Supporting Information

Table of content:

1. Synthesis of the ligands

1.1. Synthesis of dialkyl phosphonates

To a solution of the appropriate alcohol (0.43 mol, 3 equiv) in DCM (200 ml) at 0-10 °C was added PCl_3 (12.5 mL, 0.14 mol, 1 equiv) in DCM (70 ml) over the course of 1 h. Liberated HCl was removed by a constant argon stream. After completed addition, the dropping funnel was washed with additional DCM (20 mL) and the reaction mixture was stirred for 16 h. The solution was then concentrated under reduced pressure and dried under HV to yield the desired phosphonate.

Diisopropyl phosphonate **1a**: Yield 81%, colorless liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.80 (d, *J* = 687.7 Hz, 1H), 4.70 (ddd, *J* = 12.4, 6.1, 2.1 Hz, 2H), 1.33 (dd, *J* = 5.8, 3.5 Hz, 12H). ^{31}P NMR (162 MHz, $CDCl_3$) δ 4.63.

Dicyclohexyl phosphonate **1b**: Yield 91%, colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.86 (d, *J* = 688.5 Hz, 1H), 4.42 (ddt, *J* = 13.3, 8.9, 4.7 Hz, 2H), 1.91 (dd, *J* = 8.9, 2.4 Hz, 4H), 1.73 (dd, *J* = 8.9, 4.1 Hz, 4H), 1.58 – 1.47 (m, 6H), 1.41 – 1.29 (m, 4H), 1.29 – 1.20 (m, 2H). ^{31}P NMR (162 MHz, $CDCl_3$) δ 4.59.

Dipentyl phosphonate **1c**: Yield 98%, colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.79 (d, *J* = 692.3 Hz, 1H), 4.05 (dtd, *J* = 7.8, 6.6, 1.2 Hz, 4H), 1.68 (p, *J* = 7.1, 4H), 1.34 (tt, *J* = 7.1, 3.4 Hz, 8H), 0.89 (t, *J* = 7.1 Hz, 6H). ^{31}P NMR (162 MHz, $CDCl_3$) δ 7.93.

Bis(2-ethylhexyl) phosphonate **1d**: Yield 93%, colorless liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.80 (d, *J* = 690.9 Hz, 1H), 3.98 (dq, *J* = 7.2, 5.7 Hz, 4H), 1.58 (p, *J* = 6.0 Hz, 2H), 1.40 (ddd, *J* = 17.0, 14.1, 6.7 Hz, 4H), 1.35 – 1.24 (m, 12H), 0.94 – 0.87 (m, 12H). ^{31}P NMR (162 MHz, $CDCl_3$) δ 8.48.

1.2. Cross-coupling of dichloropyridine with diakyl phosphonates for the synthesis of ligands

A 50-mL round-bottom flask equipped with a rubber septa and a magnetic stirrer bar was charged with the 2,6-dichloropyridine **2** (500 mg), $Pd(OAc)_2$ (38 mg, 0.05 equiv) and dppf (187 mg, 0.1 equiv). The reaction vessel was evacuated and purged with Ar. Subsequently, toluene, corresponding $HP(O)(OR)_2$ **1** (2.4 equiv) and base Et_3N (1.13 ml, 2.4 equiv) were added via syringe. The reaction mixture was stirred at 110 °C until the reaction was complete, according to TLC. The reaction mixture was cooled and then concentrated under reduced pressure. The residue was taken up in DCM (2-5 mL) and the product was isolated by column chromatography on silica gel[30,31]

Tetraisopropyl pyridine-2,6-diylbis(phosphonate) **PO-Py-iPr**: Yield 80%, colorless crystals, m.p. 43 °C HR-ESI-MS m/z calculated for $C_{17}H_{32}NO_6P_2$ $[M+H]^+$ 408.1700, found 408,1708. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (ddd, *J* = 8.1, 5.3, 2.6 Hz, 2H), 7.88 (ddd, *J* = 7.7, 5.2, 2.4 Hz, 1H), 4.85 (dq, *J* = 12.0, 5.7 Hz, 4H), 1.38 (dd, *J* = 6.2, 2.2 Hz, 12H), 1.32 (dd, *J* = 6.2, 2.1 Hz, 12H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 153.59 (dd, *J* = 226.7, 22.1 Hz), 135.45 (t, *J* = 11.3 Hz), 128.83 (dd, *J* = 25.3, 3.1 Hz), 71.53 (d, *J* = 6.1 Hz), 23.56(s), 23.32(s). ^{31}P NMR (162 MHz, $CDCl_3$) δ 7.42. FT-IR (-P=O, cm^{-1}): 1263, 1250 (see Figures S1-S3).

Tetracyclohexyl pyridine-2,6-diylbis(phosphonate) **PO-Py-cHex**: Yield 73%, colorless crystals, m.p. 72 °C HR-ESI-MS m/z calculated for $C_{29}H_{48}NO_6P_2$ $[M+H]^+$ 568.2952, found 568,2942. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (ddd, *J* = 8.1, 5.5, 2.7 Hz, 2H), 7.83 (tt, *J* = 7.7, 5.3 Hz, 1H), 4.55

(dtd, *J* = 12.7, 8.3, 3.8 Hz, 4H), 1.91 (ddd, *J* = 31.9, 13.6, 4.3 Hz, 8H), 1.78 – 1.66 (m, 9H), 1.61 – 1.42 (m, 9H), 1.32 (ddt, *J* = 19.1, 9.3, 3.5 Hz, 6H), 1.22 (ddd, *J* = 23.6, 13.3, 3.4 Hz, 8H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 153.75 (dd, *J* = 226.9, 22.5 Hz), 135.40 (t, *J* = 11.4 Hz), 128.72 (d, *J* = 25.5 Hz), 76.29 (s), 33.07 (d, *J* = 37.1 Hz), 24.67 (s), 23.04 (s). ^{31}P NMR (162 MHz, $CDCl_3$) δ 7.36. FT-IR (-P=O, cm^{-1}): 1265, 1254 (see Figures S4-S6).

Tetrapentyl pyridine-2,6-diylbis(phosphonate) **PO-Py-C5**: Yield 75%, colorless oil. HR-ESI-MS m/z calculated for $C_{25}H_{48}NO_6P_2$ $[M+H]^+$ 520.2952, found 520,2947. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (ddd, *J* = 7.6, 5.4, 2.8 Hz, 2H), 7.89 (tt, *J* = 7.9, 5.2 Hz, 1H), 4.16 (ddq, *J* = 30.6, 9.9, 6.7 Hz, 8H), 1.68 (p, *J* = 6.7 Hz, 8H), 1.38 – 1.26 (m, 16H), 0.86 (t, *J* = 7.1 Hz, 12H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 152.62 (dd, *J* = 226.0, 22.1 Hz), 135.68 (t, *J* = 11.3 Hz), 129.26 (d, *J* = 22.1 Hz), 66.91 (d, *J* = 6.1 Hz), 29.63 (d, *J* = 5.8 Hz), 27.06 (s), 21.67 (s), 13.38 (s). ^{31}P NMR (162 MHz, $CDCl_3$) δ 9.04. FT-IR(-P=O, cm^{-1}): 1263 (see Figures S7-S9).

Tetrakis(2-ethylhexyl) pyridine-2,6-diylbis(phosphonate) **PO-Py-2EtHex**: Yield 70%, colorless oil. HR-ESI-MS m/z calculated for $C_{37}H_{72}NO_6P_2$ $[M+H]^+$ 688.4830, found 688,4821. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.06 (t, *J* = 7.8 Hz, 2H), 7.91 (ddd, *J* = 12.9, 7.9, 5.1 Hz, 1H), 4.09 (ddp, *J* = 33.6, 15.9, 6.0, 5.5 Hz, 8H), 1.60 (dp, *J* = 11.4, 6.0 Hz, 4H), 1.47 – 1.20 (m, 32H), 0.93 – 0.83 (m, 24H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 154.17 (dd, *J* = 266.7, 27.1 Hz), 135.59 (t, *J* = 11.6 Hz), 129.29 (d, *J* = 23.1 Hz), 68.93 (t, *J* = 6.6 Hz), 39.72 (d, *J* = 6.3 Hz), 29.34 (s), 28.36 (d, *J* = 4.5 Hz), 22.68 (d, *J* = 4.8 Hz), 22.45 (s), 13.51 (s), 10.34 (s). ^{31}P NMR (162 MHz, $CDCl_3$) δ 9.27. FT-IR(-P=O, cm^{-1}): 1263 (see Figures S10-S12).

