

Supplementary Information

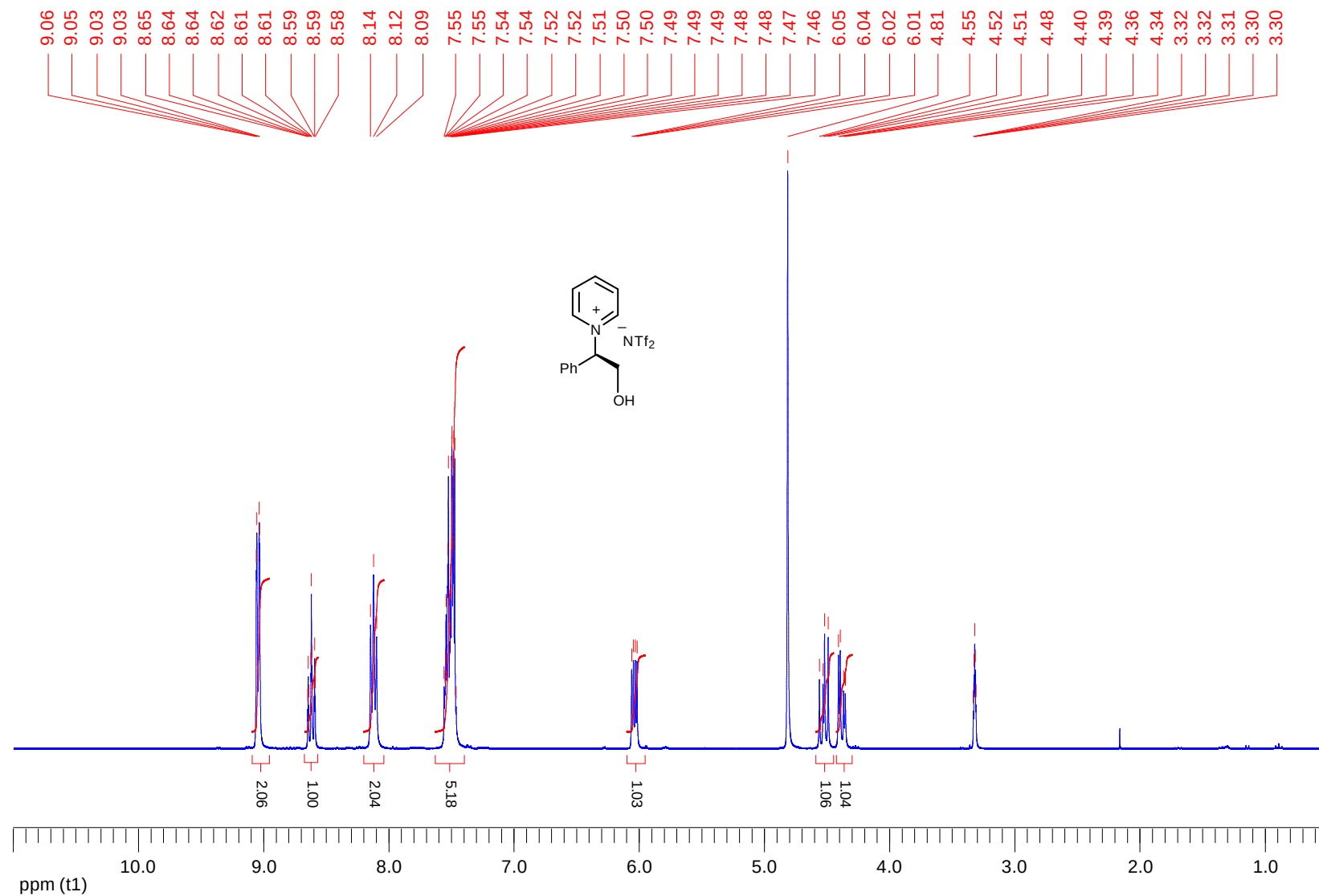
Non-occurrence of a Zincke-like process upon treatment of 1-(2,4-dinitrophenyl)-3-methylimidazolium chloride with a chiral primary amine.

