Supporting Information

Selective Preparation of Diamondoid Phosphonates

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1. NMR spectra of new compounds.

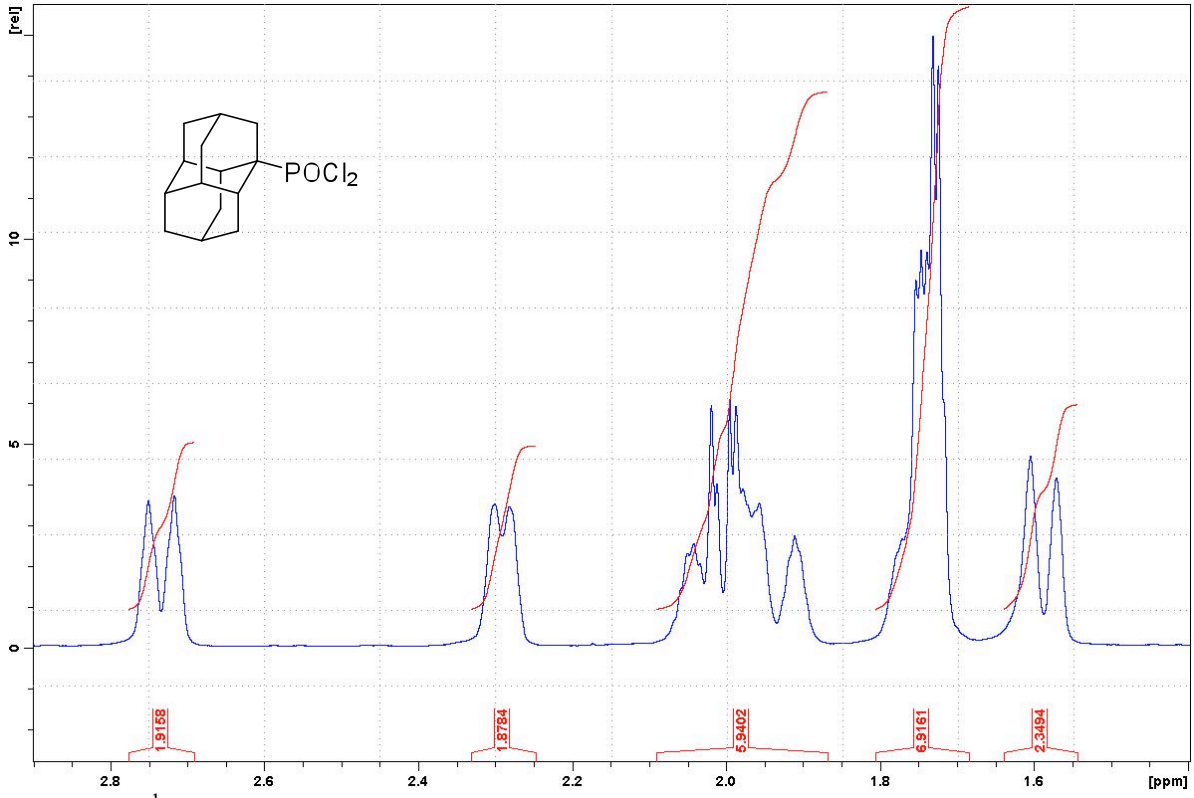


Figure 1S. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of compound **5.**

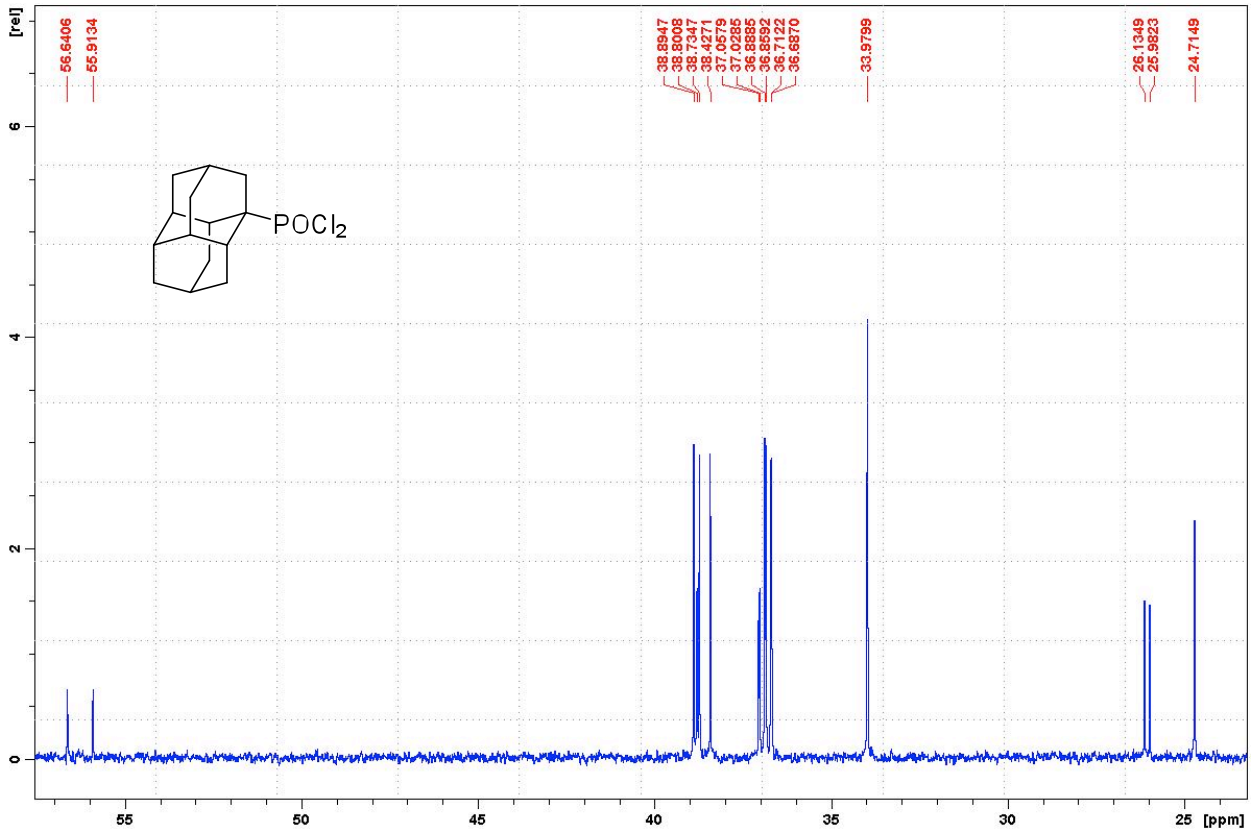


Figure 2S. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of compound **5.**

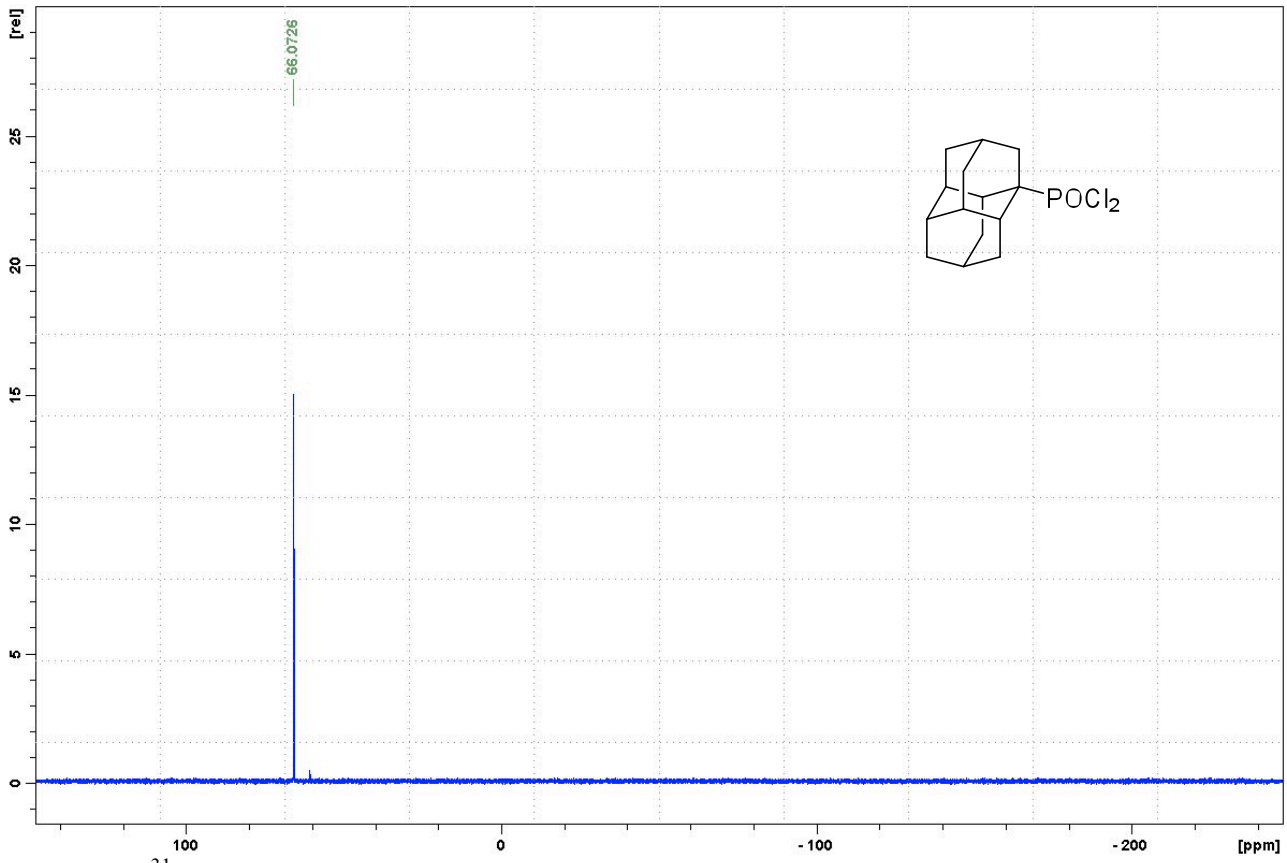


Figure 3S. ^{31}P NMR (162 MHz, $CDCl_3$) spectrum of compound **5**.

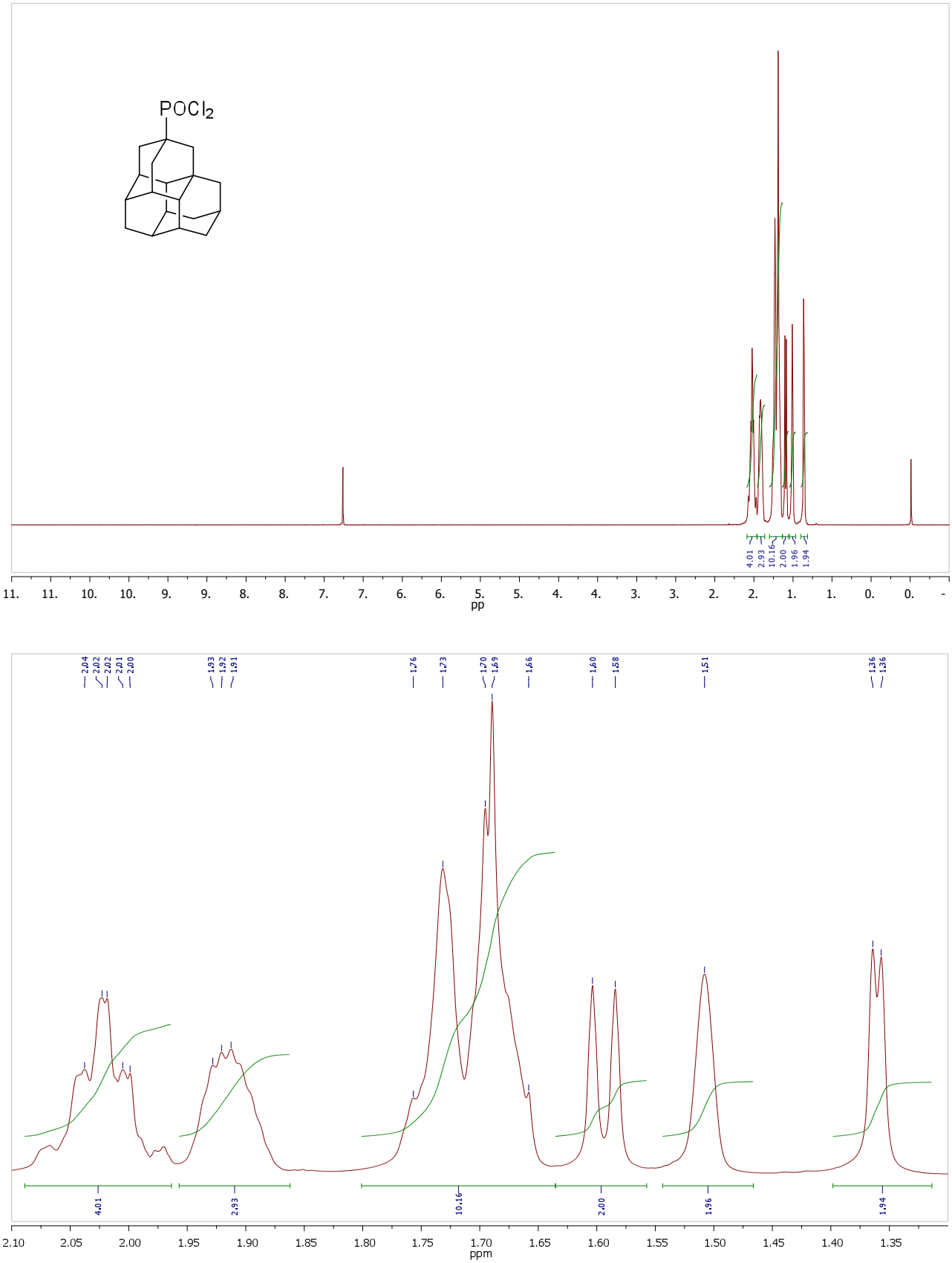


Figure 4S. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **13**.

