catalysts

MDPI

Amide-type substrates in the synthesis of *N*-protected 1-aminomethylphosphonium salts

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Supporting information

Experimental and analytical data

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4. MS spectra of unknown compounds……..….S92-S103

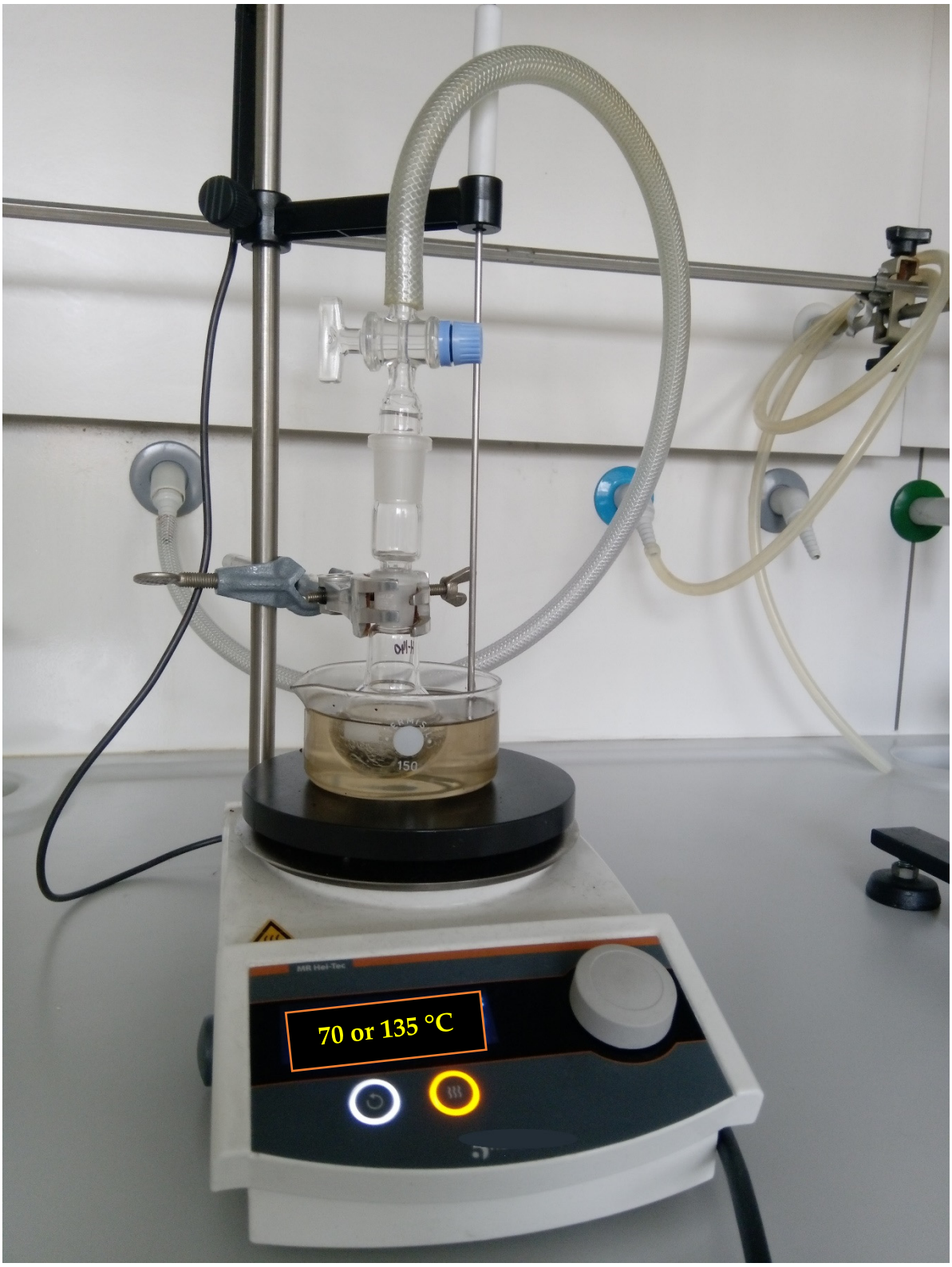
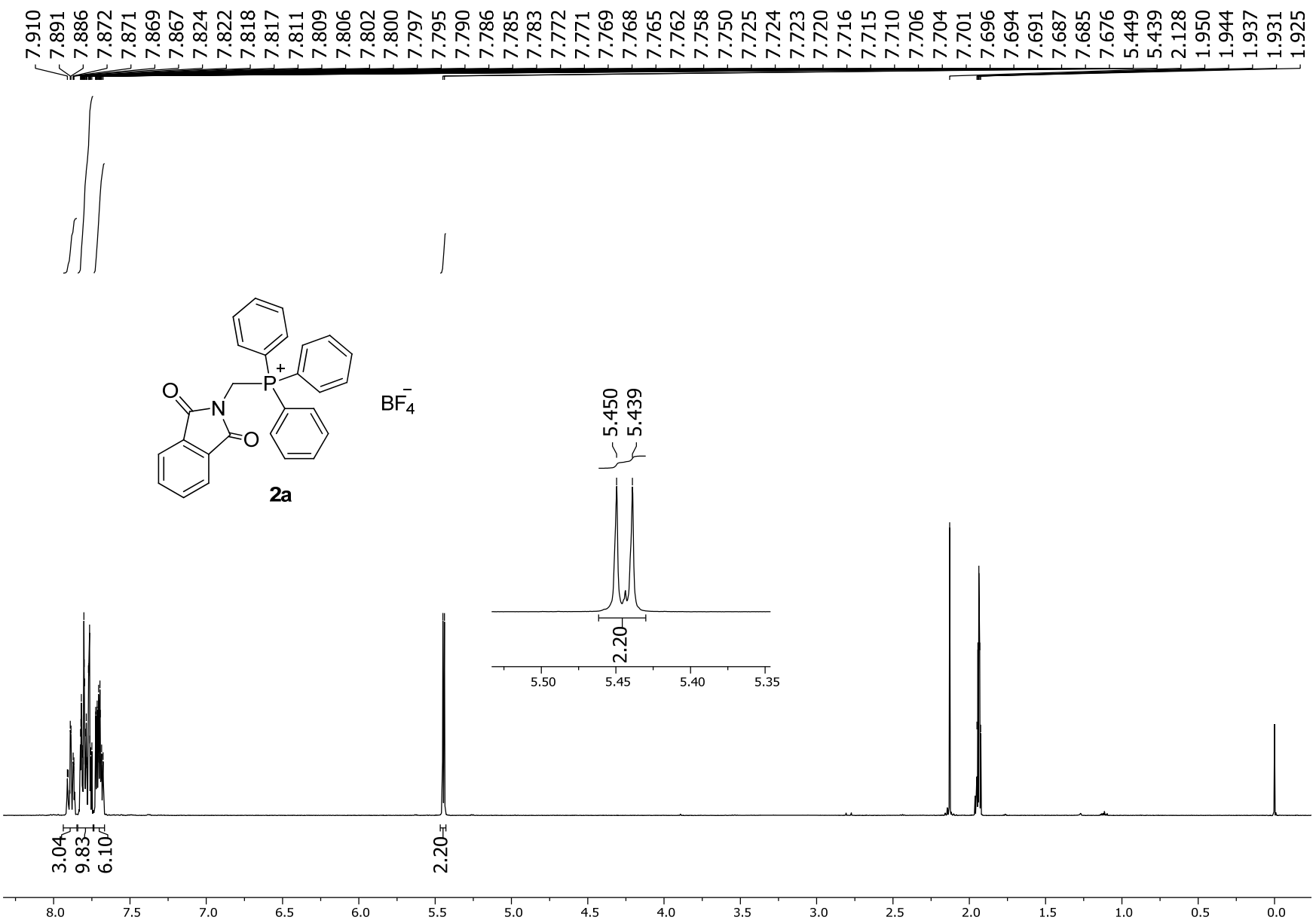
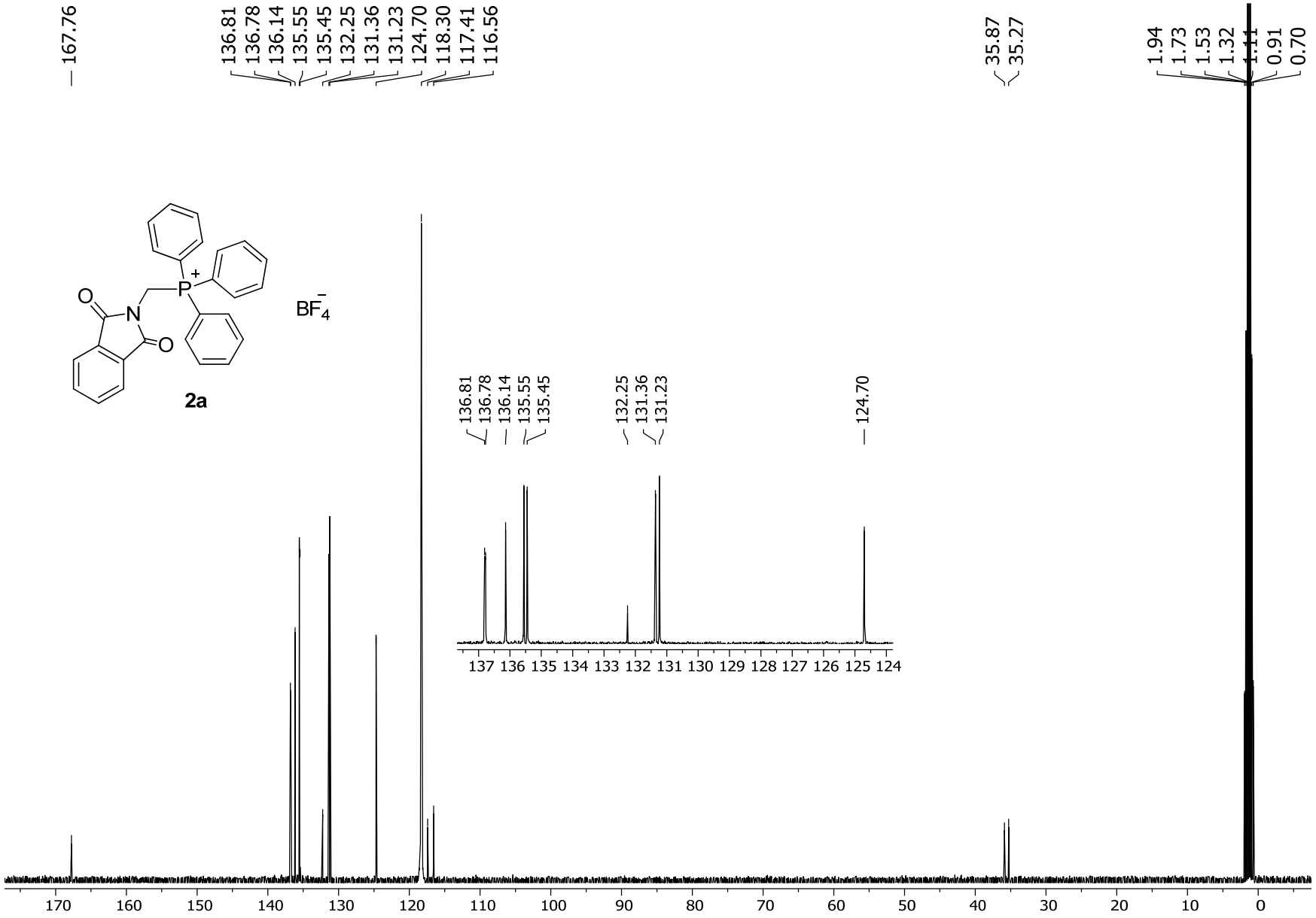


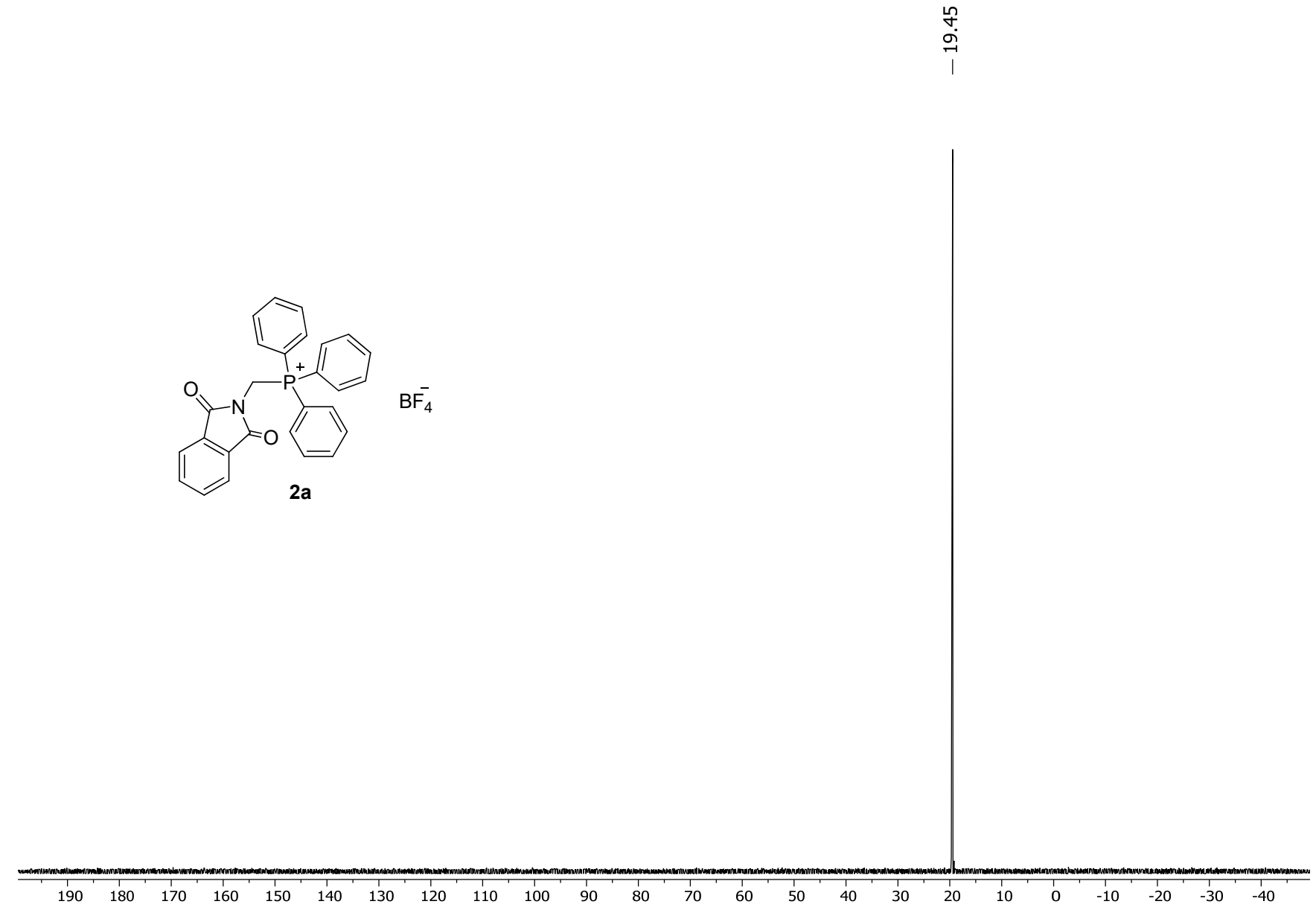
Photo S1. Apparatus for the synthesis of *N*-protected aminomethylhosphonium salts **2**. (Personal photo made by dr. J. Adamek).



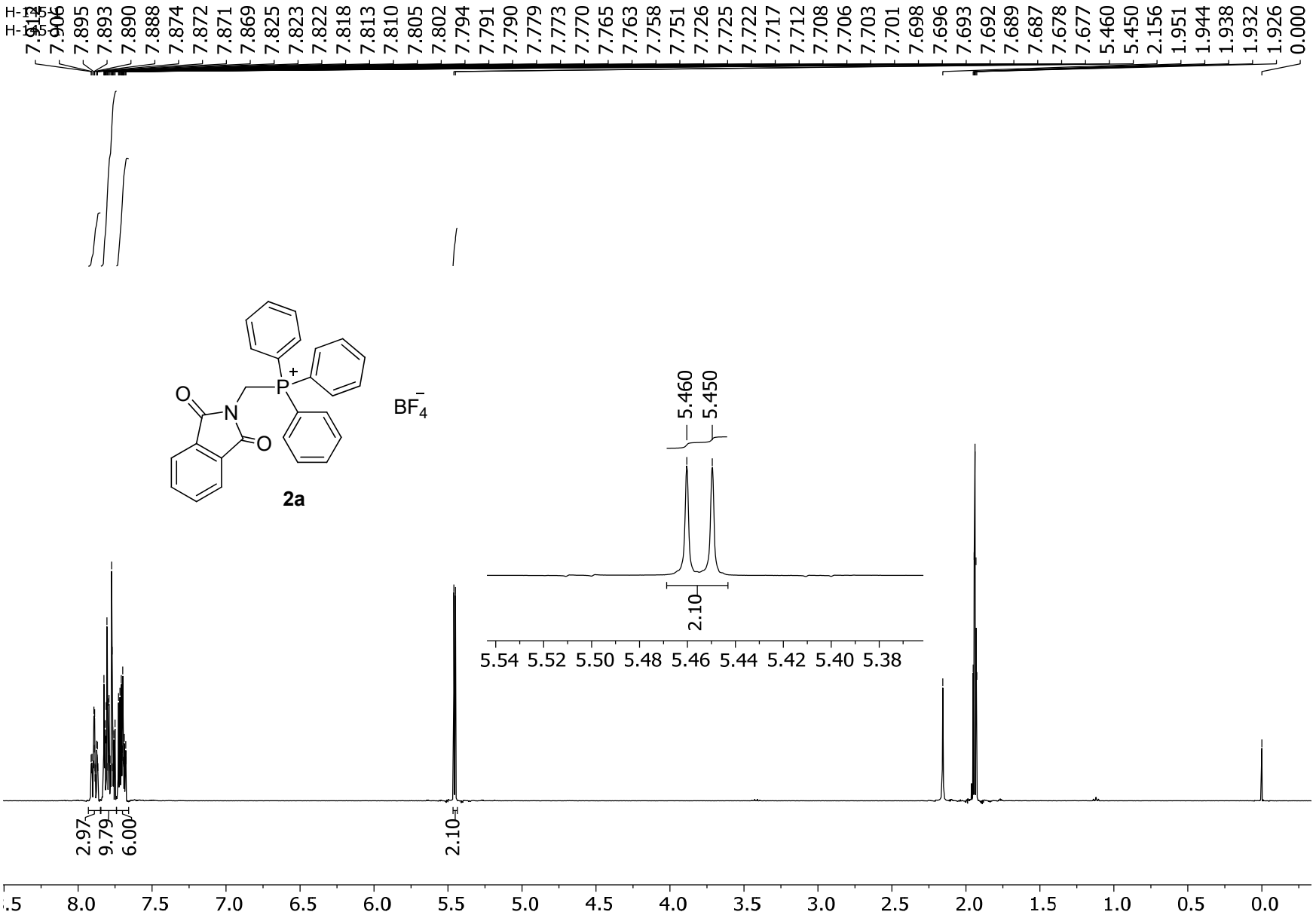
^{1}H NMR spectrum of 1-(*N*-phthalimido)methyltriphenylphosphonium tetrafluoroborate (**2a**); 400 MHz/CD_3CN/TMS; δ (ppm).



$^{13}C\{^{1}H\}$ NMR spectrum of 1-(*N*-phthalimido)methyltriphenylphosphonium tetrafluoroborate (**2a**); 100 MHz/CD_3CN/TMS; δ (ppm).

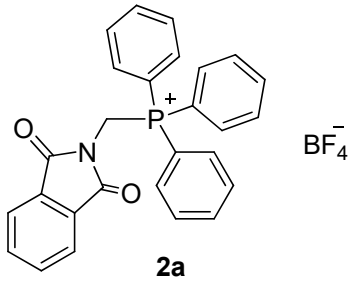


$^{31}P\{^{1}H\}$ NMR spectrum of 1-(*N*-phthalimido)methyltriphenylphosphonium tetrafluoroborate (**2a**); 161.9 MHz/CD_3CN; δ (ppm).



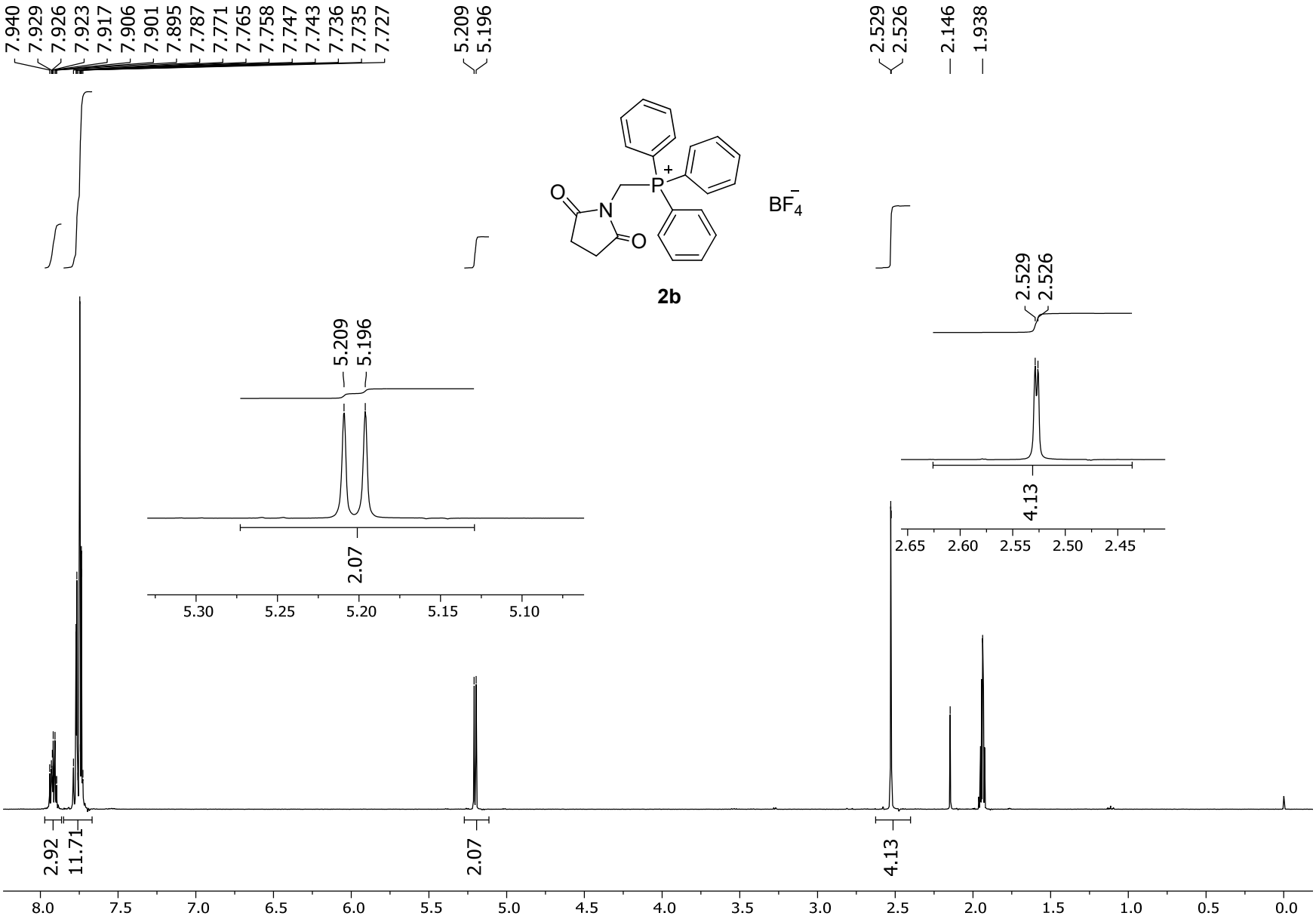
^{1}H NMR spectrum of 1-(*N*-phthalimido)methyltriphenylphosphonium tetrafluoroborate (**2a**) 5g-scale; 400 MHz/CD_3CN/TMS; δ (ppm).

H-145-1-31P
H-143-3-31P

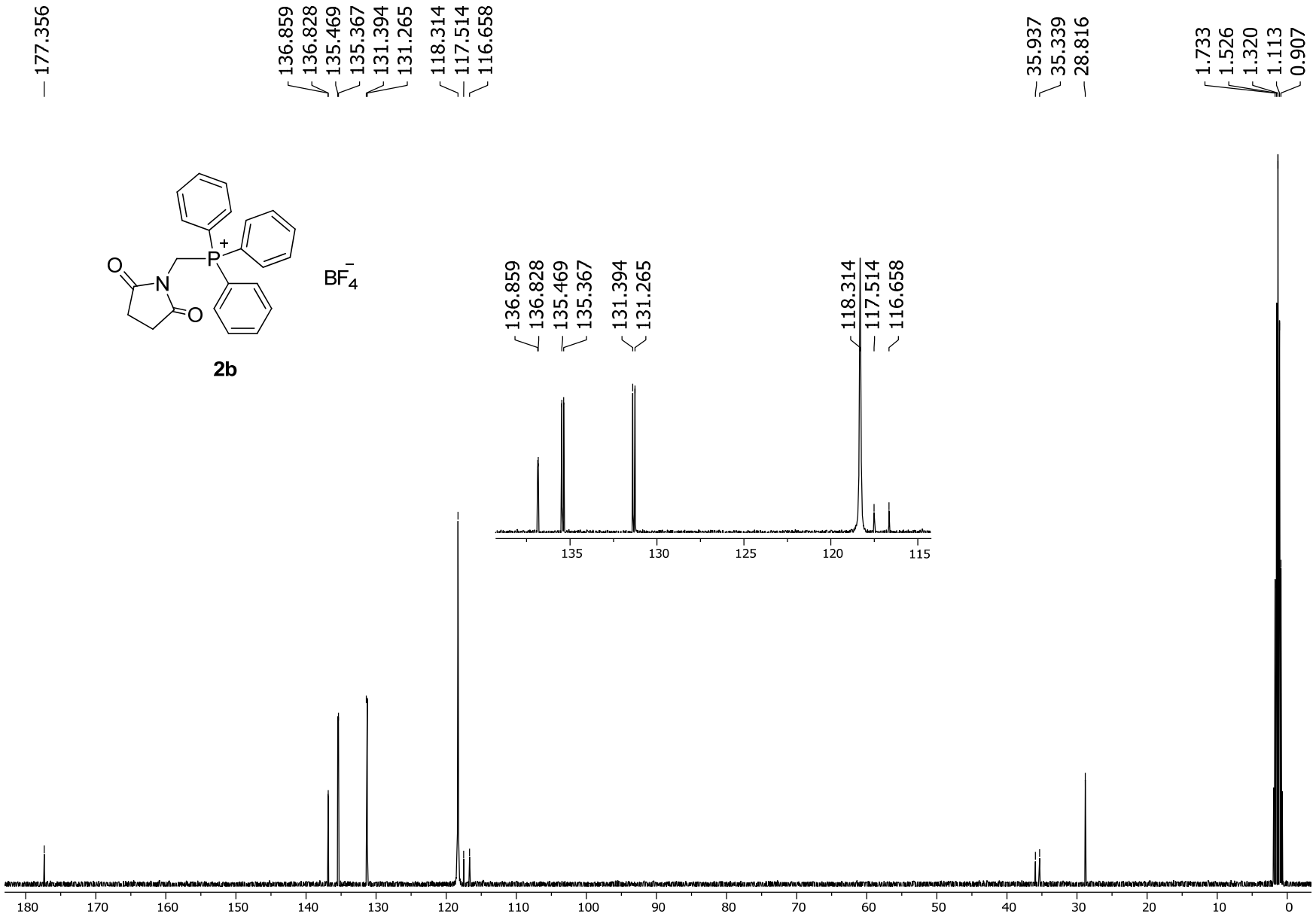


2a

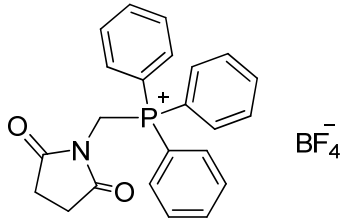
$^{31}P\{^{1}H\}$ NMR spectrum of 1-(*N*-phthalimido)methyltriphenylphosphonium tetrafluoroborate (**2a**) 5g-scale; 161.9 MHz/CD_3CN; δ (ppm).



^{1}H NMR spectrum of 1-(*N*-succinimido)methyltriphenylphosphonium tetrafluoroborate (**2b**); 400 MHz/CD_3CN/TMS; δ (ppm).

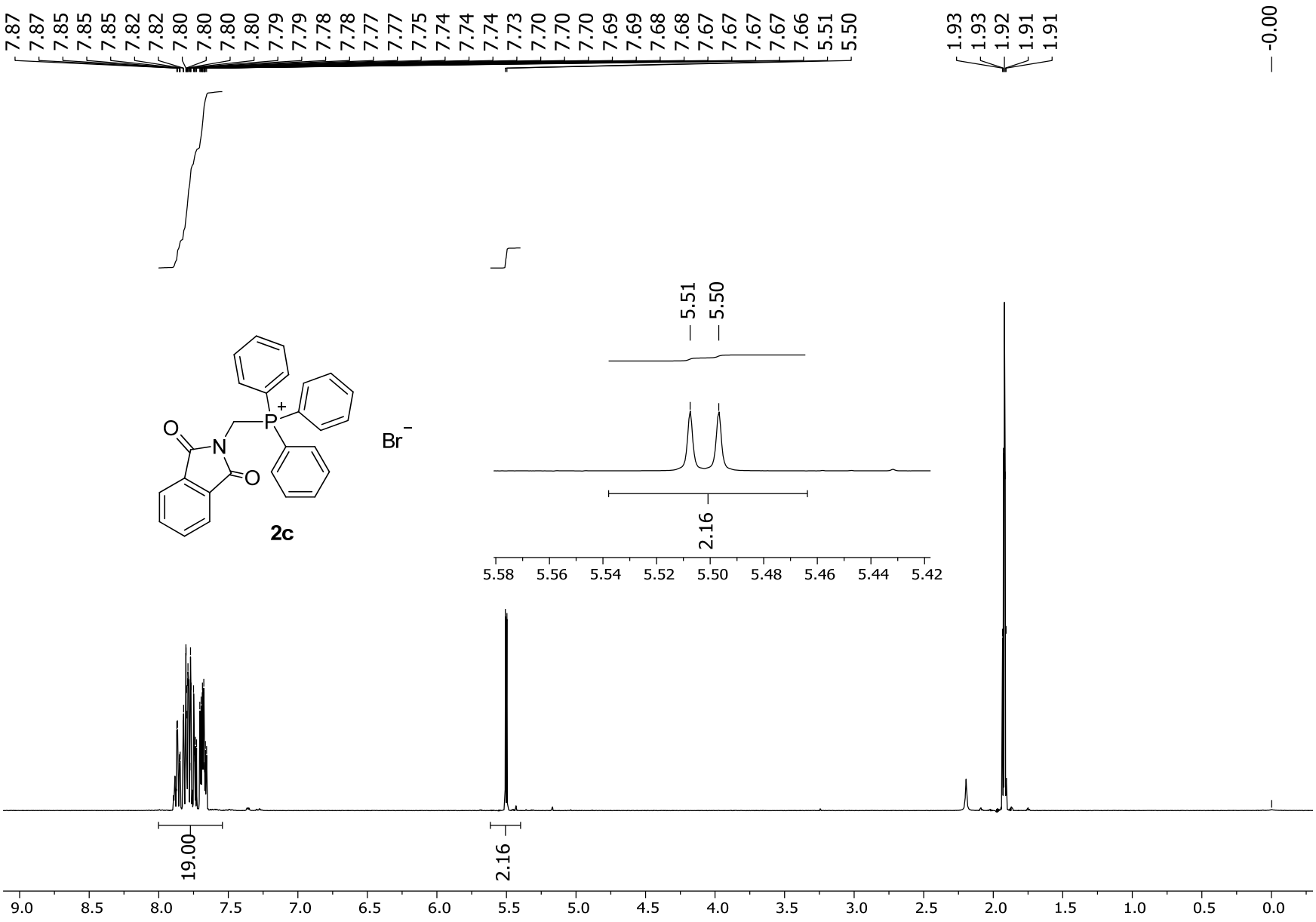


$^{13}C\{^{1}H\}$ NMR spectrum of 1-(*N*-succinimido)methyltriphenylphosphonium tetrafluoroborate (**2b**); 100 MHz/CD_3CN/TMS; δ (ppm).

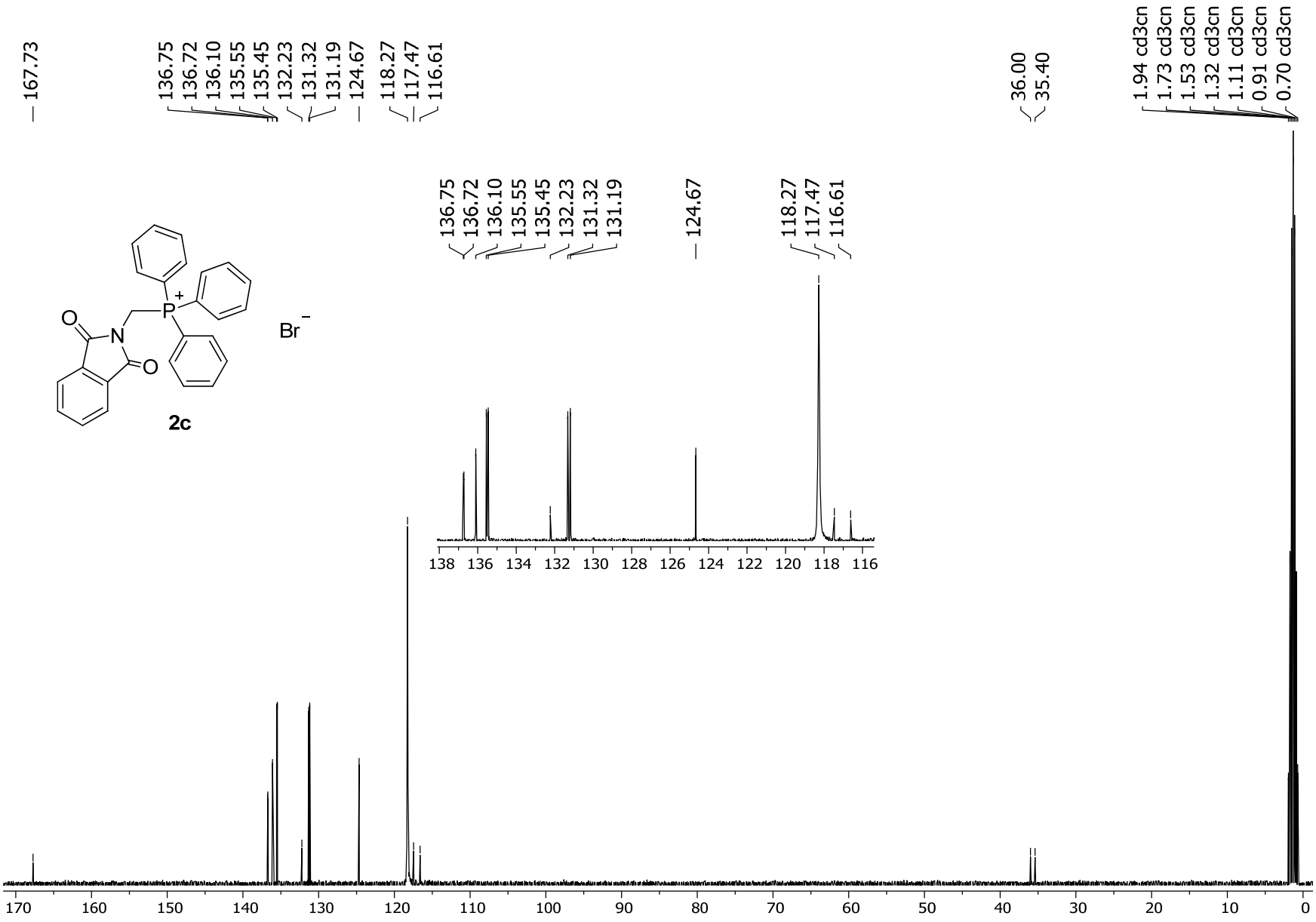


2b

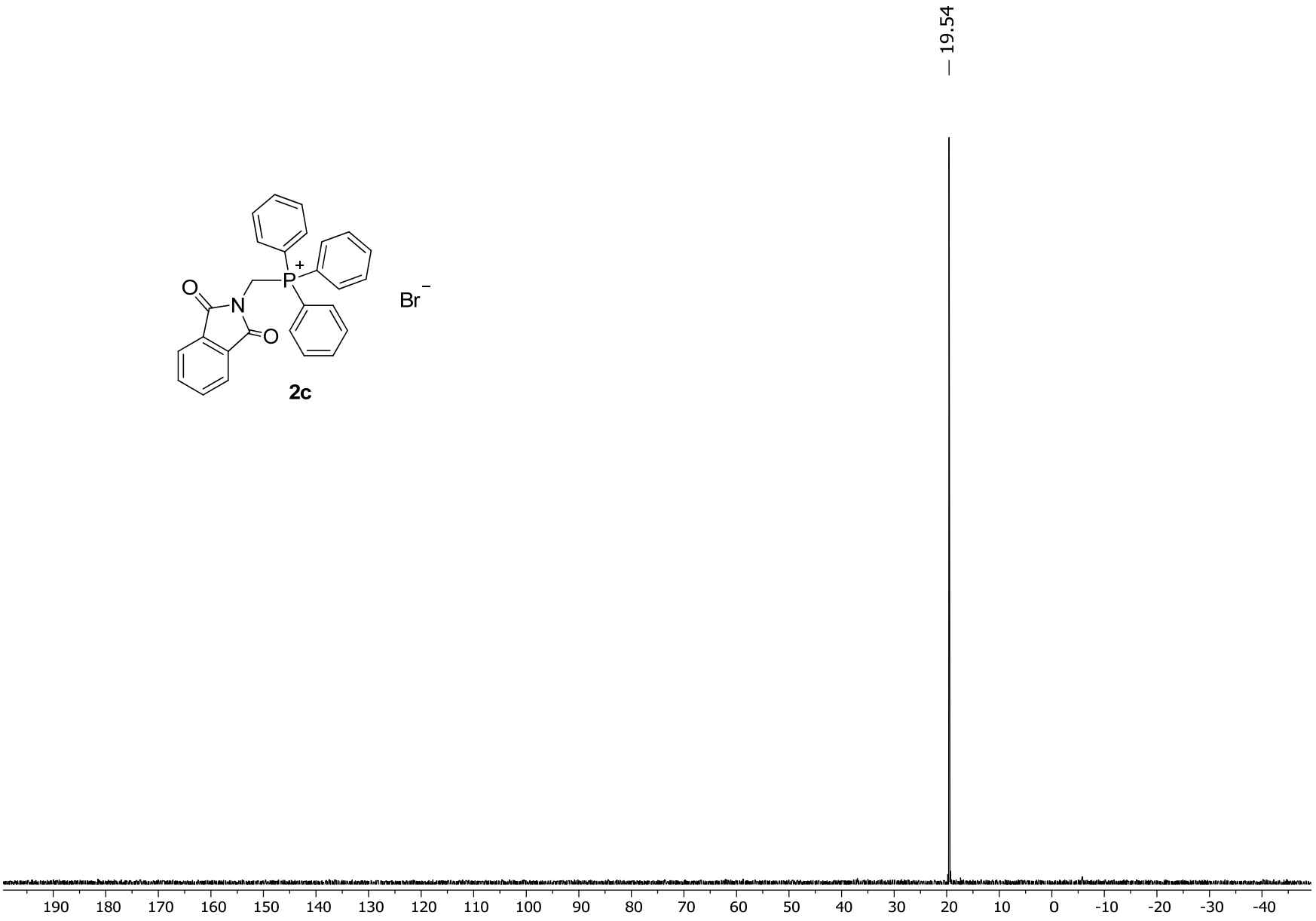
$^{31}P\{^{1}H\}$ NMR spectrum of 1-(*N*-succinimido)methyltriphenylphosphonium tetrafluoroborate (**2b**); 161.9 MHz/CD_3CN; δ (ppm).



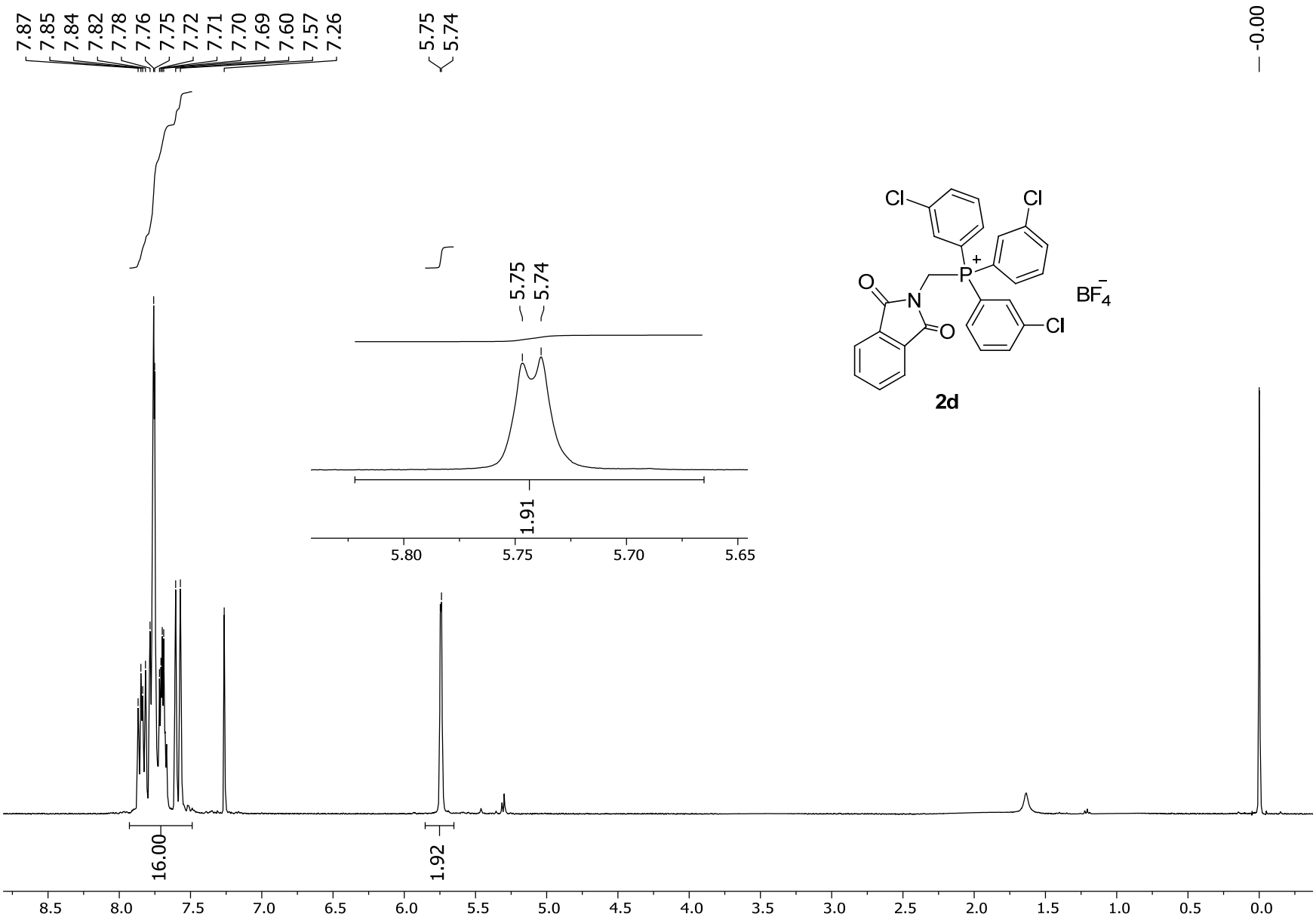
^{1}H NMR spectrum of 1-(*N*-phthalimido)methyltriphenylphosphonium bromide (**2c**); 400 MHz/CD_3CN/TMS; δ (ppm).



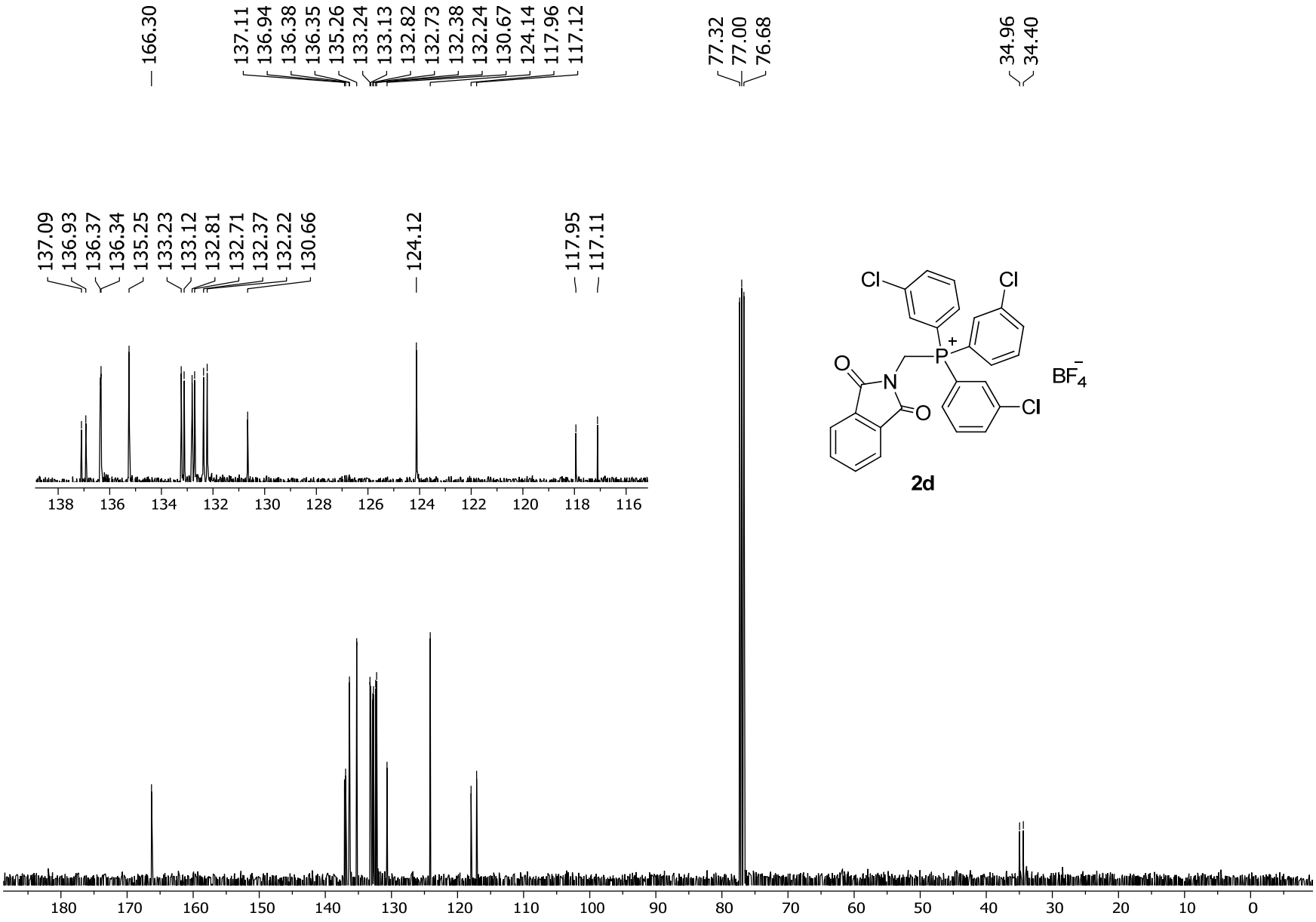
$^{13}C\{^{1}H\}$ NMR spectrum of 1-(*N*-phthalimido)methyltriphenylphosphonium bromide (**2c**); 100 MHz/CD_3CN/TMS; δ (ppm).



