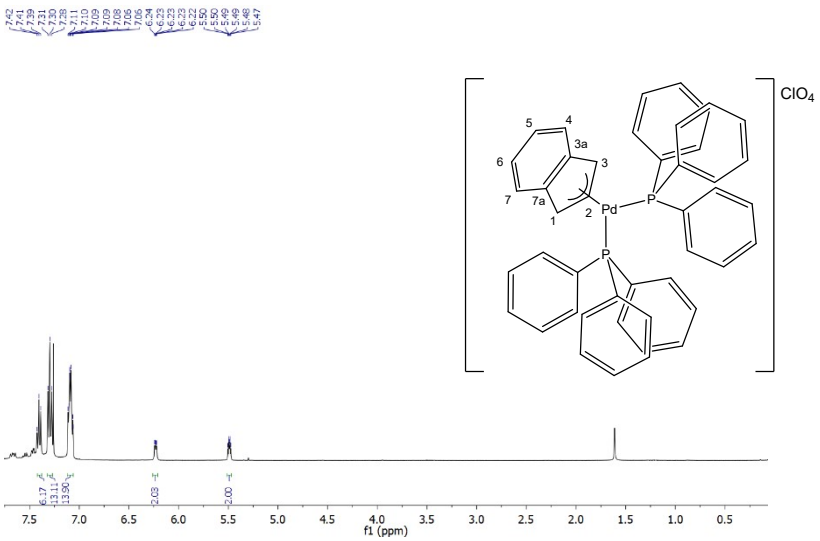
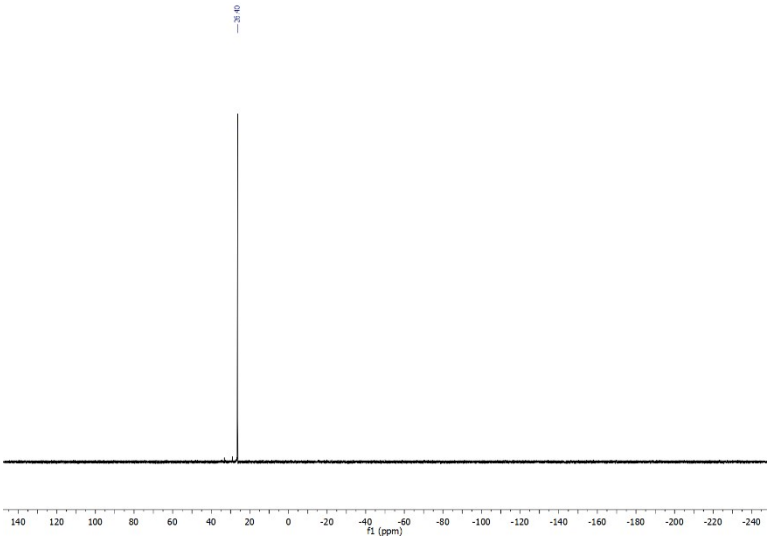
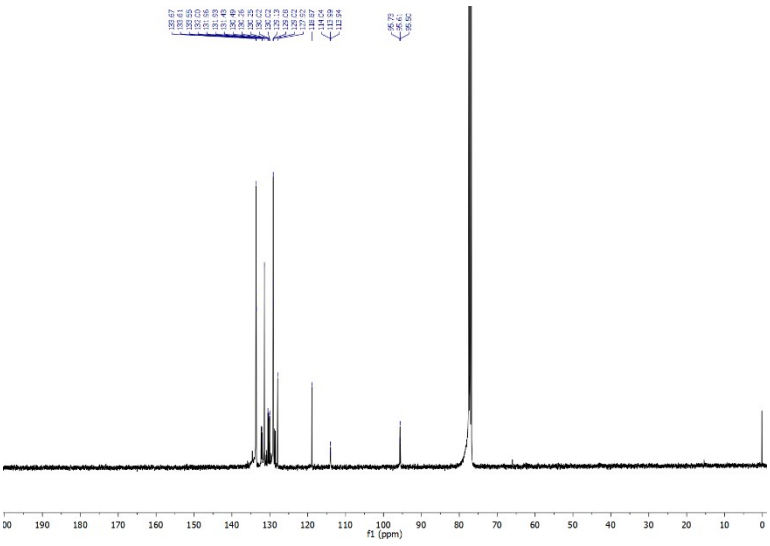


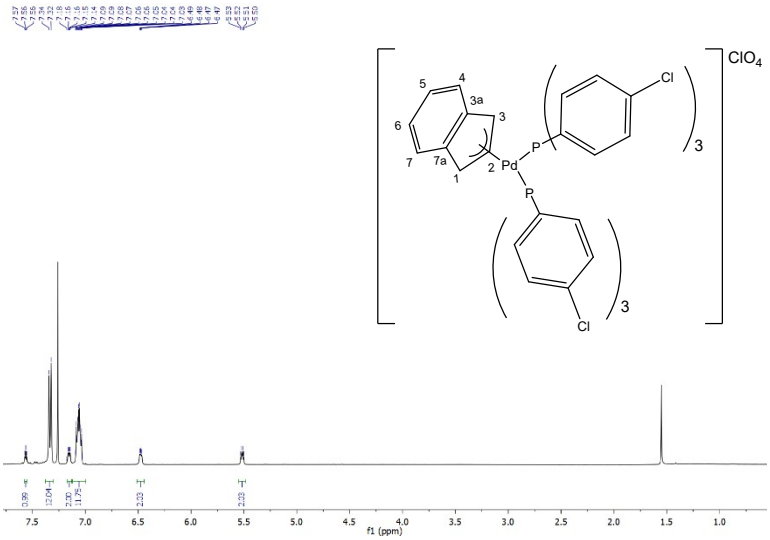
***S** 24. [1]H NMR spectra of **3a** in $CDCl_3$ at 298K*



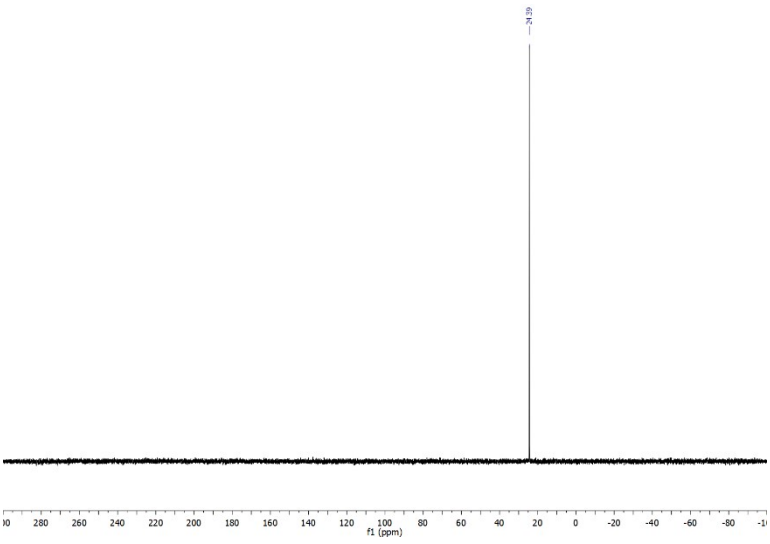
***S** 25. [31]P{[1]H} NMR spectra of **3a** in $CDCl_3$ at 298K*



***S** 26. [13]C{[1]H} NMR spectra of **3a** in $CDCl_3$ at 298K*



***S** 27. [1]H NMR spectra of **3b** in $CDCl_3$ at 298K*



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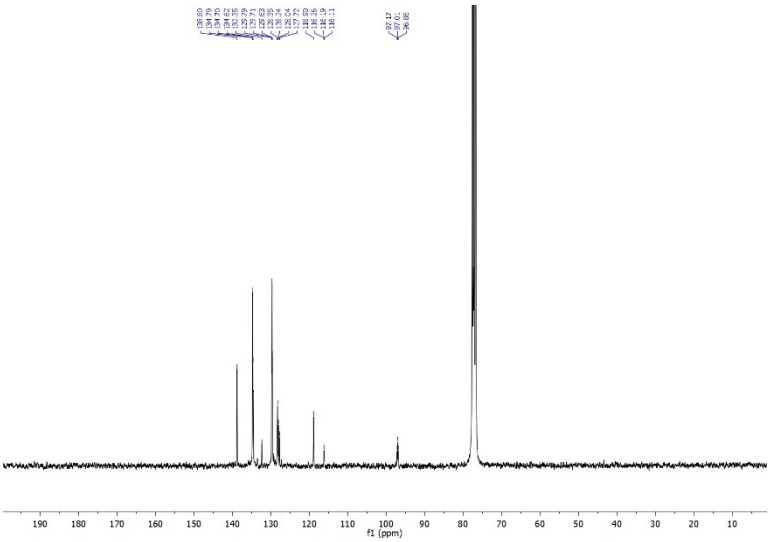

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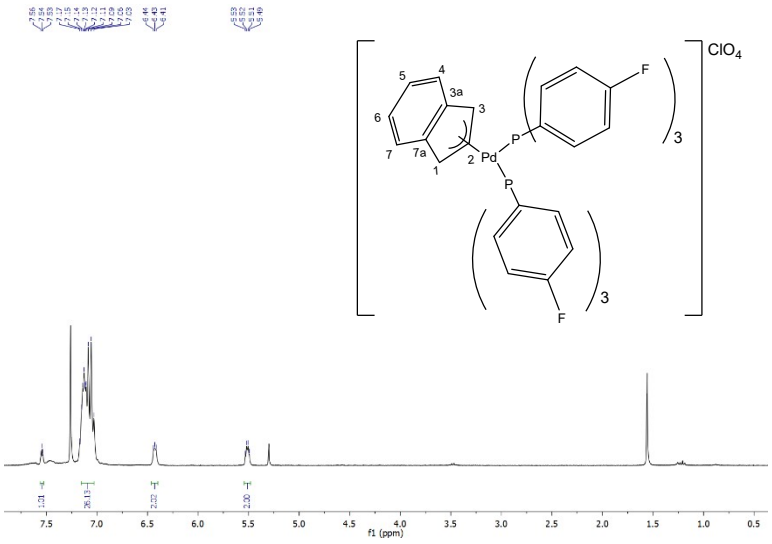

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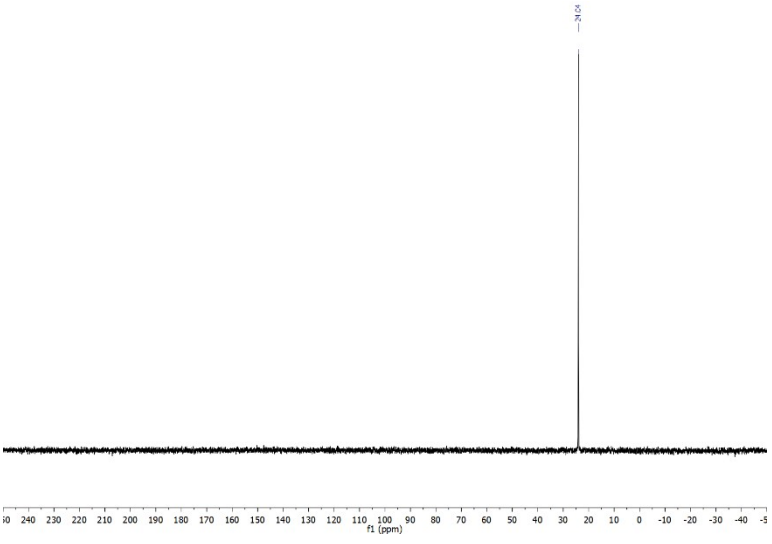

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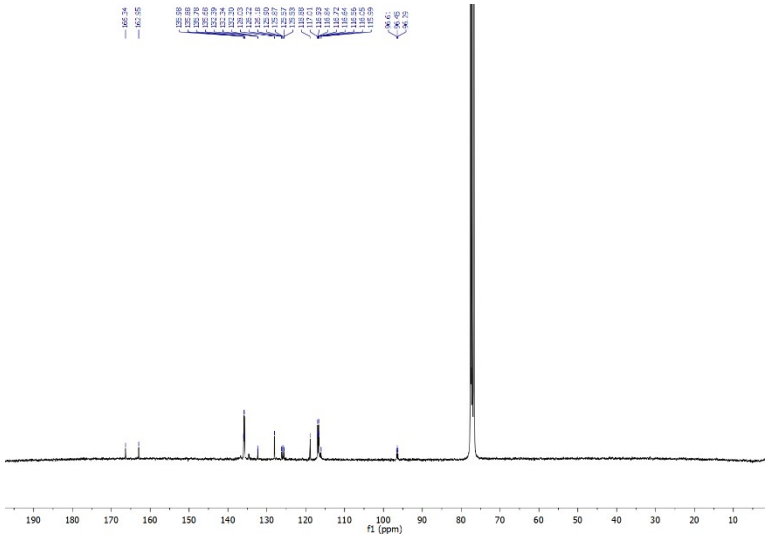

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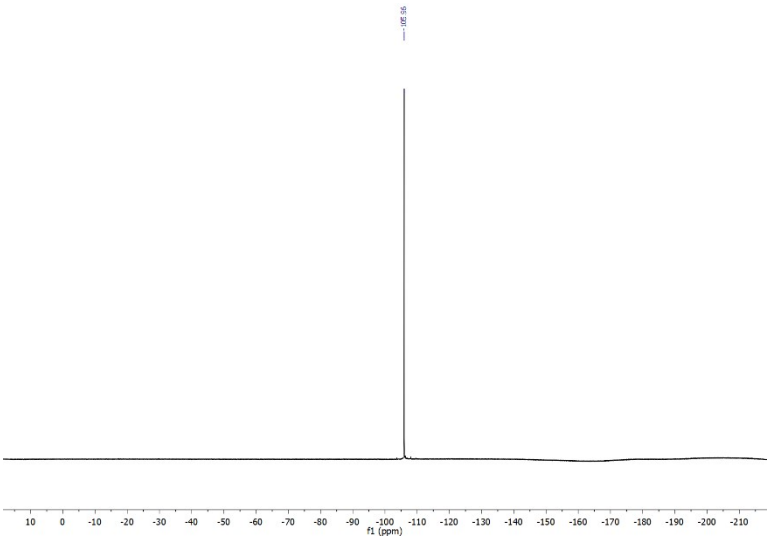
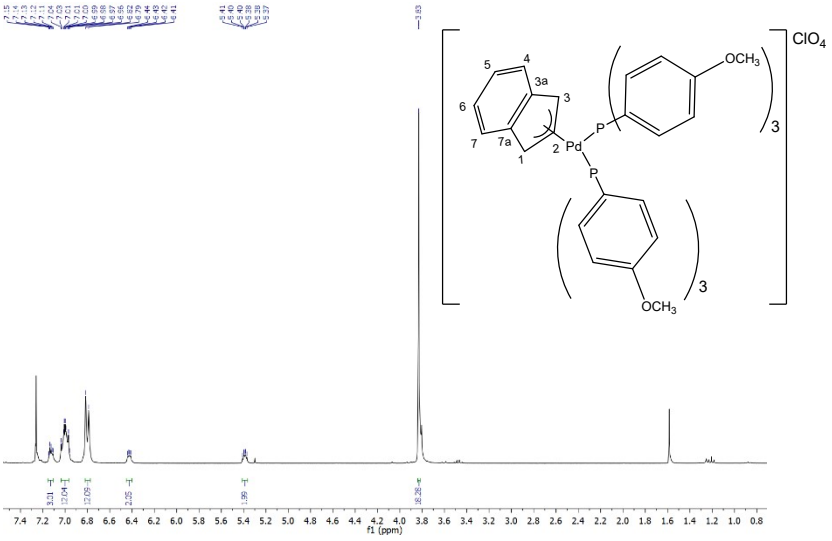


***S** 33. $^{19}F\{^{1}H\}$ NMR spectra of **3c** in $CDCl_3$ at 298K*



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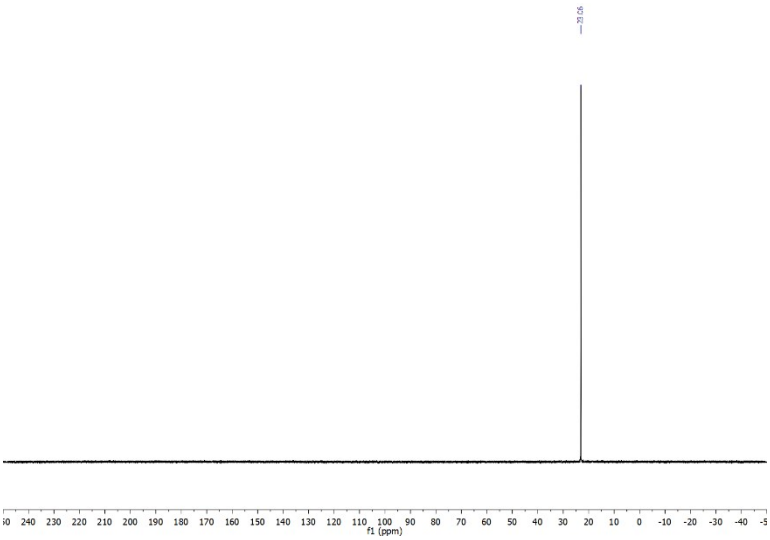

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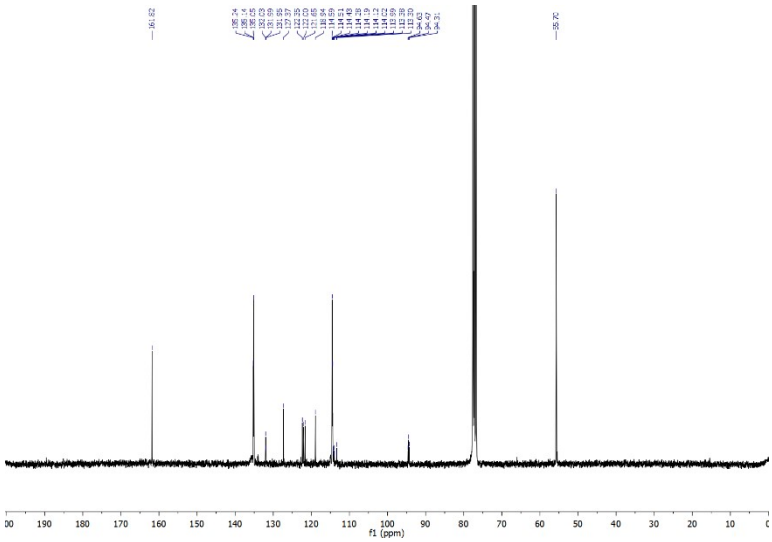

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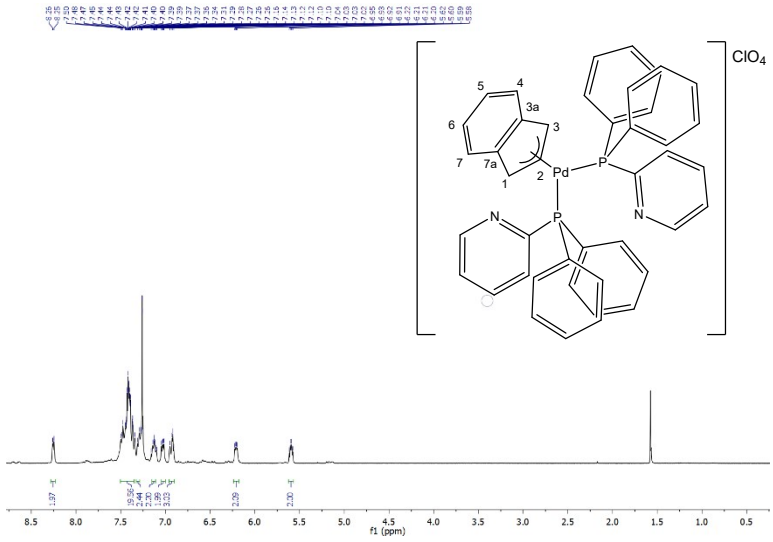

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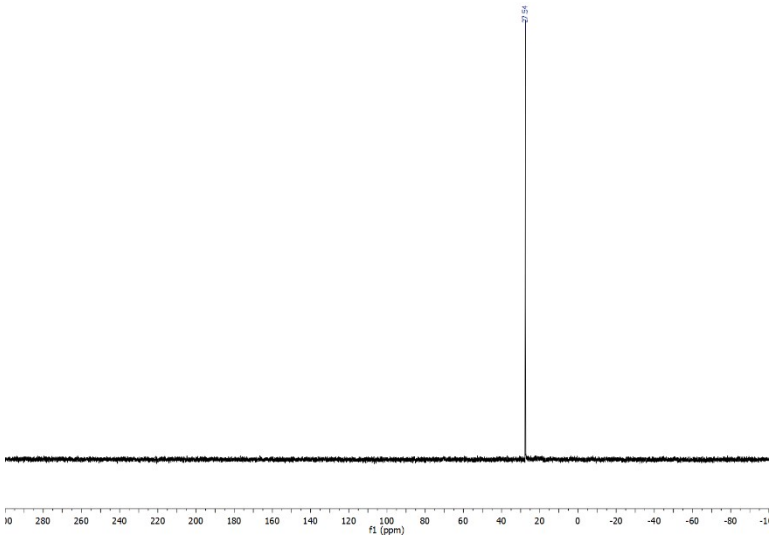

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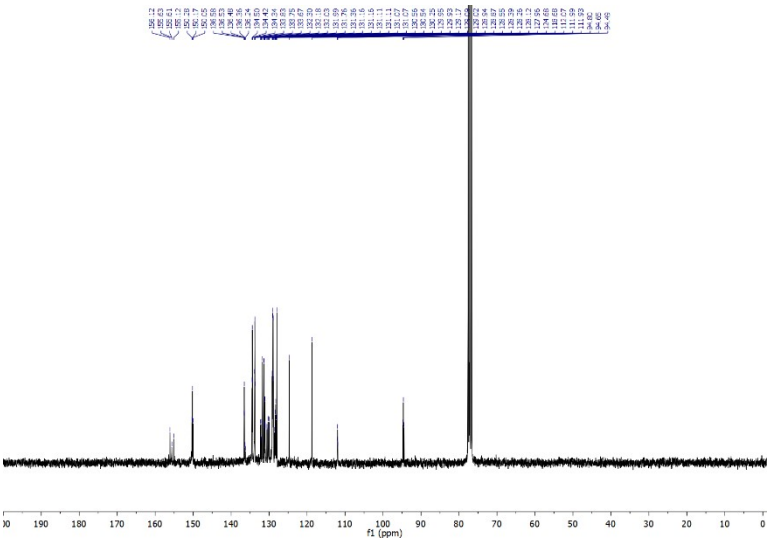

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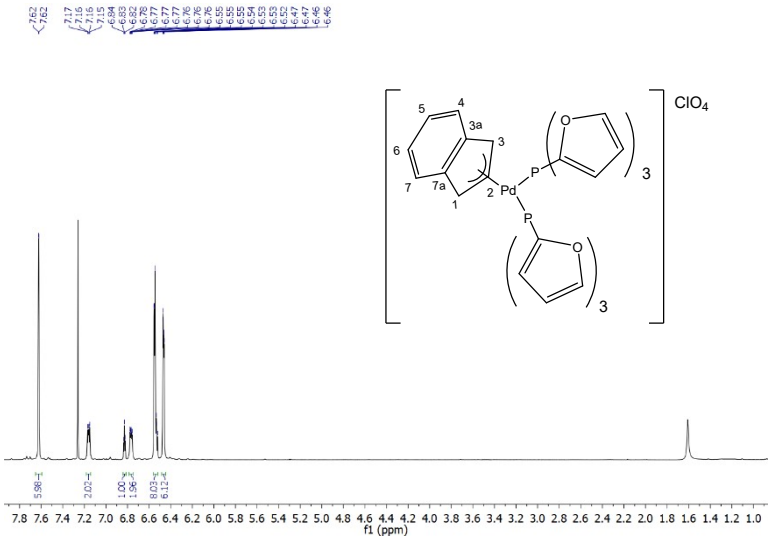

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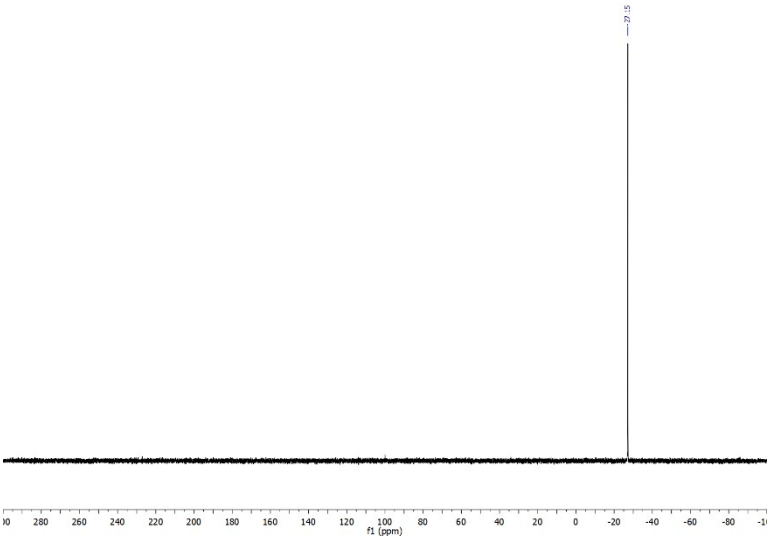

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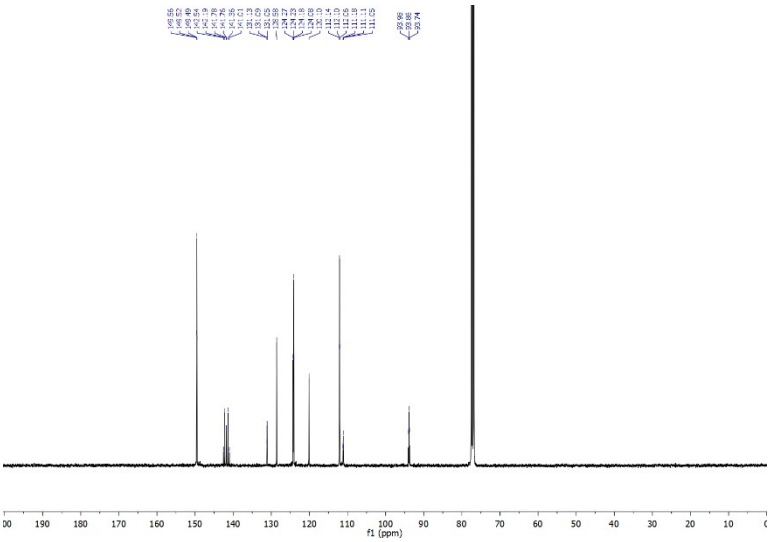

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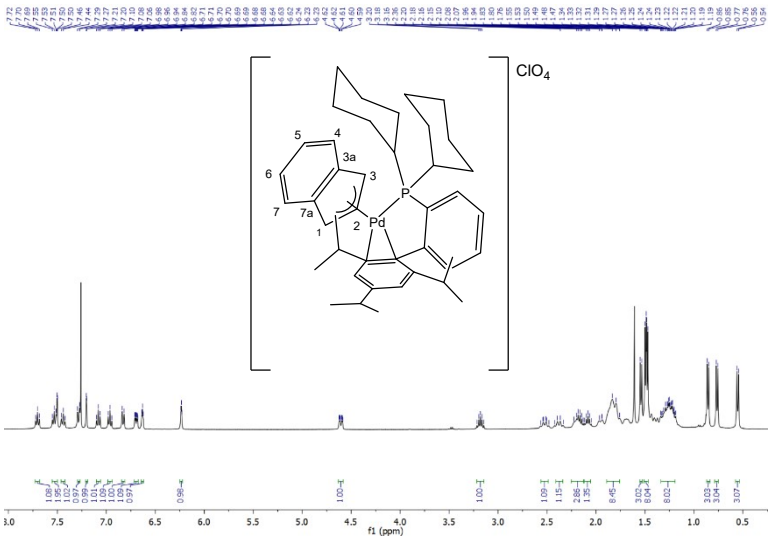
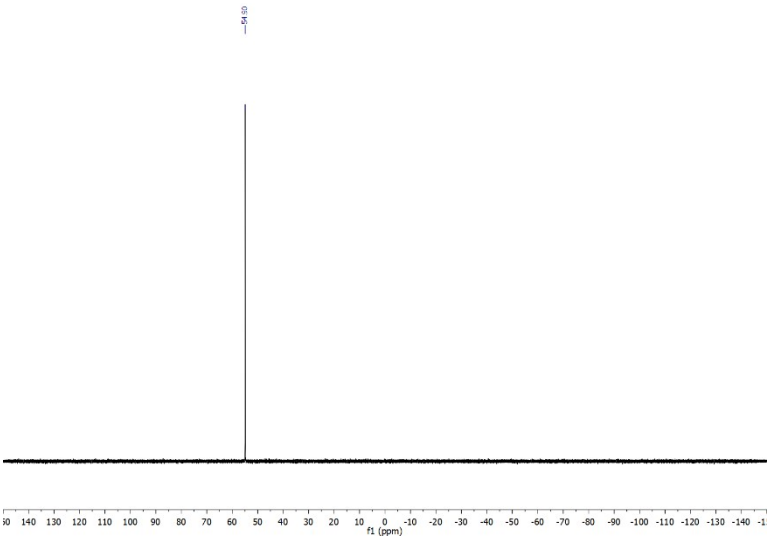