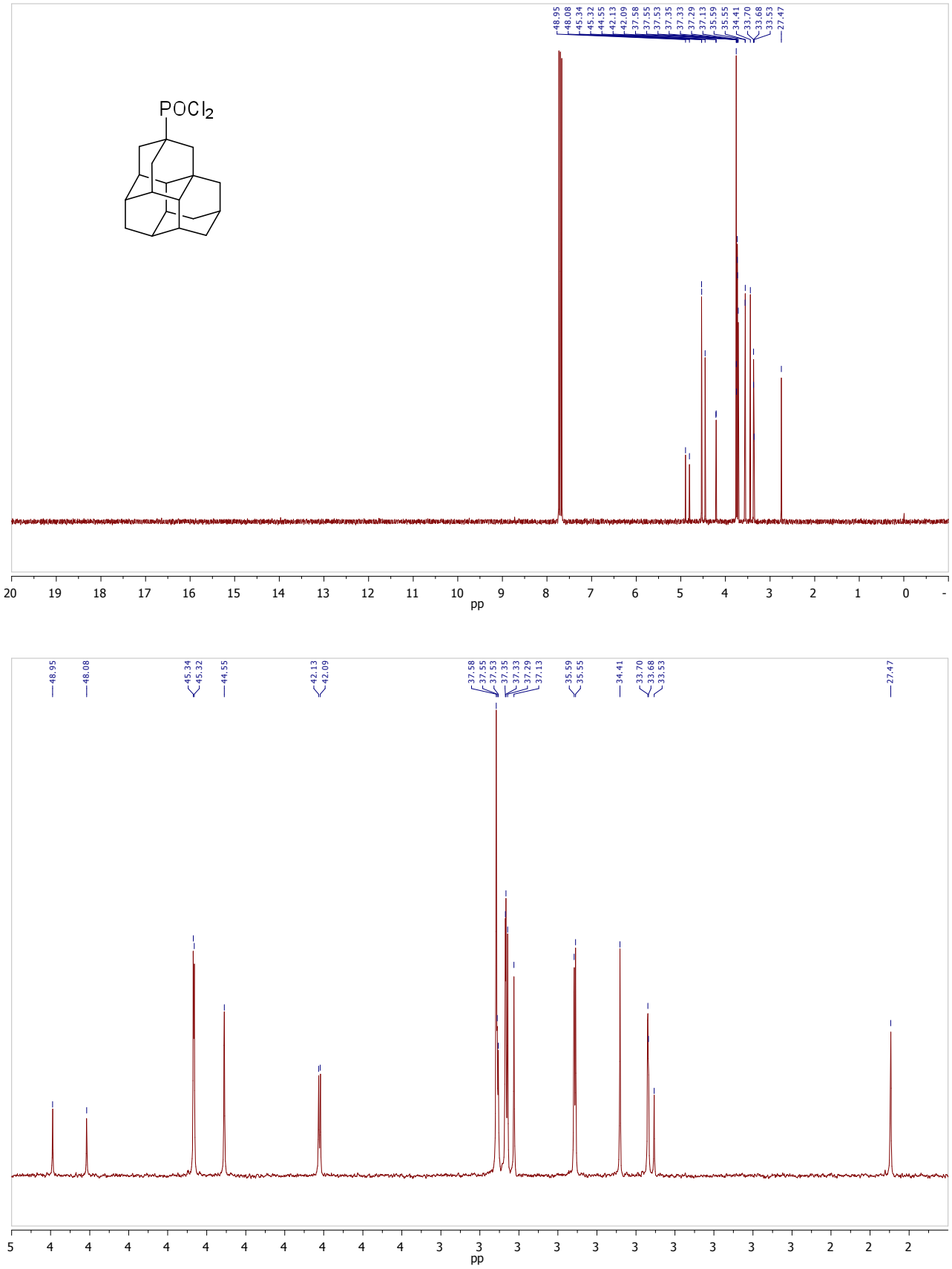


Figure 5S. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **13**.

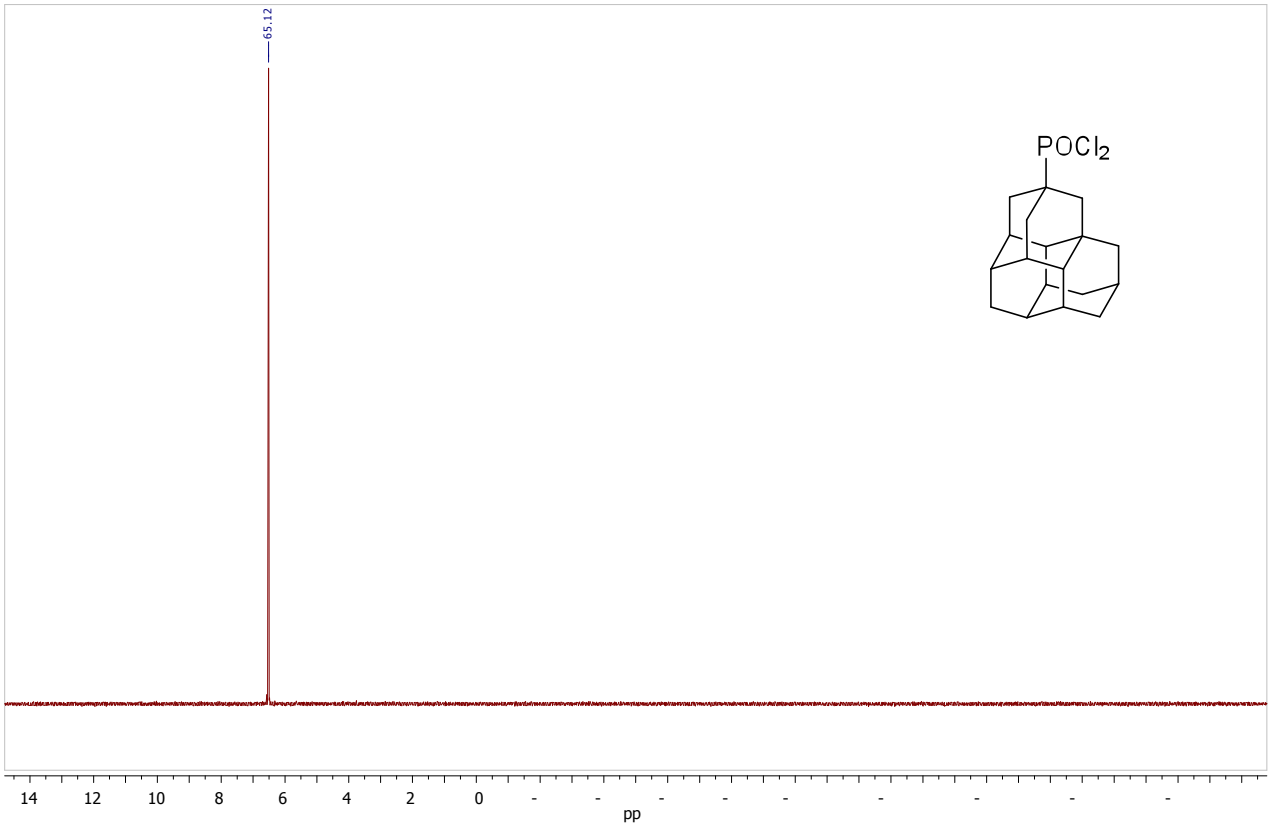


Figure 6S. ^{31}P NMR (162 MHz, $CDCl_3$) spectrum of compound **13**.

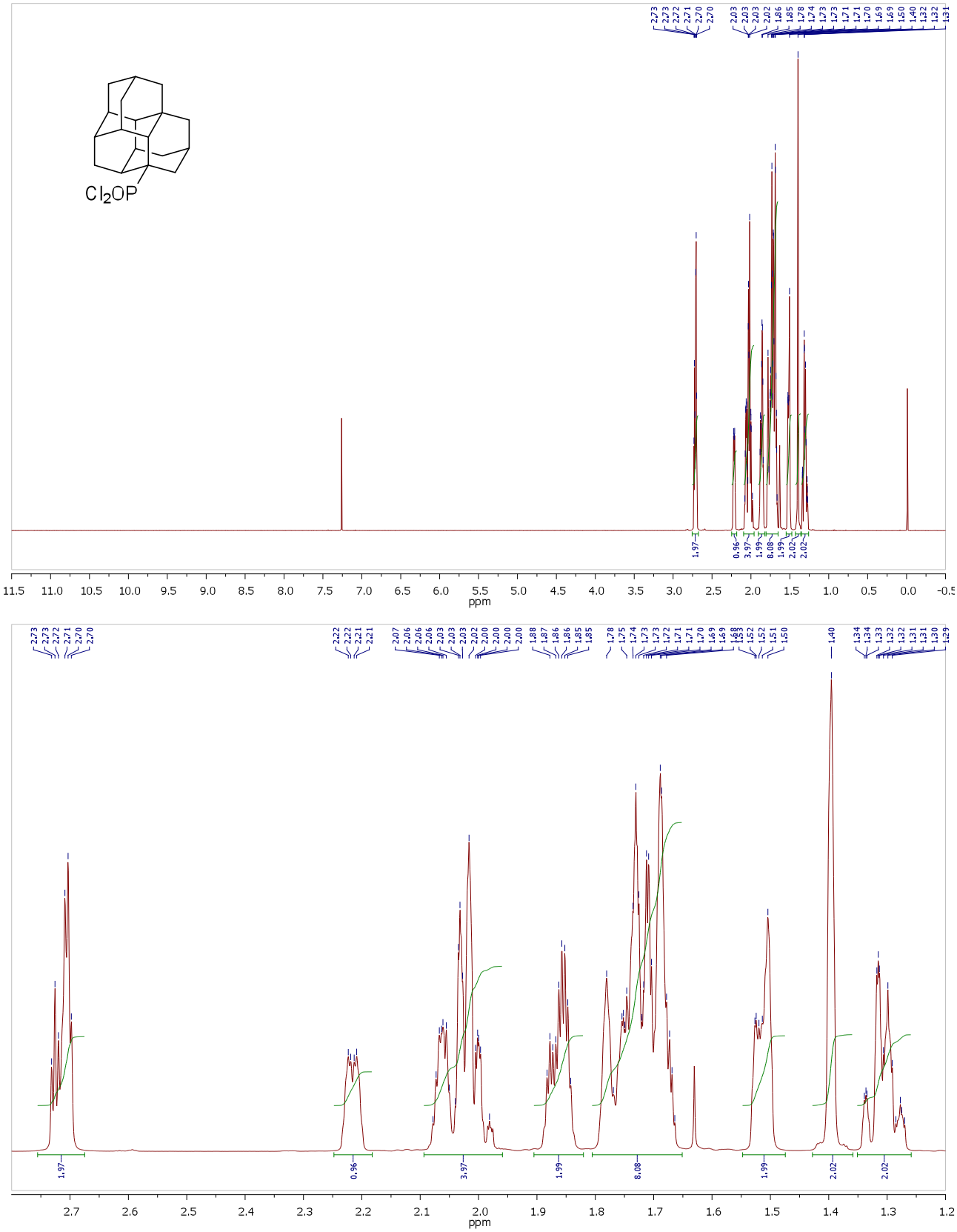


Figure 7S. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **14**.

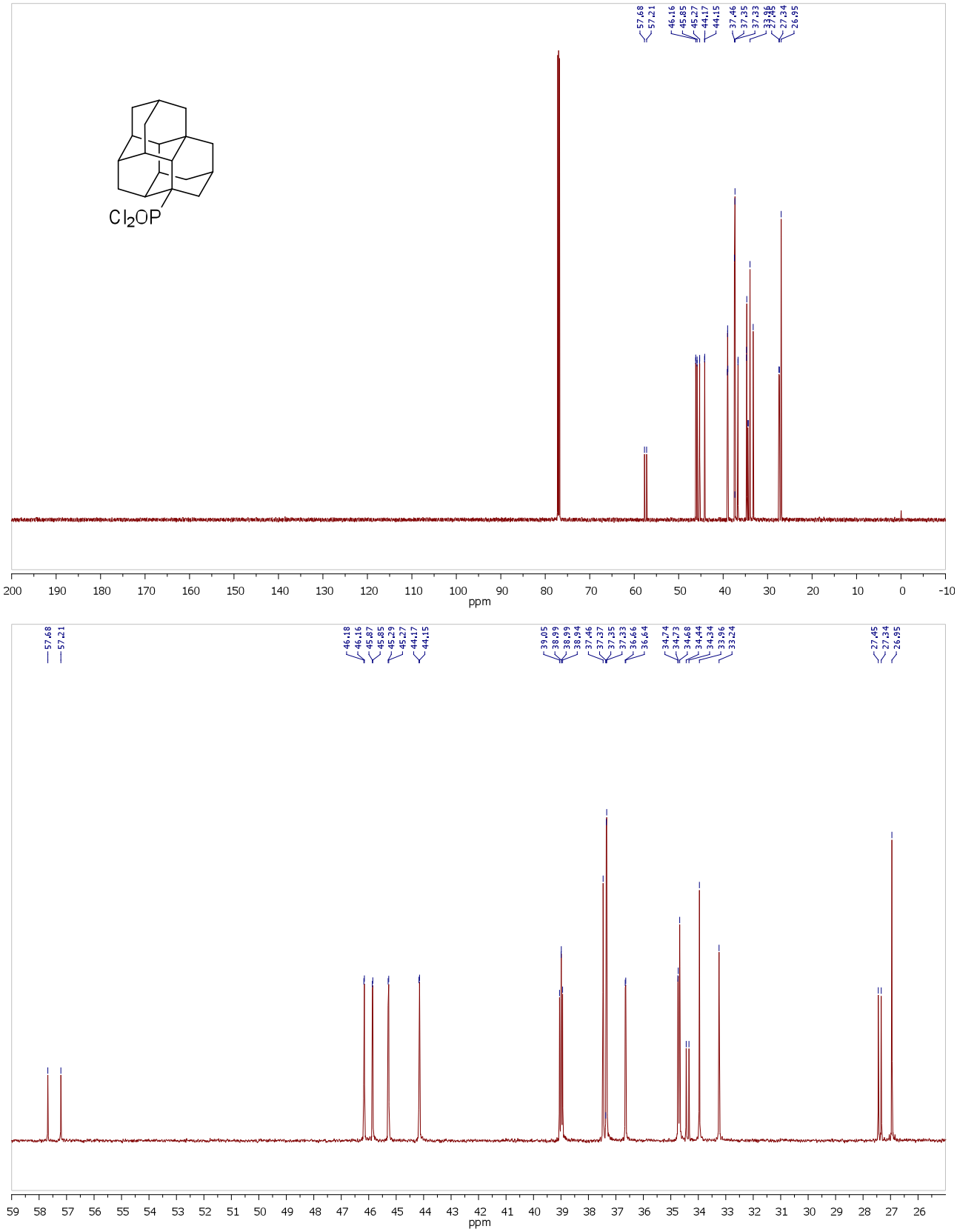


Figure 8S. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of compound **14**.