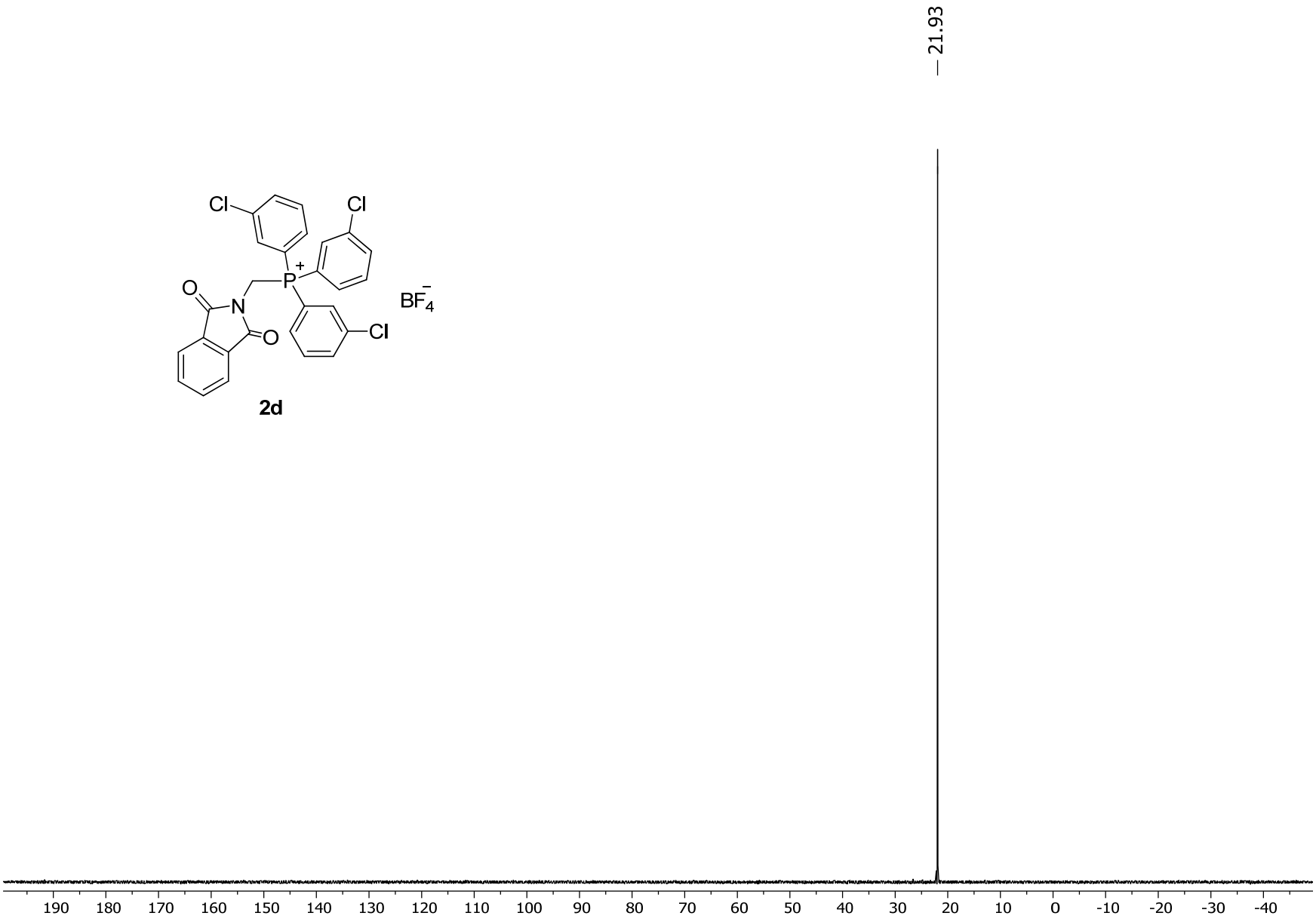
$^{31}P\{^{1}H\}$ NMR spectrum of 1-(*N*-phthalimido)methyltriphenylphosphonium bromide (**2c**); 161.9 MHz/CD_3CN; δ (ppm).



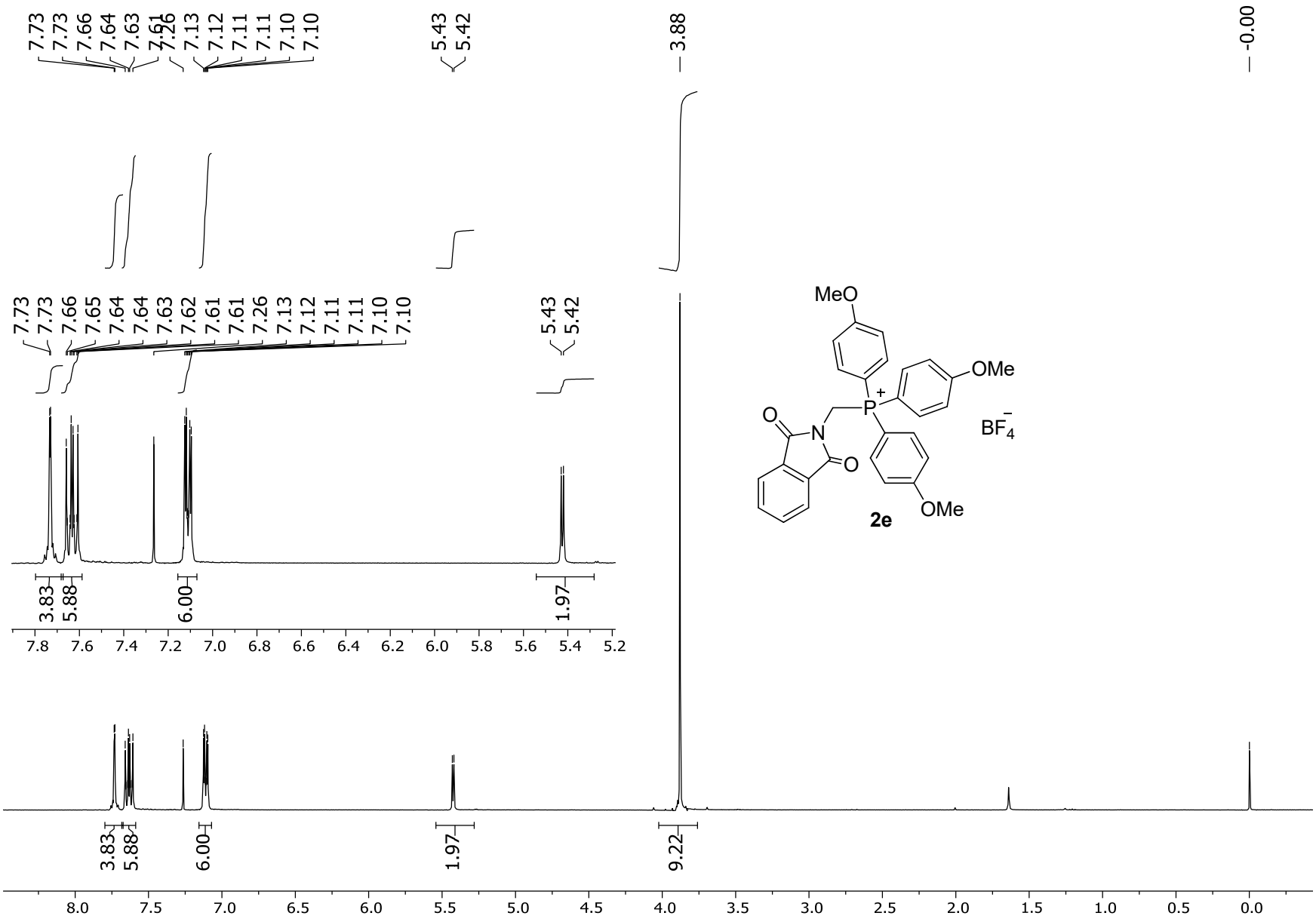
^{1}H NMR spectrum of 1-(*N*-phthalimido)methyltris(3-chlorophenyl)phosphonium tetrafluoroborate (**2d**); 400 MHz/$CDCl_3$/TMS; δ (ppm).



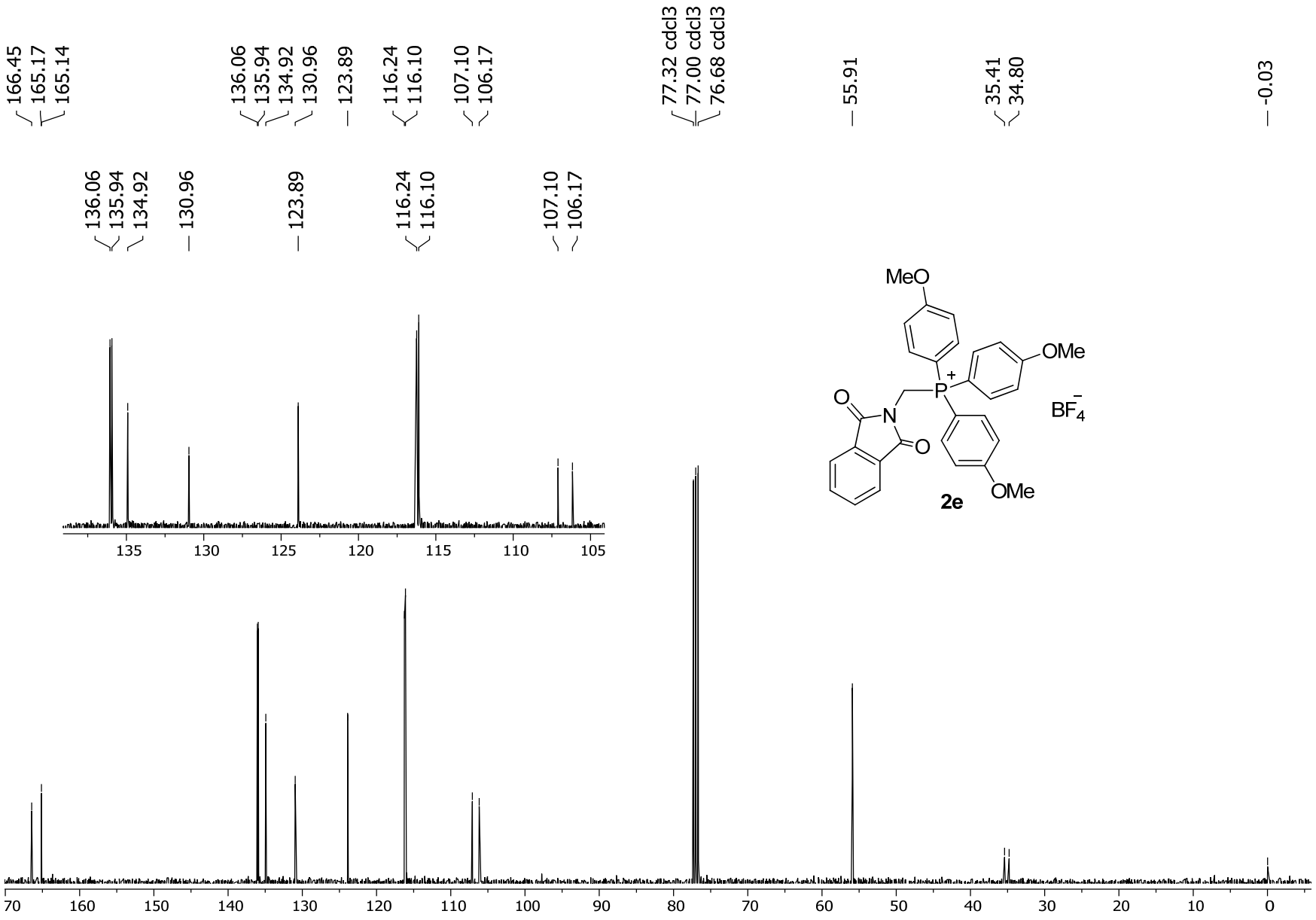
$^{13}C\{^{1}H\}$ NMR spectrum of 1-(*N*-phthalimido)methyltris(3-chlorophenyl)phosphonium tetrafluoroborate (**2d**); 100 MHz/$CDCl_3$/TMS; δ (ppm).



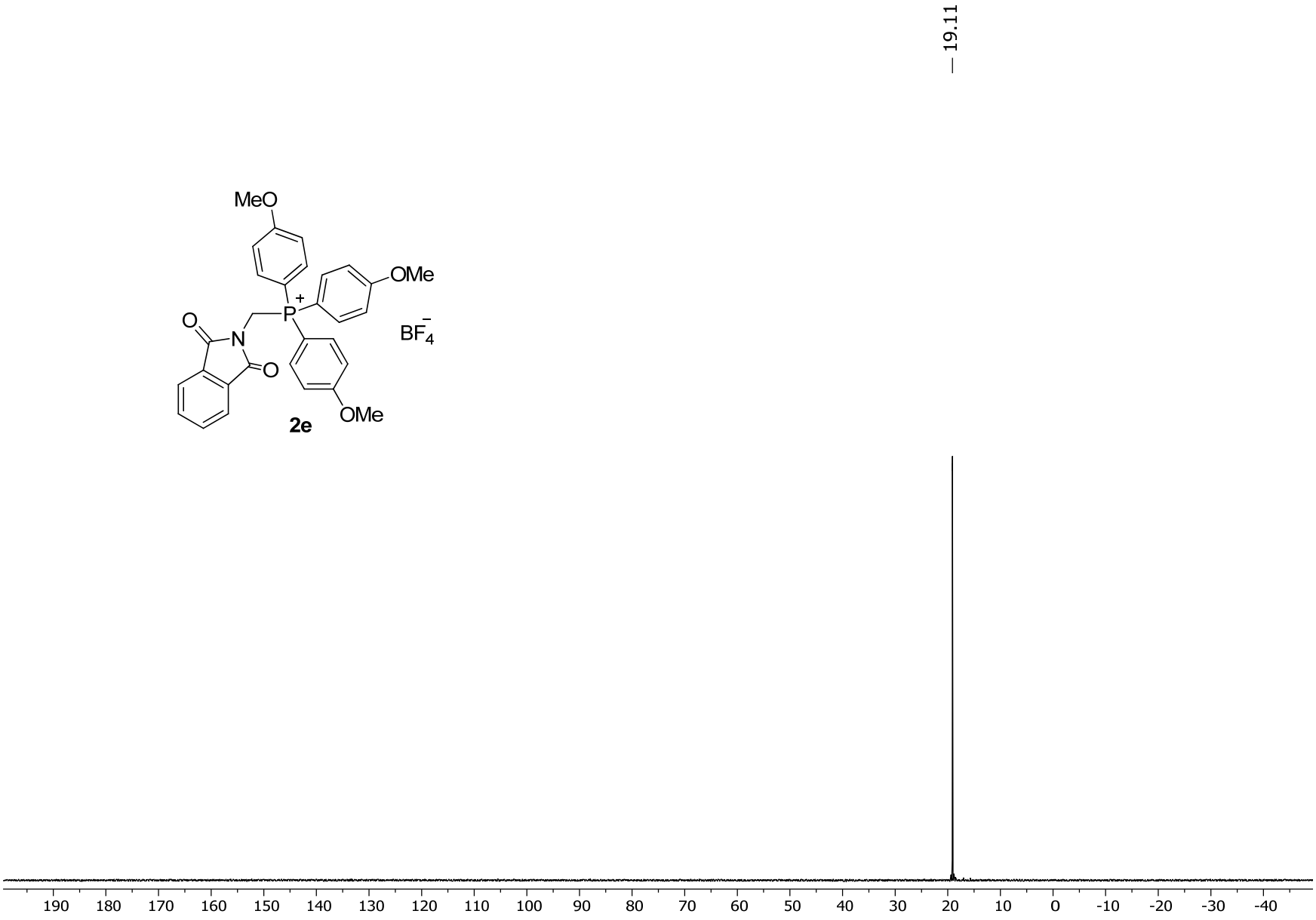
$^{31}P\{^{1}H\}$ NMR spectrum of 1-(*N*-phthalimido)methyltris(3-chlorophenyl)phosphonium tetrafluoroborate (**2d**); 161.9 MHz/$CDCl_3$; δ (ppm).



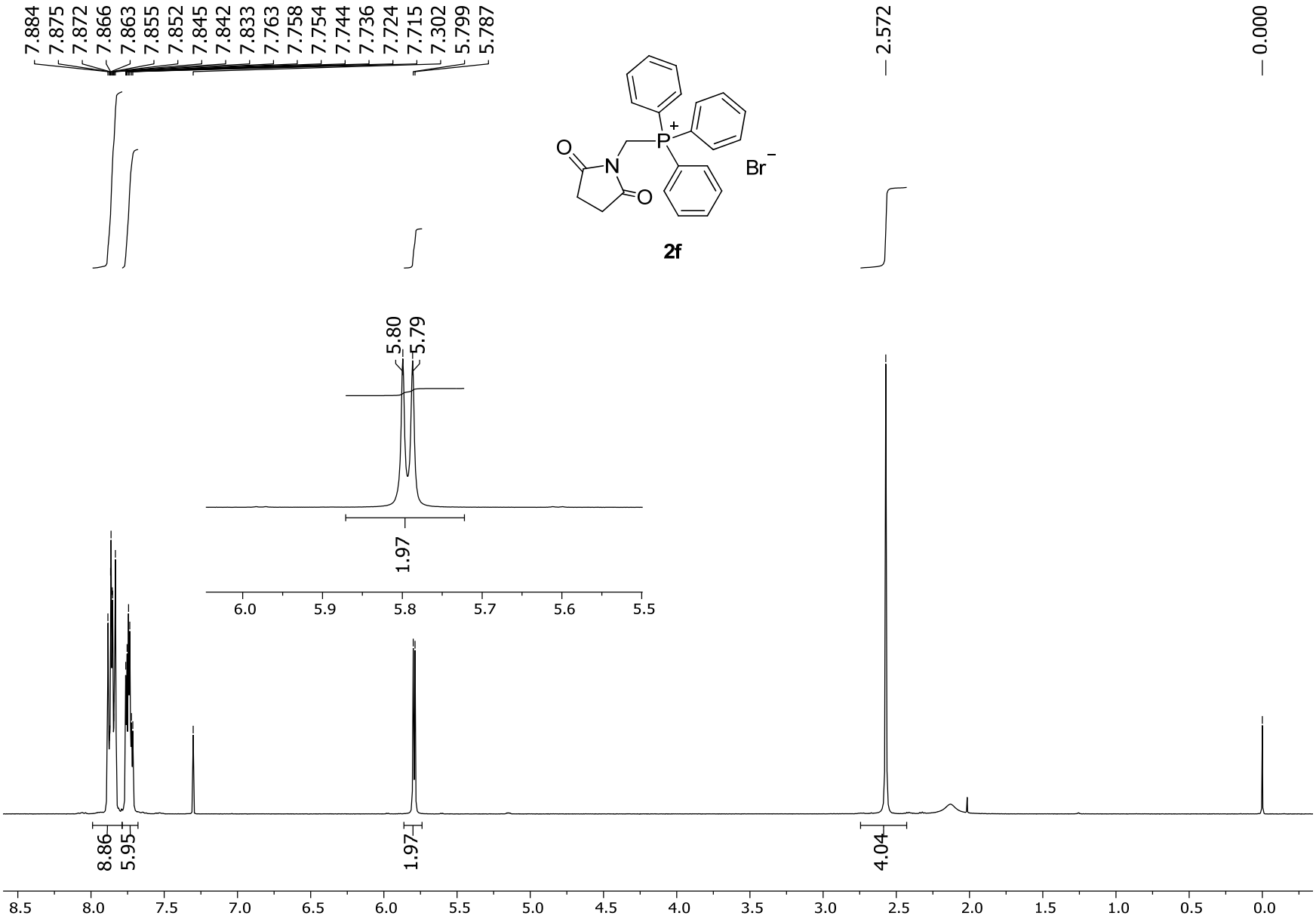
^{1}H NMR spectrum of 1-(*N*-phthalimido)methyltris(4-methoxyphenyl)phosphonium tetrafluoroborate (**2e**); 400 MHz/$CDCl_3$/TMS; δ (ppm).



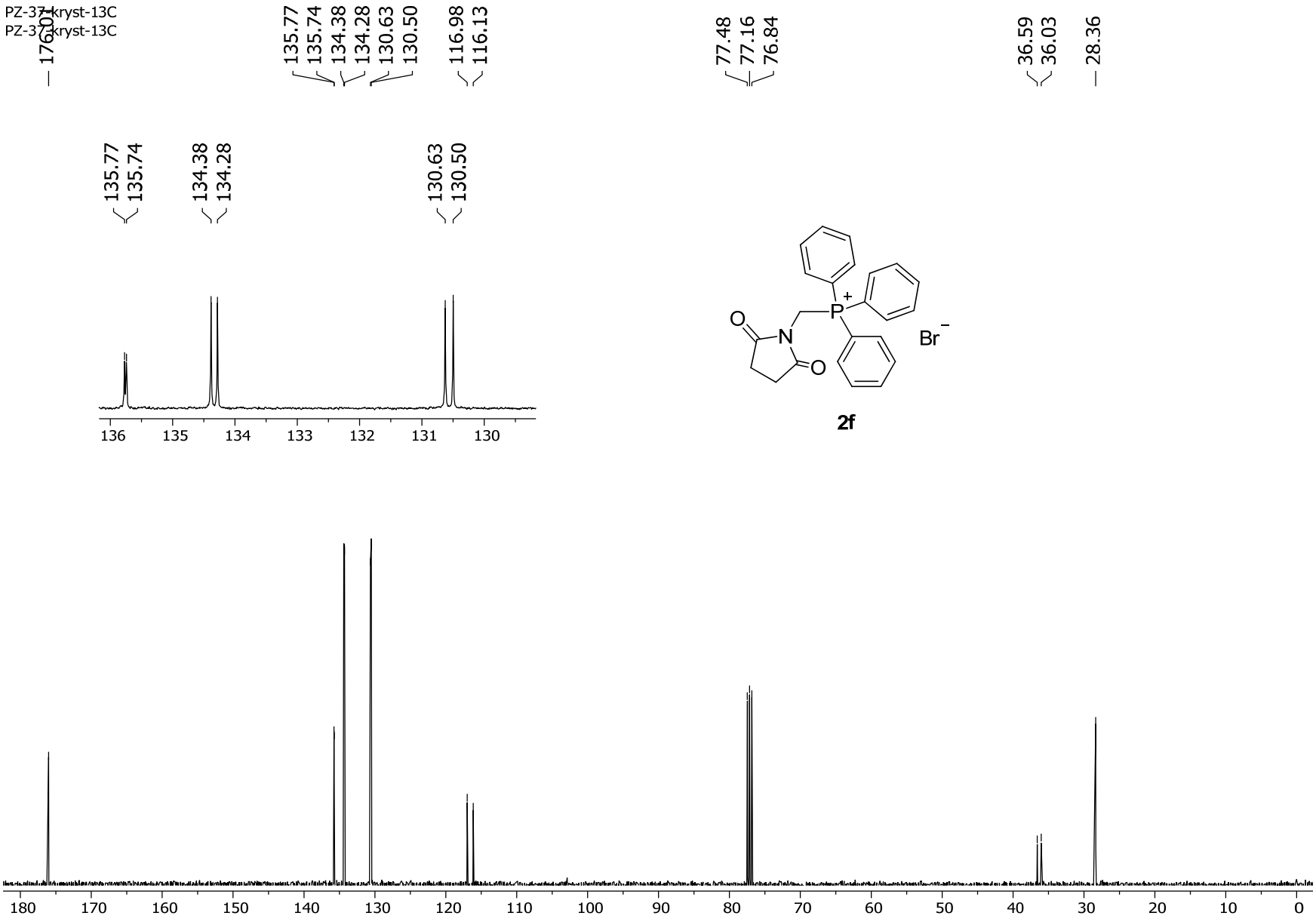
$^{13}C\{^{1}H\}$ NMR spectrum of 1-(*N*-phthalimido)methyltris(4-methoxyphenyl)phosphonium tetrafluoroborate (**2e**); 100 MHz/$CDCl_3$/TMS; δ (ppm).



$^{31}P\{^{1}H\}$ NMR spectrum of 1-(*N*-phthalimido)methyltris(4-methoxyphenyl)phosphonium tetrafluoroborate (**2e**); 161.9 MHz/$CDCl_3$; δ (ppm).

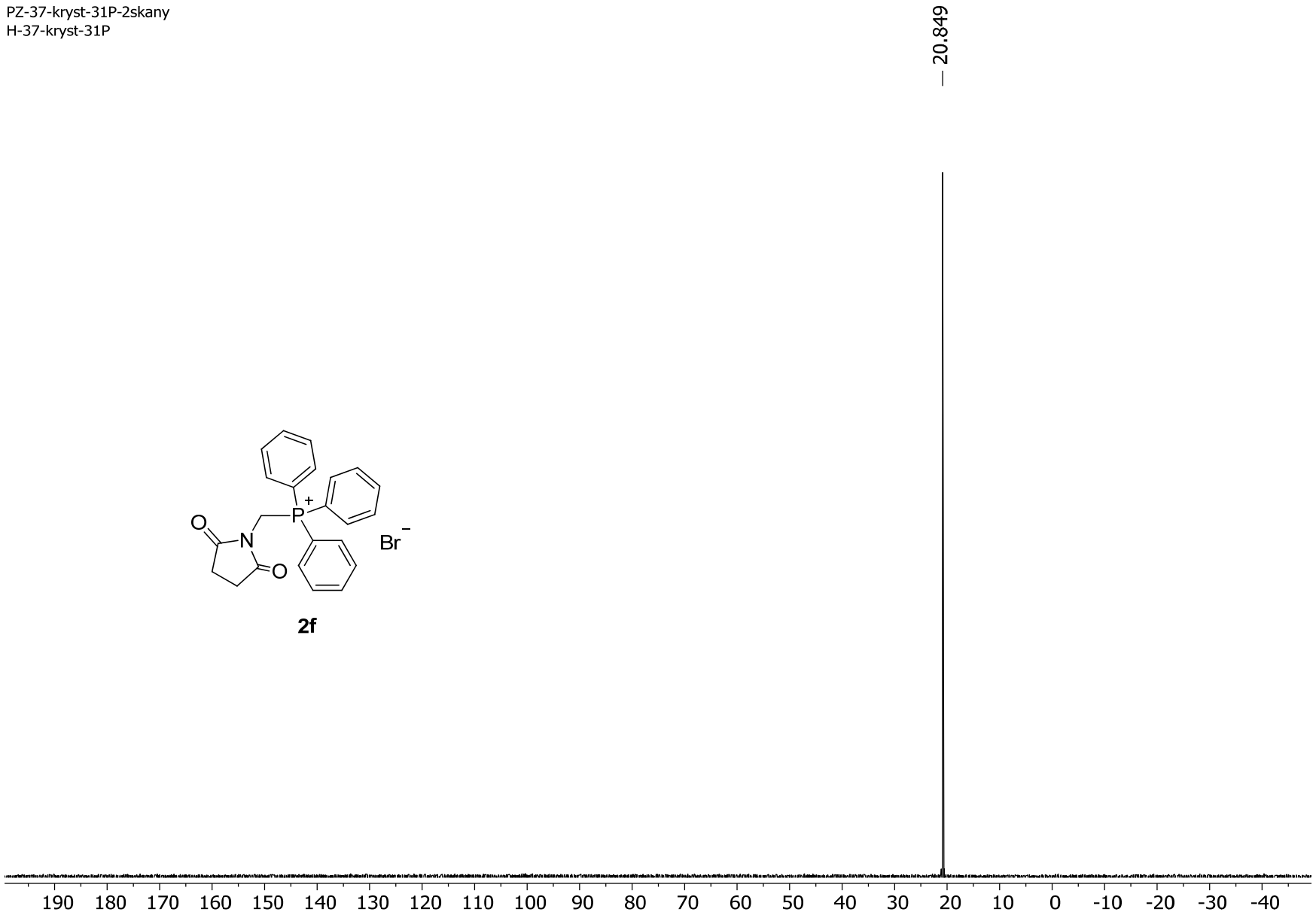


^{1}H NMR spectrum of 1-(*N*-succinimido)methyltriphenylphosphonium bromide (**2f**); 400 MHz/$CDCl_3$/TMS; δ (ppm).



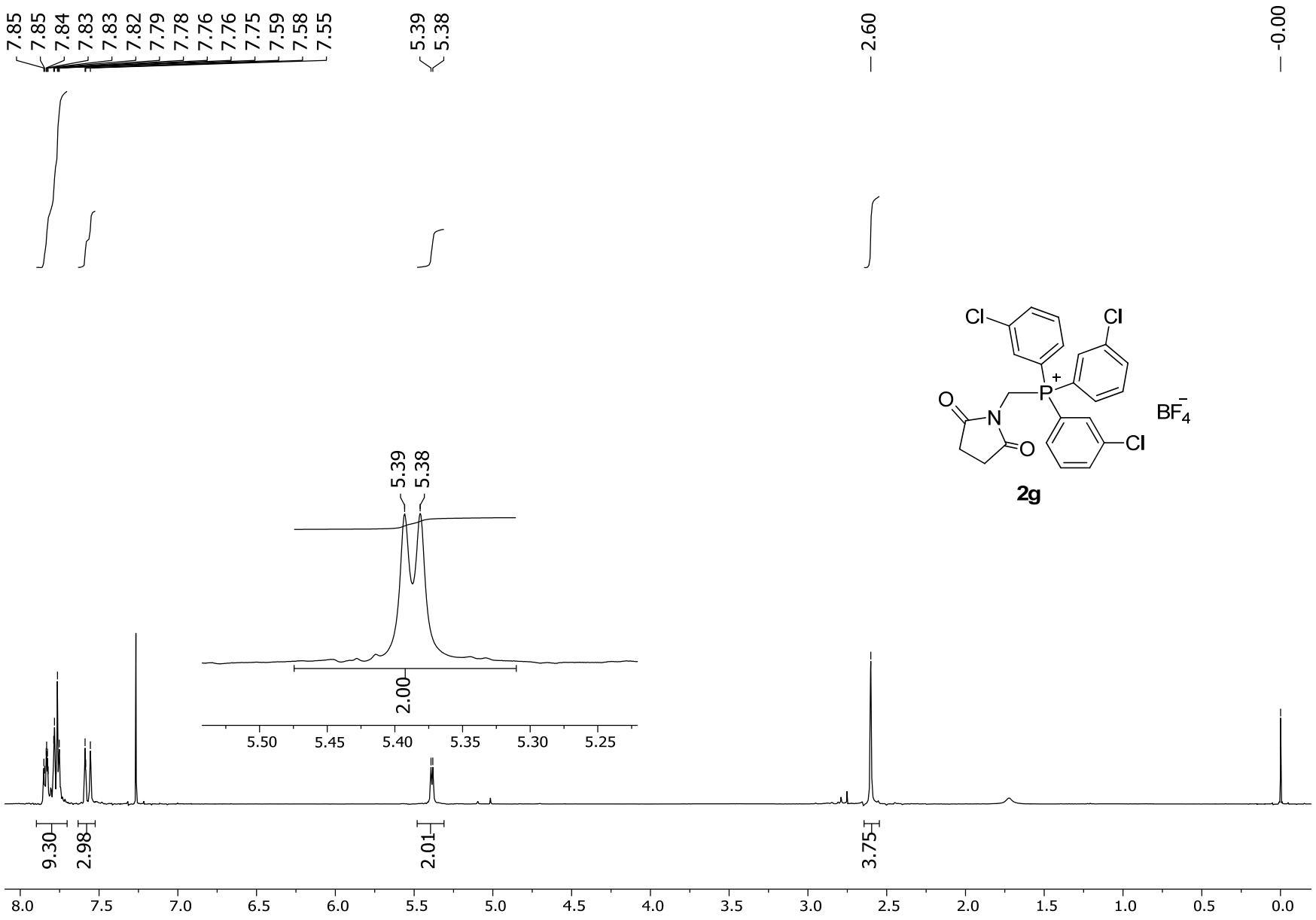
$^{13}C\{^{1}H\}$ NMR spectrum of 1-(*N*-succinimido)methyltriphenylphosphonium bromide (**2f**); 100 MHz/$CDCl_3$/TMS; δ (ppm).

PZ-37-kryst-31P-2skany
H-37-kryst-31P

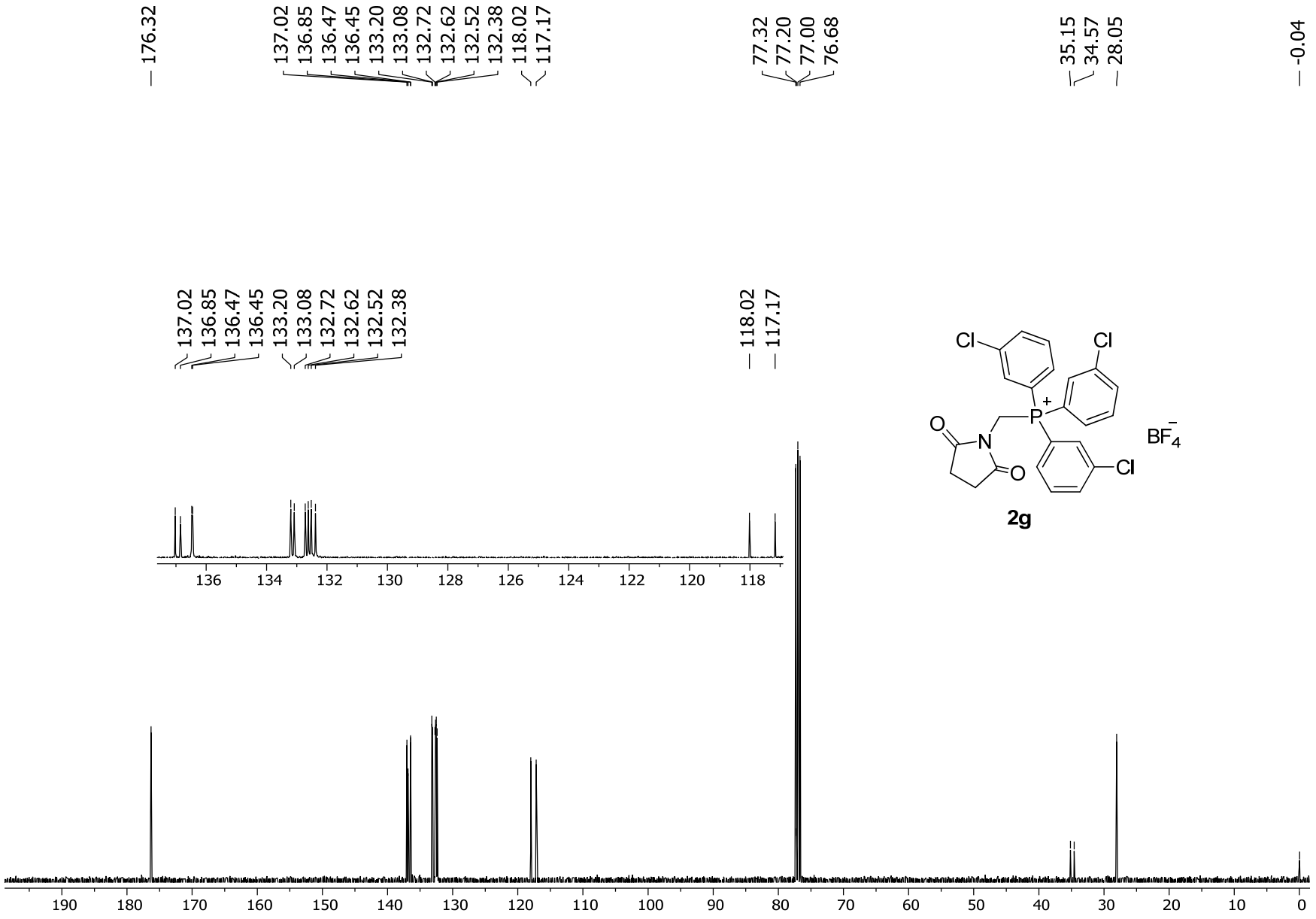


2f

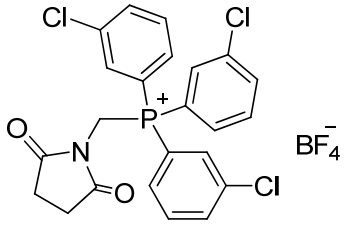
$^{31}P\{^{1}H\}$ NMR spectrum of 1-(*N*-succinimido)methyltriphenylphosphonium bromide (**2f**); 161.9 MHz/$CDCl_3$; δ (ppm).



^{1}H NMR spectrum of 1-(*N*-succinimido)methyltris(3-chlorophenyl)phosphonium tetrafluoroborate (**2g**); 400 MHz/$CDCl_3$/TMS; δ (ppm).

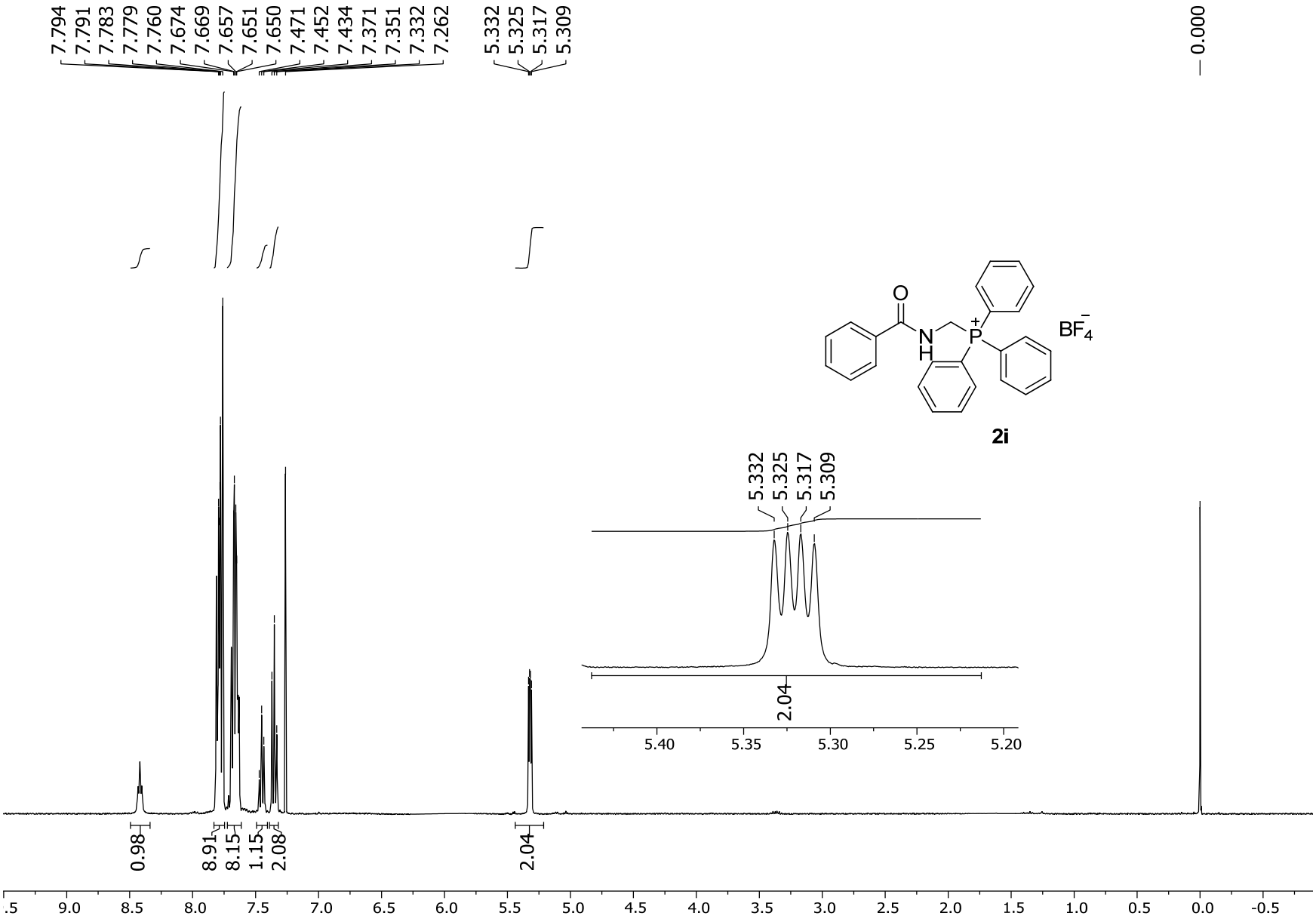


$^{13}C\{^{1}H\}$ NMR spectrum of 1-(*N*-succinimido)methyltris(3-chlorophenyl)phosphonium tetrafluoroborate (**2g**); 100 MHz/$CDCl_3$/TMS; δ (ppm).

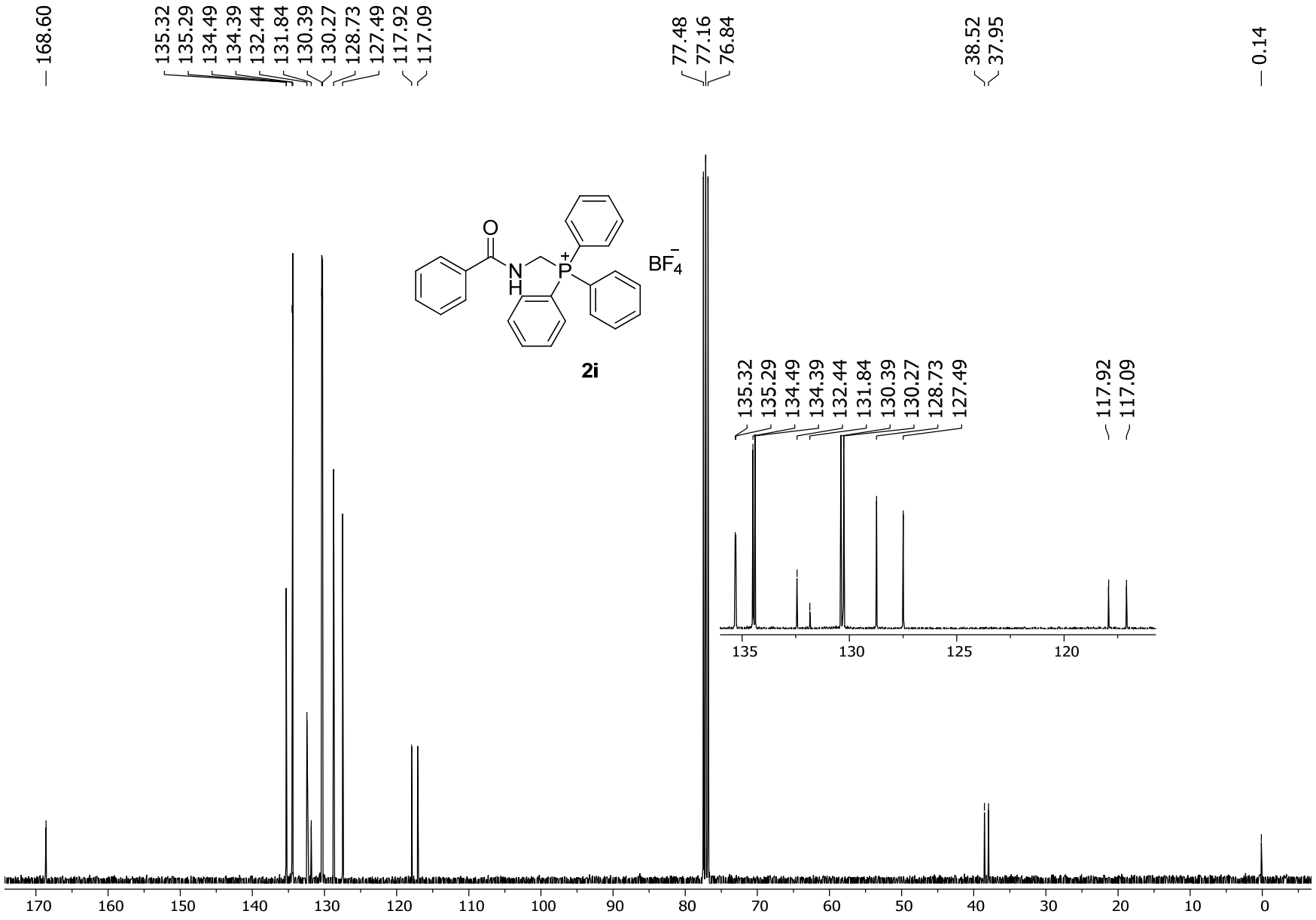


2g

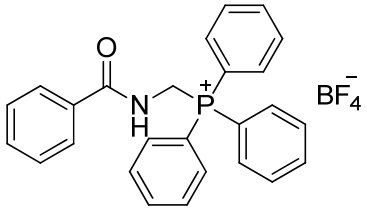
$^{31}P\{^{1}H\}$ NMR spectrum of 1-(*N*-succinimido)methyltris(3-chlorophenyl)phosphonium tetrafluoroborate (**2g**); 161.9 MHz/$CDCl_3$; δ (ppm).