2. NMR spectra for synthesized substances

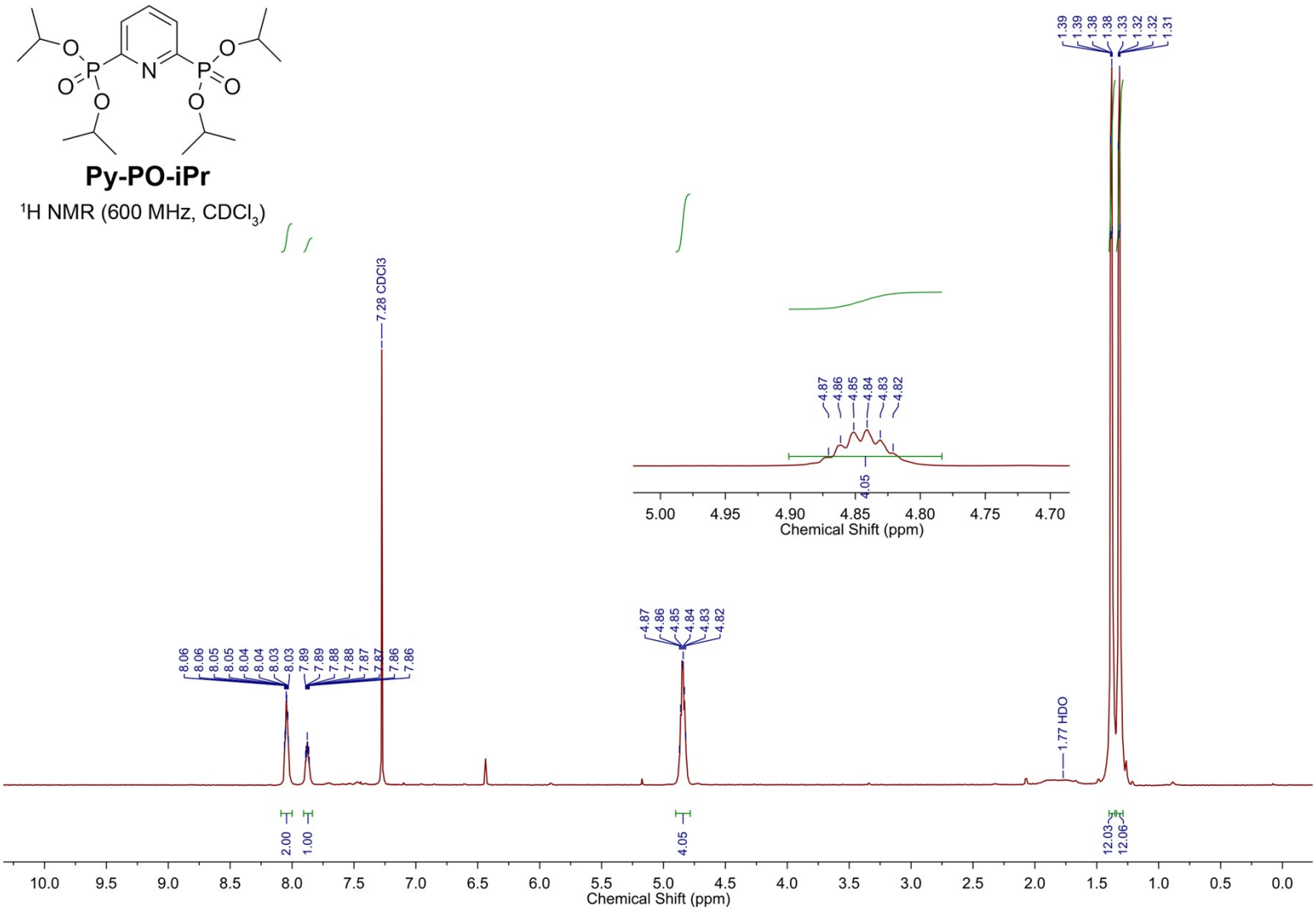

Figure S1 ^{1}H NMR spectra of the PO-Py-iPr ligand

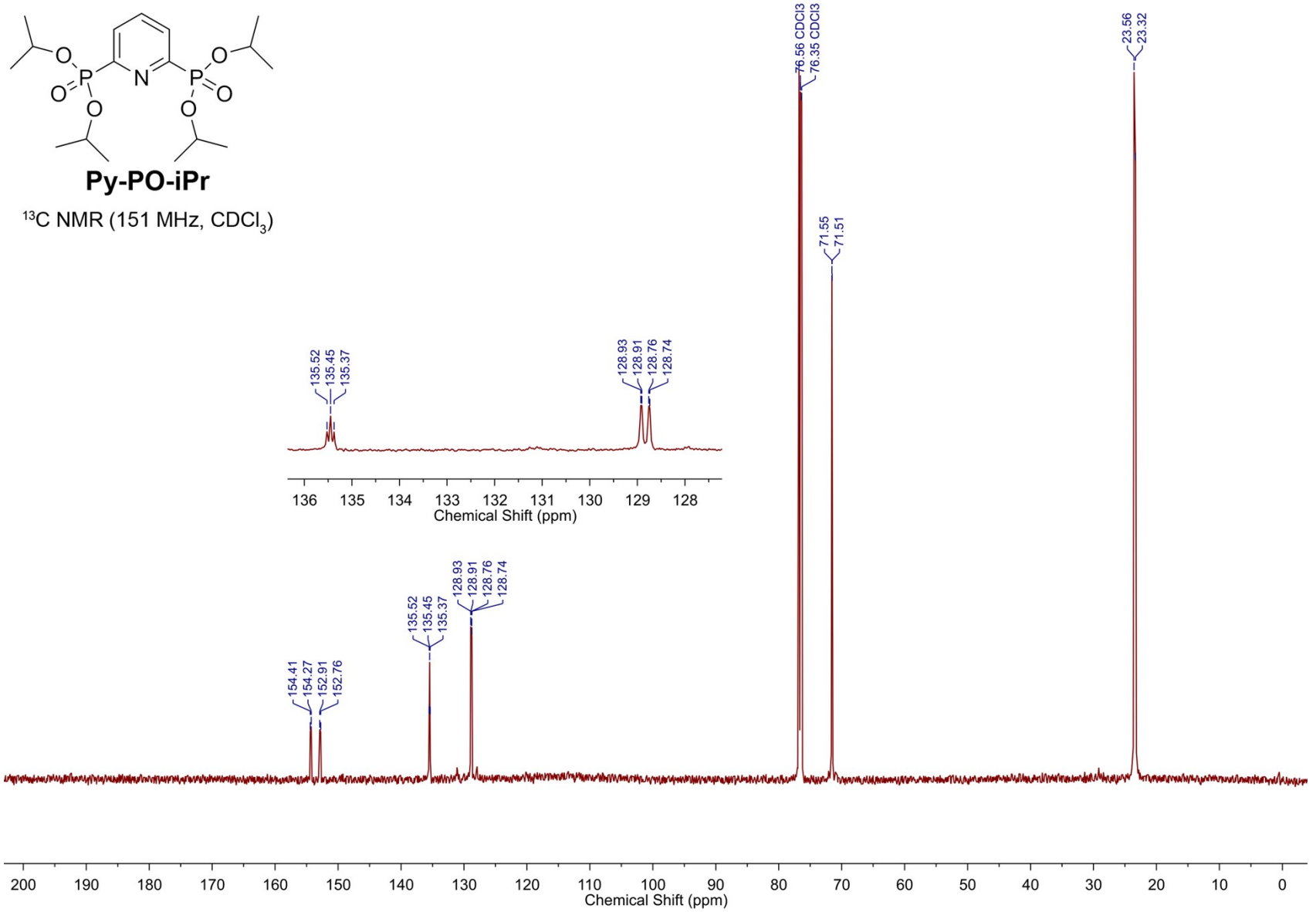

Figure S2 ^{13}C NMR spectra of the PO-Py-iPr ligand

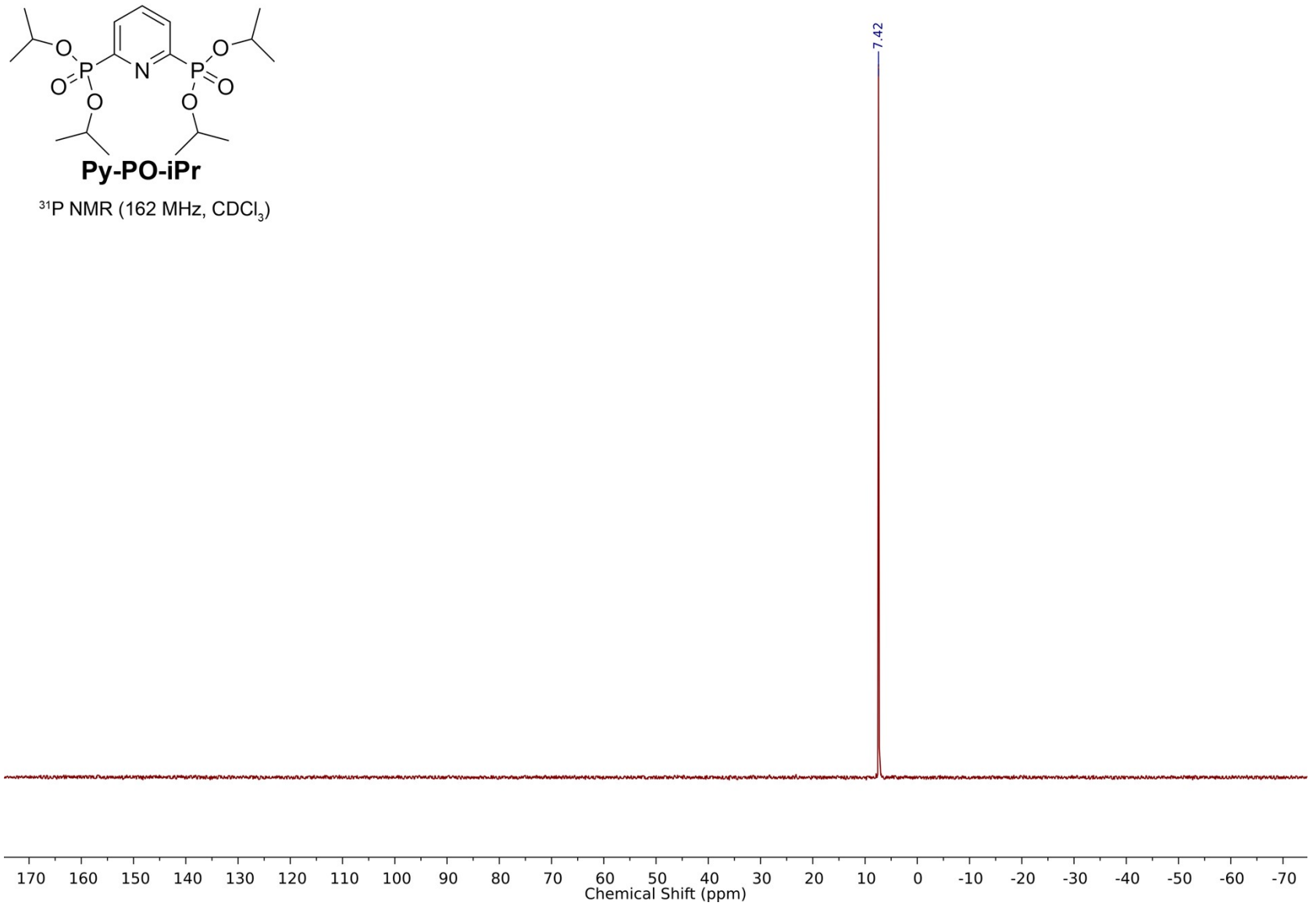

Figure S3 ^{31}P NMR spectra of the PO-Py-iPr ligand

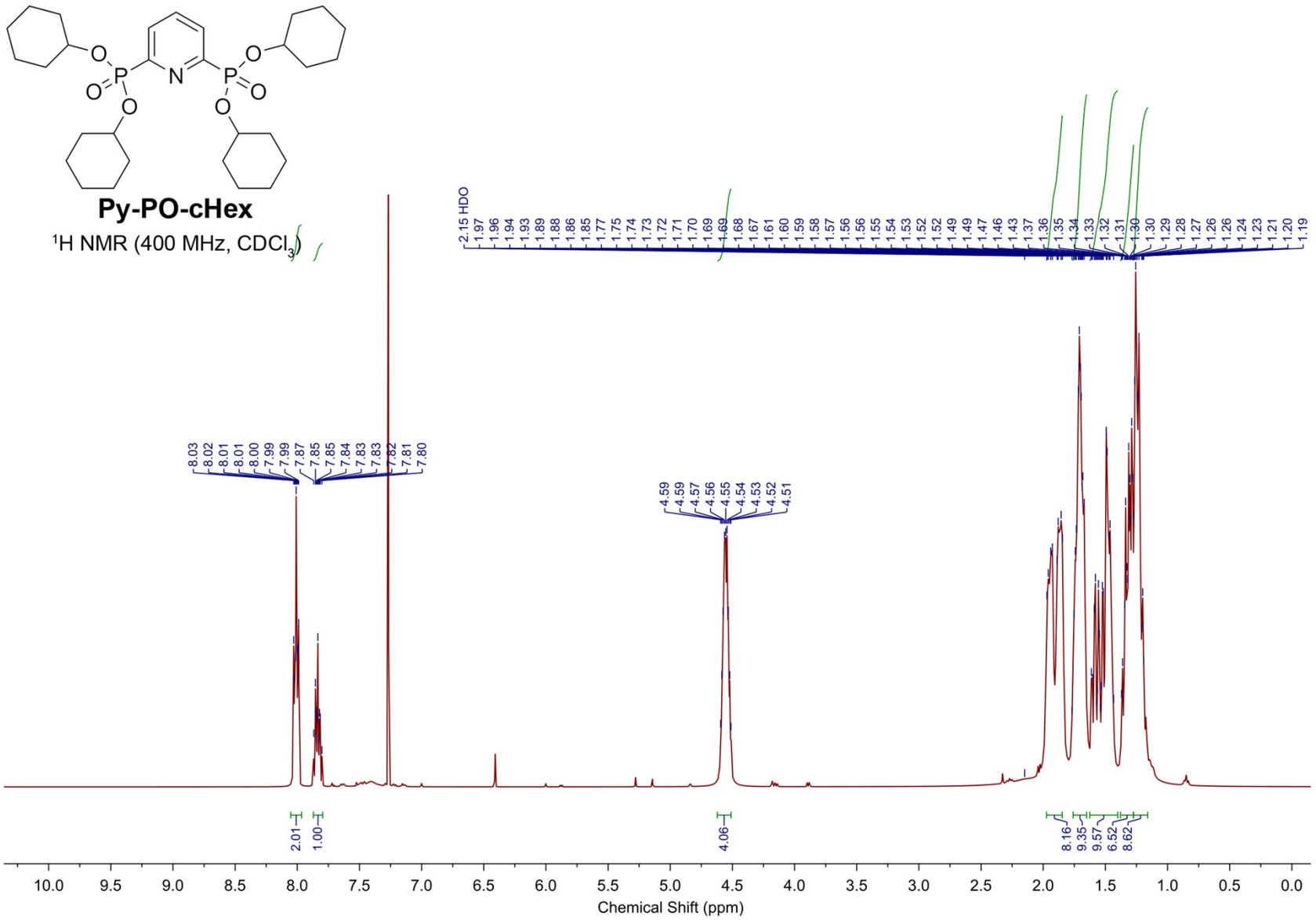

Figure S4 ^{1}H NMR spectra of the PO-Py-cHex ligand

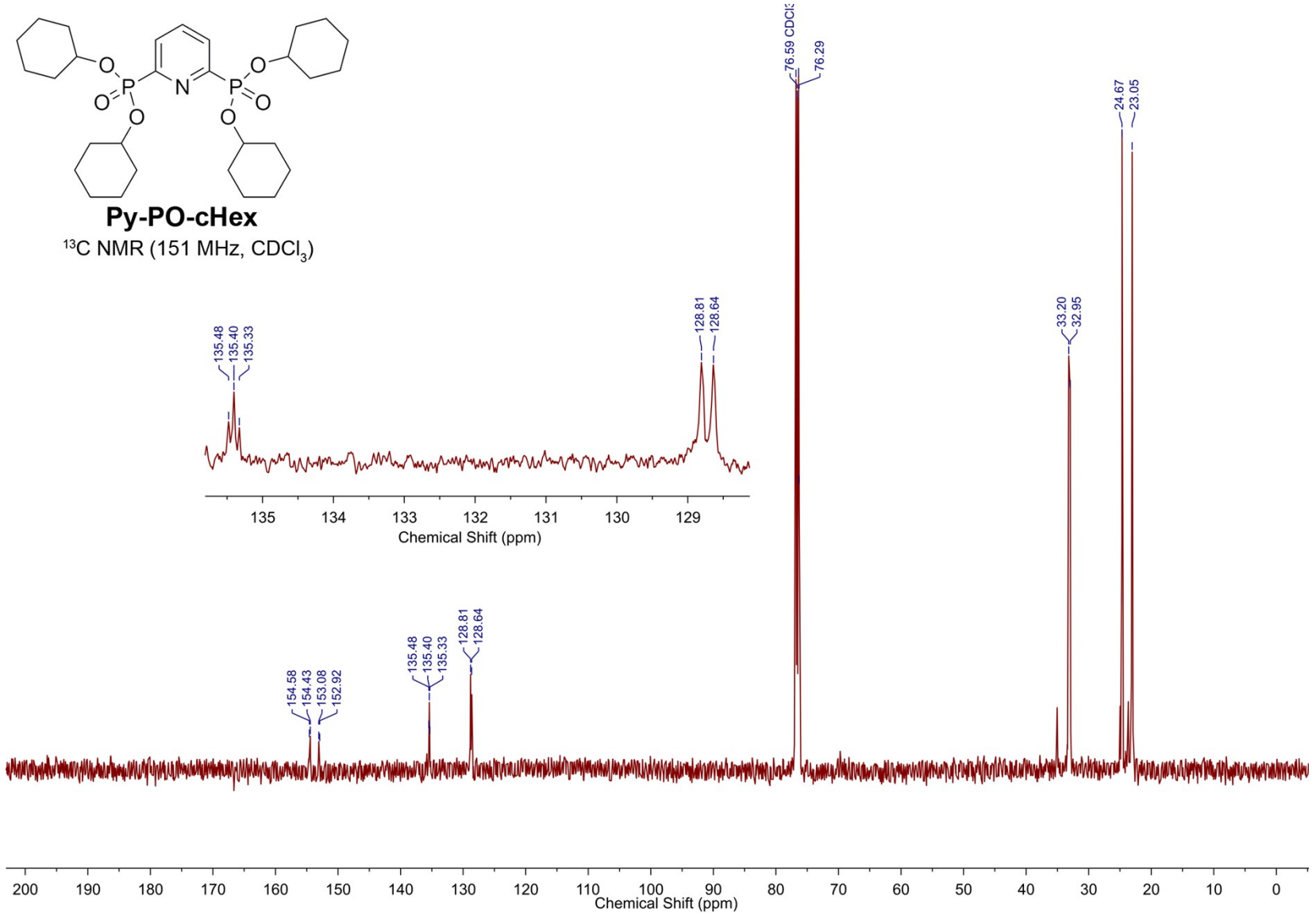

Figure S5 ^{13}C NMR spectra of the PO-Py-cHex ligand

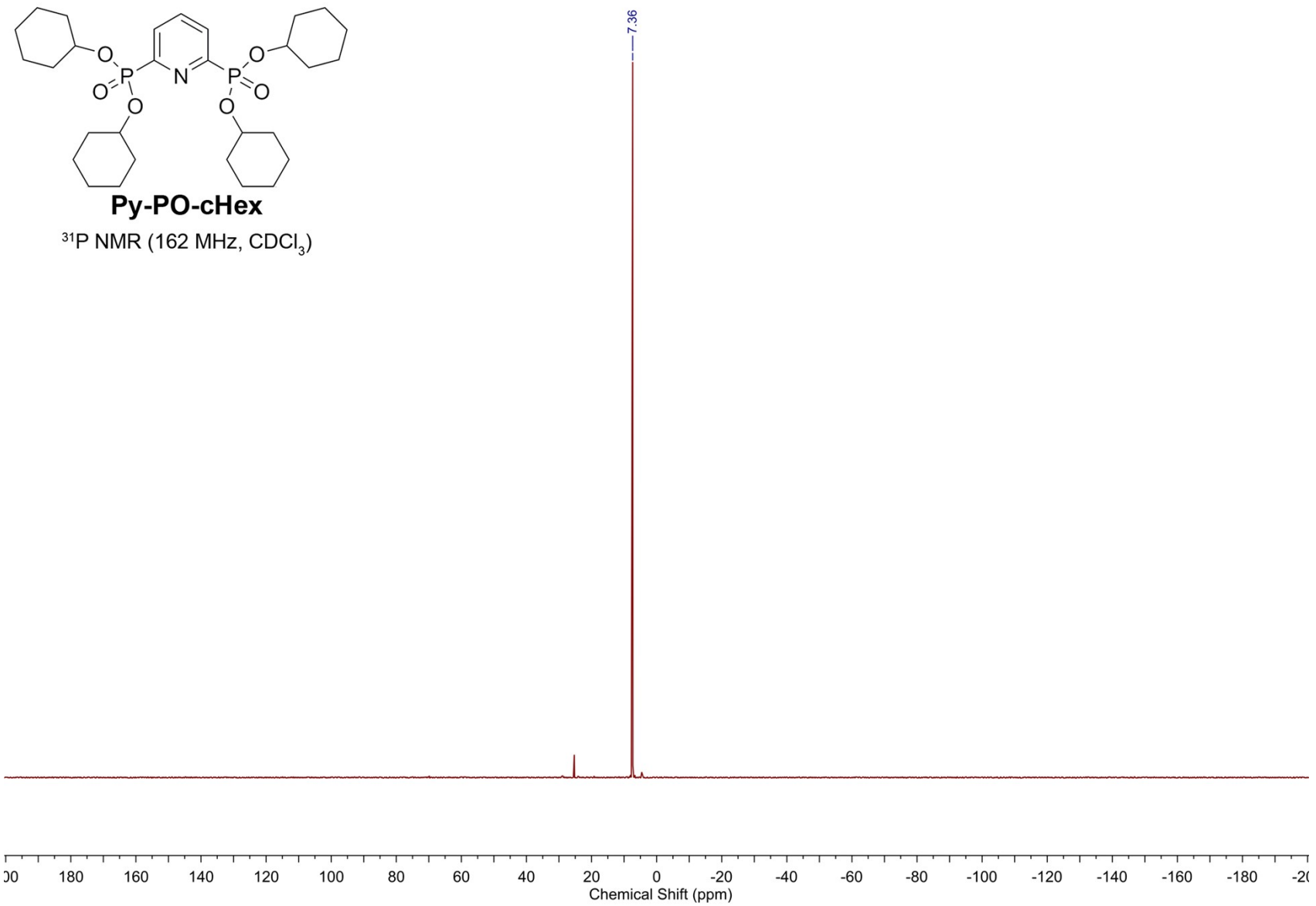