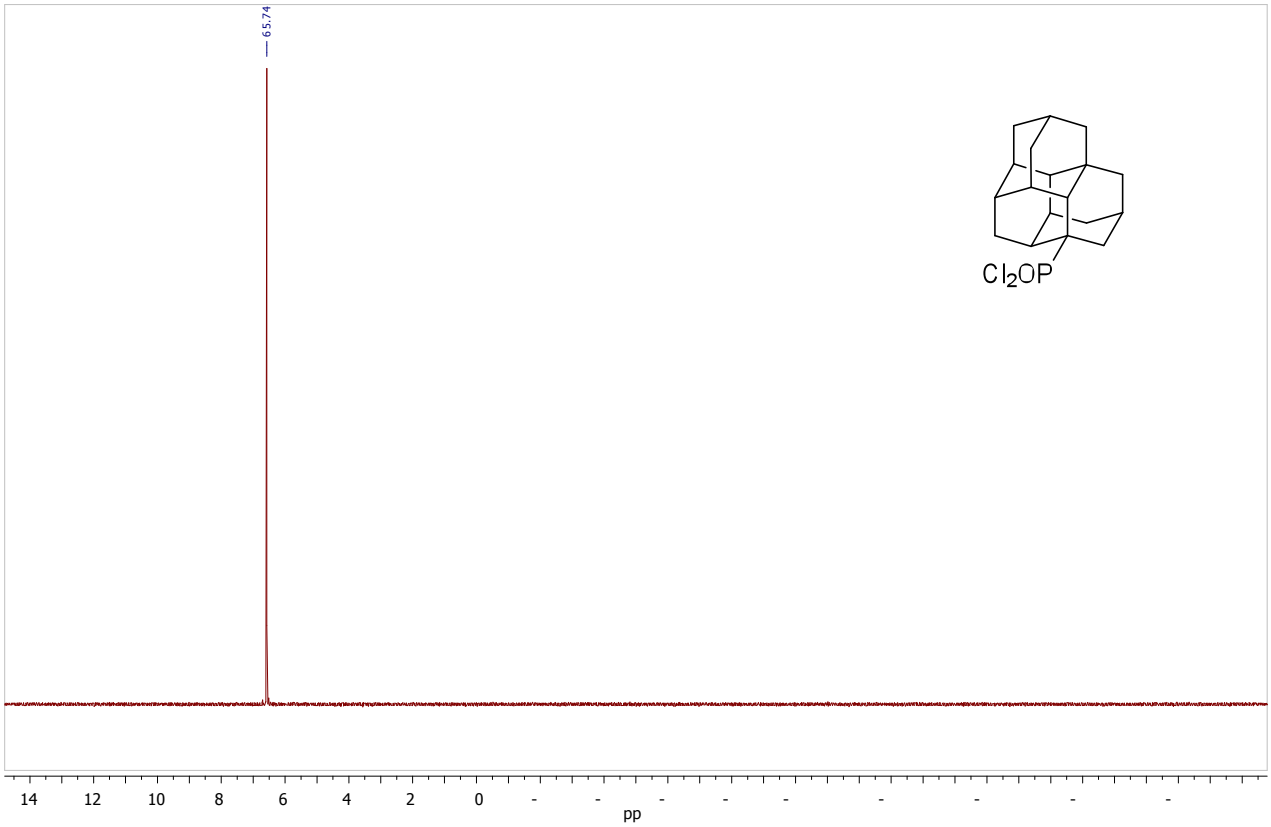


Figure 9S. ^{31}P NMR (162 MHz, $CDCl_3$) spectrum of compound **14**.

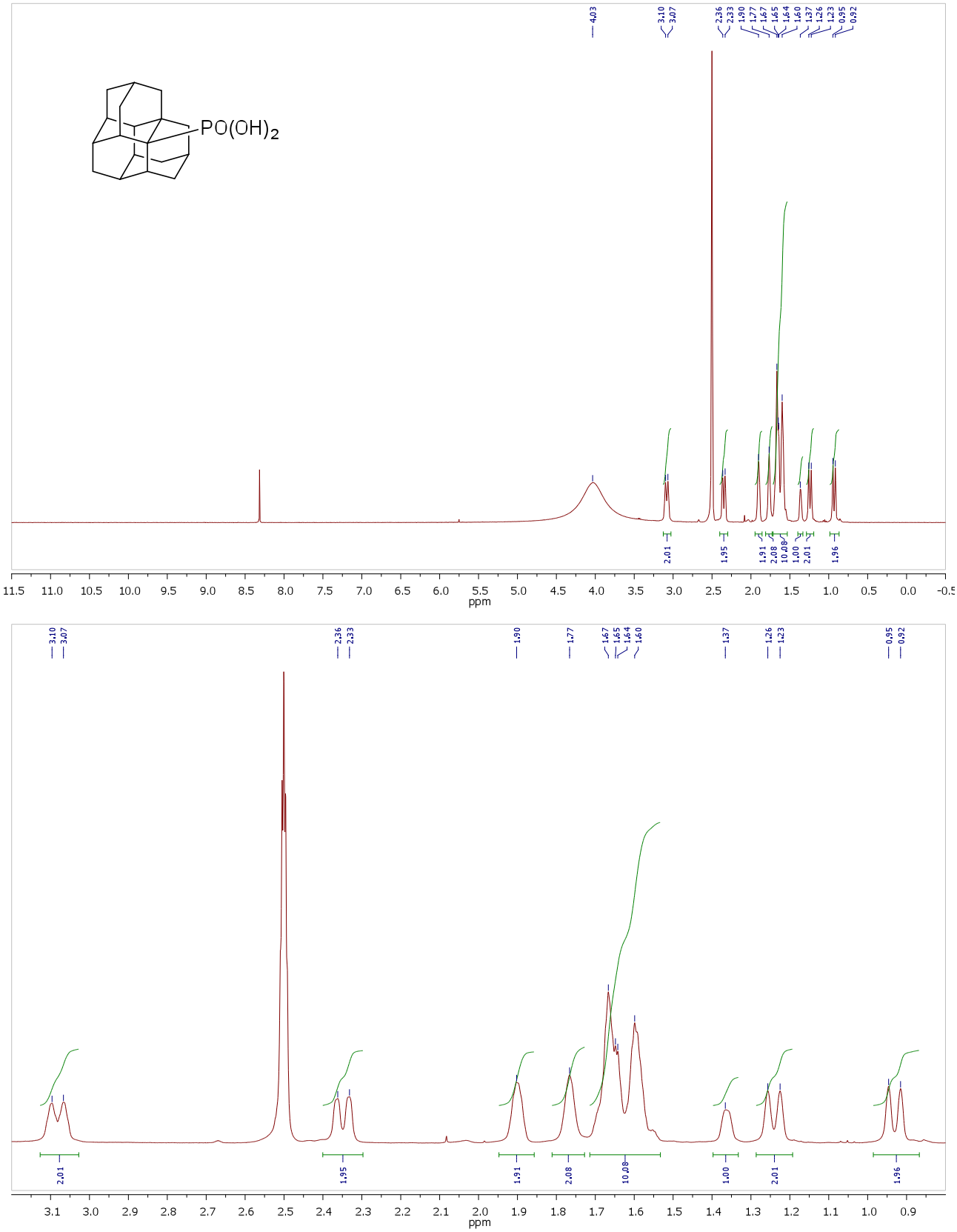


Figure 10S. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **15**.

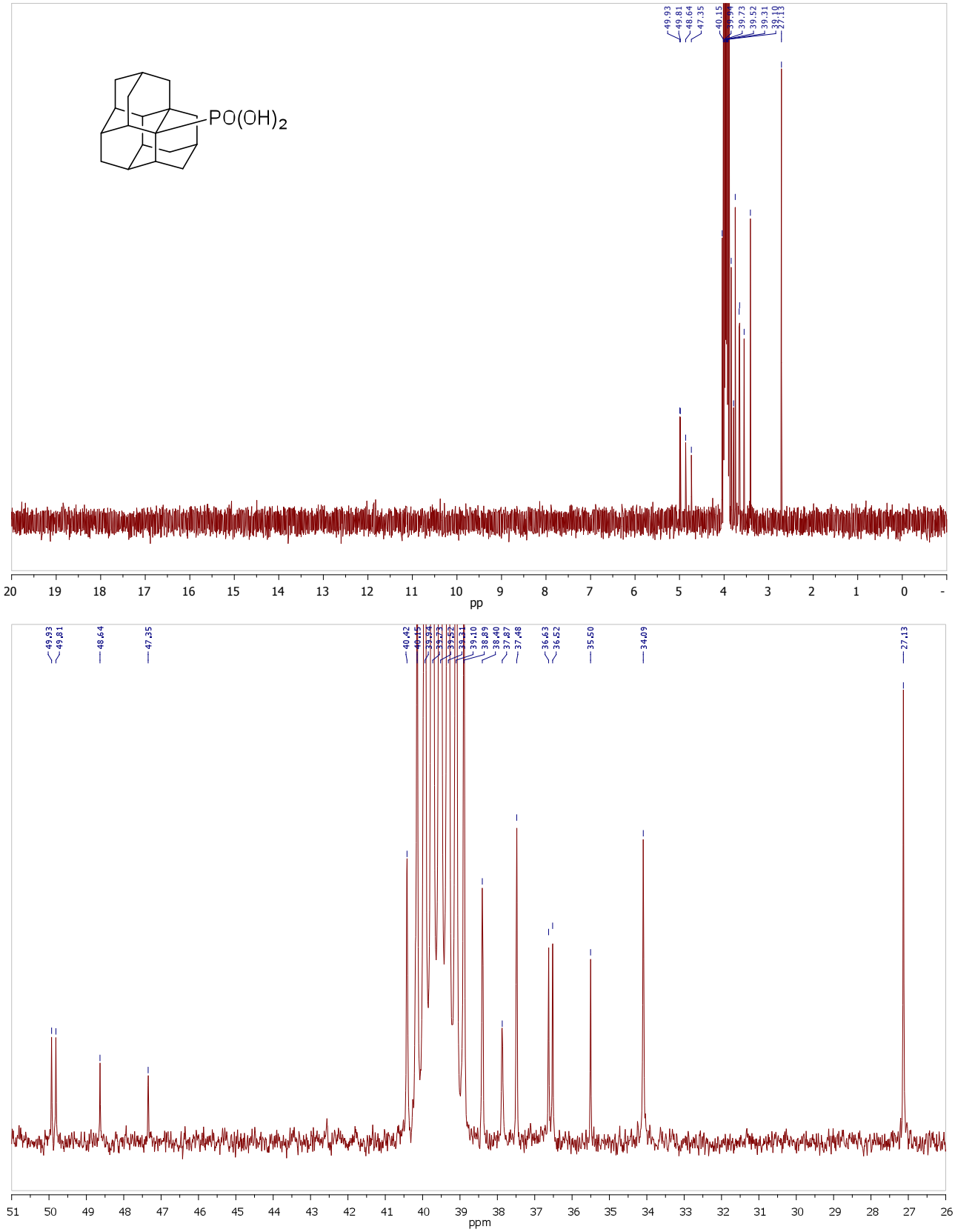


Figure 11S. ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of compound **15**.

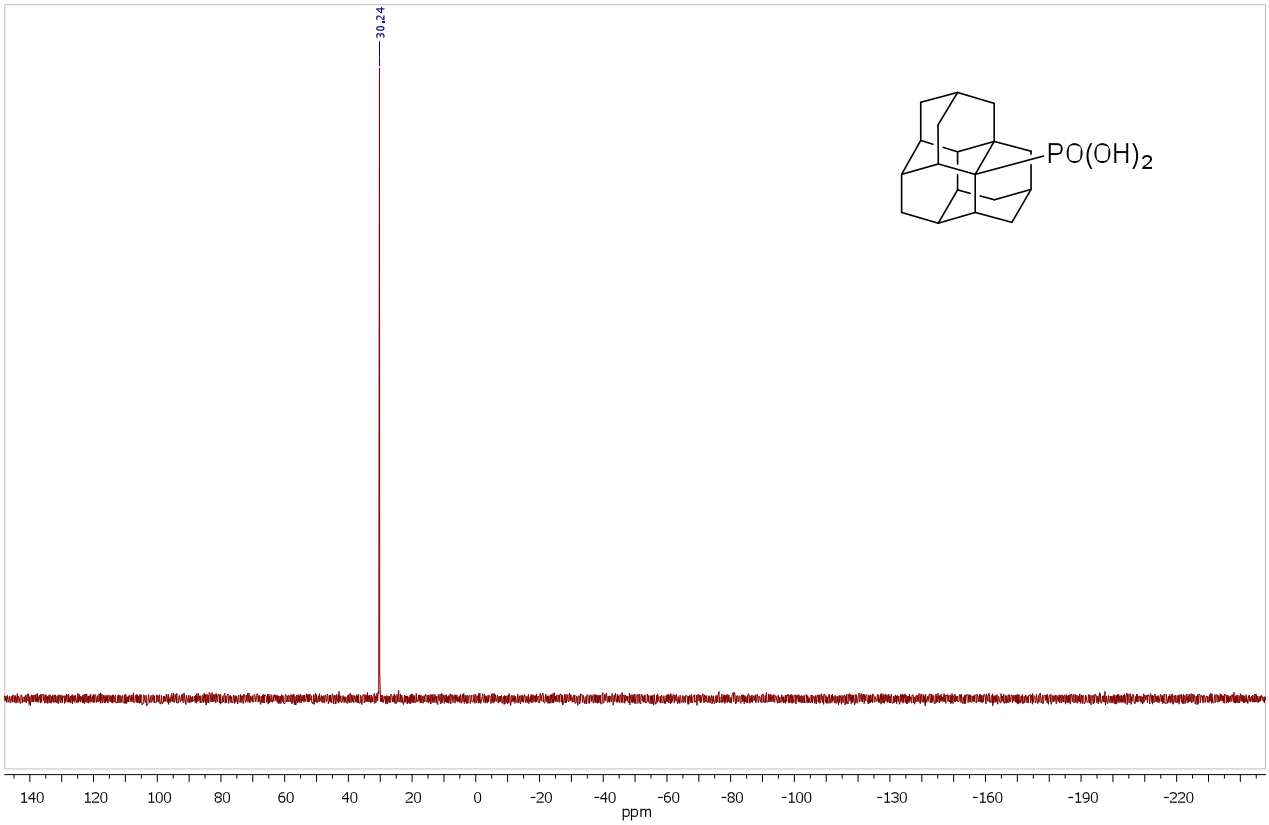


Figure 12S. ^{31}P NMR (162 MHz, DMSO-d_6) spectrum of compound **15**.