^{1}H NMR spectrum of (*N*-benzoylamino)methyltriphenylphosphonium tetrafluoroborate (**2i**); 400 MHz/$CDCl_3$/TMS; δ (ppm).

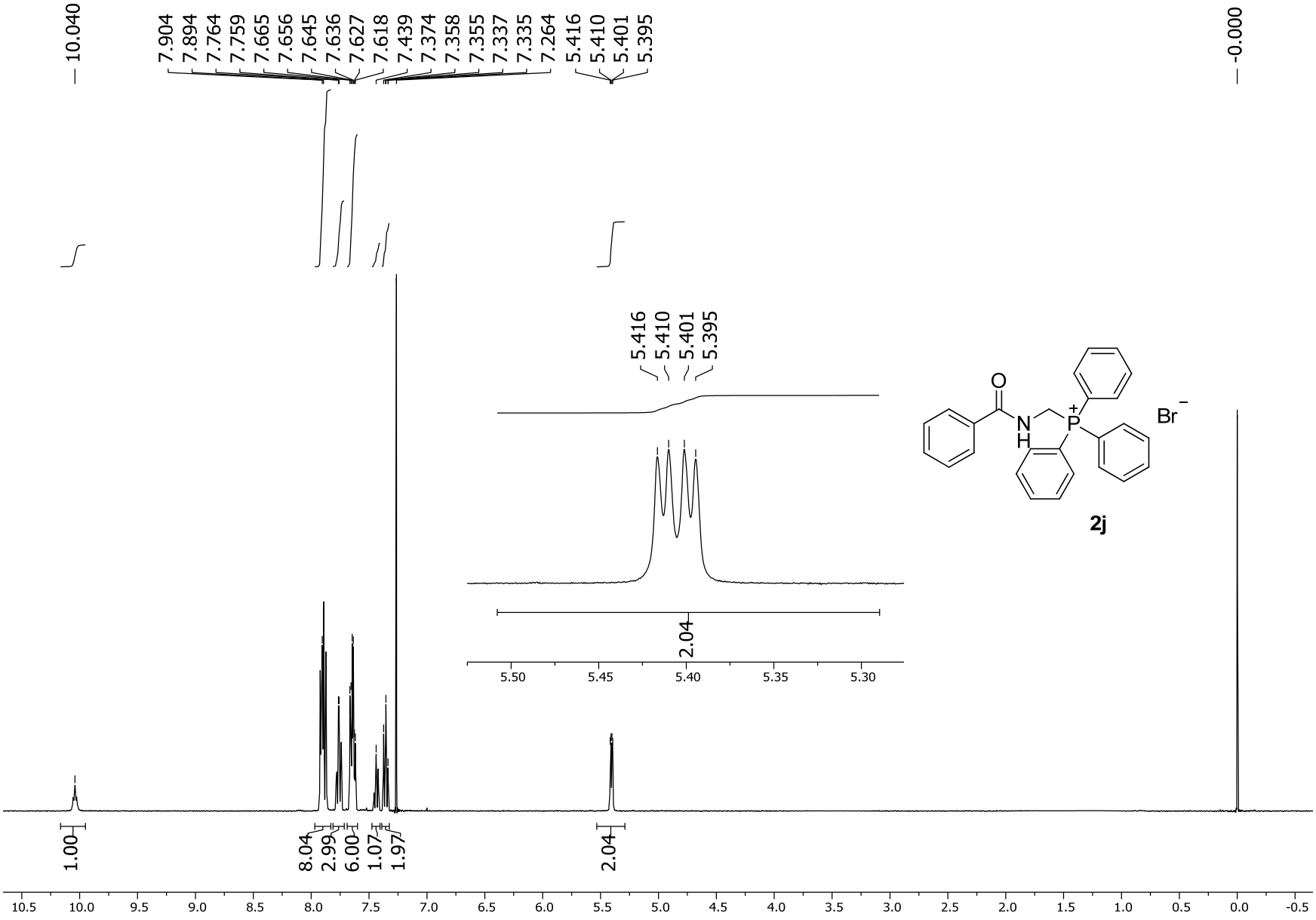


$^{13}C\{^{1}H\}$ NMR spectrum of (*N*-benzoylamino)methyltriphenylphosphonium tetrafluoroborate (**2i**); 100 MHz/$CDCl_3$/TMS; δ (ppm).

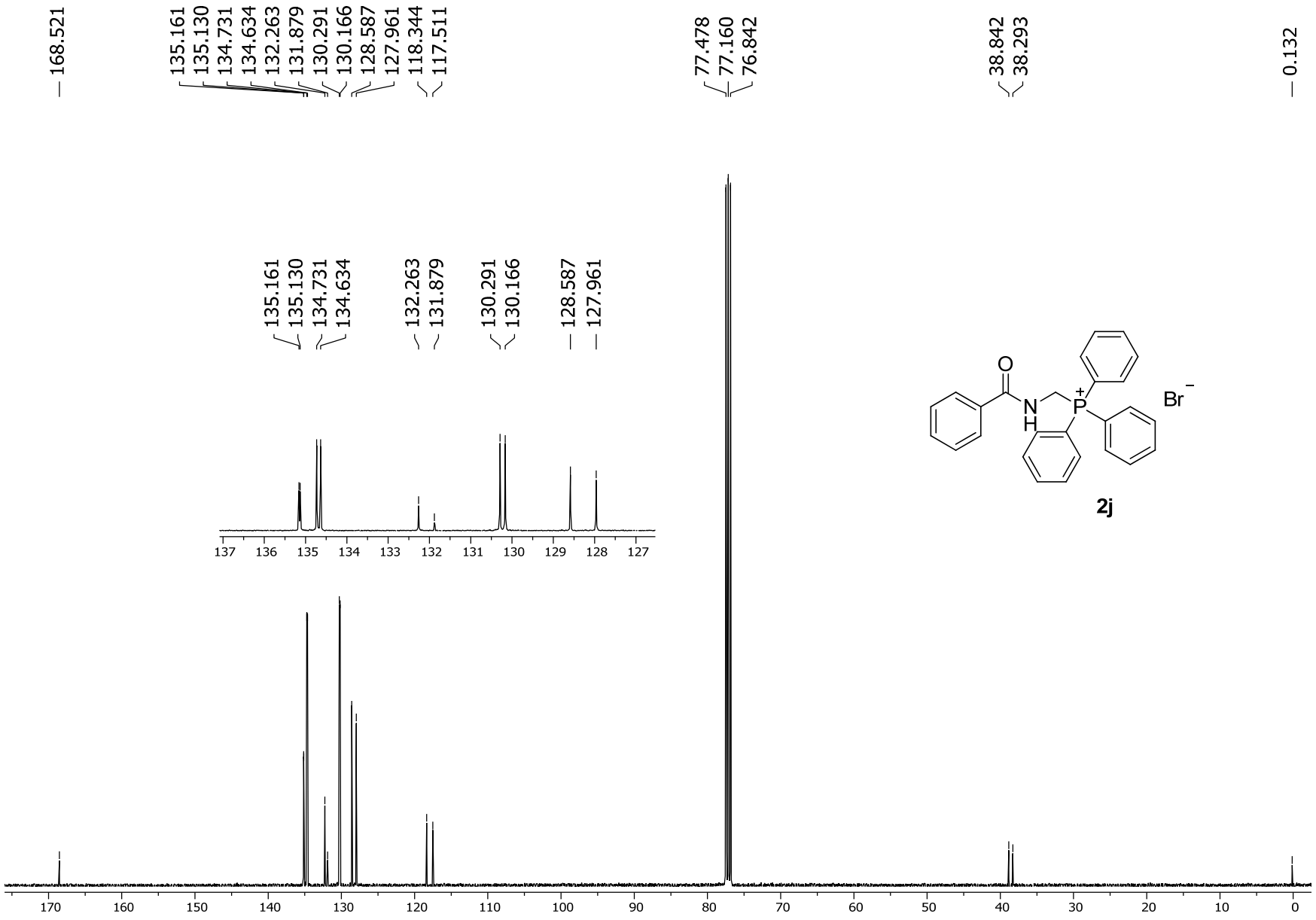


2i

$^{31}P\{^{1}H\}$ NMR spectrum of (*N*-benzoylamino)methyltriphenylphosphonium tetrafluoroborate (**2i**); 161.9 MHz/$CDCl_3$; δ (ppm).

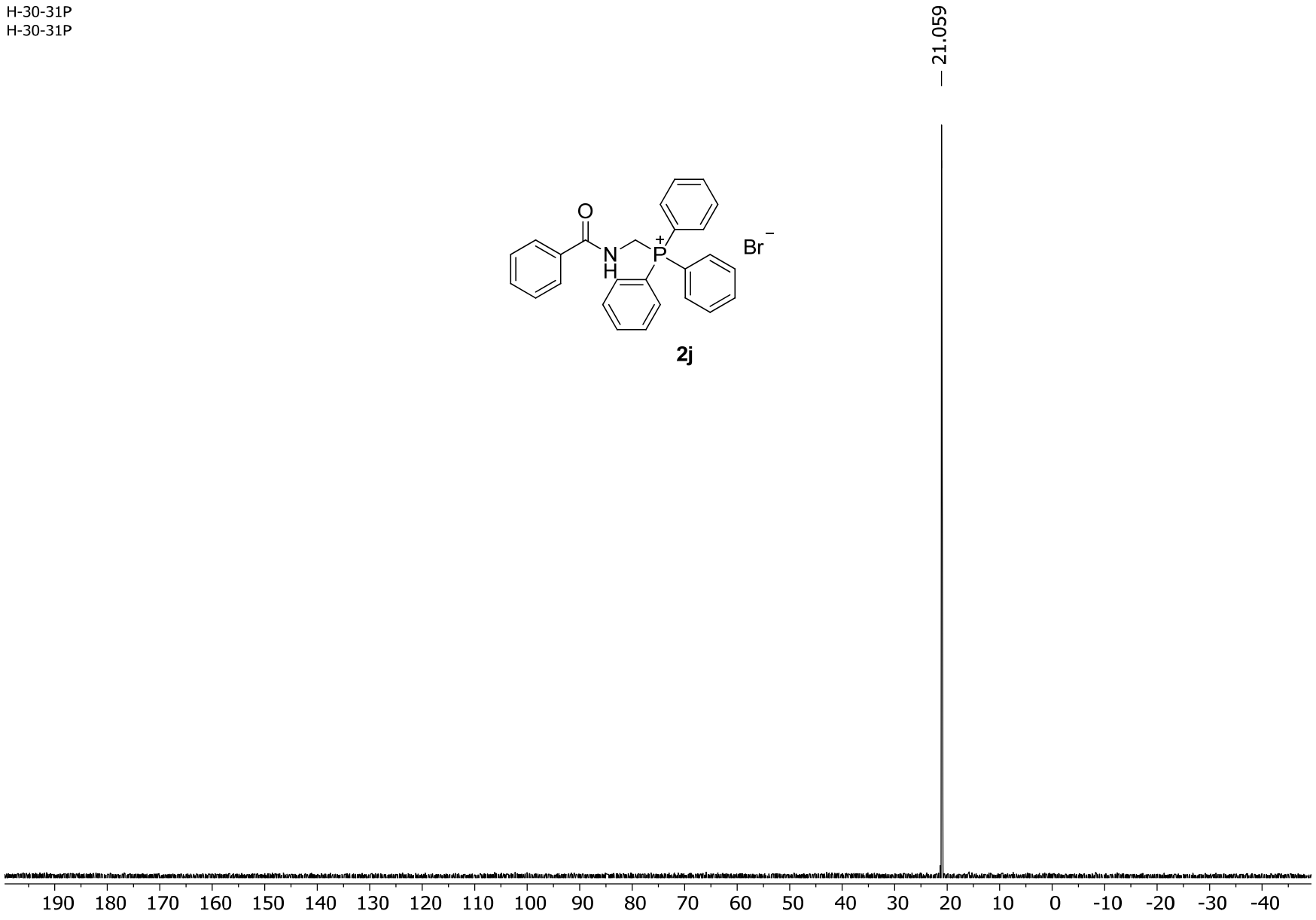


^{1}H NMR spectrum of (*N*-benzoylamino)methyltriphenylphosphonium bromide (**2j**); 400 MHz/$CDCl_3$/TMS; δ (ppm).

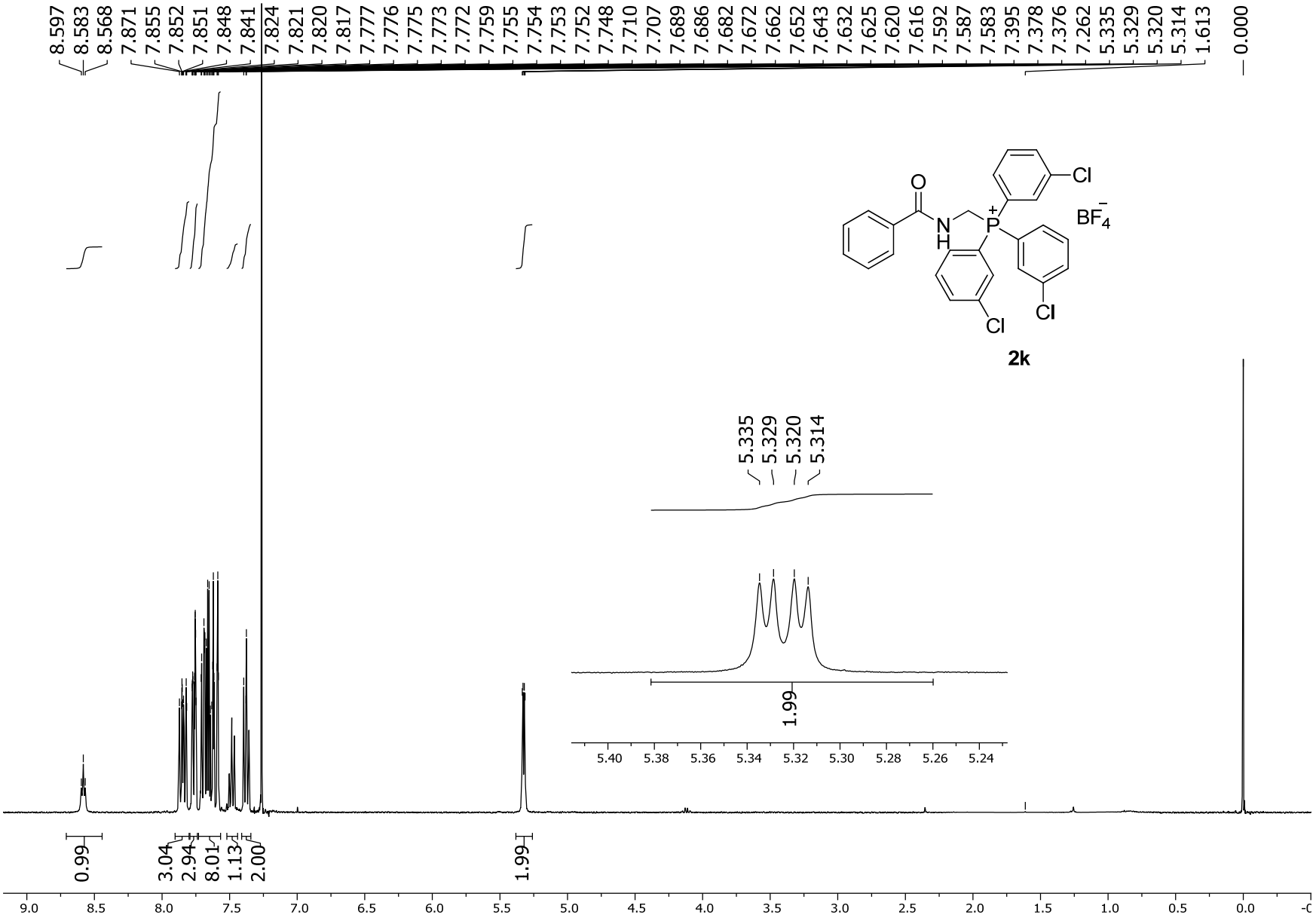


^{13}C NMR spectrum of (*N*-benzoylamino)methyltriphenylphosphonium bromide (**2j**); 100 MHz/$CDCl_3$/TMS; δ (ppm).

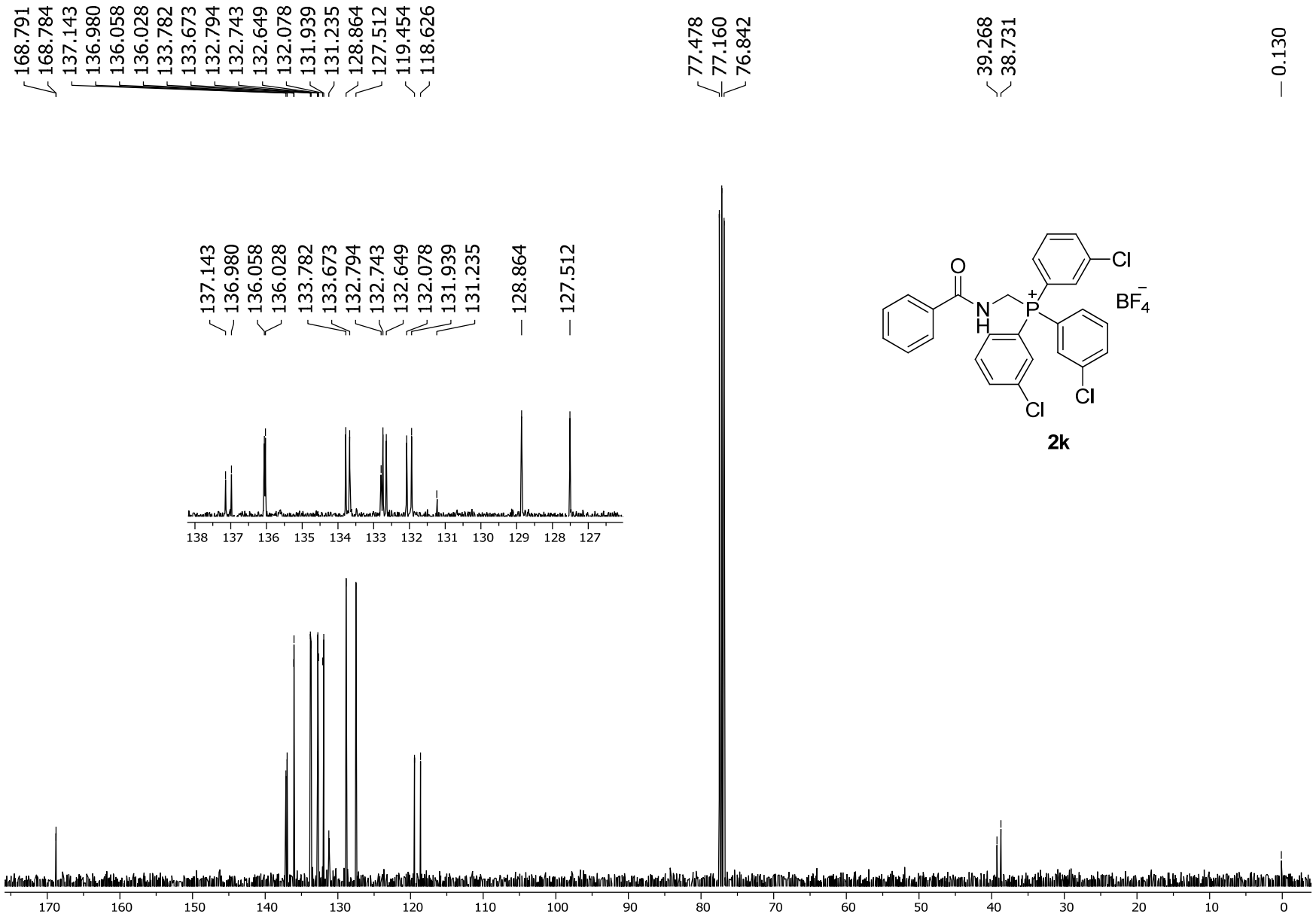
H-30-31P
H-30-31P



$^{31}P\{^{1}H\}$ NMR spectrum of (*N*-benzoylamino)methyltriphenylphosphonium bromide (**2j**); 161.9 MHz/$CDCl_3$; δ (ppm).

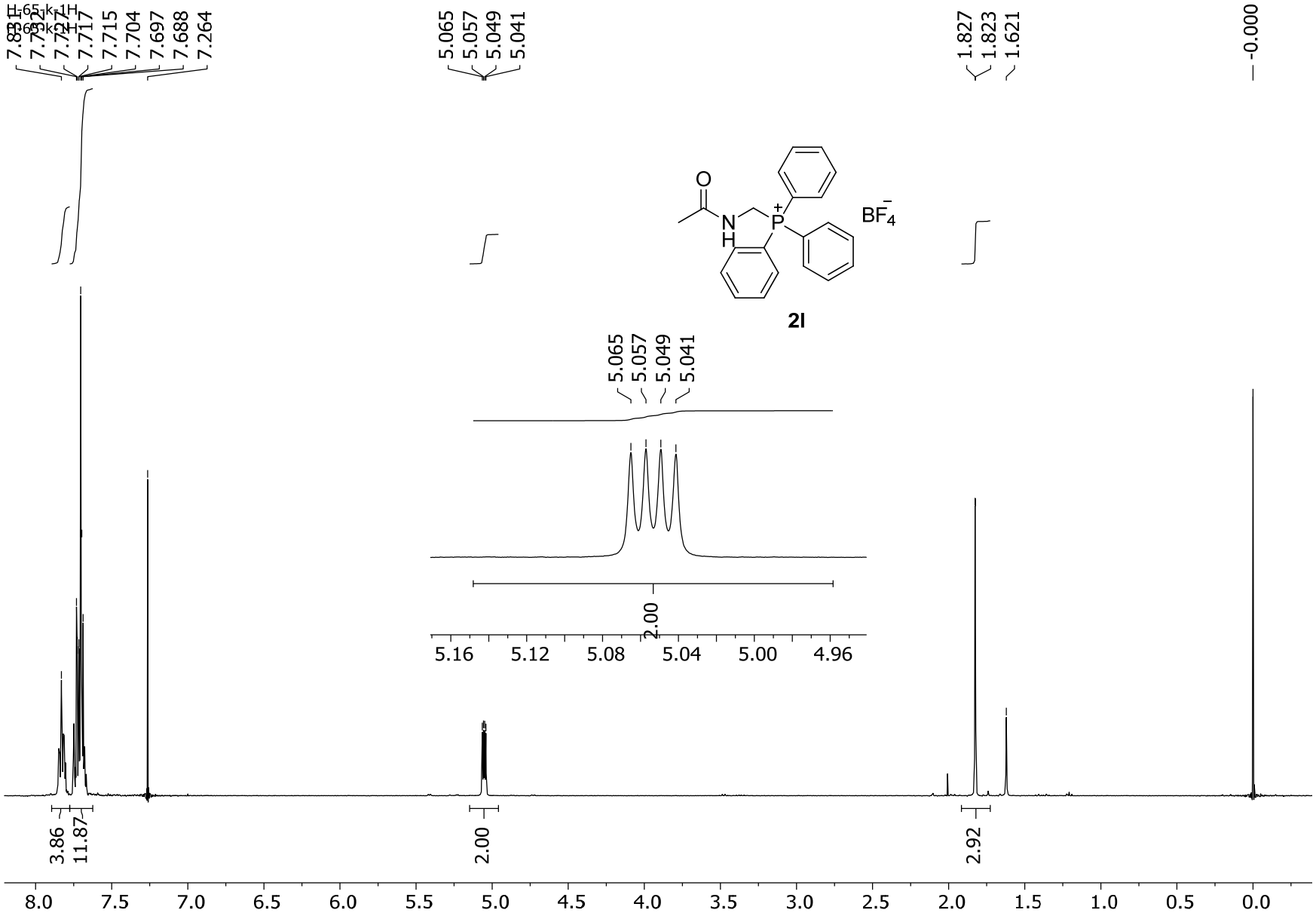


^{1}H NMR spectrum of (*N*-benzoylamino)methyltris(3-chlorophenyl)phosphonium tetrafluoroborate (**2k**); 400 MHz/$CDCl_3$/TMS; δ (ppm).

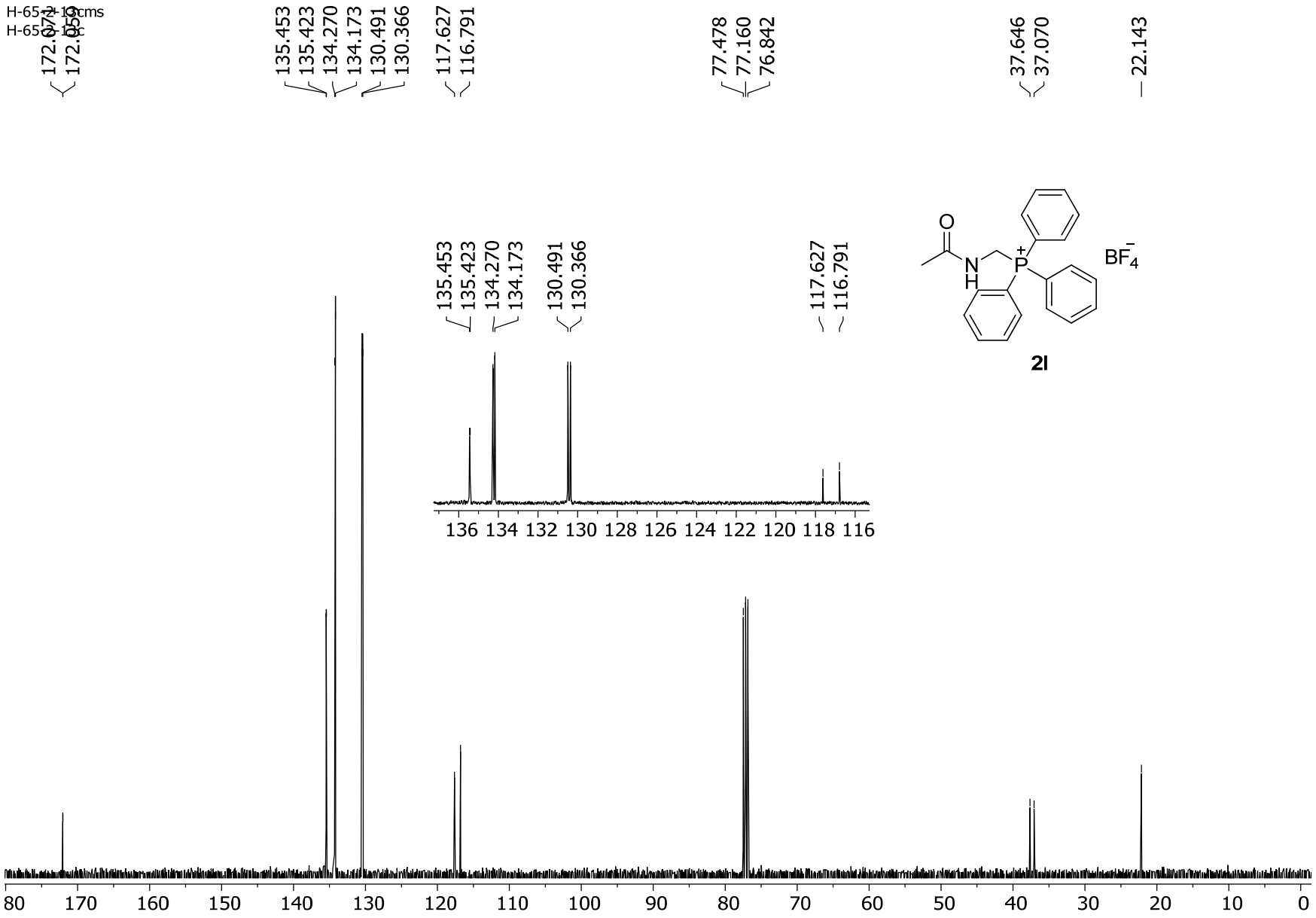


$^{13}C\{^{1}H\}$ NMR spectrum of (*N*-benzoylamino)methyltris(3-chlorophenyl)phosphonium tetrafluoroborate (**2k**); 100 MHz/$CDCl_3$/TMS; δ (ppm).

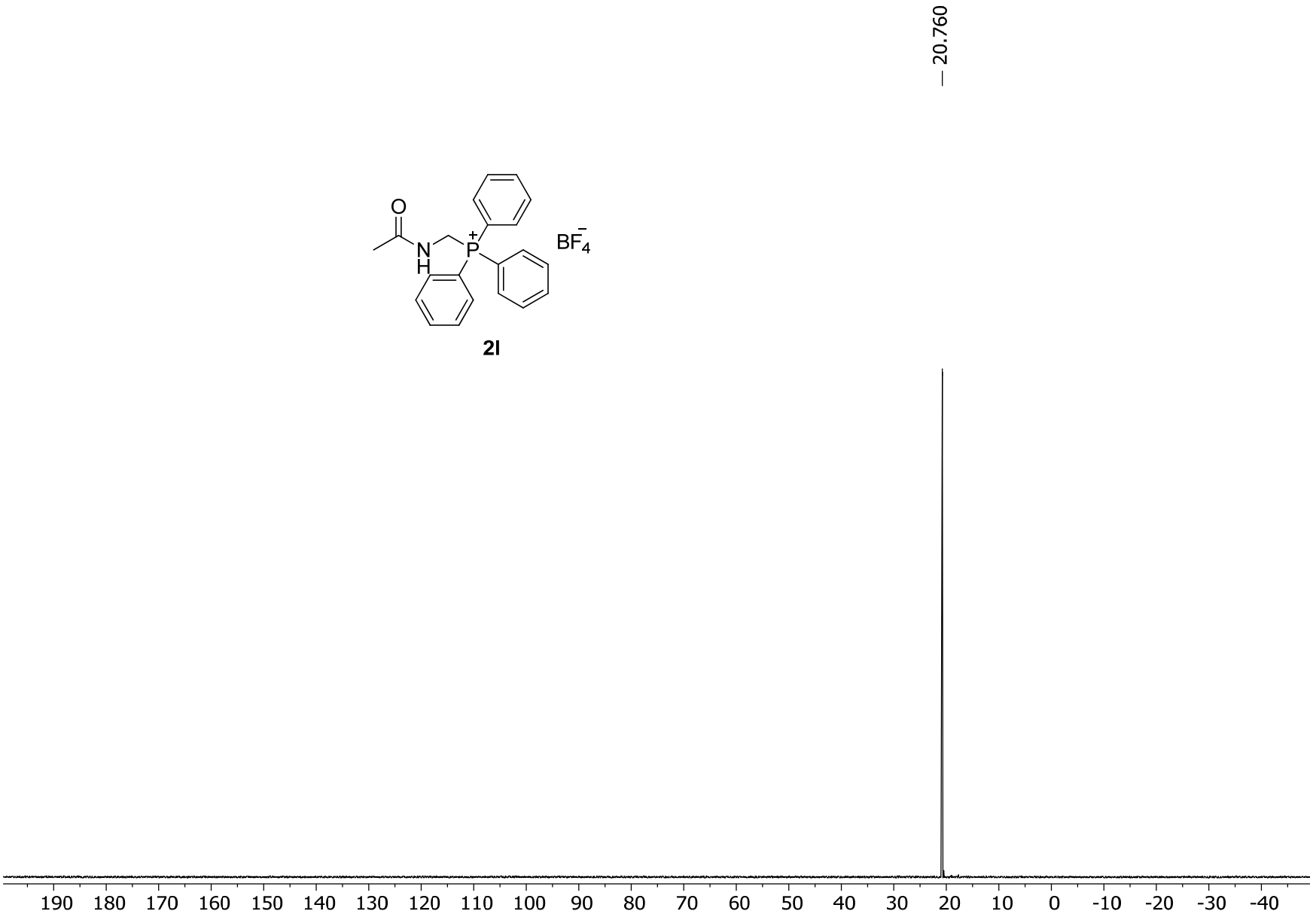
$^{31}P\{^{1}H\}$ NMR spectrum of (*N*-benzoylamino)methyltris(3-chlorophenyl)phosphonium tetrafluoroborate (**2k**); 161.9 MHz/$CDCl_3$; δ (ppm).



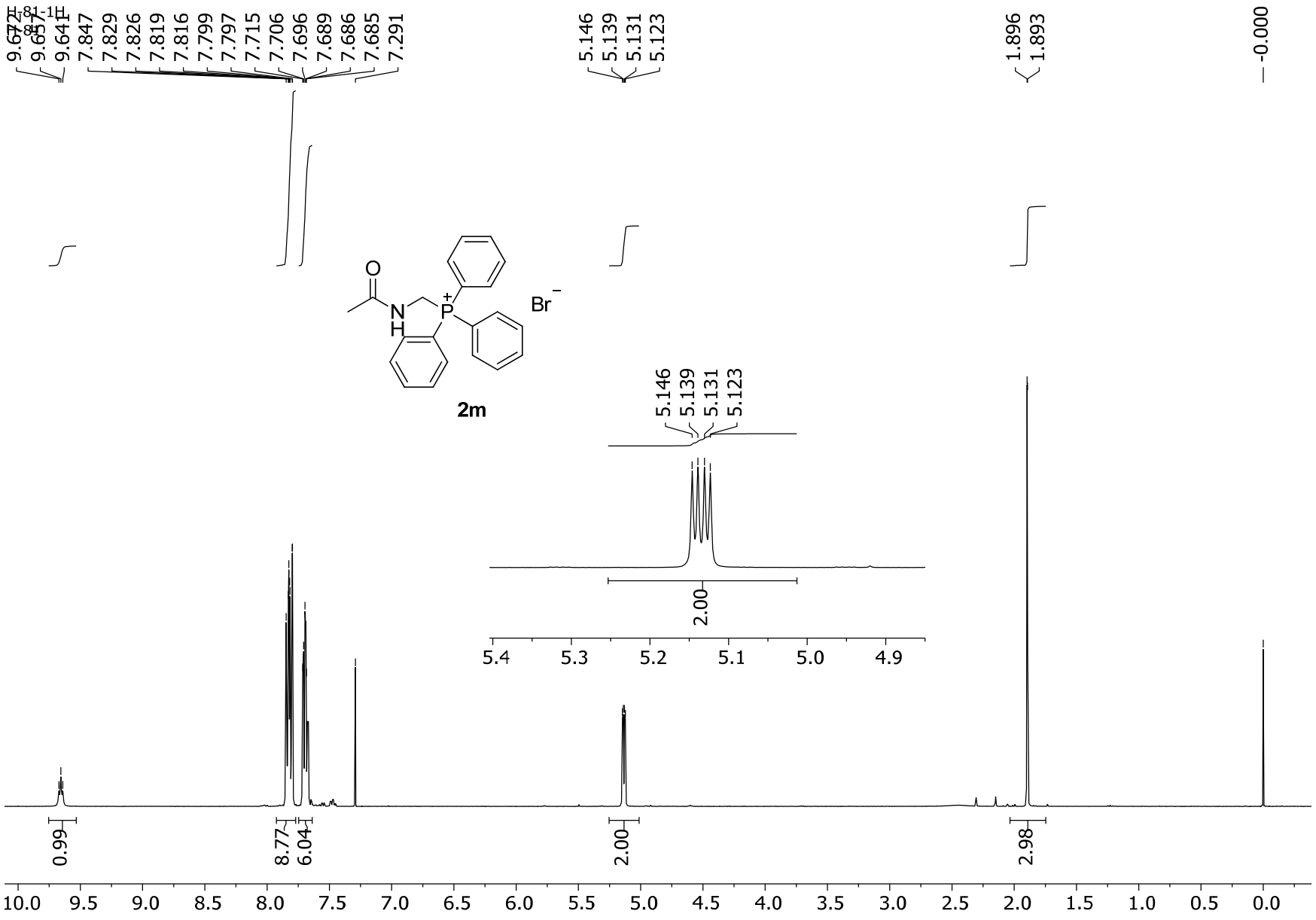
^{1}H NMR spectrum of (*N*-acetylamino)methyltriphenylphosphonium tetrafluoroborate (**2l**); 400 MHz/$CDCl_3$/TMS; δ (ppm).



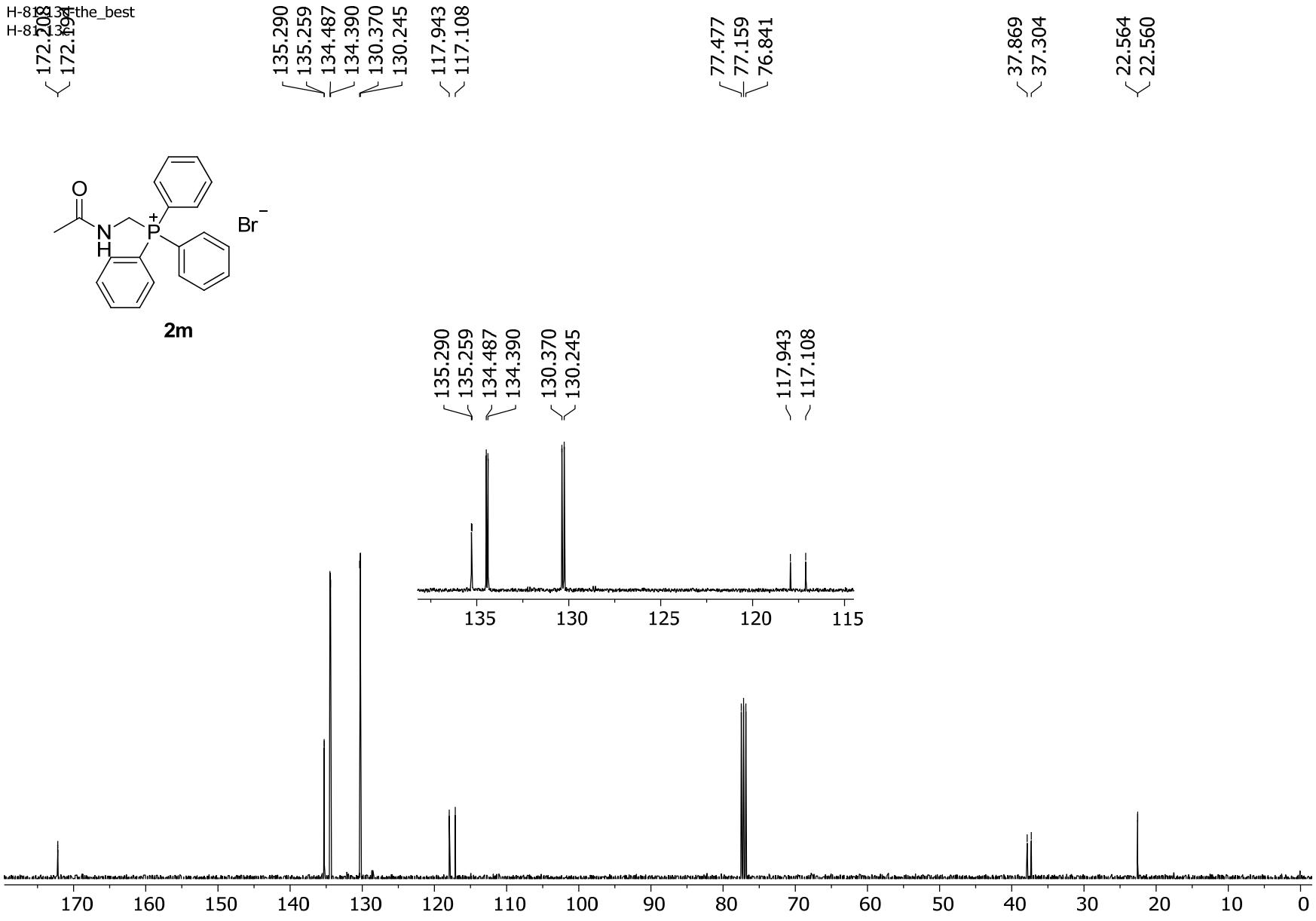
$^{13}C\{^{1}H\}$ NMR spectrum of (*N*-acetylamino)methyltriphenylphosphonium tetrafluoroborate (**2l**); 100 MHz/$CDCl_3$/TMS; δ (ppm).



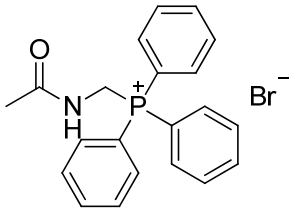
$^{31}P\{^{1}H\}$ NMR spectrum of (*N*-acetylamino)methyltriphenylphosphonium tetrafluoroborate (**2l**); 161.9 MHz/$CDCl_3$; δ (ppm).



[1]H NMR spectrum of (*N*-acetylamino)methyltriphenylphosphonium bromide (**2m**); 400 MHz/$CDCl_3$/TMS; δ (ppm).

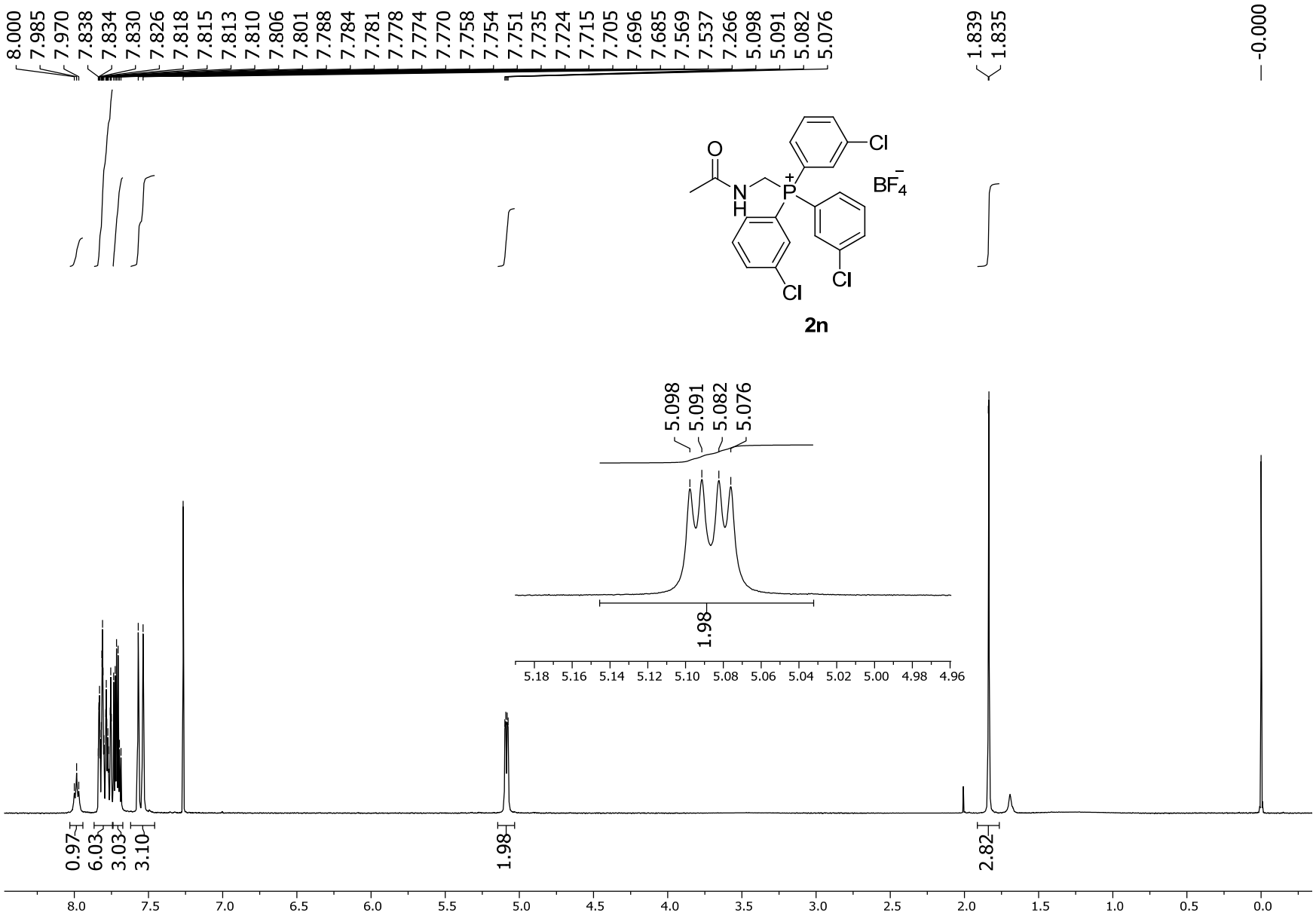


$^{13}C\{^{1}H\}$ NMR spectrum of (*N*-acetylamino)methyltriphenylphosphonium bromide (**2m**); 100 MHz/$CDCl_3$/TMS; δ (ppm).