Figure S6 ^{31}P NMR spectra of the PO-Py-cHex ligand

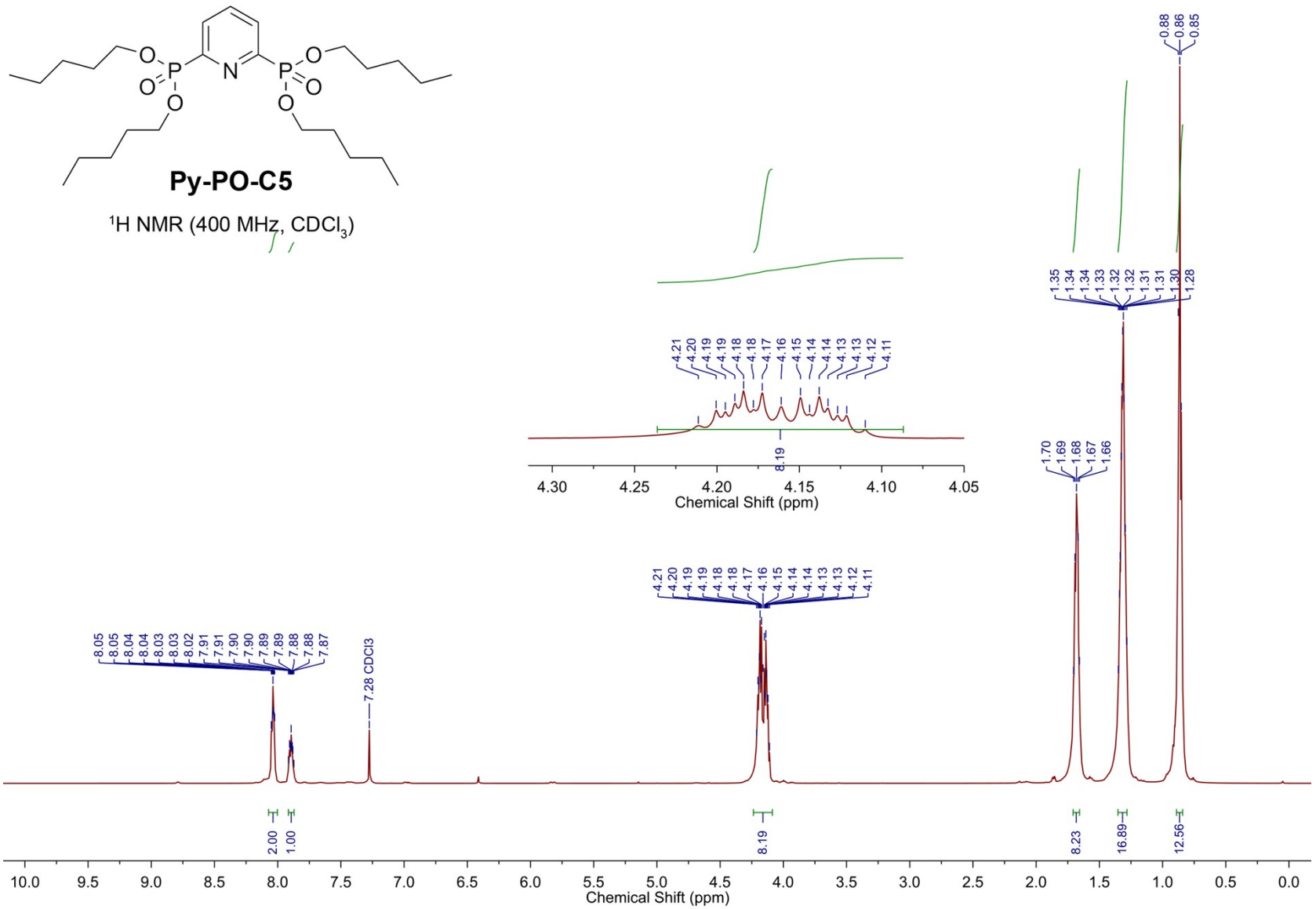

Figure S7 ^{1}H NMR spectra of the PO-Py-C5 ligand

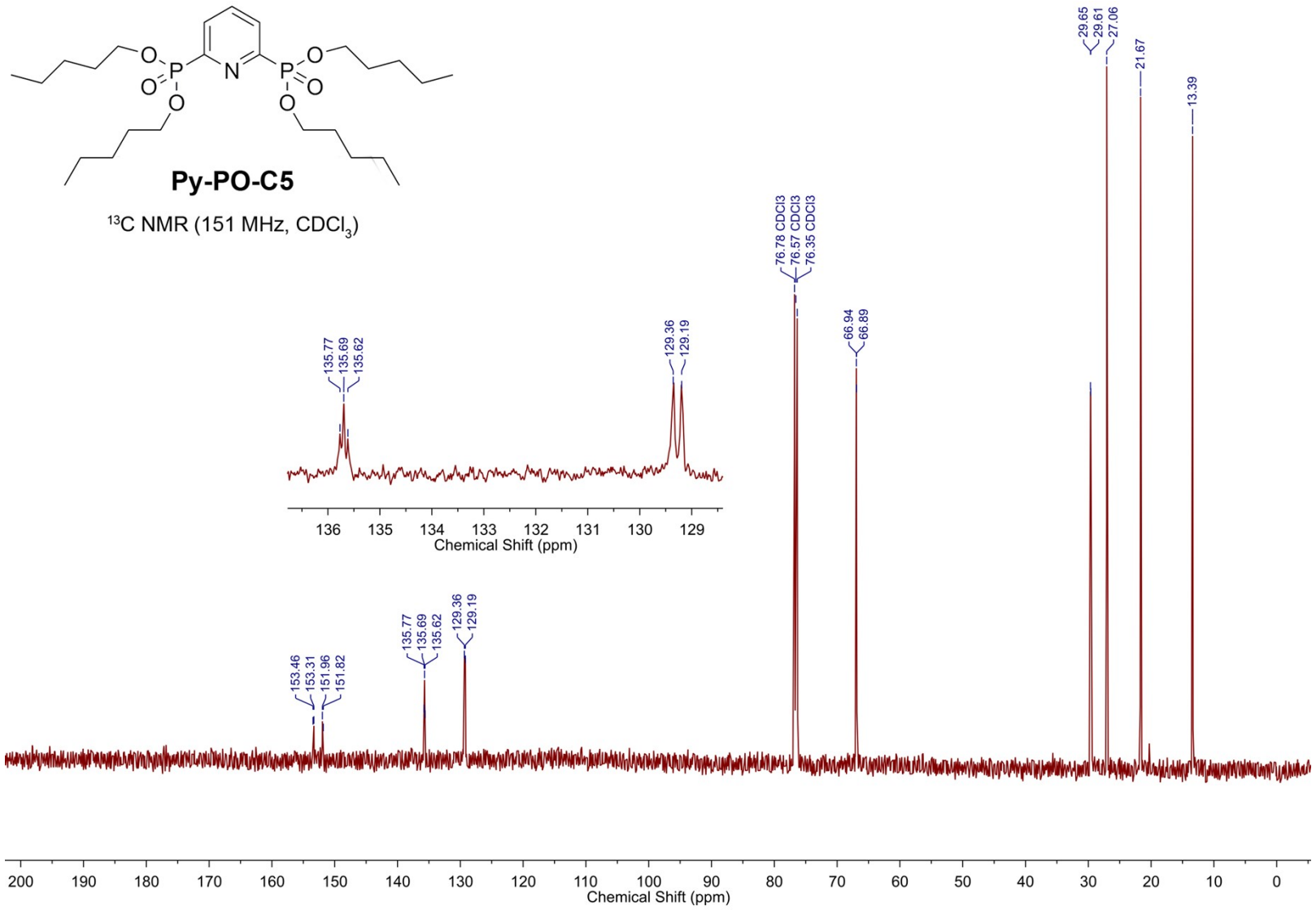

Figure S8 ^{13}C NMR spectra of the PO-Py-C5 ligand

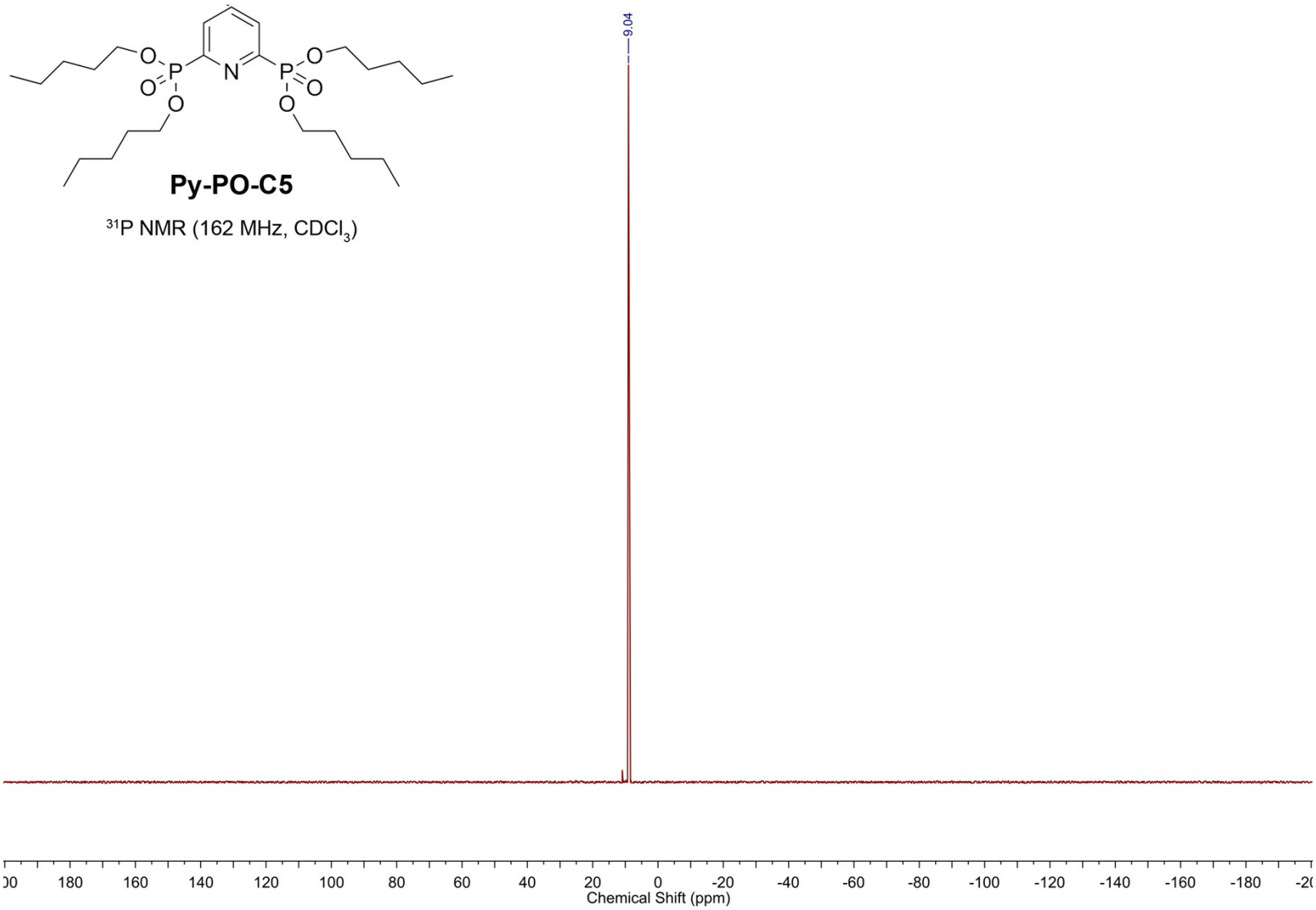

Figure S9 ^{31}P NMR spectra of the PO-Py-C5 ligand

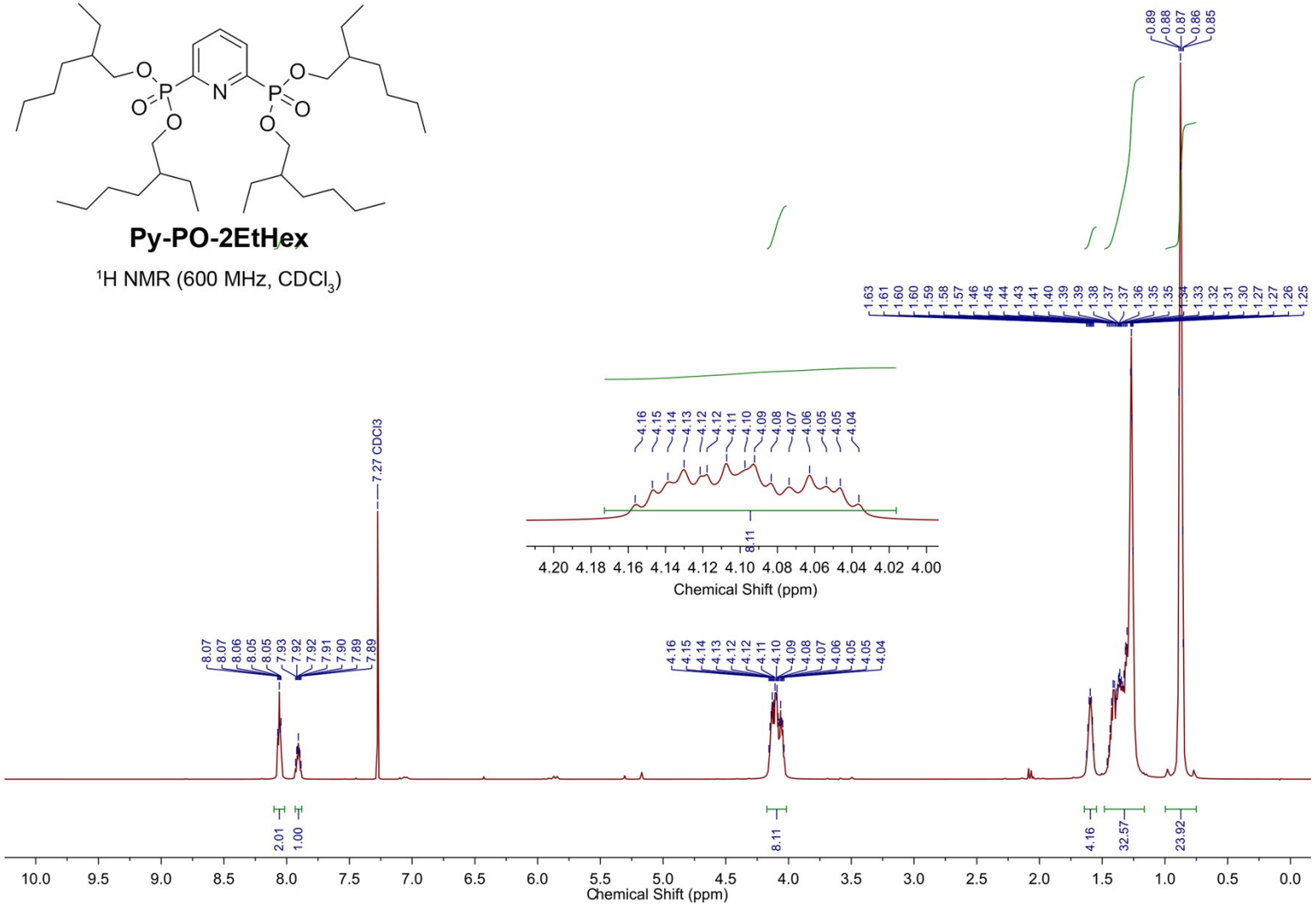

Figure S10 ^{1}H NMR spectra of the PO-Py-2EtHex ligand

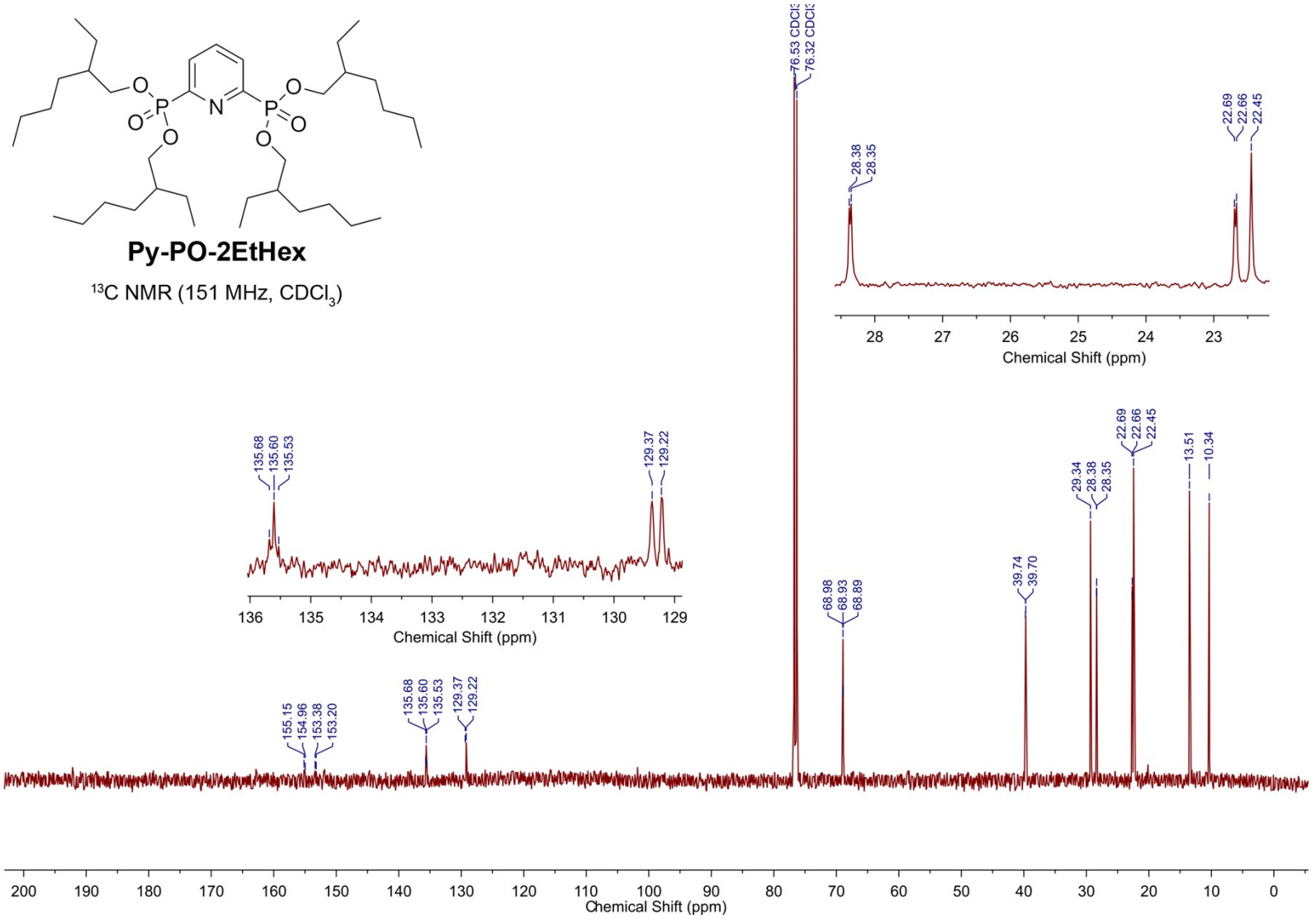

Figure S11 ^{13}C NMR spectra of the PO-Py-2EtHex ligand

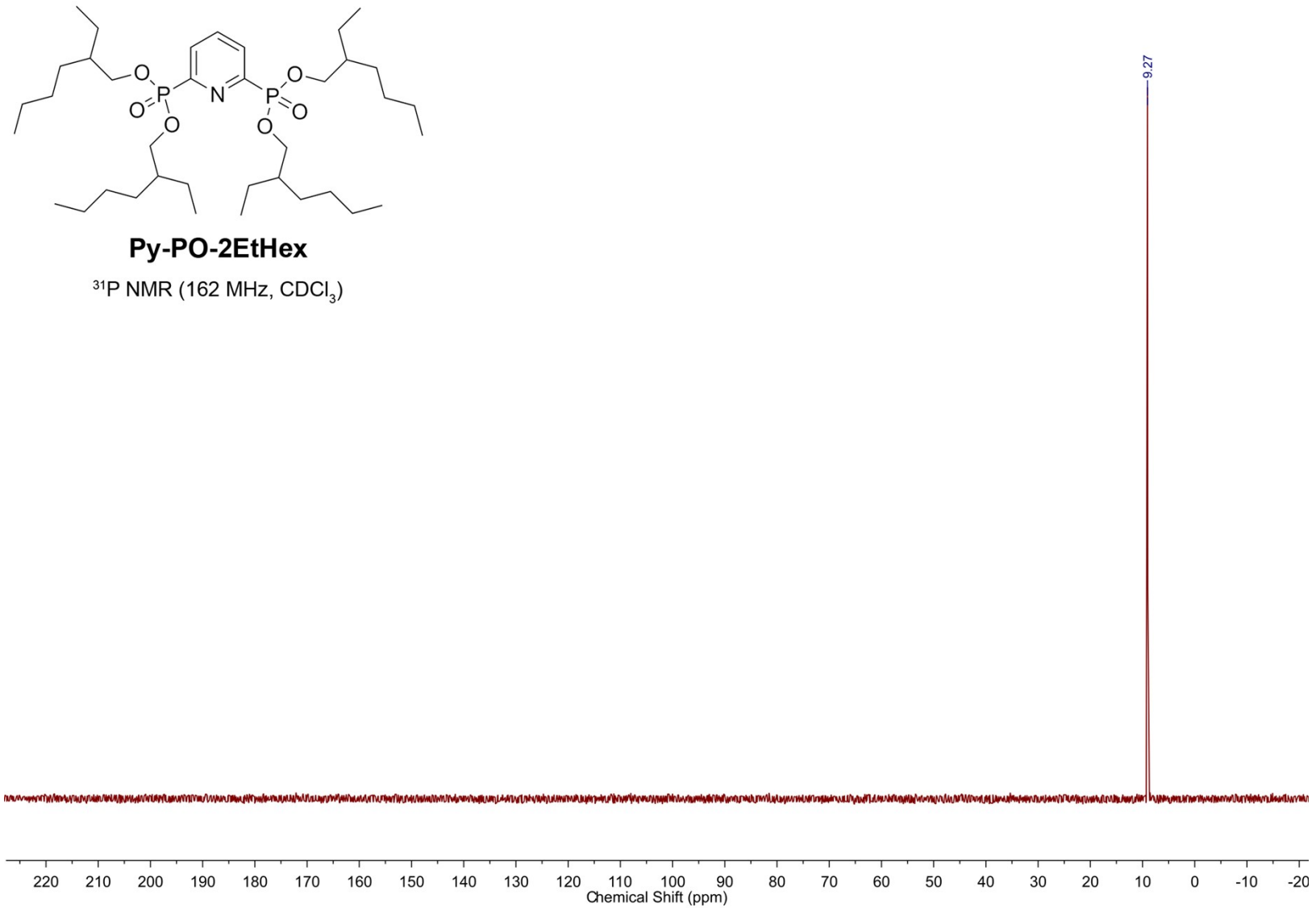