Julio Cezar Pastre ^a, Carlos Roque D. Correia ^a and Yves Génisson ^{b*}

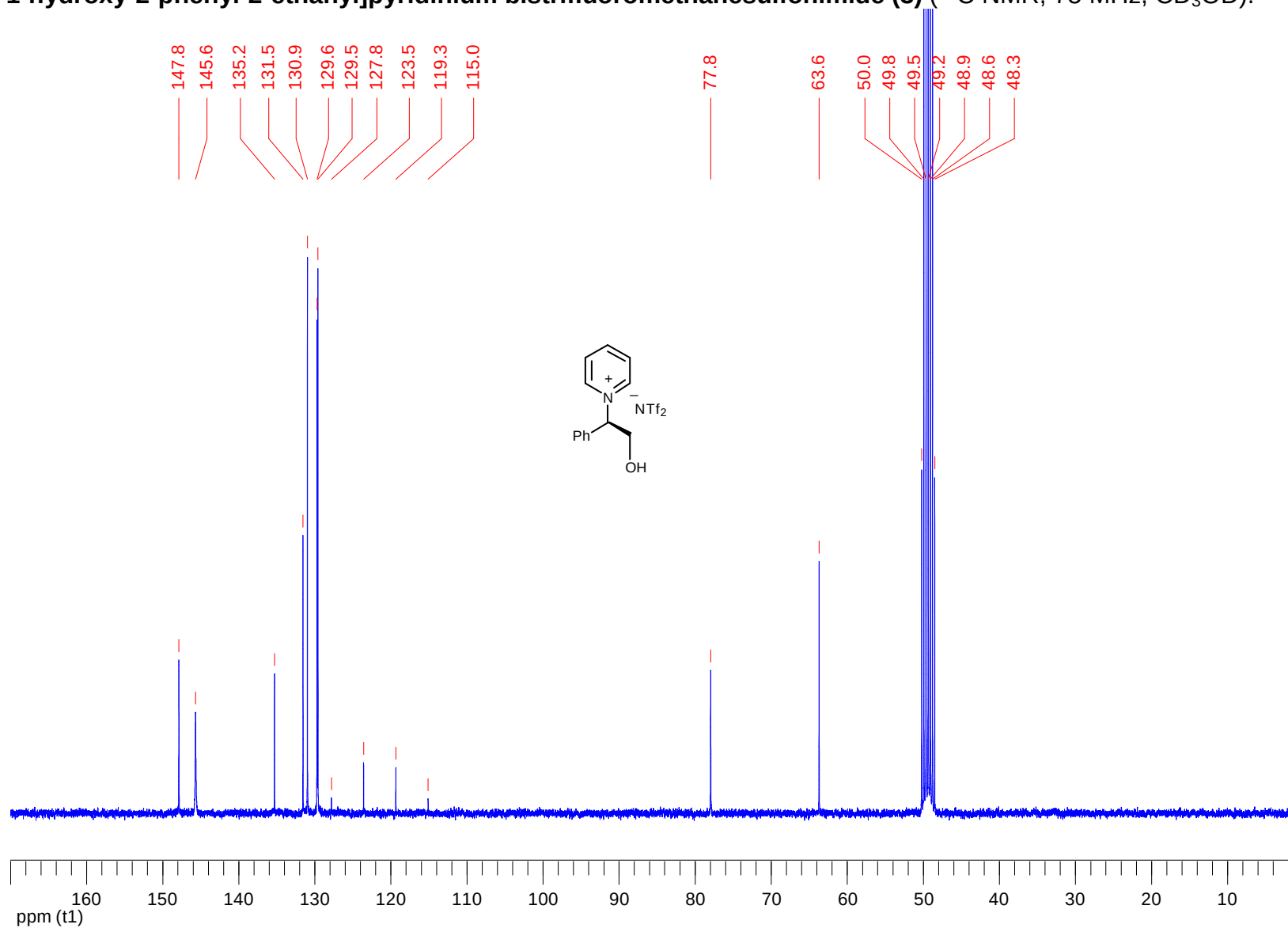
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^b *Laboratoire de Synthèse et Physicochimie de Molécules d'Intérêt Biologique UMR-CNRS 5068, Université Paul Sabatier, 118 route de Narbonne, 31062, Toulouse, France. Fax: 0033(0)561556011; Tel: 