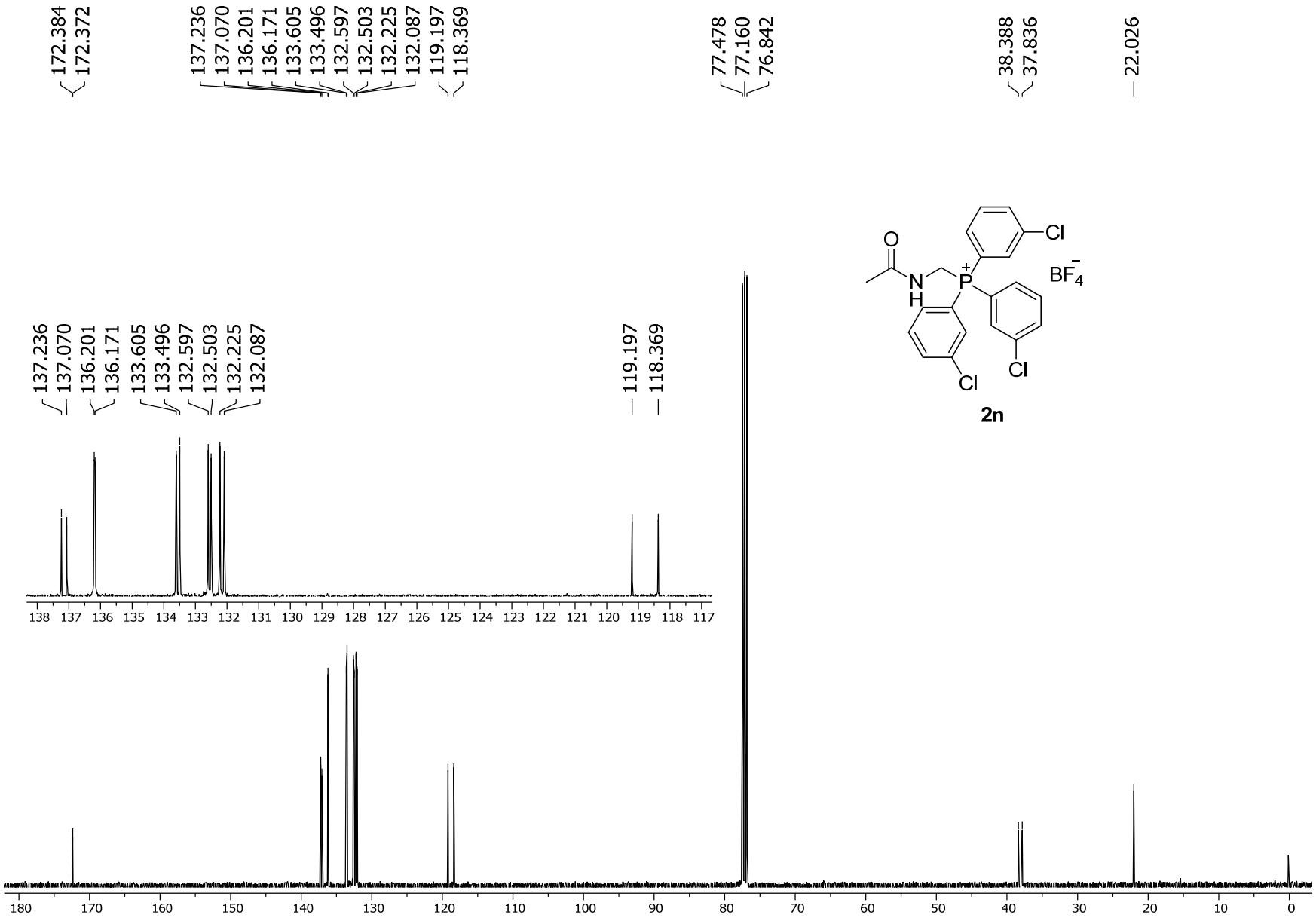


2m

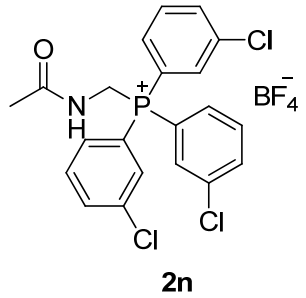
$^{31}P\{^{1}H\}$ NMR spectrum of (*N*-acetylamino)methyltriphenylphosphonium bromide (**2m**); 161.9 MHz/$CDCl_3$; δ (ppm).



^{1}H NMR spectrum of (*N*-acetylamino)methyltris(3-chlorophenyl)phosphonium tetrafluoroborate (**2n**); 400 MHz/$CDCl_3$/TMS; δ (ppm).

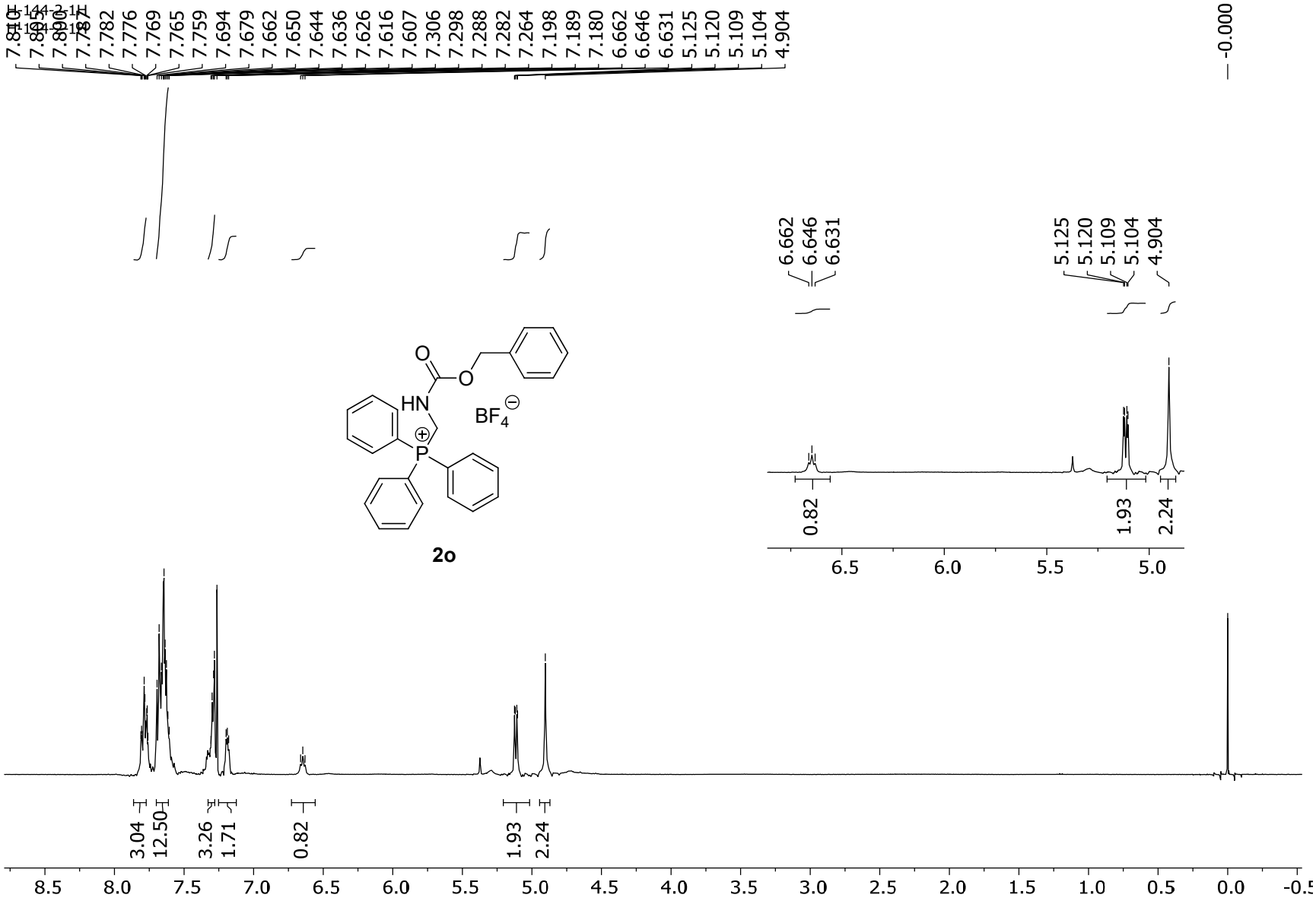


$^{13}C\{^{1}H\}$ NMR spectrum of (*N*-acetylamino)methyltris(3-chlorophenyl)phosphonium tetrafluoroborate (**2n**); 100 MHz/$CDCl_3$/TMS; δ (ppm).

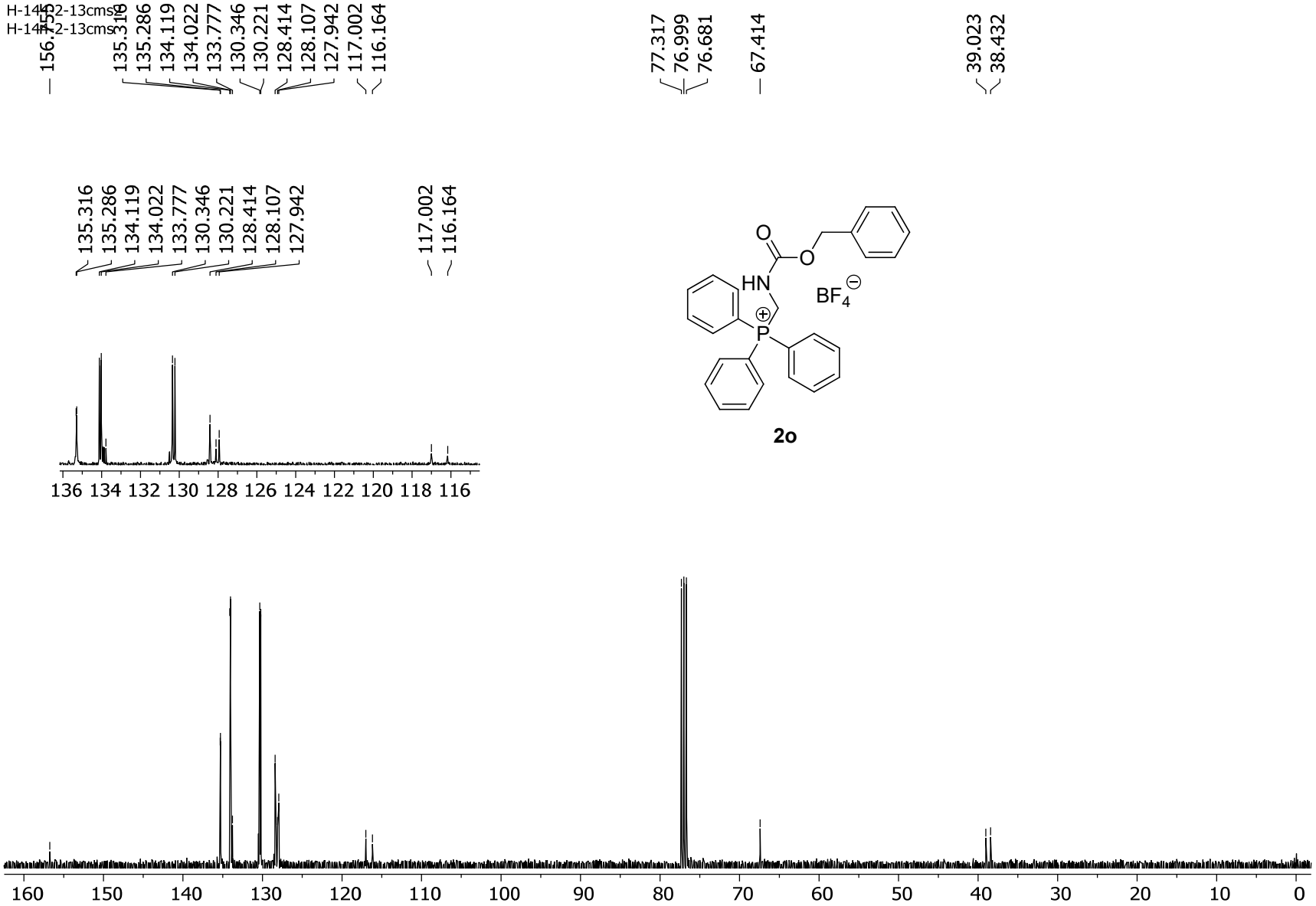


2n

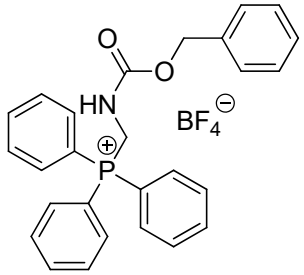
$^{31}P\{^{1}H\}$ NMR spectrum of (*N*-acetylamino)methyltris(3-chlorophenyl)phosphonium tetrafluoroborate (**2n**); 161.9 MHz/$CDCl_3$; δ (ppm).



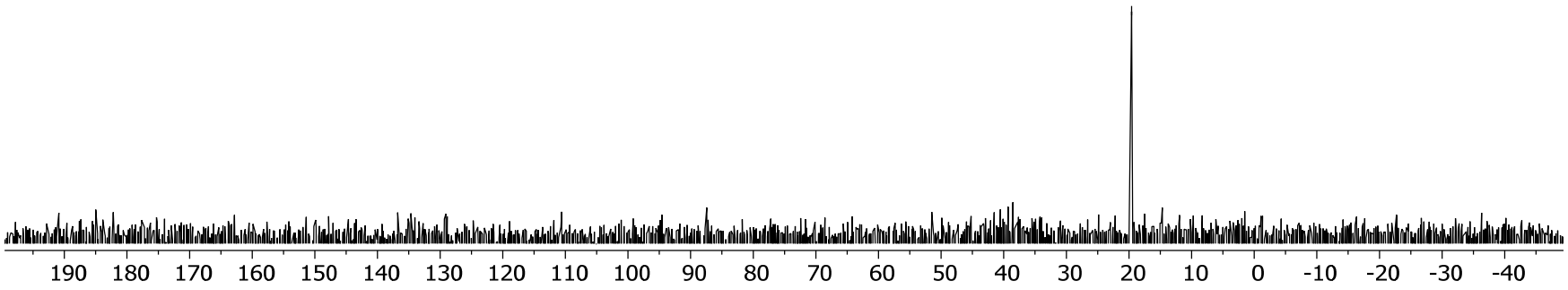
^{1}H NMR spectrum of (*N*-benzyloxycarbonylamino)methyltriphenylphosphonium tetrafluoroborate (**2o**); 400 MHz/$CDCl_3$/TMS; δ (ppm).



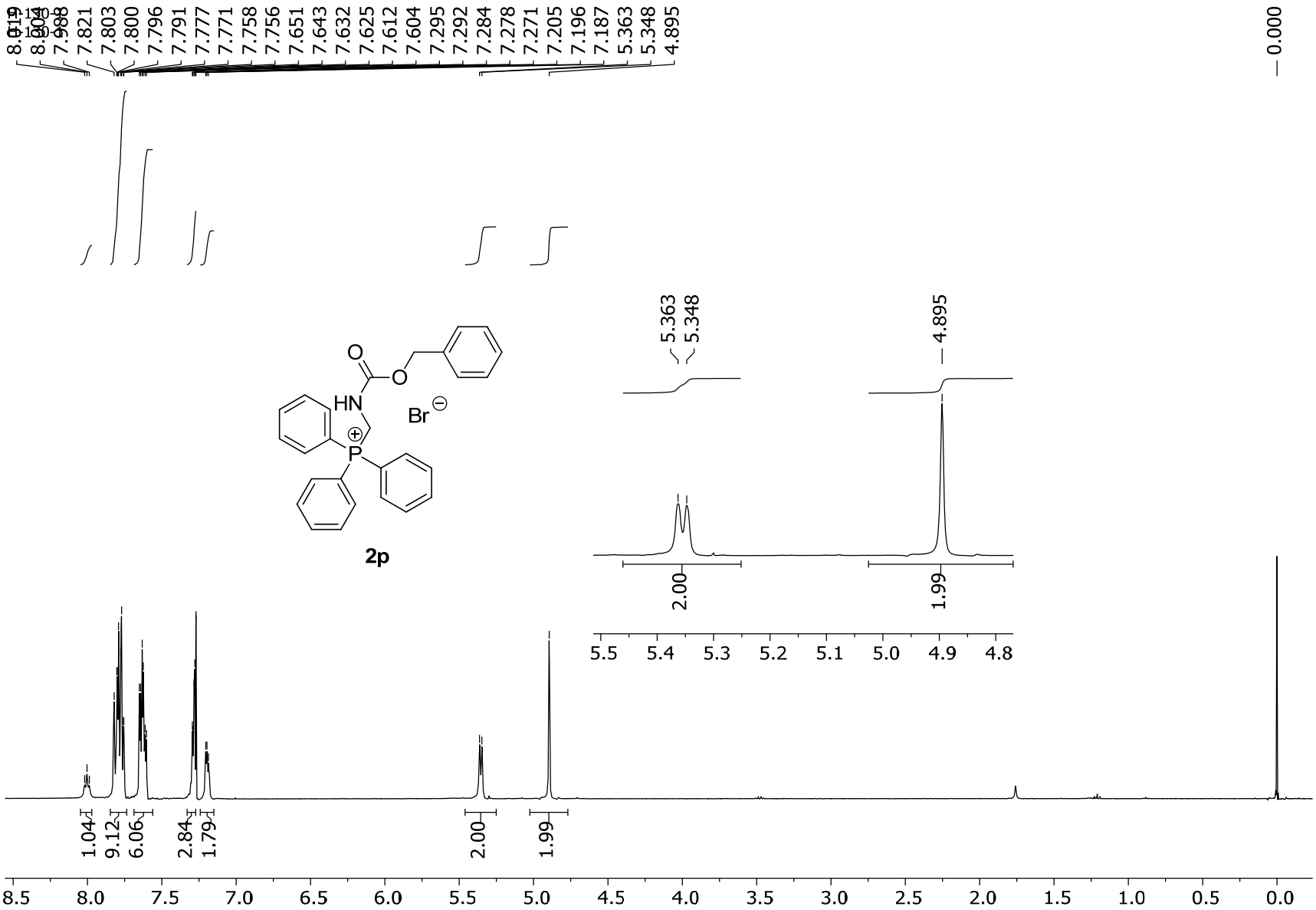
$^{13}C\{^{1}H\}$ NMR spectrum of (*N*-benzyloxycarbonylamino)methyltriphenylphosphonium tetrafluoroborate (**2o**); 100 MHz/$CDCl_3$/TMS; δ (ppm).



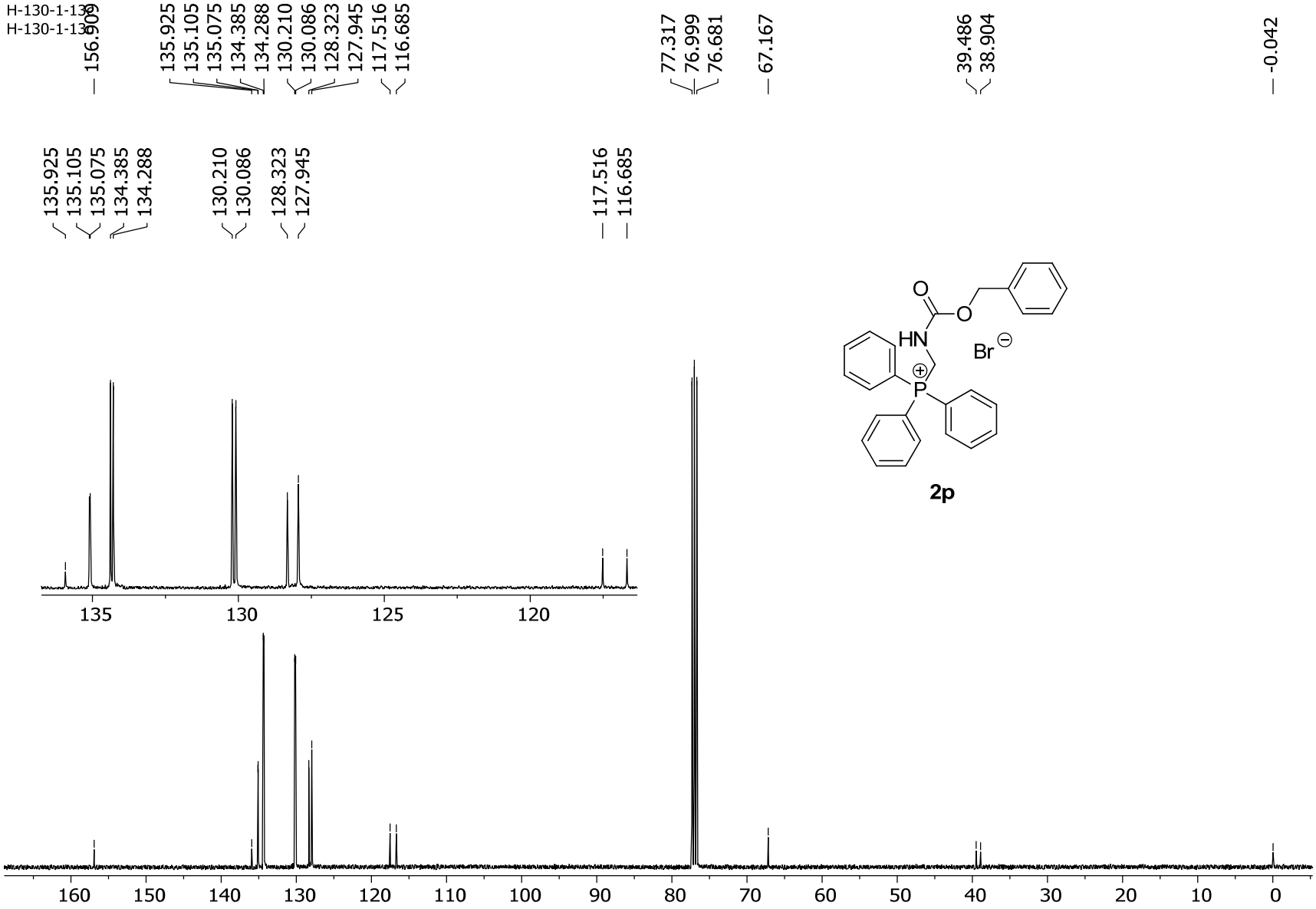
2o



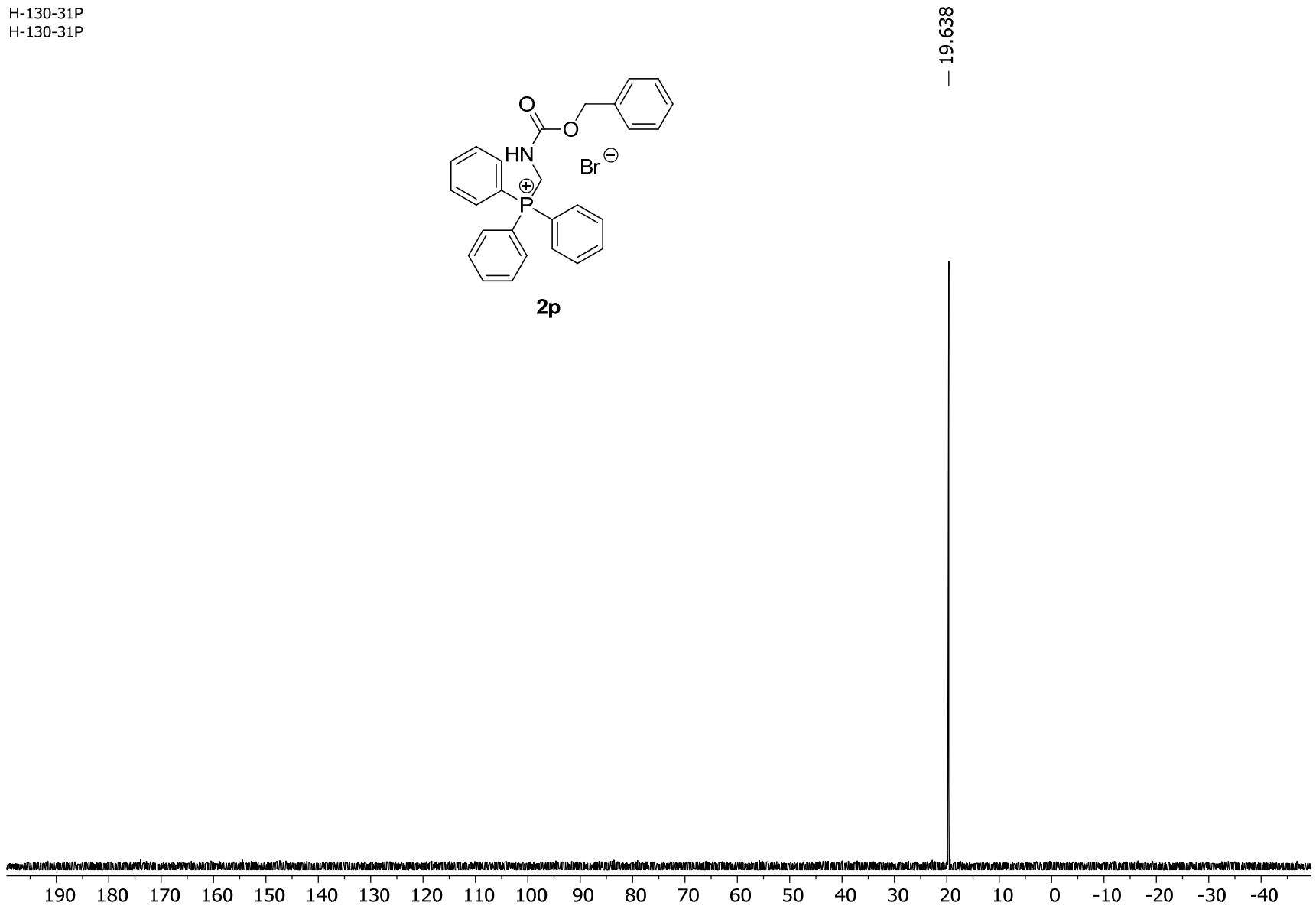
$^{31}P\{^{1}H\}$ NMR spectrum of (*N*-benzyloxycarbonylamino)methyltriphenylphosphonium tetrafluoroborate (**2o**); 161.9 MHz/$CDCl_3$; δ (ppm).



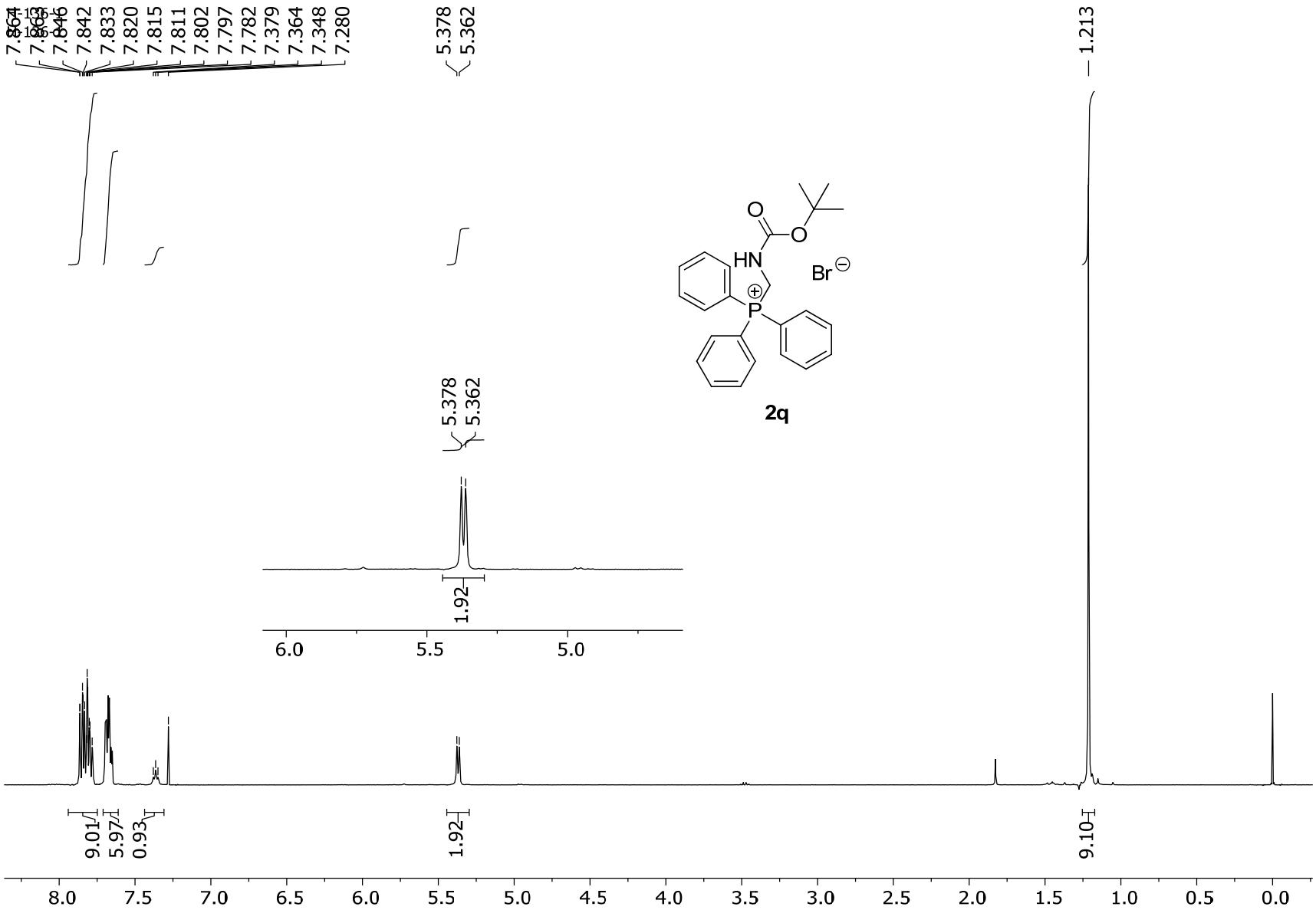
^{1}H NMR spectrum of (*N*-benzyloxycarbonylamino)methyltriphenylphosphonium bromide (**2p**); 400 MHz/$CDCl_3$/TMS; δ (ppm).



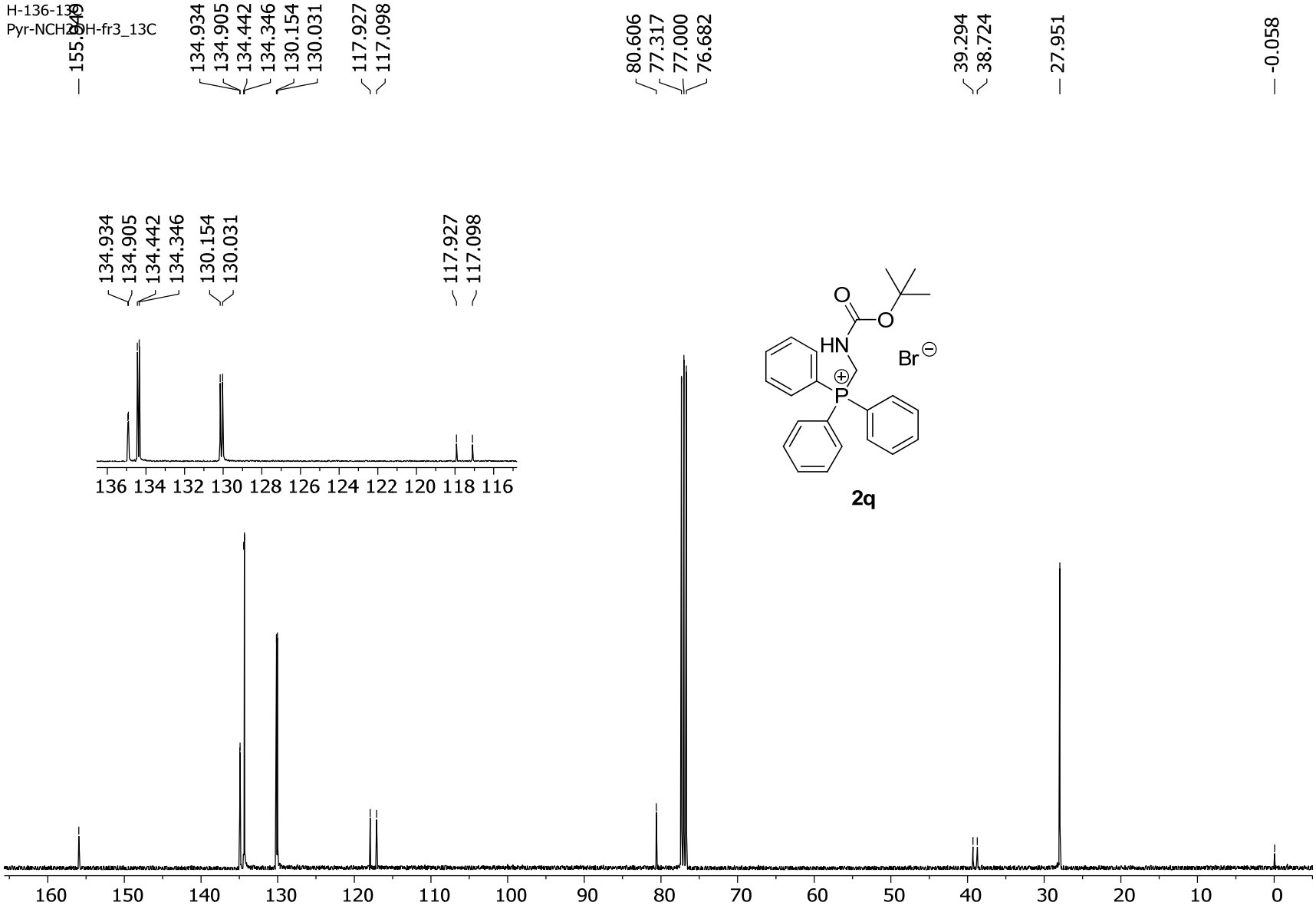
$^{13}C\{^{1}H\}$ NMR spectrum of (*N*-benzyloxycarbonylamino)methyltriphenylphosphonium bromide (**2p**); 100 MHz/$CDCl_3$/TMS; δ (ppm).



$^{31}P\{^{1}H\}$ NMR spectrum of (*N*-benzyloxycarbonylamino)methyltriphenylphosphonium bromide (**2p**); 161.9 MHz/$CDCl_3$; δ (ppm).

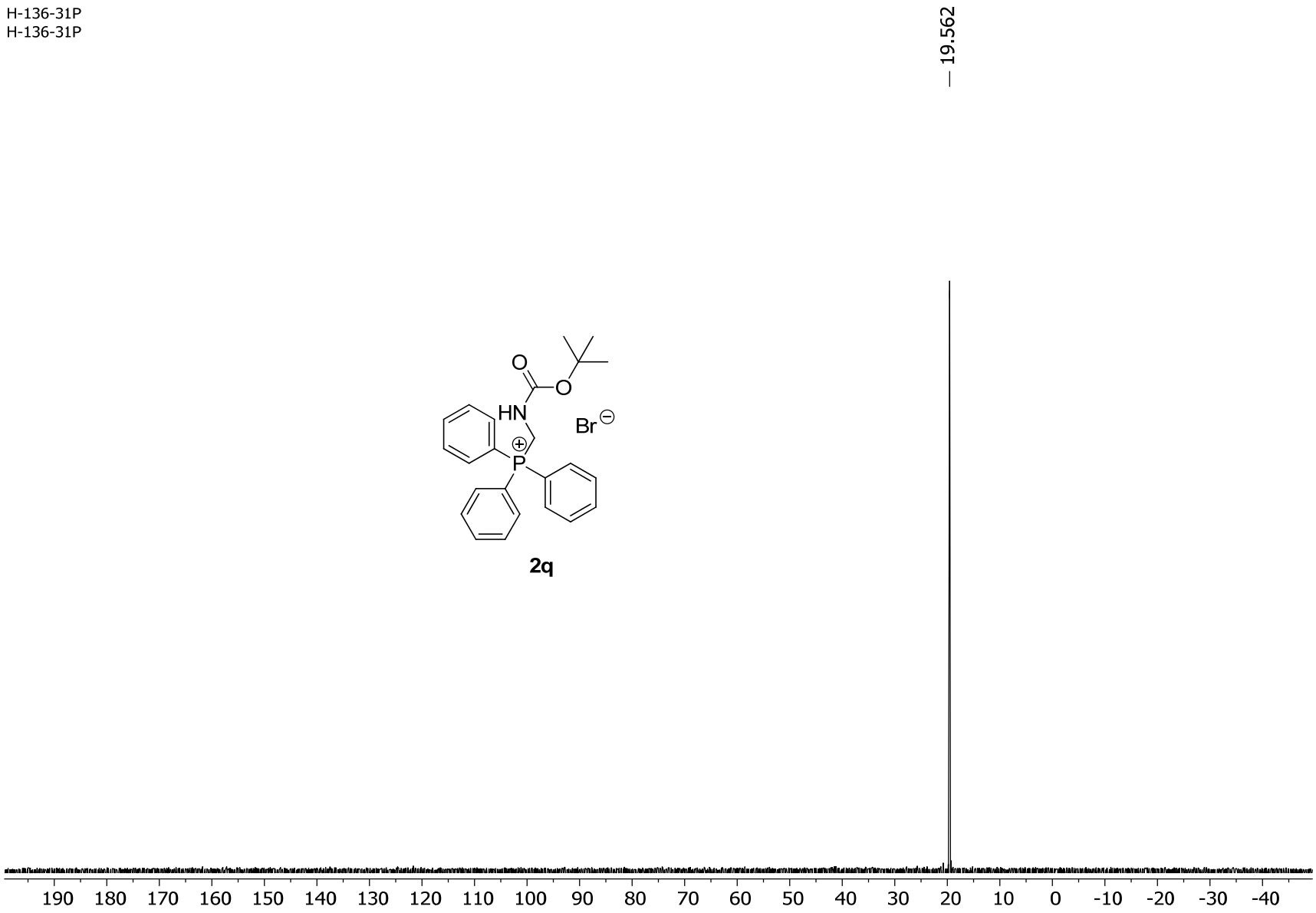


^{1}H NMR spectrum of (*N-tert*-butoxycarbonylamino)methylphosphonium bromide (**2q**); 400 MHz/$CDCl_3$/TMS; δ (ppm).

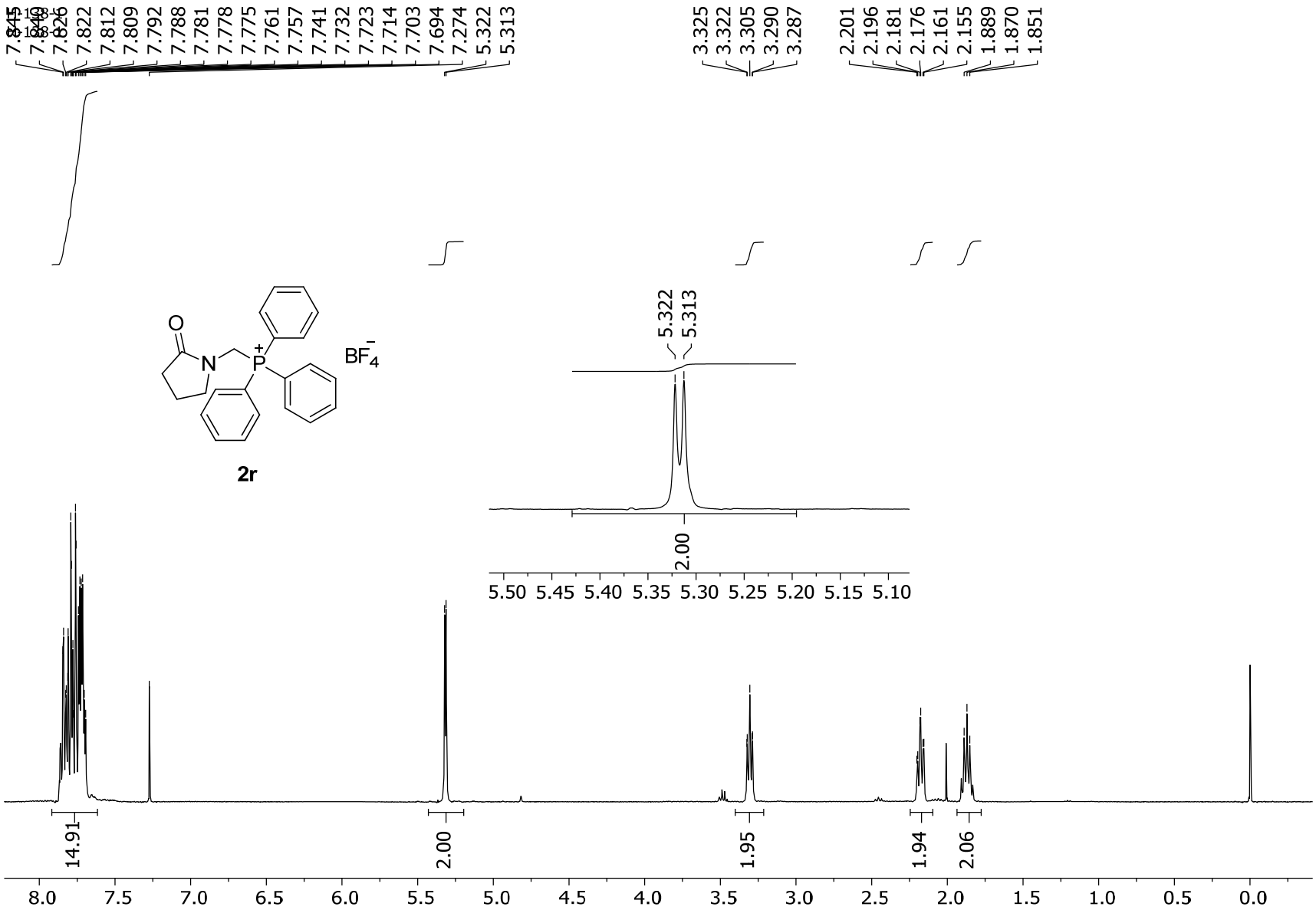


$^{13}C\{^{1}H\}$ NMR spectrum of (*N-tert*-butoxycarbonylamino)methylphosphonium bromide (**2q**); 100 MHz/$CDCl_3$/TMS; δ (ppm).

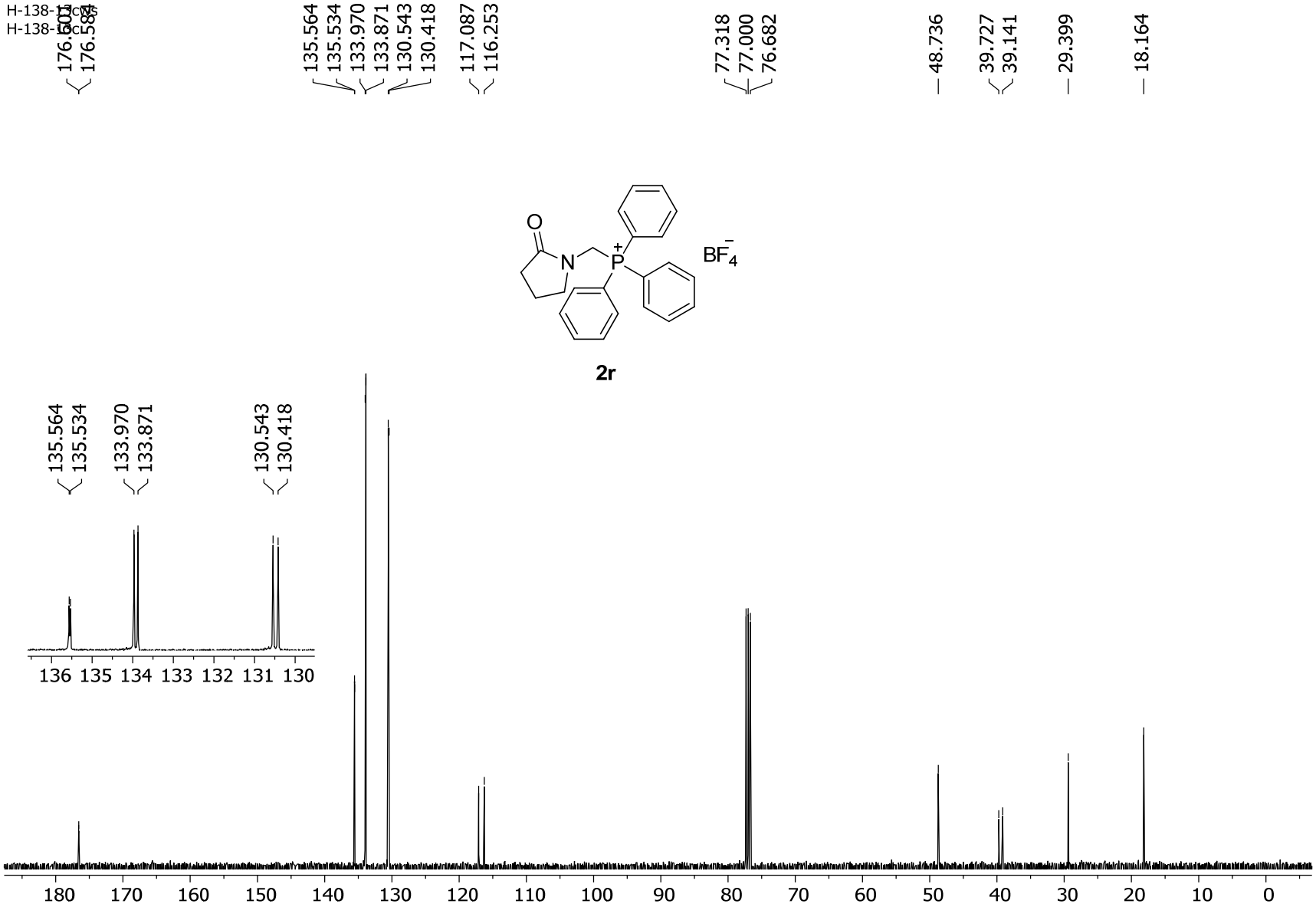
H-136-31P
H-136-31P



$^{31}P\{^{1}H\}$ NMR spectrum of (*N-tert*-butoxycarbonylamino)methylphosphonium bromide (**2q**); 161.9 MHz/$CDCl_3$; δ (ppm).

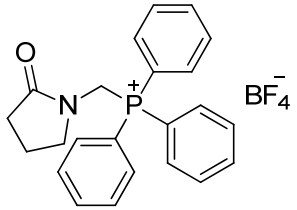


^{1}H NMR spectrum of (2-oxopyrrolidin-1-yl)methyltriphenylphosphonium tetrafluoroborate (**2r**); 400 MHz/$CDCl_3$/TMS; δ (ppm).