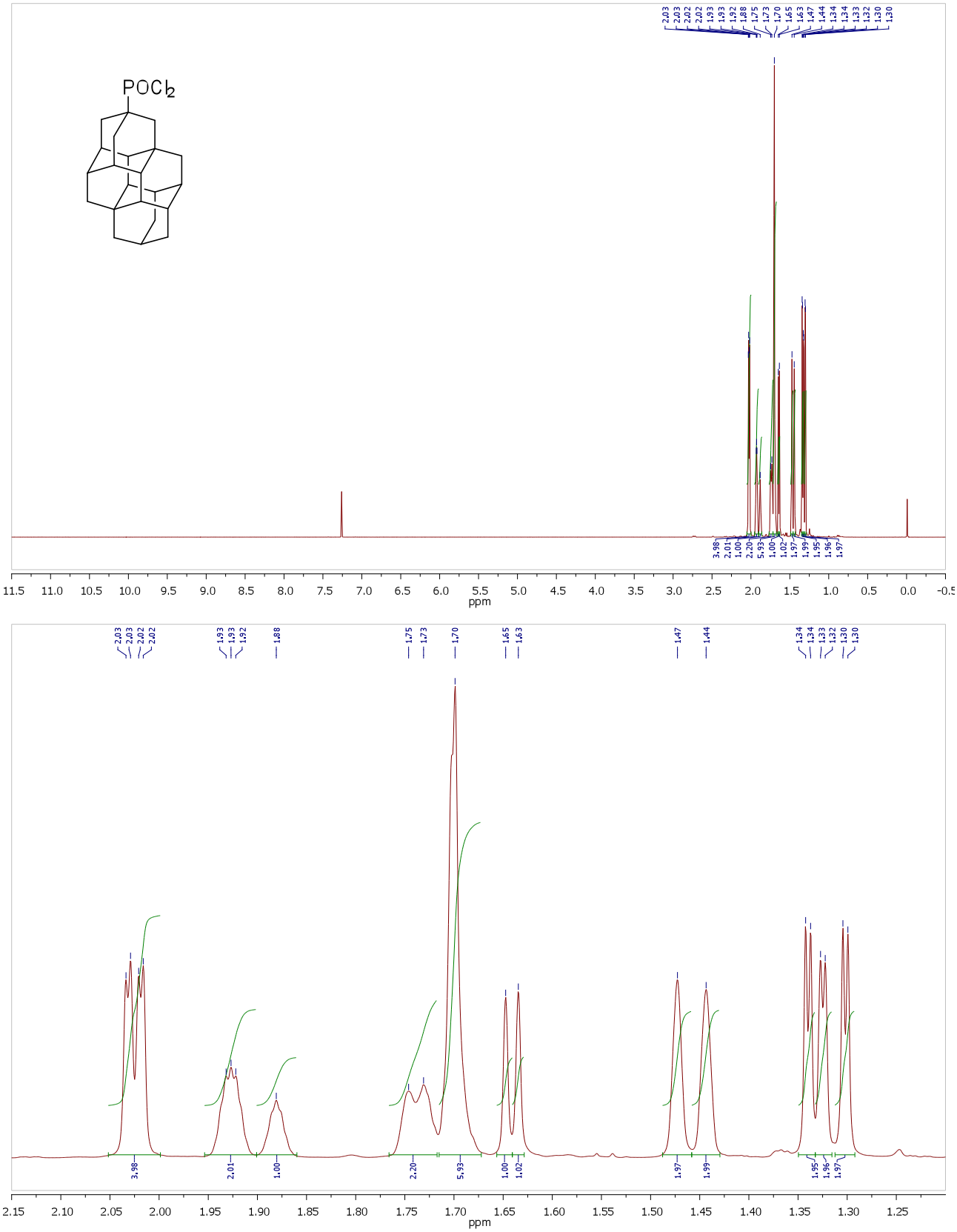


Figure 13S. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **17**.

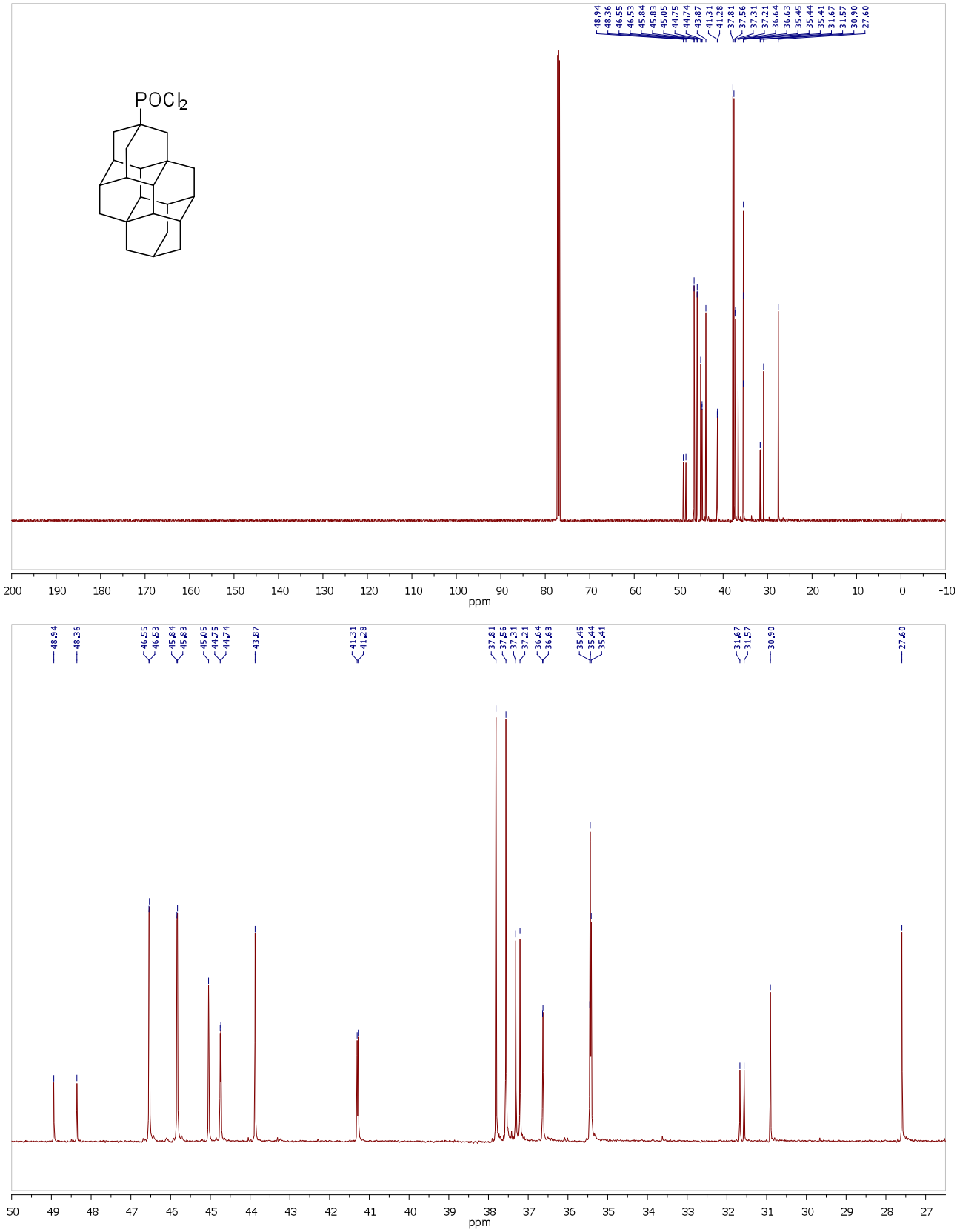


Figure 14S. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of compound **17**.

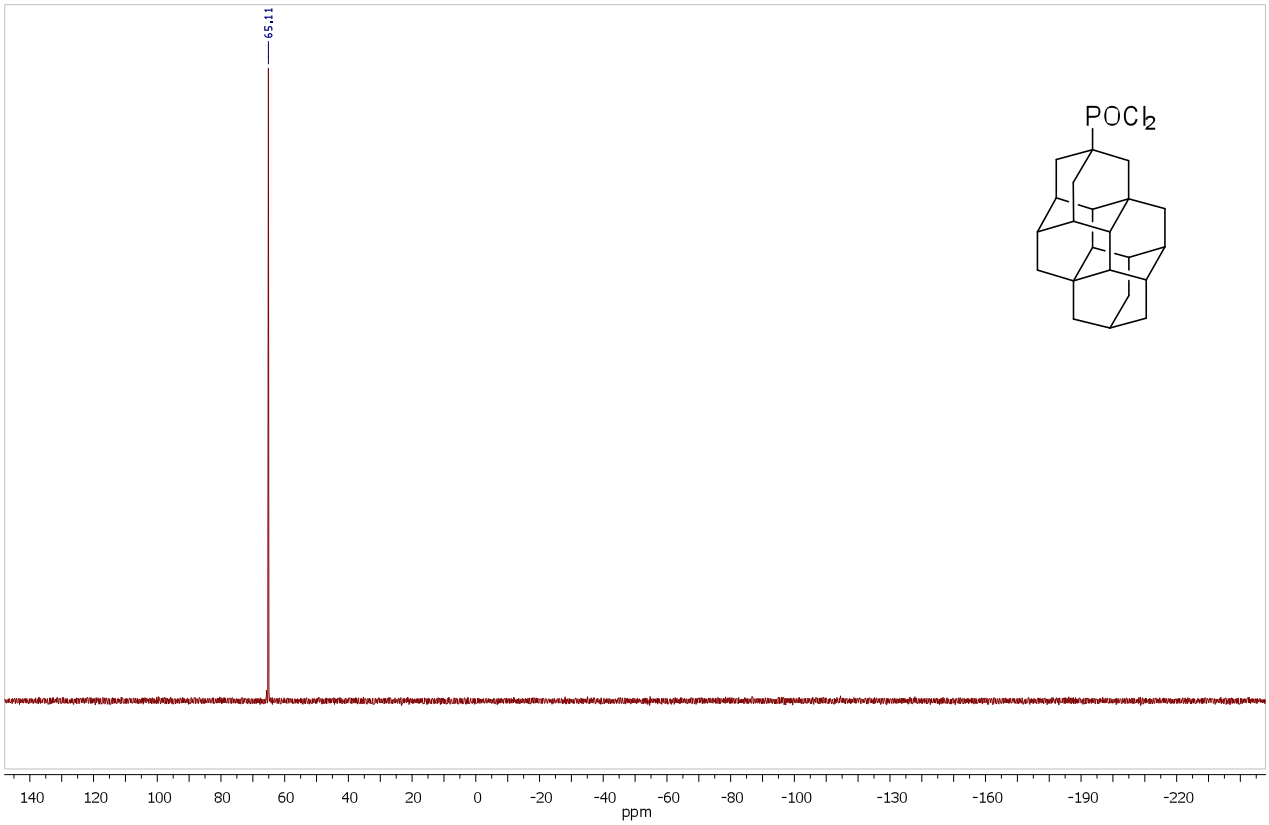
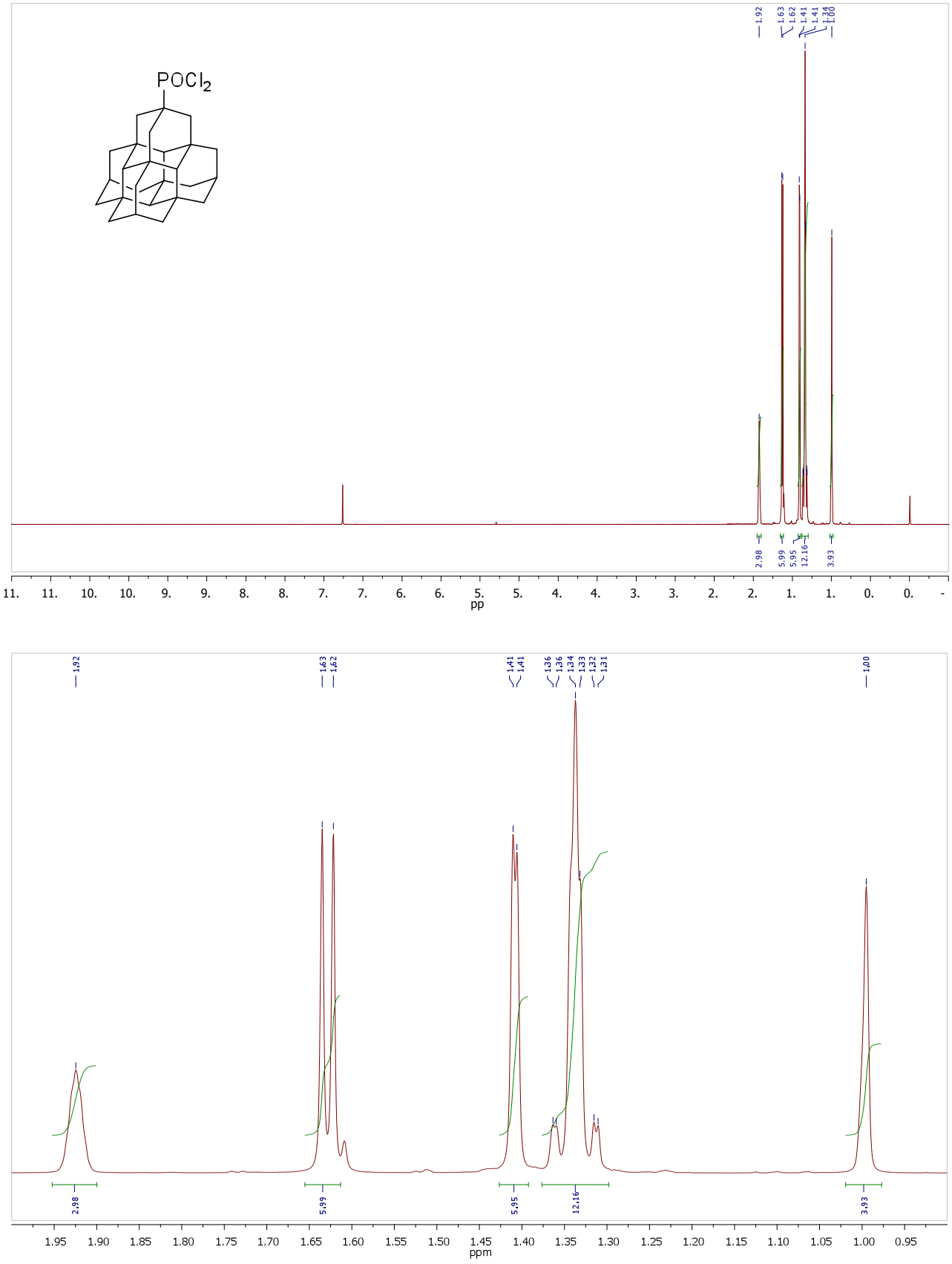


Figure 15S. ^{31}P NMR (243 MHz, $CDCl_3$) spectrum of compound **17**.