***S** 43. ^1H NMR spectra of **3h** in $CDCl_3$ at 298K*



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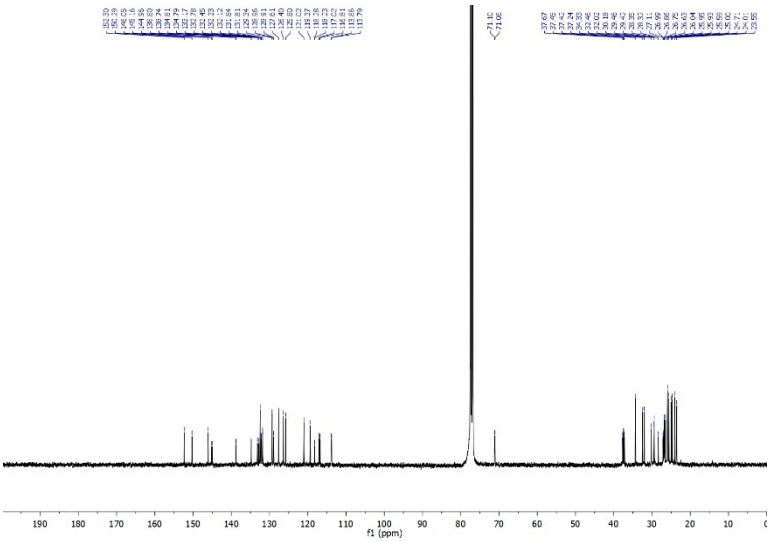
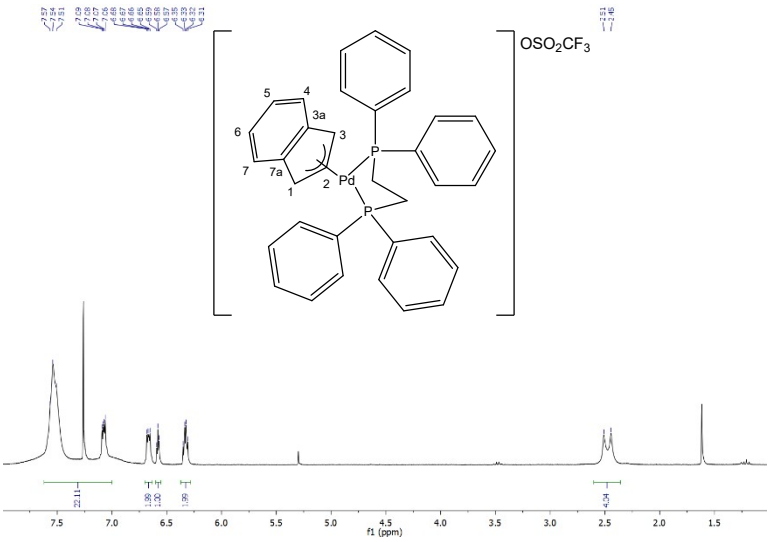
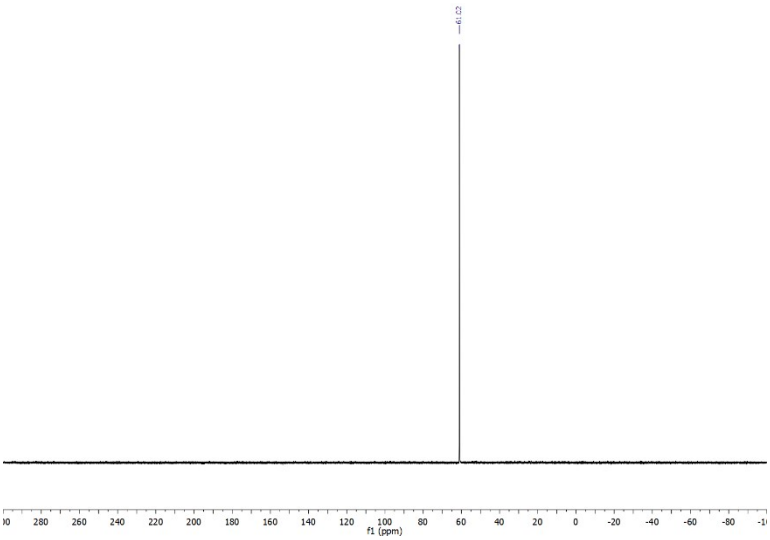


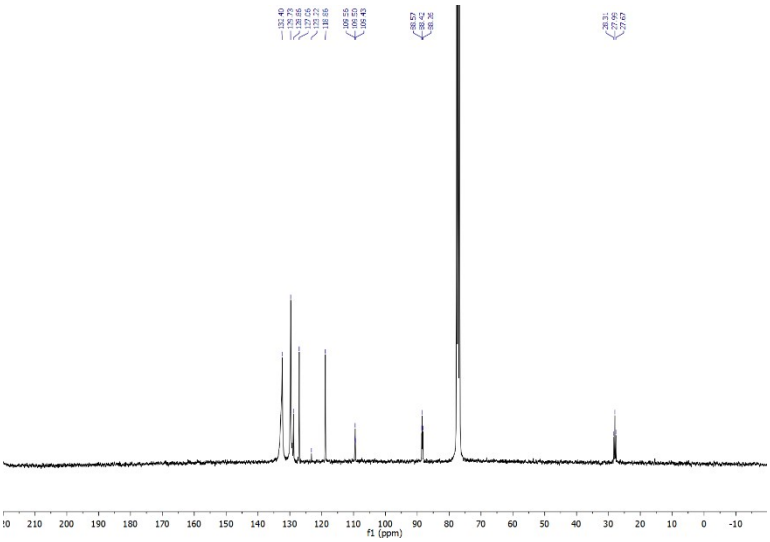
***S** 45. $^{13}C\{^1H\}$ NMR spectra of **3h** in $CDCl_3$ at 298K*



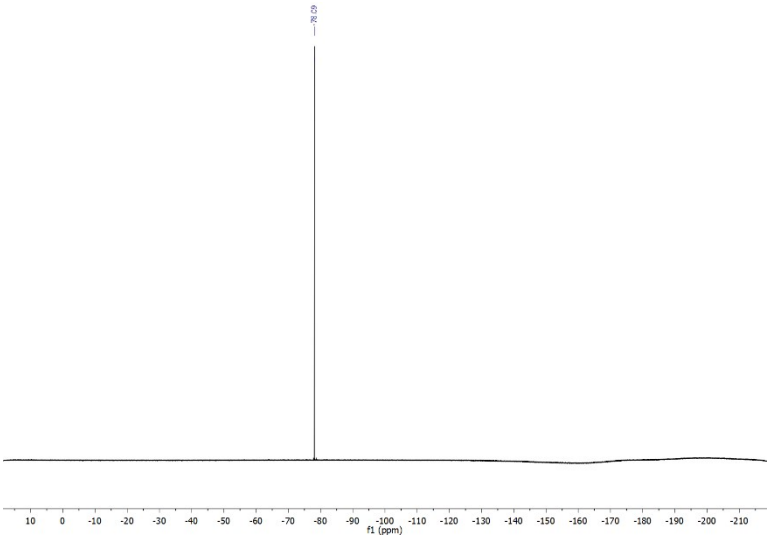
***S** 46. ^1H NMR spectra of **4** in $CDCl_3$ at 298K*



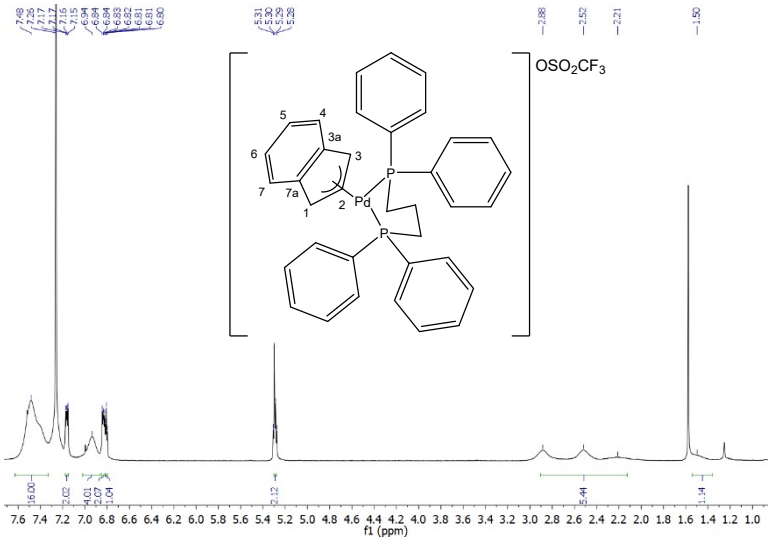
***S** 47. $^{31}P\{^1H\}$ NMR spectra of **4** in $CDCl_3$ at 298K*



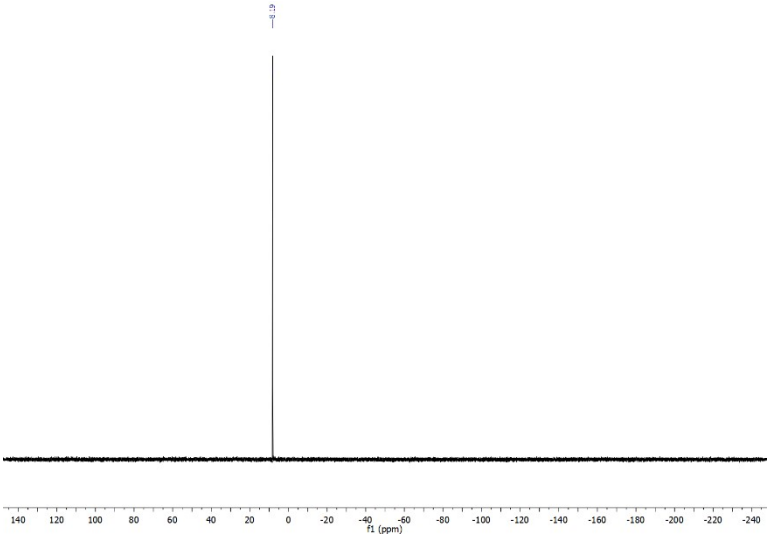
***S** 48. $^{13}C\{^{1}H\}$ NMR spectra of **4** in $CDCl_3$ at 298K*



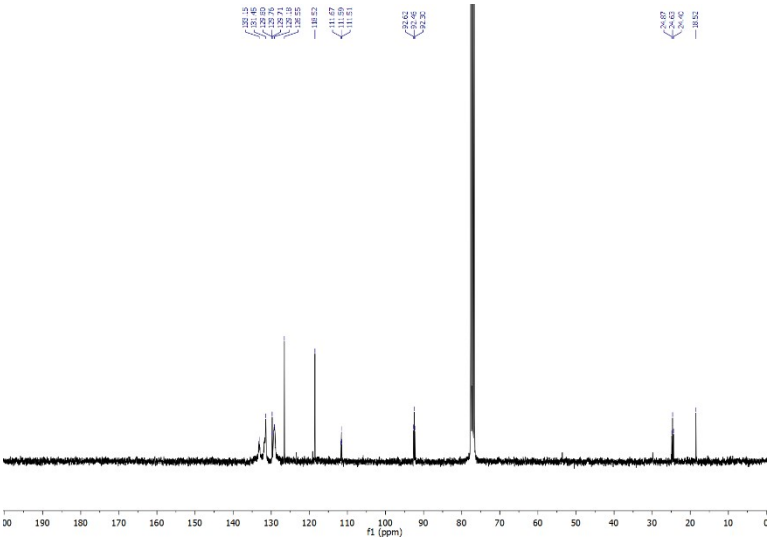
***S** 49. $^{19}F\{^{1}H\}$ NMR spectra of **4** in $CDCl_3$ at 298K*



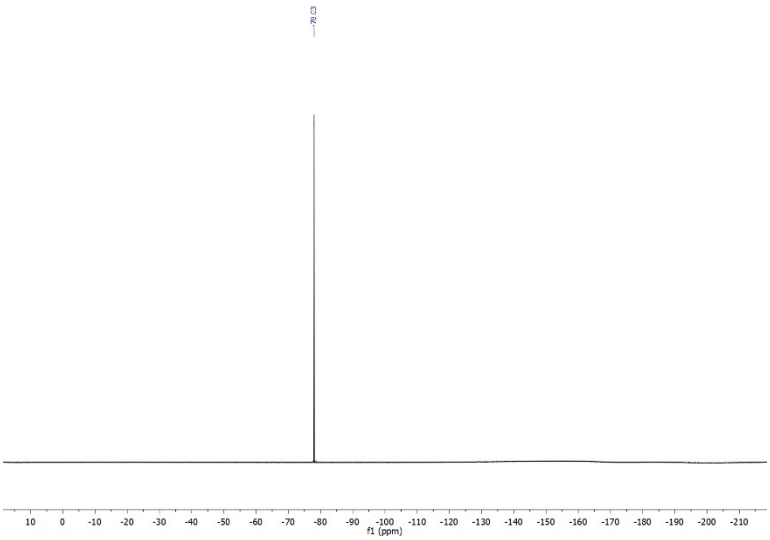
***S** 50. ^{1}H NMR spectra of **5** in $CDCl_3$ at 298K*



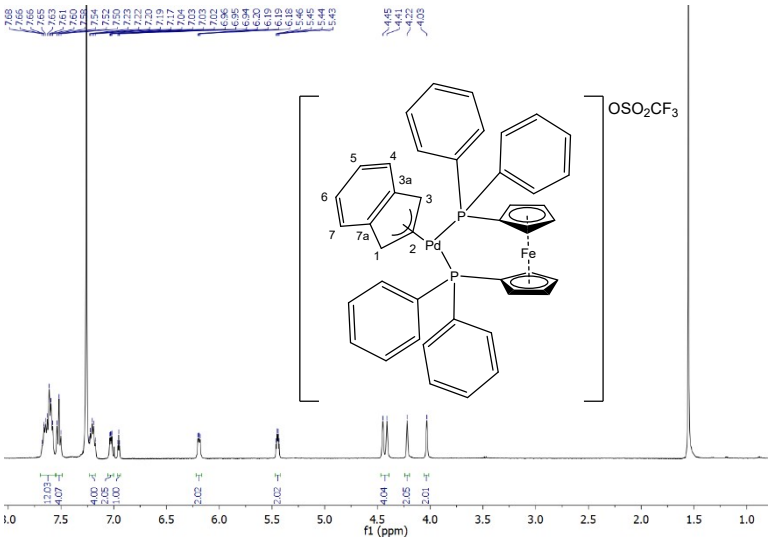
***S** 51. $^{31}P\{^{1}H\}$ NMR spectra of **5** in $CDCl_3$ at 298K*



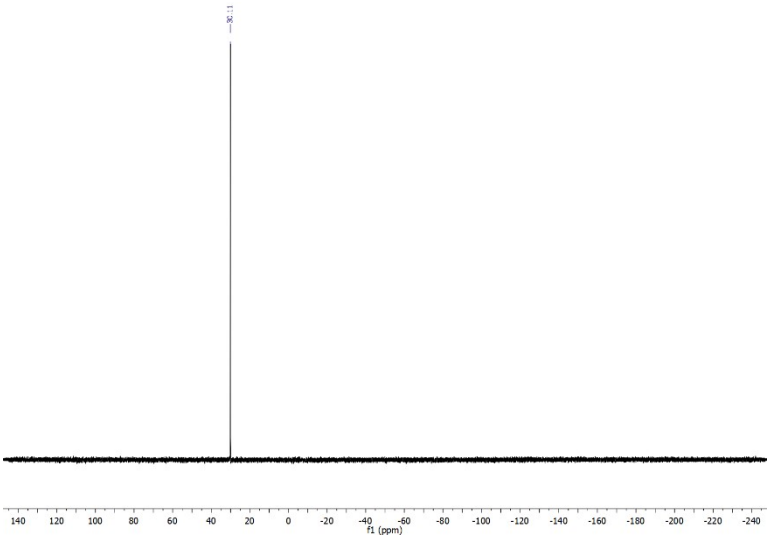
***S** 52. $^{13}C\{^{1}H\}$ NMR spectra of **5** in $CDCl_3$ at 298K*



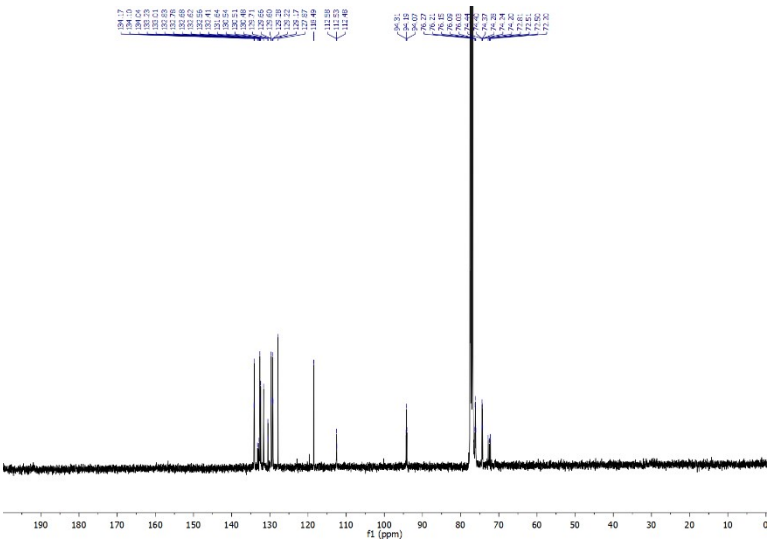
***S** 53. $^{19}F\{^{1}H\}$ NMR spectra of **5** in $CDCl_3$ at 298K*



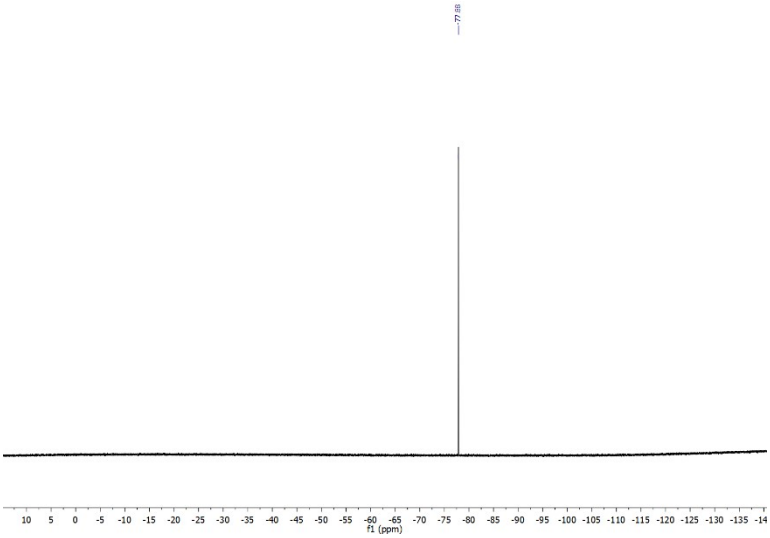
***S** 54. ^{1}H NMR spectra of **6** in $CDCl_3$ at 298K*



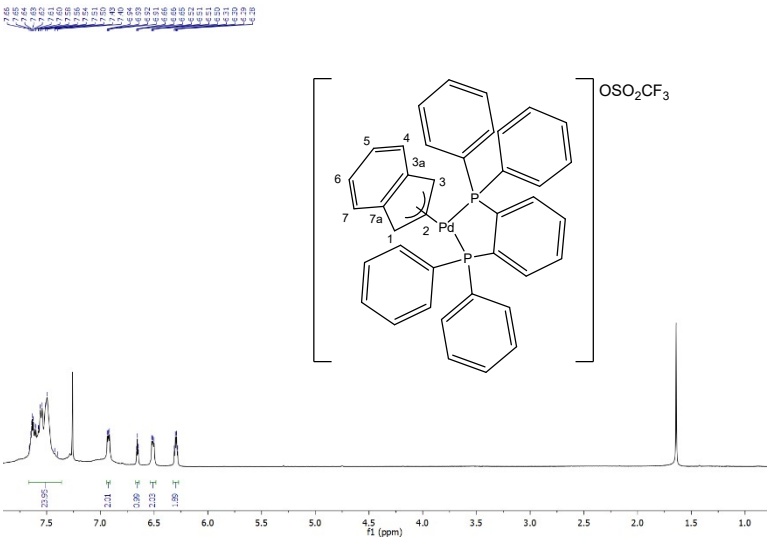
***S** 55. $^{31}P\{^{1}H\}$ NMR spectra of **6** in $CDCl_3$ at 298K*



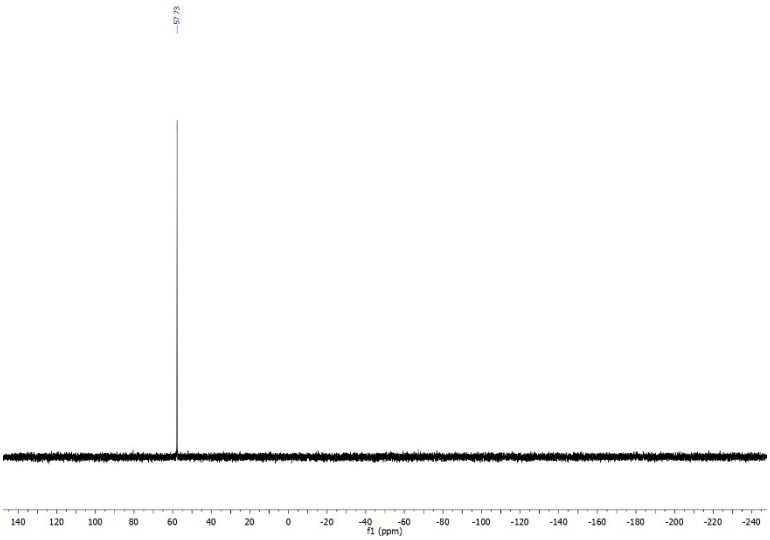
***S** 56. $^{13}C\{^{1}H\}$ NMR spectra of **6** in $CDCl_3$ at 298K*



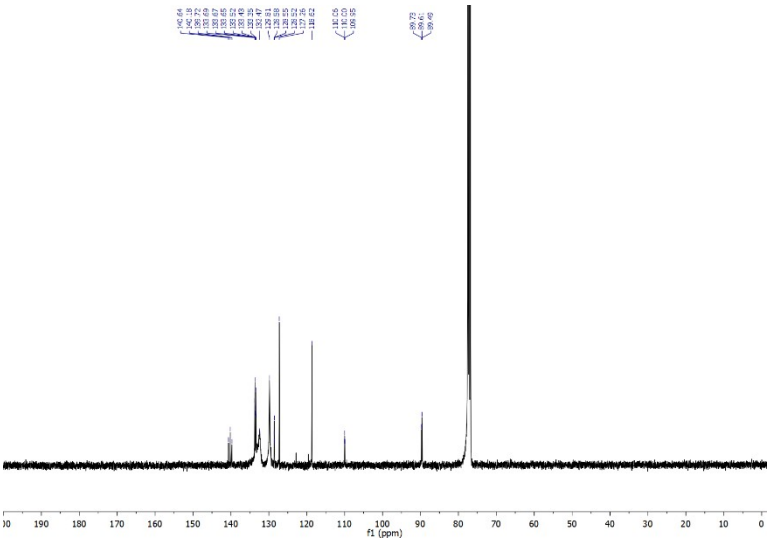
***S** 57. $^{19}F\{^{1}H\}$ NMR spectra of **6** in $CDCl_3$ at 298K*



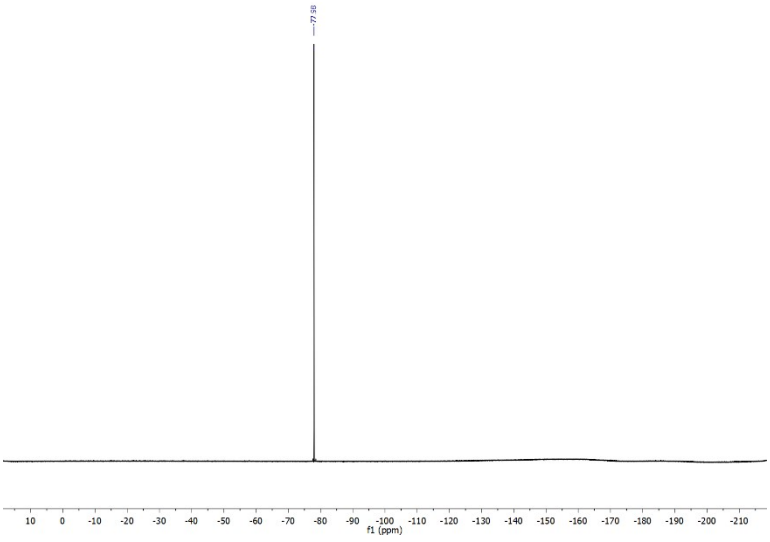
***S** 58. ^{1}H NMR spectra of **7** in $CDCl_3$ at 298K*



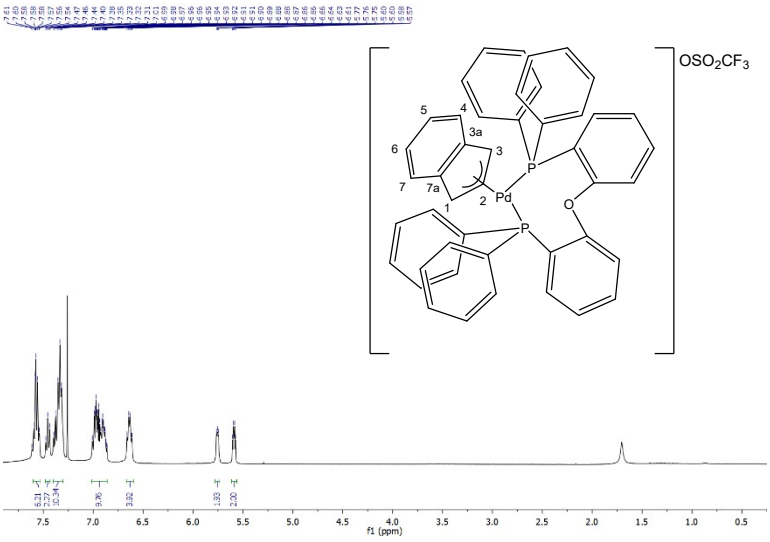
***S** 59. $^{31}P\{^{1}H\}$ NMR spectra of **7** in $CDCl_3$ at 298K*



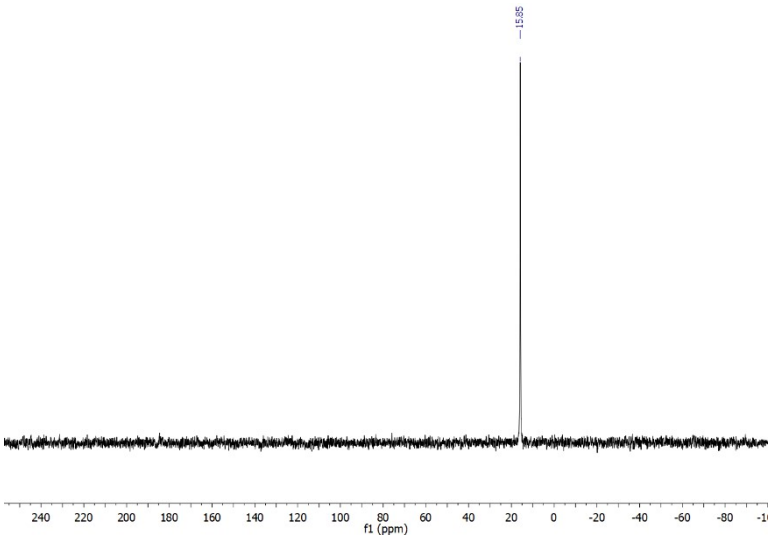
***S** 60. $^{13}C\{^1H\}$ NMR spectra of **7** in $CDCl_3$ at 298K*



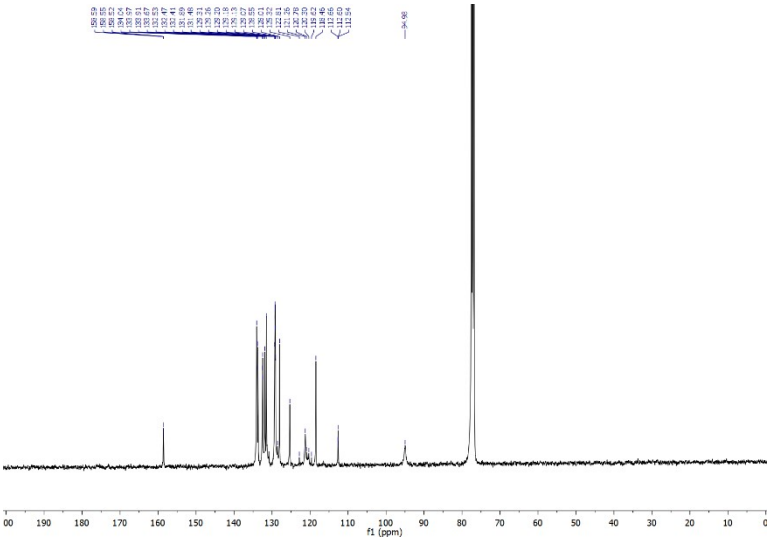
***S** 61. $^{19}F\{^1H\}$ NMR spectra of **7** in $CDCl_3$ at 298K*