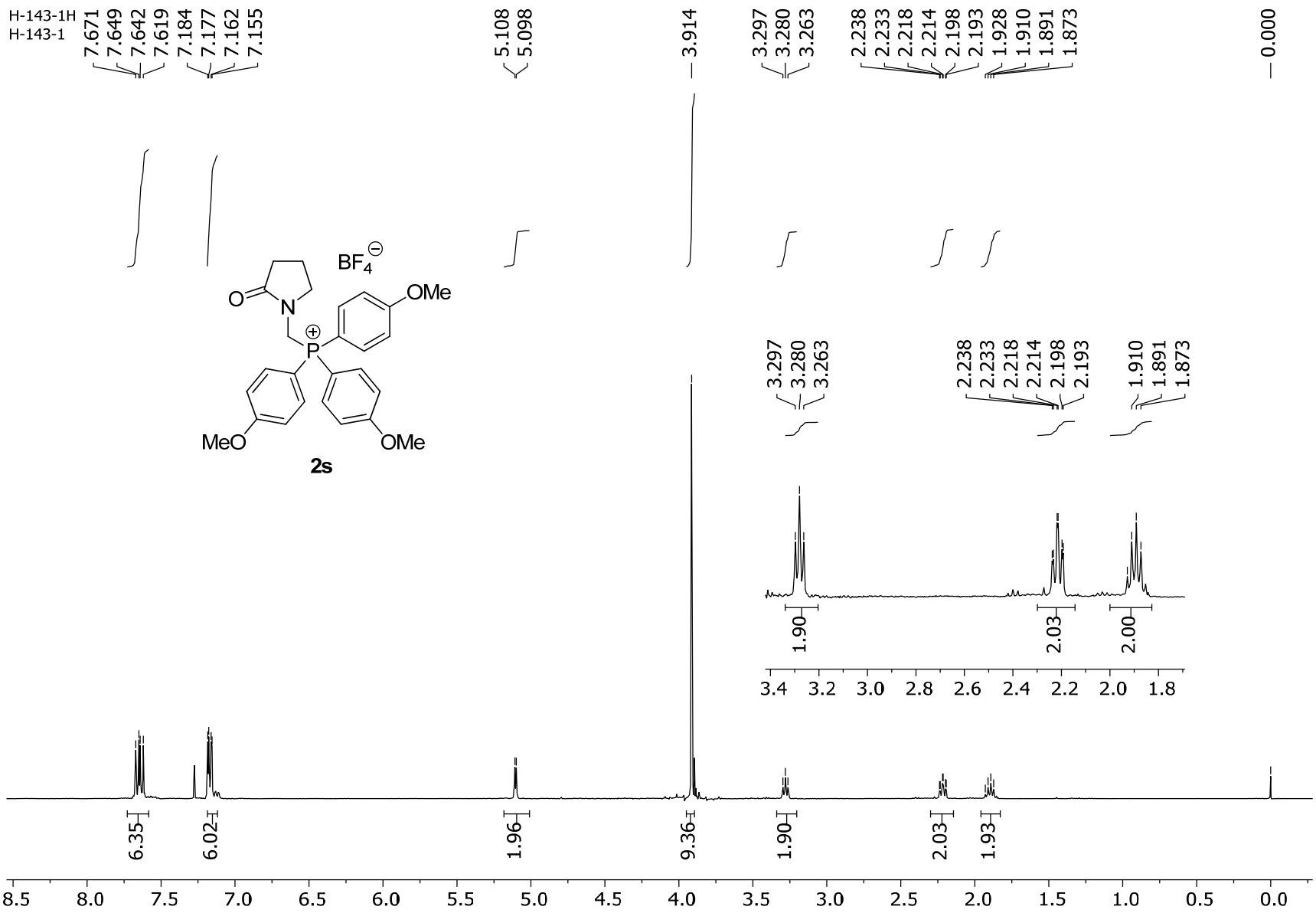
$^{13}C\{^{1}H\}$ NMR spectrum of (2-oxopyrrolidin-1-yl)methyltriphenylphosphonium tetrafluoroborate (**2r**); 100 MHz/$CDCl_3$/TMS; δ (ppm).

H-138-31P
H-138-31P

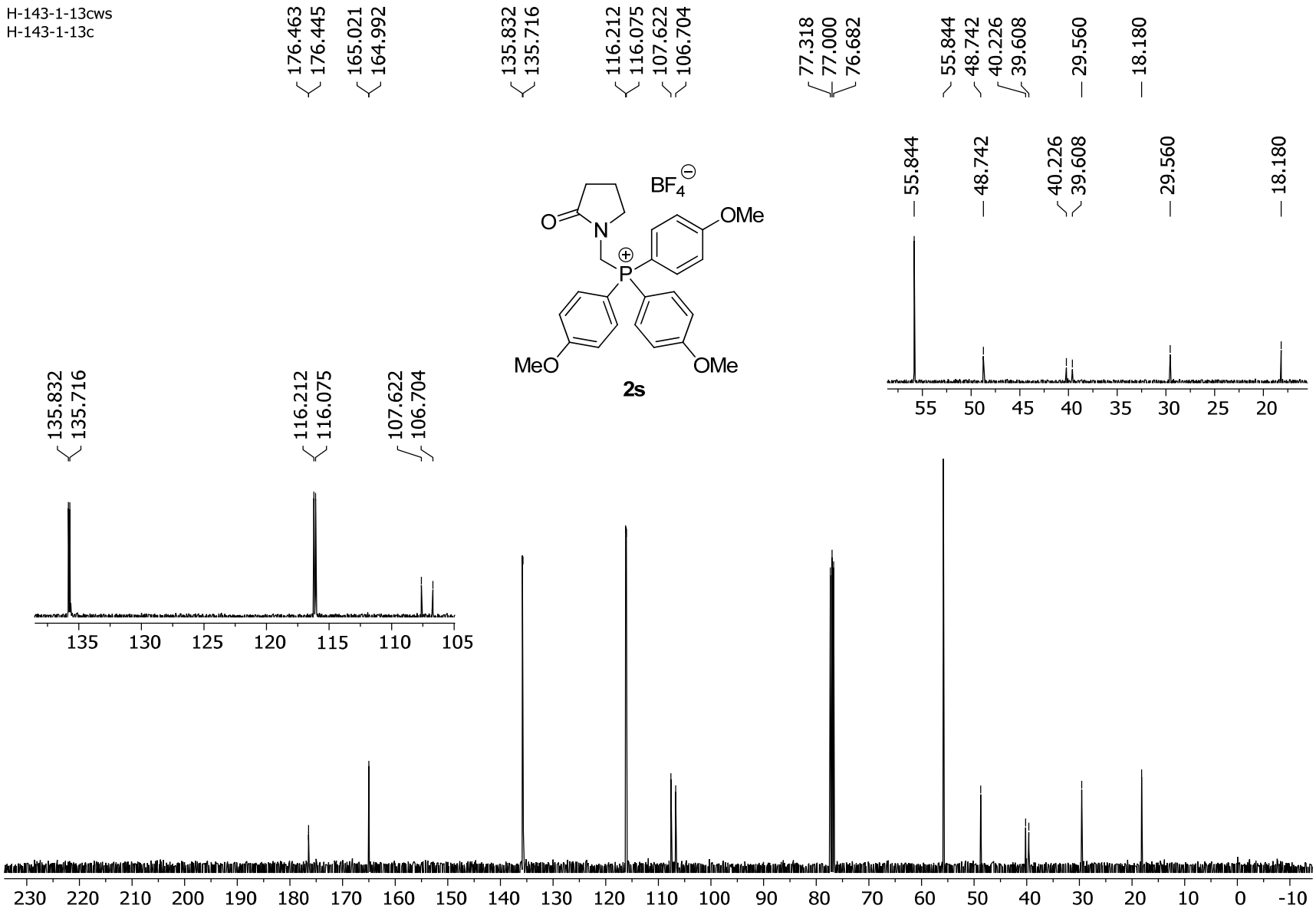


2r

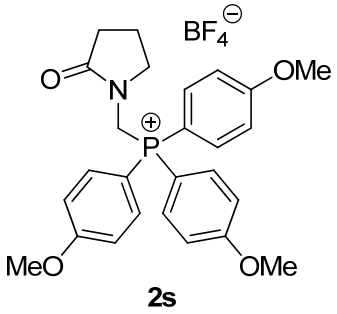
$^{31}P\{^{1}H\}$ NMR spectrum of (2-oxopyrrolidin-1-yl)methyltriphenylphosphonium tetrafluoroborate (**2r**); 161.9 MHz/$CDCl_3$; δ (ppm).



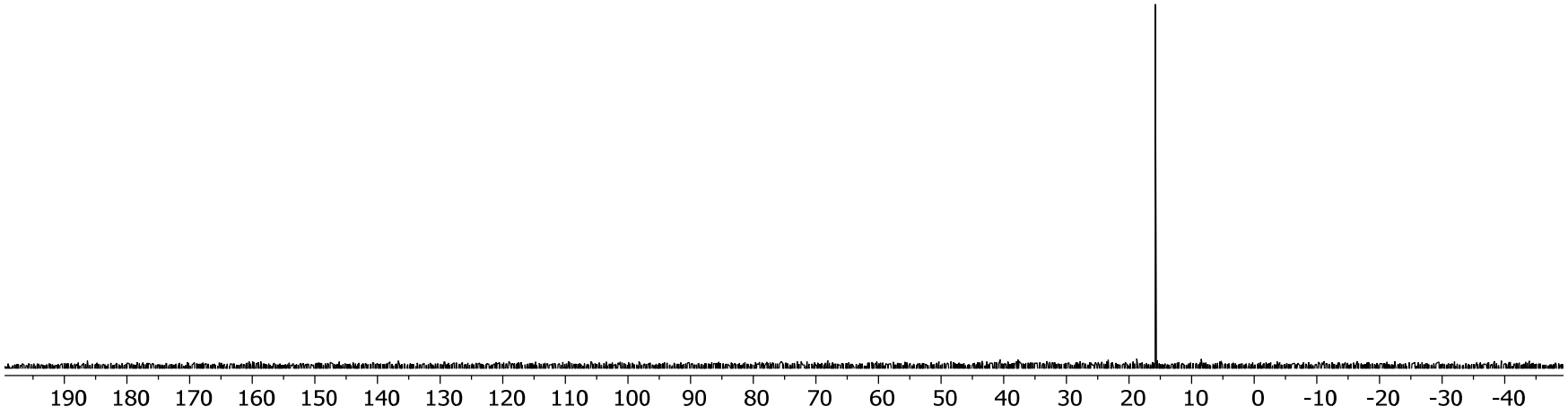
^{1}H NMR spectrum of (2-oxopyrrolidin-1-yl)methyltris(4-methoxyphenyl)phosphonium tetrafluoroborate (**2s**); 400 MHz/$CDCl_3$/TMS; δ (ppm).



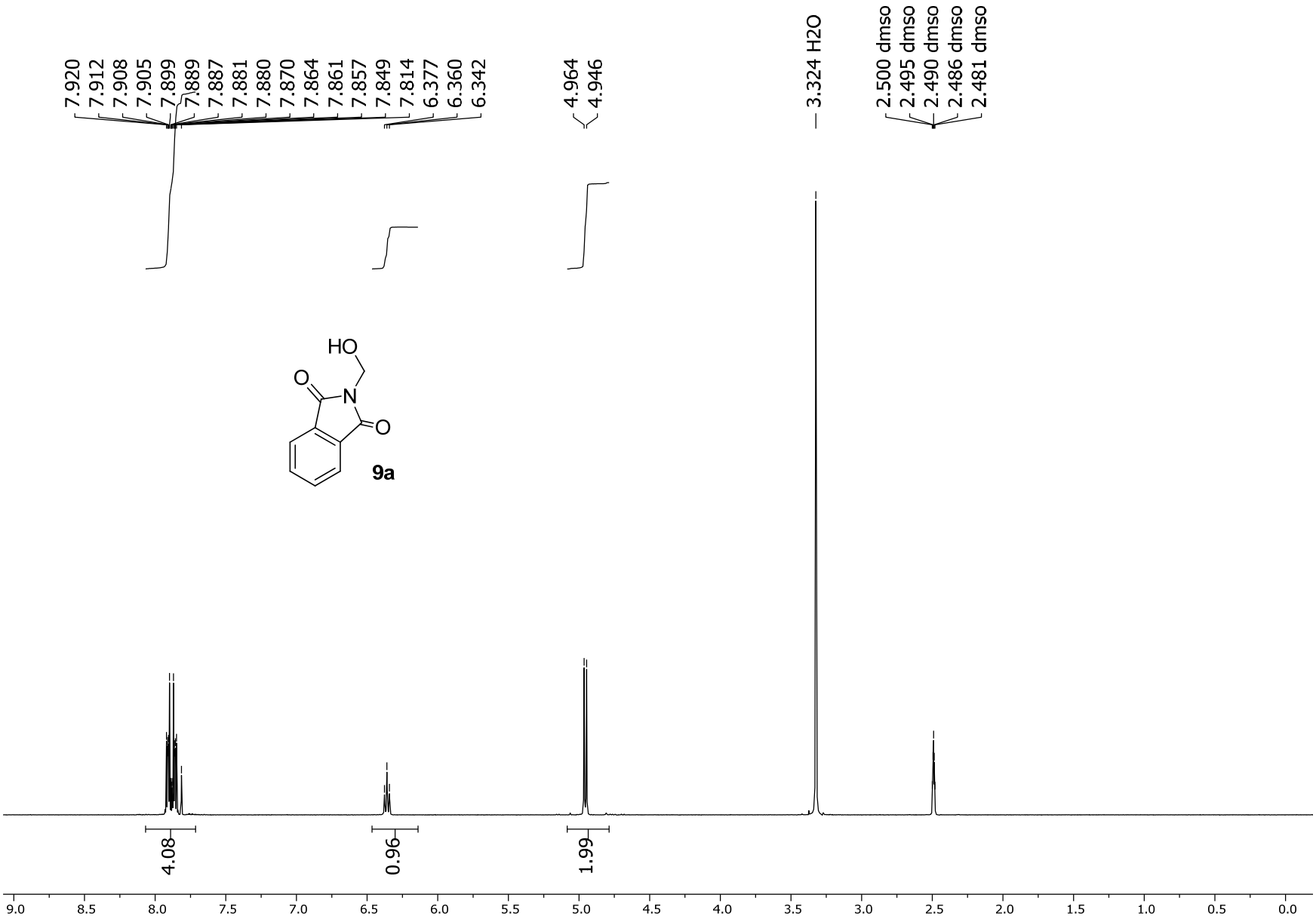
$^{13}C\{^{1}H\}$ NMR spectrum of (2-oxopyrrolidin-1-yl)methyltris(4-methoxyphenyl)phosphonium tetrafluoroborate (**2s**); 100 MHz/$CDCl_3$/TMS; δ (ppm).



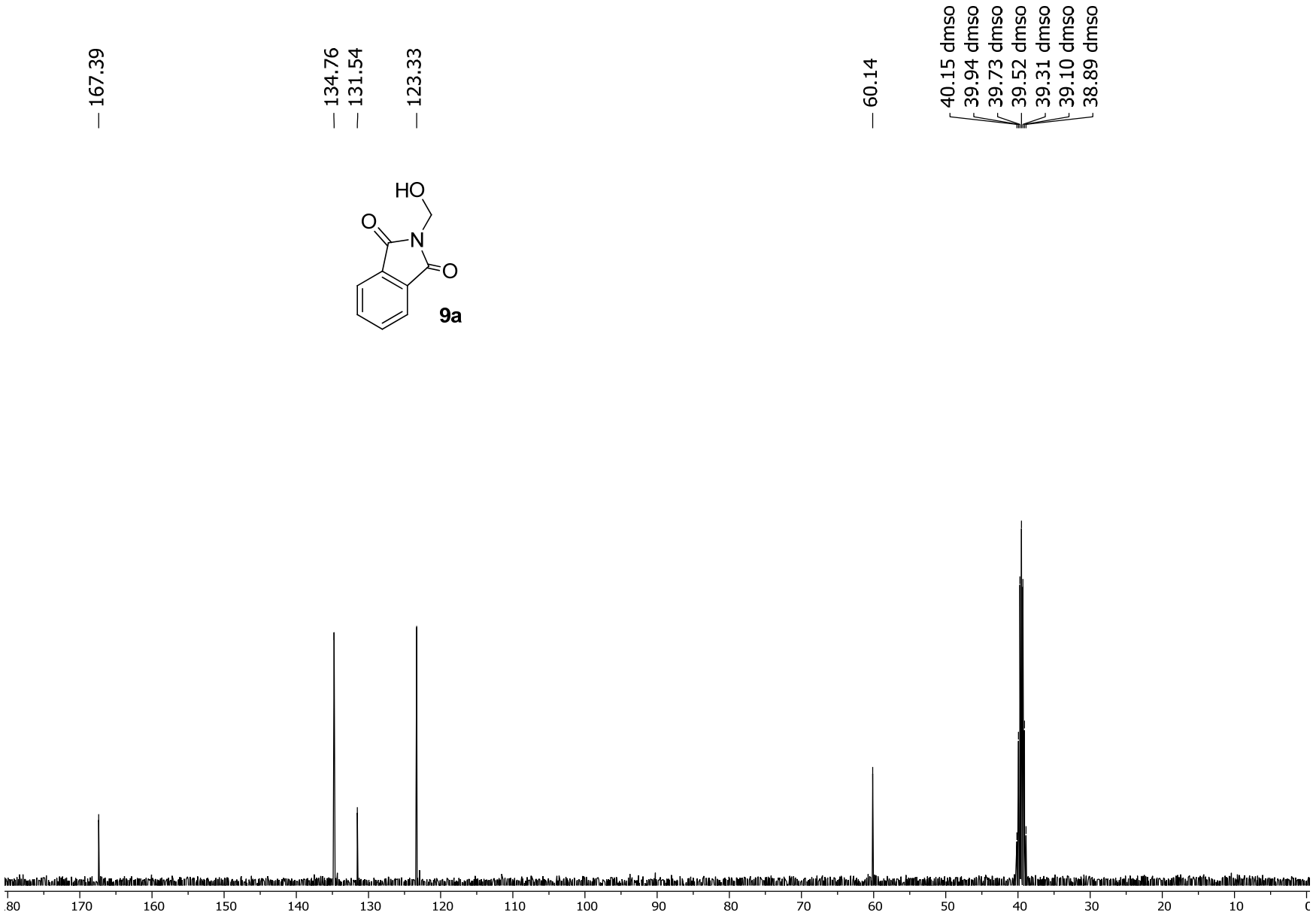
2s



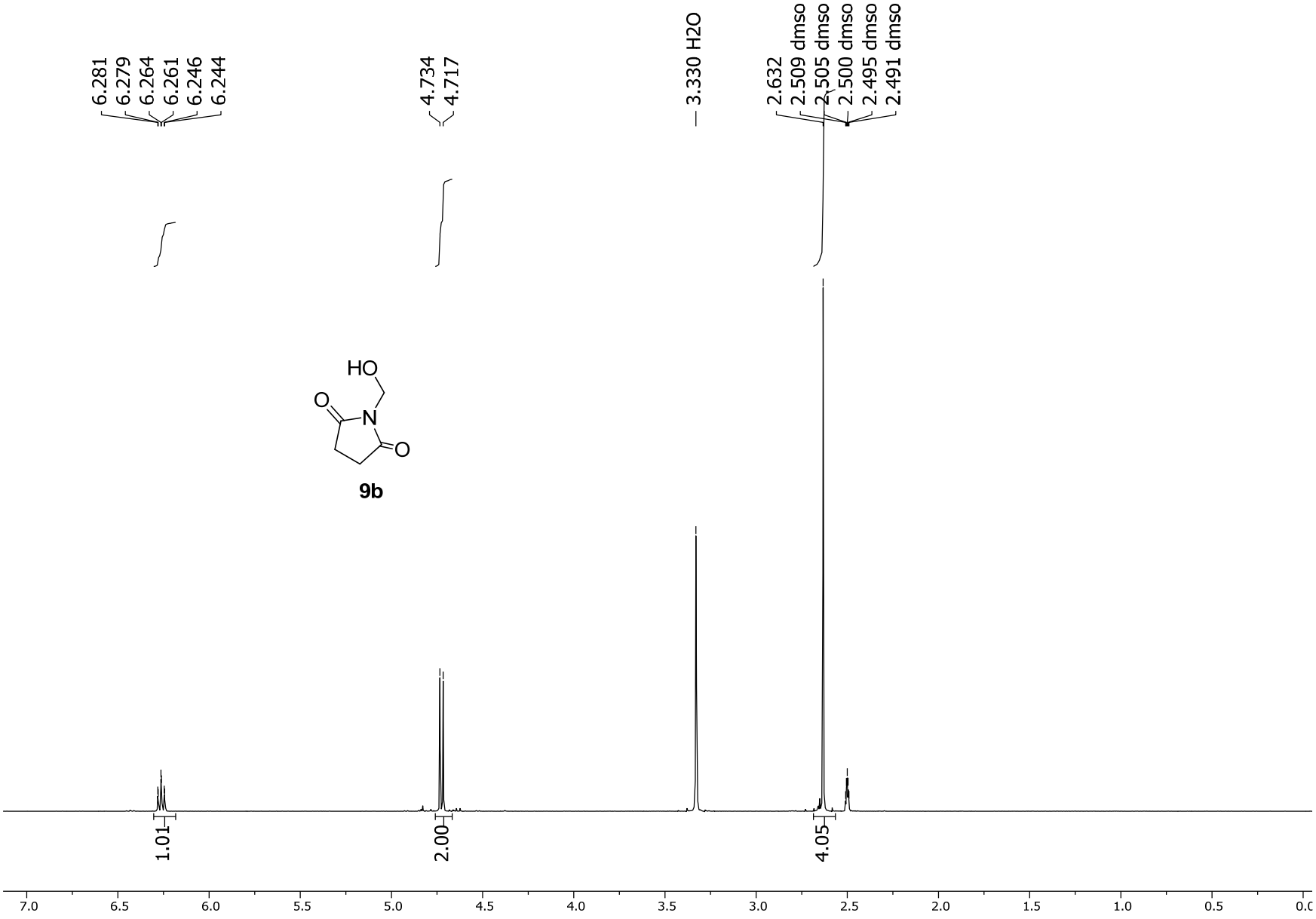
$^{31}P\{^{1}H\}$ NMR spectrum of (2-oxopyrrolidin-1-yl)methyltris(4-methoxyphenyl)phosphonium tetrafluoroborate (**2s**); 161.9 MHz/$CDCl_3$; δ (ppm).



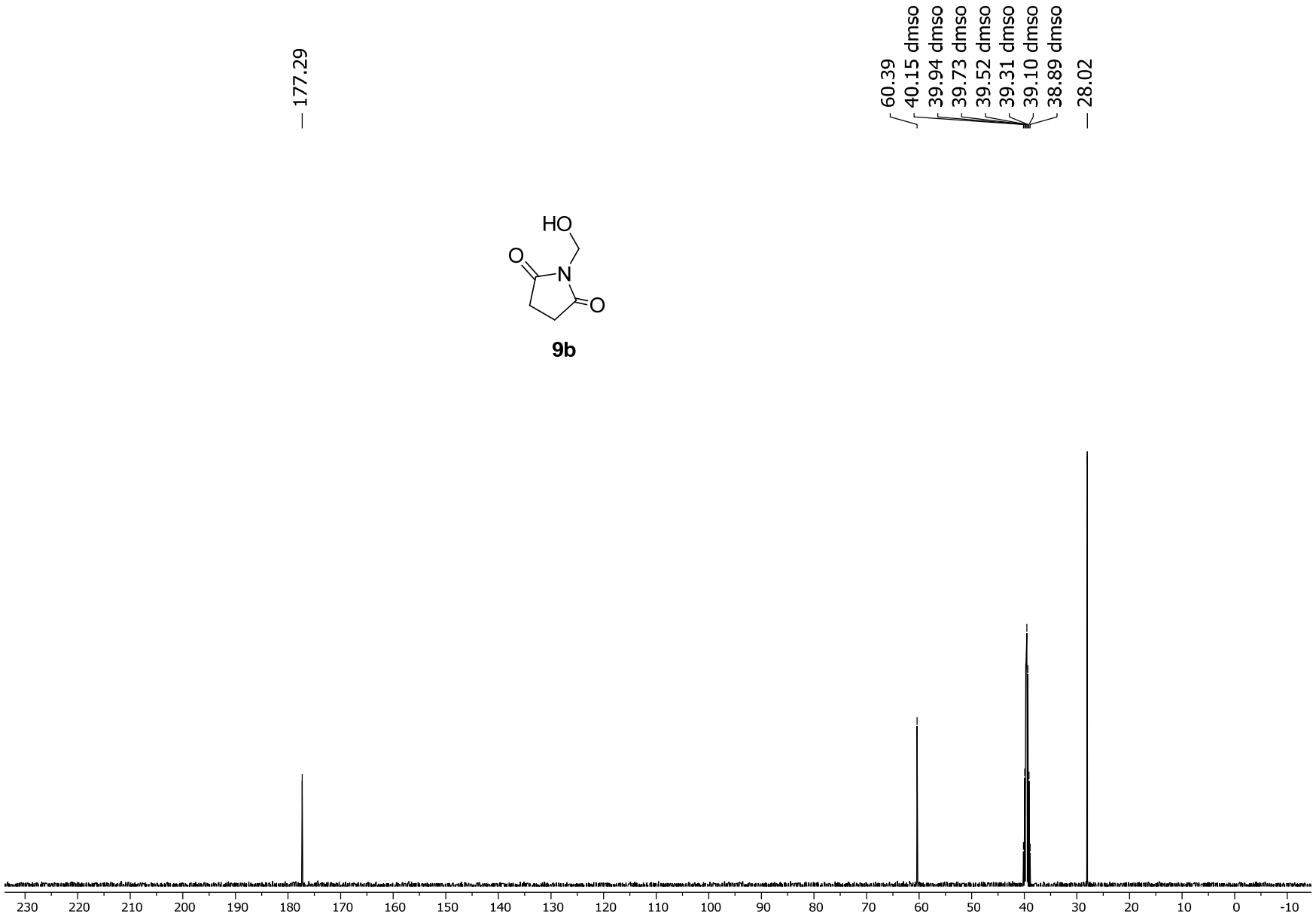
^{1}H NMR spectrum of *N*-hydroxymethylphthalimide (**9a**); 400 MHz/DMSO-d6; δ (ppm).



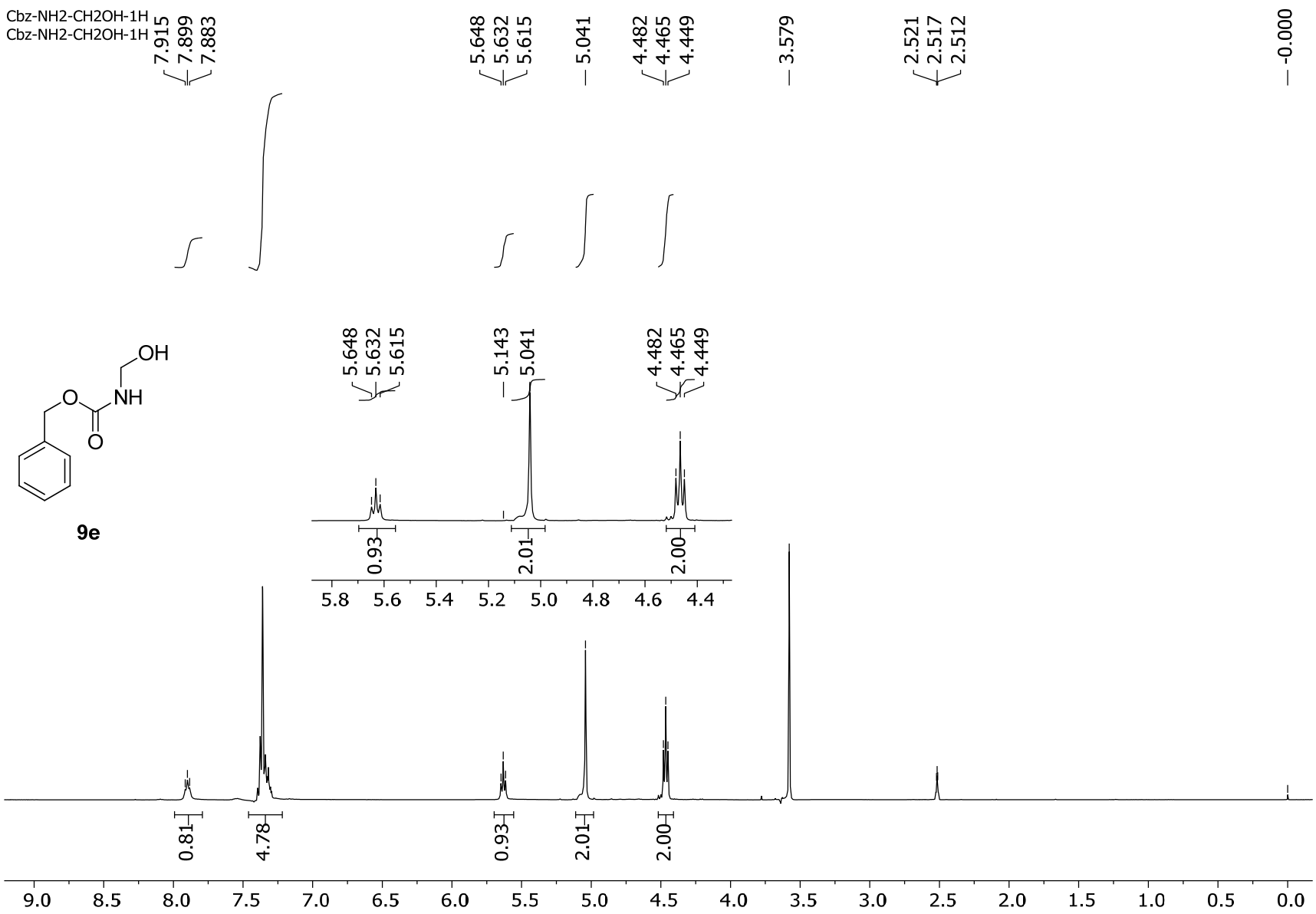
$^{13}C\{^{1}H\}$ NMR spectrum of *N*-hydroxymethylphthalimide (**9a**); 100 MHz/DMSO-d6; δ (ppm).



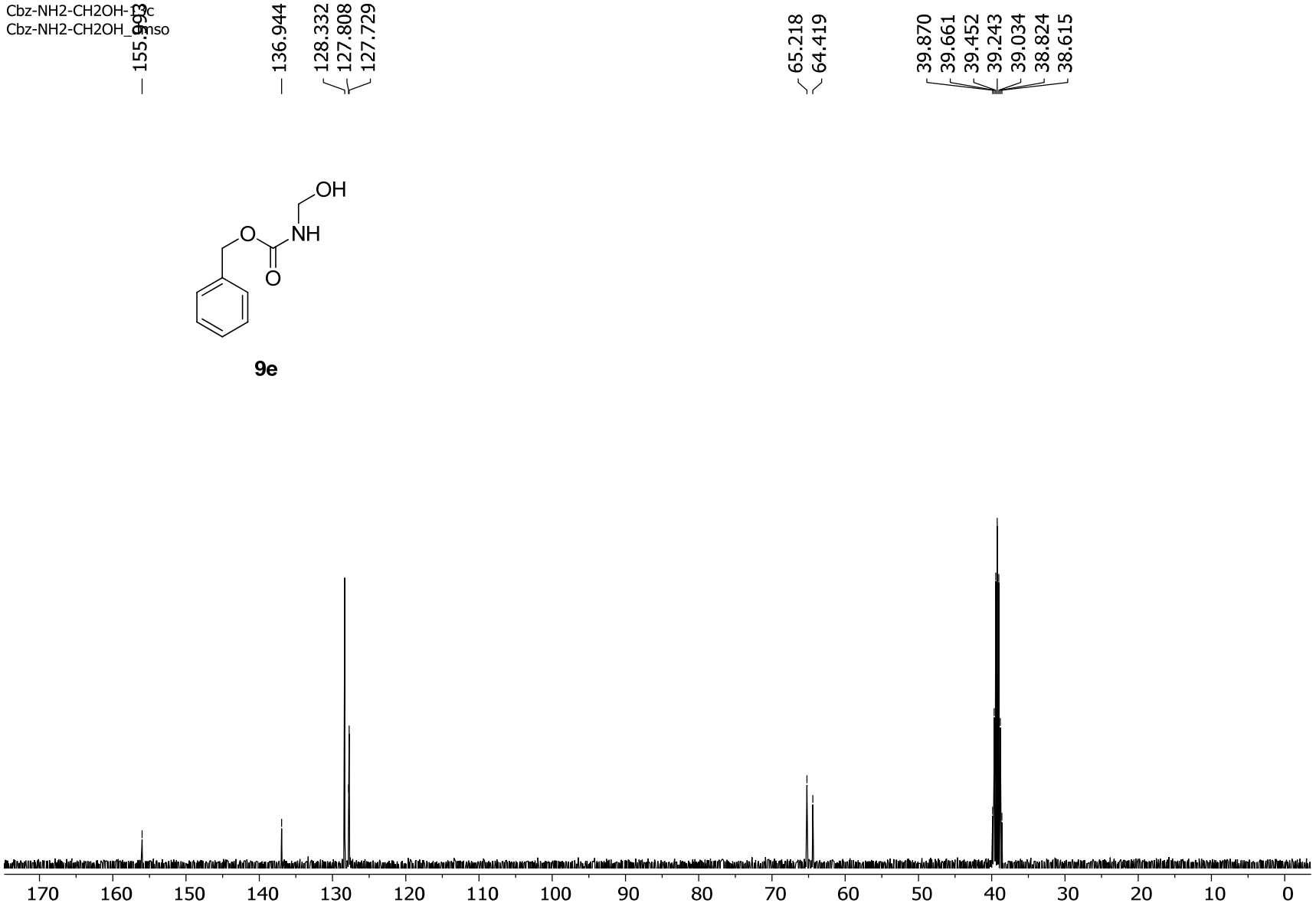
^{1}H NMR spectrum of *N*-hydroxymethylsuccinimide (**9b**); 400 MHz/DMSO-d6; δ (ppm).



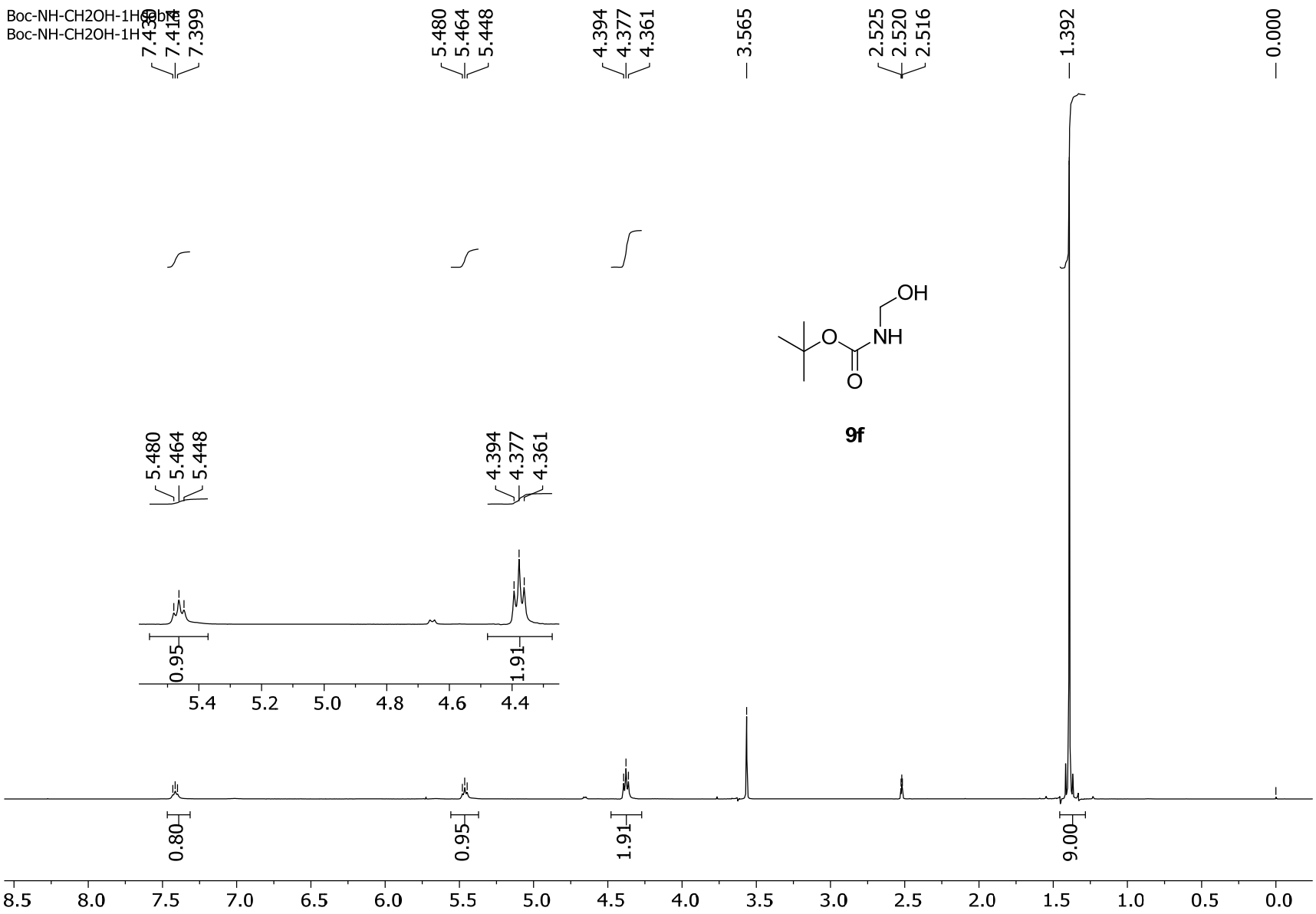
$^{13}C\{^{1}H\}$ NMR spectrum of *N*-hydroxymethylsuccinimide (**9b**); 100 MHz/DMSO-d6; δ (ppm).



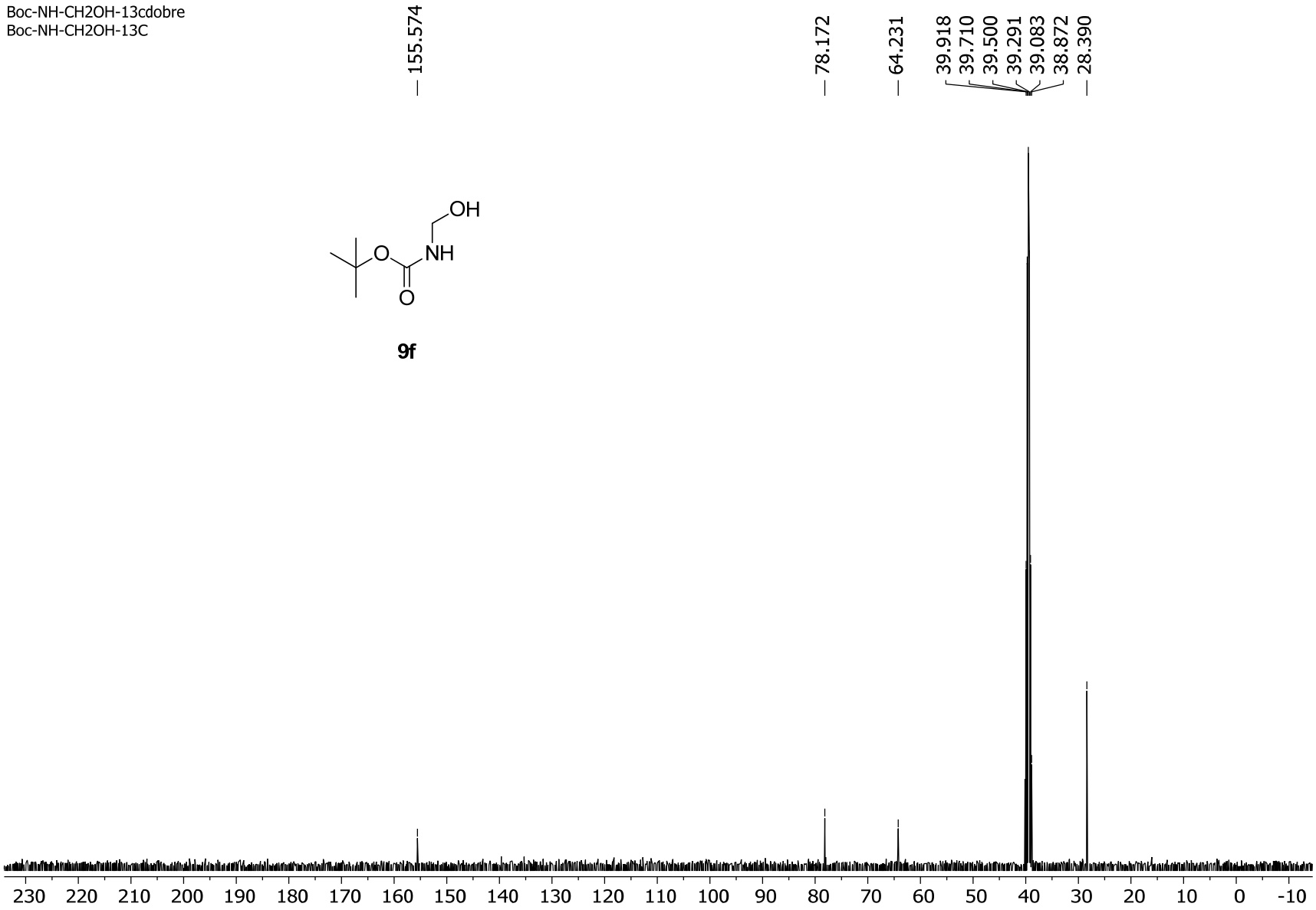
^{1}H NMR spectrum of benzyl *N*-hydroxymethylcarbamate (**9e**); 400 MHz/DMSO-d6; δ (ppm).



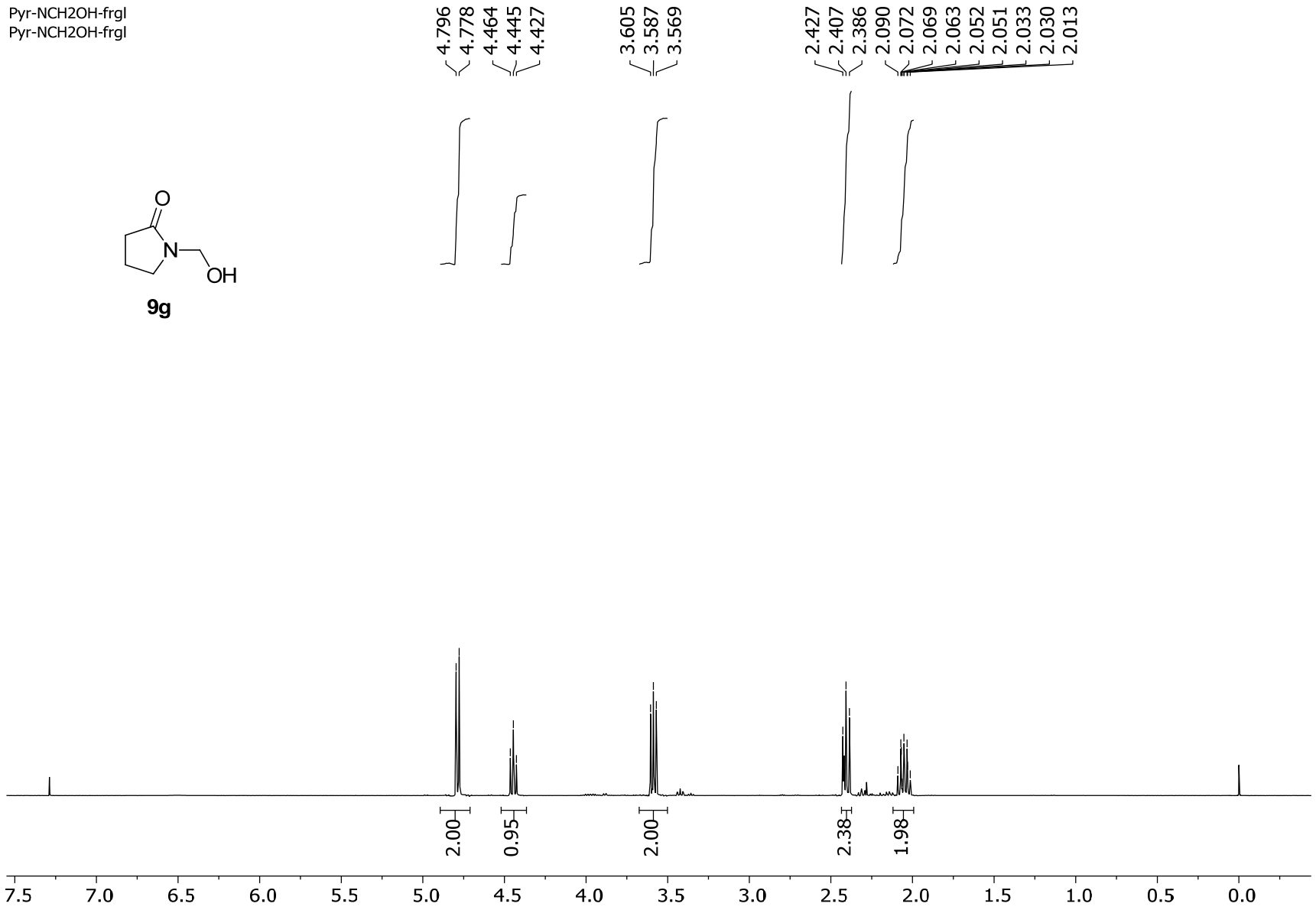
$^{13}C\{^{1}H\}$ NMR spectrum of benzyl *N*-hydroxymethylcarbamate (**9e**); 100 MHz/DMSO-d6; δ (ppm).