0033(0)561556299; E-mail: genisson@chimie.ups-tlse.fr*

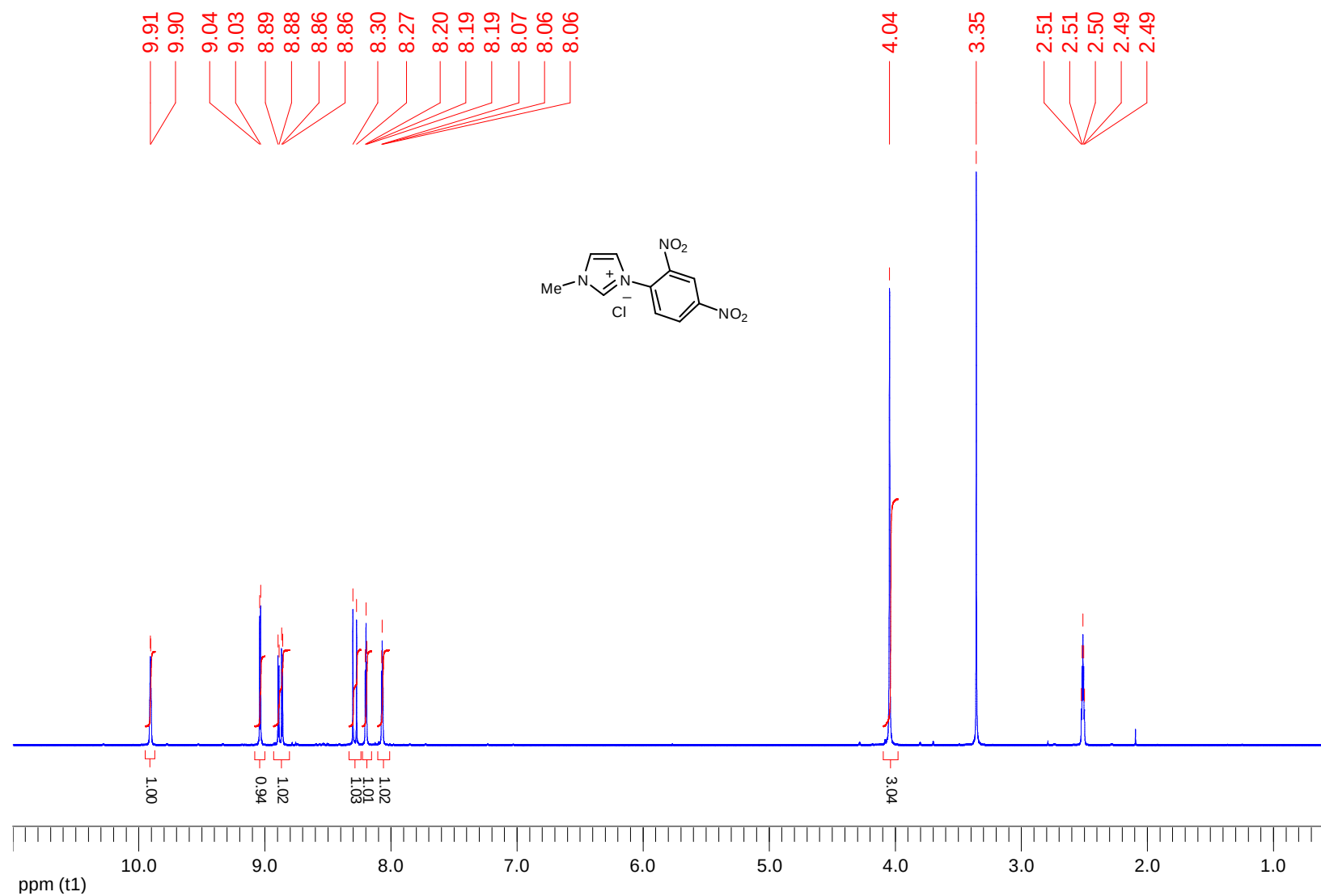
1-[(2*R*)-1-hydroxy-2-phenyl-2-ethyl]pyridinium bistrifluoromethanesulfonimide (3) (¹H NMR, 300 MHz, CD₃OD).



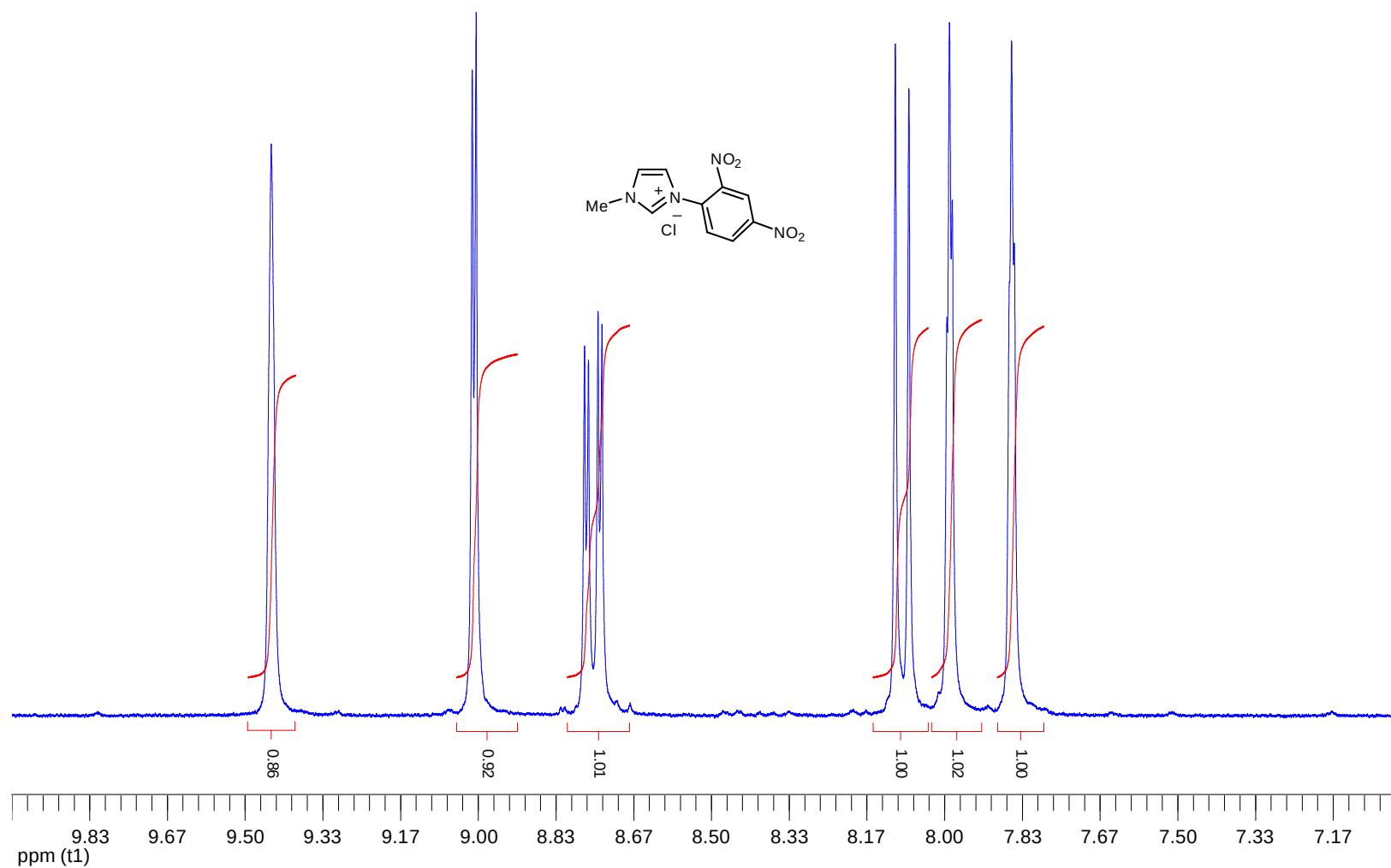
1-[(2*R*)-1-hydroxy-2-phenyl-2-ethyl]pyridinium bistrifluoromethanesulfonimide (3) (^{13}C NMR, 75 MHz, CD_3OD).