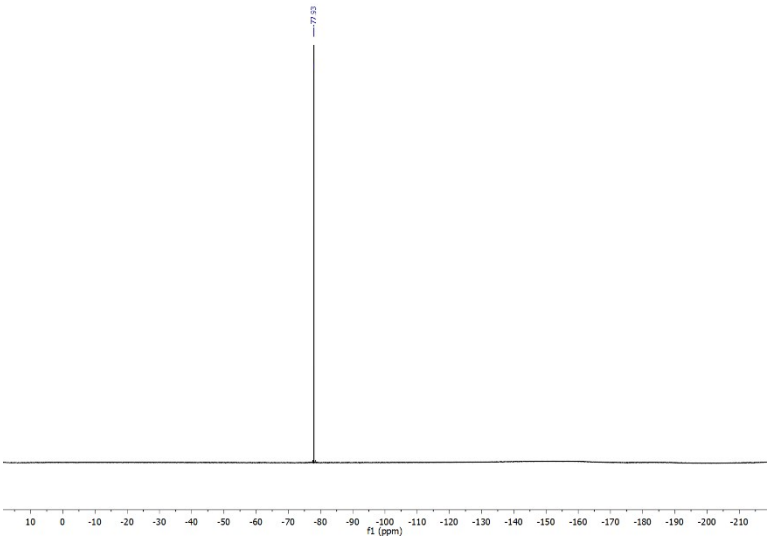
***S** 62. ^1H NMR spectra of **8** in $CDCl_3$ at 298K*



***S** 63. $^{31}P\{^{1}H\}$ NMR spectra of **8** in $CDCl_3$ at 298K*



***S** 64. $^{13}C\{^{1}H\}$ NMR spectra of **8** in $CDCl_3$ at 298K*

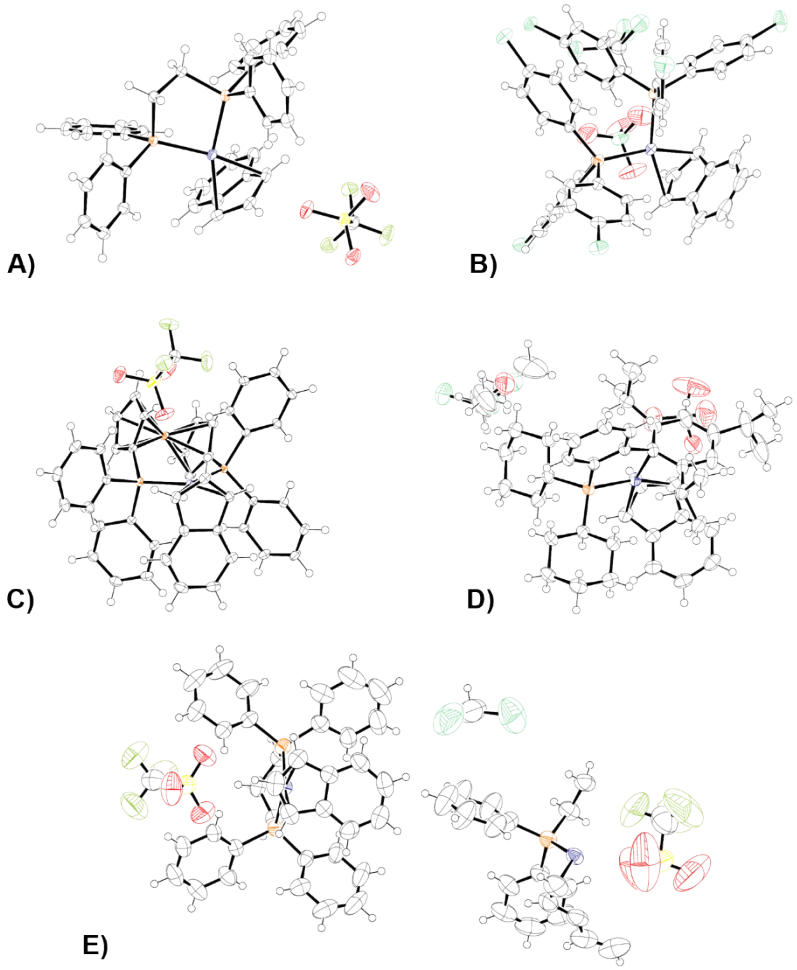


***S** 65. $^{19}F\{^{1}H\}$ NMR spectra of **8** in $CDCl_3$ at 298K*

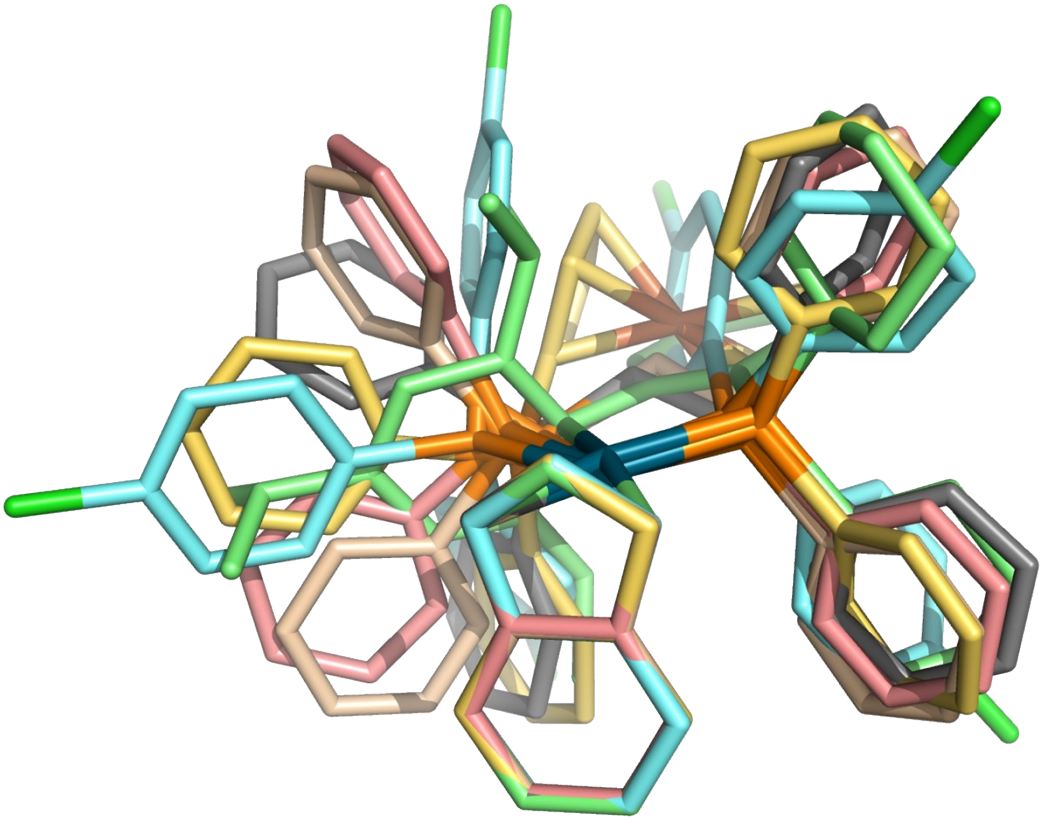
X-ray diffraction analysis - Structural characterization of 4, 5, 6, 3b and 3h

4, **6**, **3b** and **3h** crystalline forms bear one crystallographically independent palladium complex each (Figure **S** 66). Two different molecular entities are present instead in **5** asymmetric unit (ASU): one full Pd complex and an additional half, because one metal centre lies on a crystallographic mirror plane bisecting the indenyl and phosphine ligands. Each complex bear a counterion (triflate or chlorate in **5** and **3h**) that balance the palladium centre net positive charge, with a shortest Pd···O distance of ~4.5 Å. Palladium centres show square planar coordination spheres, in agreement with previously published data (Tables S2-S6). Conformations of **4**, **5**, **6**, **3b** and **3h** are well superimposable with minor phenyl sidechains rearrangements (Figure **S** 67). A clear effect on bite angles of phosphine bidentate ligands has been found: "P-Pd-P" angle increases from 86.73(2)° in **4** to 97.14(3)° **5**, extending the spacer by one methylene unit. Strong geometric constrain imposed by the rigid phenyl linker in **3h** reduces this angle to 84.54(5)°, while a lack of covalent constrain in **3b** rises the value to 100.51(2)° (or 102.17(2)°) in **6**, bearing a ferrocene based spacer). Indenyl ligand is almost perfectly perpendicular to the palladium coordination plane with almost equivalent hinge and fold angles and "slippage" of the ligand (compared to an idealised pentahapto coordination), as measured with HA, FA and ΔM···C parameters respectively[1] (Tables S2-S6).

Crystal packing show hydrophobic contacts among neighbour molecules, involving weak intermolecular π···π and CH···π interactions, among neighbour aromatic rings. Solvent molecules (chloroform or diethylether) have been found in the crystal packing of **3b**, **3h** and **5**. Chloroform molecules are bound to oxygen atoms in anions through polar contacts (with shortest $d_{CH\cdots O}$ equal to 3.237(3) Å in **3b**, 3.21(1) Å in **3h** and 3.14(1) Å in **5**, respectively).



***S** 66. Ortep representations of **4** (A), **3b** (B), **6** (C), **3h** (D) and **5** (E) asymmetric unit contents (ellipsoids dimensions correspond to 50% probability).*



***S** 67. Stick representation of **4**, **3b**, **6**, **3h** and **5** overlapped models, showing the equivalent conformations adopted by the indenyl ligand. Hydrogen atoms omitted for clarity.*

Table S1. Cristallographic data

Compound	**4**	**3b**	**6**	**3h**	**5**
Formula	$[PdC_{35}H_{31}P_2](CF_3SO_3)$	$[PdC_{45}H_{31}Cl_6P_2](ClO_4)$, $CHCl_3$	$[PdC_{43}H_{35}FeP_2](CF_3SO_3)$	$[PdC_{42}H_{56}P](ClO_4)$, $^3/_4(C_4H_{10}O)$, $^1/_4(CHCl_3)$	$[PdC_{33}H_{36}P_2](CF_3SO_3)$, $^1/_3(CHCl_3)$
M/g·mol^{-1}	769.01	1171.55	924.97	883.12	822.82
Space group	***P 2$_1$***	***P 2$_1$/n***	***P 2$_1$/c***	***P -1***	***P nma***
Crystal system	Monoclinic	Monoclinic	Monoclinic	Triclinic	Orthorhombic
a/Å	9.873(2)	11.467(2)	11.678(2)	10.196(2)	19.642(4)
b/Å	13.529(3)	34.352(7)	16.434(3)	11.919(2)	45.952(9)
c/Å	12.606(3)	12.671(3)	20.129(4)	18.601(4)	11.984(2)
α/°	90	90	90	96.61(3)	90
β/°	105.15(3)	106.03(3)	106.35(3)	101.71(3)	90
γ/°	90	90	90	100.32(3)	90
V/Å^3	1625.3(6)	4797.1(18)	3706.9(14)	2150.5(8)	10817(4)
Z	2	4	4	2	12
T/K	100(2)	100(2)	100(2)	100(2)	298(2)
D_c/g·cm^{-3}	1.571	1.622	1.657	1.364	1.516
F(000)	780	2344	1872	928	5008
μ/mm^{-1}	0.539	0.711	0.736	0.426	0.537
Measured Reflections	39534	134146	89232	117819	554682
Unique Reflections	14004	20322	16132	22062	23858
R_{int}	0.0311	0.0152	0.0147	0.0419	0.0104
Obs. Refl.ns [I≥2σ(I)]	13919	17819	15006	18285	20869
θ_{min}- θ_{max}/°	1.46 – 31.10	1.03 – 32.30	1.42 – 31.11	0.99 – 32.28	1.53 – 30.00
hkl ranges	-16,16; -22,22; -20,20	-17,17; -52,52; -19,19	-17,17; -26,26; -31,31	-17,16; -20,20; -31,32	-31,31; -74,73; -18,19
R(F^2) (Obs.Refl.ns)	0.0605	0.0387	0.0258	0.0570	0.0420
wR(F^2) (All Refl.ns)	0.2227	0.1065	0.0726	0.1602	0.1463
No. Variables	415	568	496	533	626
Goodness of fit	1.030	1.025	1.059	1.050	1.031

$\Delta\rho_{max}$; $\Delta\rho_{min}$/e·Å^{-3}	0.50; -0.85	1.39; -1.35	1.10; -1.43	1.63; -1.94	0.93; -1.94
CCDC Deposition N.	2173701	2173702	2173704	2173705	2173703

Table S2. Selected palladium coordination sphere distances and angles (Å and degrees) for **4**

4 (100 K) - $[PdC_{35}H_{31}P_2](CF_3SO_3)$			
Distances	**(Å)**	**Angles**	**(°)**
Pd_1-P1_3	2.270(1)	P1_3-Pd_1-P2_3	86.73(2)
Pd_1-P2_3	2.261(1)	C1_2-Pd_1-C3_2	61.38(7)
Pd_1-C1_2	2.214(2)	P1_3-Pd_1-C3_2	110.48(5)
Pd_1-C3_2	2.283(2)	P2_3-Pd_1-C1_2	101.61(5)
Pd_1-C2_2	2.247(2)		
C=C_Indenyl[a]	1.419(3)	HA[b]	12.31(12)
ΔM···C[b]	0.266(4)	FA[b]	11.76(12)
Pd_1···Anion[c]	4.740(2)	Pd-Indenyl Ave Planes[d]	89.06(3)

[a]Average C1=C2=C3 bond length in indenyl ligand
[b]As defined in Table 1 footnotes of Zargarian Coordination Chemistry Reviews 233-234 (2002) 157-176
[c]Shortest distance between palladium centre and anion
[d]Average angle among the mean metal coordination plane and the mean indenyl plane

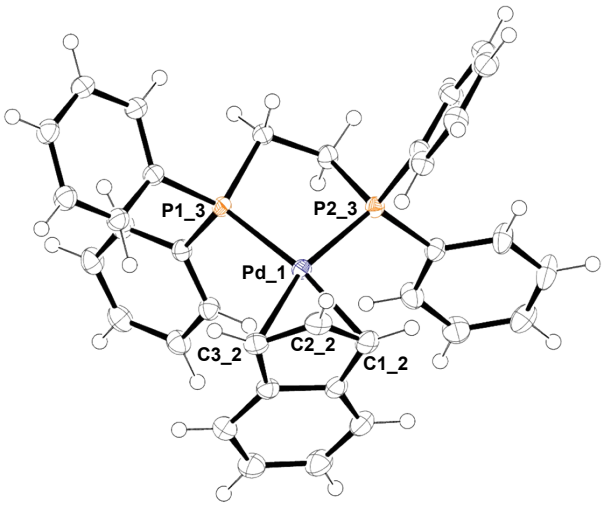


Table S3. Selected palladium coordination sphere distances and angles (Å and degrees) for **3b**

3b (100 K) - $[PdC_{45}H_{31}Cl_6P_2](ClO_4)$			
Distances	**(Å)**	**Angles**	**(°)**
Pd_1-P_3	2.285(1)	P_3-Pd_1-P_4	100.51(2)
Pd_1-P_4	2.313(1)	C1_2-Pd_1-C3_2	61.05(7)
Pd_1-C1_2	2.284(2)	P_3-Pd_1-C3_2	96.51(6)
Pd_1-C3_2	2.200(2)	P_4-Pd_1-C1_2	101.89(5)
Pd_1-C2_2	2.241(2)		
Intra π_3···π_4[a]	3.466(1)		
C=C_Indenyl[b]	1.415(3)	HA[c]	13.24(16)
ΔM···C[c]	0.298(4)	FA[c]	11.65(14)
Pd_1···Anion[d]	4.580(3)	Pd-Indenyl Ave Planes[e]	85.90(3)

[a]Intramolecular distance between ring centroids of facing phenyls
[b]Average C1=C2=C3 bond length in indenyl ligand
[c]As defined in Table 1 footnotes of Zargarian Coordination Chemistry Reviews 233-234 (2002) 157-176
[d]Shortest distance between palladium centre and anion
[e]Average angle among the mean metal coordination plane and the mean indenyl plane

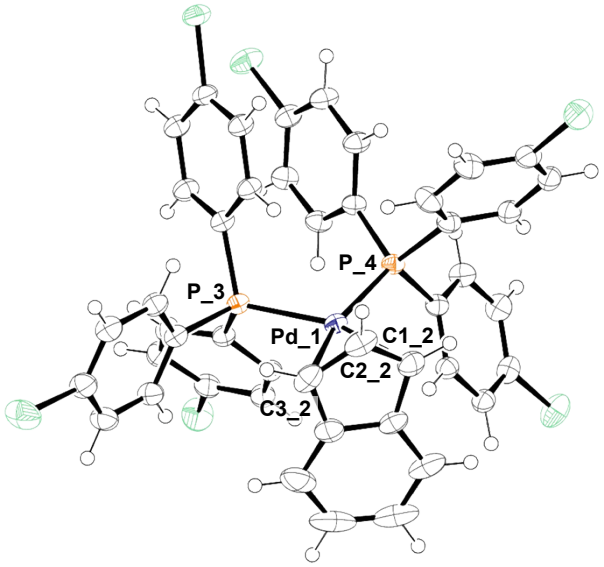


Table S4. Selected palladium coordination sphere distances and angles (Å and degrees) for **6**

6 (100 K) - $[PdC_{43}H_{35}FeP_2](CF_3SO_3)$			
Distances	**(Å)**	**Angles**	**(°)**
Pd_1-P1_3	2.273(1)	P1_3-Pd_1-P2_3	102.17(2)
Pd_1-P2_3	2.274(1)	C1_2-Pd_1-C3_2	61.28(4)
Pd_1-C1_2	2.229(1)	P1_3-Pd_1-C3_2	101.60(3)
Pd_1-C3_2	2.261(4)	P2_3-Pd_1-C1_2	95.57(3)
Pd_1-C2_2	2.243(4)	Pd Ave-Fe P Planes[e]	19.19(1)
Intra π_3···π_3[a]	3.299(1)		
Pd1-Fe	4.253(1)		
C=C_Indenyl[b]	1.418(2)	HA[c]	12.29(6)
ΔM···C[c]	0.278(2)	FA[c]	11.09(6)
Pd_1···Anion[d]	3.894(1)	Pd-Indenyl Ave Planes[f]	88.60(2)

[a]Distance between cyclopentadienyl ring centroids; distance of iron in Fe-cene is 1.650(1) Å
[b]Average C1=C2=C3 bond length in indenyl ligand
[c]As defined in Table 1 footnotes of Zargarian Coordination Chemistry Reviews 233-234 (2002) 157-176
[d]Shortest distance between palladium centre and anion
[e]Average angle among the mean metal coordination plane and the plane containing Fe and P atoms of the phosphine ligand
[f]Average angle among the mean Pd coordination plane and the mean indenyl plane

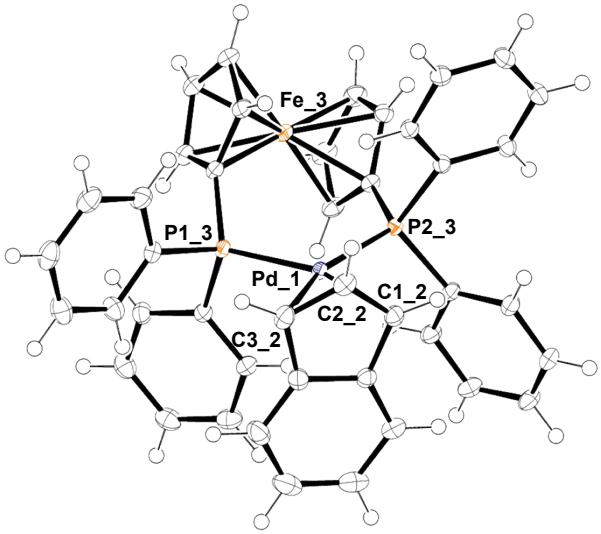


Table S5. Selected palladium coordination sphere distances and angles (Å and degrees) for **3h**

3h (100 K) - $[PdC_{42}H_{56}P](ClO_4)$			
Distances	**(Å)**	**Angles**	**(°)**
Pd_1-P_3	2.266(1)	P_3-Pd_1-C19_3	84.54(5)
Pd_1-C19_3	2.367(2)	C1_2-Pd_1-C3_2	60.62(8)
Pd_1-C1_2	2.172(2)	P_3-Pd_1-C1_2	97.65(6)
Pd_1-C3_2	2.343(2)	C19_3-Pd_1-C3_2	117.10(7)
Pd_1-C20_3	2.490(2)		
Pd_1-C2_2	2.219(2)		
C=C_Indenyl[a]	1.414(3)	HA[b]	15.25(18)
ΔM···C[b]	0.394(4)	FA[b]	15.96(17)
Pd_1···Anion[c]	4.714(4)	Pd-Indenyl Ave Planes[d]	87.60(4)

[a]Average C1=C2=C3 bond length in indenyl ligand
[b]As defined in Table 1 footnotes of Zargarian Coordination Chemistry Reviews 233-234 (2002) 157-176
[c]Shortest distance between palladium centre and anion
[d]Average angle among the mean metal coordination plane and the mean indenyl plane

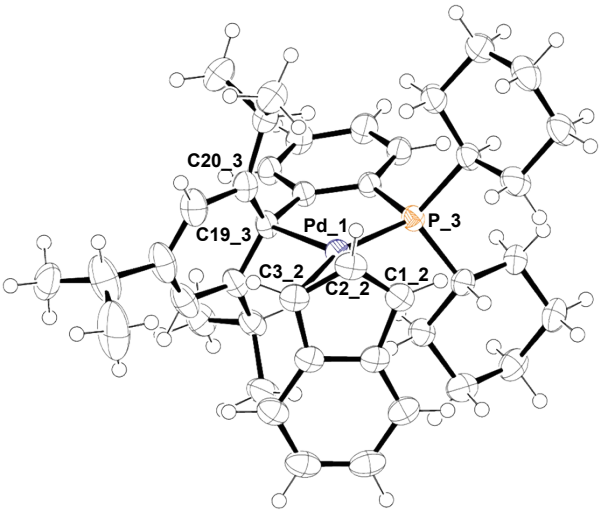
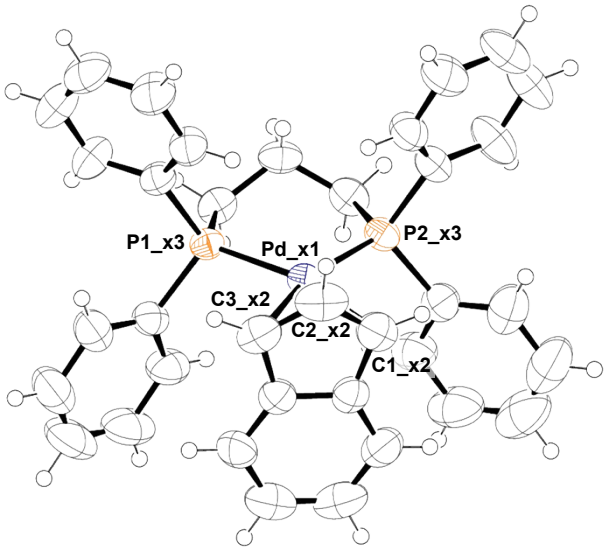


Table S6. Selected palladium coordination spheres distances and angles (Å and degrees) for **5**

5 (298 K) - $[PdC_{33}H_{36}P_2](CF_3SO_3)$							
Molecule 1x				**Molecule 2x**			
Distances	**(Å)**	**Angles**	**(°)**	**Distances**	**(Å)**	**Angles**	**(°)**
Pd_11-P1_13	2.257(1)	P1_13-Pd_11-P2_13	97.60(3)	Pd_21-P1_23	2.272(1)	P1_23-Pd_21- P1_23[e]	96.68(3)
Pd_11-P2_13	2.253(1)	C1_12-Pd_11-C3_12	61.31(8)	Pd_21-P1_23[e]	2.272(1)	C1_22-Pd_21-C1_22[e]	60.97(11)
Pd_11-C1_12	2.241(2)	P1_13-Pd_11-C3_12	101.28(6)	Pd_21-C1_22	2.254(3)	P1_23-Pd_21-C1_22[e]	101.17(8)
Pd_11-C3_12	2.248(2)	P2_13-Pd_11-C1_12	99.86(6)	Pd_21-C1_22[e]	2.254(3)	P1_23[e]-Pd_21-C1_22[e]	101.17(8)
Pd_11-C2_12	2.238(2)			Pd_21-C2_22	2.221(4)		
C=C_Indenyl[a]	1.410(4)	HA[b]	13.08(15)	C=C_Indenyl[a]	1.417(4)	HA[b]	11.84(32)
ΔM···C[b]	0.279(4)	FA[b]	10.86(14)	ΔM···C[b]	0.295(5)	FA[b]	9.47(28)
Pd_1···Anion[c]	4.896(3)	Pd-Indenyl Ave Planes[d]	88.98(3)	Pd_1···Anion[c]	4.675(7)	Pd-Indenyl Ave Planes[d]	88.27(4)

[a]Average C1=C2=C3 bond length in indenyl ligand
[b]As defined in Table 1 footnotes of Zargarian Coordination Chemistry Reviews 233-234 (2002) 157-176
[c]Shortest distance between palladium centre and anion
[d]Average angle among the mean metal coordination plane and the mean indenyl plane
[e]Symmetry generated atom for molecule bisected by crystallographic mirror plane (x, -y+1/2, z)

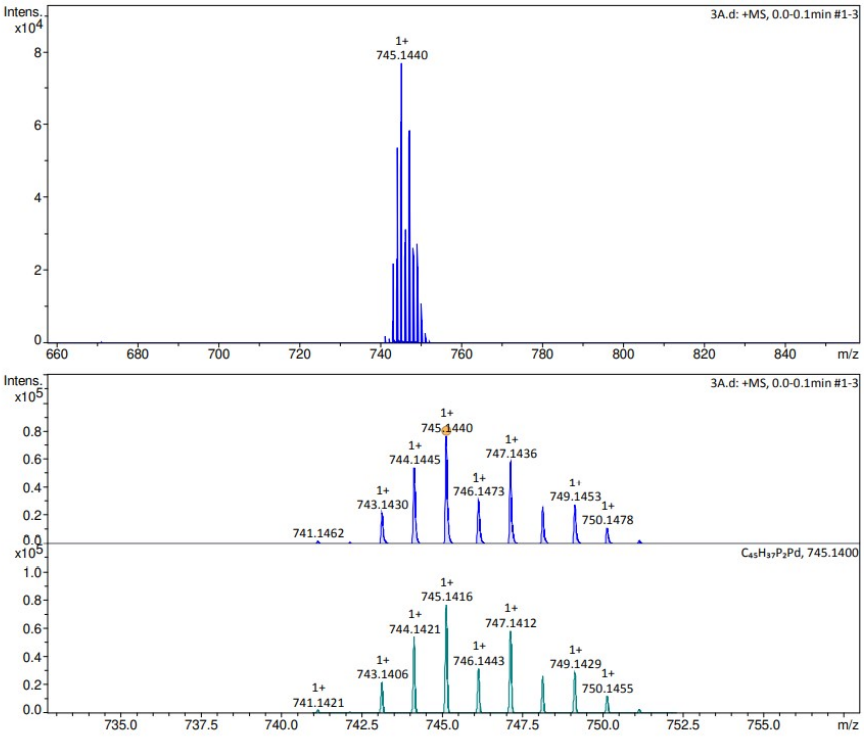


NMR hapticity evaluation

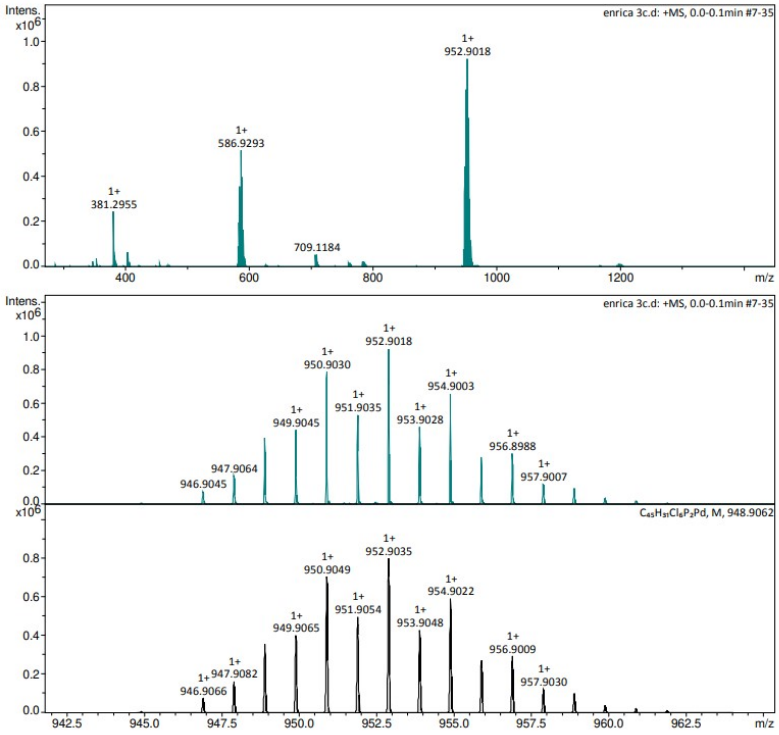
Table S7. C3a and C7a chemical shifts data and **$\Delta\delta^{13}C$** values in agreement with Marder method