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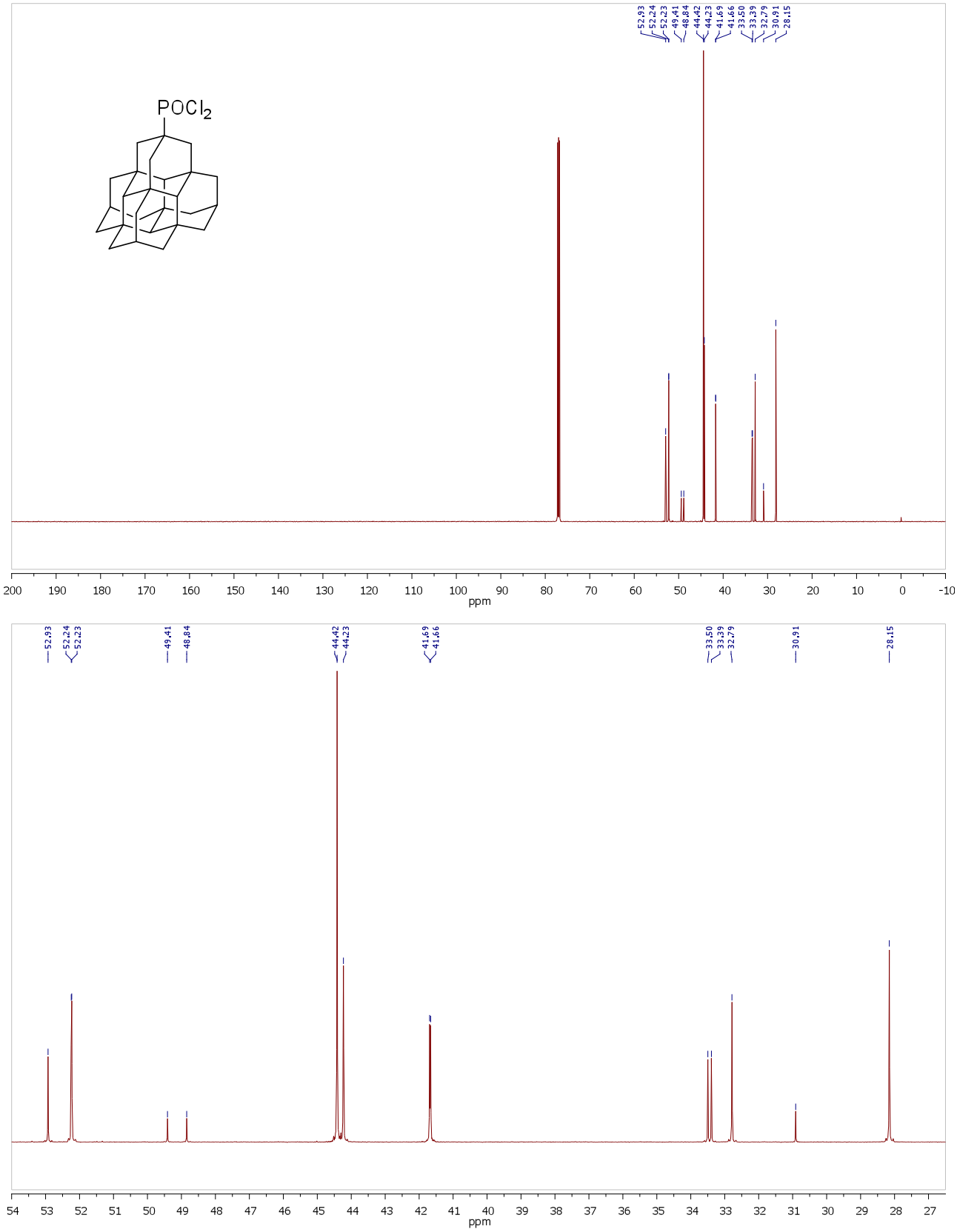

Figure 17S. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of compound **19**.

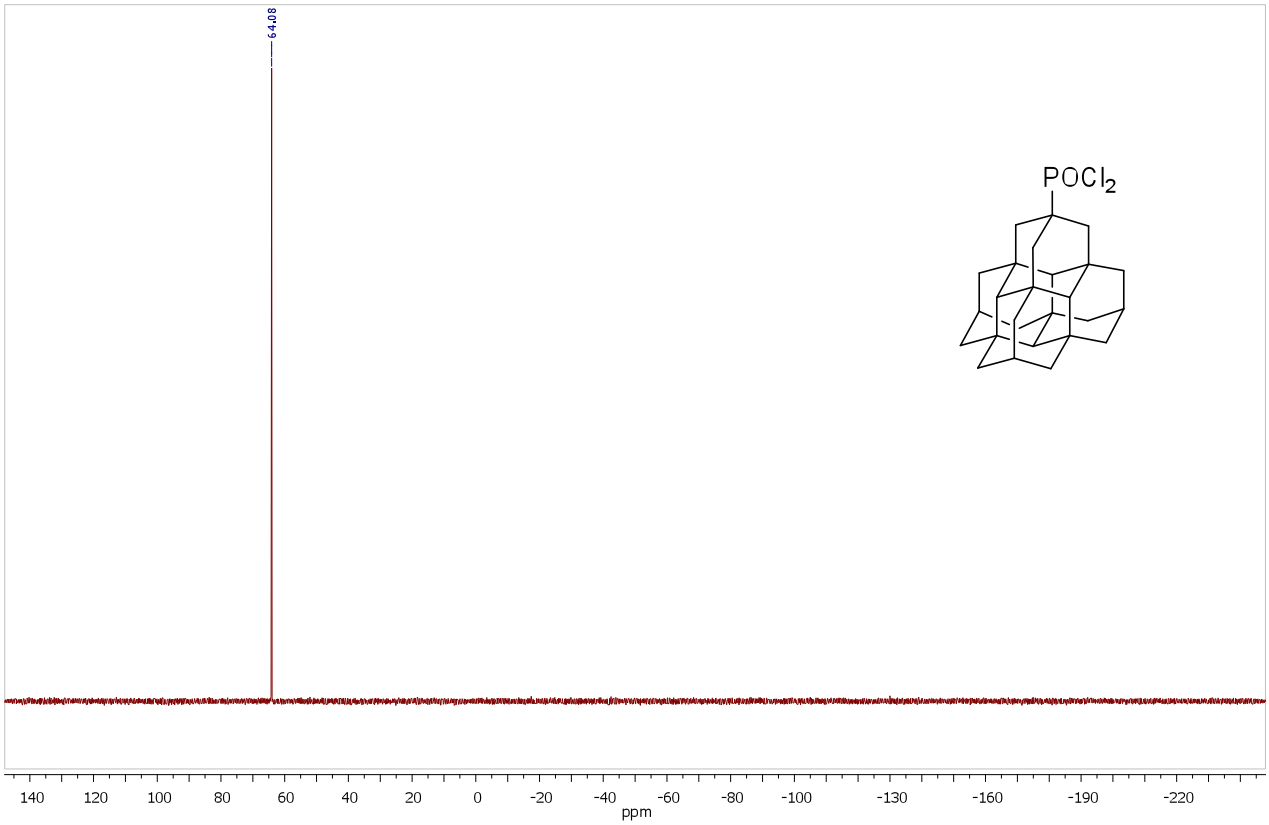

Figure 18S. ^{31}P NMR (243 MHz, $CDCl_3$) spectrum of compound **19**.

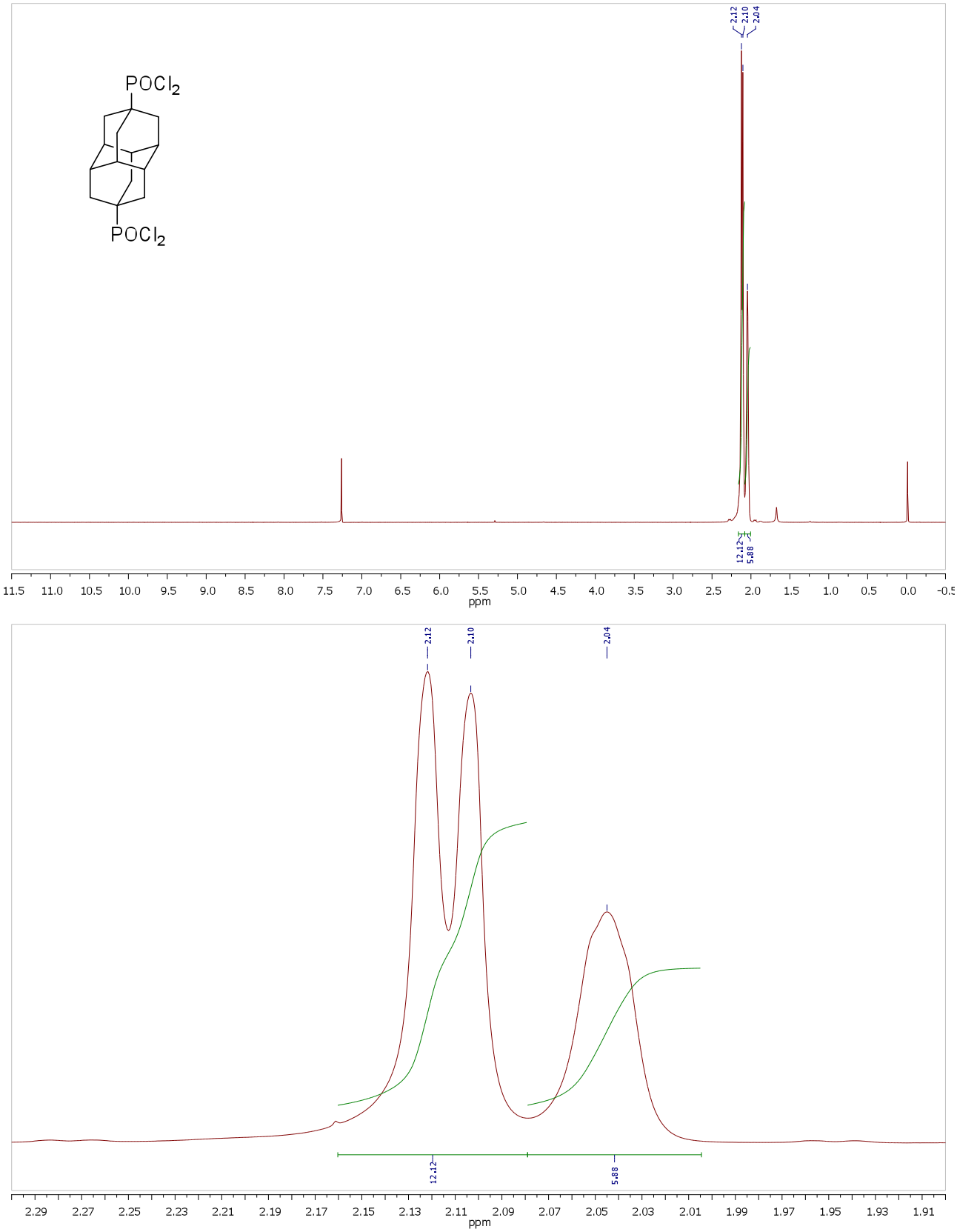

Figure 19S. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **22**.