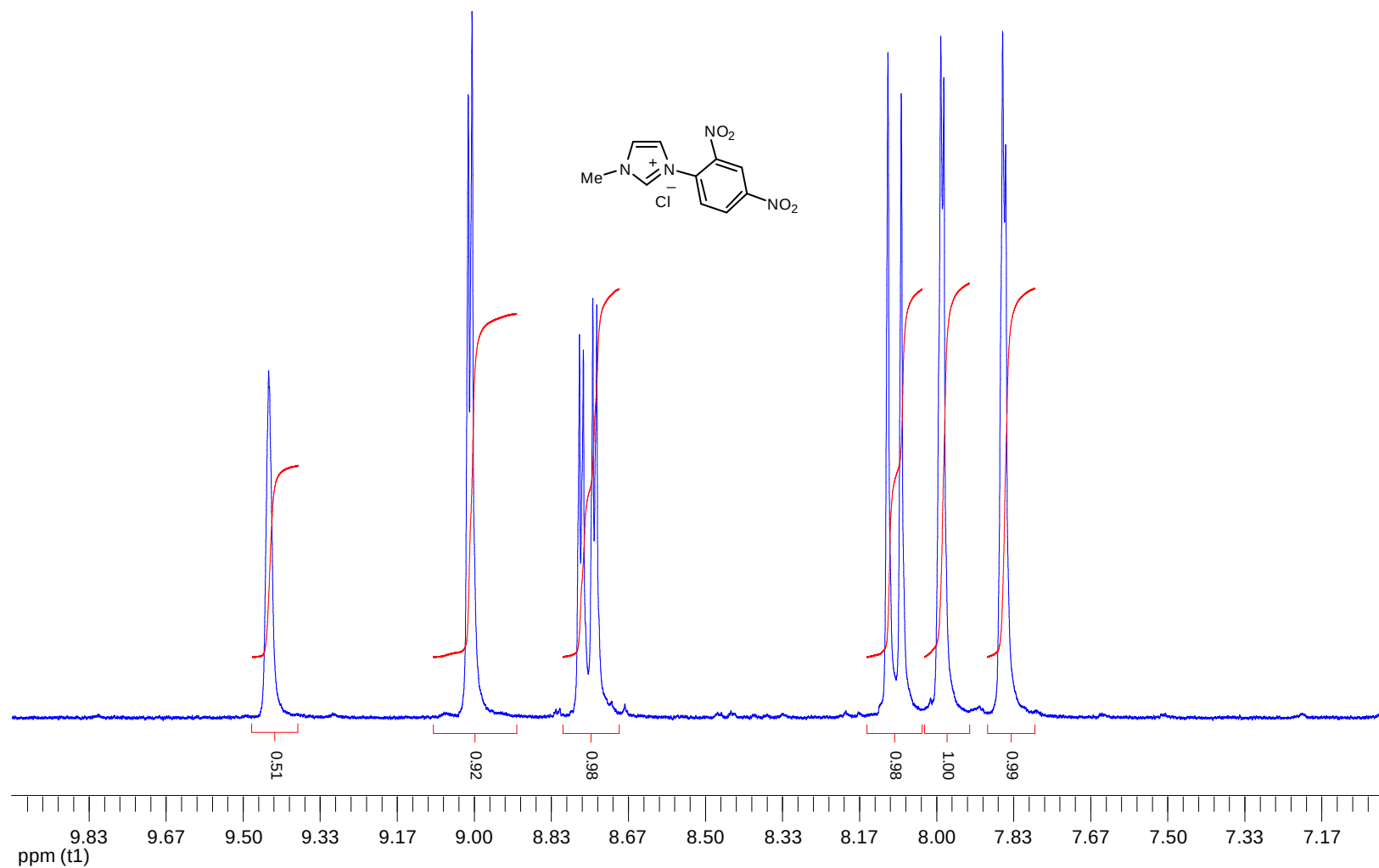
1-(2,4-dinitrophenyl)-3-methylimidazolium chloride (4) (^1H NMR, 300 MHz, DMSO- d_6).