Compound	δC3a	δC7a	$\Delta\delta^{13}C$[1]
2a	135.2	136.2	5.0
2b	134.8	135.7	4.5
2c	134.7	135.7	4.5
2d	134.8	135.6	4.5
2e	135.1	136.2	5.0
2f	132.1	134.9	2.8
2g	135.2	136.3	5.1
2h	136.4	137.4	6.2
3a	132.0	132.0	1.3
3b	132.3	132.3	1.6
3c	132.3	132.3	1.6
3e	132.0	132.0	1.3
3f	131.1	131.1	0.4
3g	131.1	131.1	0.4
3h	134.8	138.8	6.1
4	128.9	128.9	-1.8
5	129.8	129.8	-0.9
6	130.5	130.5	-0.2
7	128.6	128.6	-2.1
8	131.5	131.5	0.8

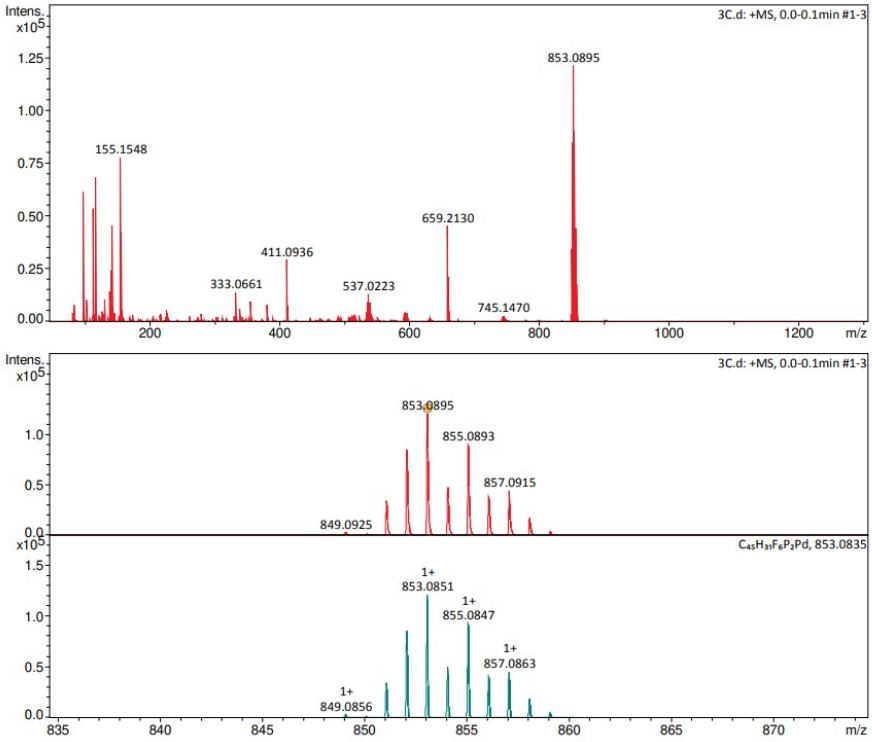
HRMS data



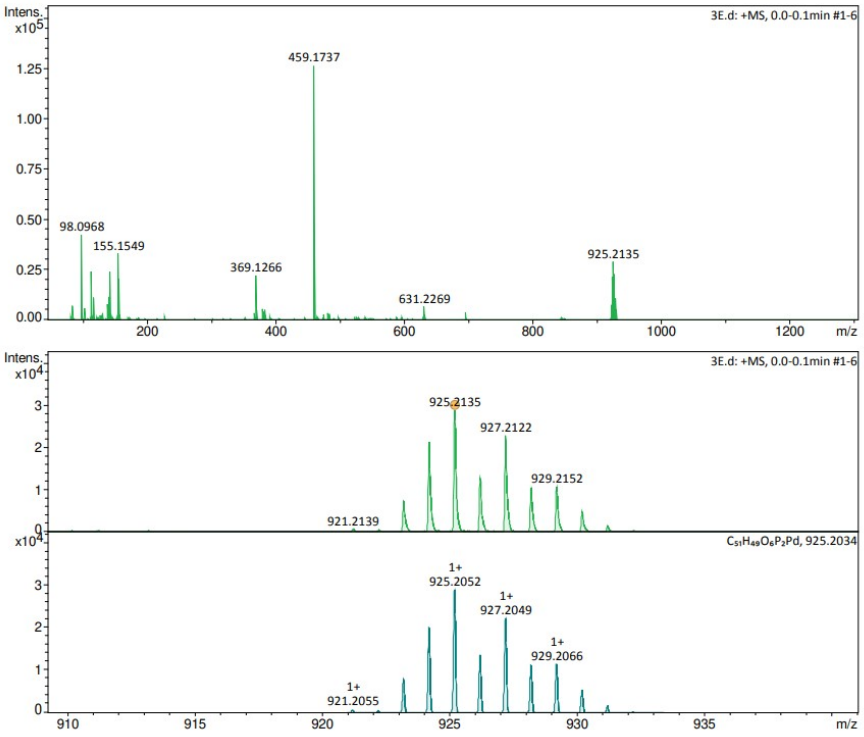
*S 68. HRMS spectra of complex **3a***



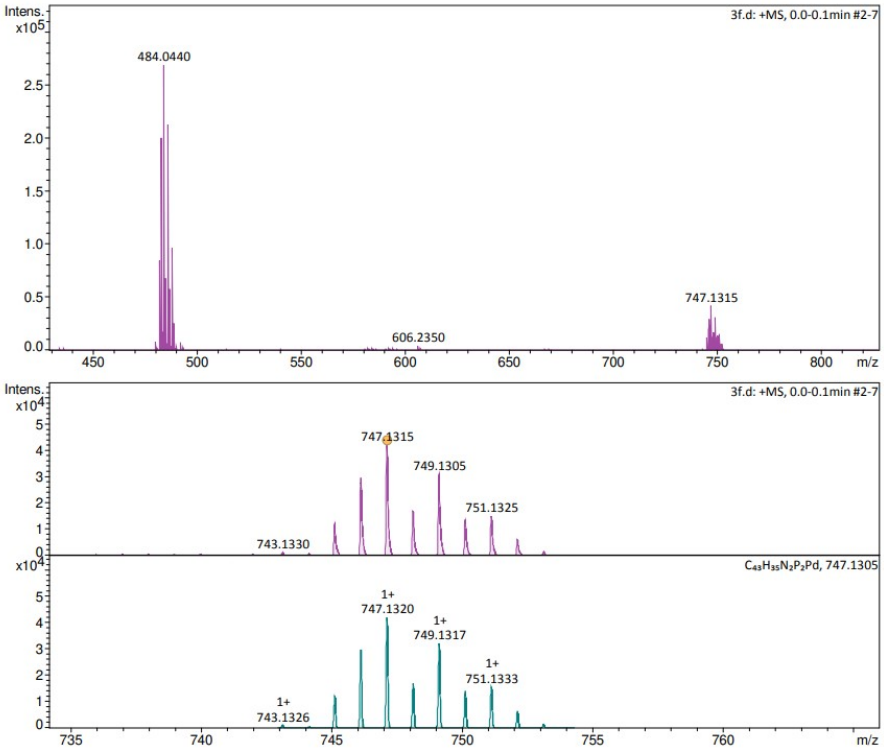
*S 69. HRMS spectra of complex **3b***



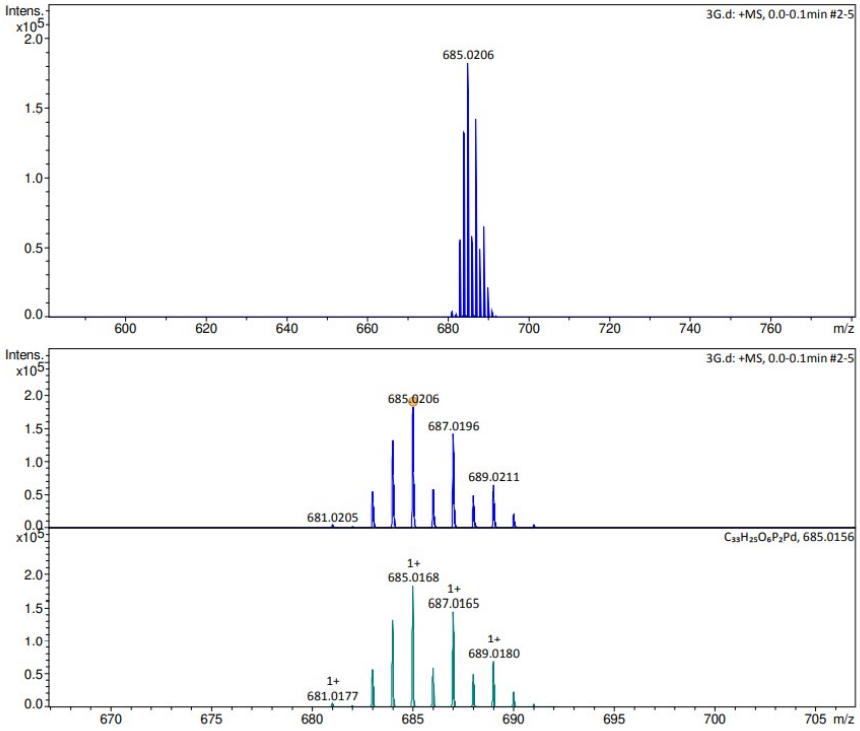
*S 70. HRMS spectra of complex **3c***



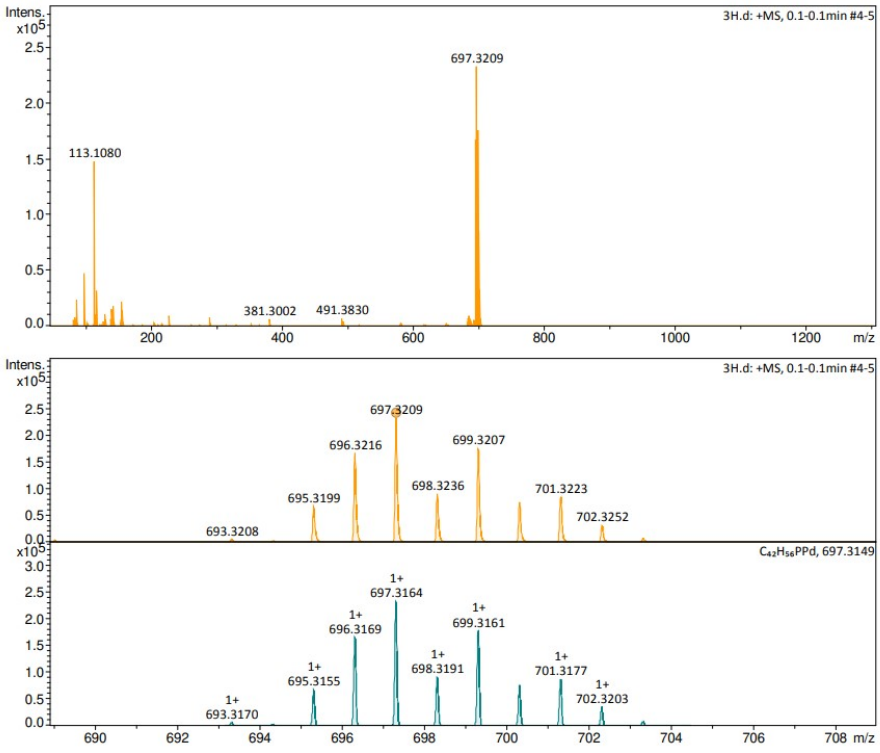
*S 71. HRMS spectra of complex **3e***



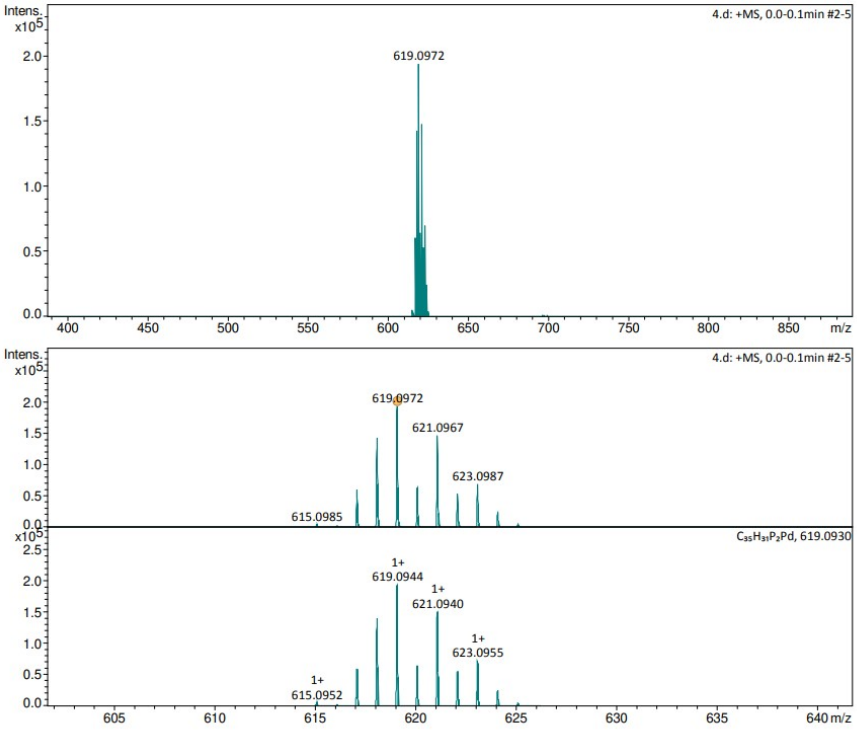
*S 72. HRMS spectra of complex **3f***



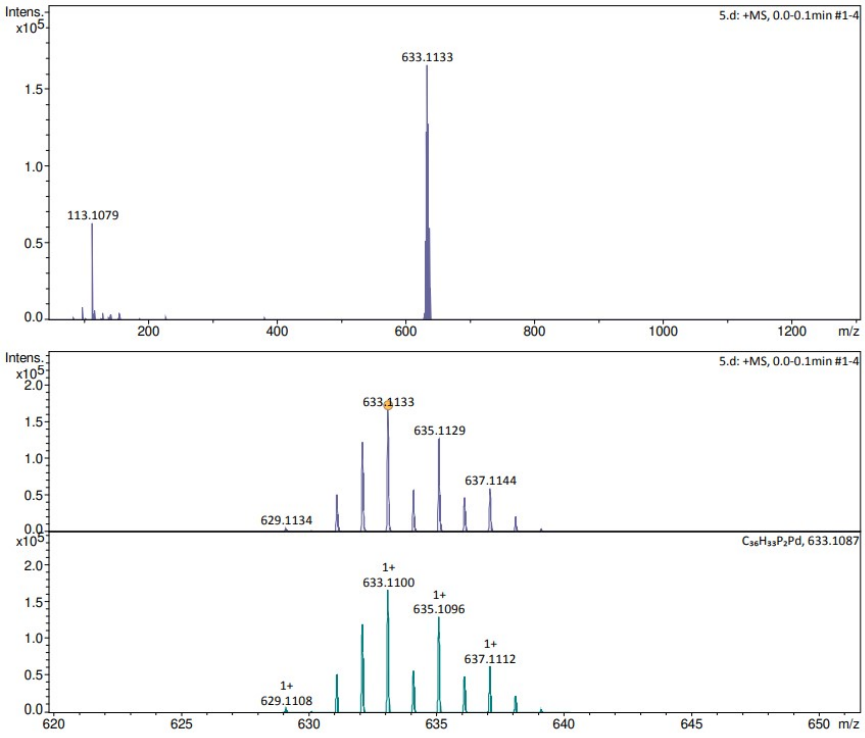
*S 73. HRMS spectra of complex **3g***



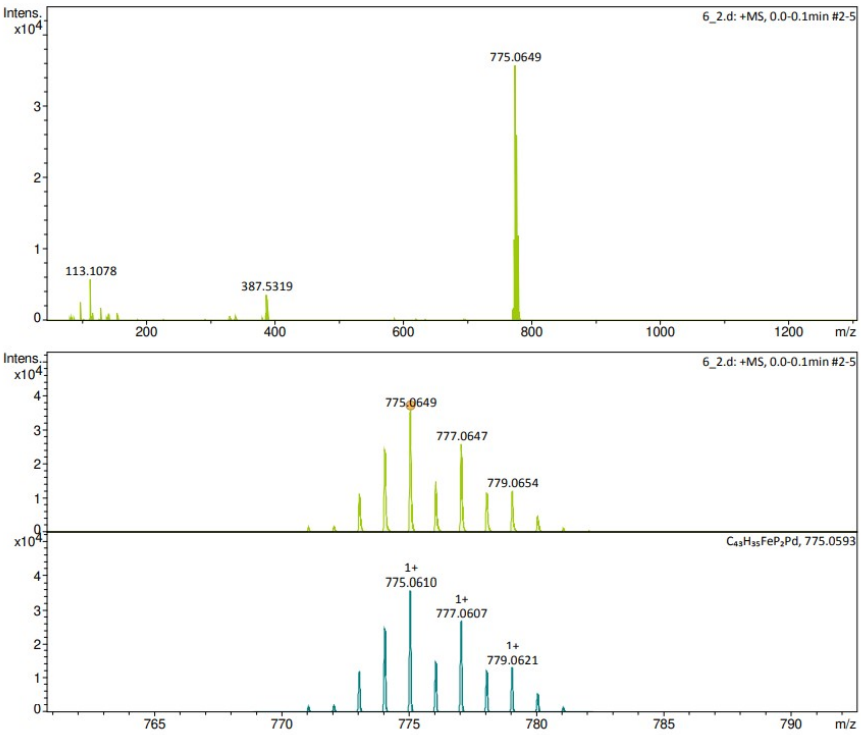
*S 74. HRMS spectra of complex **3h***



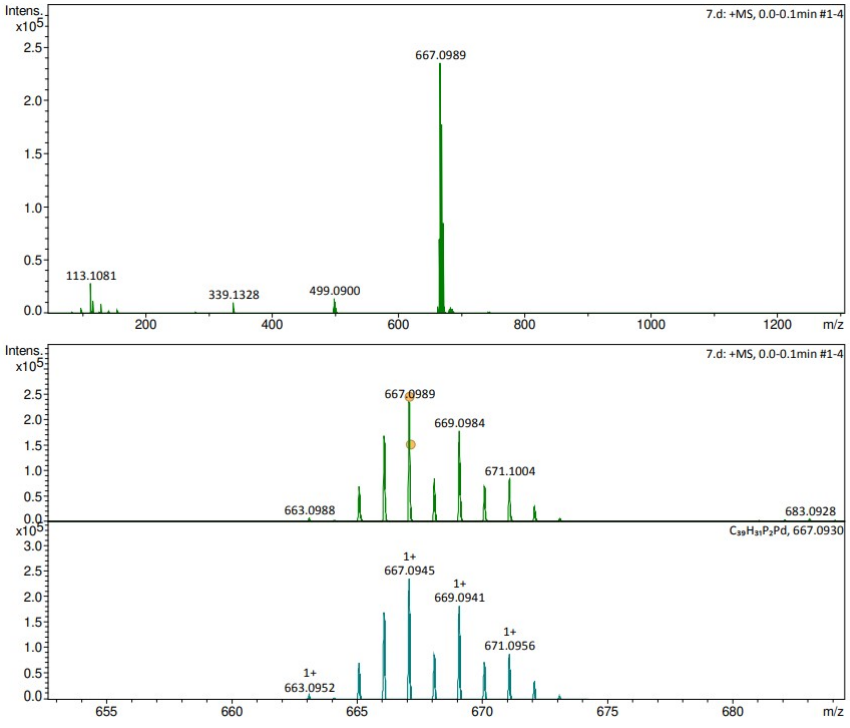
*S 75. HRMS spectra of complex **4***



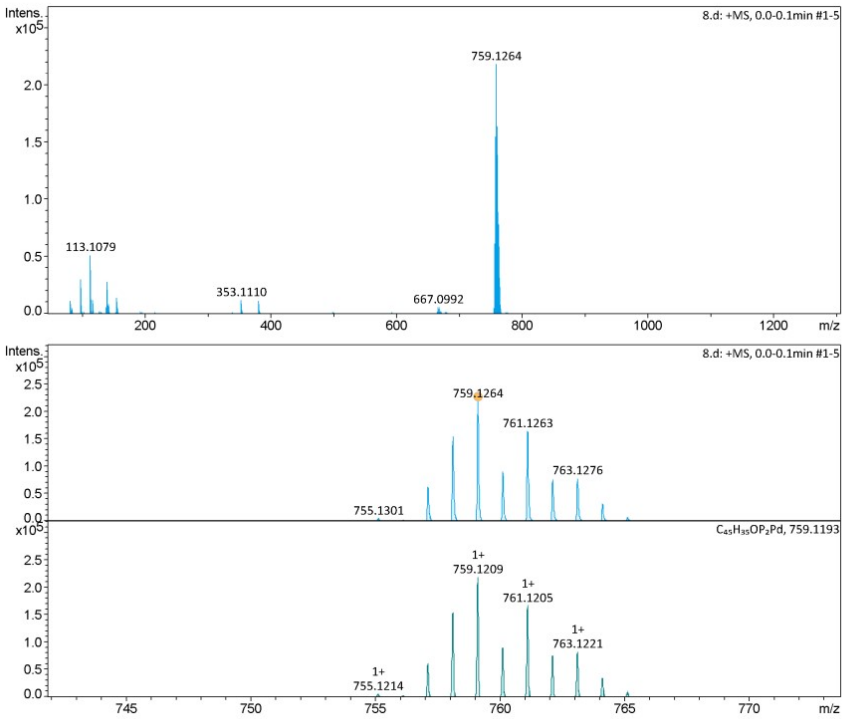
*S 76. HRMS spectra of complex **5***



*S 77. HRMS spectra of complex **6***



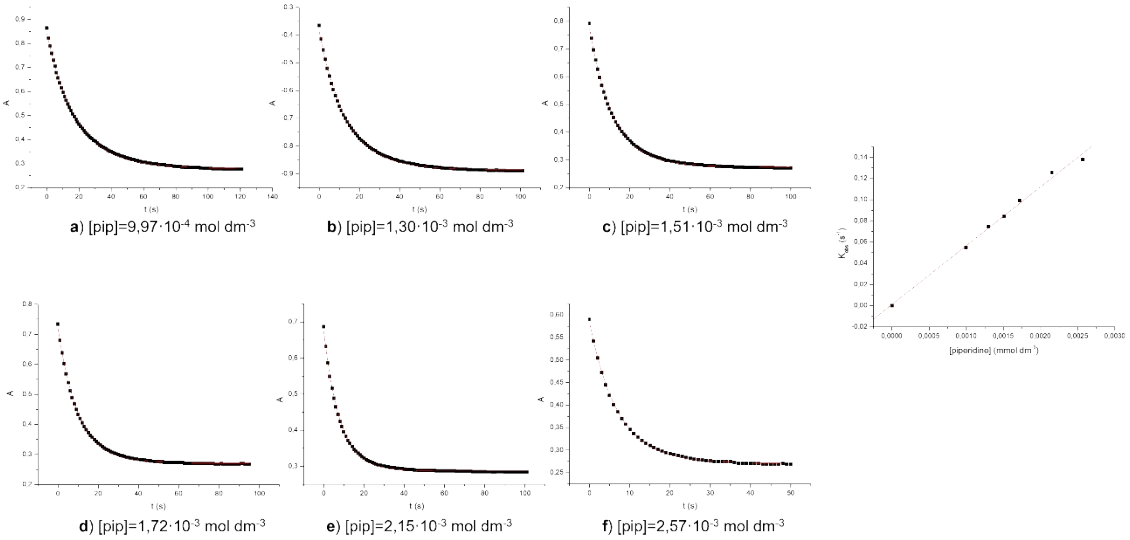
*S 78. HRMS spectra of complex **7***



*S 79. HRMS spectra of complex **8***

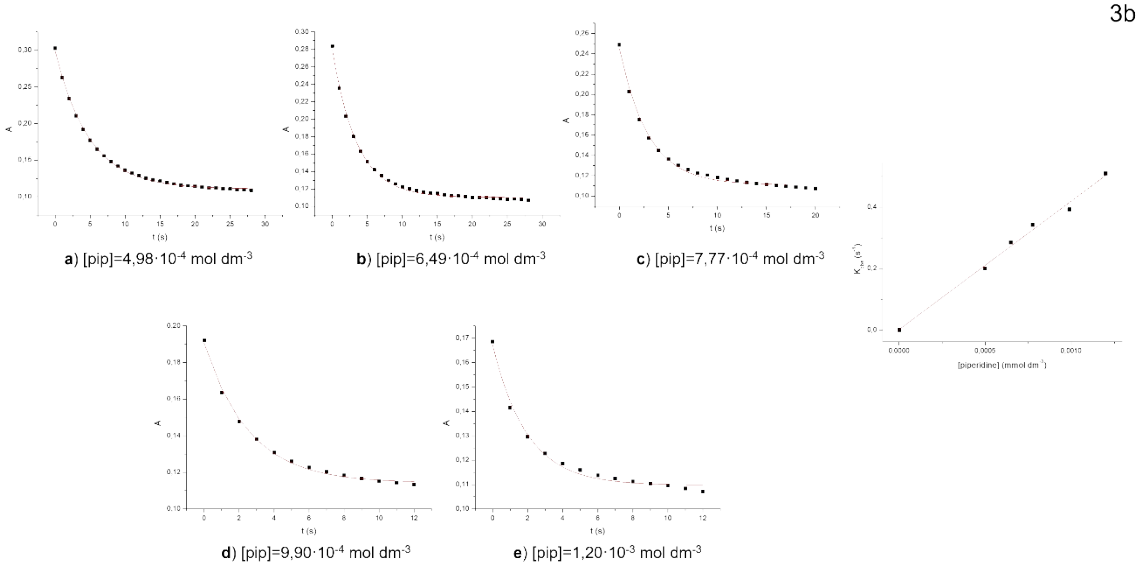
UV-Vis kinetic data

3a



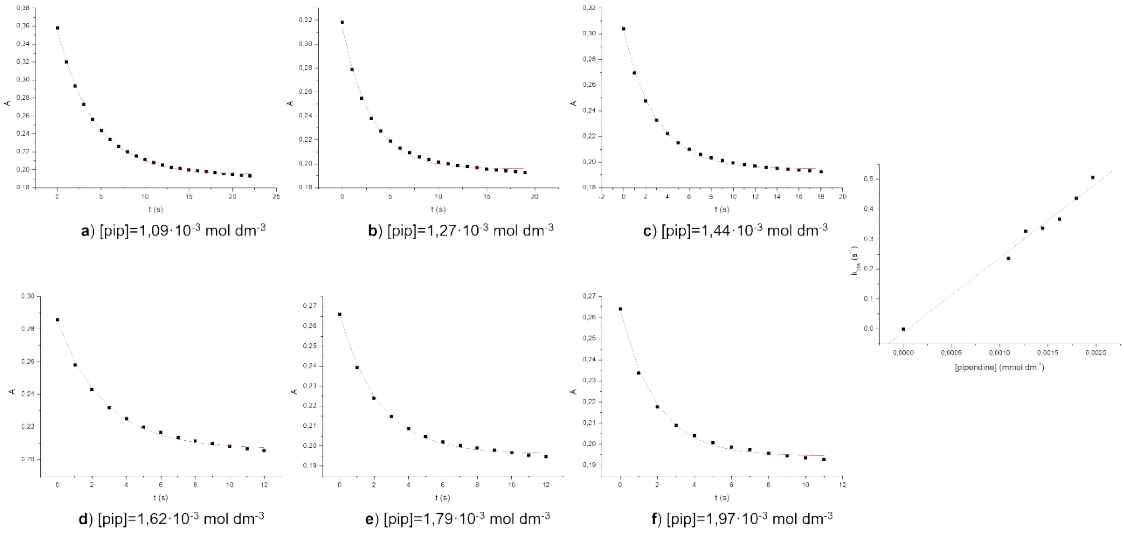
*S 80. UV-Vis Kinetic study of complex **3a***

3b



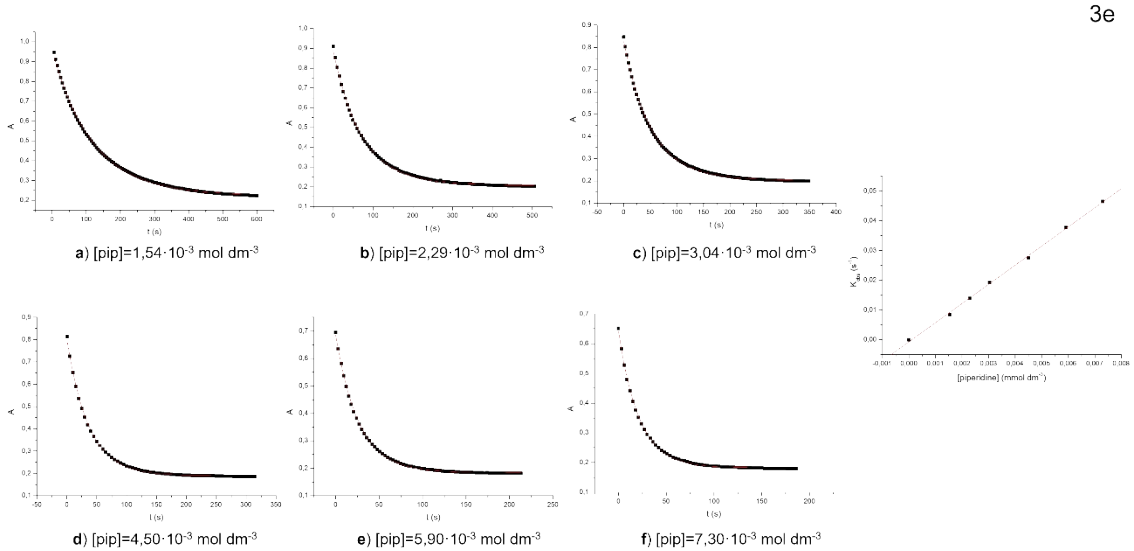
*S 81. UV-Vis Kinetic study of complex **3b***