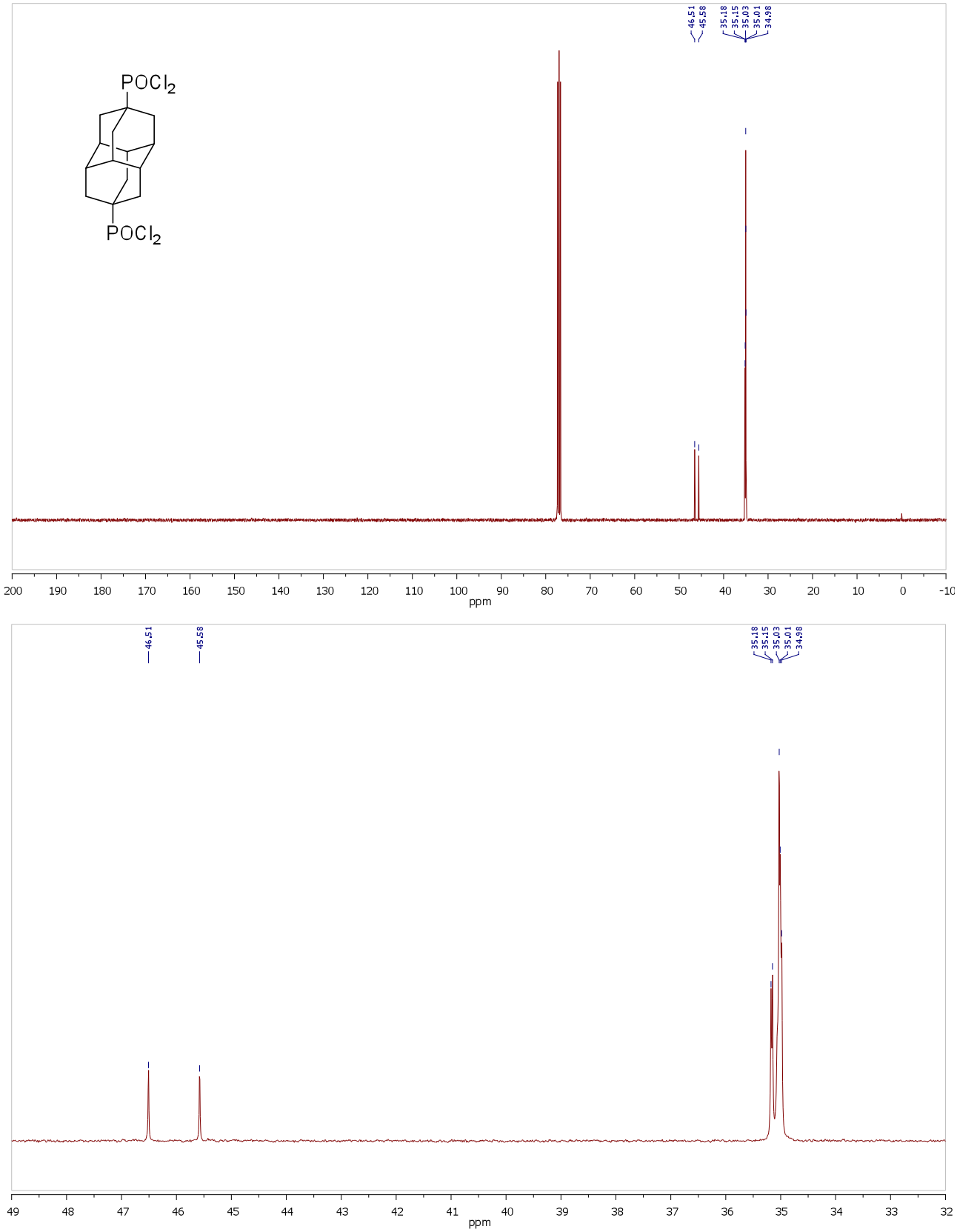

Figure 20S. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **22**.

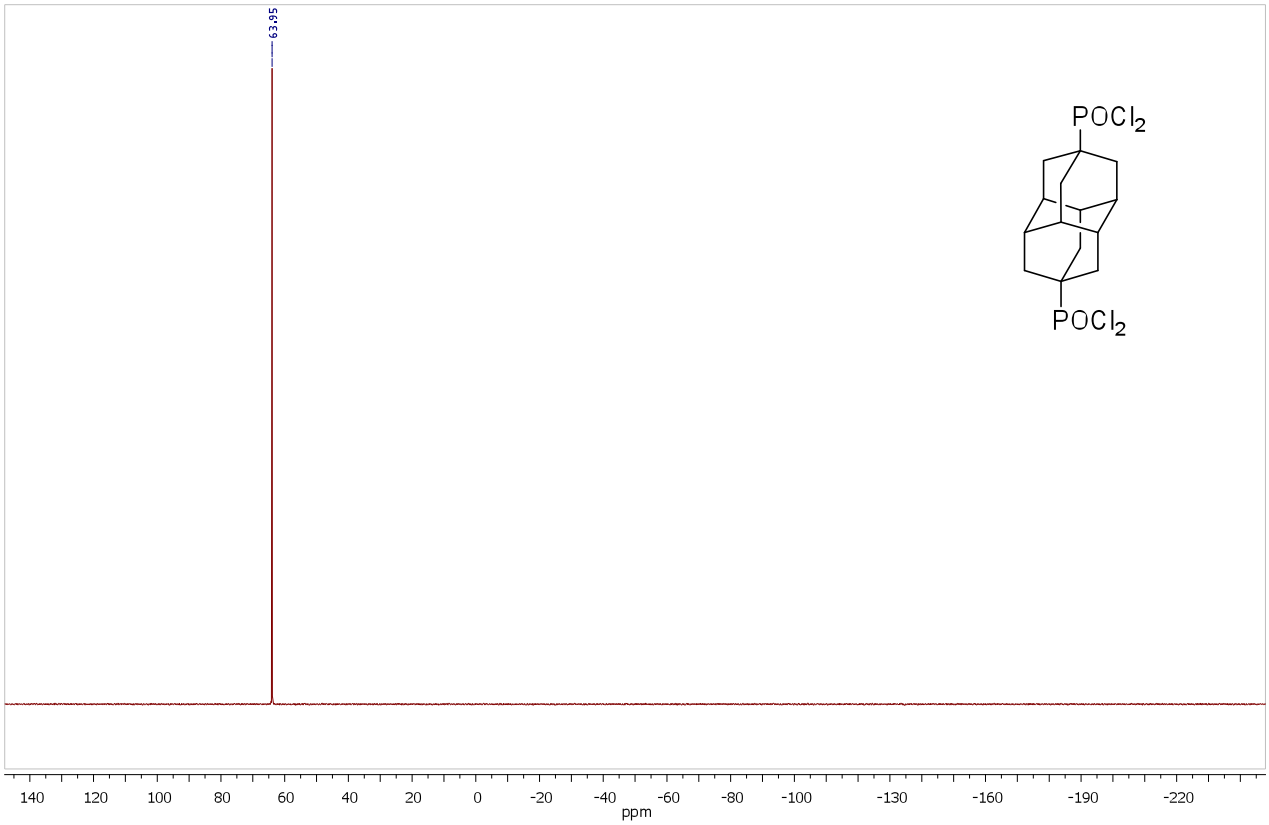

Figure 21S. ^{31}P NMR (162 MHz, $CDCl_3$) spectrum of compound **22**.

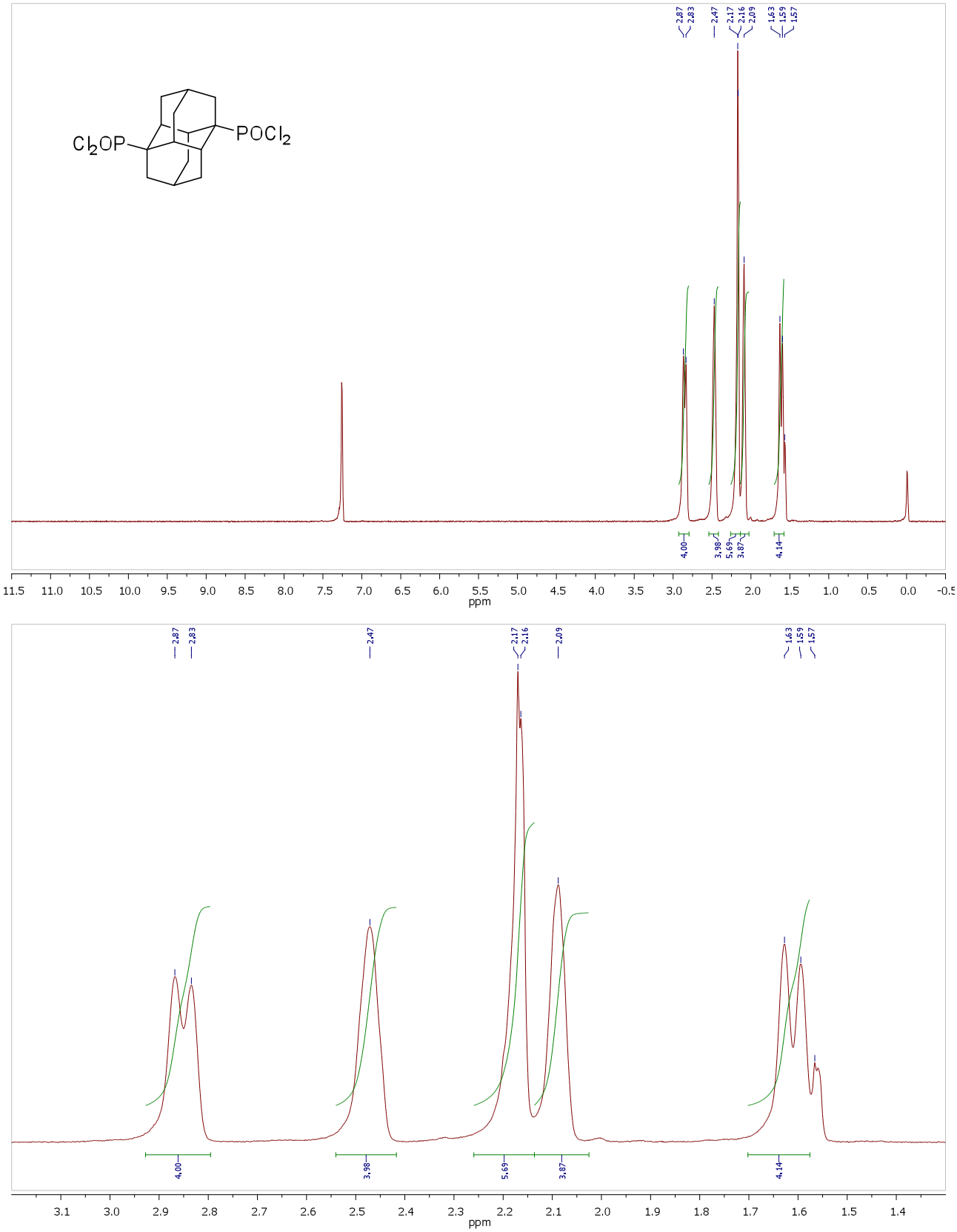

Figure 22S. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **23**.

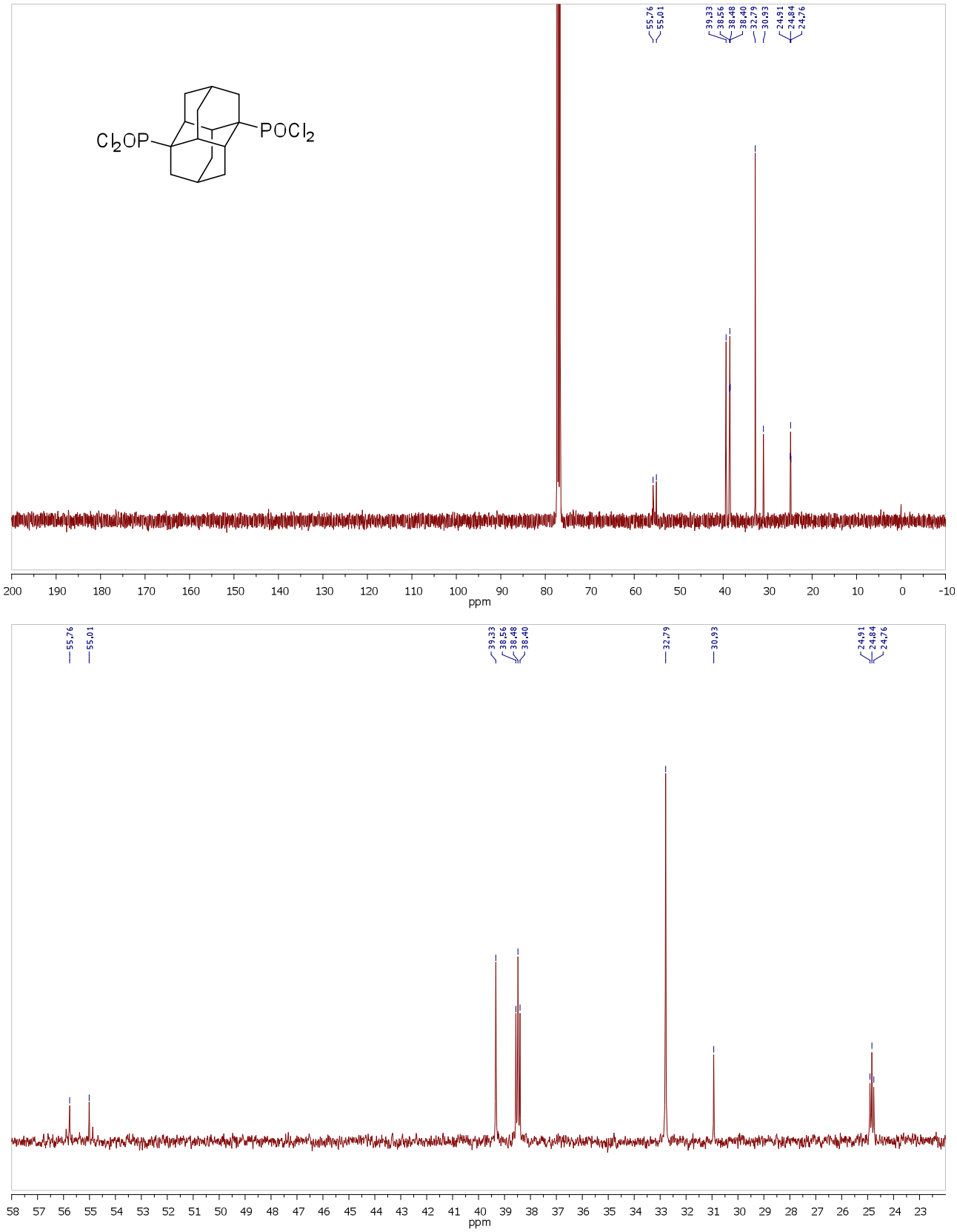

Figure 23S. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **23**.