Figure S12 ^{13}P NMR spectra of the PO-Py-2EtHex ligand

3. Extraction data for the PO-Py-R ligands;

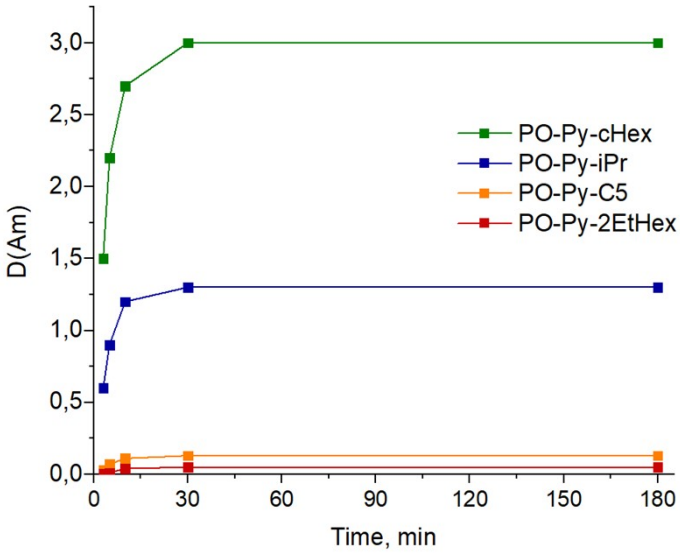

Figure S13 Kinetics of extraction of Am(III) for PO-Py-R ligands in a vortex shaker, Organic phase: c(L) = 0.05 mol L^{-1} in F-3, Aqueous phase: c(HNO3) = 3 mol L−1 with ^{152}Eu(III) and ^{241}Am(III) tracers. Temperature: 25±1 °C.

Table S1 Extraction data for PO-Py-R ligands, **Organic phase**: c(L) = 0.05 mol L^{-1} in F-3, **Aqueous phase**: c(HNO_3) = 3 mol ·L^{-1} with ^{152}Eu(III) and ^{241}Am(III) radiotracers. Temperature: 25°±1 C.