3c



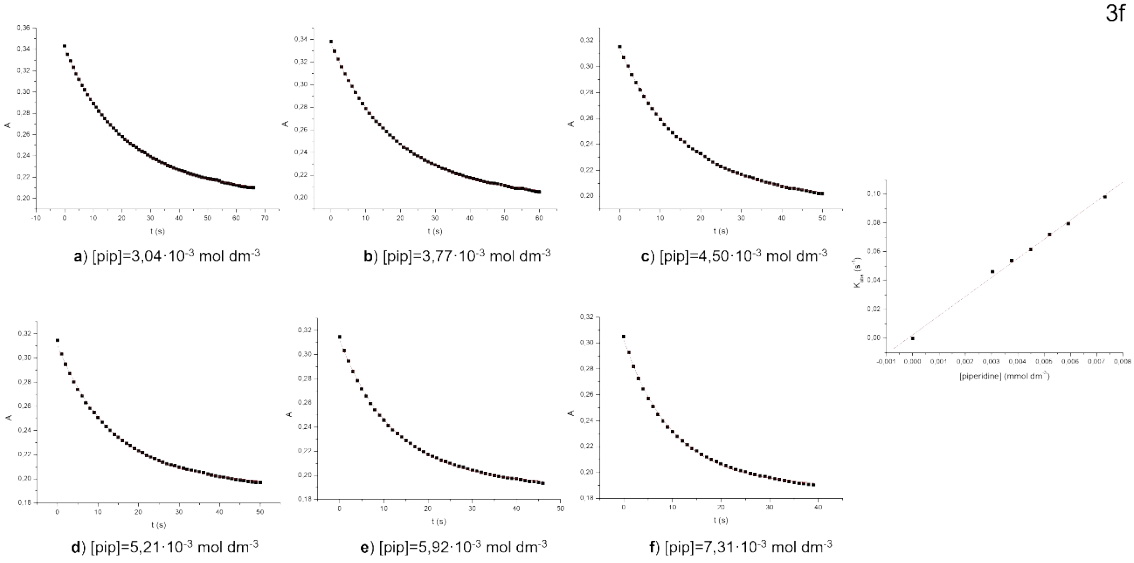
*S 82. UV-Vis Kinetic study of complex **3c***

3e



*S 83. UV-Vis Kinetic study of complex **3e***

3f

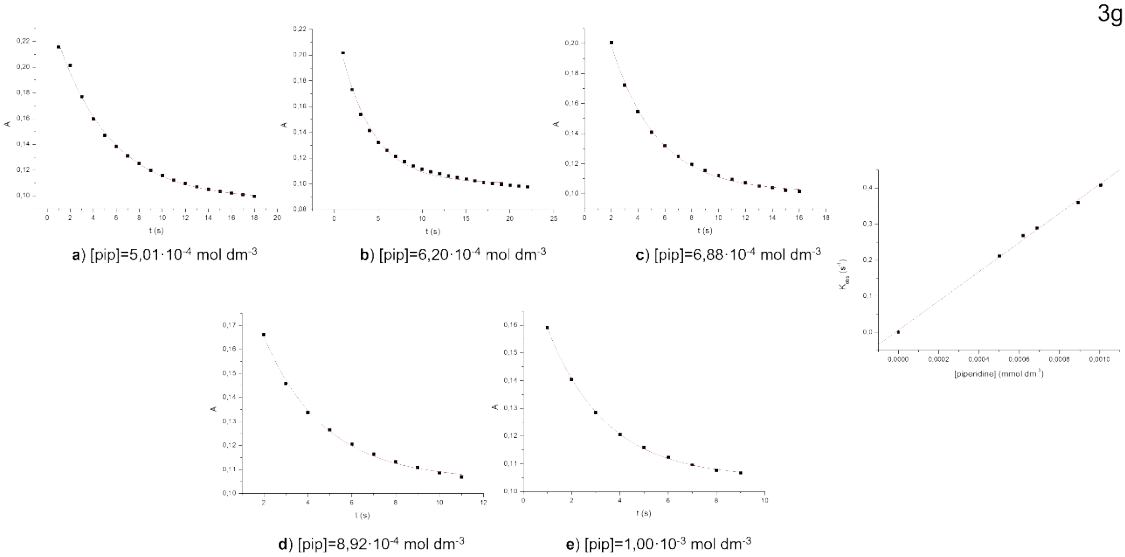


a) [pip]=3,04·10^{-3} mol dm^{-3} **b**) [pip]=3,77·10^{-3} mol dm^{-3} **c**) [pip]=4,50·10^{-3} mol dm^{-3}

d) [pip]=5,21·10^{-3} mol dm^{-3} **e**) [pip]=5,92·10^{-3} mol dm^{-3} **f**) [pip]=7,31·10^{-3} mol dm^{-3}

*S 84. UV-Vis Kinetic study of complex **3f***

3g

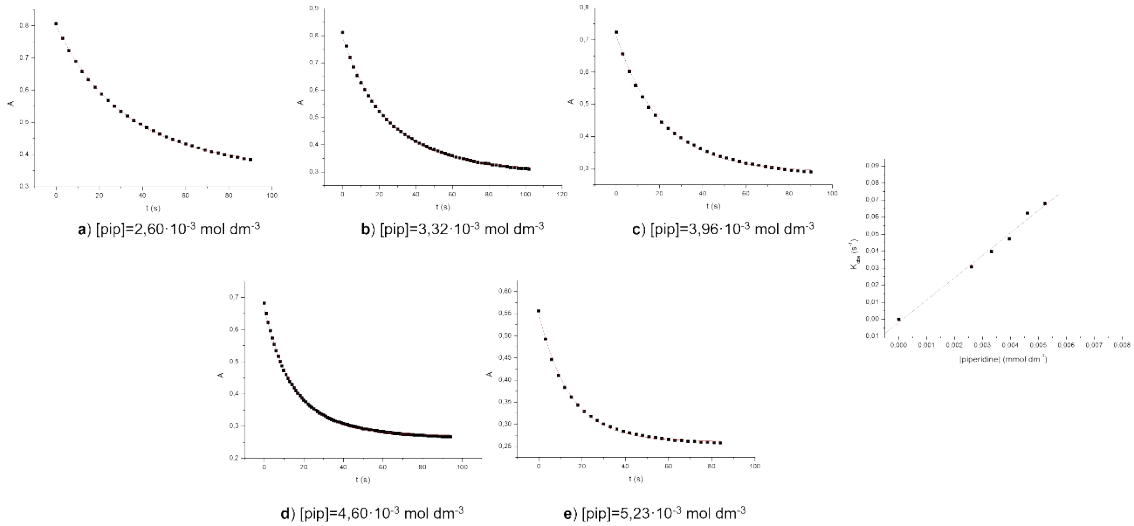


a) [pip]=5,01·10^{-4} mol dm^{-3} **b**) [pip]=6,20·10^{-4} mol dm^{-3} **c**) [pip]=6,88·10^{-4} mol dm^{-3}

d) [pip]=8,92·10^{-4} mol dm^{-3} **e**) [pip]=1,00·10^{-3} mol dm^{-3}

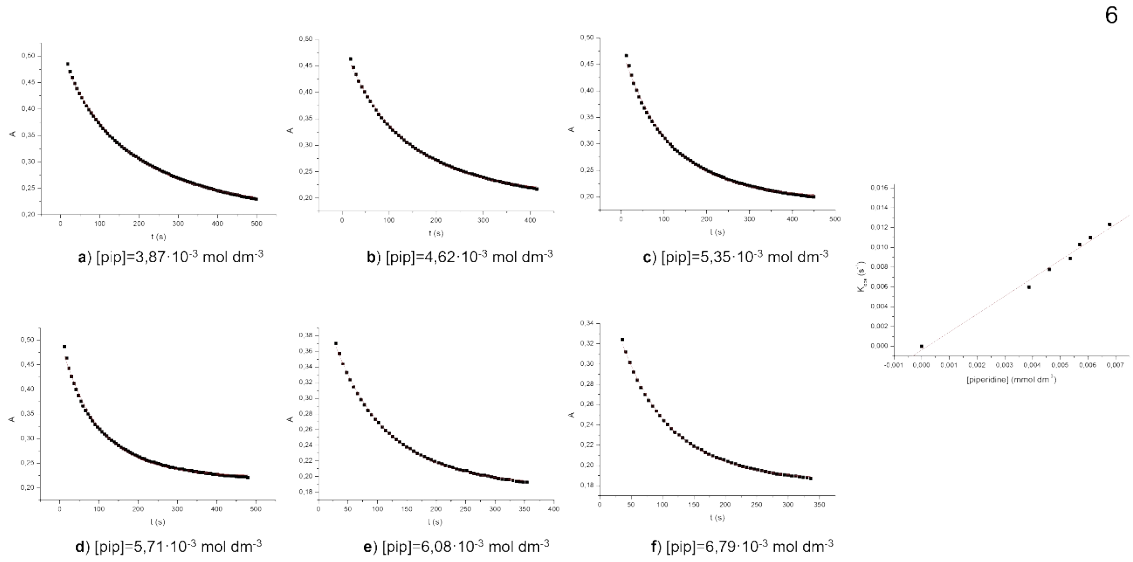
*S 85. UV-Vis Kinetic study of complex **3g***

3h



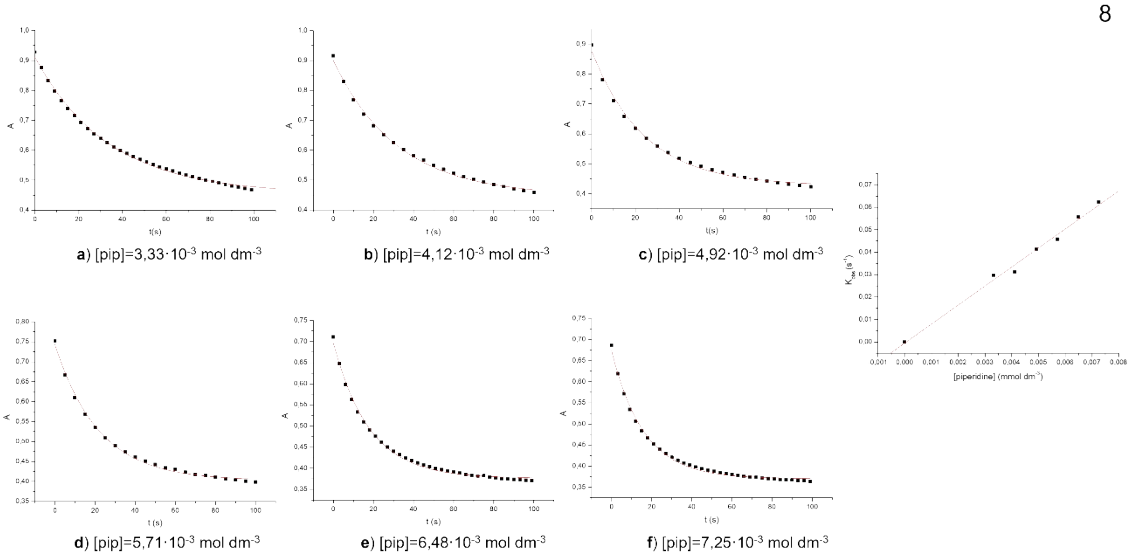
*S 86. UV-Vis Kinetic study of complex **3h***

6



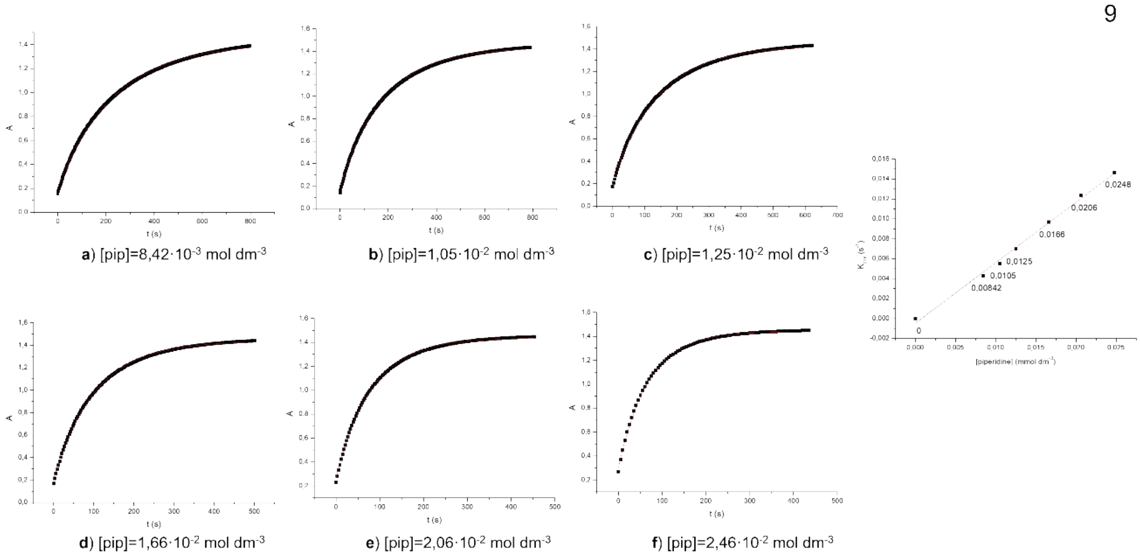
*S 87. UV-Vis Kinetic study of complex **6***

8

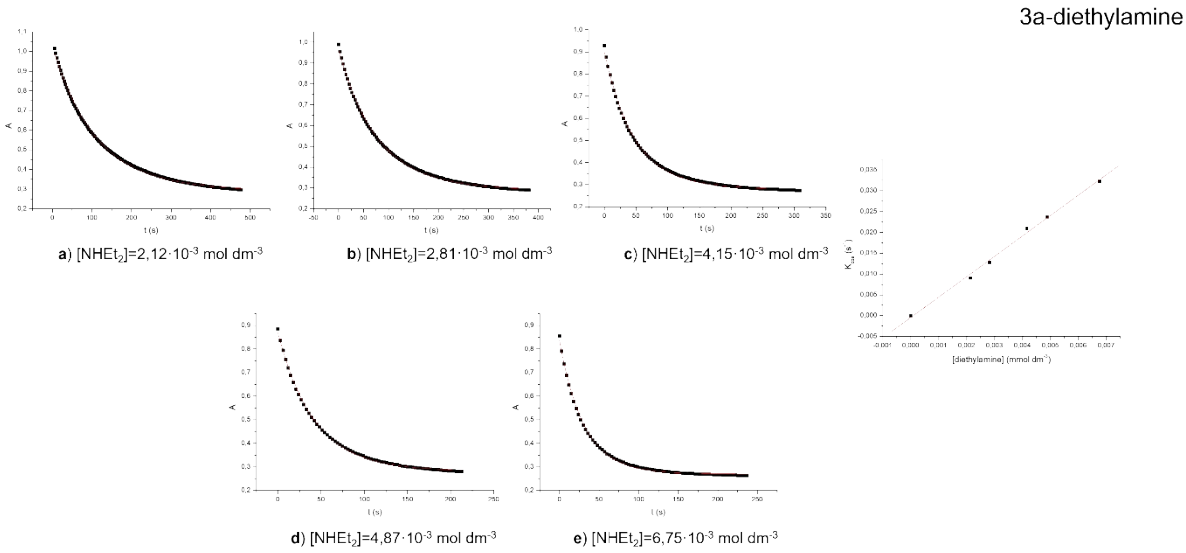


*S 88. UV-Vis Kinetic study of complex **8***

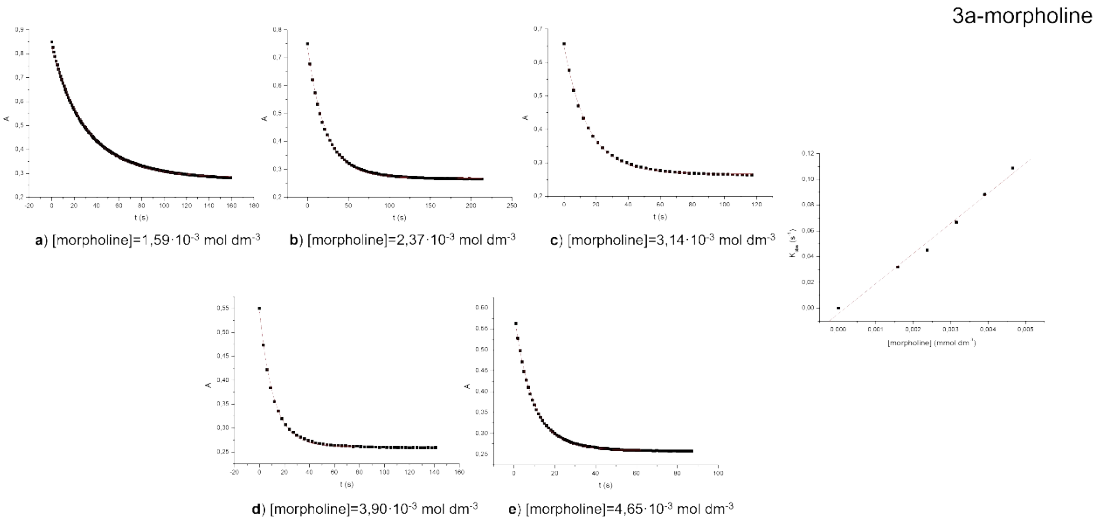
9



*S 89. UV-Vis Kinetic study of complex **9***

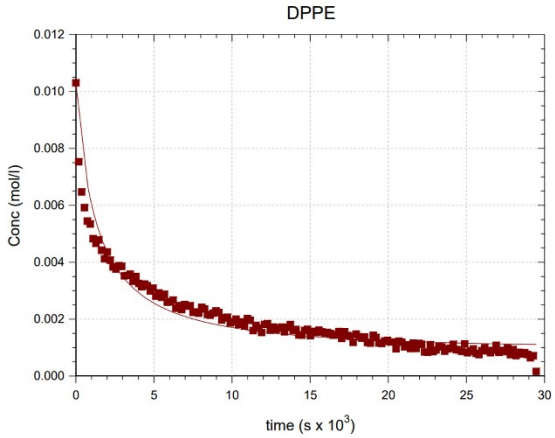


*S 90. UV-Vis Kinetic study of complex **3a** with diethylamine*



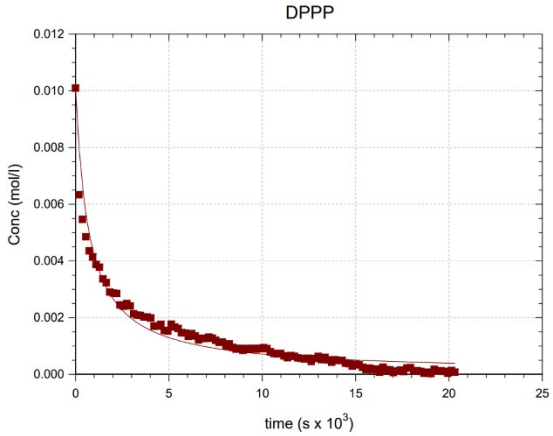
*S 91. UV-Vis Kinetic study of complex **3a** with diethylamine*

NMR kinetic data



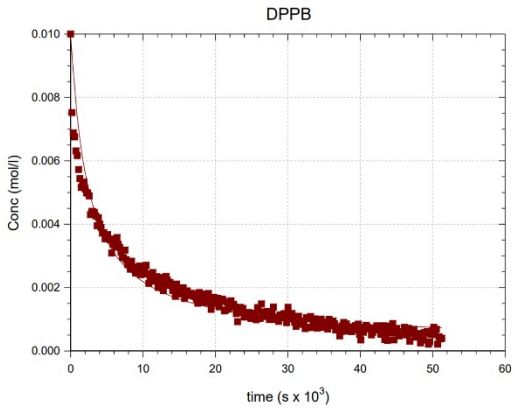
Parameter Name :	K	
Estimate Value =	0.0395408871	
Standard Deviation =	0.00156412955	
95% Range (Univar) =	0.0364518852	0.0426298890
95% Range (S-Plane) =	0.0356761707	0.0434056035

***S** 92. NMR Kinetic study of complex **4** with piperidine*



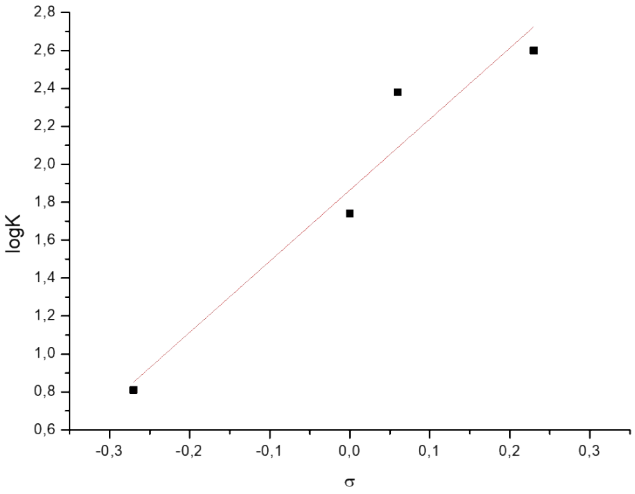
Parameter Name :	K	
Estimate Value =	0.0706646774	
Standard Deviation =	0.00343762684	
95% Range (Univar) =	0.0638521079	0.0774772469
95% Range (S-Plane) =	0.0621343472	0.0791950076

***S** 93. NMR Kinetic study of complex **5** with piperidine*

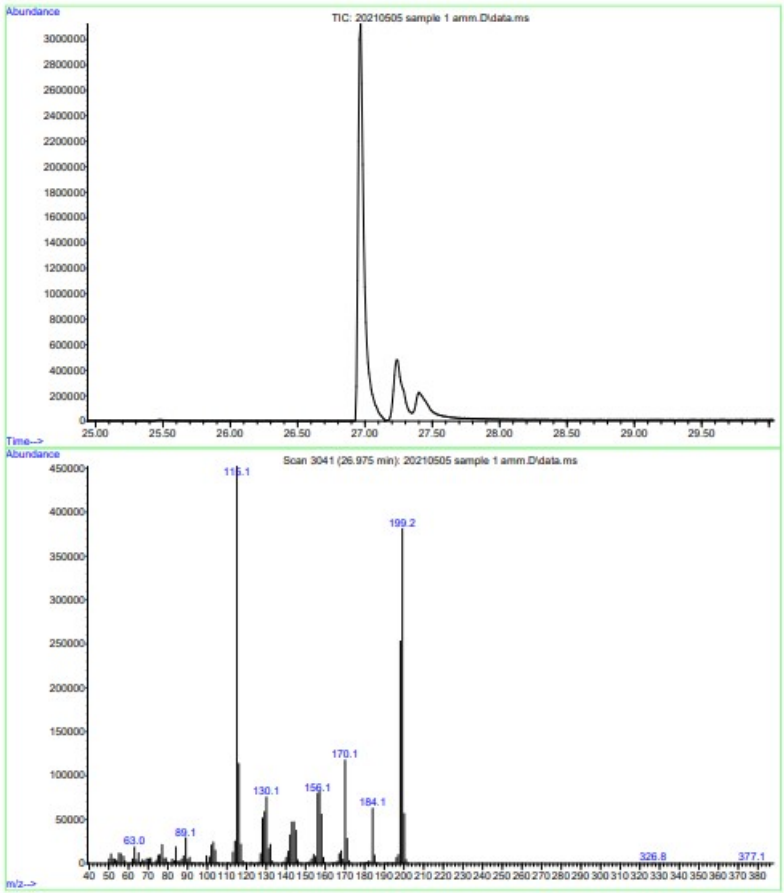


Parameter Name :	K	
Estimate Value =	0.0208041639	
Standard Deviation =	0.000615084492	
95% Range (Univar) =	0.0195933682	0.0220149596
95% Range (S-Plane) =	0.0192904736	0.0223178542

***S** 94. NMR Kinetic study of complex **7** with piperidine*



***S** 95. σ Hammett plot for aryl phosphines*



***S** 96. GC-MS spectra of kinetic study product*

Computational details

Cartesian coordinates and internal energies in gas phase (A.U.)

3b

E= -5299.80592430 A.U.

Pd	-0.137650	-0.549859	-1.466207
C	-1.801032	-3.701574	-1.706368
H	-2.887030	-3.608605	-1.641297
C	-1.136924	-4.793509	-1.147041
H	-1.713404	-5.573283	-0.644238
C	0.256073	-4.922475	-1.241343
H	0.742218	-5.801989	-0.813114
C	-1.040567	-2.739880	-2.373589
C	-1.404002	-1.485229	-3.042333
H	-2.425963	-1.153330	-3.220467
C	0.379724	-2.861449	-2.452997
C	1.029323	-3.957166	-1.885936
H	2.113149	-4.062605	-1.955344
C	0.875133	-1.668725	-3.147501
H	1.917468	-1.497422	-3.417639
C	-0.242157	-0.962809	-3.667461
H	-0.210414	-0.111264	-4.346366
P	-1.791394	0.194519	-0.072095
C	-2.004570	1.995332	-0.046549
C	-1.510140	-0.413628	1.617824
C	-3.452948	-0.415742	-0.515459
C	-1.155153	2.802814	-0.810710
C	-3.050466	2.590830	0.674230
C	-1.106782	-1.751941	1.746671
C	-1.653030	0.371112	2.764324
C	-4.114094	0.186314	-1.596904
C	-4.059990	-1.490544	0.141229
C	-1.312245	4.184984	-0.827358
H	-0.361698	2.340534	-1.404312
C	-3.211356	3.970751	0.671569
H	-3.759199	1.973313	1.231909
C	-0.852193	-2.297462	2.999236
H	-0.988552	-2.377565	0.855232
C	-1.390974	-0.164308	4.021930
H	-1.940444	1.420837	2.688590
C	-5.350878	-0.280513	-2.021349
H	-3.661977	1.038488	-2.112412
C	-5.299659	-1.967125	-0.279661
H	-3.575891	-1.960620	0.999162
C	-2.334640	4.764627	-0.074464
H	-0.651102	4.817161	-1.422239
H	-4.018929	4.441119	1.234741
C	-0.984758	-1.493012	4.133363
H	-0.537197	-3.336937	3.104857
H	-1.467814	0.456116	4.916203
C	-5.939255	-1.364473	-1.362237
H	-5.870552	0.190264	-2.857351
H	-5.778998	-2.801010	0.235692
Cl	-2.531351	6.472864	-0.079162
Cl	-0.592438	-2.135176	5.682892
Cl	-7.469096	-1.950563	-1.887624
P	1.725123	0.149475	-0.292922
C	1.569540	0.831868	1.396765

C	2.625254	1.460719	-1.177605
C	2.887690	-1.242866	-0.131769
C	1.129899	2.154376	1.551890
C	1.855333	0.076833	2.539244
C	2.298370	1.771970	-2.501979
C	3.661453	2.164884	-0.545741
C	2.445262	-2.415026	0.498329
C	4.192513	-1.191880	-0.636116
C	0.952244	2.703454	2.815769
H	0.930884	2.777308	0.679202
C	1.680981	0.616840	3.809050
H	2.227149	-0.944410	2.453288
C	2.987996	2.764591	-3.191593
H	1.486208	1.233361	-2.996565
C	4.358695	3.155329	-1.225885
H	3.924854	1.941846	0.491132
C	3.300137	-3.497907	0.665710
H	1.417082	-2.490218	0.858630
C	5.046559	-2.281711	-0.496211
H	4.554209	-0.295762	-1.144259
C	1.215053	1.923621	3.942428
H	0.606683	3.731810	2.932736
H	1.886720	0.019660	4.698753
C	4.017301	3.453298	-2.548553
H	2.733169	3.012524	-4.223149
H	5.165976	3.705385	-0.739644
C	4.600928	-3.428022	0.164010
H	2.960064	-4.406277	1.165383
H	6.063371	-2.246016	-0.890394
Cl	0.929380	2.569500	5.514682
Cl	4.870948	4.686806	-3.389192
Cl	5.657265	-4.774739	0.347279

3g

E= -2530.66985779 A.U.