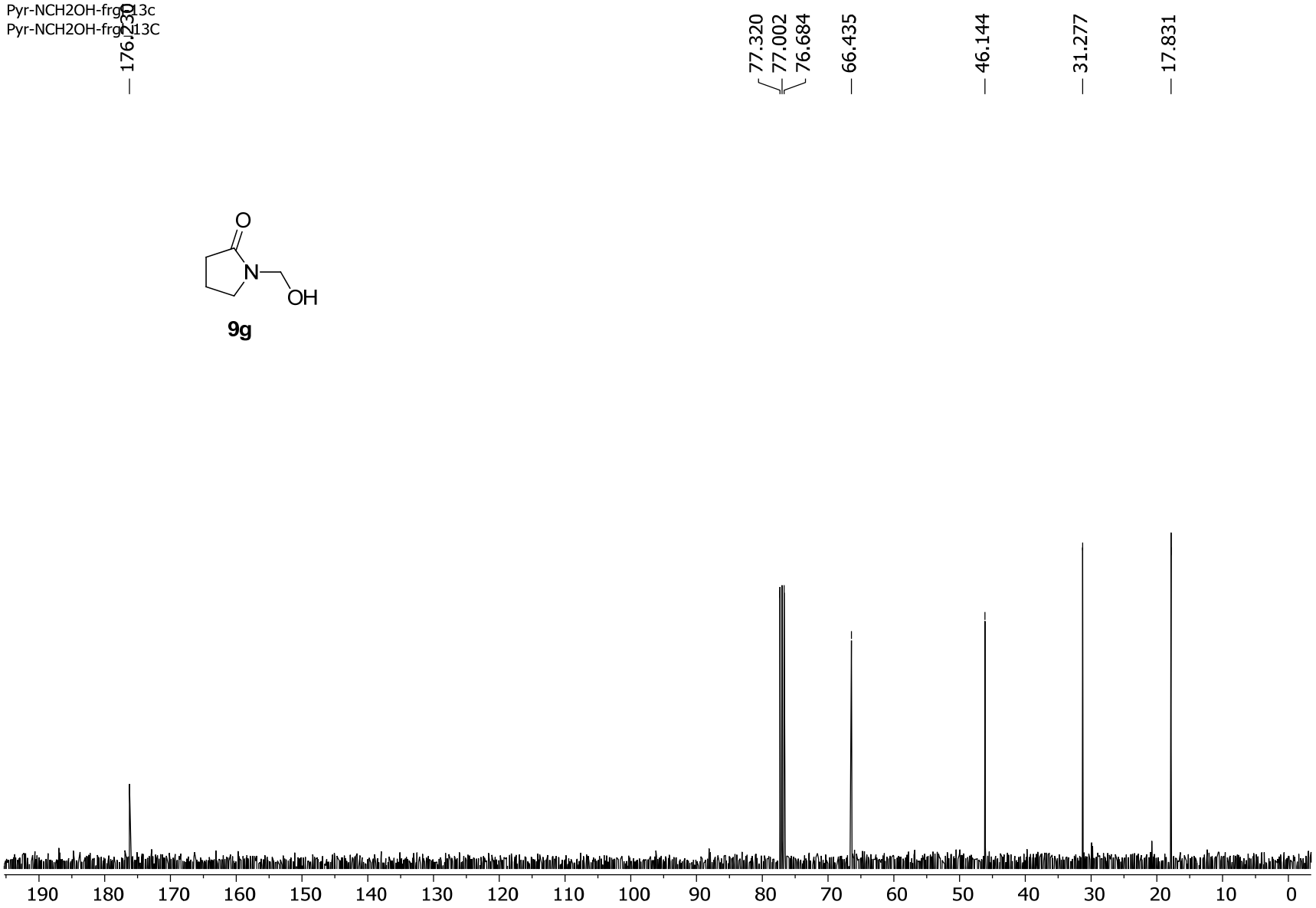
^{1}H NMR spectrum of *tert*-butyl *N*-hydroxymethylcarbamate (**9f**); 400 MHz/DMSO-d6; δ (ppm).



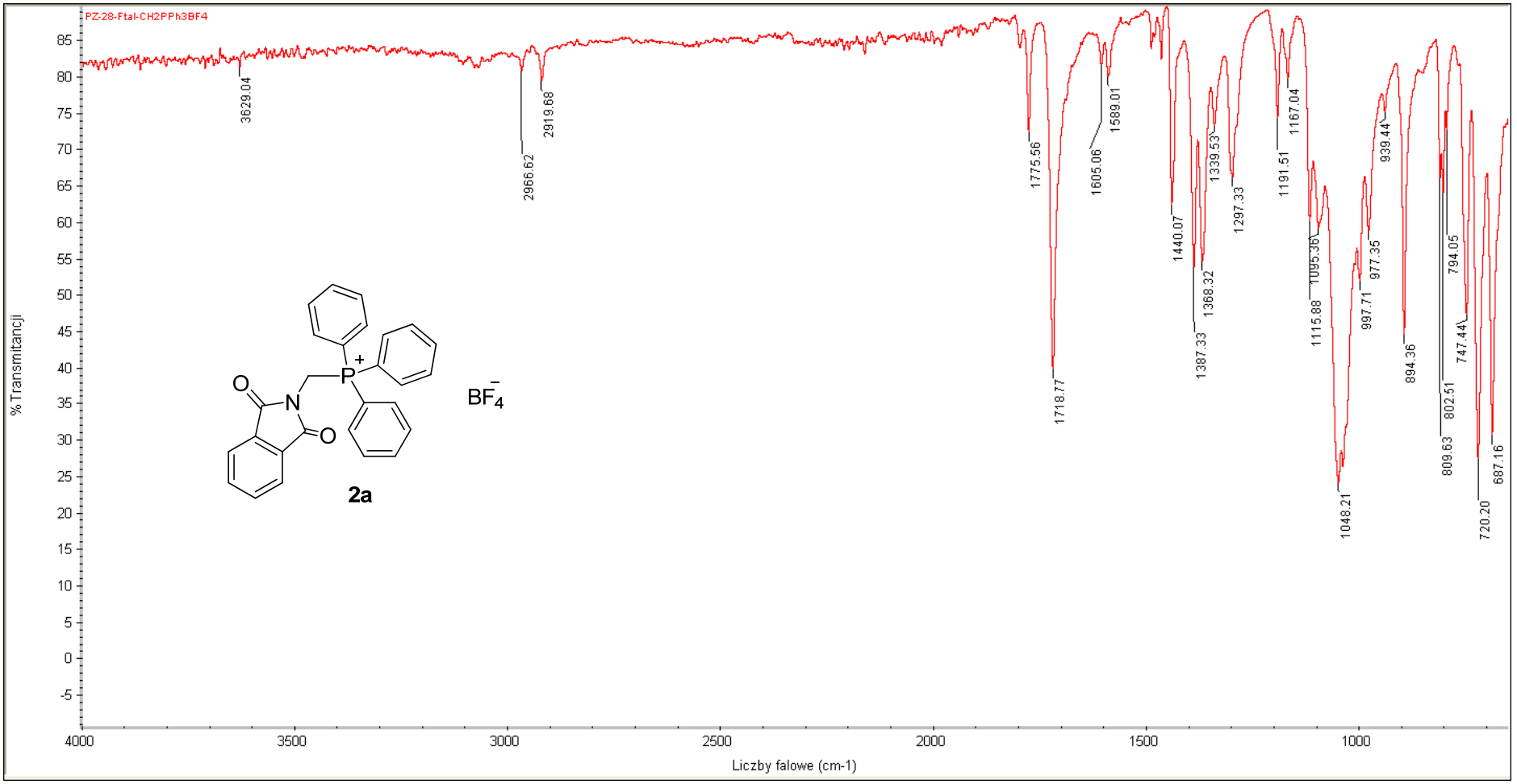
$^{13}C\{^{1}H\}$ NMR spectrum of *tert*-butyl *N*-hydroxymethylcarbamate (**9f**); 100 MHz/DMSO-d6; δ (ppm).



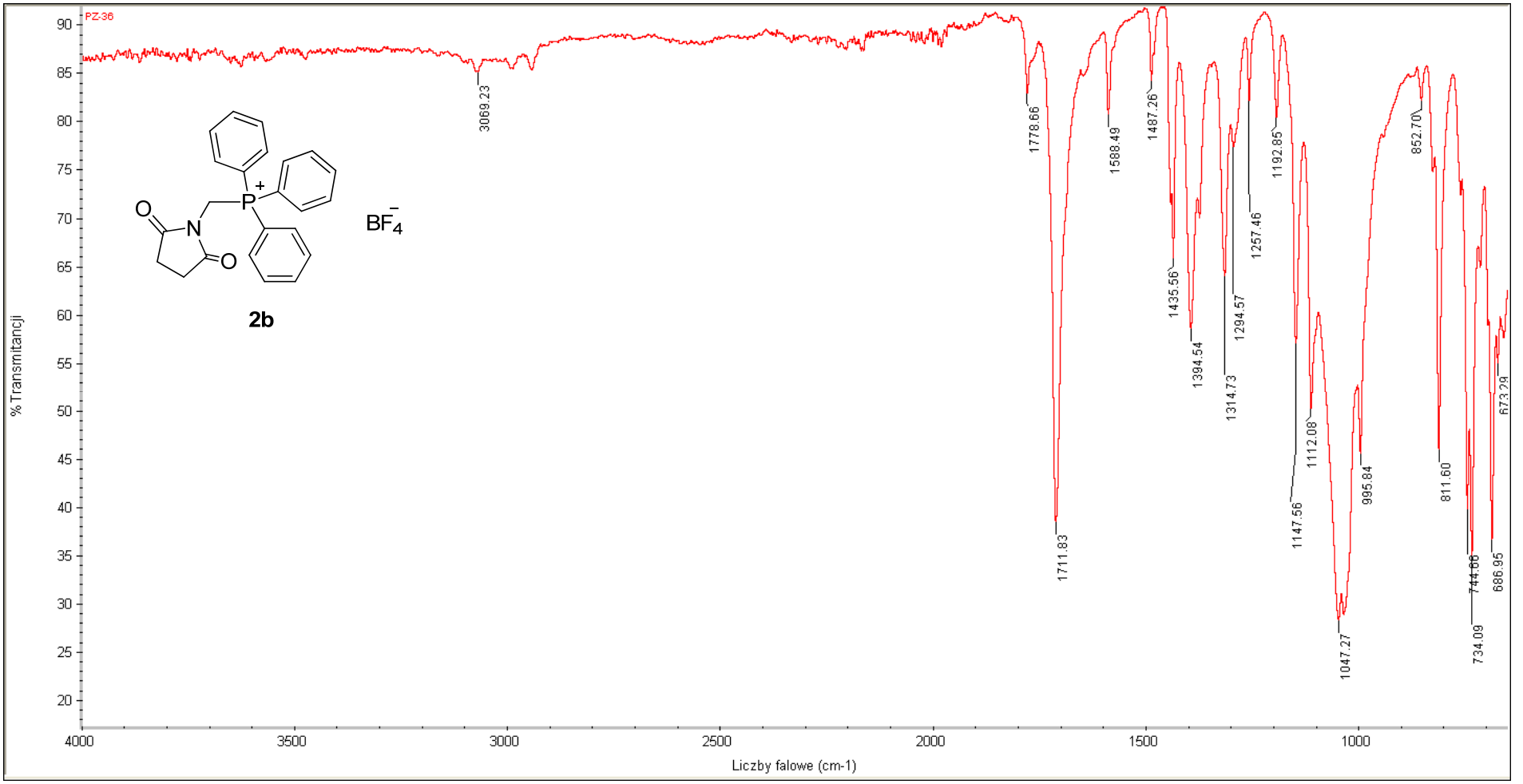
^{1}H NMR spectrum of *N*-hydroxymethyl-2-pyrrolidone (**9g**); 400 MHz/$CDCl_3$; δ (ppm).



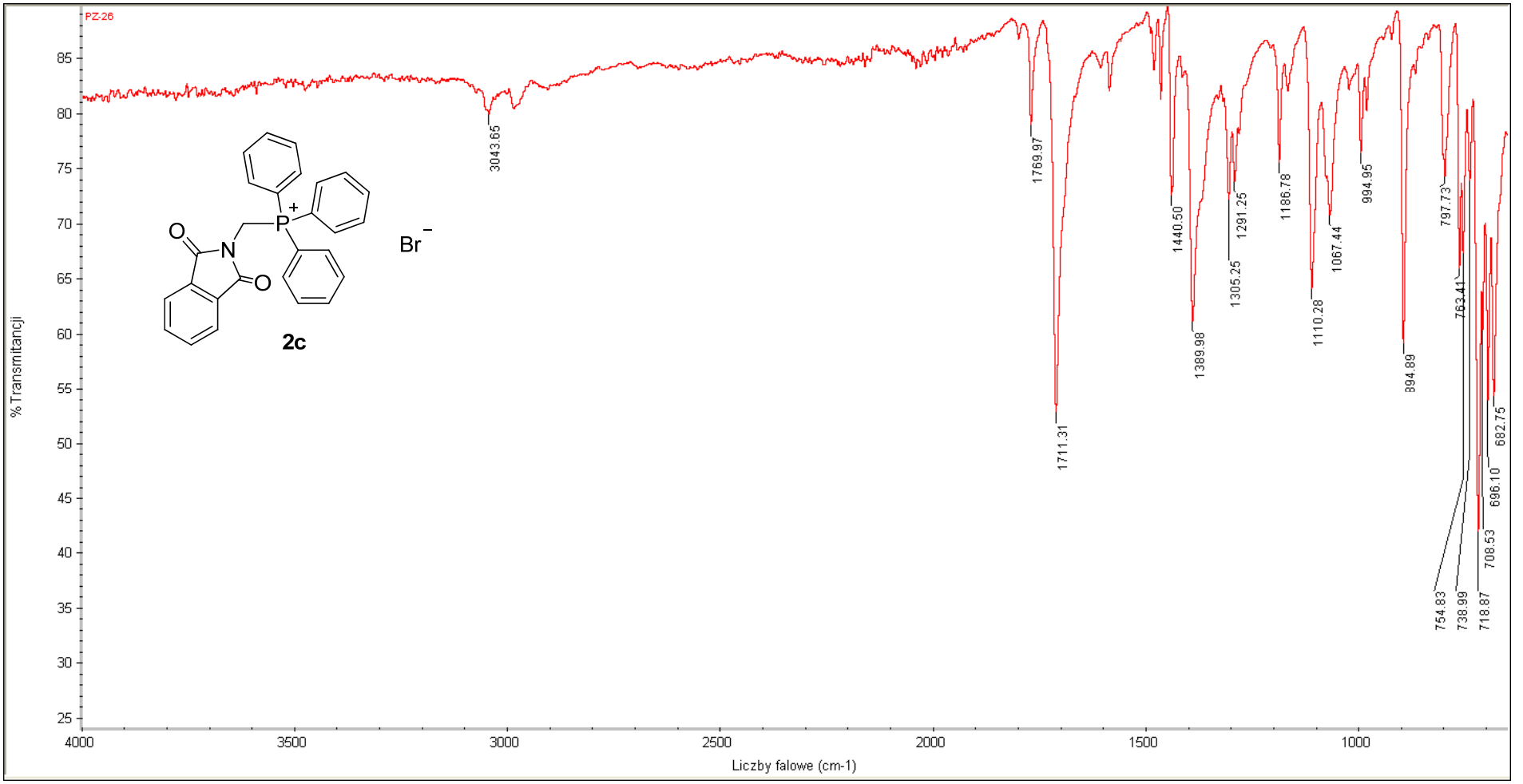
$^{13}C\{^{1}H\}$ NMR spectrum of *N*-hydroxymethyl-2-pyrrolidone (**9g**); 100 MHz/$CDCl_3$; δ (ppm).



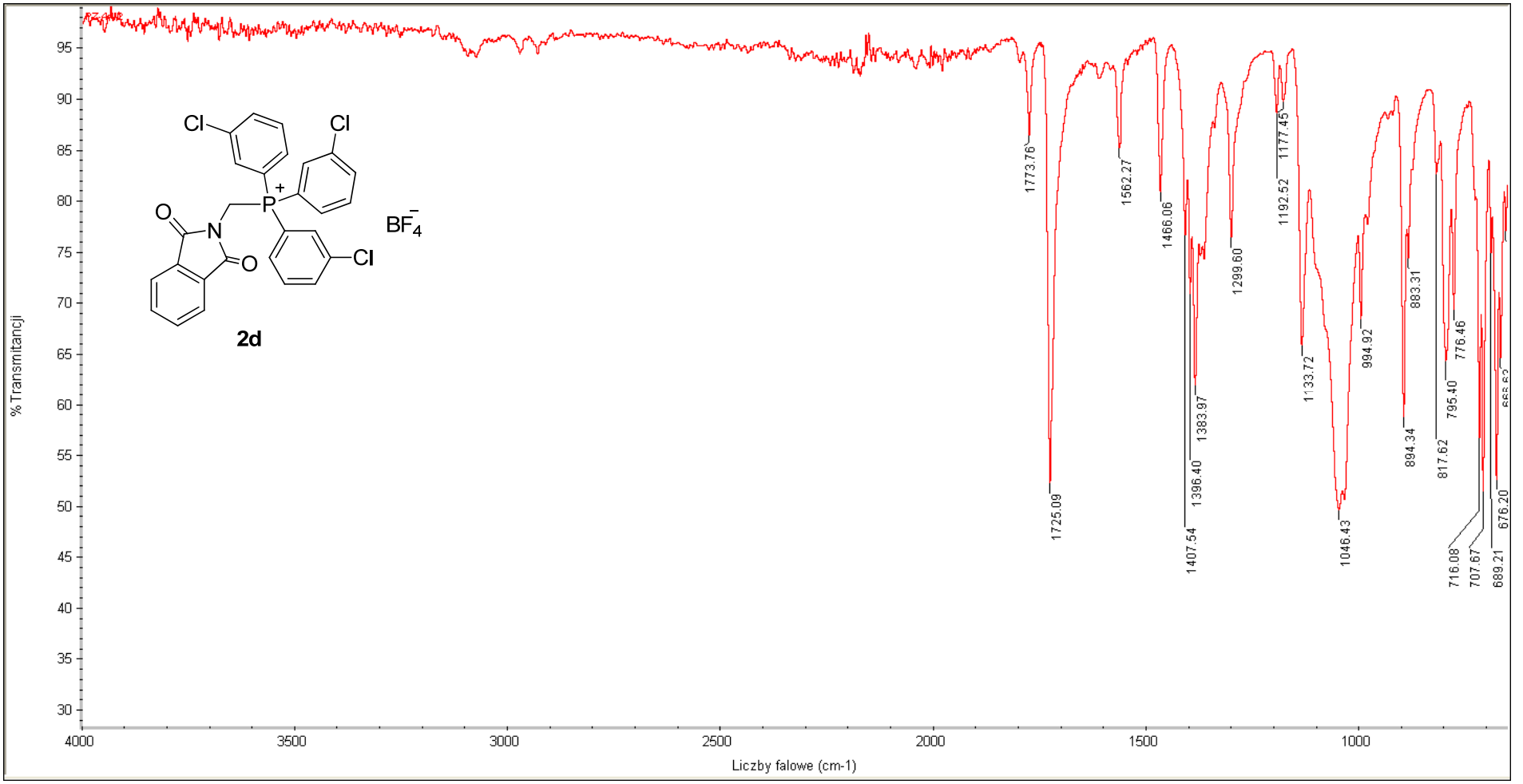
IR spectrum of 1-(*N*-phthalimido)methyltriphenylphosphonium tetrafluoroborate (**2a**); ATR (cm^{-1}).



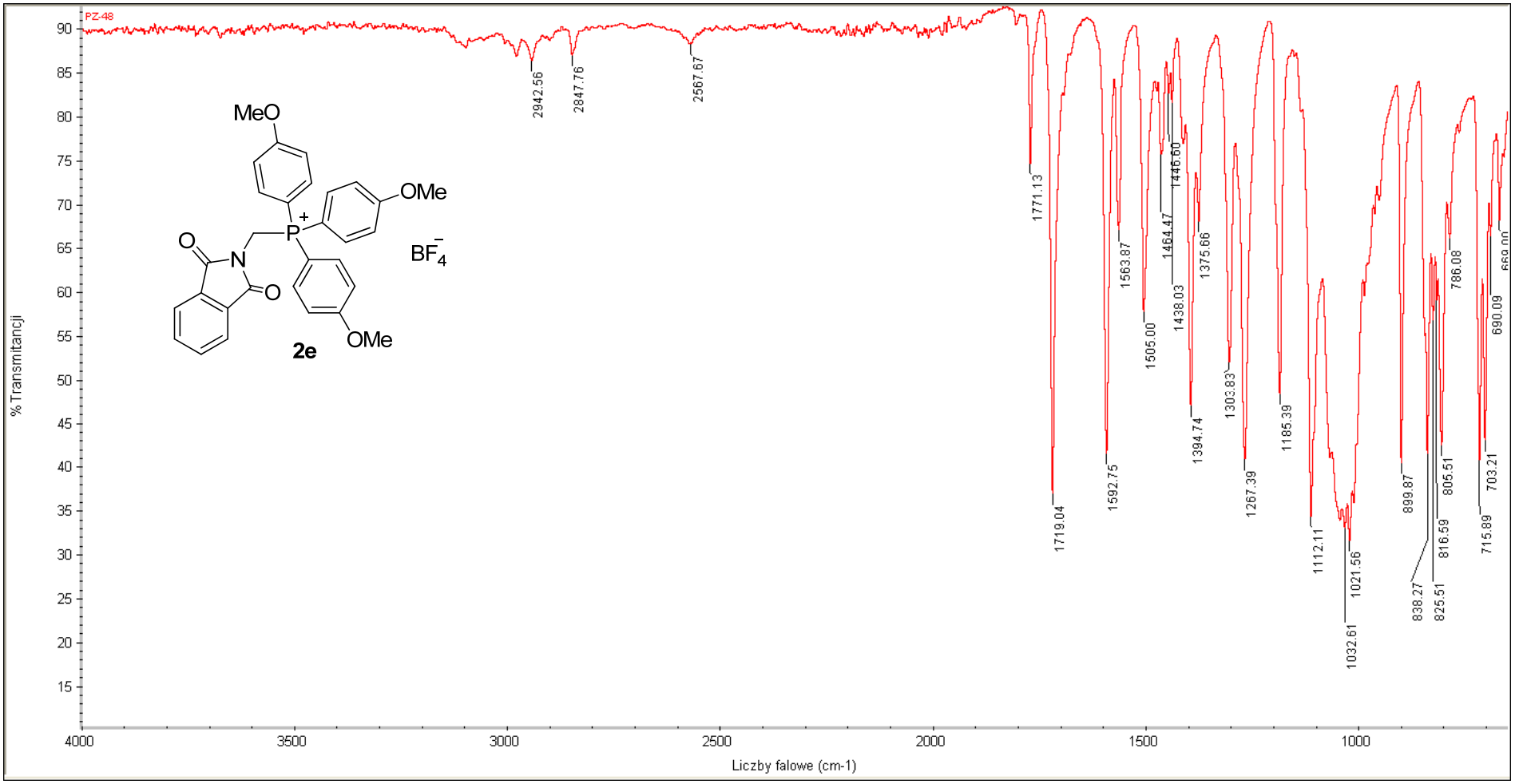
IR spectrum of 1-(*N*-succinimido)methyltriphenylphosphonium tetrafluoroborate (**2b**); ATR (cm^{-1}).



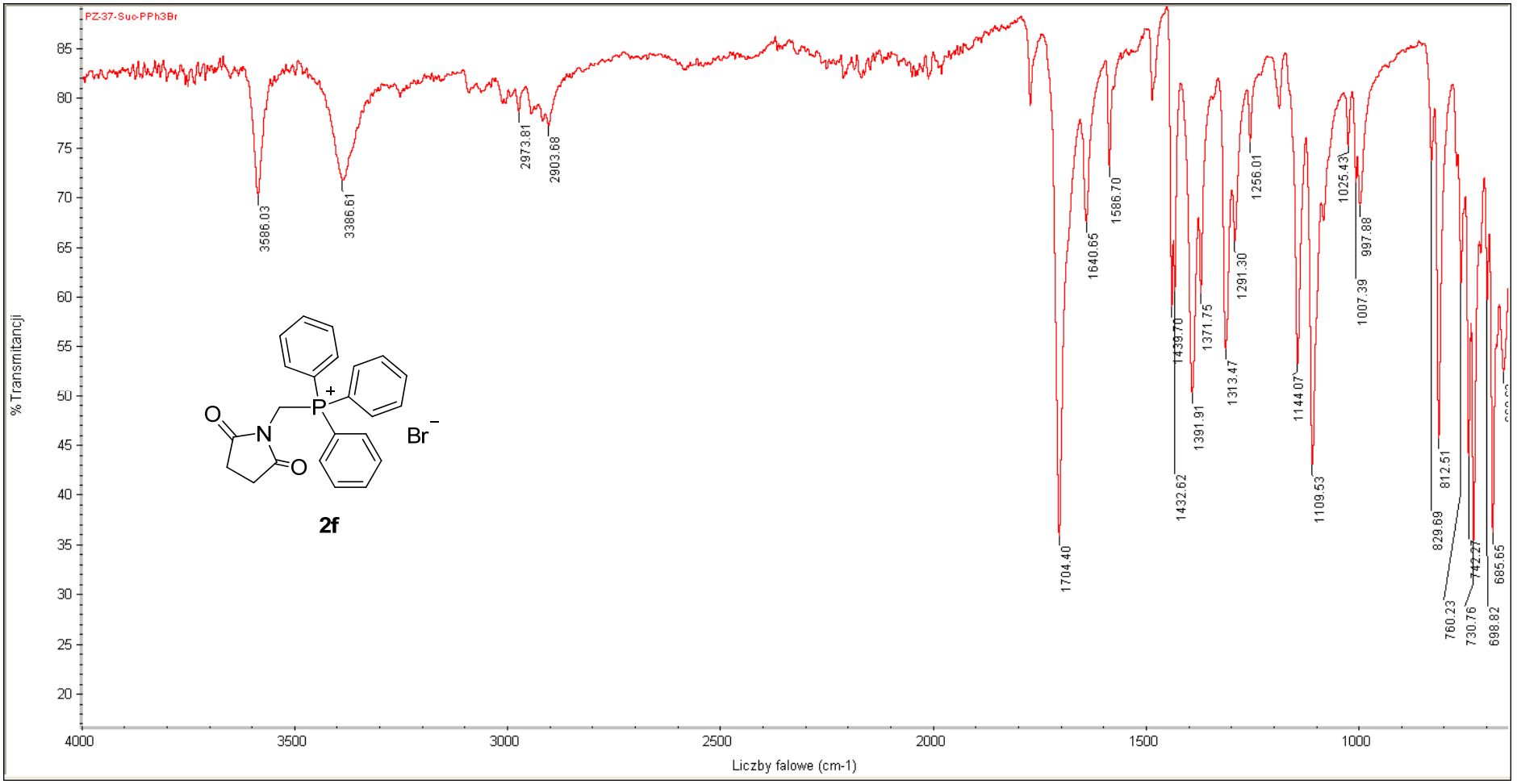
IR spectrum of 1-(*N*-phthalimido)methyltriphenylphosphonium bromide (**2c**); ATR (cm^{-1}).



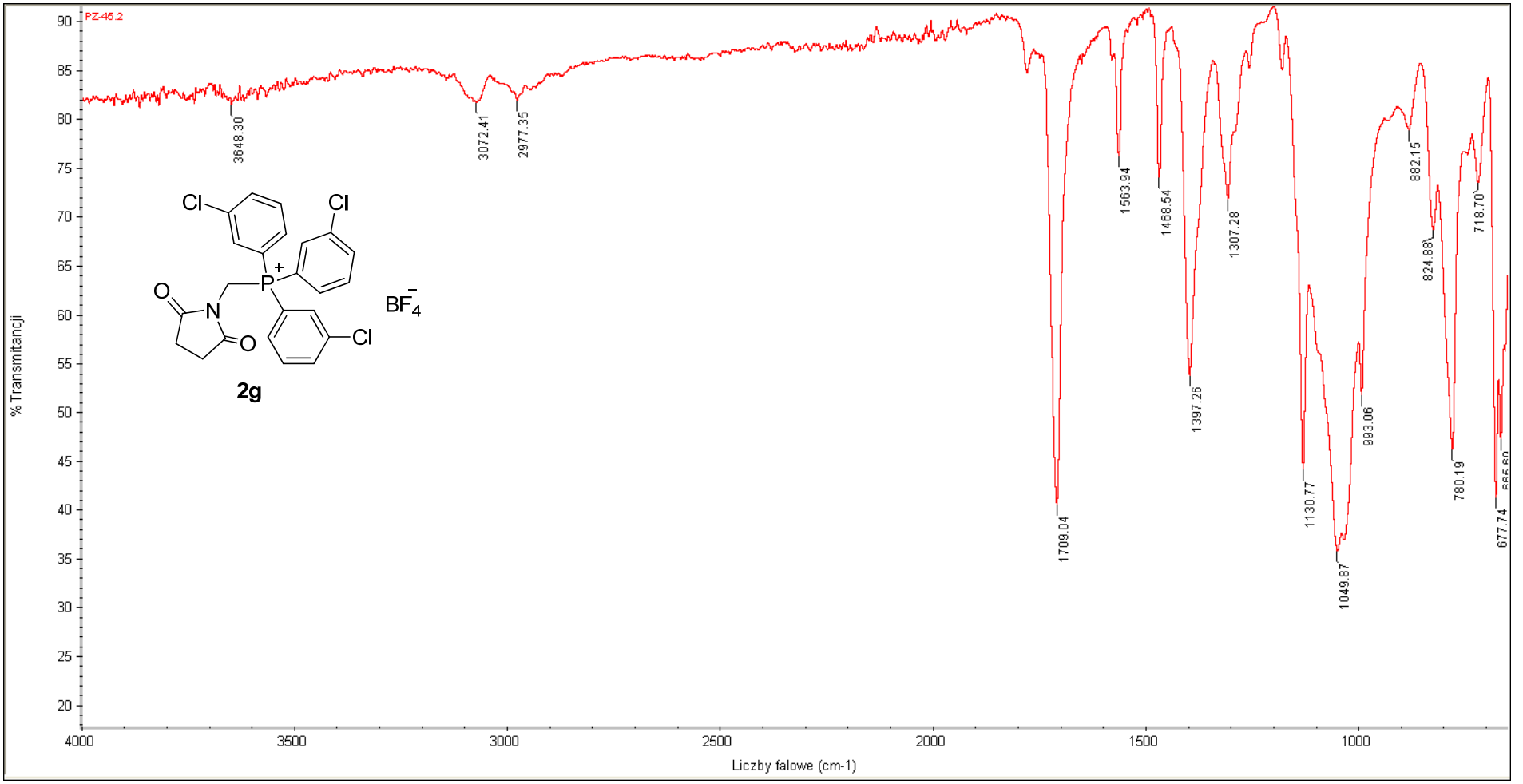
IR spectrum of 1-(*N*-phthalimido)methyltris(3-chlorophenyl)phosphonium tetrafluoroborate (**2d**); ATR (cm^{-1}).



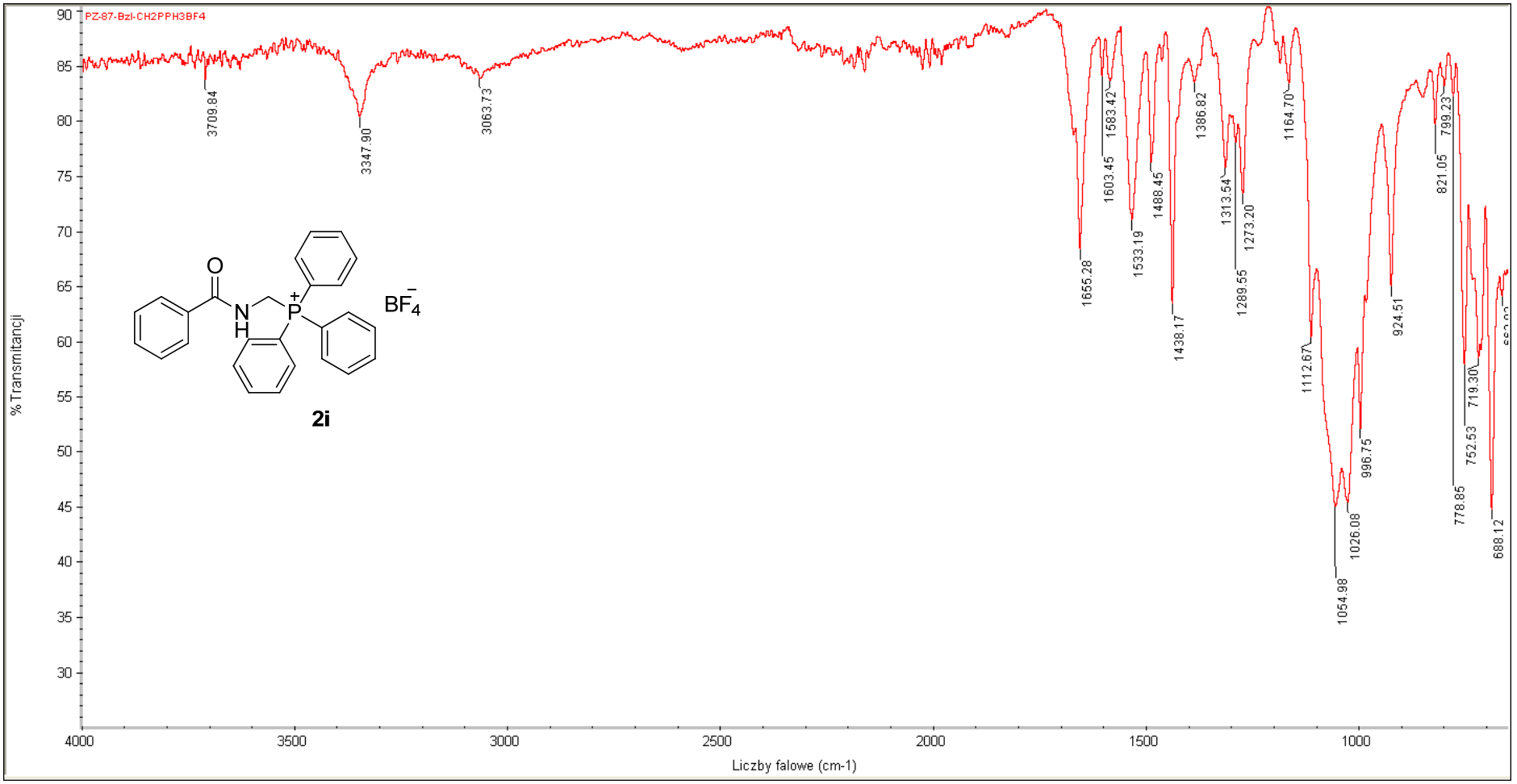
IR spectrum of 1-(*N*-phthalimido)methyltris(4-methoxyphenyl)phosphonium tetrafluoroborate (**2e**); ATR (cm^{-1}).



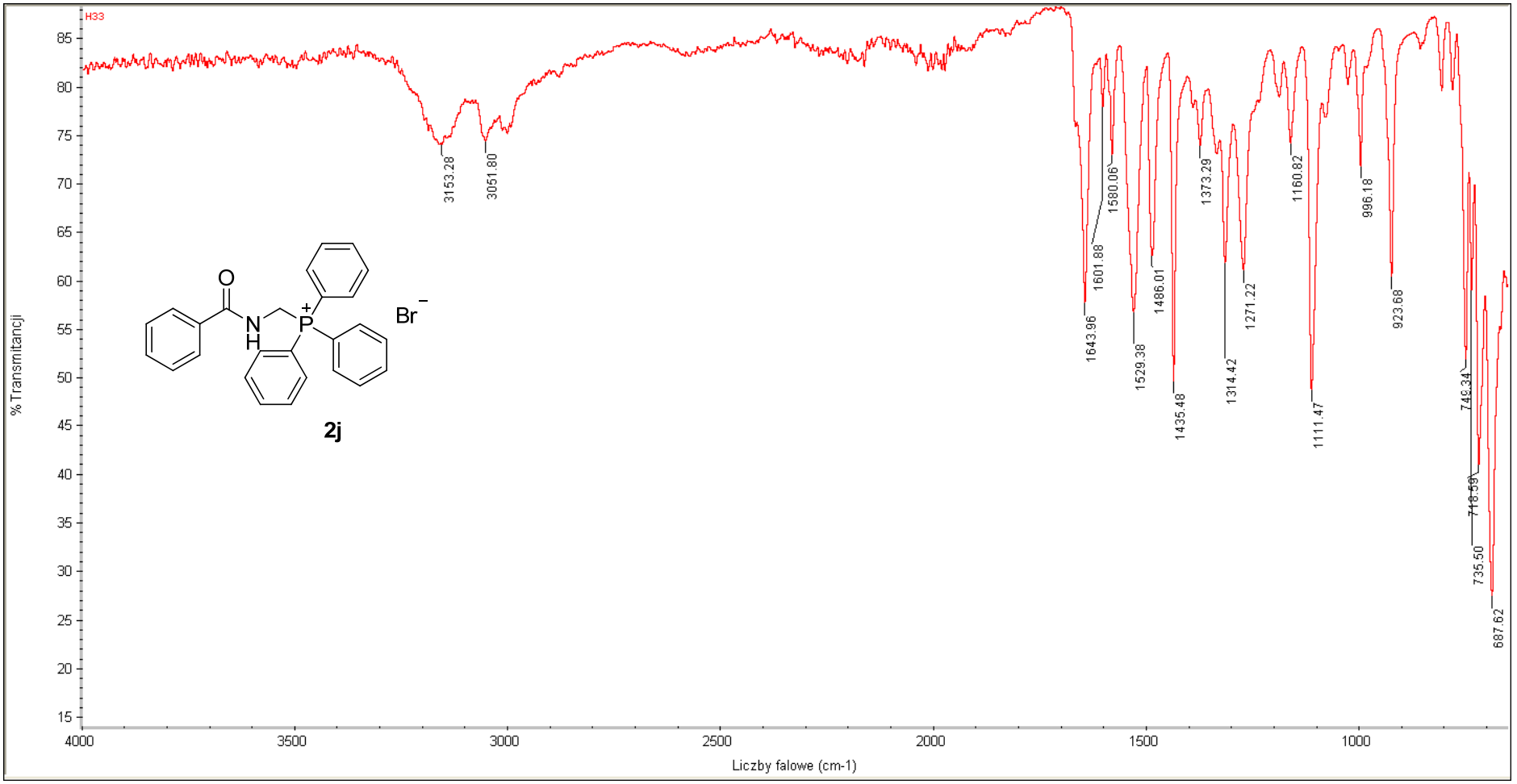
IR spectrum of 1-(*N*-succinimido)methyltriphenylphosphonium bromide (**2f**); ATR (cm^{-1}).



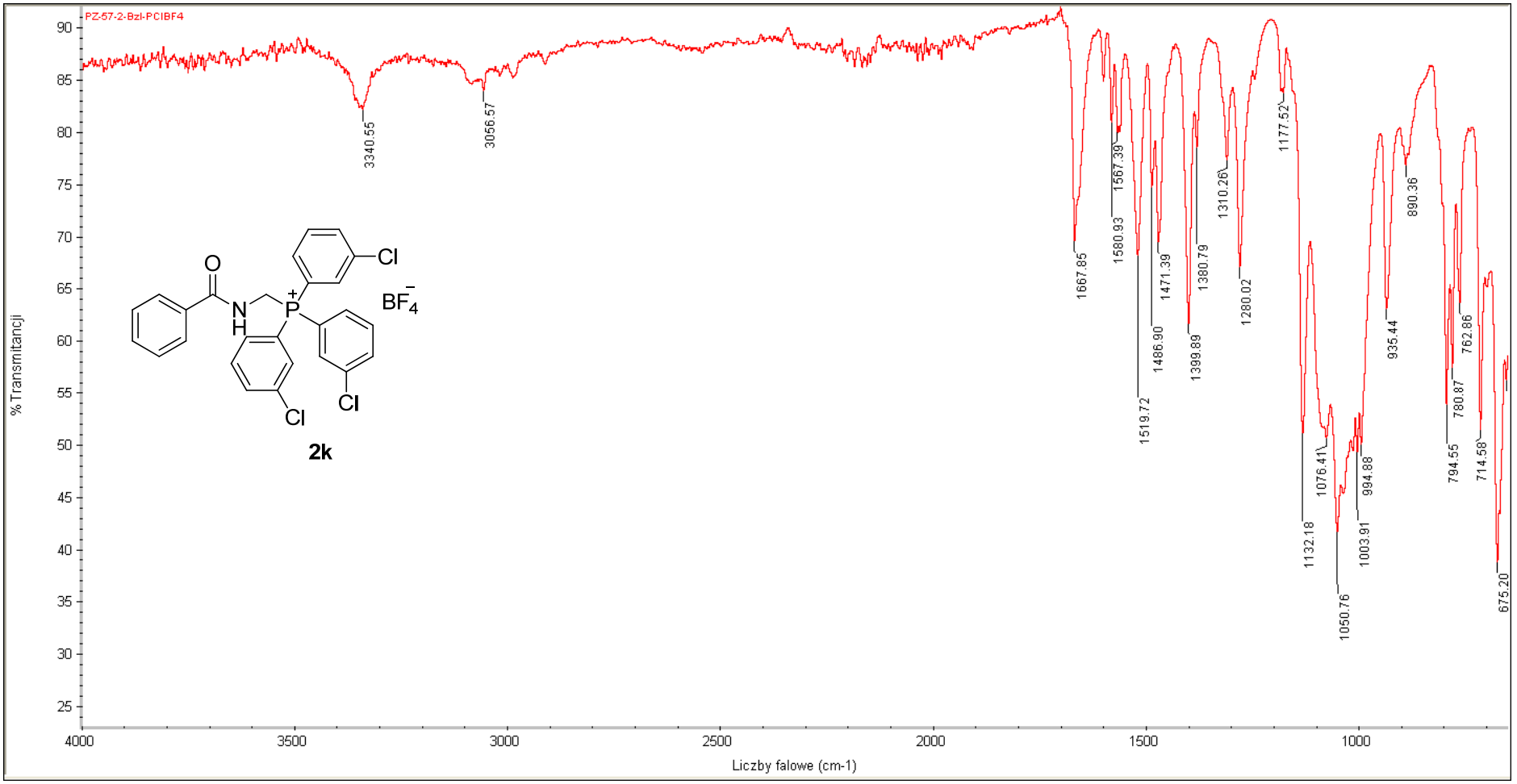
IR spectrum of 1-(*N*-succinimido)methyltris(3-chlorophenyl)phosphonium tetrafluoroborate (**2g**); ATR (cm^{-1}).



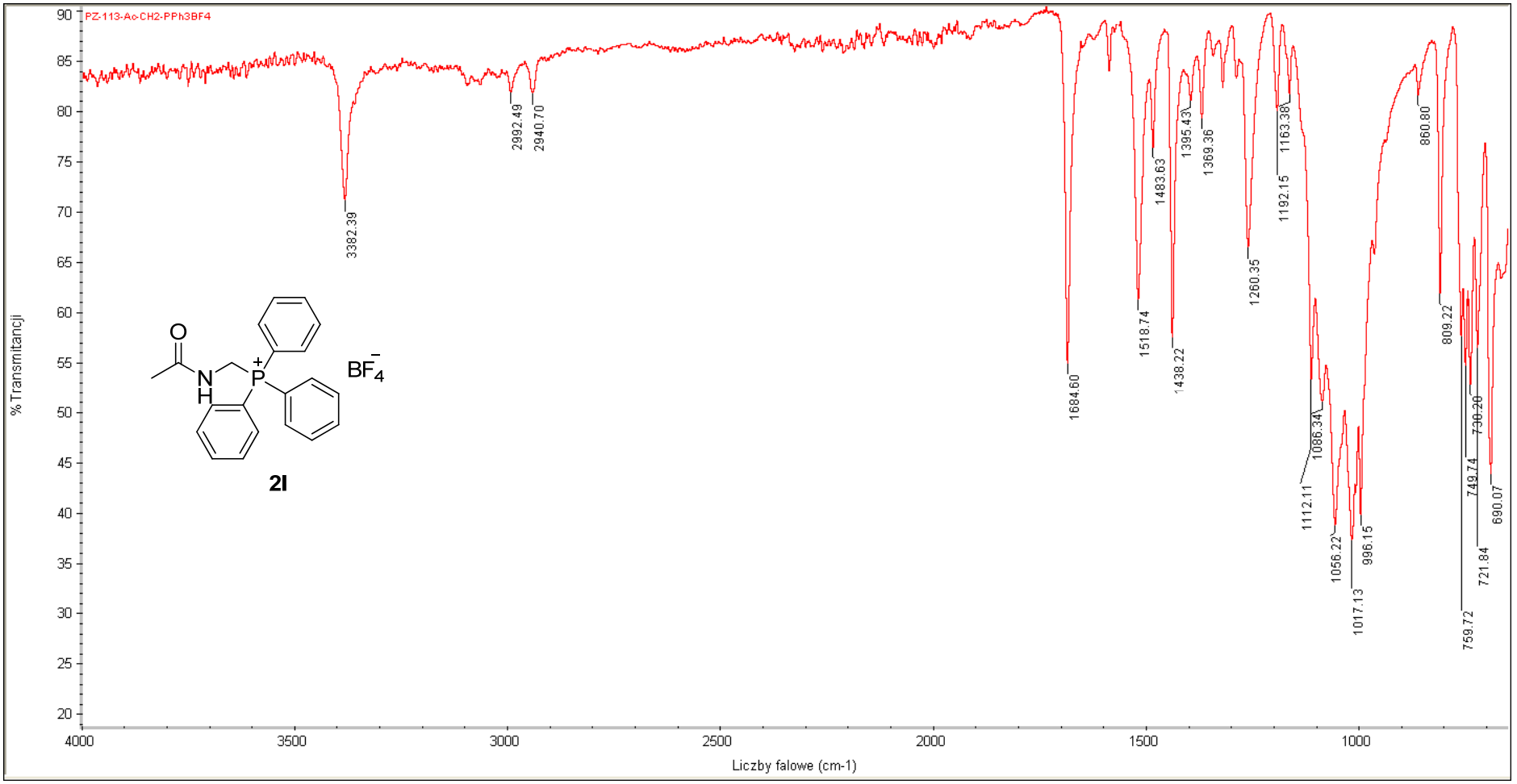
IR spectrum of (*N*-benzoylamino)methyltriphenylphosphonium tetrafluoroborate (**2i**); ATR (cm^{-1}).