Ligand	D(Am)	D(Eu)	SF(Am/Eu)
PO-Py-cHex	3.0 ± 0.3	0.29 ± 0.03	10.3
PO-Py-iPr	1.3 ± 0.2	0.28 ± 0.03	4.7
PO-Py-C5	0.13 ± 0.02	0.04 ± 0.01	3.3
PO-Py-2EtHex	0.05 ± 0.01	0.01 ± 0.005	5.0

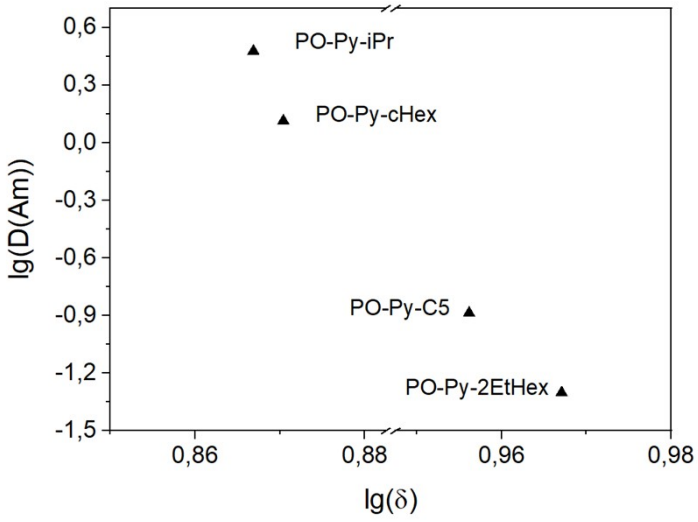

Figure S14 Dependence of the distribution ratio of Am(III) for the ligand on the chemical shift in its ^{31}P NMR spectra.

4. Liquid tension experiment

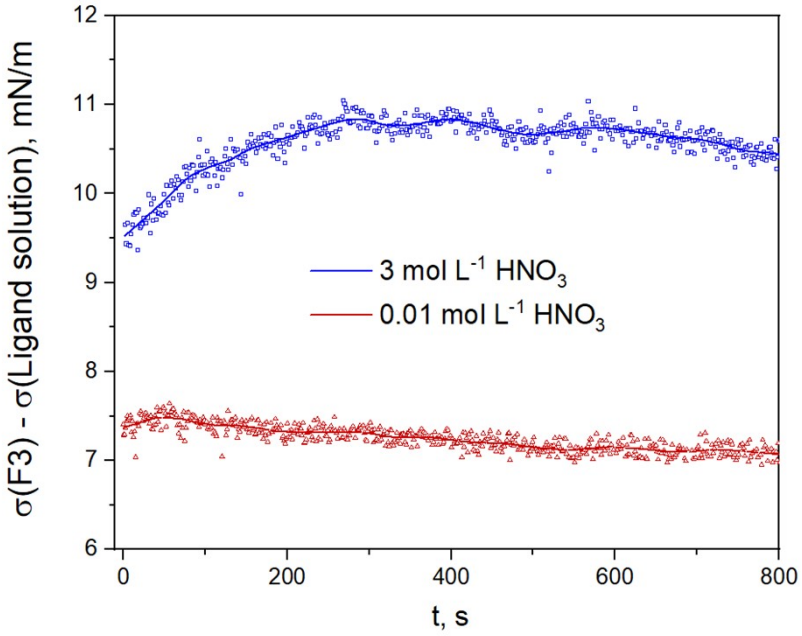

Figure S15 Changes in the surface tension of the ligands relative to that of the pure solvent over time Drop phase c(PO-Py-iPr) = 0.05 mol L^{-1} in F-3, External phase: — aqueous solution HNO_3 0.01 mol L^{-1}, — aqueous solution HNO_3 3 mol L^{-1}.

5. Spectrophotometric titration;

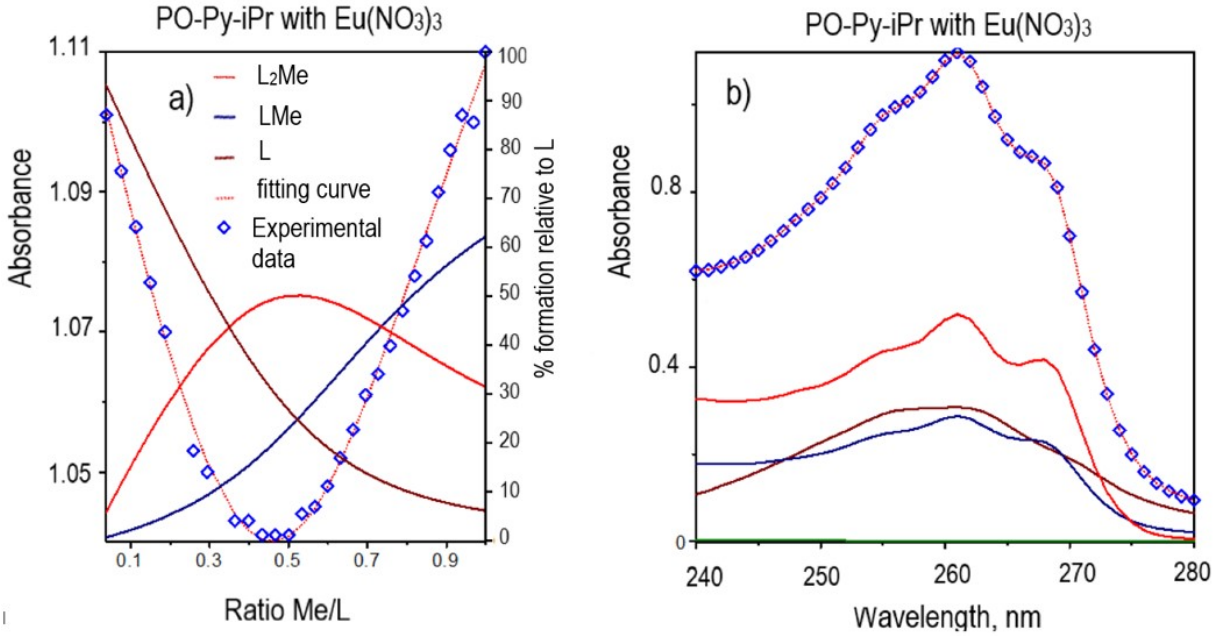

Figure S16 Experimental data (blue diamonds) ◊ obtained by spectrophotometric titration and fit (red dashed lines) ····· for PO-Py-iPr ligand and $Eu(NO_3)_3$ a) at various Me/L ratios at a wavelength of 273 nm b) full view of the spectrum

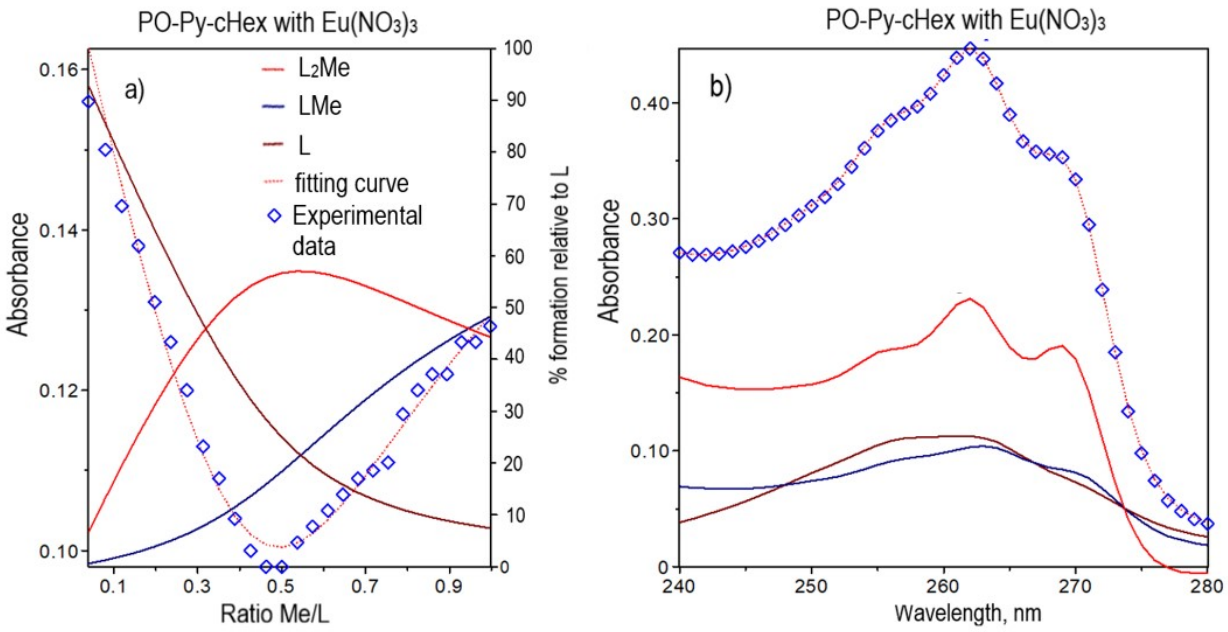

Figure S17 Experimental data (blue diamonds) ◊ obtained by spectrophotometric titration and fit (red dashed lines) ····· for PO-Py-cHex ligand and $Eu(NO_3)_3$ a) at various Me/L ratios at a wavelength of 273 nm b) full view of the spectrum

6. Free energy of complexes in nitrobenzene solution

	Am-POPyiPr-3NO3	Eu-POPyiPr -3NO3	Am-POPy2EtHex-3NO3	Eu-POPy2EtHex-3NO3
Thermal correction	0.69784	0.69808	0.969	0.9706
SCF Energy	-3292.79084	-3407.74888	-4079.24837	-4194.20658
Free Energy	-3292.093	-3407.0508	-4078.27937	-4193.23598
	Am-POPyC5-3NO3	**Eu-POPyC5-3NO3**	**Am-POPycHex-3NO3**	**Eu-POPycHex-3NO3**
Thermal correction	0.6491	0.6522	0.69784	0.69808
SCF Energy	-3607.37113	-3722.32908	-3759.86916	-3874.81781
Free Energy	-3606.72203	-3721.67688	-3759.17132	-3874.11973
	POPy2iPr	**POPy2EtHex**	**POPyC5**	**POPycHex**
Thermal correction	0.4126	0.9434	0.6230	0.6700
SCF Energy	-1855.8397	-2642.2996	-2170.4235	-2322.9069
Free Energy	-1855.4271	-2641.3562	-2169.8005	-2322.2369

7. Free energy of complexes in aqueous solution

	Am-POPy2iPr-3NO3	Eu-POPy2iPr-3NO3	Am-POPy2EtHex-3NO3	Eu-POPy2EtHex-3NO3
Thermal correction	0.6978	0.6981	0.969	0.9706
SCF Energy	-3292.8196	-3407.7560	-4079.2569	-4194.19354
Free Energy	-3292.1218	-3407.0579	-4078.2879	-4193.22294
	Am-POPyC5-3NO3	**Eu-POPyC5-3NO3**	**Am-POPycHex-**	**Eu-POPycHex-3NO3**

			3NO3	
Thermal correction	0.6491	0.6522	0.69784	0.69808
SCF Energy	-3607.39046	-3722.32641	-3759.88499	-3874.81742
Free Energy	-3606.74136	-3721.67421	-3759.18715	-3874.11934
	POPy2iPr	**POPy2EtHex**	**POPyC5**	**POPycHex**
Thermal correction	0.41264	0.94338	0.62298	0.66999
SCF Energy	-1855.83066	-2642.26869	-2170.4029	-2322.88857
Free Energy	-1855.41802	-2641.32531	-2169.77992	-2322.21858
	$[Am(H_2O)_9]^{3+}$	**$[Eu(H_2O)_9]^{3+}$**	**$[Am(NO_3)(H_2O)_7]^{2+}$**	**$[Eu(NO_3)(H_2O)_7]^{2+}$**
Thermal correction	0.16274	0.16767	0.14311	0.14213
SCF Energy	-1283.50155	-1398.49467	-1411.1319	-1526.14616
Free Energy	-1283.33881	-1398.327	-1410.98879	-1526.00403
	H_2O	**NO_3^-**		
Thermal correction	0.0035	-0.01123		
SCF Energy	-76.46024	-280.5292		
Free Energy	-76.45674	-280.54043		

8. Partial density of states of Am-5f/6d, Eu-4f/5d orbitals and the N/O-2p orbitals of the ligands in the ML(NO3)3 complexes

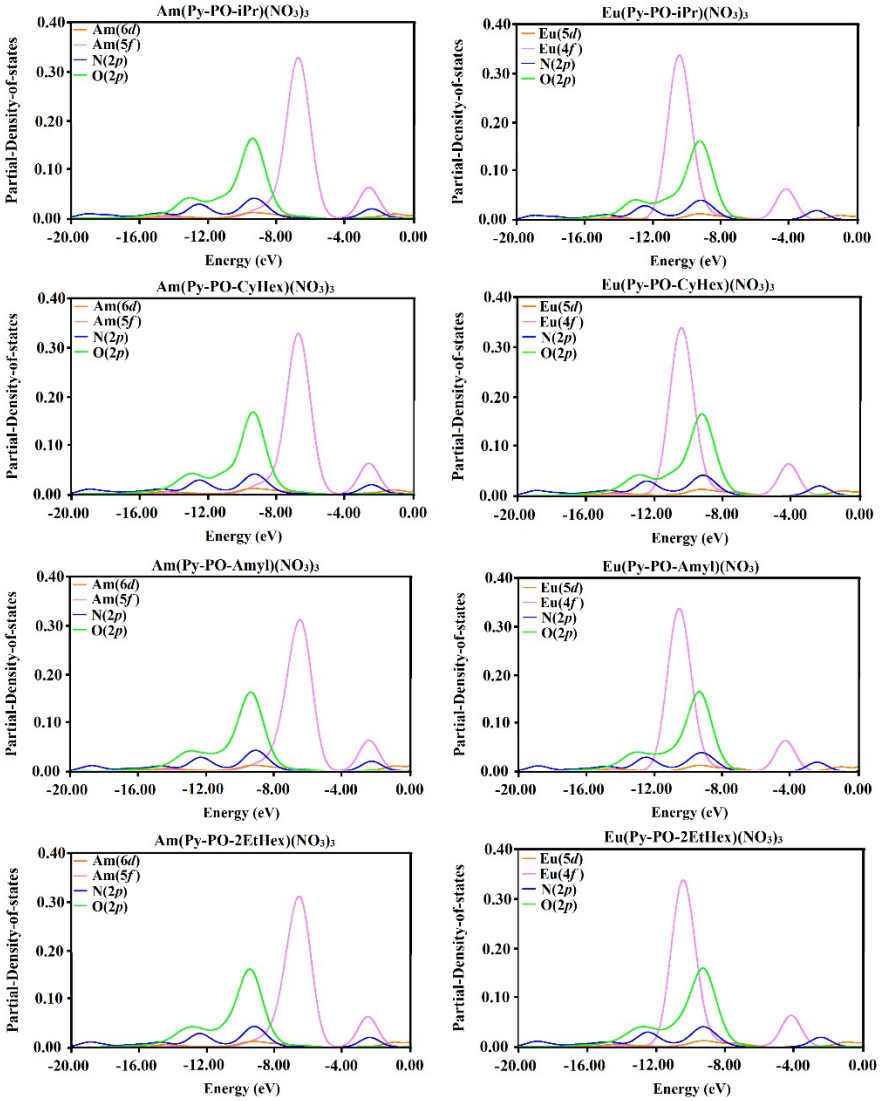

Figure S18 Partial density of states of Am-5f/6d, Eu-4f/5d orbitals and the N/O-2p orbitals of the ligands in the $ML(NO_3)_3$ complexes.