Pd	0.036896	-0.745281	-0.918444
C	-0.964841	-4.025615	0.168208
H	-2.046160	-4.174884	0.194368
C	-0.138102	-4.596739	1.135497
H	-0.576261	-5.221734	1.916769
C	1.246778	-4.383267	1.122446
H	1.866102	-4.842313	1.896090
C	-0.372979	-3.259916	-0.835530
C	-0.936191	-2.486546	-1.949104
H	-1.990178	-2.460615	-2.221226
C	1.040106	-3.060115	-0.861485
C	1.850534	-3.604004	0.135366
H	2.929336	-3.435456	0.138951
C	1.330823	-2.184416	-2.007644
H	2.330413	-1.907108	-2.338854
C	0.134652	-2.017070	-2.753469
H	0.042134	-1.515269	-3.715826
P	-1.788532	0.329907	-0.067583
C	-3.212240	0.446692	-1.161462
C	-2.391786	-0.449393	1.427409
C	-1.570894	2.053801	0.391185
O	-3.598691	-0.660113	-1.844651
C	-4.037206	1.495941	-1.469094
O	-3.604894	-0.090483	1.922163
C	-1.830969	-1.416797	2.219430
O	-0.909611	2.839301	-0.494433
C	-1.960131	2.795168	1.474525

C	-4.674424	-0.324562	-2.583757
H	-3.968714	2.504535	-1.067775
C	-4.991469	0.989030	-2.399262
C	-3.820564	-0.822656	3.028347
H	-0.864129	-1.889798	2.062535
C	-2.765780	-1.657441	3.268095
C	-0.862528	4.081451	0.019668
H	-2.519069	2.431970	2.333207
C	-1.493789	4.120829	1.229358
H	-5.107958	-1.117358	-3.188561
H	-5.809398	1.530609	-2.869031
H	-4.765411	-0.652199	3.539332
H	-2.673201	-2.365054	4.088934
H	-0.351499	4.828809	-0.582359
H	-1.611450	4.990739	1.871486
P	1.671314	0.587208	-0.040709
C	3.192066	-0.287234	0.372109
C	2.176119	1.915561	-1.124783
C	1.289069	1.377163	1.527390
O	3.871344	-0.894870	-0.631007
C	3.819957	-0.514780	1.567553
O	3.211447	2.717040	-0.764971
C	1.695936	2.294472	-2.350010
O	0.614457	0.621313	2.430213
C	1.557675	2.610359	2.057627
C	4.943857	-1.504254	-0.084509
H	3.504790	-0.145407	2.540641
C	4.964604	-1.311530	1.265606
C	3.391608	3.609441	-1.754340
H	0.864423	1.831788	-2.876987
C	2.490157	3.404385	-2.759916
C	0.437420	1.369255	3.534441
H	2.099169	3.414239	1.565759
C	0.996643	2.603342	3.368785
H	5.605137	-2.022351	-0.774858
H	5.712833	-1.683387	1.962027
H	4.198968	4.324486	-1.613698
H	2.409896	3.971916	-3.684242
H	-0.101740	0.895603	4.351196
H	1.005947	3.413583	4.094328

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C	-0.884179	-4.087157	-1.143128
H	-1.964000	-4.242846	-1.160557
C	-0.053259	-4.910396	-0.383871
H	-0.488863	-5.732189	0.188938
C	1.334756	-4.713019	-0.355097
H	1.957880	-5.383226	0.241384
C	-0.298319	-3.067265	-1.891918
C	-0.864562	-2.016304	-2.742751
H	-1.919438	-1.933369	-3.005349
C	1.116666	-2.875502	-1.874053
C	1.935457	-3.692960	-1.093043
H	3.017264	-3.546098	-1.075010
C	1.405886	-1.722173	-2.733715
H	2.406539	-1.376139	-2.988793
C	0.207365	-1.350043	-3.395155
H	0.121269	-0.613486	-4.193375
Pd	0.128902	-0.622567	-1.274775
P	1.764464	0.358015	-0.009438
P	-1.749432	0.163789	-0.183769

C	1.930890	2.149685	-0.228916
C	1.501397	-0.027410	1.747216
C	3.444203	-0.257193	-0.374040
C	-2.727449	1.271048	-1.245996
C	-2.835136	-1.243699	0.212453
C	-1.623051	1.112496	1.373763
C	1.088631	2.815734	-1.126945
C	2.943944	2.868068	0.425274
C	1.182485	-1.359655	2.056661
C	1.578269	0.916061	2.775406
C	4.076181	0.201132	-1.541113
C	4.097719	-1.195381	0.432164
C	-2.435441	1.384240	-2.610263
C	-3.795442	2.009315	-0.710866
C	-2.333792	-2.266127	1.032357
C	-4.136375	-1.351237	-0.294204
C	-1.195885	2.447173	1.309985
C	-1.945216	0.563666	2.620558
C	1.218378	4.184138	-1.342467
H	0.323421	2.249617	-1.665250
C	3.077764	4.236217	0.225750
H	3.647012	2.353767	1.085354
C	0.960074	-1.746985	3.373078
H	1.110459	-2.106385	1.258200
C	1.348654	0.539786	4.095335
H	1.792994	1.962119	2.552926
C	5.329909	-0.273310	-1.903055
H	3.587154	0.947752	-2.173212
C	5.355065	-1.679457	0.076963
H	3.636114	-1.549523	1.355339
C	-3.192658	2.210139	-3.435428
H	-1.598020	0.821201	-3.028625
C	-4.561163	2.834106	-1.524821
H	-4.029930	1.942975	0.354435
C	-3.129852	-3.350139	1.383360
H	-1.306918	-2.219139	1.401108
C	-4.931790	-2.446663	0.029201
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C	-1.065193	3.210845	2.463171
H	-0.976136	2.911037	0.347817
C	-1.820489	1.319458	3.782038
H	-2.309981	-0.460859	2.698604
C	2.207032	4.878528	-0.652789
H	0.571860	4.720225	-2.039425
H	3.854832	4.815815	0.727179
C	1.042922	-0.786111	4.377375
H	0.718279	-2.778643	3.635113
H	1.387182	1.265922	4.909277
C	5.954230	-1.215879	-1.087890
H	5.839049	0.078215	-2.802165
H	5.882977	-2.404889	0.698448
C	-4.249315	2.923702	-2.879995
H	-2.977608	2.313263	-4.500370
H	-5.395689	3.415204	-1.128437
C	-4.422767	-3.427157	0.874631
H	-2.759080	-4.147460	2.029717
H	-5.947634	-2.547550	-0.356872
C	-1.370286	2.630470	3.690270
H	-0.734911	4.250358	2.424830
H	-2.064560	0.902402	4.760580
F	2.334451	6.178790	-0.845865
F	-4.971996	3.712253	-3.654801

F	-1.222180	3.342397	4.797017
F	-5.180416	-4.462853	1.194290
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F	7.146912	-1.672106	-1.429040

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C	-0.918243	-4.049104	-0.450841
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C	-0.093380	-4.756008	0.423191
H	-0.536413	-5.476940	1.113912
C	1.295963	-4.566531	0.425061
H	1.913656	-5.143699	1.116861
C	-0.324449	-3.156131	-1.341845
C	-0.883862	-2.233073	-2.333477
H	-1.937593	-2.182515	-2.608502
C	1.091624	-2.969340	-1.346529
C	1.904150	-3.669148	-0.452478
H	2.986285	-3.522912	-0.450744
C	1.387827	-1.946086	-2.354898
H	2.390568	-1.636470	-2.646893
C	0.192489	-1.664900	-3.065996
H	0.110310	-1.039297	-3.954203
Pd	0.105754	-0.655769	-1.065207
P	1.731422	0.526111	0.024598
P	-1.764618	0.250396	-0.065395
C	1.869516	2.269606	-0.463435
C	1.502994	0.391456	1.824476
C	3.413613	-0.118176	-0.286506
C	-2.790055	1.171151	-1.258163
C	-2.808971	-1.113764	0.545421
C	-1.631880	1.431561	1.327078
C	1.005553	2.779466	-1.438692
C	2.879422	3.086839	0.064282
C	1.222071	-0.891647	2.320302
C	1.587885	1.471330	2.705024
C	4.015239	0.190740	-1.516059
C	4.083201	-0.946422	0.619002
C	-2.497727	1.127271	-2.625051
C	-3.884150	1.925036	-0.808356
C	-2.299018	-1.962966	1.538924
C	-4.077382	-1.366325	0.009637
C	-1.249500	2.748947	1.035447
C	-1.920727	1.082682	2.650129
C	1.121319	4.104476	-1.854936
H	0.241434	2.128599	-1.872963
C	2.986083	4.411999	-0.347727
H	3.594573	2.682684	0.785212
C	1.058688	-1.090886	3.688102
H	1.136027	-1.738654	1.630815
C	1.413961	1.265656	4.072887
H	1.766076	2.479018	2.327362
C	5.262937	-0.333173	-1.836843
H	3.505375	0.851723	-2.222725
C	5.334532	-1.470121	0.290651
H	3.639228	-1.178379	1.588442
C	-3.291856	1.822621	-3.536239
H	-1.636792	0.549979	-2.970607
C	-4.676530	2.614154	-1.720981
H	-4.112836	1.975632	0.259082
C	-3.069677	-3.016388	2.023324
H	-1.293829	-1.804060	1.935536

C	-4.832240	-2.439648	0.480038
H	-4.481089	-0.723162	-0.774752
C	-1.147249	3.694944	2.050162
H	-1.051852	3.050613	0.006371
C	-1.820560	2.035268	3.662667
H	-2.243900	0.072268	2.900550
C	2.104338	4.923083	-1.302006
H	0.442969	4.495753	-2.616383
H	3.770057	5.047883	0.069365
C	1.158136	-0.011371	4.566924
H	0.852486	-2.093844	4.069199
H	1.473764	2.115602	4.755842
C	5.923402	-1.170496	-0.935136
H	5.726511	-0.082866	-2.793701
H	5.854368	-2.111315	1.006080
C	-4.381380	2.564214	-3.084715
H	-3.056148	1.786471	-4.602119
H	-5.528699	3.197924	-1.366014
C	-4.336881	-3.258146	1.494297
H	-2.668654	-3.662807	2.807181
H	-5.820765	-2.629914	0.056207
C	-1.432266	3.339927	3.368327
H	-0.853589	4.718008	1.804679
H	-2.055568	1.750933	4.690616
H	2.196086	5.962067	-1.626581
H	1.028088	-0.166690	5.640259
H	6.903528	-1.581072	-1.187381
H	-5.003404	3.110518	-3.797330
H	-4.937776	-4.089751	1.868917
H	-1.361013	4.084061	4.164888

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C	-0.684739	-4.748491	0.378517
H	-1.208279	-5.423035	1.059683
C	0.716746	-4.726309	0.374942
H	1.264670	-5.382065	1.055230
C	-0.727531	-3.096636	-1.353890
C	-1.172320	-2.084166	-2.319219
H	-2.210379	-1.883259	-2.584851
C	0.700328	-3.083909	-1.365625
C	1.424858	-3.889629	-0.487223
H	2.516132	-3.868631	-0.480113
C	1.114450	-2.074476	-2.347521
H	2.145084	-1.887119	-2.646234
C	-0.040375	-1.629948	-3.043529
H	-0.055748	-0.966533	-3.907252
Pd	-0.013208	-0.674442	-1.018231
P	1.756069	0.345566	0.010491
P	-1.764921	0.402418	-0.027172
C	2.579414	1.625579	-0.979830
C	3.055358	-0.887150	0.378072
C	1.404020	1.121762	1.641352
C	-2.469098	-0.454622	1.409258
C	-3.151709	0.578991	-1.204235
C	-1.407732	2.130088	0.495881
C	1.915272	2.159171	-2.089907
C	3.856054	2.097248	-0.638164
C	4.045793	-1.149171	-0.579256
C	3.013886	-1.647480	1.553076

C	1.795051	2.416785	1.985558
N	0.726109	0.324695	2.468340
C	-1.760664	-1.520250	1.975598
C	-3.706361	-0.073584	1.951930
C	-4.160260	-0.393943	-1.245720
C	-3.146704	1.610224	-2.151704
C	-1.800560	2.668855	1.721518
N	-0.739588	2.828774	-0.423775
H	0.915979	1.795136	-2.339204
C	2.519422	3.161076	-2.847909
C	4.453053	3.099245	-1.397609
H	4.388927	1.673107	0.216981
H	4.089544	-0.563990	-1.501024
C	4.991256	-2.146099	-0.352949
C	3.969636	-2.637365	1.776468
H	2.230571	-1.463876	2.290374
H	2.331457	3.047575	1.276010
C	1.471739	2.878874	3.259886
C	0.420504	0.771493	3.681596
H	-0.801538	-1.817846	1.548270
C	-2.277871	-2.189738	3.083393
C	-4.214238	-0.741628	3.062039
H	-4.280716	0.738520	1.498127
H	-4.170696	-1.207014	-0.516009
C	-5.156678	-0.325206	-2.217020
C	-4.148928	1.673574	-3.117156
H	-2.353184	2.359993	-2.134343
H	-2.326034	2.060316	2.457996
C	-1.493108	4.003787	1.977645
C	-0.448045	4.100494	-0.172098
H	1.999884	3.572442	-3.716296
C	3.784812	3.632012	-2.501643
H	5.447919	3.462846	-1.131051
H	5.764332	-2.337329	-1.100621
C	4.958621	-2.889359	0.827686
H	3.936552	-3.218094	2.701021
H	1.759796	3.886956	3.567426
C	0.776475	2.043865	4.129029
H	-0.143350	0.086288	4.324160
H	-1.723529	-3.025601	3.515910
C	-3.499122	-1.798680	3.629134
H	-5.176717	-0.442449	3.482912
H	-5.942525	-1.083663	-2.238939
C	-5.154385	0.708356	-3.153134
H	-1.784752	4.462202	2.925568
C	-0.809470	4.738992	1.014495
H	0.108314	4.635041	-0.949869
H	4.258442	4.414820	-3.098614
H	5.706324	-3.665238	1.006563
H	0.506402	2.370651	5.135016
H	-3.903794	-2.325267	4.496627
H	-5.938292	0.760980	-3.911840
H	-0.552137	5.787325	1.177218
H	-4.142998	2.485046	-3.848343

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C	-0.826356	-4.163082	-1.299628
H	-1.907305	-4.311800	-1.287876
C	0.017814	-4.981298	-0.550884
H	-0.408914	-5.794388	0.040730
C	1.406415	-4.783269	-0.548388

H	2.039899	-5.446817	0.044830
C	-0.255255	-3.147733	-2.066598
C	-0.838673	-2.096621	-2.902857
H	-1.898172	-2.012659	-3.144569
C	1.160173	-2.952285	-2.071941
C	1.992784	-3.765870	-1.300356
H	3.073580	-3.610321	-1.295258
C	1.432618	-1.795159	-2.928754
H	2.427942	-1.441770	-3.193961
C	0.221156	-1.420752	-3.564842
H	0.119148	-0.674351	-4.351993
Pd	0.171966	-0.709368	-1.434395
P	1.809446	0.273160	-0.180300
P	-1.694244	0.042819	-0.302695
C	1.951516	2.061764	-0.403866
C	1.563978	-0.126664	1.570984
C	3.479440	-0.338248	-0.573329
C	-2.707628	1.117052	-1.359704
C	-2.727968	-1.398017	0.098297
C	-1.581969	0.995542	1.248879
C	1.097634	2.725377	-1.298328
C	2.954814	2.797485	0.237663
C	1.263471	-1.465860	1.881264
C	1.621245	0.805995	2.605595
C	4.097697	0.119878	-1.751738
C	4.148293	-1.281626	0.207534
C	-2.442723	1.237159	-2.732308
C	-3.785255	1.831599	-0.822020
C	-2.223464	-2.384761	0.964506
C	-3.993931	-1.585130	-0.461061
C	-1.127249	2.324783	1.190912
C	-1.961987	0.479670	2.489370
C	1.213571	4.088342	-1.512380
H	0.331925	2.153727	-1.830589
C	3.076995	4.168721	0.038172
H	3.667336	2.293389	0.895880
C	1.051086	-1.857301	3.191530
H	1.196593	-2.211429	1.081370
C	1.401882	0.423246	3.927545
H	1.813236	1.858004	2.388936
C	5.335387	-0.360111	-2.136297
H	3.601812	0.873254	-2.370658
C	5.397588	-1.775013	-0.171908
H	3.703236	-1.640428	1.137471
C	-3.231935	2.035459	-3.543220
H	-1.596272	0.697375	-3.162919
C	-4.588495	2.633779	-1.625687
H	-4.002543	1.765949	0.247220
C	-2.983293	-3.492168	1.297344
H	-1.219580	-2.283718	1.382645
C	-4.755221	-2.712780	-0.155957
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C	-1.033876	3.096461	2.334441
H	-0.856649	2.773941	0.234848
C	-1.878393	1.250441	3.647998
H	-2.347175	-0.537409	2.569693
C	2.198762	4.827785	-0.837133
H	0.554813	4.613870	-2.205888
H	3.865835	4.714693	0.555403
C	1.118038	-0.913461	4.230109
H	0.824406	-2.894190	3.446619
H	1.437301	1.181951	4.709284

C	5.999875	-1.320263	-1.350909
H	5.827518	-0.005695	-3.043748
H	5.895226	-2.505231	0.466262
C	-4.317002	2.741314	-2.998869
H	-3.031606	2.139081	-4.611028
H	-5.419271	3.176909	-1.175228
C	-4.259588	-3.670942	0.738568
H	-2.603736	-4.257086	1.977056
H	-5.738095	-2.828012	-0.612960
C	-1.402572	2.563853	3.580045
H	-0.683763	4.129320	2.291908
H	-2.186250	0.810498	4.596550
O	-4.915912	-4.778291	1.105434
O	-5.024237	3.487310	-3.852385
O	-1.267266	3.379679	4.636510
O	2.234297	6.137734	-1.096306
O	0.884278	-1.379511	5.464734
O	7.190997	-1.727296	-1.802570
C	-6.194661	-5.026220	0.578335
H	-6.168400	-5.127720	-0.520087
H	-6.533853	-5.972911	1.015420
H	-6.907958	-4.229750	0.850579
C	-6.125075	4.223565	-3.380491
H	-5.821439	4.967159	-2.624295
H	-6.543552	4.747396	-4.248008
H	-6.899171	3.565100	-2.951299
C	0.993505	-0.507996	6.559000
H	0.799301	-1.106278	7.457206
H	2.002573	-0.067731	6.630533
H	0.251146	0.307016	6.505459
C	-1.727128	2.955693	5.892580
H	-1.170482	2.074604	6.256617
H	-1.561741	3.789468	6.585467
H	-2.803026	2.712569	5.871801
C	3.204009	6.942109	-0.471911
H	3.037135	7.964649	-0.830560
H	3.098980	6.925242	0.626154
H	4.226374	6.629312	-0.743474
C	7.917209	-2.679657	-1.067894
H	8.846867	-2.857686	-1.621290
H	8.165664	-2.310168	-0.058408
H	7.364972	-3.630838	-0.978985

8

E= -2617.84950548 A.U.

Pd	0.041124	-0.659527	-1.101639
C	-1.095171	-3.937153	-0.214095
H	-2.180259	-4.006350	-0.119178
C	-0.252639	-4.642727	0.645847
H	-0.687939	-5.286018	1.413809
C	1.141405	-4.549602	0.535787
H	1.771809	-5.121517	1.220379
C	-0.513460	-3.144689	-1.201801
C	-1.084552	-2.237847	-2.204603
H	-2.149156	-2.140039	-2.418174
C	0.906746	-3.051710	-1.316181
C	1.738002	-3.749055	-0.439307
H	2.824410	-3.671814	-0.518406
C	1.190124	-2.106058	-2.401273
H	2.186110	-1.882146	-2.778942
C	-0.028727	-1.782731	-3.042849
H	-0.136797	-1.202572	-3.958573

P	-1.799421	0.288154	-0.099661
C	-1.571892	1.498120	1.241762
C	-2.144327	1.412220	2.514380
C	-1.882469	2.389531	3.471734
C	-1.054591	3.466005	3.159204
C	-0.490179	3.579468	1.890788
C	-0.757096	2.597003	0.942982
O	-0.274604	2.650298	-0.337489
C	2.075894	2.208230	-0.349232
C	3.378208	2.705209	-0.501992
C	3.597056	4.034399	-0.854803
C	2.516435	4.885539	-1.079532
C	1.214986	4.417835	-0.913518
C	1.005157	3.098419	-0.527637
C	-2.858803	1.173099	-1.286701
C	-2.559230	1.160060	-2.651387
C	-3.378782	1.836690	-3.553412
C	-4.495696	2.531210	-3.093517
C	-4.792153	2.555613	-1.729573
C	-3.975646	1.882932	-0.825704
C	-2.851004	-1.015214	0.616791
C	-2.408604	-1.701664	1.757005
C	-3.174857	-2.730532	2.297750
C	-4.371080	-3.107697	1.687996
C	-4.799434	-2.449365	0.535768
C	-4.048341	-1.402615	0.002755
P	1.759024	0.436513	-0.021004
C	3.366937	-0.346992	-0.396405
C	3.871734	-0.248360	-1.702510
C	5.066565	-0.872673	-2.041750
C	5.765601	-1.612693	-1.084464
C	5.270182	-1.711180	0.212525
C	4.076062	-1.076800	0.561224
C	1.567839	0.242574	1.777860
C	1.120278	-1.000832	2.247400
C	0.979869	-1.217820	3.614996
C	1.262611	-0.191176	4.517480
C	1.706365	1.044686	4.051240
C	1.870762	1.261258	2.683860
H	-2.798576	0.574608	2.760286
H	-2.331269	2.310238	4.463519
H	-0.850173	4.235014	3.907434
H	0.151848	4.424050	1.635962
H	4.230723	2.039808	-0.354932
H	4.618973	4.401805	-0.966689
H	2.685721	5.922281	-1.378281
H	0.348803	5.063015	-1.071582
H	-1.669209	0.631364	-3.000719
H	-3.139483	1.826640	-4.619039
H	-5.137036	3.062916	-3.800068
H	-5.663421	3.106162	-1.367968
H	-4.206223	1.911828	0.242501
H	-1.462438	-1.426802	2.227147
H	-2.828573	-3.248151	3.195152
H	-4.970089	-3.917877	2.109672
H	-5.733729	-2.743260	0.052297
H	-4.402506	-0.880287	-0.888674
H	3.327065	0.328030	-2.456159
H	5.456603	-0.783874	-3.058218
H	6.701525	-2.107484	-1.353035
H	5.817666	-2.280408	0.967033
H	3.701840	-1.152197	1.583722

H	0.891636	-1.804365	1.539614
H	0.643967	-2.192351	3.977145
H	1.140392	-0.357800	5.590062
H	1.930313	1.848012	4.756361
H	2.228037	2.227902	2.322478

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E= -2590.57891427 A.U.

Pd	-0.057248	-0.775908	-1.032388
C	-1.478024	-3.941023	-0.206788
H	-2.569456	-3.923525	-0.185368
C	-0.750297	-4.712746	0.698688
H	-1.280961	-5.320959	1.434604
C	0.651314	-4.735583	0.672067
H	1.189870	-5.361220	1.387398
C	-0.772396	-3.201880	-1.157584
C	-1.207295	-2.282982	-2.214701
H	-2.245168	-2.110895	-2.498007
C	0.655393	-3.218218	-1.177608
C	1.369647	-3.982598	-0.256104
H	2.460906	-3.996113	-0.267174
C	1.081395	-2.296972	-2.235867
H	2.116056	-2.142476	-2.542477
C	-0.068475	-1.905200	-2.972119
H	-0.079101	-1.328398	-3.896298
Fe	-0.023789	1.422383	2.540740
C	-1.615177	0.527042	1.711690
C	-0.880799	-0.414550	2.508757
H	-0.421596	-1.328425	2.131374
C	-0.856727	0.066595	3.844929
H	-0.348635	-0.405303	4.684358
C	-1.571753	1.296587	3.885937
H	-1.696825	1.933612	4.760020
C	-2.045534	1.585447	2.577526
H	-2.589216	2.479058	2.278301
C	2.015323	1.362451	2.603116
H	2.621737	0.547152	2.990069
C	1.547735	2.479921	3.344598
H	1.720927	2.652947	4.405478
C	0.785516	3.307009	2.474365
H	0.268625	4.224298	2.751176
C	0.768105	2.704571	1.189207
H	0.253343	3.088110	0.311086
C	1.526466	1.488003	1.260733
P	-1.811420	0.336313	-0.068349
P	1.733540	0.348240	-0.128355
C	-3.397525	-0.541143	-0.259052
C	-3.860149	-1.404211	0.739847
H	-3.312164	-1.501219	1.679606
C	-5.030046	-2.137167	0.539839
H	-5.391210	-2.803634	1.326356
C	-5.739773	-2.014826	-0.652948
H	-6.656459	-2.588606	-0.805690
C	-5.283051	-1.150031	-1.649382
H	-5.843221	-1.042900	-2.580973
C	-4.116712	-0.415771	-1.456092
H	-3.766998	0.265007	-2.237277
C	-2.121707	1.983518	-0.769890
C	-3.261294	2.712802	-0.403239
H	-3.993198	2.279560	0.283340
C	-3.474026	3.981949	-0.934283
H	-4.361760	4.549014	-0.645420

C	-2.561943	4.524601	-1.841453
H	-2.734719	5.519696	-2.257534
C	-1.440689	3.792313	-2.227821
H	-0.732820	4.207184	-2.948766
C	-1.222704	2.522007	-1.697232
H	-0.348109	1.941316	-2.002328
C	2.601983	1.372569	-1.359739
C	3.554073	2.312957	-0.942659
H	3.766273	2.442067	0.121664
C	4.227985	3.083998	-1.885090
H	4.970125	3.815018	-1.556763
C	3.954804	2.926718	-3.245013
H	4.483793	3.536311	-3.981051
C	3.005350	1.996492	-3.664049
H	2.787614	1.875299	-4.727484
C	2.328992	1.221140	-2.723420
H	1.576616	0.495932	-3.043889
C	2.967628	-0.861851	0.455112
C	4.164561	-1.066871	-0.241225
H	4.397360	-0.463543	-1.121556
C	5.068575	-2.034377	0.195165
H	6.001347	-2.186448	-0.352419
C	4.793643	-2.792972	1.332338
H	5.510743	-3.540879	1.677749
C	3.599246	-2.596397	2.024593
H	3.372450	-3.194917	2.909728
C	2.681127	-1.649220	1.579334
H	1.737372	-1.523246	2.112394

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E= -2159.97383643 A.U.

Pd	-0.028340	0.217824	0.939394
P	-1.635026	0.562933	-0.627012
C	-0.822136	1.511789	-1.991430
H	-1.476747	1.529456	-2.876289
H	-0.679560	2.550774	-1.654369
C	-2.142615	-0.982665	-1.436462
C	-3.145999	-0.983023	-2.416858
H	-3.681107	-0.060622	-2.659263
C	-3.471642	-2.164703	-3.075205
H	-4.254562	-2.163547	-3.836731
C	-2.801962	-3.349829	-2.761791
H	-3.063773	-4.275241	-3.279803
C	-1.807509	-3.354239	-1.786293
H	-1.288759	-4.280445	-1.529372
C	-1.476589	-2.173210	-1.122742
H	-0.705492	-2.178583	-0.348010
C	-3.152258	1.441039	-0.174632
C	-4.265934	0.711329	0.264452
H	-4.242745	-0.381413	0.259530
C	-5.408357	1.378243	0.698149
H	-6.275467	0.804736	1.032938
C	-5.447749	2.772405	0.701131
H	-6.346493	3.292968	1.038925
C	-4.339322	3.501651	0.272808
H	-4.367231	4.593412	0.274205
C	-3.191723	2.841412	-0.159168
H	-2.328597	3.428507	-0.481163
P	1.460413	0.675122	-0.705040
C	0.518563	0.853319	-2.287303
H	1.112373	1.432513	-3.010054
H	0.373016	-0.154347	-2.706917

C	2.691189	-0.635250	-0.934822
C	2.303376	-1.857243	-1.502839
H	1.291359	-1.997109	-1.890917
C	3.205955	-2.915367	-1.564289
H	2.899881	-3.861128	-2.016619
C	4.491900	-2.770611	-1.044686
H	5.197961	-3.602567	-1.092399
C	4.875943	-1.562183	-0.463620
H	5.882613	-1.445405	-0.056292
C	3.981363	-0.495851	-0.406231
H	4.290112	0.448902	0.047460
C	2.360742	2.236485	-0.506781
C	3.288682	2.651420	-1.473966
H	3.507220	2.019407	-2.339422
C	3.949022	3.866749	-1.324215
H	4.673776	4.187000	-2.075915
C	3.688068	4.673558	-0.214539
H	4.209149	5.626894	-0.101368
C	2.768064	4.264784	0.748400
H	2.565796	4.895407	1.616789
C	2.104566	3.046993	0.604406
H	1.380057	2.715020	1.353328
C	-1.169846	-2.924108	2.248570
H	-2.250739	-3.007021	2.380359
C	-0.417485	-4.014971	1.821795
H	-0.913320	-4.970762	1.638047
C	0.968097	-3.908456	1.620457
H	1.528084	-4.780653	1.276064
C	-0.507669	-1.720715	2.506663
C	-0.986534	-0.393591	2.901132
H	-2.016991	-0.150101	3.159279
C	0.909324	-1.624266	2.339135
C	1.643630	-2.715991	1.866215
H	2.720387	-2.636898	1.701088
C	1.290173	-0.246129	2.658989
H	2.315223	0.119850	2.715770
C	0.141487	0.422438	3.167540
H	0.118523	1.422958	3.597949

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E= -2199.22013987 A.U.