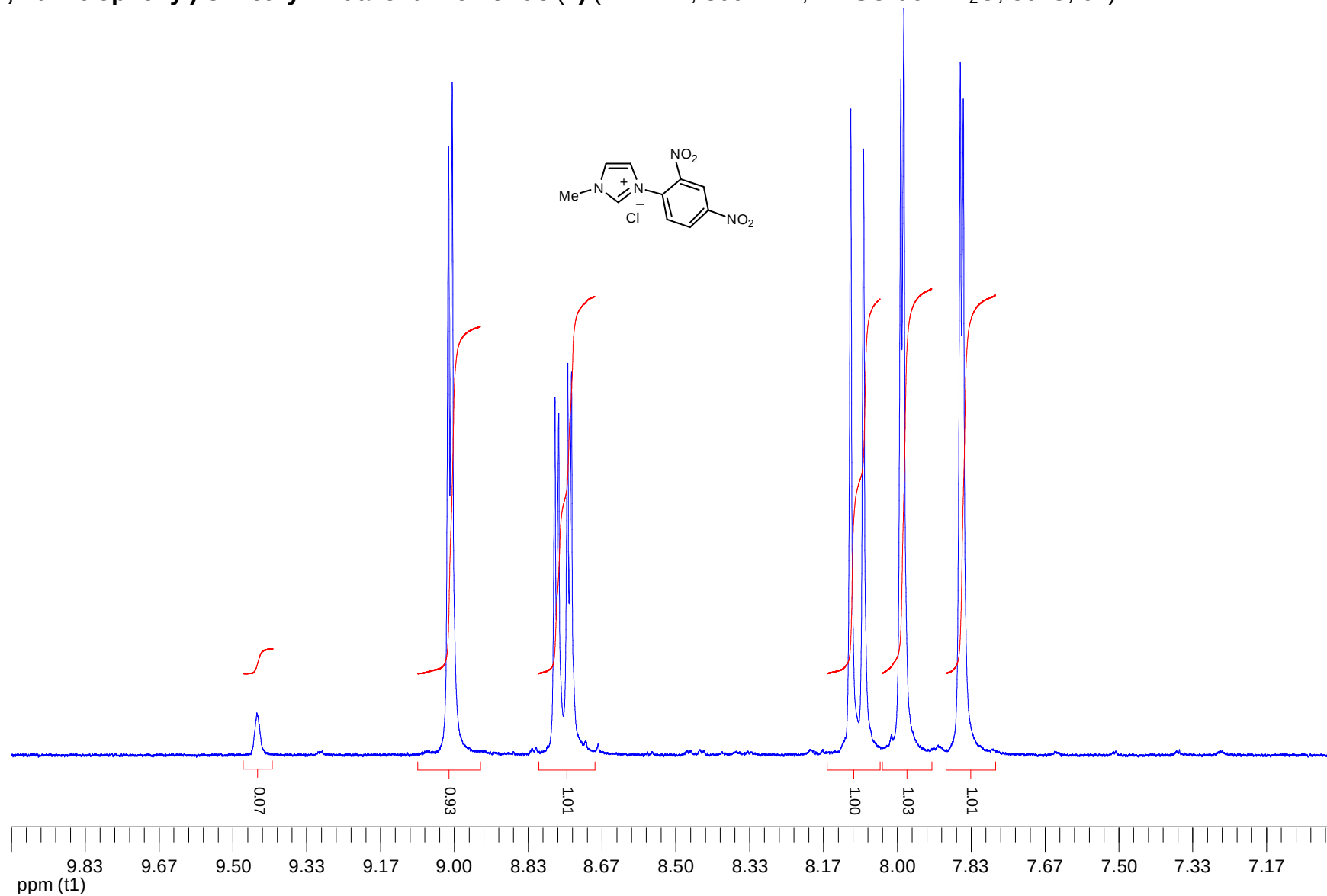
1-(2,4-dinitrophenyl)-3-methylimidazolium chloride (4) (^1H NMR, 300 MHz, DMSO- d_6 + D_2O , r.t.).