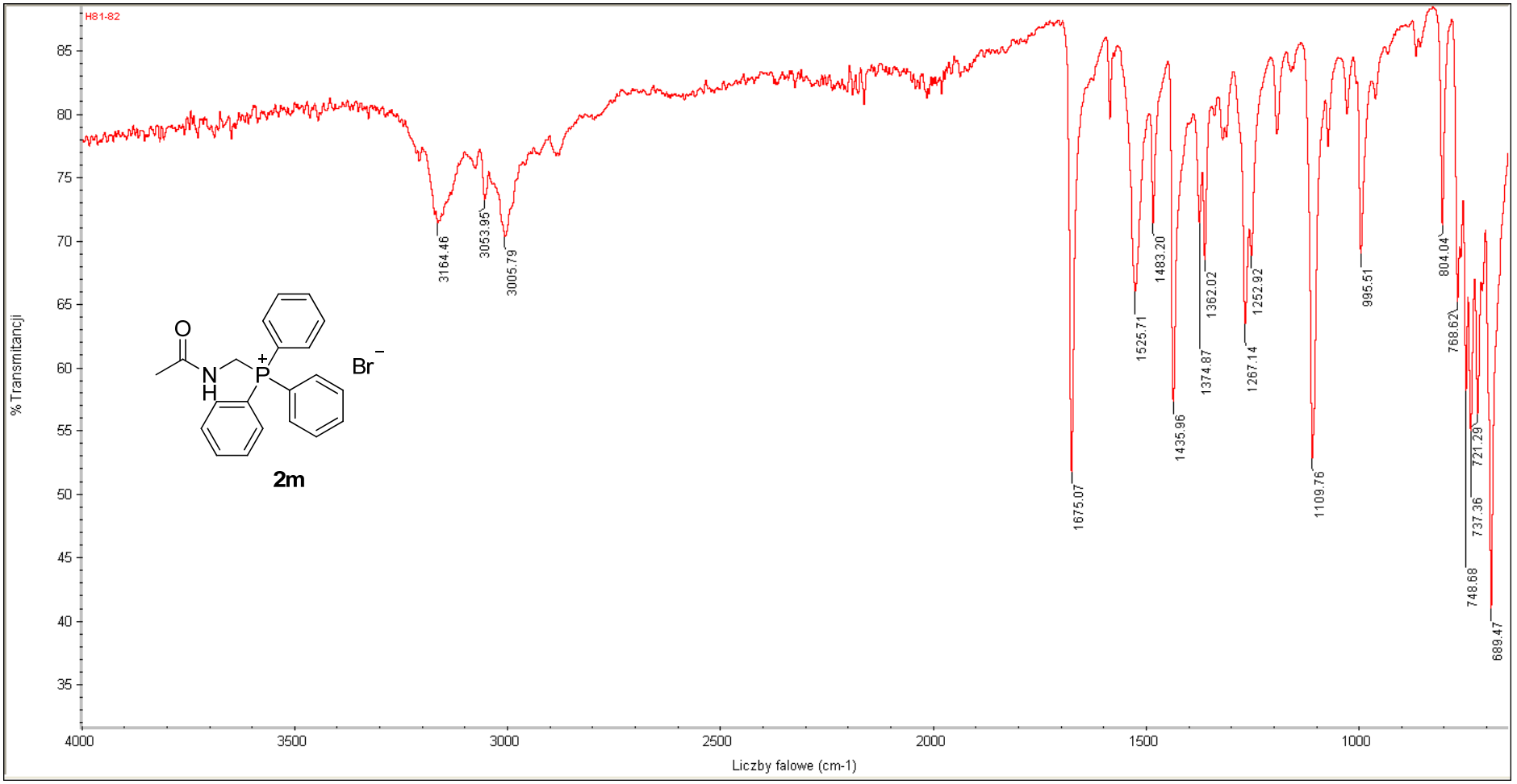
IR spectrum of (*N*-benzoylamino)methyltriphenylphosphonium bromide (**2j**); ATR (cm^{-1}).



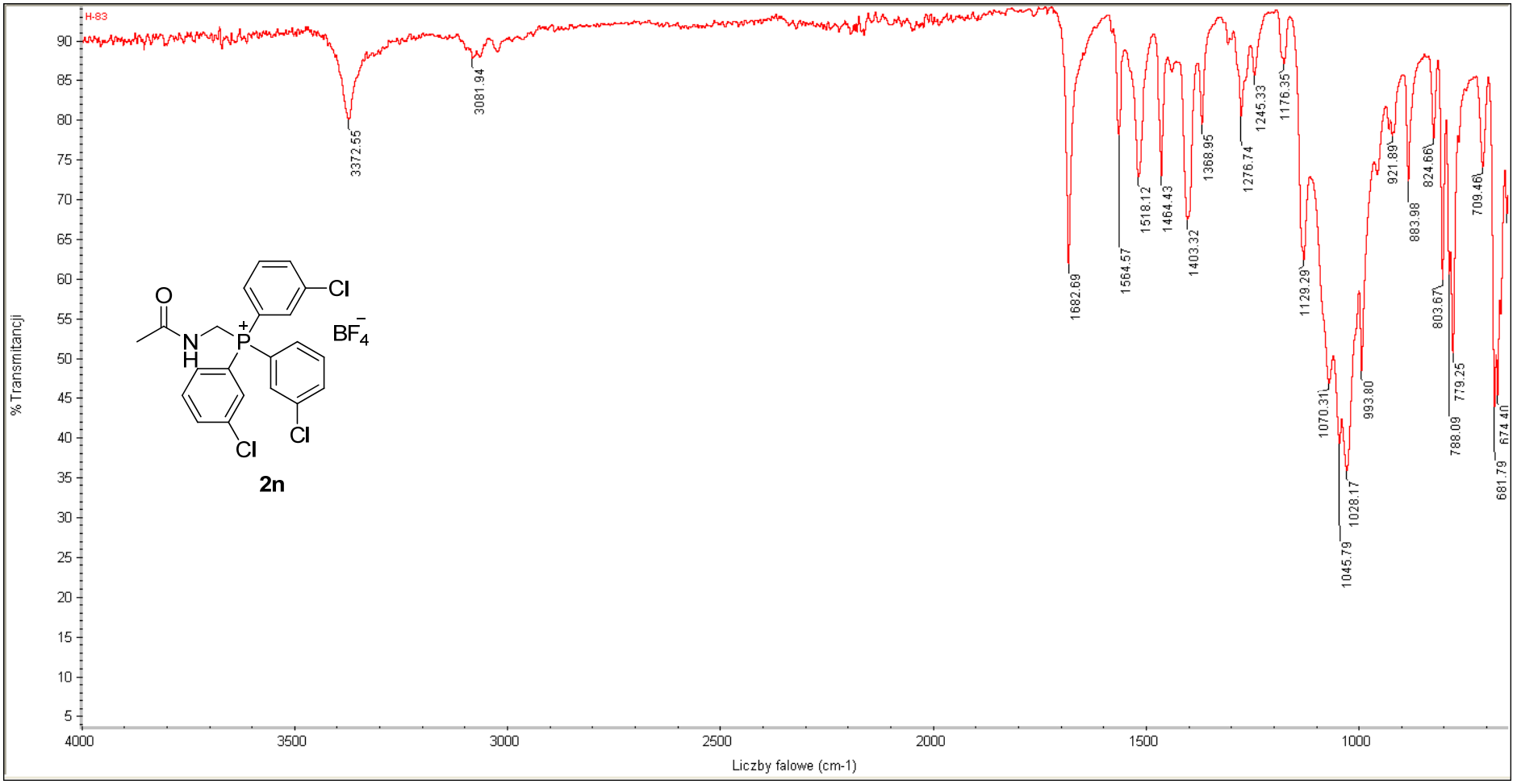
IR spectrum of (*N*-benzoylamino)methyltris(3-chlorophenyl)phosphonium tetrafluoroborate (**2k**); ATR (cm^{-1}).



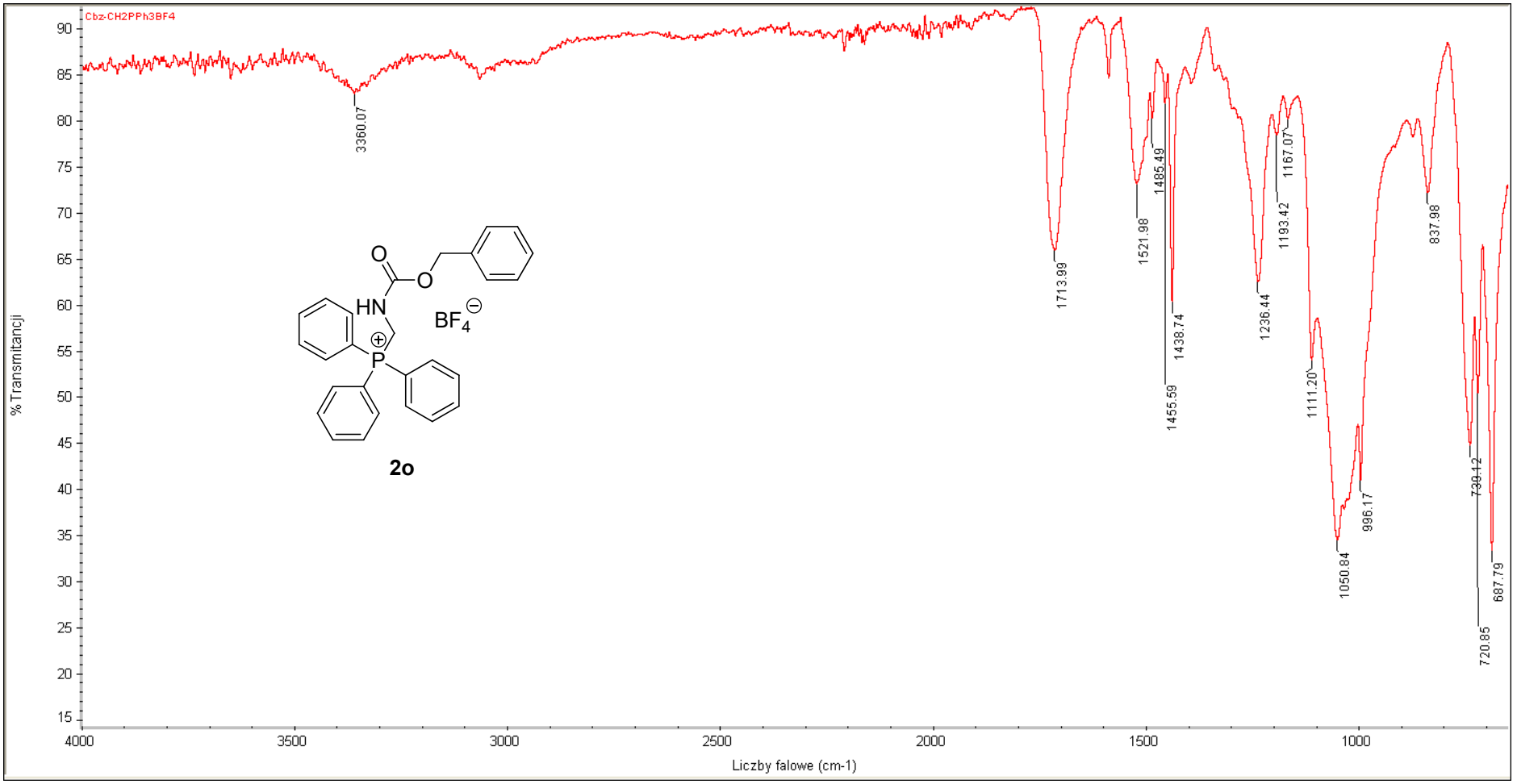
IR spectrum of (*N*-acetylamino)methyltriphenylphosphonium tetrafluoroborate (**2l**); ATR (cm^{-1}).



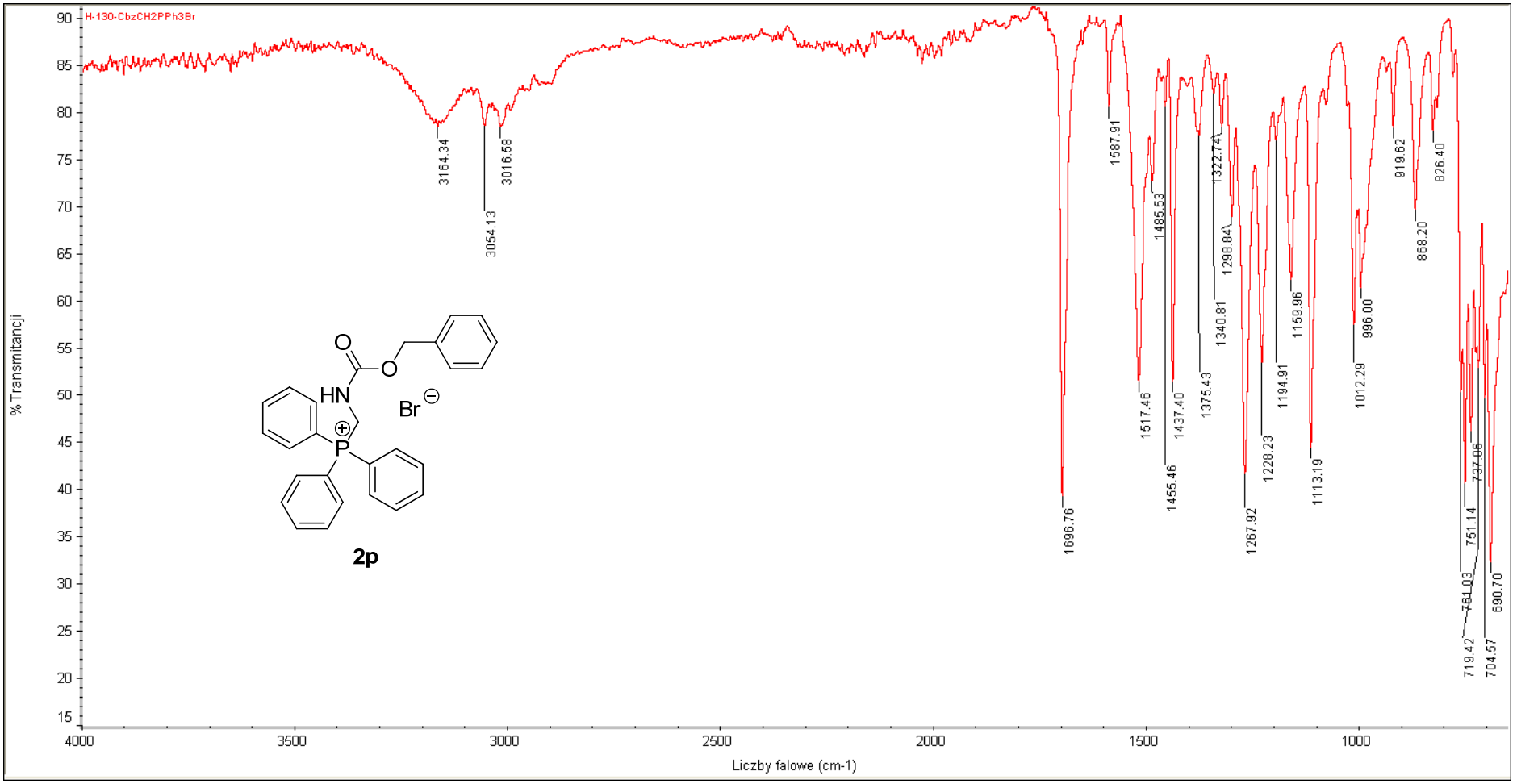
IR spectrum of (*N*-acetylamino)methyltriphenylphosphonium bromide (**2m**); ATR (cm^{-1}).



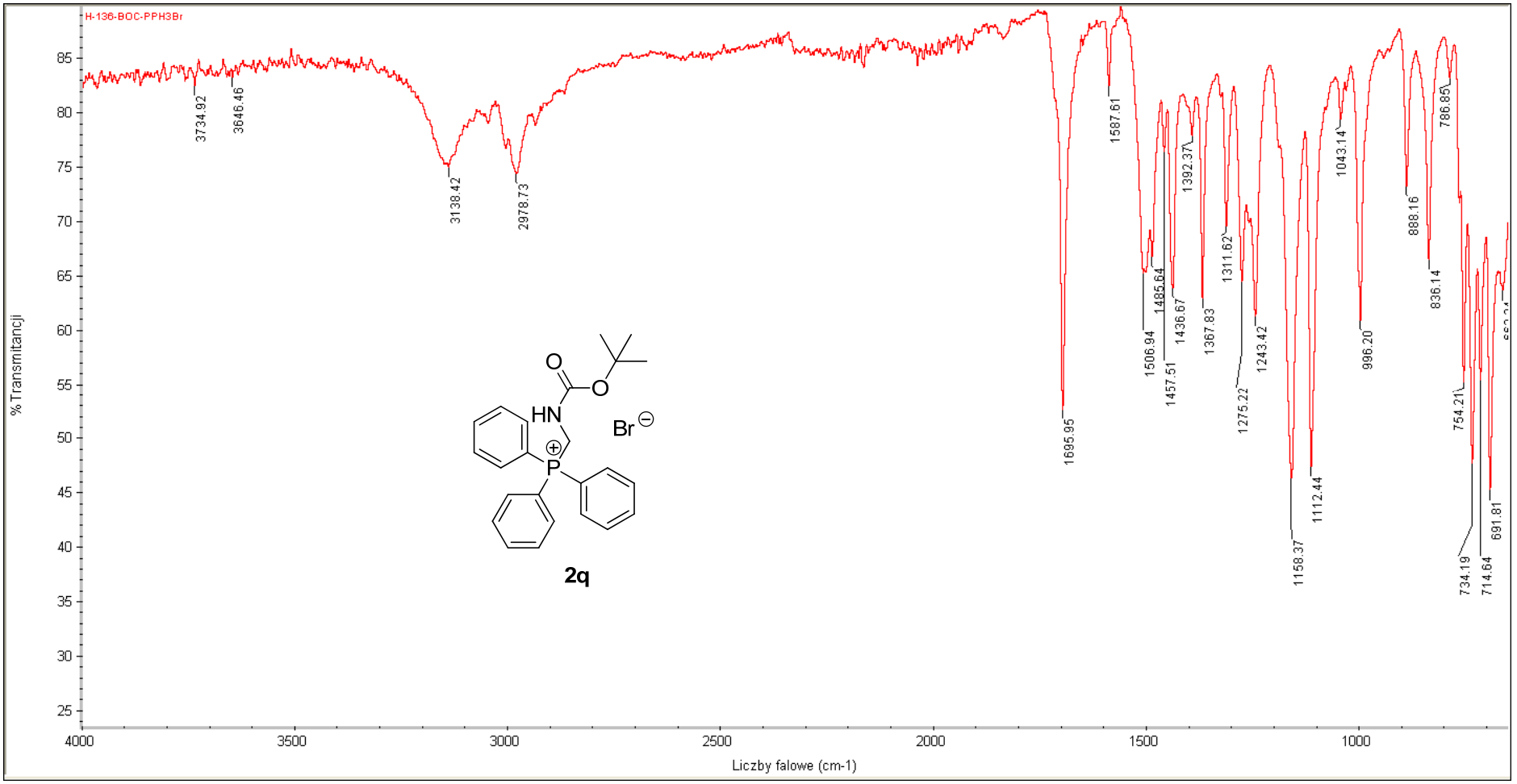
IR spectrum of (*N*-acetylamino)methyltris(3-chlorophenyl)phosphonium tetrafluoroborate (**2n**); ATR (cm^{-1}).



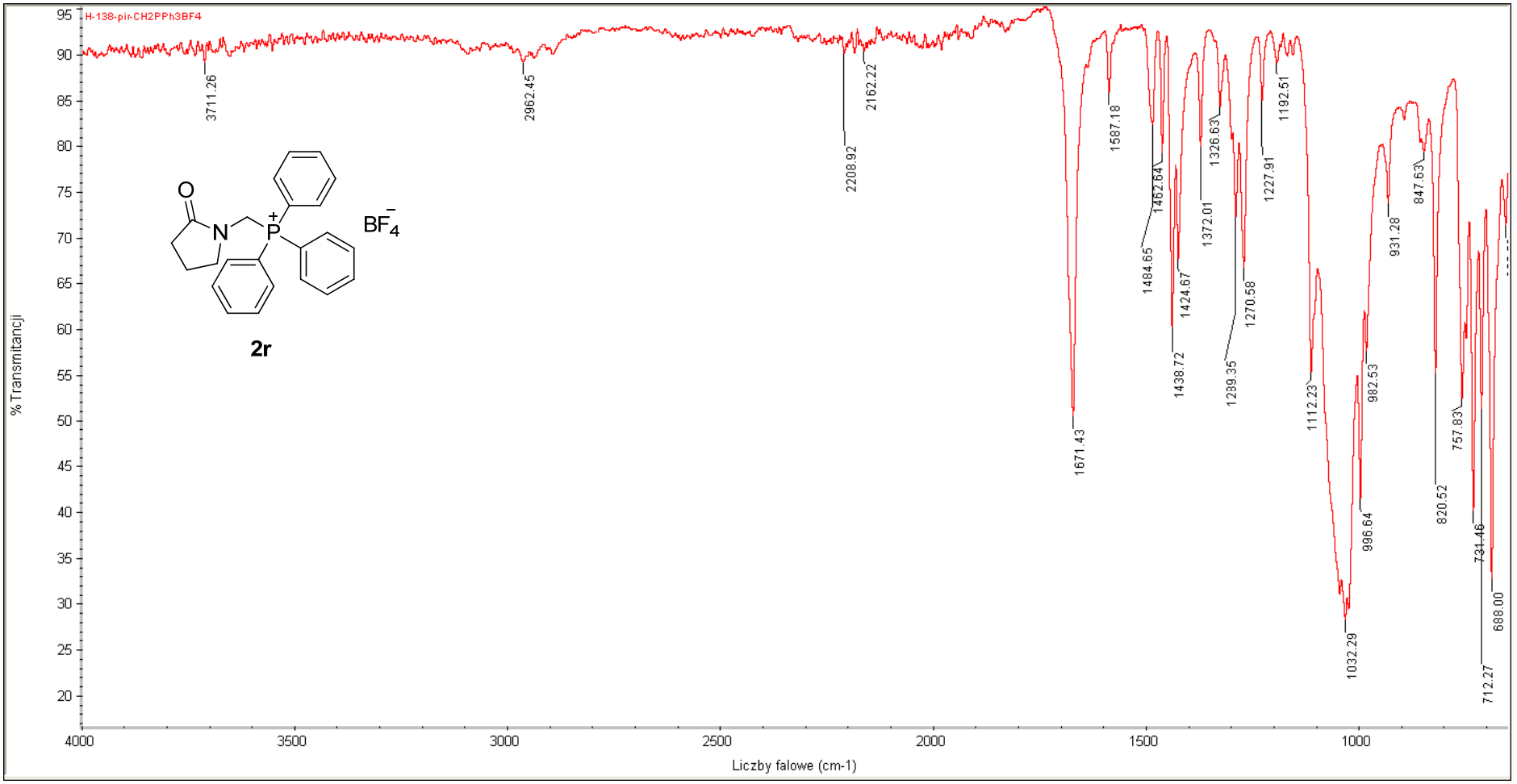
IR spectrum of (*N*-benzyloxycarbonylamino)methyltriphenylphosphonium tetrafluoroborate (**2o**); ATR (cm^{-1}).



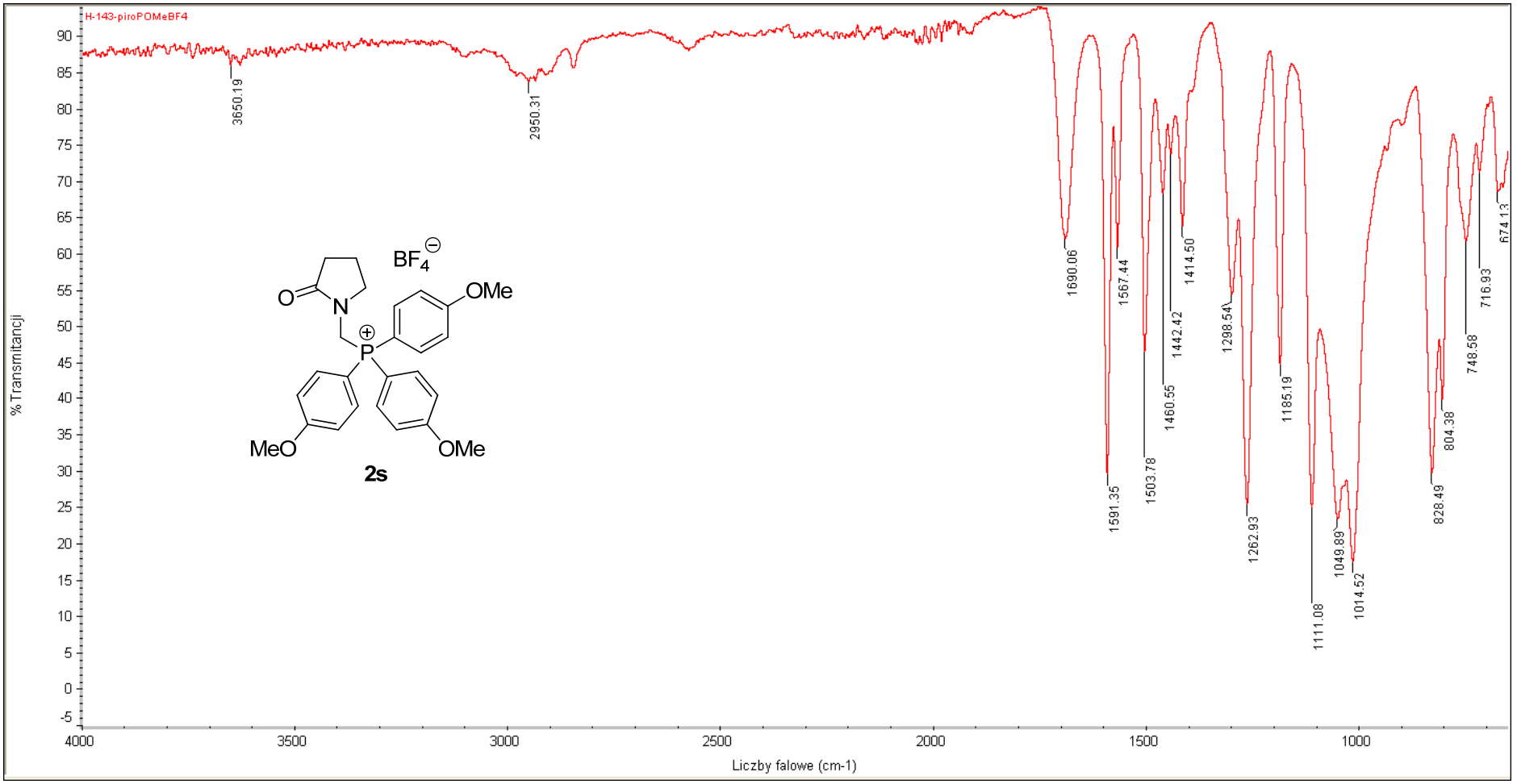
IR spectrum of (*N*-benzyloxycarbonylamino)methyltriphenylphosphonium bromide (**2p**); ATR (cm^{-1}).



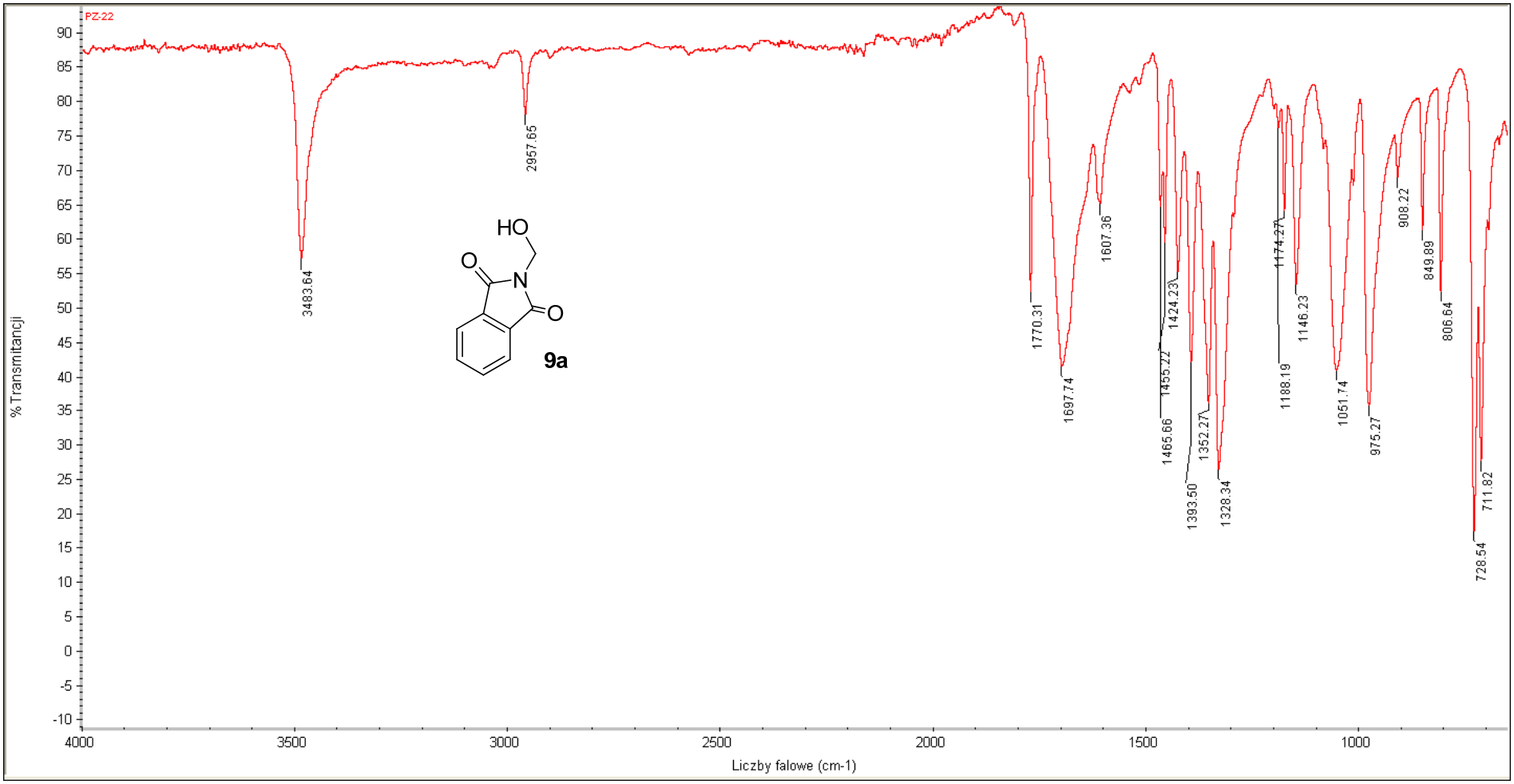
IR spectrum of (*N-tert*-butoxycarbonylamino)methylphosphonium bromide (**2q**); ATR (cm^{-1}).



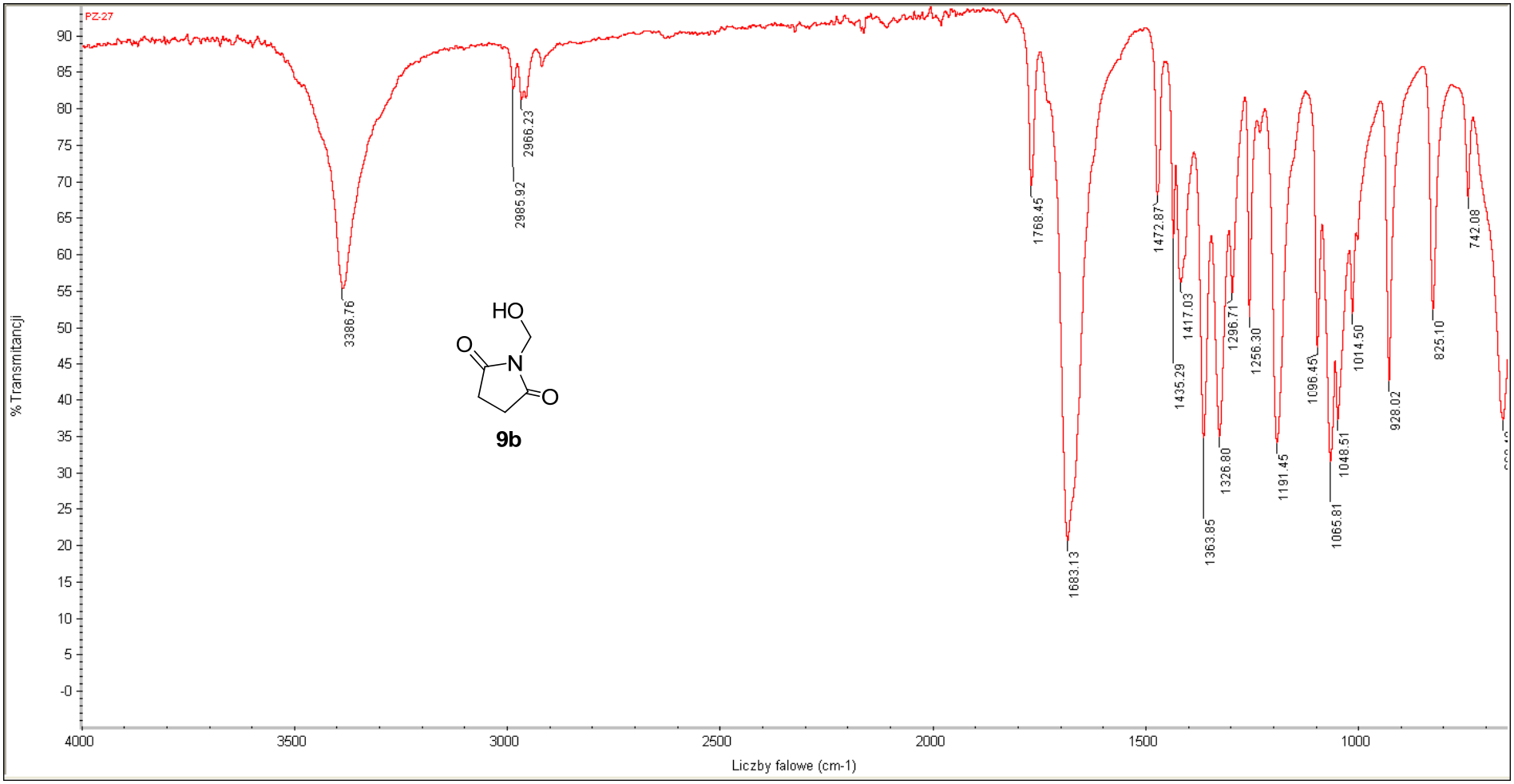
IR spectrum of 1-(2-oxopyrrolidin-1-yl)methyltriphenylphosphonium tetrafluoroborate (**2r**); ATR (cm^{-1}).



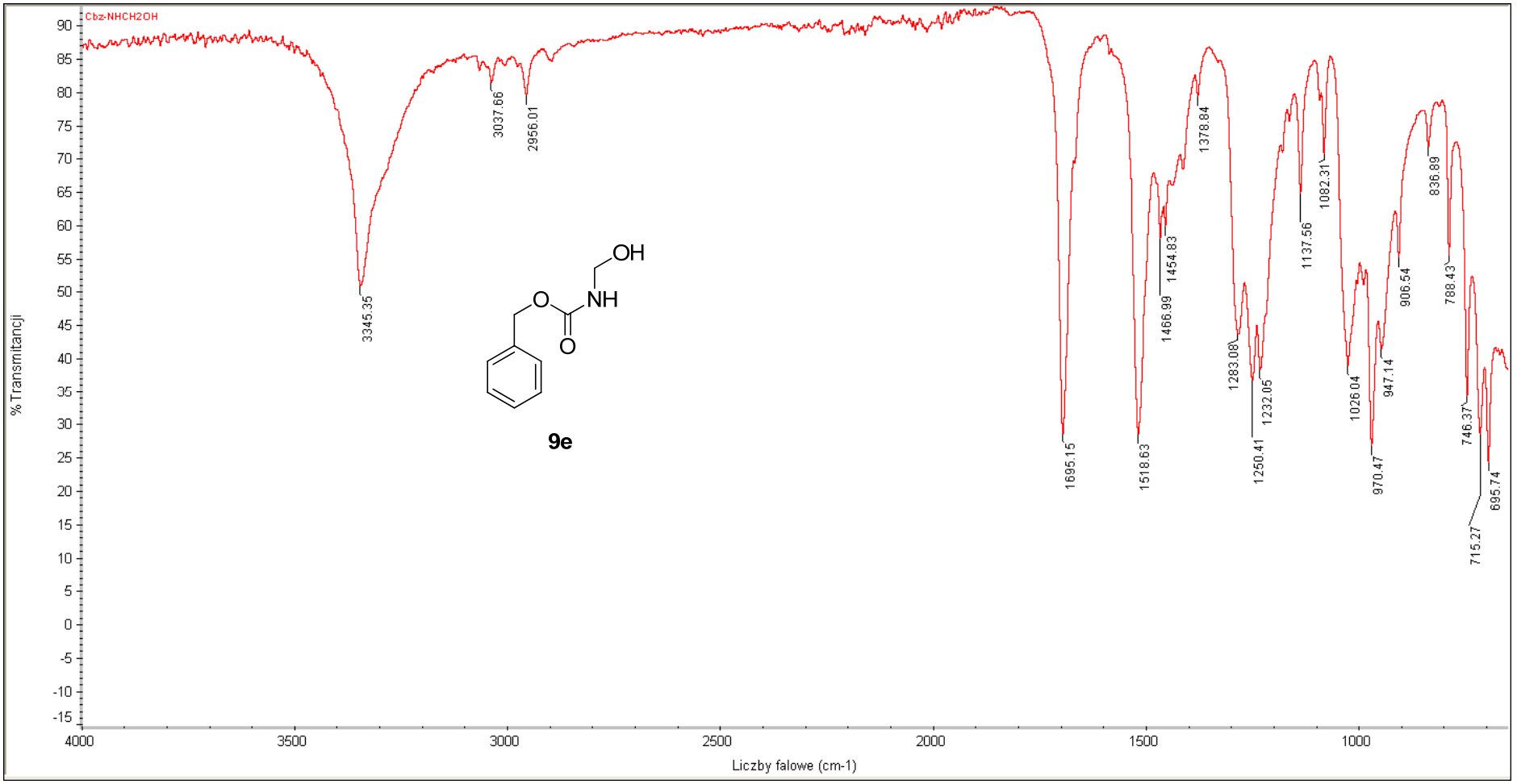
IR spectrum of (2-oxopyrrolidin-1-yl)methyltris(4-methoxyphenyl)phosphonium tetrafluoroborate (**2s**); ATR (cm^{-1}).



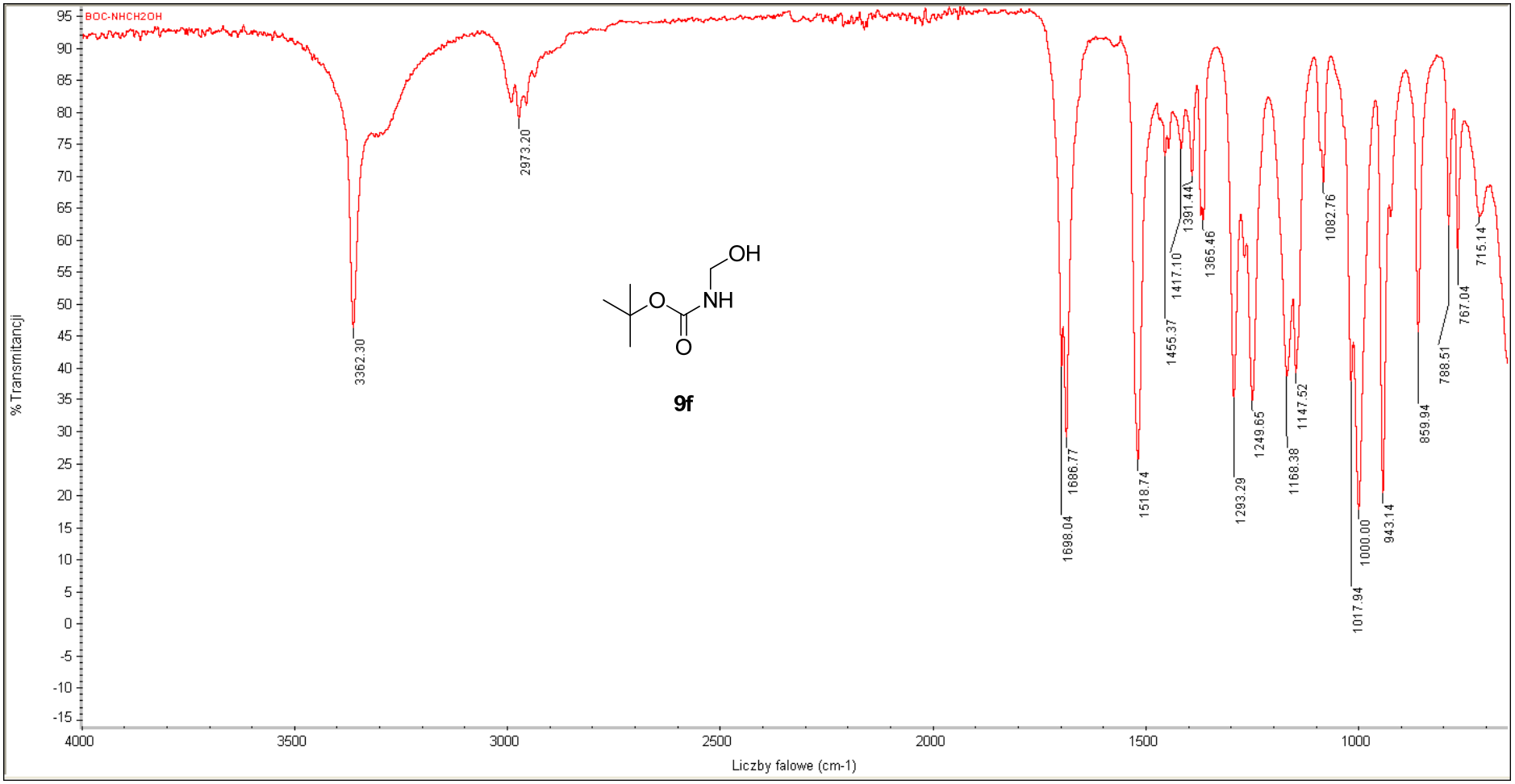
IR spectrum of *N*-hydroxymethylphthalimide (**9a**); ATR (cm^{-1}).



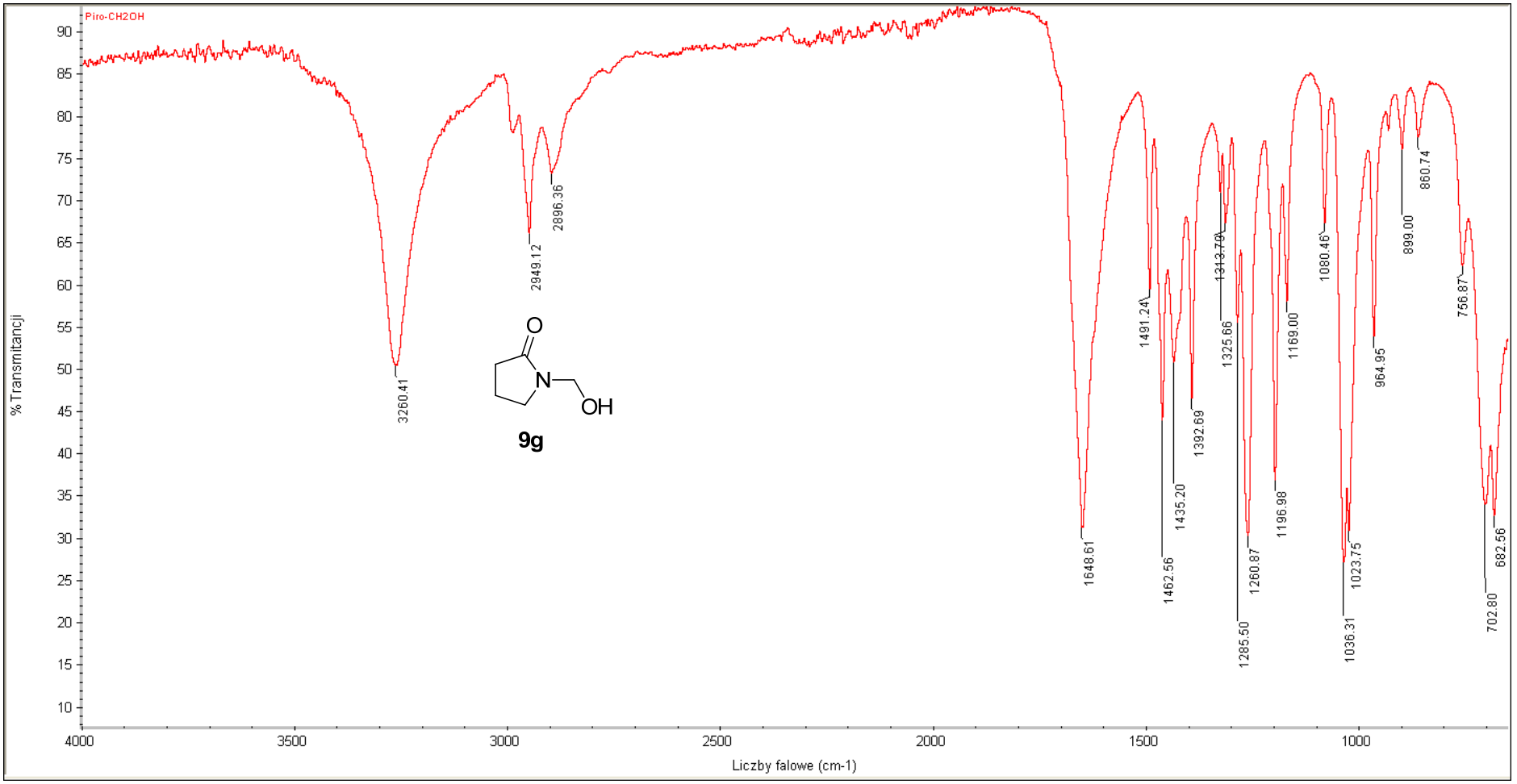
IR spectrum of *N*-hydroxymethylsuccinimide (**9b**); ATR (cm^{-1}).



IR spectrum of benzyl *N*-hydroxymethylcarbamate (**9e**); ATR (cm^{-1}).