Pd	0.020892	-1.139012	0.084639
C	-1.226921	-0.784333	3.479732
H	-2.314168	-0.841976	3.571464
C	-0.484385	0.064675	4.298099
H	-0.995722	0.673256	5.047358
C	0.913041	0.138421	4.190068
H	1.466236	0.807466	4.852850
C	-0.545627	-1.577978	2.553275
C	-1.006160	-2.526904	1.536016
H	-2.041099	-2.840759	1.400212
C	0.878062	-1.512358	2.453630
C	1.606728	-0.641058	3.267342
H	2.694515	-0.582427	3.187944
C	1.278537	-2.432556	1.384987
H	2.308715	-2.661869	1.113301
C	0.132476	-3.173296	0.988010
H	0.122955	-4.019930	0.302461
C	1.242781	0.103129	-2.868152
H	2.107270	0.573893	-3.361529
H	1.204337	-0.936268	-3.232729
C	-0.039680	0.854153	-3.211653

H	0.011879	1.872708	-2.794951
H	-0.069882	0.979759	-4.305754
C	-1.342871	0.176226	-2.795934
H	-1.395085	-0.847501	-3.202269
H	-2.209745	0.711482	-3.215317
C	1.778974	1.728572	-0.513241
C	1.304872	2.073622	0.757638
H	0.850016	1.310812	1.394466
C	1.412452	3.385819	1.211876
H	1.036487	3.645652	2.203418
C	1.988166	4.359696	0.398918
H	2.066793	5.390414	0.752005
C	2.469106	4.020291	-0.866744
H	2.926854	4.782124	-1.501517
C	2.369680	2.709075	-1.323016
H	2.760884	2.455364	-2.311232
C	3.264457	-0.734136	-0.978105
C	4.322106	-0.081332	-0.336652
H	4.177408	0.916721	0.082935
C	5.565141	-0.706363	-0.236438
H	6.388663	-0.192839	0.264630
C	5.758255	-1.976088	-0.775605
H	6.733678	-2.461139	-0.697367
C	4.703297	-2.630791	-1.414579
H	4.851838	-3.627255	-1.836518
C	3.458386	-2.017378	-1.509864
H	2.630547	-2.547327	-1.990262
C	-1.933026	1.639083	-0.314697
C	-2.003059	1.758016	1.080001
H	-1.877145	0.873399	1.708988
C	-2.210294	3.000124	1.669401
H	-2.266678	3.080007	2.757366
C	-2.331123	4.138987	0.872434
H	-2.483290	5.117156	1.334154
C	-2.260926	4.027791	-0.514726
H	-2.360678	4.916506	-1.141552
C	-2.071483	2.781452	-1.110371
H	-2.037478	2.714714	-2.199092
C	-3.269290	-0.855442	-0.950733
C	-3.319637	-2.233472	-1.201944
H	-2.393873	-2.790148	-1.377327
C	-4.543347	-2.895815	-1.218099
H	-4.579070	-3.968982	-1.418241
C	-5.721626	-2.189738	-0.969761
H	-6.681193	-2.711451	-0.974287
C	-5.673992	-0.821051	-0.712934
H	-6.595232	-0.268052	-0.516826
C	-4.452035	-0.149535	-0.706228
H	-4.420628	0.923819	-0.505601
P	1.608638	0.010263	-1.069856
P	-1.651663	-0.021583	-0.993896

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E= -2312.12739129 A.U.

Pd	0.009012	-0.378461	-1.295324
C	-1.434383	-3.668493	-1.307300
H	-2.526503	-3.662867	-1.295986
C	-0.718234	-4.642848	-0.616240
H	-1.257127	-5.419421	-0.069014
C	0.684987	-4.653910	-0.623123
H	1.216505	-5.440510	-0.083076
C	-0.722611	-2.703669	-2.024721

C	-1.150332	-1.541445	-2.809094
H	-2.184808	-1.293855	-3.047399
C	0.706316	-2.714441	-2.032566
C	1.408994	-3.691130	-1.322283
H	2.501334	-3.713005	-1.334431
C	1.142336	-1.558605	-2.821602
H	2.177717	-1.331549	-3.075642
C	-0.003674	-0.986488	-3.436710
H	-0.003312	-0.189547	-4.179451
P	1.505905	0.674583	0.057735
P	-1.510793	0.645562	0.051803
C	3.128850	1.138160	-0.598483
C	4.273796	1.121976	0.207024
H	4.210418	0.787683	1.245405
C	5.497061	1.527577	-0.324287
H	6.391256	1.512120	0.302678
C	5.579714	1.949570	-1.650305
H	6.540799	2.264792	-2.062713
C	4.438938	1.964562	-2.454660
H	4.505949	2.291408	-3.494614
C	3.215565	1.554906	-1.933523
H	2.320048	1.553099	-2.561782
C	1.794462	-0.245537	1.596359
C	1.410872	0.256932	2.843898
H	0.985893	1.259236	2.927616
C	1.555565	-0.532934	3.982808
H	1.249312	-0.139824	4.954436
C	2.083373	-1.818581	3.881931
H	2.194256	-2.434823	4.776968
C	2.466711	-2.321745	2.637744
H	2.876317	-3.330923	2.555583
C	2.317244	-1.541979	1.495763
H	2.593993	-1.946845	0.519343
C	0.683083	2.226308	0.560352
C	-0.723354	2.222556	0.542004
C	-1.428643	3.367786	0.913349
H	-2.521005	3.375220	0.876479
C	-0.730778	4.511912	1.302685
H	-1.281569	5.413029	1.581201
C	0.663407	4.513839	1.324207
H	1.203216	5.415846	1.620444
C	1.374865	3.372001	0.953737
H	2.467808	3.378826	0.953383
C	-1.765828	-0.255967	1.609123
C	-2.312856	0.378448	2.732334
H	-2.633084	1.421868	2.677880
C	-2.439520	-0.320453	3.928957
H	-2.865407	0.174778	4.804366
C	-2.019458	-1.649434	4.010895
H	-2.116296	-2.192795	4.953648
C	-1.473875	-2.281614	2.895549
H	-1.136910	-3.318348	2.957653
C	-1.343122	-1.587245	1.695315
H	-0.899596	-2.079273	0.826258
C	-3.138097	1.069627	-0.618281
C	-4.310266	0.495174	-0.115436
H	-4.265660	-0.190510	0.733711
C	-5.537795	0.804509	-0.700626
H	-6.452554	0.356962	-0.306008
C	-5.598296	1.682560	-1.780570
H	-6.562073	1.924013	-2.234250
C	-4.428051	2.253348	-2.286089

H	-4.475206	2.940535	-3.133696
C	-3.199124	1.944270	-1.713427
H	-2.281975	2.384691	-2.115397

TS-3b

E= -5551.25033717 A.U.

N	-4.912133	-1.551078	-1.258010
C	-5.312016	-0.711174	-2.382172
C	-5.808727	-1.448821	-0.110159
C	-6.761479	-0.923022	-2.801248
H	-5.164648	0.337891	-2.067682
H	-4.622683	-0.900622	-3.217946
C	-7.272466	-1.674759	-0.470896
H	-5.685833	-0.435816	0.310210
H	-5.472692	-2.164909	0.652580
C	-7.698251	-0.757739	-1.610808
H	-7.011519	-0.215601	-3.607360
H	-6.872955	-1.935433	-3.228458
H	-7.419213	-2.730025	-0.761805
H	-7.890927	-1.507572	0.424662
H	-7.671091	0.290011	-1.262414
H	-8.738275	-0.963396	-1.905452
H	-4.802961	-2.523289	-1.548318
Pd	-0.428989	-0.468683	-0.726654
C	-2.919300	-2.467378	1.402799
H	-3.608751	-1.853916	1.987304
C	-2.402873	-3.655941	1.927560
H	-2.700898	-3.982464	2.926150
C	-1.518470	-4.437950	1.178305
H	-1.137073	-5.371419	1.598443
C	-2.539408	-2.086532	0.117714
C	-2.963402	-0.959801	-0.729253
H	-3.425074	-0.052170	-0.344560
C	-1.594252	-2.854046	-0.621202
C	-1.091370	-4.038908	-0.090753
H	-0.363528	-4.635968	-0.644391
C	-1.289127	-2.124174	-1.862757
H	-0.743767	-2.556395	-2.701610
C	-2.176880	-1.007203	-1.930227
H	-2.320745	-0.355335	-2.790901
P	-0.588740	1.498649	0.456907
C	0.053759	2.978375	-0.377087
C	0.181622	1.368026	2.101962
C	-2.336106	1.947038	0.774805
C	0.663846	2.838275	-1.628421
C	-0.102778	4.261384	0.167304
C	-0.039564	0.170995	2.801417
C	1.013197	2.340001	2.663627
C	-3.075428	2.500384	-0.281568
C	-3.004219	1.577942	1.947088
C	1.150210	3.948196	-2.312354
H	0.749686	1.842291	-2.072496
C	0.384642	5.376787	-0.503260
H	-0.623408	4.396920	1.118787
C	0.543613	-0.044558	4.044423
H	-0.665665	-0.610656	2.357973
C	1.613813	2.127633	3.901356
H	1.231166	3.263106	2.124638
C	-4.455032	2.646610	-0.187198
H	-2.569349	2.806201	-1.201319
C	-4.387498	1.714097	2.049723
H	-2.448049	1.170375	2.793790

C	1.017926	5.213435	-1.738924
H	1.627880	3.842045	-3.287640
H	0.272235	6.377283	-0.082530
C	1.379614	0.935451	4.583631
H	0.375466	-0.974273	4.590688
H	2.293206	2.869799	4.323324
C	-5.109137	2.227013	0.972953
H	-5.030117	3.074886	-1.010038
H	-4.910143	1.419318	2.961347
Cl	1.624343	6.592722	-2.571210
Cl	2.176042	0.642562	6.084551
Cl	-6.832411	2.314927	1.060370
P	1.835045	-0.939689	-0.593932
C	2.913125	0.118561	0.443468
C	2.667646	-0.869371	-2.213152
C	2.096413	-2.634266	0.022655
C	3.244644	1.392385	-0.039630
C	3.363824	-0.255341	1.713812
C	1.908860	-0.733395	-3.380469
C	4.065086	-0.941279	-2.310884
C	1.607741	-2.961013	1.295740
C	2.687874	-3.637918	-0.752938
C	3.977239	2.284329	0.734023
H	2.936657	1.698087	-1.040404
C	4.096789	0.629609	2.498720
H	3.153391	-1.249239	2.109170
C	2.524346	-0.677472	-4.628002
H	0.819992	-0.665155	-3.304638
C	4.690223	-0.890054	-3.550529
H	4.673716	-1.032623	-1.407593
C	1.751733	-4.244053	1.808327
H	1.092032	-2.206720	1.894257
C	2.802494	-4.936370	-0.262704
H	3.060796	-3.413129	-1.754259
C	4.385565	1.902469	2.011983
H	4.226207	3.276926	0.355203
H	4.428070	0.341569	3.497660
C	3.914694	-0.758168	-4.706308
H	1.936757	-0.568555	-5.540914
H	5.776833	-0.946855	-3.632707
C	2.341186	-5.232508	1.020245
H	1.381534	-4.492517	2.803901
H	3.256177	-5.722098	-0.868871
Cl	5.226379	3.028817	3.013816
Cl	4.686714	-0.686305	-6.243792
Cl	2.467626	-6.841114	1.629047

TS-3g

E= -2782.11294558 A.U.

P	0.563428	1.904199	0.028867
C	-0.234269	3.240623	-0.883572
C	0.361027	2.357662	1.755790
C	2.304087	2.256409	-0.269995
O	-1.568560	3.128124	-1.118653
C	0.239080	4.394762	-1.445936
O	0.553410	3.646140	2.142405
C	0.031590	1.591247	2.842372
O	2.815373	1.812626	-1.445029
C	3.289838	2.853763	0.469461
C	-1.948926	4.212752	-1.822972
H	1.269184	4.742822	-1.415841
C	-0.882459	5.028586	-2.059346

C	0.349880	3.705516	3.469760
H	-0.171171	0.522830	2.826622
C	0.026630	2.473381	3.963158
C	4.125332	2.117188	-1.462739
H	3.169935	3.306126	1.450469
C	4.479902	2.760407	-0.312715
H	-3.001986	4.270460	-2.087198
H	-0.894233	5.968931	-2.605949
H	0.461919	4.684998	3.928973
H	-0.193244	2.228117	4.999851
H	4.673929	1.815343	-2.351550
H	5.471421	3.123110	-0.051676
P	1.783124	-1.395551	-0.358540
C	1.664561	-3.130582	0.126019
C	2.665188	-1.446178	-1.918446
C	3.001648	-0.784088	0.819344
O	0.876809	-3.934068	-0.630383
C	2.176503	-3.837130	1.180563
O	3.821897	-2.152179	-2.019335
C	2.361696	-0.878235	-3.126517
O	2.507347	-0.295253	1.986341
C	4.365682	-0.665475	0.808806
C	0.892001	-5.162442	-0.071749
H	2.844402	-3.450733	1.946946
C	1.669130	-5.165404	1.049197
C	4.260127	-2.031312	-3.284745
H	1.495597	-0.253771	-3.333190
C	3.406473	-1.258484	-4.018957
C	3.546590	0.141560	2.719232
H	5.026411	-0.982596	0.006321
C	4.719232	-0.058385	2.050329
H	0.319661	-5.930900	-0.585466
H	1.866704	-6.015852	1.698008
H	5.184369	-2.552077	-3.524152
H	3.507620	-1.000674	-5.070745
H	3.301682	0.570848	3.687585
H	5.716816	0.199335	2.398744
Pd	-0.177455	-0.218432	-0.427116
N	-4.805808	-0.078063	-0.113894
C	-5.367958	0.879755	-1.059263
C	-5.136041	-1.464068	-0.424487
H	-5.090584	0.144854	0.840621
C	-6.875187	0.725128	-1.222879
H	-4.863943	0.709640	-2.026908
H	-5.099245	1.895662	-0.729075
C	-6.636578	-1.686737	-0.571677
H	-4.620324	-1.712755	-1.368120
H	-4.703142	-2.104242	0.358793
C	-7.235664	-0.712866	-1.580596
H	-7.233670	1.427745	-1.991343
H	-7.373774	1.012590	-0.280088
H	-7.123333	-1.554629	0.411073
H	-6.820546	-2.730267	-0.870760
H	-6.847789	-0.945938	-2.588193
H	-8.328129	-0.833875	-1.633405
C	-2.215666	-0.507026	-1.214128
C	-1.630946	-1.747629	-0.815736
C	-2.741264	0.159369	-0.056974
H	-2.332824	-0.154933	-2.238394
C	-1.854761	-1.894078	0.636655
H	-1.357493	-2.568462	-1.477662
C	-2.459257	-0.697195	1.109365

H	-2.877506	1.239395	-0.004139
C	-1.520698	-2.906133	1.536312
C	-2.731963	-0.514011	2.461096
C	-1.804815	-2.716047	2.890804
H	-1.041478	-3.825853	1.195811
H	-3.183629	0.413889	2.822133
C	-2.399240	-1.537221	3.352887
H	-1.554392	-3.504741	3.603892
H	-2.605143	-1.417227	4.418607

TS-3a

E= -2795.39602569 A.U.

Pd	0.243610	-0.212432	-0.478657
C	2.274655	-0.412865	-1.252370
C	1.652713	-1.699739	-1.200295
C	1.875714	-2.242337	0.148085
C	2.462982	-1.216739	0.941001
C	2.755966	-0.081081	0.055579
C	2.722751	-1.417672	2.293954
H	3.155475	-0.621486	2.905881
C	2.432347	-2.666580	2.851501
H	2.641598	-2.851647	3.907166
C	1.887246	-3.687335	2.063342
H	1.677915	-4.658778	2.517050
C	1.590758	-3.485313	0.712986
H	1.137432	-4.278864	0.115034
H	2.940852	0.936808	0.395802
H	1.383309	-2.311837	-2.060099
H	2.442838	0.184219	-2.148284
P	-0.277738	1.956678	0.146354
C	1.234713	2.908155	0.554219
C	-1.343834	2.141723	1.615548
C	-1.039259	2.945621	-1.178521
C	2.066305	3.324314	-0.496325
C	1.638370	3.127277	1.875395
C	-1.165139	1.216547	2.651888
C	-2.355830	3.103376	1.718833
C	-1.628589	2.293921	-2.267034
C	-1.053653	4.347311	-1.120798
C	3.278226	3.953840	-0.225643
H	1.756050	3.162780	-1.532457
C	2.859304	3.748490	2.141778
H	0.993703	2.822062	2.702692
C	-1.986797	1.246915	3.775461
H	-0.391168	0.450723	2.563796
C	-3.178610	3.128930	2.843190
H	-2.524025	3.814833	0.908281
C	-2.249296	3.030852	-3.273533
H	-1.601495	1.204151	-2.322680
C	-1.673693	5.079724	-2.129030
H	-0.568803	4.866795	-0.290083
C	3.681073	4.162999	1.095136
H	3.909760	4.290247	-1.051445
H	3.161186	3.922942	3.177159
C	-2.998699	2.201368	3.869631
H	-1.848254	0.507513	4.567009
H	-3.972657	3.875828	2.914166
C	-2.276393	4.422006	-3.202917
H	-2.712693	2.511829	-4.115180
H	-1.683285	6.170910	-2.079549
P	-1.781326	-1.337489	-0.391767
C	-2.240758	-1.824409	1.305611

C	-1.734835	-2.911436	-1.319756
C	-3.249348	-0.452932	-1.021246
C	-1.218275	-2.064505	2.230389
C	-3.574699	-2.006845	1.691084
C	-1.233551	-2.896565	-2.629599
C	-2.142830	-4.124635	-0.756179
C	-3.775275	0.590580	-0.245874
C	-3.791415	-0.706812	-2.285830
C	-1.522305	-2.482654	3.523021
H	-0.176716	-1.920330	1.936407
C	-3.876334	-2.411170	2.989963
H	-4.381535	-1.827350	0.977088
C	-1.161821	-4.072257	-3.370807
H	-0.887362	-1.954437	-3.065309
C	-2.052296	-5.304074	-1.495985
H	-2.527483	-4.152387	0.265416
C	-4.814370	1.374945	-0.734754
H	-3.374263	0.791087	0.749075
C	-4.830130	0.086712	-2.773055
H	-3.411056	-1.529982	-2.893900
C	-2.852636	-2.650276	3.906741
H	-0.713531	-2.672297	4.232528
H	-4.919282	-2.544414	3.286008
C	-1.567364	-5.280733	-2.801712
H	-0.779074	-4.048462	-4.393757
H	-2.368055	-6.248166	-1.046196
C	-5.339155	1.131262	-2.003944
H	-5.212052	2.184798	-0.118961
H	-5.249069	-0.121846	-3.760200
N	4.893985	-0.325724	-0.015318
C	5.216716	-1.636447	-0.560114
C	5.461120	0.779227	-0.775609
C	6.716410	-1.838967	-0.747288
H	4.698882	-1.717545	-1.532335
H	4.782495	-2.402709	0.099555
C	6.967982	0.648361	-0.968520
H	4.957845	0.785571	-1.758951
H	5.194705	1.722799	-0.274680
C	7.320821	-0.707131	-1.571589
H	6.897062	-2.815762	-1.222439
H	7.203060	-1.879491	0.243603
H	7.469177	0.763989	0.009175
H	7.330001	1.472145	-1.603665
H	6.931243	-0.759191	-2.604133
H	8.412649	-0.823567	-1.646516
H	5.166205	-0.270317	0.966236
H	-3.654431	2.219457	4.743034
H	-2.761770	5.000443	-3.992405
H	4.629897	4.661286	1.306917
H	-1.501442	-6.206170	-3.378177
H	-3.094045	-2.970358	4.923071
H	-6.151703	1.750595	-2.390149

TS-3f

E= -2827.41757065 A.U.

Pd	0.250508	-0.248705	-0.468680
P	-0.255090	1.897126	0.190008
P	-1.790120	-1.298689	-0.427515
C	-0.583585	3.090514	-1.142448
C	1.165486	2.612597	1.102371
C	-1.665124	2.058735	1.363758
C	-2.092823	-2.301479	1.061139

C	-1.997538	-2.455315	-1.828184
C	-3.250019	-0.183215	-0.542927
C	-0.782591	2.604240	-2.439106
C	-0.646017	4.471384	-0.901357
C	2.128959	3.365554	0.415681
C	1.394576	2.263021	2.439809
C	-2.728120	2.947284	1.193058
N	-1.598249	1.199091	2.383389
C	-1.331994	-2.042718	2.206590
C	-3.082035	-3.296529	1.095336
C	-1.507069	-3.763754	-1.709892
C	-2.514956	-2.024468	-3.055513
C	-4.340317	-0.241139	0.328315
N	-3.157925	0.714955	-1.526615
H	-0.741276	1.526844	-2.614018
C	-1.053448	3.488363	-3.482727
C	-0.918251	5.350129	-1.946014
H	-0.471662	4.861531	0.105106
H	1.968370	3.637689	-0.630240
C	3.296108	3.771097	1.062320
C	2.560497	2.676937	3.081042
H	0.657551	1.656187	2.970070
H	-2.760944	3.620242	0.336160
C	-3.749080	2.940408	2.141172
C	-2.574583	1.199417	3.284409
H	-0.562384	-1.268001	2.177207
C	-1.567160	-2.761251	3.378072
C	-3.309782	-4.013407	2.266353
H	-3.671269	-3.514743	0.200801
H	-1.100917	-4.111210	-0.757020
C	-1.548799	-4.629960	-2.799273
C	-2.555264	-2.897549	-4.141054
H	-2.877853	-1.000339	-3.161485
H	-4.371124	-0.975574	1.134109
C	-5.379054	0.668179	0.140487
C	-4.152839	1.578429	-1.700215
H	-1.207659	3.103734	-4.493468
C	-1.124381	4.858437	-3.236604
H	-0.965428	6.424563	-1.754668
H	4.033019	4.368796	0.520096
C	3.515715	3.428949	2.396511
H	2.721993	2.410837	4.128575
H	-4.598072	3.620571	2.038777
C	-3.674437	2.054375	3.211122
H	-2.483654	0.474953	4.101096
H	-0.964993	-2.556684	4.266233
C	-2.554153	-3.743959	3.409648
H	-4.079906	-4.787816	2.288038
H	-1.172987	-5.650362	-2.693580
C	-2.073952	-4.199712	-4.017690
H	-6.248836	0.652492	0.801700
C	-5.291628	1.593828	-0.894987
H	-4.031633	2.301192	-2.514934
H	-1.335282	5.550534	-4.055272
H	4.425943	3.755547	2.904653
H	-4.454456	2.016786	3.973872
H	-2.734283	-4.309944	4.326713
H	-2.109057	-4.881176	-4.870562
H	-6.085335	2.321437	-1.075124
H	-2.968241	-2.554907	-5.092642
N	4.865434	-0.381142	-0.181034
C	5.443700	0.690117	-0.982732

C	5.162268	-1.715201	-0.685467
H	5.150792	-0.298550	0.795251
C	6.946646	0.528454	-1.177507
H	4.933262	0.670212	-1.961880
H	5.195599	1.652784	-0.508495
C	6.657076	-1.946533	-0.871689
H	4.636788	-1.816788	-1.651055
H	4.716401	-2.449669	0.002049
C	7.274646	-0.852184	-1.736080
H	7.317609	1.324360	-1.842127
H	7.454860	0.669631	-0.206835
H	7.148331	-1.963010	0.117607
H	6.819559	-2.940963	-1.315603
H	6.879154	-0.932659	-2.764449
H	8.364108	-0.987962	-1.811897
C	2.247092	-0.560085	-1.317370
C	1.594759	-1.814703	-1.100273
C	2.809391	-0.104284	-0.077620
H	2.380895	-0.067841	-2.280160
C	1.852261	-2.207133	0.296684
H	1.262425	-2.500164	-1.880260
C	2.500196	-1.118501	0.944211
H	2.993583	0.945273	0.150636
C	1.533681	-3.353272	1.022746
C	2.787108	-1.158364	2.304769
C	1.848023	-3.395268	2.383131
H	1.041303	-4.201153	0.542393
H	3.262419	-0.307242	2.799362
C	2.454333	-2.310103	3.023941
H	1.605283	-4.290653	2.959795
H	2.676837	-2.367416	4.091527

TS-4

E= -2411.40916530 A.U.

N	-4.125388	-1.349682	-0.724213
C	-4.966606	-0.343193	-1.366000
C	-4.038294	-2.598233	-1.477625
H	-4.453962	-1.539766	0.224047
C	-6.364838	-0.863663	-1.674927
H	-4.456878	-0.048968	-2.299878
H	-4.999477	0.547494	-0.719011
C	-5.410753	-3.181311	-1.788043
H	-3.497101	-2.369672	-2.411208
H	-3.414305	-3.299981	-0.904382
C	-6.296738	-2.154156	-2.484539
H	-6.931813	-0.086708	-2.210925
H	-6.902628	-1.044238	-0.727141
H	-5.887510	-3.510926	-0.847723
H	-5.288474	-4.083980	-2.406236
H	-5.885893	-1.935639	-3.486213
H	-7.306565	-2.560373	-2.645763
C	-1.569923	-0.624799	-1.658978
C	-0.625790	-1.701360	-1.630862
C	-2.294093	-0.592120	-0.410568
H	-1.815559	-0.018014	-2.530293
C	-0.791544	-2.391259	-0.342757
H	-0.127771	-2.130395	-2.499857
C	-1.723804	-1.651912	0.439971
H	-2.730931	0.321629	-0.002544
C	-0.184911	-3.526730	0.199410
C	-2.008175	-2.011271	1.755315
C	-0.500291	-3.897486	1.506617

H	0.531341	-4.109573	-0.383773
H	-2.698330	-1.417390	2.361041
C	-1.388549	-3.144911	2.285798
H	-0.033469	-4.786595	1.936507
H	-1.602353	-3.452123	3.311698
Pd	0.224983	0.000388	-0.592363
P	2.490101	-0.056426	-0.225383
C	2.948678	1.664056	0.292944
H	3.961575	1.678140	0.724192
H	2.951869	2.292377	-0.613545
C	2.936305	-1.047653	1.241051
C	4.275097	-1.332930	1.542075
H	5.069727	-1.011868	0.862832
C	4.594065	-2.035973	2.700253
H	5.638596	-2.258200	2.930019
C	3.582434	-2.459262	3.564542
H	3.837190	-3.011616	4.471975
C	2.249468	-2.188505	3.263292
H	1.452824	-2.533749	3.926107
C	1.924518	-1.489878	2.101152
H	0.877290	-1.302680	1.847282
C	3.690533	-0.547223	-1.495413
C	3.528492	-1.818478	-2.064844
H	2.699789	-2.453271	-1.737453
C	4.413367	-2.269639	-3.037641
H	4.284479	-3.263373	-3.472313
C	5.460819	-1.450061	-3.462448
H	6.152916	-1.801616	-4.230825
C	5.621228	-0.182605	-2.907836
H	6.439364	0.460842	-3.239086
C	4.741814	0.270223	-1.924023
H	4.887224	1.264238	-1.496884
P	0.224920	1.966791	0.568475
C	1.917389	2.173414	1.293927
H	2.093186	3.226581	1.559958
H	1.961214	1.584188	2.223880
C	-0.959352	2.035160	1.946671
C	-0.738125	1.250657	3.087991
H	0.189071	0.683539	3.199991
C	-1.703653	1.178411	4.088481
H	-1.514307	0.574678	4.978995
C	-2.905731	1.873994	3.956231
H	-3.659979	1.819922	4.744475
C	-3.137173	2.645387	2.817860
H	-4.073004	3.199353	2.712627
C	-2.171561	2.727249	1.815803
H	-2.356716	3.342039	0.931452
C	-0.031470	3.480211	-0.405741
C	-0.007115	4.747397	0.195099
H	0.128778	4.842448	1.276216
C	-0.170720	5.889560	-0.582557
H	-0.154307	6.874954	-0.111517
C	-0.354864	5.776432	-1.962359
H	-0.480458	6.675679	-2.569765
C	-0.377612	4.520437	-2.564696
H	-0.518366	4.432104	-3.644235
C	-0.217960	3.372889	-1.788252
H	-0.230461	2.379790	-2.247140

TS-9

E= -2181.94957665 A.U.

N	4.546204	-1.250033	-0.332197

C	5.143384	-1.004893	-1.641971
C	4.445522	-2.670272	-0.004447
H	5.066099	-0.753977	0.393098
C	6.493889	-1.687459	-1.814120
H	4.429747	-1.386967	-2.393146
H	5.219563	0.083517	-1.791543
C	5.776552	-3.401561	-0.131069
H	3.705377	-3.103832	-0.699273
H	4.028997	-2.763619	1.010595
C	6.390782	-3.177339	-1.508117
H	6.859727	-1.516743	-2.838521
H	7.229416	-1.216363	-1.137997
H	6.468092	-3.038990	0.650286
H	5.621942	-4.474055	0.064636
H	5.761147	-3.665106	-2.273412
H	7.380570	-3.653836	-1.571152
C	1.874213	-0.994932	-1.341106
C	0.942603	-2.059353	-1.123111
C	2.655291	-0.425312	-0.310111
H	1.984992	-0.581766	-2.349456
H	0.481966	-2.530576	-1.995728
H	3.064749	0.577464	-0.444671
Pd	0.065115	-0.293377	-0.397187
P	-2.107250	-0.773791	0.161568
C	-2.620275	0.531850	1.374667
H	-3.714549	0.528118	1.498356
H	-2.167959	0.276375	2.347239
C	-3.262928	-0.527929	-1.225660
C	-4.571322	-1.025692	-1.180570
H	-4.902029	-1.621539	-0.325569
C	-5.447010	-0.773766	-2.233393
H	-6.465107	-1.167985	-2.198206
C	-5.025541	-0.023818	-3.332185
H	-5.715511	0.169910	-4.156614
C	-3.723182	0.470558	-3.383172
H	-3.389362	1.050641	-4.246383
C	-2.840522	0.214485	-2.335630
H	-1.810500	0.582934	-2.375801
C	-2.586327	-2.361389	0.901121
C	-2.296322	-3.525511	0.174282
H	-1.799555	-3.447409	-0.796645
C	-2.643893	-4.773382	0.680164
H	-2.422050	-5.674294	0.103759
C	-3.271303	-4.874038	1.923241
H	-3.540251	-5.854551	2.322343
C	-3.554571	-3.722673	2.653746
H	-4.047775	-3.797432	3.625479
C	-3.217779	-2.467913	2.145586
H	-3.458842	-1.577270	2.728737
P	-0.314298	1.814838	0.494424
C	-2.125958	1.893169	0.901169
H	-2.320563	2.666563	1.659374
H	-2.639800	2.191300	-0.028216
C	0.015278	3.336794	-0.441767
C	-0.672802	4.534687	-0.202888
H	-1.444923	4.587420	0.568180
C	-0.376564	5.672162	-0.950406
H	-0.917554	6.601881	-0.760609
C	0.606181	5.624479	-1.939105
H	0.834528	6.518156	-2.524229
C	1.289804	4.434998	-2.186560
H	2.051540	4.393690	-2.968304

C	0.991795	3.294477	-1.444548
H	1.505951	2.350966	-1.647748
C	0.504681	2.014237	2.115207
C	0.928573	3.253023	2.609236
H	0.799174	4.156652	2.009200
C	1.528922	3.336215	3.864695
H	1.860443	4.306409	4.241701
C	1.706235	2.189421	4.637399
H	2.173755	2.260578	5.622063
C	1.292316	0.950382	4.148487
H	1.435063	0.048306	4.748078
C	0.703551	0.860821	2.889452
H	0.402108	-0.114447	2.492512
H	1.071580	-2.726855	-0.262875
H	2.504636	-0.740552	0.725436

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E= -1930.51500739 A.U.