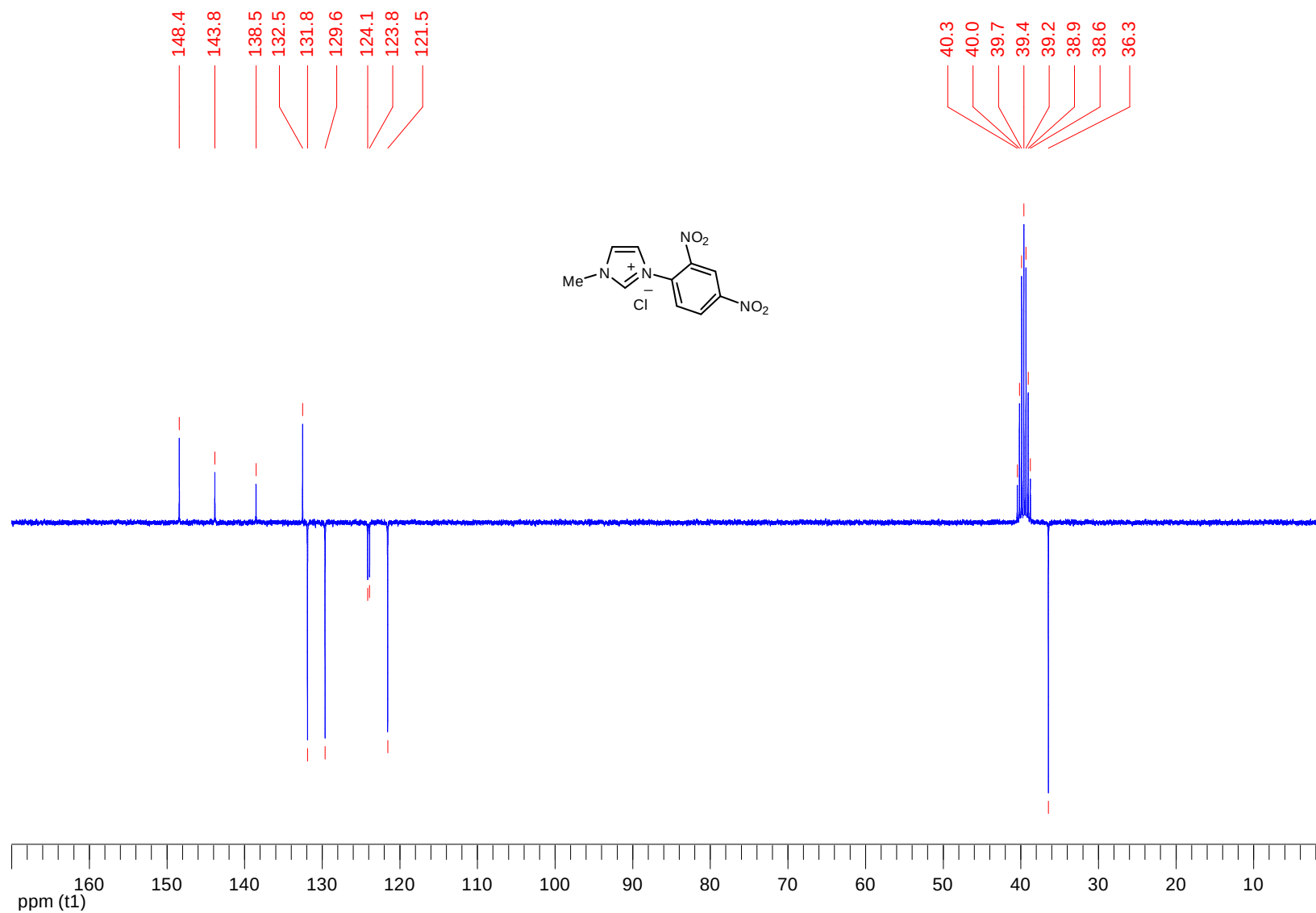
1-(2,4-dinitrophenyl)-3-methylimidazolium chloride (4) (^1H NMR, 300 MHz, DMSO- d_6 + D_2O , 50 $^\circ\text{C}$, 30 min.).



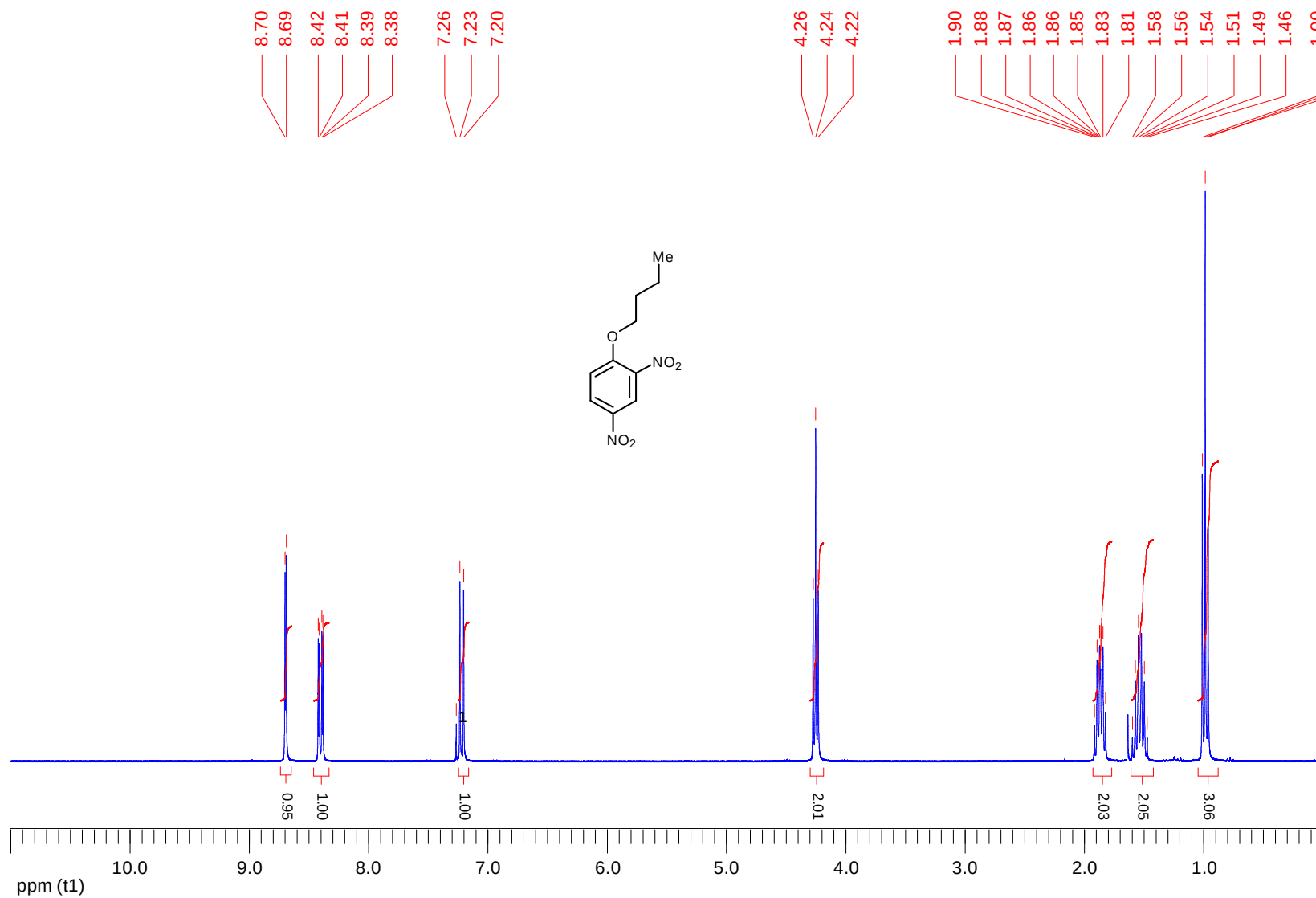