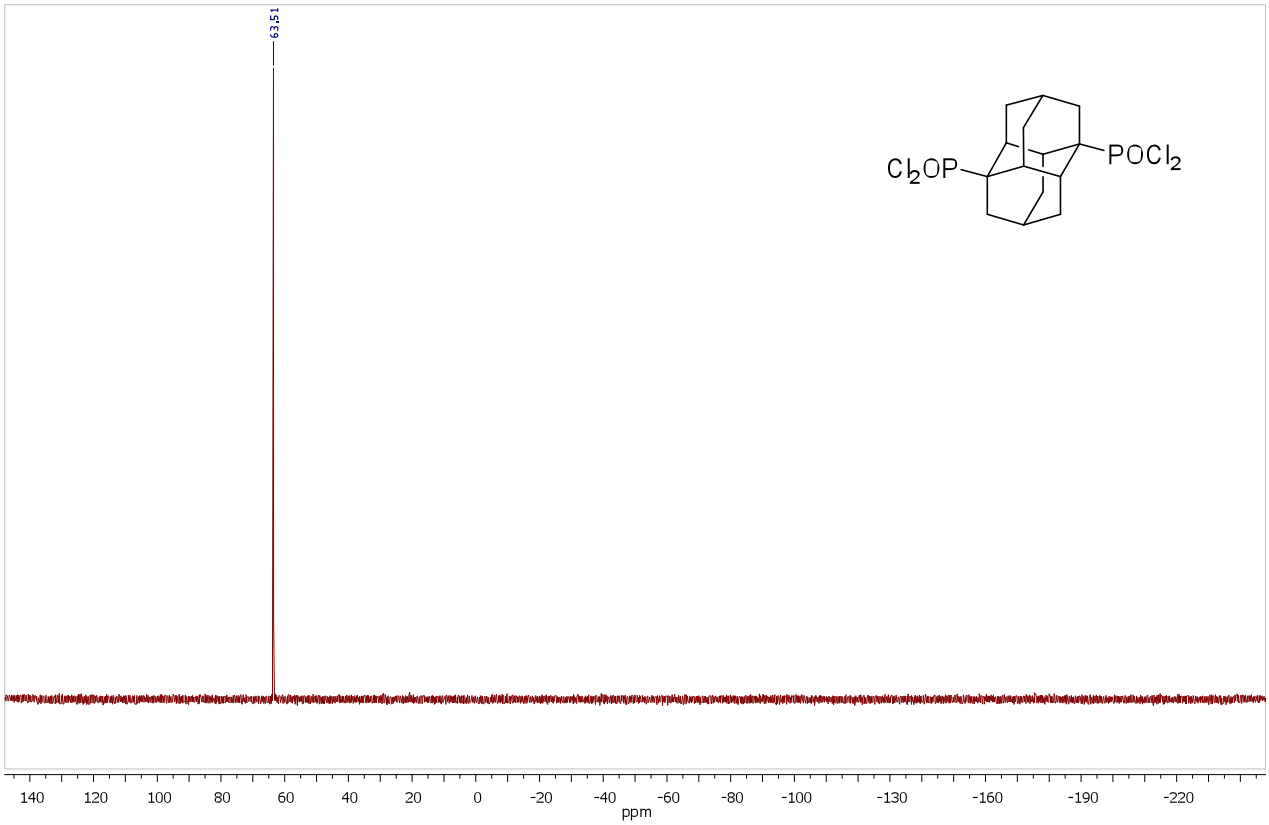

Figure 24S. ^{31}P NMR (162 MHz, $CDCl_3$) spectrum of compound **23**.

2. **The X-Ray crystal stricture data**

Compound **5**: Summary of Data CCDC 983769
Compound **17**: Summary of Data CCDC 981439
Compound **19**: Summary of Data CCDC 981440

Crystals were obtained as described in the Experimental section. For compound **5** the intensity data were collected at 100 K. The structure was solved with the olex2.solve structure solution program, using the charge flipping solution method. The model was refined with full-matrix least-squares methods based on F^2 (SHELXL)[1] with the aid of the Olex2 program.[2] All non-hydrogen atoms were refined with anisotropic thermal parameters. Hydrogen atoms were included in their calculated positions and refined with a riding model. The structure was refined as a 2-component inversion twin.

The X-ray crystallographic data for **17** and **19** were collected at 193 K. Mo Kα radiation (λ= 0.71069 Å) and a graphite monochromator was used. Cell parameters were refined by using up to 5000 reflections. A sphere of data was collected with the φ-oscillation mode (frame widths: 0.7^0, 1.0^0; number of frames: 265, 190; Irradiation times/frame: 30, and 5 min for **17** and **19** resp.) No absorption corrections were applied. The structures were solved by direct methods in SHELXS97 (all non H-atoms). The H-atoms were found by difference Fourier syntheses. The structures were refined using full-matrix least squares in SHELXL.[1] Refinement was done with F^2. All non-H atoms were treated anisotropically. All H-atoms were found in the difference Fourier syntheses and were refined isotropically.

Crystallographic data are reported in Tables 1S–10S.

Table S1. Crystal data and structure refinement for diamantane 1-phosphonic dichloride (**5**).

Identification code	(5)
Empirical formula	$C_{14}H_{19}Cl_2OP$
Formula weight	305.16
Temperature/K	100
Crystal system	monoclinic
Space group	$P2_1$
a/Å	6.547(3)
b/Å	14.435(7)
c/Å	7.735(4)
α/°	90
β/°	108.659(18)
γ/°	90
Volume/Å^3	692.5(6)
Z	2
ϱ_{calc}mg/mm^3	1.463
m/mm^{-1}	0.569
F(000)	320.0
Crystal size/mm^3	0.58 × 0.22 × 0.08
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection	5.558 to 54.974°
Index ranges	-8 ≤ h ≤ 8, -18 ≤ k ≤ 18, -9 ≤ l ≤ 10
Reflections collected	11813
Independent reflections	3153 [R_{int} = 0.0451, R_{sigma} = 0.0407]
Data/restraints/parameters	3153/1/164
Goodness-of-fit on F^2	1.092
Final R indexes [I>=2σ (I)]	R_1 [a] = 0.0370, wR_2 [b] = 0.0831
Final R indexes [all data]	R_1 [a] = 0.0457, wR_2 [b] = 0.0889
Largest diff. peak/hole / e Å^{-3}	0.48/-0.36
Flack parameter	0.10(11)
N° CCDC	983769

[a] $R1=S(||F_o|-|F_c||)/S|F_o|$. [b] $wR2=[Sw(F_o^2-F_c^2)^2/S[w(F_o^2)^2]^{1/2}$ where $w=1/[s^2(Fo^2+(0.0369P)^2+0.22P]$

Table S2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for diamantane 1-phosphonic dichloride (**5**). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C4	515(5)	2554(2)	5873(5)	26.3(7)
C5	859(7)	4098(3)	7528(5)	37.8(9)
C7	4131(5)	2817(2)	5440(4)	25.9(7)
C8	3793(6)	2933(2)	8637(4)	31.5(8)
C9	397(7)	3562(3)	2500(5)	44.1(10)
C10	3655(6)	3873(2)	5249(5)	31.8(8)
C11	3005(5)	2415(2)	6784(4)	21.6(6)
C12	-318(6)	2102(3)	3958(5)	38.2(9)
C13	69(6)	3610(2)	5675(5)	28.9(7)
C14	858(7)	2522(3)	2709(5)	41.9(10)
C15	3296(6)	2363(3)	3541(5)	37.1(8)
C16	1210(6)	4020(3)	4385(5)	32.5(8)
C17	4469(7)	4366(3)	7097(6)	40.1(9)
C18	3305(7)	3972(3)	8359(5)	36.6(9)
O6	3002(5)	513.0(19)	5726(5)	49.0(8)
P1	3641.7(13)	1180.5(6)	7217.1(13)	29.9(2)
Cl2	2440.2(17)	817.4(7)	9240.5(15)	45.8(3)
Cl3	6871.0(15)	1121.3(8)	8502.6(17)	55.9(3)

Table S3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for diamantane 1-phosphonic dichloride (**5**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C4	22.2(16)	24.4(16)	34.1(17)	-0.1(13)	11.7(13)	-1.7(13)
C5	55(3)	28.5(18)	37.1(19)	-0.6(15)	24.7(19)	10.4(18)
C7	20.0(16)	31.7(17)	27.4(15)	-0.1(13)	9.4(12)	-1.9(13)
C8	40(2)	29.5(18)	22.1(15)	-2.9(13)	6.4(14)	0.0(16)
C9	43(2)	60(3)	26.5(19)	9.5(18)	6.6(16)	9(2)
C10	35.6(19)	29.5(18)	34.3(18)	6.2(15)	16.7(15)	-4.0(15)
C11	23.3(16)	17.8(14)	24.0(15)	-1.8(12)	8.2(12)	-0.5(12)
C12	24.1(18)	37(2)	45(2)	-11.7(16)	-0.1(15)	-6.0(16)
C13	28.2(18)	26.3(17)	34.4(17)	4.7(14)	12.9(14)	7.9(14)
C14	41(2)	55(3)	23.5(17)	-10.4(16)	2.8(15)	1.3(19)
C15	41(2)	47(2)	27.3(17)	-5.7(16)	17.2(15)	4.8(18)
C16	39(2)	29.7(17)	30.9(17)	8.7(14)	13.5(15)	3.3(16)
C17	44(2)	24.5(18)	48(2)	-2.3(16)	9.6(18)	-7.9(16)
C18	53(2)	27.6(18)	27.9(17)	-7.8(14)	10.9(16)	0.9(17)
O6	56.9(19)	28.1(14)	63.8(19)	-12.4(13)	21.7(15)	1.7(13)
P1	25.4(4)	21.1(4)	43.8(5)	1.2(4)	11.8(3)	2.2(4)
Cl2	48.3(5)	37.6(5)	56.7(6)	18.9(4)	24.3(4)	4.2(4)
Cl3	24.6(4)	47.1(6)	89.7(8)	16.1(6)	9.3(4)	7.5(5)

Table S4. Bond Lengths for diamantane 1-phosphonic dichloride (**5**).

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C4	C11	1.569(4)	C9	C16	1.533(5)
C4	C12	1.548(5)	C10	C16	1.539(5)
C4	C13	1.551(5)	C10	C17	1.532(5)
C5	C13	1.530(5)	C11	P1	1.836(3)
C5	C18	1.534(6)	C12	C14	1.539(6)
C7	C10	1.554(5)	C13	C16	1.543(5)
C7	C11	1.565(4)	C14	C15	1.536(6)
C7	C15	1.540(5)	C17	C18	1.527(6)
C8	C11	1.551(4)	O6	P1	1.458(3)
C8	C18	1.534(5)	P1	Cl2	2.0325(16)
C9	C14	1.529(6)	P1	Cl3	2.0298(15)

Table S5. Bond Angles for diamantane 1-phosphonic dichloride (**5**).

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C12	C4	C11	111.9(3)	C5	C13	C16	109.9(3)
C12	C4	C13	108.8(3)	C16	C13	C4	109.0(3)
C13	C4	C11	107.8(3)	C9	C14	C12	109.4(3)
C13	C5	C18	109.4(3)	C9	C14	C15	109.5(3)
C10	C7	C11	107.7(3)	C15	C14	C12	109.9(3)
C15	C7	C10	109.1(3)	C14	C15	C7	109.9(3)
C15	C7	C11	112.2(3)	C9	C16	C10	110.5(3)
C18	C8	C11	110.4(3)	C9	C16	C13	110.9(3)
C14	C9	C16	109.0(3)	C10	C16	C13	108.5(3)
C16	C10	C7	109.0(3)	C18	C17	C10	109.1(3)
C17	C10	C7	111.6(3)	C8	C18	C5	108.5(3)
C17	C10	C16	110.1(3)	C17	C18	C5	110.8(3)
C4	C11	P1	110.4(2)	C17	C18	C8	109.3(3)
C7	C11	C4	107.2(2)	C11	P1	Cl2	105.64(11)
C7	C11	P1	110.7(2)	C11	P1	Cl3	105.67(11)
C8	C11	C4	110.1(3)	O6	P1	C11	120.41(17)
C8	C11	C7	110.3(3)	O6	P1	Cl2	110.78(15)
C8	C11	P1	108.1(2)	O6	P1	Cl3	110.51(14)
C14	C12	C4	109.9(3)	Cl3	P1	Cl2	102.17(7)
C5	C13	C4	111.3(3)				

Table S6. Torsion Angles for diamantane 1-phosphonic dichloride (**5**).

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C4	C11	P1	O6	56.9(3)	C11	C8	C18	C5	60.7(4)
C4	C11	P1	Cl2	-69.4(2)	C11	C8	C18	C17	-60.2(4)
C4	C11	P1	Cl3	-177.22(18)	C12	C4	C11	C7	56.2(3)
C4	C12	C14	C9	-61.2(4)	C12	C4	C11	C8	176.2(3)
C4	C12	C14	C15	59.1(4)	C12	C4	C11	P1	-64.5(3)
C4	C13	C16	C9	59.4(4)	C12	C4	C13	C5	-180.0(3)
C4	C13	C16	C10	-62.1(4)	C12	C4	C13	C16	-58.6(4)
C5	C13	C16	C9	-178.4(3)	C12	C14	C15	C7	-59.4(4)
C5	C13	C16	C10	60.1(4)	C13	C4	C11	C7	-63.4(3)
C7	C10	C16	C9	-59.6(4)	C13	C4	C11	C8	56.6(3)
C7	C10	C16	C13	62.2(4)	C13	C4	C11	P1	175.9(2)
C7	C10	C17	C18	-61.3(4)	C13	C4	C12	C14	60.2(4)
C7	C11	P1	O6	-61.7(3)	C13	C5	C18	C8	-61.2(4)
C7	C11	P1	Cl2	172.01(19)	C13	C5	C18	C17	58.8(4)
C7	C11	P1	Cl3	64.2(2)	C14	C9	C16	C10	60.4(4)
C8	C11	P1	O6	177.4(2)	C14	C9	C16	C13	-60.0(4)
C8	C11	P1	Cl2	51.1(2)	C15	C7	C10	C16	58.7(3)
C8	C11	P1	Cl3	-56.7(2)	C15	C7	C10	C17	-179.5(3)
C9	C14	C15	C7	60.8(4)	C15	C7	C11	C4	-56.6(3)
C10	C7	C11	C4	63.5(3)	C15	C7	C11	C8	-176.5(3)
C10	C7	C11	C8	-56.5(3)	C15	C7	C11	P1	63.9(3)
C10	C7	C11	P1	-176.0(2)	C16	C9	C14	C12	60.1(4)
C10	C7	C15	C14	-59.7(4)	C16	C9	C14	C15	-60.3(4)
C10	C17	C18	C5	-58.8(4)	C16	C10	C17	C18	59.8(4)
C10	C17	C18	C8	60.7(4)	C17	C10	C16	C9	177.7(3)
C11	C4	C12	C14	-58.8(4)	C17	C10	C16	C13	-60.5(4)
C11	C4	C13	C5	-58.4(4)	C18	C5	C13	C4	61.6(4)
C11	C4	C13	C16	63.0(3)	C18	C5	C13	C16	-59.3(4)
C11	C7	C10	C16	-63.3(3)	C18	C8	C11	C4	-59.4(4)
C11	C7	C10	C17	58.5(4)	C18	C8	C11	C7	58.8(4)
C11	C7	C15	C14	59.5(4)	C18	C8	C11	P1	179.9(3)

Table S7. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for diamantane 1-phosphonic dichloride (5).