C	0.002961	0.686473	3.367884
C	1.236202	0.075765	3.065785
C	-1.213141	0.030262	3.091179
H	-0.016498	1.768219	3.546686
H	2.158901	0.656492	3.133088
H	-2.153796	0.580301	3.166909
Pd	-0.006892	0.107692	1.276313
P	1.563326	0.026182	-0.397281
C	0.647237	-0.371696	-1.957855
H	1.264505	-0.114886	-2.831798
H	0.487704	-1.461907	-1.979677
C	2.345088	1.629383	-0.729329
C	3.167087	1.813636	-1.851138
H	3.377642	0.980338	-2.527222
C	3.732983	3.059996	-2.101144
H	4.375904	3.199174	-2.972998
C	3.480424	4.129537	-1.239685
H	3.925728	5.106507	-1.440664
C	2.663767	3.952871	-0.124864
H	2.467113	4.789085	0.549508
C	2.097382	2.705166	0.131281
H	1.455843	2.556047	1.004194
C	2.873593	-1.217738	-0.248301
C	4.216948	-0.863925	-0.081700
H	4.515239	0.186691	-0.091626
C	5.179249	-1.856788	0.096613
H	6.227207	-1.576056	0.222336
C	4.808454	-3.199658	0.113260
H	5.566122	-3.974201	0.250631
C	3.467652	-3.555258	-0.040789
H	3.173720	-4.606993	-0.022524
C	2.501047	-2.569895	-0.214138
H	1.450206	-2.858199	-0.316648
P	-1.582999	-0.003794	-0.389573
C	-0.680452	0.371920	-1.962569
H	-1.303390	0.095465	-2.826722
H	-0.521710	1.461454	-2.007572
C	-2.991688	1.134898	-0.320632
C	-2.756657	2.509973	-0.465863
H	-1.748090	2.884103	-0.663973
C	-3.808635	3.413253	-0.349297
H	-3.621500	4.482310	-0.471408
C	-5.097371	2.954519	-0.074087
H	-5.921646	3.665104	0.017973

C	-5.331362	1.590287	0.086885
H	-6.338435	1.228972	0.306206
C	-4.283901	0.678877	-0.034183
H	-4.475968	-0.389022	0.091875
C	-2.236944	-1.675662	-0.656200
C	-3.069489	-1.955001	-1.750009
H	-3.375546	-1.155769	-2.430815
C	-3.523273	-3.252539	-1.965602
H	-4.174165	-3.465502	-2.816393
C	-3.149526	-4.279182	-1.096186
H	-3.508165	-5.296316	-1.269143
C	-2.323407	-4.008101	-0.007497
H	-2.033954	-4.809837	0.675308
C	-1.868336	-2.708859	0.213200
H	-1.222541	-2.488215	1.067643
H	1.354622	-1.010829	3.152932
H	-1.288273	-1.057254	3.206170

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E= -5551.26729959 A.U.

N	-4.659803	1.409769	1.078862
C	-5.126817	0.494305	2.162245
C	-5.654855	1.455728	-0.035179
C	-6.507233	0.872767	2.664808
H	-5.109484	-0.517175	1.730052
H	-4.386374	0.538022	2.967688
C	-7.035668	1.854981	0.445695
H	-5.661547	0.446283	-0.473524
H	-5.268499	2.158185	-0.781209
C	-7.530272	0.922271	1.540729
H	-6.793233	0.143082	3.437348
H	-6.455177	1.851507	3.174731
H	-7.013997	2.897976	0.808838
H	-7.709533	1.848017	-0.424150
H	-7.673691	-0.089393	1.124331
H	-8.507391	1.252909	1.921438
H	-4.587436	2.355313	1.476077
Pd	-0.365628	0.369377	0.865519
C	-2.994062	3.005948	-1.259902
H	-3.682774	2.561481	-1.983278
C	-2.407500	4.244935	-1.540520
H	-2.655418	4.765204	-2.467862
C	-1.506485	4.815546	-0.640132
H	-1.057052	5.784097	-0.871251
C	-2.674882	2.360389	-0.068638
C	-3.231580	1.092749	0.546623
H	-3.391663	0.254622	-0.147305
C	-1.703182	2.903870	0.805444
C	-1.134273	4.145799	0.526300
H	-0.383124	4.574177	1.193090
C	-1.420676	1.941711	1.881783
H	-0.997166	2.245035	2.840700
C	-2.264153	0.803531	1.668935
H	-2.512884	0.083941	2.449938
P	-0.582216	-1.634212	-0.252033
C	0.084410	-3.107089	0.580902
C	0.107940	-1.597219	-1.939375
C	-2.345495	-2.092043	-0.492344
C	0.805390	-2.932251	1.767289
C	-0.138541	-4.405949	0.101693
C	-0.186264	-0.466897	-2.718241
C	0.967279	-2.569456	-2.458004

C	-3.056013	-2.561808	0.622750
C	-3.048992	-1.830734	-1.673148
C	1.325673	-4.026111	2.452823
H	0.948596	-1.920208	2.158130
C	0.379100	-5.506081	0.775038
H	-0.730322	-4.564161	-0.803811
C	0.349939	-0.316529	-3.991633
H	-0.831109	0.319277	-2.311344
C	1.523083	-2.421697	-3.725928
H	1.239541	-3.441776	-1.861783
C	-4.435319	-2.728884	0.575496
H	-2.521495	-2.796203	1.547607
C	-4.435100	-1.979252	-1.729444
H	-2.516704	-1.499498	-2.567167
C	1.115647	-5.309218	1.946808
H	1.888682	-3.894219	3.378143
H	0.214164	-6.519316	0.405152
C	1.214997	-1.294847	-4.484875
H	0.126720	0.563876	-4.596642
H	2.224172	-3.162126	-4.114144
C	-5.124031	-2.405389	-0.596431
H	-4.983912	-3.105925	1.441019
H	-4.980886	-1.767258	-2.650671
Cl	1.758383	-6.670296	2.784177
Cl	1.954485	-1.077432	-6.028259
Cl	-6.852570	-2.504434	-0.627143
P	1.857012	0.987181	0.520642
C	2.918719	-0.090120	-0.518301
C	2.867451	1.168690	2.028324
C	1.930143	2.617434	-0.298583
C	3.299899	-1.331597	0.010607
C	3.305977	0.231392	-1.822480
C	2.234583	1.201989	3.275369
C	4.264216	1.276897	1.969518
C	1.239174	2.772353	-1.508451
C	2.568003	3.728293	0.262282
C	4.024771	-2.242223	-0.747868
H	3.035566	-1.595489	1.036435
C	4.026579	-0.675532	-2.595889
H	3.046095	1.198784	-2.254733
C	2.972768	1.349963	4.446419
H	1.146712	1.104059	3.322572
C	5.012306	1.425630	3.131291
H	4.775838	1.238046	1.004350
C	1.206342	3.996796	-2.161999
H	0.707834	1.922685	-1.942019
C	2.516499	4.969259	-0.369803
H	3.106189	3.635136	1.207947
C	4.370271	-1.913429	-2.059114
H	4.313339	-3.209901	-0.334173
H	4.304901	-0.432747	-3.622680
C	4.360689	1.462588	4.367092
H	2.483614	1.373518	5.421399
H	6.099490	1.509811	3.091204
C	1.836387	5.096502	-1.579354
H	0.667179	4.115435	-3.102743
H	3.002864	5.840421	0.072158
Cl	5.200201	-3.069371	-3.039218
Cl	5.284850	1.640692	5.811069
Cl	1.724879	6.641575	-2.344076

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E= -2782.12824376 A.U.

P	0.152066	1.902902	0.072159
C	-0.818271	3.168859	-0.783161
C	-0.415603	2.064088	1.776618
C	1.778306	2.679286	0.127501
O	-2.090866	2.843460	-1.141127
C	-0.530207	4.437426	-1.204520
O	-0.594287	3.295435	2.323415
C	-0.733126	1.100787	2.698720
O	2.562984	2.478201	-0.960890
C	2.475326	3.377075	1.077409
C	-2.614901	3.909050	-1.784209
H	0.412307	4.959036	-1.054520
C	-1.704062	4.919209	-1.859482
C	-1.019092	3.123892	3.587371
H	-0.667910	0.026312	2.538707
C	-1.125742	1.794450	3.882451
C	3.758215	3.043627	-0.715588
H	2.099858	3.682759	2.050577
C	3.769644	3.613585	0.524177
H	-3.639215	3.806747	-2.134287
H	-1.850433	5.891057	-2.325723
H	-1.208131	4.030499	4.157637
H	-1.442673	1.364480	4.830146
H	4.498712	2.958101	-1.506969
H	4.601888	4.136113	0.990155
P	2.107607	-1.085601	-0.397922
C	2.309262	-2.863928	-0.131999
C	3.228582	-0.749628	-1.761511
C	2.981358	-0.414081	1.032092
O	1.805200	-3.682554	-1.088056
C	2.824952	-3.608302	0.893904
O	4.501784	-1.224216	-1.733101
C	3.019234	-0.057768	-2.923829
O	2.207049	-0.091792	2.101169
C	4.284914	-0.086882	1.293999
C	2.009601	-4.954357	-0.686575
H	3.299995	-3.218350	1.791041
C	2.626147	-4.975363	0.529703
C	5.105920	-0.832796	-2.869003
H	2.091718	0.434293	-3.207290
C	4.247780	-0.109408	-3.646580
C	3.006441	0.440186	3.042204
H	5.124010	-0.237084	0.619468
C	4.299340	0.471906	2.606892
H	1.679718	-5.732749	-1.370157
H	2.917098	-5.859191	1.093250
H	6.139711	-1.145766	-2.995243
H	4.464674	0.324082	-4.620255
H	2.519330	0.753007	3.962404
H	5.159098	0.851824	3.154132
Pd	-0.032179	-0.267905	-0.646143
N	-4.398810	-0.570649	-0.150824
C	-4.932656	0.675978	-0.770949
C	-4.792688	-1.785521	-0.925055
H	-4.834147	-0.661603	0.775095
C	-6.442526	0.617308	-0.899940
H	-4.442523	0.765174	-1.751163
H	-4.590993	1.518629	-0.153771
C	-6.301306	-1.877256	-1.045997
H	-4.306941	-1.695235	-1.906315
H	-4.352643	-2.649415	-0.408471

C	-6.890057	-0.618469	-1.670928
H	-6.783234	1.540866	-1.391629
H	-6.898026	0.622473	0.106718
H	-6.743324	-2.050615	-0.048177
H	-6.543342	-2.769053	-1.643008
H	-6.556187	-0.538411	-2.719864
H	-7.987831	-0.677275	-1.696427
C	-2.057703	-0.603132	-1.130925
C	-1.359234	-1.854524	-1.114755
C	-2.886872	-0.474606	0.123795
H	-2.336474	-0.069172	-2.042461
C	-1.597375	-2.475579	0.201579
H	-1.061456	-2.428796	-1.993729
C	-2.454669	-1.649766	0.959893
H	-2.784744	0.492323	0.639776
C	-1.090163	-3.642752	0.773867
C	-2.792764	-1.958897	2.270832
C	-1.440182	-3.957989	2.088285
H	-0.411882	-4.288764	0.213947
H	-3.434812	-1.298558	2.863561
C	-2.279426	-3.130163	2.838040
H	-1.039135	-4.867062	2.542596
H	-2.528520	-3.393549	3.867831

Pro-3a

E= -2795.41459924 A.U.

Pd	0.146342	-0.183509	-0.675775
C	2.157043	-0.574137	-1.140203
C	1.379810	-1.739301	-1.452179
C	1.513736	-2.689232	-0.340967
C	2.338846	-2.125340	0.656669
C	2.886025	-0.809169	0.164714
C	2.569955	-2.777464	1.860967
H	3.185429	-2.324823	2.645806
C	1.991705	-4.035986	2.065615
H	2.160891	-4.568857	3.003314
C	1.195998	-4.609458	1.069876
H	0.748624	-5.591062	1.242667
C	0.945358	-3.948278	-0.134365
H	0.297166	-4.395634	-0.891067
H	2.789309	0.017658	0.886342
H	1.098107	-2.055961	-2.457807
H	2.565164	0.109460	-1.889175
P	0.099543	2.003319	0.073894
C	1.769822	2.719395	0.346712
C	-0.745848	2.261068	1.674809
C	-0.659813	3.190763	-1.083281
C	2.533671	3.093802	-0.770350
C	2.330316	2.847906	1.623043
C	-0.627030	1.240646	2.627651
C	-1.549822	3.371612	1.957562
C	-1.524215	2.696608	-2.066902
C	-0.423189	4.571017	-1.002389
C	3.813857	3.616865	-0.609918
H	2.105642	3.003351	-1.772789
C	3.622383	3.356245	1.779986
H	1.743367	2.578954	2.504857
C	-1.294546	1.328021	3.846407
H	-0.031990	0.354166	2.394885
C	-2.224591	3.452437	3.174547
H	-1.670978	4.164739	1.217152
C	-2.161882	3.570942	-2.945145

H	-1.699479	1.620633	-2.135733
C	-1.058670	5.440903	-1.884042
H	0.266855	4.965735	-0.252020
C	4.363787	3.751061	0.667530
H	4.382161	3.935865	-1.487428
H	4.038378	3.469881	2.784122
C	-2.099198	2.433563	4.118857
H	-1.206249	0.515486	4.570599
H	-2.858901	4.316944	3.383765
C	-1.931554	4.941877	-2.852876
H	-2.841664	3.174985	-3.702664
H	-0.871578	6.515086	-1.816564
P	-1.985119	-1.068808	-0.334006
C	-2.263412	-1.506593	1.420248
C	-2.245499	-2.660061	-1.203075
C	-3.437042	-0.054322	-0.786477
C	-1.180380	-2.035430	2.135250
C	-3.500655	-1.365618	2.057103
C	-1.807489	-2.766690	-2.530431
C	-2.808107	-3.776861	-0.576795
C	-3.675779	1.124800	-0.064235
C	-4.244678	-0.357885	-1.887005
C	-1.332839	-2.420489	3.463752
H	-0.209834	-2.143504	1.645825
C	-3.646582	-1.737419	3.393313
H	-4.354753	-0.961399	1.509860
C	-1.939948	-3.966758	-3.223697
H	-1.349668	-1.900065	-3.016266
C	-2.924087	-4.983007	-1.267391
H	-3.147566	-3.708237	0.458844
C	-4.706853	1.980407	-0.436654
H	-3.049843	1.377804	0.794605
C	-5.269551	0.510608	-2.264554
H	-4.077871	-1.277374	-2.452174
C	-2.566438	-2.266345	4.098081
H	-0.481258	-2.840008	4.004609
H	-4.615238	-1.618102	3.884099
C	-2.492040	-5.080796	-2.588940
H	-1.603080	-4.037316	-4.260621
H	-3.357980	-5.852272	-0.767761
C	-5.502816	1.679243	-1.542783
H	-4.881943	2.893957	0.136141
H	-5.894910	0.264338	-3.125859
N	4.407887	-0.939102	-0.015385
C	4.809460	-1.943684	-1.043846
C	5.052722	0.383731	-0.250226
C	6.316976	-2.103730	-1.073145
H	4.417698	-1.576289	-2.002121
H	4.286643	-2.878776	-0.800775
C	6.562960	0.258460	-0.284530
H	4.653727	0.758107	-1.203307
H	4.702628	1.065609	0.537026
C	7.016855	-0.771016	-1.312266
H	6.568976	-2.833156	-1.857216
H	6.660675	-2.548891	-0.121965
H	6.932794	-0.018978	0.719147
H	6.982681	1.252631	-0.498744
H	6.777832	-0.408305	-2.326869
H	8.108718	-0.896707	-1.274435
H	4.753612	-1.291696	0.885130
H	-2.638410	2.497809	5.066684
H	-2.429278	5.627739	-3.542402

H	5.362497	4.175608	0.794868
H	-2.585697	-6.026708	-3.127342
H	-2.687218	-2.561759	5.143038
H	-6.307897	2.355325	-1.839453

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E= -2827.43471164 A.U.

Pd	-0.156221	-0.214478	0.747032
P	-0.125016	1.937298	-0.076045
P	1.981889	-1.027163	0.377052
C	0.568206	3.221819	1.015236
C	-1.791715	2.604937	-0.478713
C	0.792322	2.125609	-1.663116
C	1.898816	-2.325371	-0.908328
C	2.891213	-1.790959	1.764837
C	3.253760	0.135018	-0.276590
C	1.286246	2.814252	2.144583
C	0.421255	4.590646	0.743704
C	-2.534589	3.227247	0.536446
C	-2.376137	2.443372	-1.742585
C	1.833180	3.038699	-1.847298
N	0.419471	1.258196	-2.610786
C	1.104442	-2.054739	-2.032781
C	2.561300	-3.553192	-0.812133
C	2.167761	-2.213657	2.884709
C	4.279232	-1.979969	1.732278
C	3.938260	-0.042563	-1.481134
N	3.472797	1.170905	0.535648
H	1.406634	1.747574	2.345398
C	1.860811	3.764565	2.988368
C	0.997732	5.535533	1.587093
H	-0.150433	4.918026	-0.128964
H	-2.096082	3.355171	1.529513
C	-3.812203	3.719409	0.279510
C	-3.658551	2.935307	-1.994693
H	-1.813170	1.943334	-2.533892
H	2.120259	3.720328	-1.046626
C	2.500502	3.043848	-3.069395
C	1.055679	1.277975	-3.778535
H	0.561382	-1.106428	-2.096054
C	1.008604	-2.987258	-3.060932
C	2.448173	-4.490416	-1.839524
H	3.167568	-3.781203	0.067371
H	1.089544	-2.041306	2.912429
C	2.817114	-2.832484	3.951363
C	4.926863	-2.594655	2.800715
H	4.858239	-1.643348	0.868715
H	3.724001	-0.901453	-2.119095
C	4.904191	0.899605	-1.831887
C	4.396233	2.062065	0.197147
H	2.421435	3.438982	3.867433
C	1.719480	5.122277	2.709306
H	0.882139	6.600185	1.371265
H	-4.364330	4.228184	1.073711
C	-4.376783	3.583856	-0.990365
H	-4.089711	2.826293	-2.993083
H	3.324460	3.740133	-3.242243
C	2.105598	2.150479	-4.060118
H	0.720087	0.553343	-4.528614
H	0.389297	-2.768255	-3.933847
C	1.681320	-4.206277	-2.967803
H	2.968524	-5.447632	-1.757393

H	2.244547	-3.158145	4.822895
C	4.196911	-3.024058	3.909735
H	5.465216	0.792400	-2.763593
C	5.147360	1.969736	-0.976332
H	4.543711	2.897160	0.891657
H	2.169247	5.866218	3.371208
H	-5.370402	3.988496	-1.197221
H	2.601820	2.121562	-5.031930
H	1.599717	-4.940807	-3.772557
H	4.708462	-3.503476	4.747563
H	5.901773	2.723673	-1.210017
H	6.009496	-2.737386	2.769528
N	-4.444661	-0.938178	0.167501
C	-5.071644	0.375385	0.486460
C	-4.819183	-1.987645	1.160454
H	-4.825265	-1.244598	-0.735833
C	-6.581181	0.255517	0.559072
H	-4.644243	0.698559	1.446049
H	-4.741366	1.092058	-0.277660
C	-6.325882	-2.141912	1.230610
H	-4.394196	-1.667655	2.121691
H	-4.310548	-2.912642	0.856510
C	-7.011194	-0.818733	1.550572
H	-6.990156	1.240113	0.830732
H	-6.980201	0.026354	-0.445667
H	-6.701278	-2.542838	0.271674
H	-6.557755	-2.904687	1.988758
H	-6.741275	-0.503766	2.573401
H	-8.104418	-0.937983	1.538802
C	-2.157791	-0.627370	1.223270
C	-1.376833	-1.806953	1.469981
C	-2.929924	-0.813292	-0.063371
H	-2.543098	0.023158	2.013146
C	-1.549168	-2.712346	0.323405
H	-1.107623	-2.174754	2.462192
C	-2.412668	-2.115380	-0.616976
H	-2.851383	0.033687	-0.763384
C	-0.996353	-3.963860	0.050186
C	-2.716340	-2.737297	-1.821366
C	-1.319731	-4.597389	-1.150197
H	-0.311537	-4.435441	0.757962
H	-3.367406	-2.258949	-2.561098
C	-2.168226	-3.996635	-2.083458
H	-0.887190	-5.575412	-1.371857
H	-2.393481	-4.505807	-3.022527

Pro-4

E= -2411.42307886 A.U.

N	-3.874328	-1.119049	-0.819739
C	-4.642805	0.149209	-0.967277
C	-4.010962	-1.996421	-2.019344
H	-4.289233	-1.633216	-0.033407
C	-6.109243	-0.134094	-1.231003
H	-4.178471	0.697611	-1.799905
H	-4.482167	0.732588	-0.048940
C	-5.469566	-2.311588	-2.288910
H	-3.549069	-1.450989	-2.853638
H	-3.408269	-2.894798	-1.827568
C	-6.296674	-1.041076	-2.441243
H	-6.628441	0.826484	-1.366533
H	-6.557548	-0.599904	-0.334816
H	-5.871847	-2.933089	-1.468548

H	-5.524547	-2.933763	-3.194550
H	-5.983290	-0.505418	-3.353965
H	-7.360291	-1.286852	-2.574097
C	-1.538874	-0.392505	-1.537581
C	-0.598583	-1.429773	-1.879723
C	-2.413440	-0.866745	-0.400185
H	-1.911565	0.343870	-2.255327
C	-0.774532	-2.520870	-0.909716
H	-0.179075	-1.591700	-2.874604
C	-1.790437	-2.173999	0.008554
H	-2.514804	-0.149112	0.428651
C	-0.104743	-3.736299	-0.752269
C	-2.111799	-2.989167	1.086145
C	-0.447621	-4.567685	0.315077
H	0.690952	-4.024638	-1.442502
H	-2.875179	-2.692233	1.813421
C	-1.434609	-4.204134	1.235578
H	0.078718	-5.516452	0.442834
H	-1.672846	-4.865575	2.070884
Pd	0.322797	0.118889	-0.732895
P	2.522949	-0.064669	-0.008043
C	2.836823	1.457901	1.015266
H	3.717133	1.318204	1.661232
H	3.055849	2.280630	0.313339
C	2.731067	-1.394843	1.231635
C	3.995292	-1.821779	1.657815
H	4.896806	-1.398450	1.206891
C	4.107734	-2.797037	2.645344
H	5.096708	-3.129467	2.969187
C	2.961746	-3.351781	3.217326
H	3.054488	-4.117375	3.991162
C	1.701409	-2.938141	2.790950
H	0.800185	-3.383077	3.218277
C	1.585149	-1.968852	1.795646
H	0.598157	-1.667405	1.430935
C	3.970683	-0.212885	-1.099274
C	3.852824	-1.077104	-2.196231
H	2.905146	-1.596145	-2.367070
C	4.925069	-1.264854	-3.063255
H	4.825476	-1.943126	-3.913681
C	6.120695	-0.577494	-2.852708
H	6.960331	-0.717866	-3.537185
C	6.241026	0.294565	-1.772366
H	7.174549	0.837705	-1.608526
C	5.172749	0.475805	-0.894703
H	5.287059	1.159026	-0.050409
P	0.126568	1.873713	0.729979
C	1.601778	1.782157	1.851266
H	1.724728	2.722595	2.409855
H	1.416167	0.981091	2.584932
C	-1.348988	1.749689	1.794263
C	-1.437925	0.714635	2.738787
H	-0.576891	0.070265	2.934737
C	-2.627807	0.483102	3.425335
H	-2.675219	-0.317727	4.167229
C	-3.750423	1.273971	3.174541
H	-4.679253	1.099266	3.722503
C	-3.672156	2.301216	2.233900
H	-4.540663	2.937079	2.043952
C	-2.481749	2.537727	1.545621
H	-2.429732	3.347507	0.813572
C	0.154958	3.583511	0.110252

C	0.074305	4.687897	0.970746
H	-0.054928	4.538257	2.046544
C	0.149408	5.978812	0.456565
H	0.084523	6.837167	1.129142
C	0.311173	6.176644	-0.916541
H	0.373995	7.191533	-1.315953
C	0.393850	5.083586	-1.776371
H	0.523276	5.238352	-2.849835
C	0.313408	3.788382	-1.265000
H	0.378694	2.919865	-1.927405

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E= -2181.96347685 A.U.

N	4.231705	-1.477428	-0.417896
C	4.923064	-1.042650	-1.666380
C	4.070894	-2.960545	-0.373435
H	4.841614	-1.220111	0.366788
C	6.275241	-1.714368	-1.808285
H	4.249667	-1.308110	-2.493839
H	5.000753	0.053567	-1.630177
C	5.410043	-3.661703	-0.499422
H	3.390248	-3.216259	-1.197741
H	3.560220	-3.202062	0.569481
C	6.148641	-3.231756	-1.760426
H	6.726854	-1.380505	-2.754358
H	6.950181	-1.363140	-1.007088
H	6.026231	-3.448517	0.392681
H	5.230372	-4.747129	-0.492402
H	5.597571	-3.584068	-2.649281
H	7.142018	-3.701315	-1.802388
C	1.896469	-0.882985	-1.264486
C	0.986487	-1.987515	-1.327767
C	2.905173	-0.726273	-0.183785
H	2.117055	-0.341114	-2.192215
H	0.594887	-2.297637	-2.301762
H	3.203616	0.323922	-0.049951
Pd	0.008481	-0.324529	-0.516363
P	-2.178470	-0.668727	0.150853
C	-2.483540	0.560060	1.512984
H	-3.562441	0.650134	1.714582
H	-2.002988	0.167380	2.424680
C	-3.429531	-0.180694	-1.088403
C	-4.775965	-0.545479	-0.965948
H	-5.096462	-1.186640	-0.140284
C	-5.706245	-0.104246	-1.903691
H	-6.754499	-0.396090	-1.806562
C	-5.301802	0.704637	-2.966351
H	-6.034596	1.047954	-3.700215
C	-3.962020	1.066476	-3.096499
H	-3.641076	1.692235	-3.932422
C	-3.026481	0.619833	-2.164909
H	-1.969377	0.883613	-2.271420
C	-2.783982	-2.256024	0.807256
C	-2.507727	-3.404691	0.051981
H	-1.938015	-3.310585	-0.877017
C	-2.951461	-4.652190	0.479214
H	-2.739602	-5.539985	-0.121103
C	-3.660437	-4.769727	1.675723
H	-4.003797	-5.749714	2.014831
C	-3.928766	-3.634969	2.437789
H	-4.483692	-3.722846	3.374673
C	-3.497585	-2.380778	2.005228

H	-3.727909	-1.502396	2.611217
P	-0.140853	1.729475	0.540600
C	-1.894306	1.914789	1.137121
H	-1.951713	2.617085	1.982652
H	-2.453057	2.355068	0.293972
C	0.239864	3.319031	-0.258868
C	-0.311224	4.538331	0.158366
H	-1.006794	4.572502	1.000184
C	0.025767	5.720194	-0.497817
H	-0.409908	6.666557	-0.169383
C	0.915657	5.696251	-1.571734
H	1.175779	6.624782	-2.085041
C	1.464052	4.486702	-1.995907
H	2.150686	4.465362	-2.845331
C	1.122985	3.302751	-1.345539
H	1.524946	2.342957	-1.684017
C	0.843042	1.723642	2.087122
C	1.505496	2.852355	2.583069
H	1.448801	3.800568	2.043464
C	2.244894	2.771328	3.762975
H	2.758140	3.658922	4.140431
C	2.325681	1.568395	4.462528
H	2.898970	1.511872	5.390737
C	1.672331	0.436785	3.972719
H	1.731055	-0.509032	4.517091
C	0.945133	0.510377	2.787073
H	0.454559	-0.383090	2.386431
H	1.036665	-2.794329	-0.586629
H	2.543768	-1.102779	0.783937

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