9. Geometrical structure data (.xyz files) of 8 $ML(NO_3)_3$ complexes (M=Am, Eu, L= PO-Py-cHex, PO-Py-2EtHex, PO-Py-iPr, and PO-Py-C5).

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Am(PO-Py-cHex)$(NO_3)_3$-opted

C	1.01410700	-0.07960200	-2.07296000
C	1.07474700	-0.20907900	-3.46290200
C	-0.12094600	-0.31077100	-4.17352900
C	-1.32799600	-0.31097100	-3.47458400
C	-1.29734600	-0.18537700	-2.08231200
N	-0.14782400	-0.04974300	-1.40064900
H	-0.11143600	-0.40324900	-5.25559000
H	2.03447800	-0.23115400	-3.96832200
H	-2.27711900	-0.41463800	-3.99035000
P	-2.80168300	-0.28864800	-1.03491100
P	2.48772800	0.02602800	-0.99653900

O	2.08152200	-0.07805500	0.44877500
O	-2.39883600	-0.06496700	0.39456600
Am	-0.17717100	0.36551700	1.38979100
N	0.36541900	-2.49893400	1.93047800
O	-0.28854000	-2.11894800	0.88510500
O	0.72217700	-1.56702500	2.72702800
N	-0.04586100	3.15563800	0.35809300
O	-1.15786000	2.52368100	0.48805000
O	0.99287700	2.52077200	0.75877000
N	-0.90516000	1.06029700	4.09602100
O	0.26157300	1.30248900	3.59852300
O	-1.74641200	0.53072700	3.27291800
O	0.01461600	4.26911100	-0.13103000
O	-1.18778600	1.31636100	5.24329100
O	0.62282500	-3.67335300	2.13275800
O	3.49474400	-1.12526000	-1.46097400
O	3.16180600	1.37376600	-1.48503400
O	-3.87001200	0.69988100	-1.66995600
O	-3.48341800	-1.68773600	-1.35398400
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C	5.45176600	1.88685800	-0.75935200
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H	3.63381100	2.09201600	0.41441200
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H	5.62197200	0.85604900	-0.42588800
C	4.56356900	4.66623700	-0.23692600
H	3.88953800	3.78625900	-2.10799500
H	2.62231700	3.90428600	-0.87043500
C	6.05573000	4.32501200	-0.36779400
H	7.38676000	2.61708500	-0.10966700
H	6.12762100	2.74640600	1.11248100
H	4.37032600	5.68938600	-0.57986200
H	4.27172300	4.63420000	0.82213000
H	6.65650500	5.00672300	0.24669600
H	6.37441100	4.47640200	-1.40965900
C	3.58681700	-2.42646400	-0.76369800
C	2.47454000	-3.36500200	-1.22754700
C	4.97594800	-2.98108600	-1.06247300
H	3.48395200	-2.22299000	0.30681000
C	2.64900500	-4.76118500	-0.60089000
H	2.51180600	-3.43477000	-2.32398500
H	1.49694500	-2.95679900	-0.94589600
C	5.14764500	-4.36963400	-0.42115600
H	5.09834800	-3.05361600	-2.15186900
H	5.73829100	-2.28324600	-0.69695400
C	4.04542000	-5.33831900	-0.87659900
H	1.87206500	-5.43019600	-0.98953700
H	2.47731300	-4.69058800	0.48070100
H	6.13896000	-4.76626400	-0.67067000
H	5.11650900	-4.27107600	0.67317700
H	4.16034300	-6.30462000	-0.37073200
H	4.15659700	-5.53178100	-1.95397900
C	-3.75369400	2.16799700	-1.48880500
C	-4.32246900	2.81544600	-2.74574200
C	-4.49547200	2.59302100	-0.22617100
H	-2.69226400	2.41598400	-1.38265000

C	-4.29172800	4.34941800	-2.61152300
H	-5.35539700	2.46781400	-2.88244400
H	-3.75257400	2.49052800	-3.62521000
C	-4.44908300	4.12556200	-0.08892200
H	-5.53592600	2.24702300	-0.29821200
H	-4.04266600	2.11379000	0.64672000
C	-5.01294500	4.81994800	-1.33835600
H	-4.74260800	4.80332300	-3.50233100
H	-3.24646100	4.68832100	-2.58096400
H	-5.00796100	4.42858200	0.80417300
H	-3.40728200	4.43445700	0.07097100
H	-4.92481500	5.90885000	-1.23984800
H	-6.08667300	4.59748900	-1.42659900
C	-3.23796400	-2.88916700	-0.52128700
C	-4.58847500	-3.53804200	-0.24404500
C	-2.28388300	-3.82365300	-1.25809600
H	-2.78126100	-2.55647900	0.41426000
C	-4.39060000	-4.83021100	0.57064600
H	-5.07590200	-3.76611200	-1.20180800
H	-5.23485500	-2.83360000	0.29166000
C	-2.07980600	-5.11641400	-0.44723000
H	-2.70771900	-4.05394400	-2.24566700
H	-1.32211900	-3.32286300	-1.41235100
C	-3.41993900	-5.79699300	-0.12674800
H	-5.36206900	-5.31175700	0.73425300
H	-3.99790800	-4.57425400	1.56474200
H	-1.42995500	-5.79956300	-1.00806000
H	-1.54577200	-4.87043400	0.48014200
H	-3.25337400	-6.68021900	0.50191800
H	-3.87706000	-6.15711500	-1.06041500

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Eu(PO-Py-cHex)(NO_3)$_3$-opted

C	1.09508900	-0.13167200	-1.99792600
C	1.14816500	-0.21770200	-3.39180700
C	-0.04898800	-0.18823400	-4.10633600
C	-1.25513500	-0.10662300	-3.40969400
C	-1.21631500	-0.03019300	-2.01526900
N	-0.06237400	-0.01831700	-1.32832600
H	-0.04326700	-0.24451300	-5.19087600
H	2.10383700	-0.30961000	-3.89699000
H	-2.20733700	-0.10967000	-3.92991100
P	-2.70716100	-0.03662000	-0.95260900
P	2.56379200	-0.23076300	-0.91299700
O	2.14011200	-0.31416100	0.52761600
O	-2.28984400	0.10208200	0.48376100
Eu	-0.05301500	0.33906200	1.40954100
N	0.31328000	-2.49181300	1.95037300
O	-0.28775200	-2.08303300	0.88515700
O	0.62514300	-1.58197000	2.79045500
N	0.26733700	3.06561300	0.34513900
O	-0.88244100	2.57967800	0.63935700
O	1.26251900	2.29958600	0.59843800
N	-0.58614400	1.24795500	4.04155800
O	0.57607100	1.34985100	3.49239800
O	-1.50194200	0.74114500	3.29051600
O	0.40060900	4.16660400	-0.15933100

O	-0.80059300	1.60855500	5.17648600
O	0.56825800	-3.66916300	2.13300700
O	3.40897900	-1.49126500	-1.41071200
O	3.42064800	1.02196100	-1.36806200
O	-3.70043200	1.06950600	-1.52347200
O	-3.44141200	-1.39180100	-1.33529600
C	4.26864900	1.81490500	-0.44717000
C	5.69372700	1.26915400	-0.47577700
C	4.18133600	3.26501800	-0.90743800
H	3.83448600	1.71844000	0.55175000
C	6.62238000	2.15609000	0.37383300
H	6.04059900	1.25211700	-1.51784600
H	5.70905400	0.23409300	-0.11319500
C	5.11544500	4.14847600	-0.06072200
H	4.47567100	3.31591700	-1.96519200
H	3.14500600	3.60628400	-0.82677400
C	6.55995900	3.62492900	-0.07315400
H	7.64917100	1.77593100	0.31174800
H	6.32652800	2.08406200	1.43028300
H	5.07552500	5.17943000	-0.43148500
H	4.74574200	4.17647700	0.97403000
H	7.19320300	4.24287600	0.57530700
H	6.97071400	3.71195800	-1.08993300
C	3.35682600	-2.81306900	-0.74872600
C	2.19518300	-3.64008700	-1.29725400
C	4.71111800	-3.46787000	-1.00063700
H	3.21625700	-2.63253900	0.32148400
C	2.23162900	-5.06953700	-0.72313100
H	2.27523500	-3.66880400	-2.39327900
H	1.24215300	-3.16577400	-1.03693600
C	4.74119900	-4.88921900	-0.41194400
H	4.88300100	-3.50848600	-2.08498500
H	5.50602400	-2.84769600	-0.57018900
C	3.58977300	-5.74554600	-0.96075900
H	1.42442400	-5.65924800	-1.17382500
H	2.01630800	-5.02312900	0.35187000
H	5.70929000	-5.35511000	-0.63171300
H	4.66278900	-4.83184000	0.68296200
H	3.60315100	-6.73813600	-0.49419200
H	3.73818600	-5.90285300	-2.03957600
C	-3.46554500	2.51744300	-1.30014200
C	-3.98858500	3.24674900	-2.53188800
C	-4.15913400	2.96368700	-0.01770000
H	-2.38765600	2.67668600	-1.19593300
C	-3.82936600	4.76812800	-2.35310600
H	-5.04801300	2.99067300	-2.66898400
H	-3.45406300	2.90239900	-3.42604500
C	-3.98593000	4.48267000	0.16330600
H	-5.22523500	2.70561000	-0.08695600
H	-3.73778400	2.42430400	0.83569600
C	-4.49953200	5.25832200	-1.05964500
H	-4.24783000	5.28444600	-3.22562000
H	-2.75944500	5.01840800	-2.32309300
H	-4.51084000	4.80415500	1.07046800
H	-2.92085000	4.69887200	0.32131400
H	-4.32009700	6.33269800	-0.93023800
H	-5.58872900	5.12899800	-1.14378300

C	-3.99551000	-2.31909700	-0.32123900
C	-5.47451400	-2.51948000	-0.63593600
C	-3.19943600	-3.61920300	-0.37253100
H	-3.87287600	-1.84684500	0.65839900
C	-6.08926100	-3.55996300	0.31820100
H	-5.56611800	-2.86430400	-1.67480400
H	-6.00321000	-1.56166400	-0.56501200
C	-3.81883300	-4.65922500	0.57925200
H	-3.21909200	-3.99799800	-1.40412700
H	-2.15610000	-3.42386800	-0.10347300
C	-5.30979200	-4.88403200	0.28472900
H	-7.14086700	-3.72266200	0.05330300
H	-6.08405300	-3.16115000	1.34277700
H	-3.26319600	-5.60089100	0.50044100
H	-3.69865400	-4.31648700	1.61674100
H	-5.73647200	-5.59042900	1.00739000
H	-5.41976200	-5.34485200	-0.70809000

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Am(PO-Py-iPr)-opted

C	-1.24877400	-1.52079600	1.51789000
C	-1.35574300	-2.46823000	2.53989300
C	-0.18450900	-2.98929200	3.08818400
C	1.04744800	-2.57383600	2.58144700
C	1.06029400	-1.63027500	1.55179600
N	-0.06493700	-1.09886900	1.04840100
H	-0.23067800	-3.71929500	3.89089500
H	-2.33205900	-2.78404600	2.89203800
H	1.97909400	-2.97475200	2.96674500
P	2.57978400	-1.08677900	0.69203900
P	-2.68315200	-0.77607800	0.66357300
O	-2.22273700	0.08687400	-0.47859100
O	2.26977800	0.03200500	-0.26166100
Am	0.06697100	1.03814200	-0.78069200
N	-0.55633500	-0.74004800	-3.04699800
O	0.13484700	-1.15932400	-2.04090700
O	-0.79325700	0.51786300	-3.06404900
N	-0.20547000	2.31153000	1.89944000
O	0.92871200	1.91498300	1.43859700
O	-1.19301700	2.18889200	1.09280600
N	0.91101200	3.41878000	-2.18541100
O	-0.29435700	3.24819600	-1.75792600
O	1.72934200	2.46170300	-1.89902600
O	-0.33175900	2.75057800	3.02746100
O	1.24942400	4.40260200	-2.80170200
O	-0.96278900	-1.49759500	-3.90755800
O	-3.63133400	-1.98131100	0.21403600
O	-3.45503000	-0.07824900	1.85890100
O	3.68153400	-0.76798000	1.79873000
O	3.08707900	-2.44201300	0.03548000
C	-4.28106500	1.14790900	1.70694200
C	-4.07305100	1.95025200	2.97979600
C	-5.72322100	0.72923500	1.45912000
H	-3.87799800	1.69560400	0.85178800
H	-3.02231100	2.22889400	3.09019300
H	-4.67023500	2.86774900	2.93180900

H	-4.39386500	1.37608100	3.85632200
H	-5.81598900	0.13264900	0.54612900
H	-6.10422800	0.13945000	2.29974500
H	-6.35070000	1.62070300	1.34920300
C	-3.65272400	-2.51706200	-1.16938700
C	-5.02738000	-3.14470000	-1.33794000
C	-2.50292200	-3.49545400	-1.36540400
H	-3.53749300	-1.66334500	-1.84228900
H	-5.81812600	-2.40984600	-1.15913300
H	-5.13350300	-3.52566300	-2.35912900
H	-5.16193800	-3.97910800	-0.64101600
H	-1.53238800	-2.99482000	-1.29731000
H	-2.55421200	-4.30376000	-0.62708500
H	-2.56688900	-3.93421200	-2.36667900
C	3.81490000	-2.47312400	-1.25826300
C	2.99232300	-3.32999900	-2.20702000
C	5.21186200	-3.00450700	-0.97578500
H	3.86106300	-1.44629700	-1.63195600
H	2.00136600	-2.89301200	-2.36053600
H	3.49875000	-3.39358900	-3.17679900
H	2.88087900	-4.34512500	-1.80960600
H	5.73887300	-2.36323600	-0.26261300
H	5.16303500	-4.01830300	-0.56394000
H	5.79020000	-3.03697100	-1.90581000
C	3.82575000	0.57507200	2.42683300
C	4.80133700	1.39271700	1.59433500
C	4.29518300	0.31188300	3.84846300
H	2.84302000	1.05384200	2.42788500
H	4.41657300	1.54358100	0.58224400
H	4.93996400	2.37685000	2.05555800
H	5.77604600	0.89457500	1.54040000
H	3.56740400	-0.29329700	4.39837800
H	5.25760400	-0.21149500	3.84914300
H	4.41745000	1.26330700	4.37681700