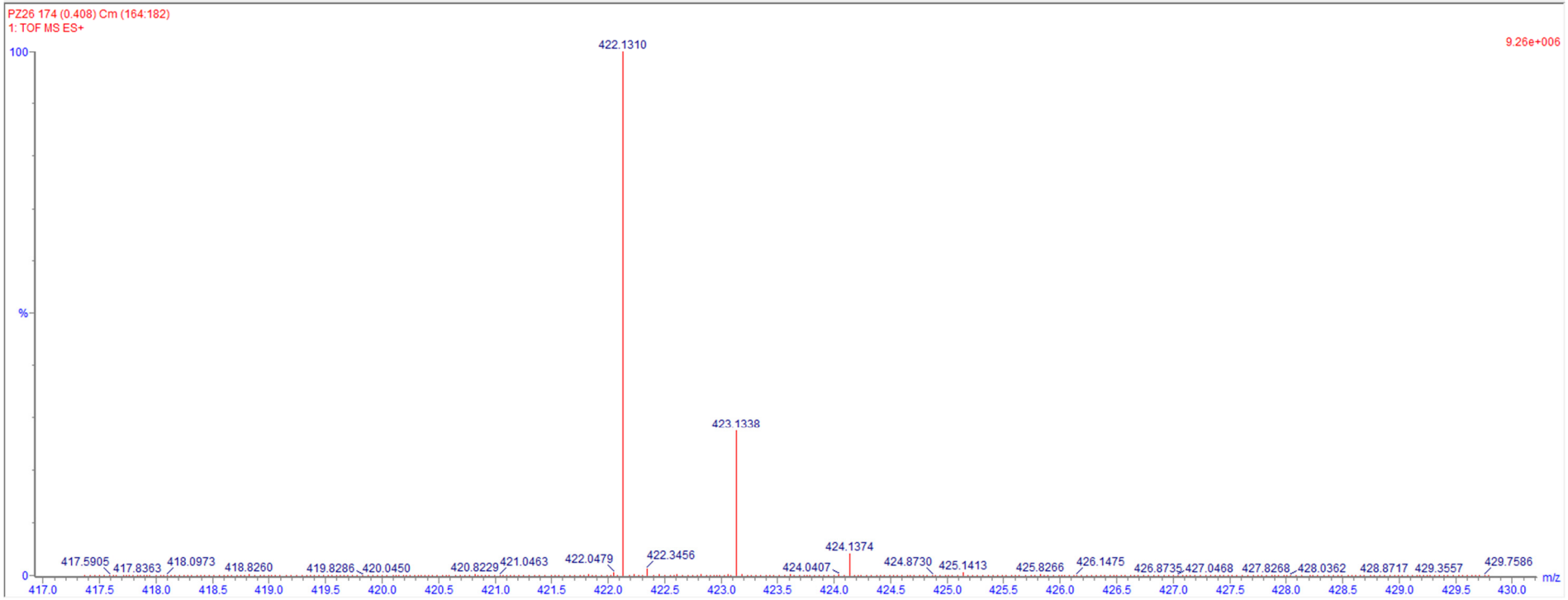
IR spectrum of *tert*-butyl *N*-hydroxymethylcarbamate (**9f**); ATR (cm^{-1}).



IR spectrum of *N*-hydroxymethyl-2-pyrrolidone (**9g**); ATR (cm^{-1}).

Tolerance = 50.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
2477 formula(e) evaluated with 203 results within limits (up to 3 closest results for each mass)
Elements Used:

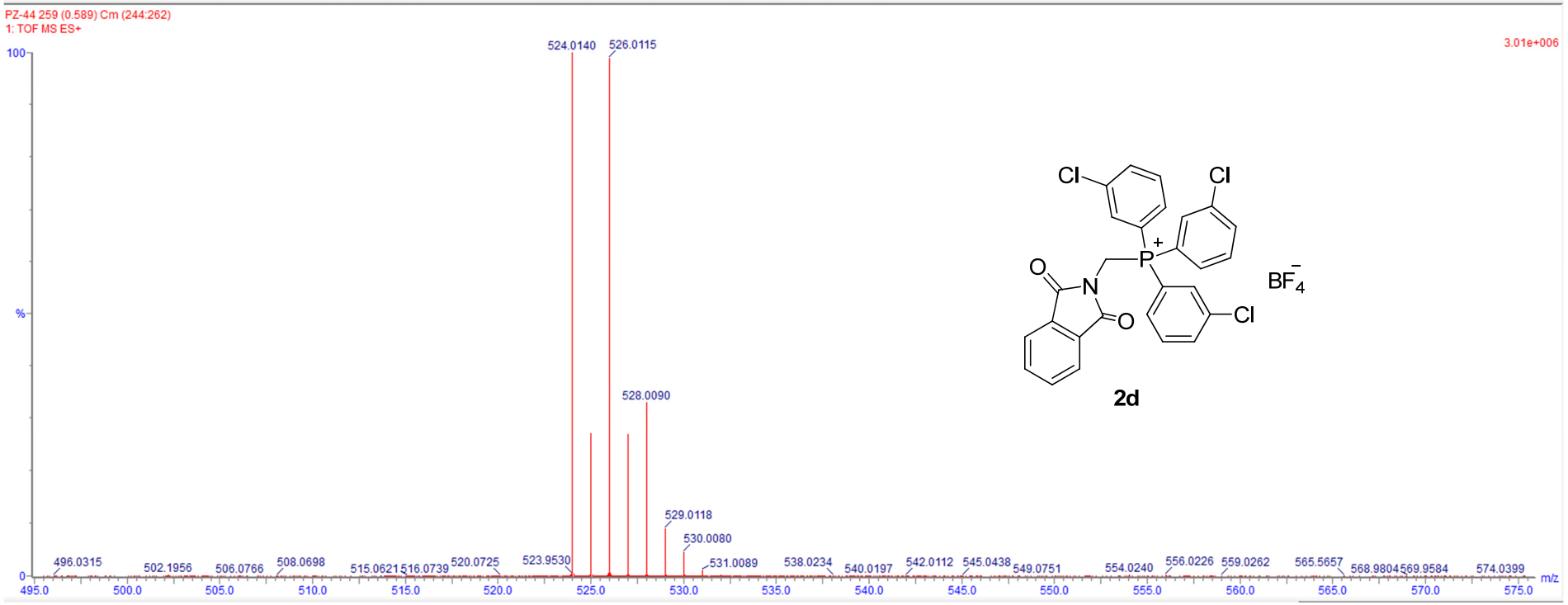
Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Na	P	S	Cl
422.1310	100.00	422.1310	0.0	0.0	18.5	C27 H21 N O2 P	550.7	0.336	71.43	27	21	1	2		1		
		422.1312	-0.2	-0.5	18.5	C28 H21 N O Cl	551.7	1.333	26.36	28	21	1	1				1
		422.1314	-0.4	-0.9	1.5	C18 H33 N Na P Cl3	554.2	3.813	2.21	18	33	1		1	1		3



MS spectrum of 1-(*N*-phthalimido)methyltriphenylphosphonium bromide (**2c**).

Multiple Mass Analysis: 2 mass(es) processed
Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
36 formula(e) evaluated with 13 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	P	Cl
524.0140	100.00	524.0141	-0.1	-0.2	18.5	C27 H18 N O2 P Cl3	454.0	2.480	8.38	27	18	1	2	1	3
		523.9777	36.3	69.3	19.5	C26 H14 N O3 P Cl3	453.2	1.655	19.11	26	14	1	3	1	3
		524.0505	-36.5	-69.7	17.5	C28 H22 N O P Cl3	455.6	4.030	1.78	28	22	1	1	1	3
		523.9566	57.4	109.5	24.5	C29 H10 N O P Cl3	456.8	5.263	0.52	29	10	1	1	1	3
		524.0716	-57.6	-109.9	12.5	C25 H26 N O3 P Cl3	451.9	0.354	70.21	25	26	1	3	1	3
526.0115	98.94	525.9933	18.2	34.6	18.5	C26 H16 N O3 P Cl3	479.5	1.120	32.63	26	16	1	3	1	3
		526.0297	-18.2	-34.6	17.5	C27 H20 N O2 P Cl3	480.9	2.530	7.97	27	20	1	2	1	3
		525.9722	39.3	74.7	23.5	C29 H12 N O P Cl3	483.0	4.691	0.92	29	12	1	1	1	3

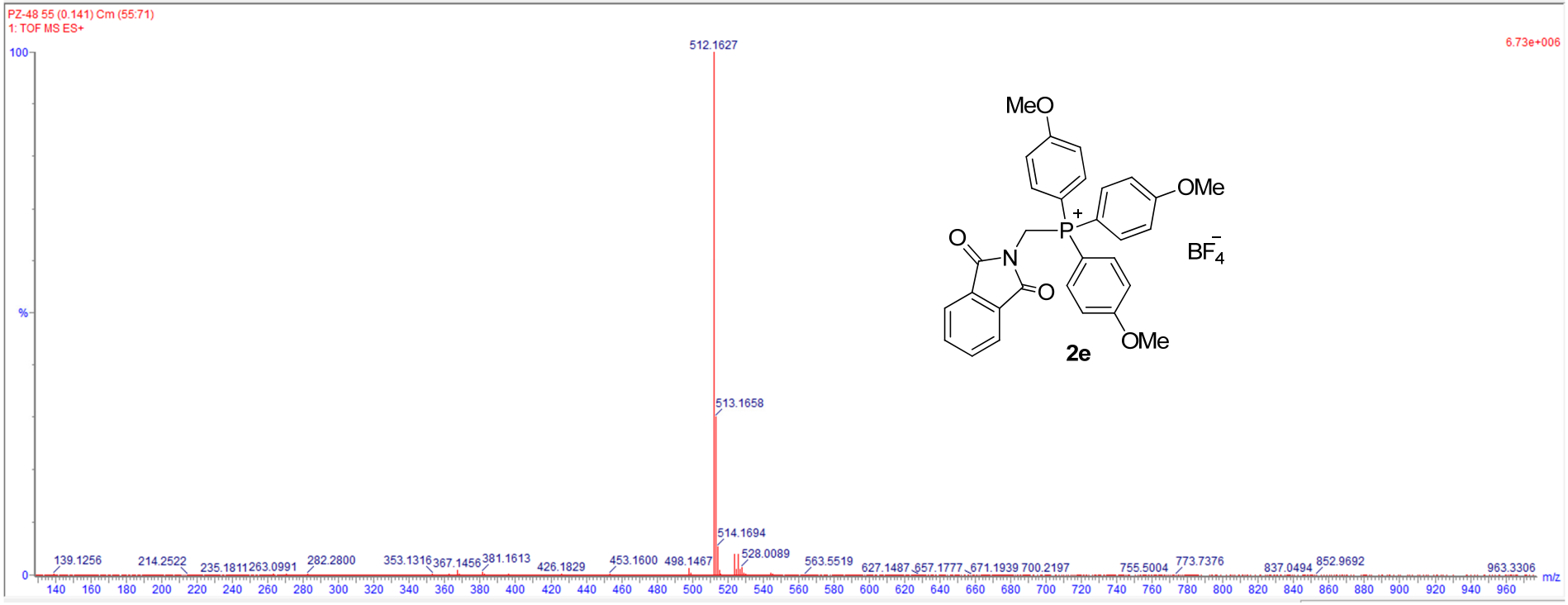


2d

MS spectrum of 1-(*N*-phthalimido)methyltris(3-chlorophenyl)phosphonium tetrafluoroborate (**2d**).

Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
27 formula(e) evaluated with 10 results within limits (up to 5 closest results for each mass)
Elements Used:

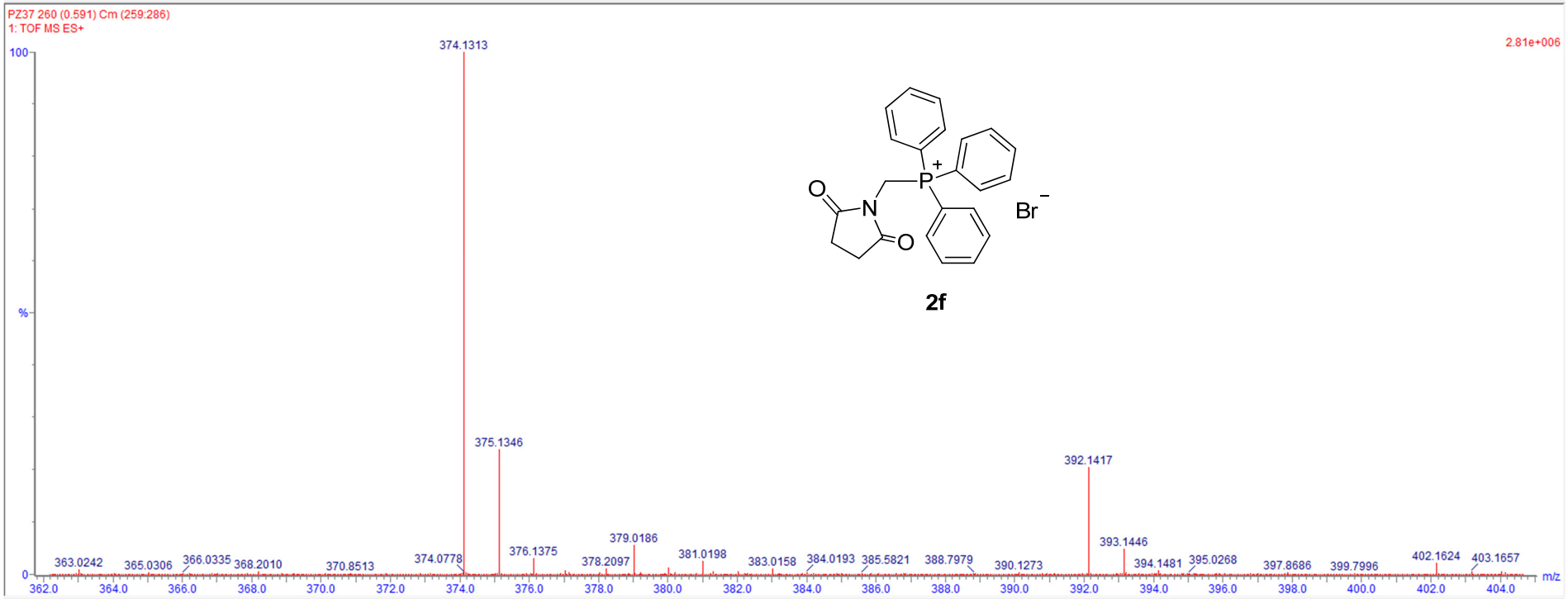
Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	P
512.1627	100.00	512.1627	0.0	0.0	18.5	C30 H27 N O5 P	544.7	0.387	67.90	30	27	1	5	1
		512.1779	-15.2	-29.7	22.5	C34 H27 N O2 P	547.2	2.883	5.60	34	27	1	2	1
		512.1416	21.1	41.2	23.5	C33 H23 N O3 P	546.9	2.583	7.55	33	23	1	3	1
		512.1991	-36.4	-71.1	17.5	C31 H31 N O4 P	546.0	1.746	17.45	31	31	1	4	1
		512.2143	-51.6	-100.7	21.5	C35 H31 N O P	548.5	4.197	1.50	35	31	1	1	1



MS spectrum of 1-(*N*-phthalimido)methyltris(4-methoxyphenyl)phosphonium tetrafluoroborate (**2e**).

Tolerance = 50.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
2432 formula(e) evaluated with 195 results within limits (up to 3 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Na	P	S	Cl
374.1313	100.00	374.1310	0.3	0.8	14.5	C23 H21 N O2 P	498.0	0.243	78.40	23	21	1	2		1		
		374.1312	0.1	0.3	14.5	C24 H21 N O Cl	499.3	1.570	20.80	24	21	1	1				1
		374.1314	-0.1	-0.3	-2.5	C14 H33 N Na P Cl3	502.5	4.830	0.80	14	33	1		1	1		3

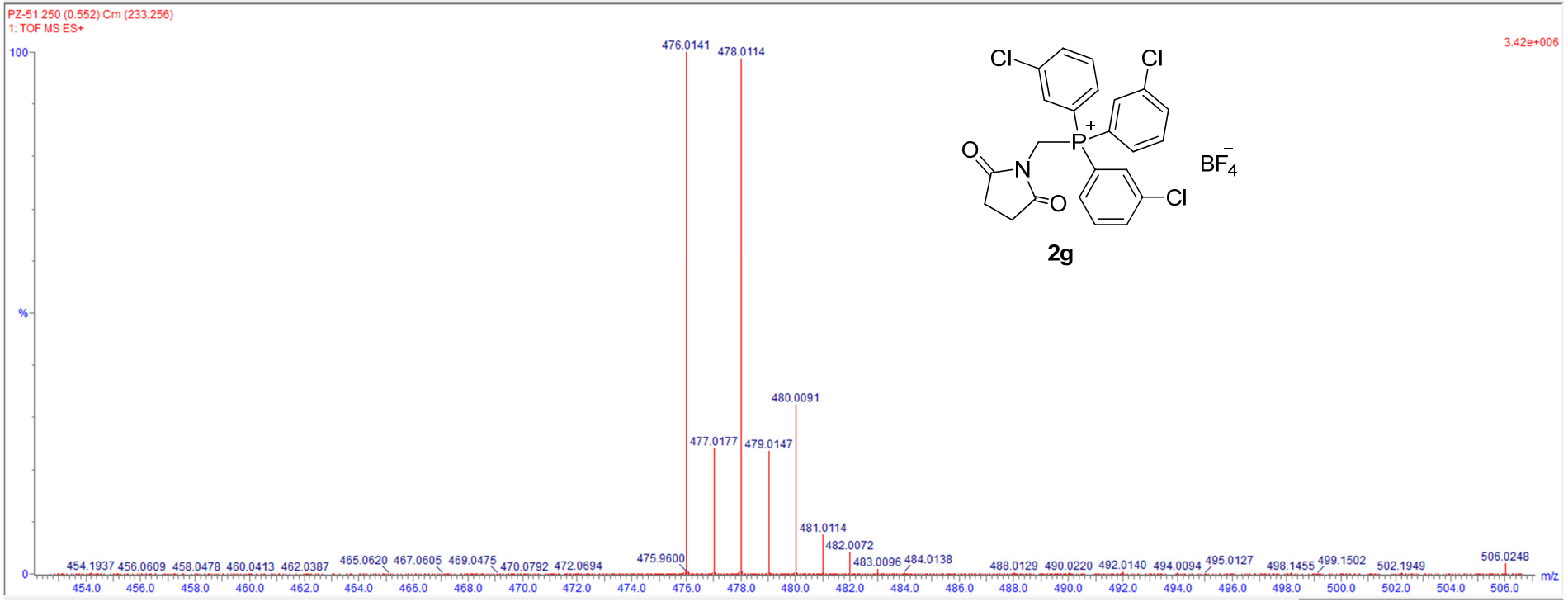


2f

MS spectrum of 1-(*N*-succinimido)methyltriphenylphosphonium bromide (**2f**).

Multiple Mass Analysis: 2 mass(es) processed
Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
55 formula(e) evaluated with 22 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	P	Cl
476.0141	100.00	476.0141	0.0	0.0	14.5	C23 H18 N O2 P Cl3	439.9	3.446	3.19	23	18	1	2	1	3
		475.9988	15.3	32.1	10.5	C19 H18 N O5 P Cl3	441.9	5.449	0.43	19	18	1	5	1	3
		476.0352	-21.1	-44.3	9.5	C20 H22 N O4 P Cl3	440.6	4.085	1.68	20	22	1	4	1	3
		476.0505	-36.4	-76.5	13.5	C24 H22 N O P Cl3	442.2	5.709	0.33	24	22	1	1	1	3
		475.9777	36.4	76.5	15.5	C22 H14 N O3 P Cl3	436.5	0.058	94.37	22	14	1	3	1	3
478.0114	98.74	478.0145	-3.1	-6.5	9.5	C19 H20 N O5 P Cl3	472.6	3.807	2.22	19	20	1	5	1	3
		477.9933	18.1	37.9	14.5	C22 H16 N O3 P Cl3	469.0	0.158	85.40	22	16	1	3	1	3
		478.0297	-18.3	-38.3	13.5	C23 H20 N O2 P Cl3	471.8	2.953	5.22	23	20	1	2	1	3

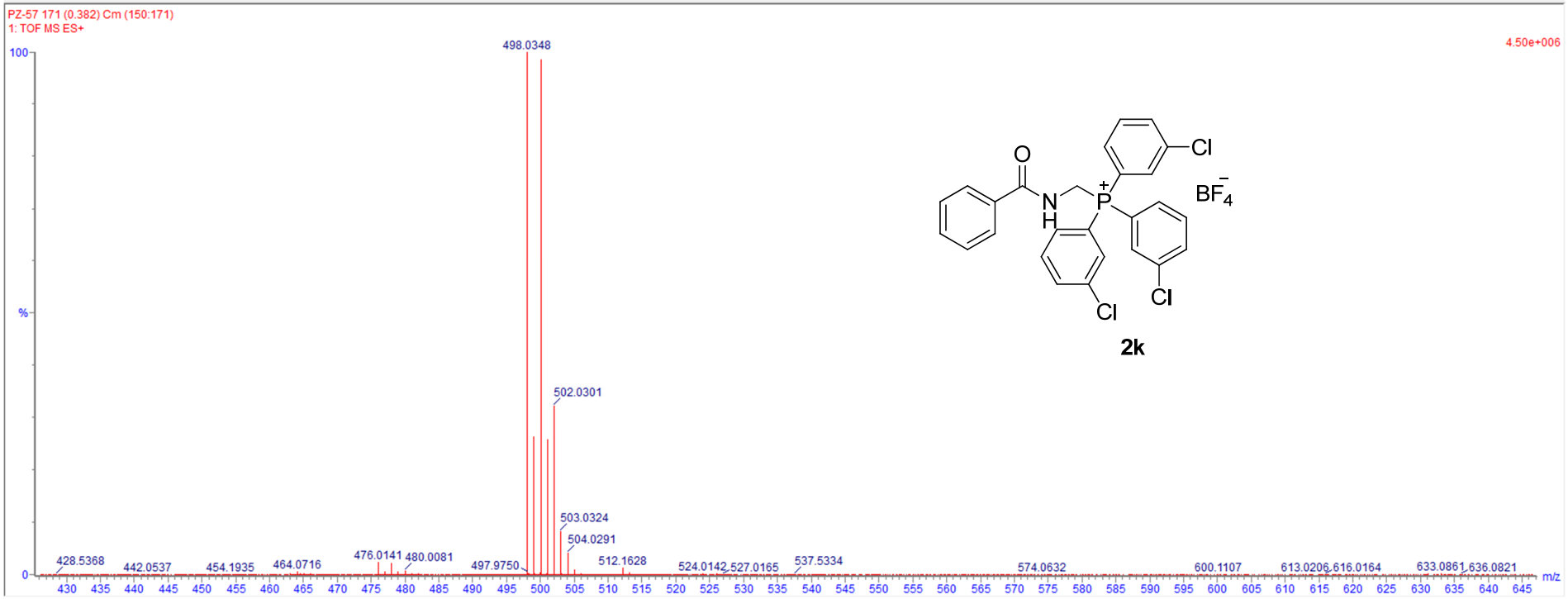


2g

MS spectrum of 1-(*N*-succinimido)methyltris(3-chlorophenyl)phosphonium tetrafluoroborate (**2g**).

Multiple Mass Analysis: 2 mass(es) processed
Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
56 formula(e) evaluated with 22 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	P	Cl
498.0348	100.00	498.0348	0.0	0.0	16.5	C26 H20 N O P Cl3	474.3	4.987	0.68	26	20	1	1	1	3
		498.0196	15.2	30.5	12.5	C22 H20 N O4 P Cl3	472.9	3.569	2.82	22	20	1	4	1	3
		498.0559	-21.1	-42.4	11.5	C23 H24 N O3 P Cl3	469.3	0.056	94.54	23	24	1	3	1	3
		497.9984	36.4	73.1	17.5	C25 H16 N O2 P Cl3	473.3	3.990	1.85	25	16	1	2	1	3
		498.0771	-42.3	-84.9	6.5	C20 H28 N O5 P Cl3	476.1	6.833	0.11	20	28	1	5	1	3
500.0323	98.60	500.0352	-2.9	-5.8	11.5	C22 H22 N O4 P Cl3	495.6	4.018	1.80	22	22	1	4	1	3
		500.0505	-18.2	-36.4	15.5	C26 H22 N O P Cl3	497.8	6.218	0.20	26	22	1	1	1	3
		500.0141	18.2	36.4	16.5	C25 H18 N O2 P Cl3	496.3	4.785	0.84	25	18	1	2	1	3

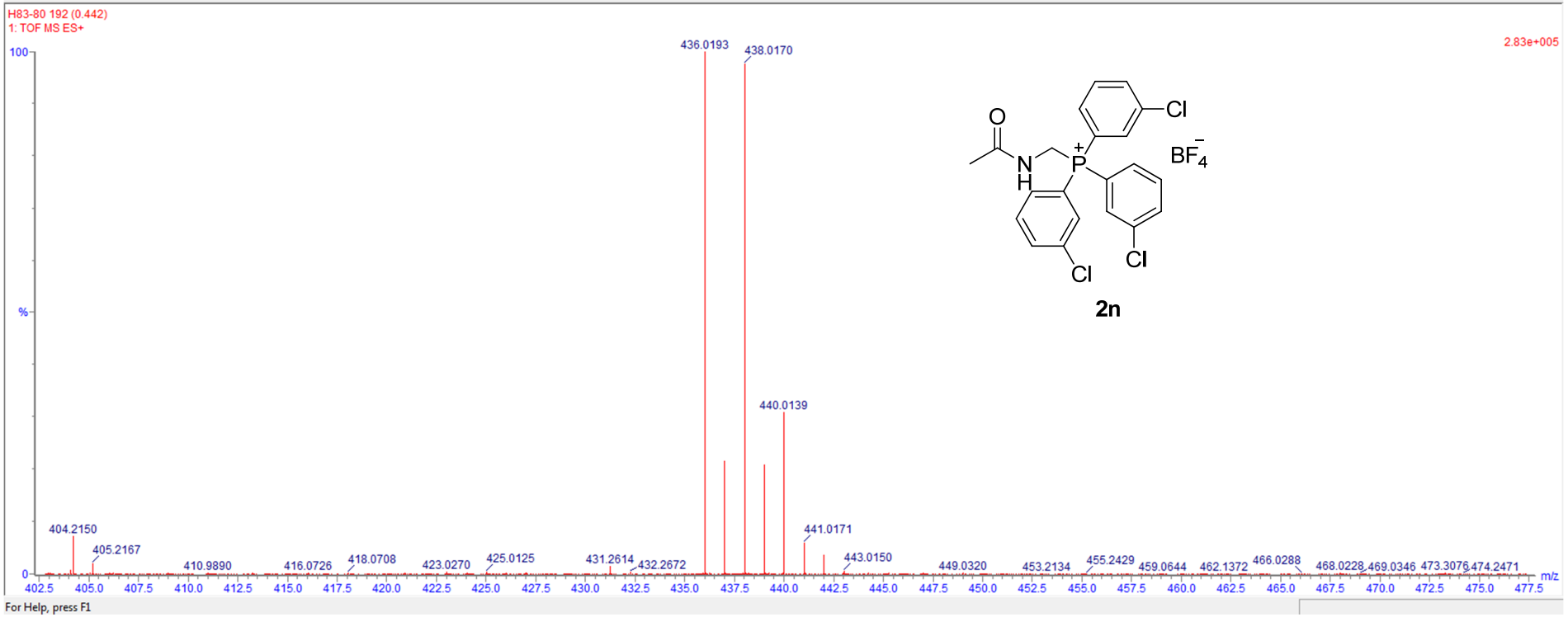


2k

MS spectrum of (*N*-benzoylamino)methyltris(3-chlorophenyl)phosphonium tetrafluoroborate (**2k**).

Multiple Mass Analysis: 2 mass(es) processed
Tolerance = 50.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
4939 formula(e) evaluated with 403 results within limits (up to 3 closest results for each mass)
Elements Used:

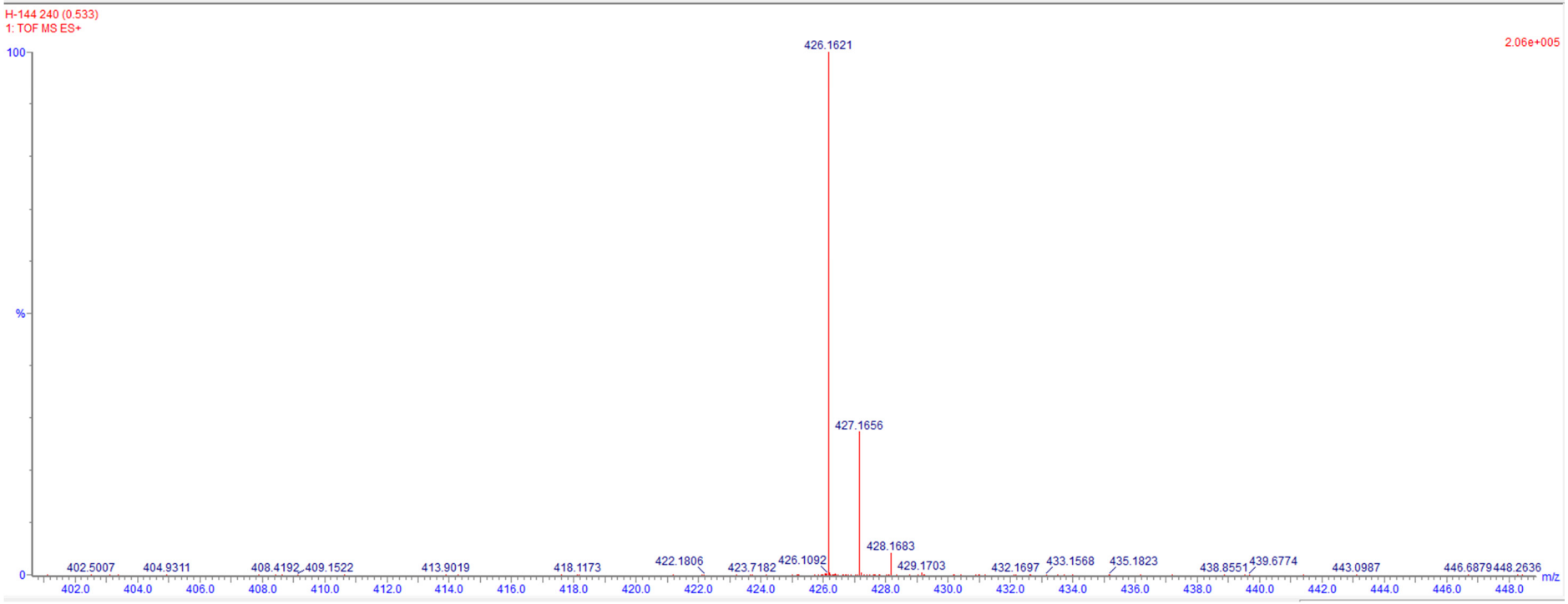
Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Na	P	S	Cl
436.0193	100.00	436.0192	0.1	0.2	12.5	C21 H18 N O P Cl3	245.1	0.028	97.21	21	18	1	1		1		3
		436.0197	-0.4	-0.9	27.5	C30 H7 N Na S	250.4	5.300	0.50	30	7	1		1		1	
		436.0197	-0.4	-0.9	21.5	C25 H11 N O3 P S	248.9	3.777	2.29	25	11	1	3		1	1	
438.0170	97.67	438.0171	-0.1	-0.2	4.5	C15 H21 N O4 Na P Cl3	312.6	0.324	72.29	15	21	1	4	1	1		3
		438.0169	0.1	0.2	21.5	C25 H9 N O5 Cl	313.8	1.512	22.04	25	9	1	5				1
		438.0167	0.3	0.7	27.5	C29 H5 N O3 Na	315.2	2.870	5.67	29	5	1	3	1			



MS spectrum of (*N*-acetylamino)methyltris(3-chlorophenyl)phosphonium tetrafluoroborate (**2n**).

Tolerance = 50.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
524 formula(e) evaluated with 58 results within limits (up to 3 closest results for each mass)
Elements Used:

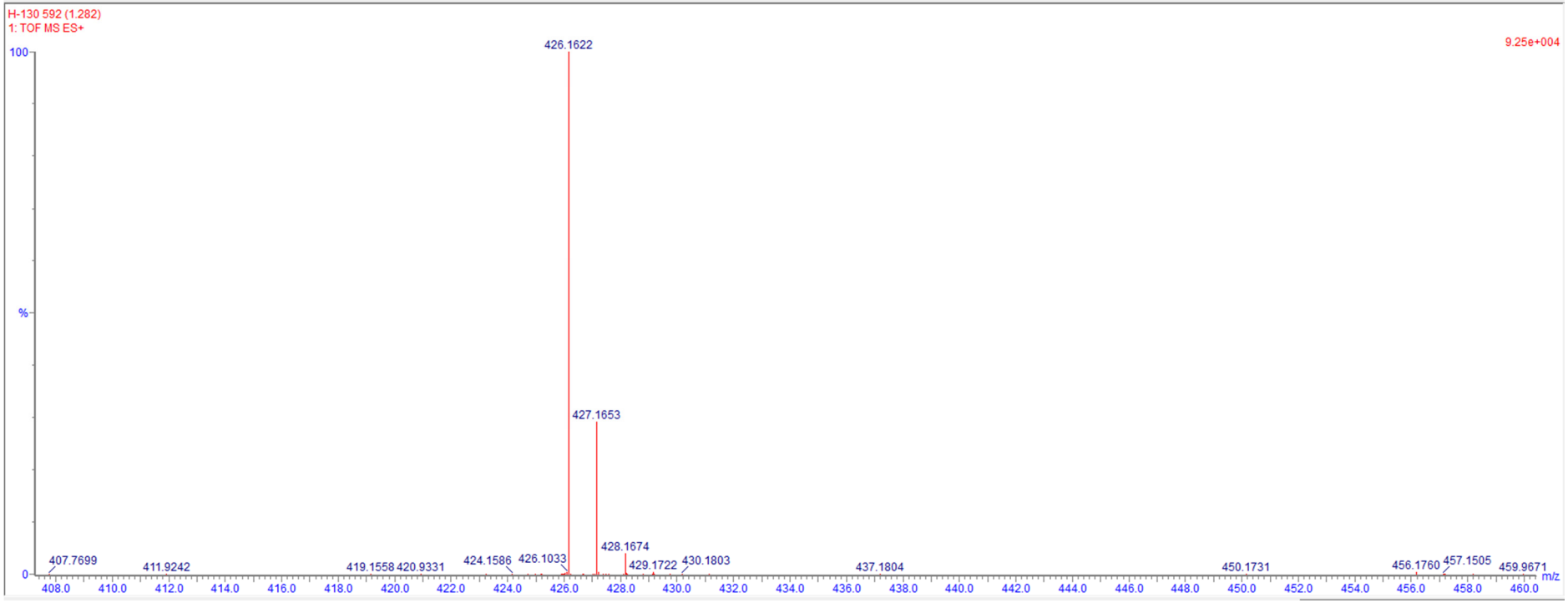
Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	P
426.1621	100.00	426.1623	-0.2	-0.5	16.5	C27 H25 N O2 P	198.9	0.014	98.56	27	25	1	2	1
		426.1615	0.6	1.4	4.5	C11 H25 N9 O7 P	206.0	7.084	0.08	11	25	9	7	1
		426.1641	-2.0	-4.7	3.5	C15 H29 N3 O9 P	203.2	4.301	1.35	15	29	3	9	1



MS spectrum of (*N*-benzyloxycarbonylamino)methyltriphenylphosphonium tetrafluoroborate (**2o**).

Tolerance = 50.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
524 formula(e) evaluated with 58 results within limits (up to 3 closest results for each mass)
Elements Used:

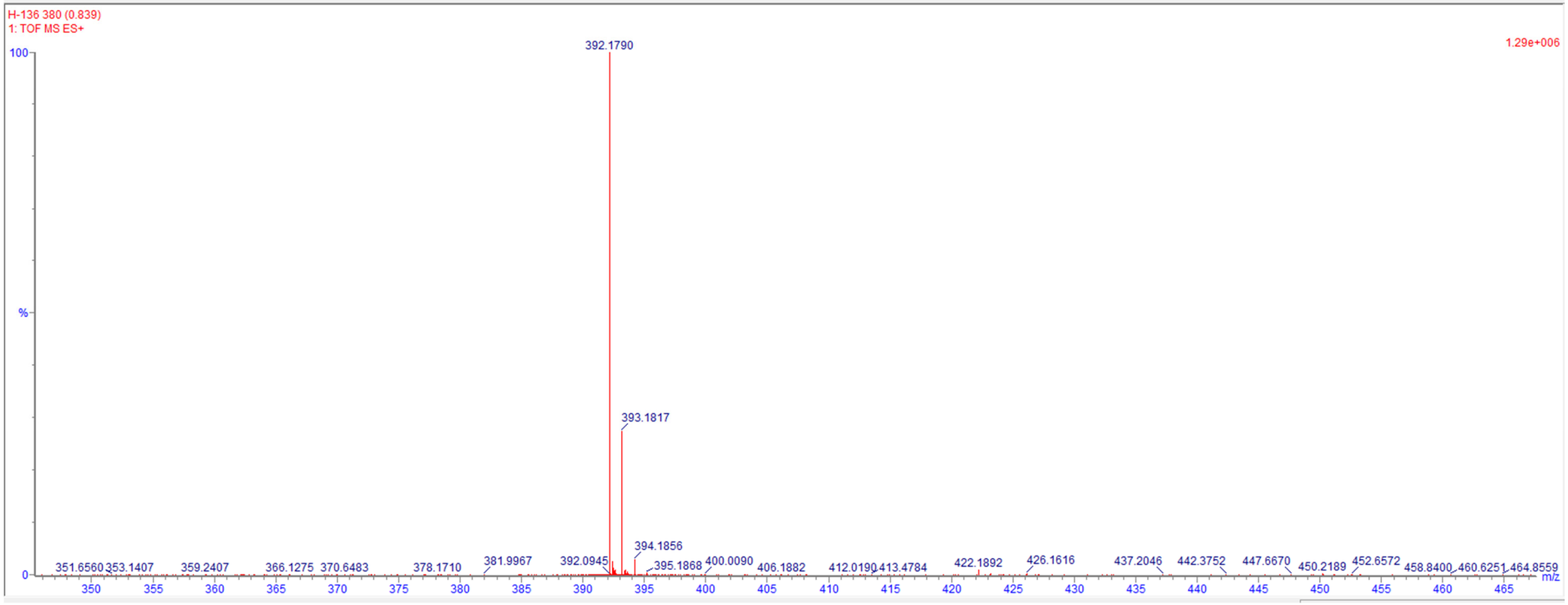
Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	P
426.1622	100.00	426.1623	-0.1	-0.2	16.5	C27 H25 N O2 P	76.3	0.000	99.97	27	25	1	2	1
		426.1615	0.7	1.6	4.5	C11 H25 N9 O7 P	86.9	10.596	0.00	11	25	9	7	1
		426.1641	-1.9	-4.5	3.5	C15 H29 N3 O9 P	84.7	8.395	0.02	15	29	3	9	1



MS spectrum of (*N*-benzyloxycarbonylamino)methyltriphenylphosphonium bromide (**2p**).

Tolerance = 50.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
523 formula(e) evaluated with 59 results within limits (up to 3 closest results for each mass)
Elements Used:

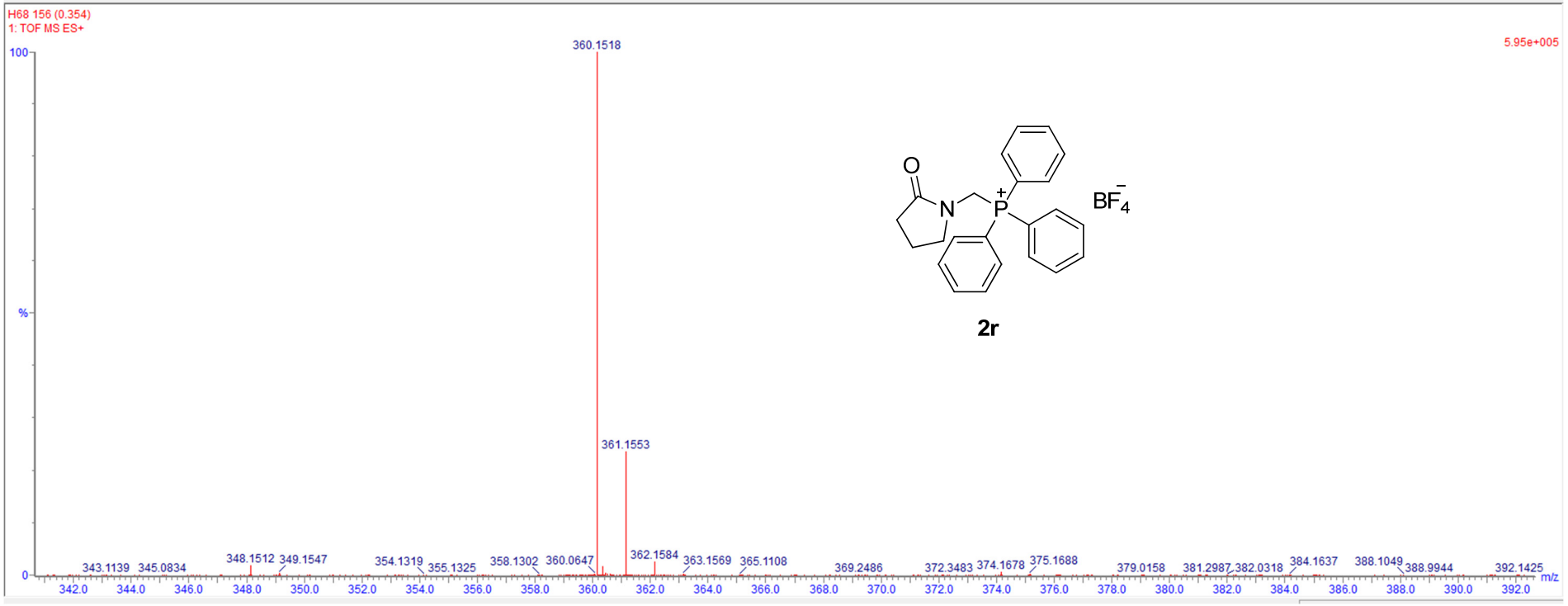
Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	P
392.1790	100.00	392.1779	1.1	2.8	12.5	C24 H27 N O2 P	419.9	0.000	99.97	24	27	1	2	1
		392.1798	-0.8	-2.0	-0.5	C12 H31 N3 O9 P	428.1	8.257	0.03	12	31	3	9	1
		392.1771	1.9	4.8	0.5	C8 H27 N9 O7 P	430.0	10.174	0.00	8	27	9	7	1



MS spectrum of (*N-tert*-butoxycarbonylamino)methylphosphonium bromide (**2q**).

Tolerance = 50.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
2407 formula(e) evaluated with 185 results within limits (up to 3 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Na	P	S	Cl
360.1518	100.00	360.1517	0.1	0.3	13.5	C23 H23 N O P	375.6	0.526	59.07	23	23	1	1		1		
		360.1519	-0.1	-0.3	13.5	C24 H23 N Cl	376.8	1.732	17.69	24	23	1					1
		360.1527	-0.9	-2.5	5.5	C18 H28 N O Na P S	376.6	1.460	23.23	18	28	1	1	1	1	1	

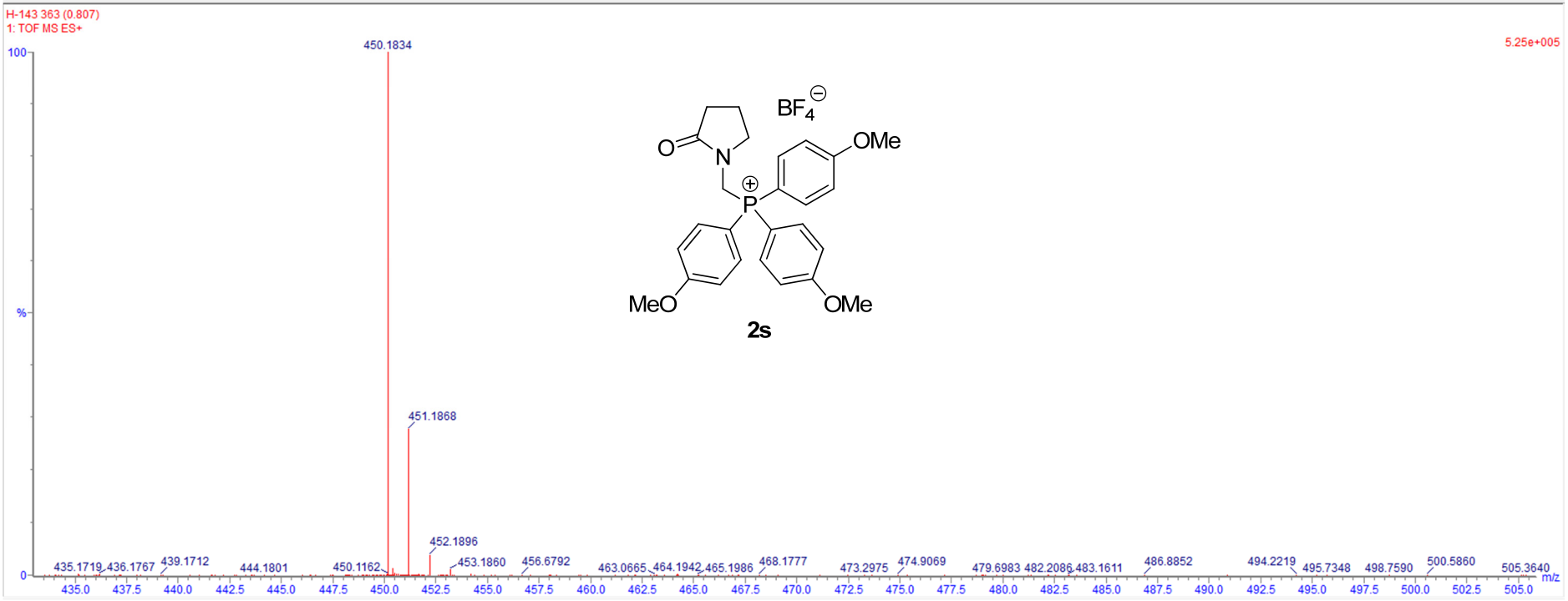


2r

MS spectrum of 1-(2-oxopyrrolidin-1-yl)methyltriphenylphosphonium tetrafluoroborate (**2r**).

Tolerance = 50.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
524 formula(e) evaluated with 58 results within limits (up to 3 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	P
450.1834	100.00	450.1834	0.0	0.0	13.5	C26 H29 N O4 P	331.6	0.042	95.91	26	29	1	4	1
		450.1848	-1.4	-3.1	18.5	C27 H25 N5 P	334.8	3.199	4.08	27	25	5		1
		450.1826	0.8	1.8	1.5	C10 H29 N9 O9 P	340.8	9.247	0.01	10	29	9	9	1



2s

MS spectrum of 2-oxopyrrolidin-1-yl)methyltris(4-methoxyphenyl)phosphonium tetrafluoroborate (**2s**).