1-(2,4-dinitrophenyl)-3-methylimidazolium chloride (4) (^1H NMR, 300 MHz, DMSO- d_6 + D_2O , 50 $^\circ\text{C}$, 6h).



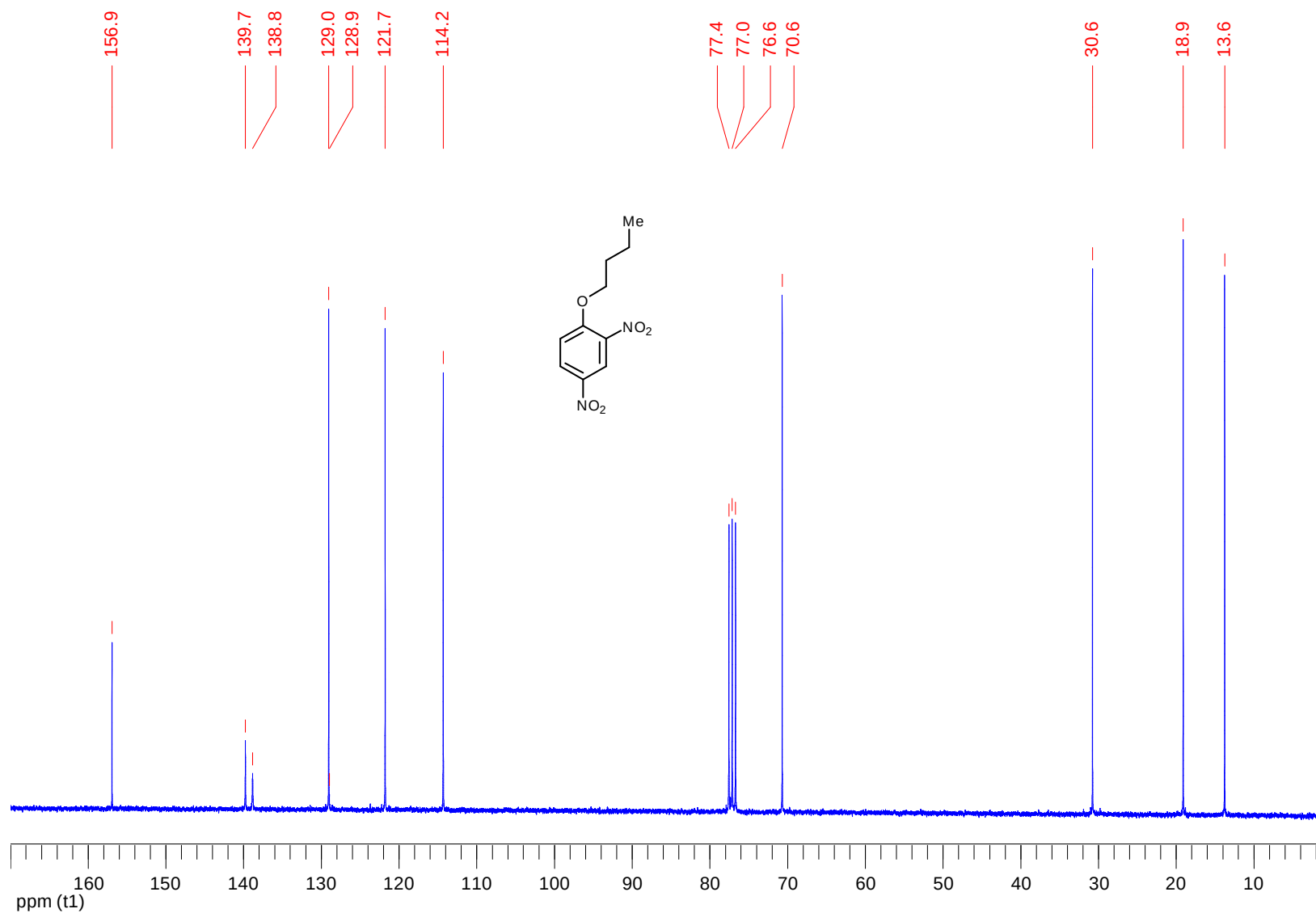
1-(2,4-dinitrophenyl)-3-methylimidazolium chloride (4) (^{13}C NMR, 75 MHz, DMSO-d₆).