Atom	***x***	***y***	***z***	**U(eq)**
H4	-262	2280	6673	32
H5A	129	3832	8355	45
H5B	506	4766	7372	45
H7	5722	2718	5962	31
H8A	3063	2676	9472	38
H8B	5365	2840	9204	38
H9A	-1172	3668	1948	53
H9B	1136	3836	1687	53
H10	4400	4144	4421	38
H12A	-63	1426	4065	46
H12B	-1889	2208	3421	46
H13	-1519	3712	5128	35
H14	327	2220	1483	50
H15A	4048	2634	2735	44
H15B	3602	1690	3648	44
H16	907	4700	4247	39
H17A	6043	4273	7644	48
H17B	4188	5040	6930	48
H18	3823	4295	9564	44

Table S8. Final atomic coordinates for **17**

	x	y	z	U_{equiv} or U_{iso}
P1	0.82765(4)	0.27945(8)	0.97341(3)	0.01782(15)
Cl1	0.70463(4)	0.11473(9)	0.95832(3)	0.03107(17)
Cl2	0.77728(4)	0.57070(8)	0.96963(3)	0.02695(16)
O1	0.87493(13)	0.2340(3)	1.03590(8)	0.0299(4)
C1	1.05457(15)	0.3583(3)	0.72369(11)	0.0185(4)
C2	0.90344(13)	0.2483(3)	0.77978(10)	0.0128(4)
C3	0.99599(17)	0.3970(3)	0.66002(11)	0.0230(5)
C4	1.00444(14)	-0.0096(3)	0.72092(10)	0.0160(4)
C5	0.90827(15)	0.2503(3)	0.65795(10)	0.0202(4)
C6	1.15082(15)	0.0963(4)	0.78752(12)	0.0243(5)
C7	0.93512(16)	0.0193(3)	0.90174(11)	0.0184(4)
C8	1.0591(2)	0.3612(4)	0.60131(13)	0.0301(5)
C9	0.89848(14)	0.2434(3)	0.90162(10)	0.0150(4)
C10	0.83978(14)	0.2848(3)	0.83820(10)	0.0156(4)
C11	1.09339(14)	0.1354(3)	0.72397(11)	0.0181(4)
C12	0.84519(15)	0.2870(3)	0.71631(11)	0.0193(4)
C13	1.00014(15)	-0.0130(3)	0.84386(10)	0.0169(4)
C14	0.99234(14)	0.3929(3)	0.78320(10)	0.0157(4)
C15	0.94202(14)	0.0248(3)	0.78005(10)	0.0142(4)
C16	1.15494(17)	0.0993(4)	0.66440(13)	0.0265(5)
C17	0.98693(15)	0.3897(3)	0.90569(11)	0.0187(4)
C18	1.00877(19)	-0.0077(4)	0.59842(12)	0.0267(5)
C19	1.04998(15)	0.3538(3)	0.84712(11)	0.0184(4)
C20	1.09587(18)	0.1387(4)	0.60165(12)	0.0273(5)
C21	0.94551(16)	0.0280(3)	0.65721(11)	0.0194(4)
C22	1.08809(15)	0.1324(3)	0.84630(11)	0.0202(5)
H1	0.8850(16)	-0.069(3)	0.7777(11)	0.011(5)
H2	0.8793(18)	-0.074(4)	0.8986(12)	0.022(6)
H3	0.7866(17)	0.195(4)	0.7143(11)	0.014(5)
H4	1.0250(17)	-0.153(4)	0.8453(12)	0.018(6)
H5	1.1252(19)	0.107(4)	0.8840(14)	0.026(6)
H6	0.8717(18)	0.277(4)	0.6182(13)	0.023(6)
H7	0.7840(17)	0.190(3)	0.8366(11)	0.015(6)
H8	1.0296(17)	-0.154(4)	0.7220(12)	0.021(6)
H9	0.8201(18)	0.425(4)	0.8371(13)	0.024(6)
H10	1.110(2)	0.450(4)	0.7262(14)	0.032(7)
H11	1.105(2)	0.443(4)	0.8487(13)	0.028(7)
H12	1.0227(18)	0.363(4)	0.9436(13)	0.022(6)
H13	0.9677(18)	0.532(4)	0.7807(12)	0.021(6)
H14	1.175(2)	-0.040(4)	0.6651(14)	0.032(7)
H15	0.8901(18)	-0.064(4)	0.6566(12)	0.021(6)
H16	0.9712(19)	-0.006(4)	0.9388(14)	0.026(6)
H17	1.115(2)	0.449(5)	0.6022(15)	0.042(8)
H18	0.8242(18)	0.429(4)	0.7162(13)	0.025(6)
H19	1.209(2)	0.183(4)	0.7897(14)	0.034(7)
H20	0.973(2)	0.015(4)	0.5601(15)	0.031(7)
H21	1.0247(19)	0.391(4)	0.5597(15)	0.030(7)
H22	1.215(2)	0.185(4)	0.6687(14)	0.035(7)
H23	0.965(2)	0.523(5)	0.9087(14)	0.037(8)
H24	1.174(2)	-0.042(5)	0.7901(13)	0.033(7)
H25	0.972(2)	0.538(4)	0.6596(14)	0.031(7)
H26	1.137(2)	0.108(5)	0.5664(16)	0.044(8)
H27	1.031(2)	-0.152(5)	0.5981(14)	0.039(8)

Table S9. Final atomic coordinates for **19**

	x	y	z	U_{equiv} or U_{iso}
P1	0.04670(6)	0.2500	0.79723(5)	0.02059(16)
Cl1	0.01052(5)	0.12474(4)	0.91170(4)	0.03515(16)
O1	0.21109(18)	0.2500	0.78350(17)	0.0326(4)
C1	-0.4284(2)	0.2500	0.52133(17)	0.0107(3)
C2	-0.1244(2)	0.2500	0.63566(18)	0.0133(3)
C3	-0.41391(14)	0.15104(10)	0.43446(13)	0.0111(3)
C4	-0.2355(2)	0.2500	0.32246(17)	0.0113(3)
C5	-0.2908(2)	0.2500	0.66311(18)	0.0132(3)
C6	-0.55318(15)	0.14901(11)	0.29227(13)	0.0131(3)
C7	-0.24688(15)	0.14928(11)	0.40740(13)	0.0115(3)
C8	-0.5940(2)	0.2500	0.54806(19)	0.0162(4)
C9	-0.7310(2)	0.2500	0.4065(2)	0.0183(4)
C10	-0.71782(16)	0.15056(13)	0.32159(15)	0.0187(3)
C11	-0.3714(2)	0.2500	0.17822(18)	0.0134(3)
C12	-0.53590(17)	0.04981(12)	0.20813(15)	0.0193(3)
C13	-0.37104(18)	0.04972(12)	0.18006(14)	0.0201(3)
C14	-0.11049(15)	0.14976(11)	0.55005(13)	0.0137(3)
C15	-0.23381(16)	0.05028(11)	0.32173(14)	0.0179(3)
C16	-0.35766(18)	0.14943(13)	0.09558(14)	0.0196(3)
C17	-0.5368(2)	0.2500	0.20908(18)	0.0127(3)
H1	-0.127(3)	0.2500	0.302(3)	0.018(6)
H2	-0.301(2)	0.1862(16)	0.718(2)	0.021(4)
H3	-0.624(3)	0.2500	0.118(3)	0.021(6)
H4	-0.130(2)	0.0536(17)	0.306(2)	0.026(5)
H5	-0.419(2)	0.0861(16)	0.490(2)	0.019(4)
H6	-0.237(2)	-0.0152(17)	0.377(2)	0.026(5)
H7	-0.361(2)	-0.0146(17)	0.125(2)	0.027(5)
H8	-0.838(4)	0.2500	0.423(3)	0.032(7)
H9	-0.809(3)	0.1486(18)	0.233(2)	0.032(5)
H10	-0.116(2)	0.0861(17)	0.605(2)	0.024(4)
H11	-0.549(2)	-0.0114(18)	0.258(2)	0.029(5)
H12	-0.619(3)	0.0494(19)	0.121(2)	0.038(6)
H13	-0.442(3)	0.1476(18)	0.007(2)	0.031(5)
H14	-0.728(3)	0.0871(19)	0.376(2)	0.032(5)
H15	-0.009(3)	0.1492(17)	0.533(2)	0.028(5)
H16	-0.253(3)	0.1499(18)	0.076(2)	0.035(5)
H17	-0.602(3)	0.1861(17)	0.605(2)	0.031(5)

Table 1S10. Crystallographic data for **17** and **19**

	17	**19**
	[121]tetramantane-dichlorophosphonat	[1(2,3)4]pentamantane-dichlorophosphonat
emp. form.	$C_{22}H_{27}Cl_2OP$	$C_{26}H_{31}Cl_2OP$
form. wt.	409.34	461.38
T (K)	193(2)	193(2)
cryst. syst.	monoclinic	monoclinic
space group	$P2_1/n$	$P2_1/m$
a (Å)	13.7657(10)	8.5927(10)
b (Å)	6.5028(6)	12.5125(11)
c (Å)	20.5800(14)	9.8811(11)
α (°)	90.0	90
β (°)	91.615(8)	107.977(13)
γ (°)	90.0	90
Z	4	2
V (Å^3)	1841.5(2)	1010.51(19)
D_{calc} (Mg/m^3)	1.476	1.516
F (000)	864	488
R_1	0.034	0.0361
wR_2	0.996	0.1140
N – total	12826	9249
N – indep.	3483	2528
N – obsd.	2537	2115
variables	343	216

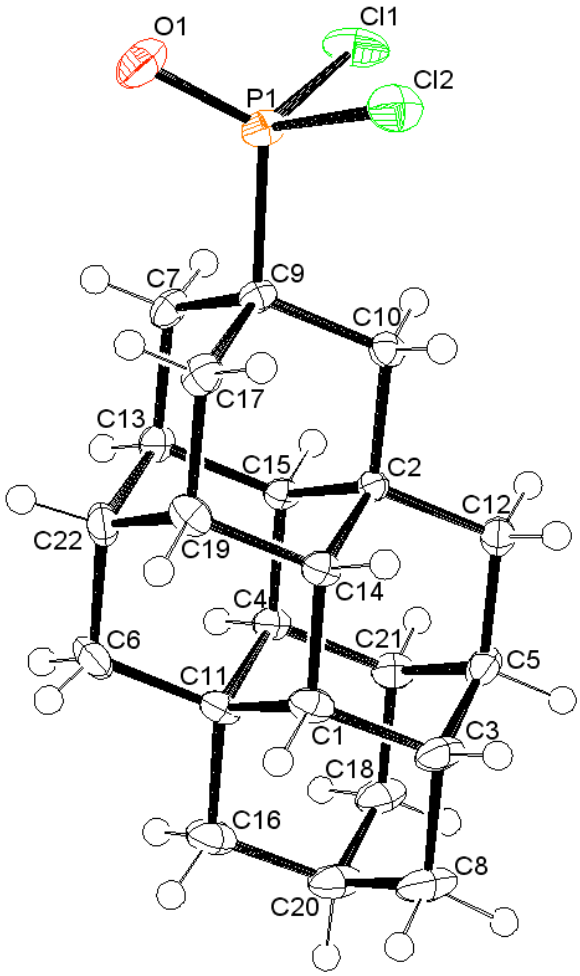

Figure 25S. The ORTEP-Plot of **17.**

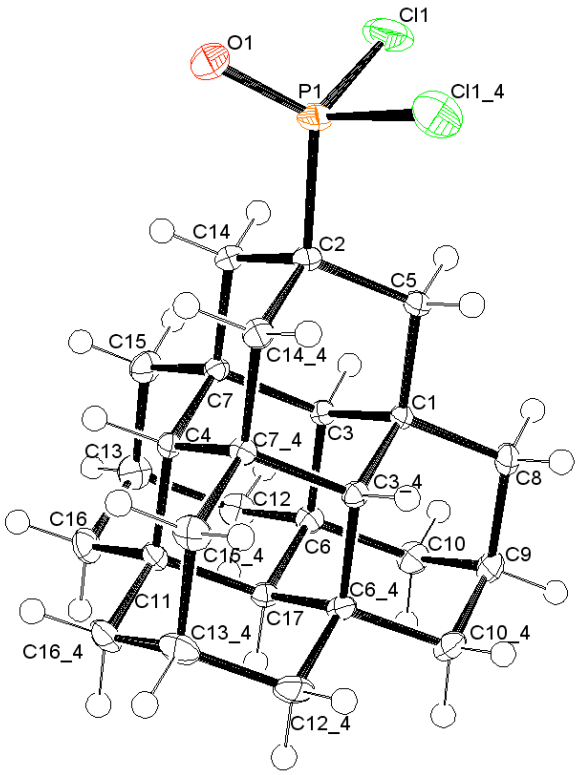

Figure 26S. The ORTEP-plot of compound **19**.

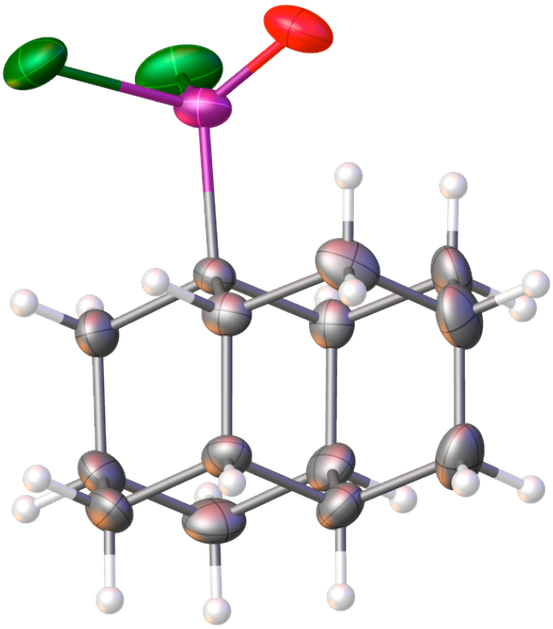

Figure 27S. The ORTEP-plot of compound **5**.

Additional References

(1) Sheldrick, G. M. *Acta Crystallographica Section A* **2008**, *64*, 112–122.
(2) Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. *J. Appl. Crystallogr.* **2009**, *42*, 339–341.