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Eu(PO-Py-iPr)-opted

C	-1.19936400	-1.00981900	1.78128200
C	-1.27630100	-1.64723400	3.02279800
C	-0.08931500	-1.99305500	3.66763100
C	1.12935300	-1.72629600	3.04187200
C	1.11287700	-1.09471000	1.79677000
N	-0.02782400	-0.72257100	1.19426600
H	-0.11337400	-2.47842600	4.63882100
H	-2.24214000	-1.86329600	3.46710000
H	2.07207100	-2.00519900	3.50078500
P	2.60035400	-0.79461200	0.77712000
P	-2.65386300	-0.54601100	0.77414100
O	-2.21691500	0.02487000	-0.54628600
O	2.24171300	0.03284000	-0.42396700
Eu	0.04112400	0.86138300	-1.05770400
N	-0.58476700	-1.32378400	-2.85298900
O	0.09713600	-1.50977600	-1.77222600

O	-0.81268100	-0.10366900	-3.15418800
N	-0.09742600	2.69243300	1.24709700
O	1.02419200	2.32049800	0.74761200
O	-1.13567800	2.26457200	0.62859200
N	0.69569400	2.88096600	-2.93742700
O	-0.46349100	2.80036100	-2.37907500
O	1.55248600	2.00201700	-2.54458500
O	-0.17233800	3.38256800	2.24711100
O	0.96047200	3.72412000	-3.76368500
O	-0.98810300	-2.25574300	-3.52361500
O	-3.54191800	-1.86786700	0.64303200
O	-3.47633600	0.38839500	1.75509600
O	3.73500500	-0.19723400	1.72312800
O	3.10283800	-2.27270100	0.47973700
C	-4.22719200	1.59359800	1.31893800
C	-4.01211000	2.63729100	2.40165800
C	-5.68192900	1.19906100	1.10832700
H	-3.77270600	1.92775300	0.38367600
H	-2.95163300	2.88645900	2.48581200
H	-4.56185500	3.54871000	2.14130600
H	-4.38247900	2.27600400	3.36768200
H	-5.78025200	0.43457200	0.33086200
H	-6.11585600	0.81025100	2.03578500
H	-6.25927400	2.07673900	0.79700200
C	-3.58642000	-2.69984400	-0.58414700
C	-4.95805700	-3.35641800	-0.57826600
C	-2.43009300	-3.68952000	-0.57853900
H	-3.49257800	-2.01896500	-1.43404300
H	-5.75233300	-2.60417200	-0.55472100
H	-5.07972500	-3.95999700	-1.48390600
H	-5.07204600	-4.01118400	0.29257100
H	-1.46552600	-3.17880100	-0.65267300
H	-2.45455100	-4.30571000	0.32750800
H	-2.51183900	-4.34840500	-1.44955200
C	3.77780300	-2.63951300	-0.79087100
C	2.91023000	-3.68749900	-1.46962300
C	5.17778400	-3.11397000	-0.43218000
H	3.82309300	-1.73843000	-1.40911100
H	1.92047300	-3.28186500	-1.69860100
H	3.38171500	-4.00243700	-2.40751000
H	2.79962300	-4.56854200	-0.82744800
H	5.73980400	-2.32626900	0.07895100
H	5.13204300	-3.99107100	0.22227300
H	5.71928500	-3.39073200	-1.34356400
C	3.89218400	1.26213300	1.97839900
C	4.81225200	1.84095900	0.91456400
C	4.43667200	1.37043400	3.39342400
H	2.90437700	1.72501300	1.90794600
H	4.37526000	1.72572900	-0.08083700

H	4.95691500	2.91103700	1.10008300
H	5.79130100	1.34904100	0.93959000
H	3.74562500	0.92578500	4.11666800
H	5.40468800	0.86442800	3.47730800
H	4.57272500	2.42528800	3.65435800

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Am(PO-Py-Amyl)$(NO_3)_3$-opted

C	-1.27265100	0.73486100	-2.02490200
C	-1.29089100	1.10399800	-3.37316000
C	-0.07521100	1.24947200	-4.04058000
C	1.11236000	1.03138000	-3.34240400
C	1.03265500	0.67647000	-1.99361800
N	-0.13407000	0.52686800	-1.35056300
H	-0.05325600	1.53363400	-5.08840500
H	-2.23489100	1.27167100	-3.88107600
H	2.07850500	1.14658800	-3.82173500
P	2.47746700	0.38690100	-0.92198600
P	-2.78501300	0.48713200	-1.03087000
O	-2.44236600	0.19122500	0.40165700
O	2.04099400	0.35818500	0.51644900
Am	-0.19933800	-0.16330800	1.42083800
N	-0.97043800	2.62387900	2.01940200
O	-0.39254700	2.35020400	0.90515300
O	-1.01444100	1.66196300	2.86928100
N	-1.10590600	-2.83158900	0.56466100
O	-0.32000500	-2.09568300	-0.15197700
O	-1.48452200	-2.32217400	1.66921200
N	1.09447400	-1.66909600	3.55226500
O	0.21013500	-0.74508600	3.74125000
O	1.42778000	-1.85283300	2.32623100
O	-1.46793400	-3.93188400	0.18543200
O	1.57386500	-2.30200600	4.46652900
O	-1.45776900	3.71629800	2.24627000
O	-3.70299300	1.77528300	-1.24990700
O	-3.54187700	-0.66428500	-1.82099400
O	3.24973300	-0.92582100	-1.39693400
O	3.44741000	1.57084800	-1.36128800
C	-4.32849200	-1.69941200	-1.13133200
C	-4.10103100	-3.02565100	-1.83595100
H	-5.37402800	-1.37987400	-1.17687900
H	-4.00984100	-1.74161600	-0.08653800
C	-4.86012600	-4.16726800	-1.14380500
H	-4.41520700	-2.93650000	-2.88423800
H	-3.02749400	-3.24630800	-1.82880500
C	-4.66225900	-5.51920300	-1.84248700
H	-4.51405500	-4.24745300	-0.10448600
H	-5.93438900	-3.93227900	-1.10297100
H	-4.99289600	-5.44063300	-2.88818900

H	-3.58895700	-5.74937000	-1.87305200
C	-3.55459100	2.94973500	-0.37256400
C	-4.30146700	4.10817400	-1.00817200
H	-2.49185500	3.17426200	-0.24769800
H	-3.96914000	2.68308100	0.60302800
C	-4.26426900	5.35705600	-0.11400200
H	-3.85287200	4.33043200	-1.98559500
H	-5.34031400	3.80712100	-1.19565400
C	-4.94675900	6.57233800	-0.75589500
H	-4.74982500	5.13189900	0.84594500
H	-3.22158200	5.60603200	0.12754300
H	-4.45363100	6.80192700	-1.71124500
H	-5.98689600	6.31642100	-1.00314400
C	4.71920300	1.79127500	-0.67083600
C	5.34523800	3.05346500	-1.23848900
H	5.35265700	0.91391100	-0.83708200
H	4.51393500	1.88805600	0.39988000
C	6.69375900	3.37322200	-0.57735200
H	5.47727100	2.92783700	-2.32107900
H	4.64755800	3.88823500	-1.09547000
C	7.34562000	4.64533200	-1.13649000
H	6.55425800	3.48515900	0.50752600
H	7.38075400	2.52498400	-0.71250000
H	7.48254400	4.53397400	-2.22132800
H	6.65886900	5.49230500	-1.00029400
C	2.97223500	-2.24770200	-0.79778200
C	4.02775900	-3.21263000	-1.30669700
H	1.96367400	-2.54893600	-1.09395200
H	2.99762400	-2.14278800	0.28936300
C	3.81582300	-4.62464000	-0.73951100
H	3.99551100	-3.23859300	-2.40388500
H	5.02108300	-2.83919900	-1.02477400
C	4.86953200	-5.62867700	-1.22630700
H	3.83093800	-4.58450500	0.35860800
H	2.81509300	-4.98471000	-1.01732800
H	4.85546200	-5.66507600	-2.32500300
H	5.86945600	-5.26881100	-0.94535000
C	-4.92438900	7.81320700	0.14267700
H	-3.89617100	8.11052800	0.38176400
H	-5.41476700	8.66502600	-0.34209600
H	-5.44229600	7.62491500	1.09084600
C	-5.41189800	-6.66300800	-1.15186200
H	-6.49284300	-6.47558600	-1.13145300
H	-5.24882900	-7.61527300	-1.66929800
H	-5.07632500	-6.78511300	-0.11509400
C	4.65567000	-7.03767400	-0.66363100
H	3.67713000	-7.43698100	-0.95667900
H	5.42206700	-7.73195900	-1.02647500
H	4.69722000	-7.03678800	0.43222700

C	8.69194400	4.96639200	-0.47973000
H	9.41084200	4.15131100	-0.62826000
H	9.13111200	5.87828700	-0.89933700
H	8.58045100	5.11717000	0.60091200

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Eu(PO-Py-Amyl)$(NO_3)_3$-opted

C	0.28903600	1.15682500	-1.96268500
C	0.23501600	1.20478000	-3.35864100
C	-0.09303700	0.03880300	-4.04999200
C	-0.32279500	-1.13849100	-3.33571300
C	-0.23696700	-1.09770300	-1.94299800
N	0.04007000	0.03290100	-1.27552600
H	-0.15770800	0.04369400	-5.13401000
H	0.43929900	2.13234200	-3.88302000
H	-0.55928600	-2.06801000	-3.84266200
P	-0.36733700	-2.56645100	-0.86094300
P	0.74709900	2.57383600	-0.89839800
O	0.69107500	2.17294000	0.54800100
O	-0.39590200	-2.16944600	0.58819500
Eu	-0.32324300	0.14767700	1.41464600
N	2.24515400	-1.03667500	2.04403300
O	2.04143400	-0.46108000	0.91137600
O	1.28239200	-0.96178300	2.88280800
N	-2.87158700	0.82955300	0.05251800
O	-2.53135500	-0.38454600	0.27735900
O	-2.05986000	1.71553800	0.50116400
N	-1.31387300	0.93609600	3.95251400
O	-0.37266100	1.57637800	3.35090900
O	-1.79262000	-0.07142100	3.30283000
O	-3.88171200	1.12337200	-0.56282900
O	-1.72582700	1.25833600	5.04348200
O	3.28491100	-1.61997400	2.29397900
O	2.19637100	3.03969800	-1.38882700
O	-0.19467000	3.74979300	-1.38448300
O	-1.60084700	-3.43932000	-1.36825700
O	0.90330500	-3.40595000	-1.32340600
C	-0.98730600	4.59333600	-0.47196800
C	-2.40183900	4.70180400	-1.01258100
H	-0.47848900	5.56137700	-0.44335900
H	-0.97152500	4.14188700	0.52160100
C	-3.26581800	5.62598100	-0.14144600
H	-2.36590100	5.07997300	-2.04299100
H	-2.84337100	3.69991900	-1.03633600
C	-4.70953600	5.73805900	-0.65038800
H	-3.27671200	5.24627900	0.88996300
H	-2.81604300	6.62934400	-0.09834400
H	-4.70103900	6.11157600	-1.68439500
H	-5.15277500	4.73401300	-0.68968700

C	3.39829600	2.45655600	-0.77883400
C	4.59033300	2.86420200	-1.62698300
H	3.28893600	1.36843500	-0.72308000
H	3.47122200	2.84233100	0.24148600
C	5.91156900	2.33970600	-1.04629300
H	4.45040000	2.48377100	-2.64743700
H	4.61728500	3.95920000	-1.69758700
C	7.13335200	2.73923700	-1.88488200
H	6.03716100	2.71641000	-0.02102600
H	5.86924600	1.24399800	-0.96521100
H	7.00695700	2.36346400	-2.91011700
H	7.17456500	3.83463900	-1.96432800
C	1.71843800	-4.18956100	-0.38559600
C	3.16077000	-3.71721900	-0.46369700
H	1.60579500	-5.23294900	-0.69400400
H	1.31554100	-4.06891800	0.62337700
C	4.07309900	-4.51905100	0.47578700
H	3.50978300	-3.80630900	-1.50113100
H	3.19675600	-2.65633100	-0.19177900
C	5.52657800	-4.02789400	0.44633800
H	3.69309400	-4.43856800	1.50323500
H	4.04023000	-5.58617800	0.20860400
H	5.90657400	-4.07560700	-0.58454800
H	5.54411500	-2.96999000	0.73856600
C	-2.92566300	-3.39583100	-0.72528900
C	-3.85131600	-4.28968700	-1.53117400
H	-3.26721700	-2.35917400	-0.69424500
H	-2.80526700	-3.75248800	0.30140700
C	-5.26004700	-4.34263500	-0.92153800
H	-3.90302300	-3.91438700	-2.56172300
H	-3.42343900	-5.29941400	-1.58100100
C	-6.22399800	-5.23040600	-1.72044200
H	-5.19903600	-4.71301600	0.11196000
H	-5.67134500	-3.32526900	-0.85765100
H	-6.28640800	-4.85818900	-2.75278700
H	-5.80969900	-6.24636500	-1.78663500
C	8.45260700	2.21732200	-1.30660300
H	8.45362400	1.12215400	-1.24603300
H	9.30508200	2.51803500	-1.92595000
H	8.62243600	2.60449900	-0.29458000
C	-5.58087900	6.65188500	0.21731400
H	-5.17820600	7.67202000	0.25020600
H	-6.60464100	6.71021900	-0.16947900
H	-5.63523600	6.28376000	1.24900100
C	-7.62848400	-5.28814800	-1.11100000
H	-8.08122300	-4.29034500	-1.06310600
H	-8.29294200	-5.92800900	-1.70255800
H	-7.60160900	-5.68849600	-0.09020800
C	6.44769900	-4.83114100	1.37008500

H	6.46939900	-5.89142400	1.08813000
H	7.47653200	-4.45530100	1.33117800
H	6.11072100	-4.77082400	2.41185500

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Am(PO-Py-2EtHex)$(NO_3)_3$-opted

C	-1.23952200	0.55818400	-1.70729500
C	-1.31078500	0.79562600	-3.08308200
C	-0.12657600	0.80254600	-3.81922900
C	1.08294000	0.58270900	-3.16053600
C	1.05718200	0.36420800	-1.78080900
N	-0.08008700	0.34712600	-1.07129800
H	-0.14535100	0.98078800	-4.89021100
H	-2.27046100	0.96707900	-3.55911100
H	2.02607000	0.59161100	-3.69628500
P	2.53927600	0.08808700	-0.75610400
P	-2.70479500	0.51003300	-0.62006700
O	-2.31736600	0.24980300	0.80747000
O	2.16960400	0.18298500	0.69782200
Am	-0.04025000	-0.16470900	1.74241800
N	-0.61582400	2.69774900	2.20058300
O	-0.12793700	2.32051400	1.07390500
O	-0.67291600	1.79237900	3.10976100
N	-1.07361100	-2.84021300	1.11263100
O	-0.32006400	-2.16924100	0.29942300
O	-1.38816100	-2.23859300	2.19210500
N	1.29558600	-1.59108300	3.90518400
O	0.46644100	-0.61413000	4.07515900
O	1.55590500	-1.86992600	2.67954100
O	-1.45821000	-3.96176000	0.84282300
O	1.79268000	-2.18653800	4.83537100
O	-1.01208900	3.83404300	2.38822800
O	-3.52517300	1.86150800	-0.85009500
O	-3.59465500	-0.60270100	-1.32819900
O	3.23396700	-1.28678200	-1.16924100
O	3.53680600	1.19523100	-1.31700600
C	-4.68412000	-1.27152300	-0.60732700
C	-5.13786800	-2.47931600	-1.42472900
H	-5.49211200	-0.54323600	-0.48360200
H	-4.30958900	-1.56752000	0.37774600
C	-6.43027200	-3.02558100	-0.77716200
H	-5.38850600	-2.10412500	-2.42839500
C	-7.11047800	-4.17428600	-1.53441700
H	-6.20033800	-3.35872800	0.24583500
H	-7.15260400	-2.20185700	-0.67550100
H	-7.29386900	-3.86965100	-2.57553200
H	-6.43897200	-5.04145200	-1.58008500
C	-3.30768700	3.03861400	0.00960000
C	-4.14675300	4.19505700	-0.52732400

H	-2.24209200	3.27946700	0.00475400
H	-3.59977700	2.76344800	1.02704000
C	-3.77614700	5.45363600	0.29081600
H	-3.83511700	4.35611900	-1.57052700
C	-4.40622300	6.76635900	-0.19447200
H	-4.05720500	5.28741700	1.34099600
H	-2.68322400	5.56646500	0.29125200
H	-4.17503500	6.91449900	-1.26011700
H	-5.50060100	6.70863800	-0.12207500
C	4.82880800	1.42583000	-0.66501800
C	5.50486500	2.62656400	-1.32373500
H	5.42938200	0.51611400	-0.77483800
H	4.63906900	1.60769200	0.39677200
C	6.74689600	2.98521500	-0.47717100
H	4.79125900	3.46096300	-1.26197500
C	7.50971700	4.24473900	-0.91172500
H	6.43249700	3.11534800	0.56845700
H	7.43953300	2.12971500	-0.48250900
H	7.91014900	4.11195900	-1.92570300
H	6.81463900	5.09553300	-0.96180500
C	2.91120200	-2.55440000	-0.47962000
C	3.92365300	-3.61244700	-0.90903800
H	1.88878700	-2.83248800	-0.75221700
H	2.94901500	-2.36971900	0.59576100
C	3.67211800	-4.86064200	-0.03131000
H	4.92196700	-3.21633700	-0.66914900
C	4.66498800	-6.01746800	-0.21080600
H	3.68348300	-4.55323700	1.02373100
H	2.65424600	-5.22967400	-0.22623400
H	4.60642000	-6.41070400	-1.23475800
H	5.69225200	-5.64554600	-0.08039800
C	-3.92063500	7.98599400	0.60159600
H	-2.82589300	8.05140700	0.53134900
H	-4.14716900	7.83608100	1.66644500
C	-8.43700400	-4.60689800	-0.89366100
H	-9.11768600	-3.74461700	-0.85143300
H	-8.25545700	-4.90269500	0.14920500
C	4.41481100	-7.16647600	0.77629800
H	3.38487700	-7.53003000	0.65399600
H	4.48029500	-6.78161800	1.80340100
C	8.66666900	4.59259000	0.03603000
H	9.35479900	3.73743900	0.09593800
H	8.27189800	4.73748800	1.05139900
C	-4.54457900	9.30214600	0.12572600
H	-5.63764200	9.27993900	0.21765000
H	-4.17884300	10.15238500	0.71255700
H	-4.30564800	9.49695600	-0.92733900
C	-9.11681300	-5.75913500	-1.64070800
H	-8.47492300	-6.64827100	-1.66655300

H	-10.06038600	-6.04367800	-1.16152000
H	-9.34024300	-5.48227900	-2.67857200
C	5.39314100	-8.33293400	0.60275900
H	6.42990100	-8.00797400	0.75572600
H	5.18747200	-9.13590800	1.31964000
H	5.32628000	-8.76123100	-0.40525100
C	9.44069200	5.84259300	-0.39530900
H	8.78520400	6.72132100	-0.43368200
H	10.25641000	6.06615900	0.30129100
H	9.87978000	5.71338800	-1.39232500
C	-4.00642800	-3.53303300	-1.55004500
C	-3.91200800	-4.19534900	-2.93034700
H	-4.13605700	-4.29895600	-0.77439700
H	-3.04117200	-3.06193200	-1.33581900
H	-3.10159500	-4.93260900	-2.95014900
H	-4.83761100	-4.70950700	-3.20986300
H	-3.70223400	-3.44892400	-3.70689700
C	-5.66024900	3.85734200	-0.50995200
C	-6.44139900	4.38157600	-1.72209700
H	-6.10495700	4.24406900	0.41741200
H	-5.78315100	2.76835300	-0.47568800
H	-7.50266500	4.11722400	-1.64760800
H	-6.37601500	5.47018400	-1.81772300
H	-6.05498000	3.94433200	-2.65106000
C	5.81875100	2.34778700	-2.81634300
C	5.60807800	3.55123900	-3.74441300
H	5.17686800	1.53161700	-3.16958900
H	6.85113800	1.98205300	-2.90621000
H	5.84913000	3.29163300	-4.78179300
H	4.56311200	3.88351000	-3.71780700
H	6.23162500	4.40540100	-3.46256200
C	3.85181300	-3.88594300	-2.43308300
C	5.20695900	-4.17075600	-3.09415000
H	3.41173000	-3.01317800	-2.93053800
H	3.16256600	-4.72193600	-2.61661300
H	5.08716600	-4.35405900	-4.16845200
H	5.88357100	-3.31518600	-2.97699100
H	5.70361900	-5.04492300	-2.66176500

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Eu(PO-Py-2EtHex)$(NO_3)_3$-opted

C	1.35769200	-0.16474800	-1.55349800
C	1.44020800	-0.22643600	-2.94737100
C	0.27520600	-0.04119600	-3.69113600
C	-0.93409400	0.16268800	-3.02516100
C	-0.92472300	0.20151300	-1.62954500
N	0.20187300	0.06505100	-0.91370100
H	0.30617000	-0.07027100	-4.77619100
H	2.39359300	-0.41087000	-3.43080000

H	-1.86427700	0.28165200	-3.57055300
P	-2.42180500	0.33517900	-0.59196900
P	2.77012500	-0.46487400	-0.43232200
O	2.36865100	-0.28866400	1.00305700
O	-2.05679100	0.38219300	0.86250200
Eu	0.20633900	0.58542000	1.77543700
N	0.42696500	-2.20467200	2.51005600
O	-0.09714400	-1.85457500	1.38772800
O	0.67458800	-1.25146700	3.32767100
N	0.73177000	3.10923900	0.34185900
O	-0.45676200	2.72499000	0.64749300
O	1.67082800	2.34693900	0.75972400
N	-0.26065000	1.83660400	4.27716400
O	0.91412300	1.74410900	3.75525500
O	-1.21611400	1.35514900	3.55905300
O	0.94164800	4.11281800	-0.31348700
O	-0.45207200	2.34476300	5.35864400
O	0.68329900	-3.36828900	2.76366700
O	3.31523700	-1.93201800	-0.76531800
O	3.87420000	0.50871300	-1.02750900
O	-3.31778700	1.54588800	-1.11675000
O	-3.22275900	-0.95903200	-1.07406400
C	5.06054800	0.89558400	-0.25486600
C	5.69710100	2.11249000	-0.92283100
H	5.73903500	0.03632200	-0.24982300
H	4.74353300	1.11692900	0.76877000
C	7.09355600	2.32116300	-0.29562500
H	5.83549200	1.85018100	-1.98264000
C	7.93877700	3.43188000	-0.93438900
H	6.97300700	2.53697100	0.77675300
H	7.65721800	1.37811900	-0.35619600
H	8.03090500	3.24644100	-2.01485100
H	7.42735900	4.39776900	-0.83030300
C	2.87814800	-3.09060800	0.03546700
C	3.25032200	-4.36919900	-0.71000800
H	1.79994100	-3.02197900	0.19838800
H	3.38026400	-3.02380300	1.00479500
C	2.64799900	-5.55574100	0.07764500
H	2.75556100	-4.32004400	-1.69200400
C	2.77728300	-6.92925000	-0.59531300
H	3.12037800	-5.59702000	1.07010000
H	1.58418900	-5.35323000	0.26440600
H	2.35986000	-6.88181400	-1.61236300
H	3.83693900	-7.19460100	-0.71000800
C	-4.40162700	-1.40904200	-0.33118000
C	-4.77473300	-2.81394500	-0.80062600
H	-5.21031800	-0.69413400	-0.52238500
H	-4.15464600	-1.39887700	0.73421300
C	-5.88294300	-3.33963200	0.13952000

H	-3.87960000	-3.43750000	-0.66261800
C	-6.33254800	-4.78849300	-0.09656400
H	-5.52968200	-3.25282400	1.17714600
H	-6.75975200	-2.67861900	0.06001700
H	-6.78332000	-4.88549700	-1.09331000
H	-5.45511400	-5.45137800	-0.08713500
C	-3.41890200	2.84291800	-0.42277800
C	-4.50789000	3.65934800	-1.11332400
H	-2.44146000	3.32815800	-0.46308300
H	-3.66132500	2.63916100	0.62295300
C	-4.78554600	4.90788700	-0.24535100
H	-5.41608900	3.03790200	-1.12117300
C	-5.94228500	5.79604300	-0.72366700
H	-4.99946600	4.58143000	0.78256700
H	-3.86847900	5.51266200	-0.18663300
H	-5.71636000	6.20461700	-1.71792300
H	-6.84947300	5.18464900	-0.83991900
C	2.06944700	-8.04308700	0.18911700
H	1.00641600	-7.78761600	0.30082700
H	2.47937400	-8.08441900	1.20791800
C	9.34060200	3.54026400	-0.31817400
H	9.86020500	2.57755700	-0.42738500
H	9.24772400	3.71469700	0.76308900
C	-6.23694100	6.95938200	0.23434100
H	-5.32955800	7.56774800	0.35477000
H	-6.46806800	6.55799800	1.23109000
C	-7.34232200	-5.27208800	0.95395500
H	-8.21165600	-4.59909000	0.95781500
H	-6.89102700	-5.19200100	1.95280100
C	2.19927800	-9.41947300	-0.47177200
H	3.25093000	-9.71835500	-0.56374000
H	1.68369100	-10.19208500	0.10987200
H	1.76709500	-9.41771100	-1.48030700
C	10.18875400	4.65262400	-0.94379000
H	9.71375700	5.63304900	-0.81564500
H	11.18311300	4.70215400	-0.48566400
H	10.32542500	4.48970600	-2.02011700
C	-7.39076700	7.84928600	-0.23927300
H	-8.32007200	7.27457900	-0.33777400
H	-7.57842600	8.66742500	0.46518200
H	-7.17275800	8.29550800	-1.21756400
C	-7.81173000	-6.71157100	0.71859800
H	-6.96825100	-7.41248800	0.74181100
H	-8.52796300	-7.02763800	1.48534000
H	-8.30143500	-6.81505200	-0.25769000
C	4.77687600	3.35879400	-0.82692100
C	4.70699400	4.19128200	-2.11309700
H	5.11742100	3.99194400	0.00406100
H	3.75992000	3.05216200	-0.56311600

H	4.03254500	5.04442900	-1.98130900
H	5.68704800	4.57880000	-2.41369000
H	4.32009600	3.58950600	-2.94520100
C	4.78119800	-4.47600100	-0.93339000
C	5.18487300	-5.05929400	-2.29388600
H	5.22254900	-5.07492300	-0.12473000
H	5.22545400	-3.47707800	-0.85046700
H	6.27567600	-5.11481700	-2.38783100
H	4.78636900	-6.06734600	-2.44750900
H	4.81334700	-4.42912000	-3.11144600
C	-5.16202600	-2.82207800	-2.30175700
C	-4.70420800	-4.06918000	-3.06944800
H	-4.71810500	-1.94518800	-2.78804200
H	-6.25089400	-2.70387400	-2.39443800
H	-5.00933500	-4.01428900	-4.12098500
H	-3.61150700	-4.16011200	-3.04388000
H	-5.12086600	-4.99030800	-2.65042000
C	-4.12213200	3.98970200	-2.57920600
C	-5.28538700	3.90276200	-3.57588900
H	-3.34188800	3.29286900	-2.90881000
H	-3.67019900	4.99024800	-2.61719900
H	-4.95134100	4.14790600	-4.59096800
H	-5.70187800	2.88818100	-3.59822300
H	-6.10040300	4.58751500	-3.32064600

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10. Full information of reference (Gaussian 09 D.01).

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci,G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian,A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09, Revision D.01, Gaussian, Inc., Wallingford CT, 2013.