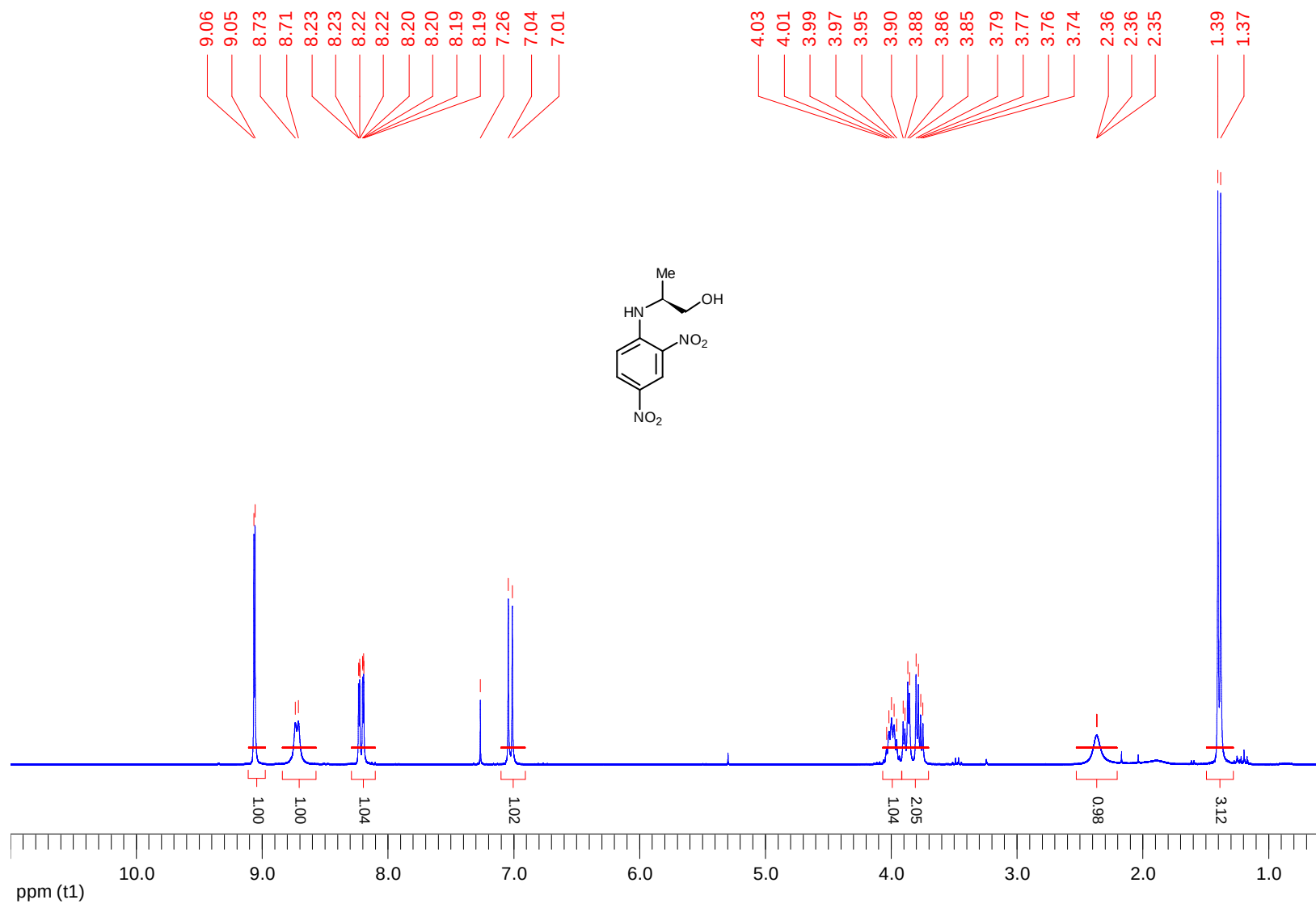
1-butoxy-2,4-dinitrobenzene (6) (^1H NMR, 300 MHz, CDCl_3).



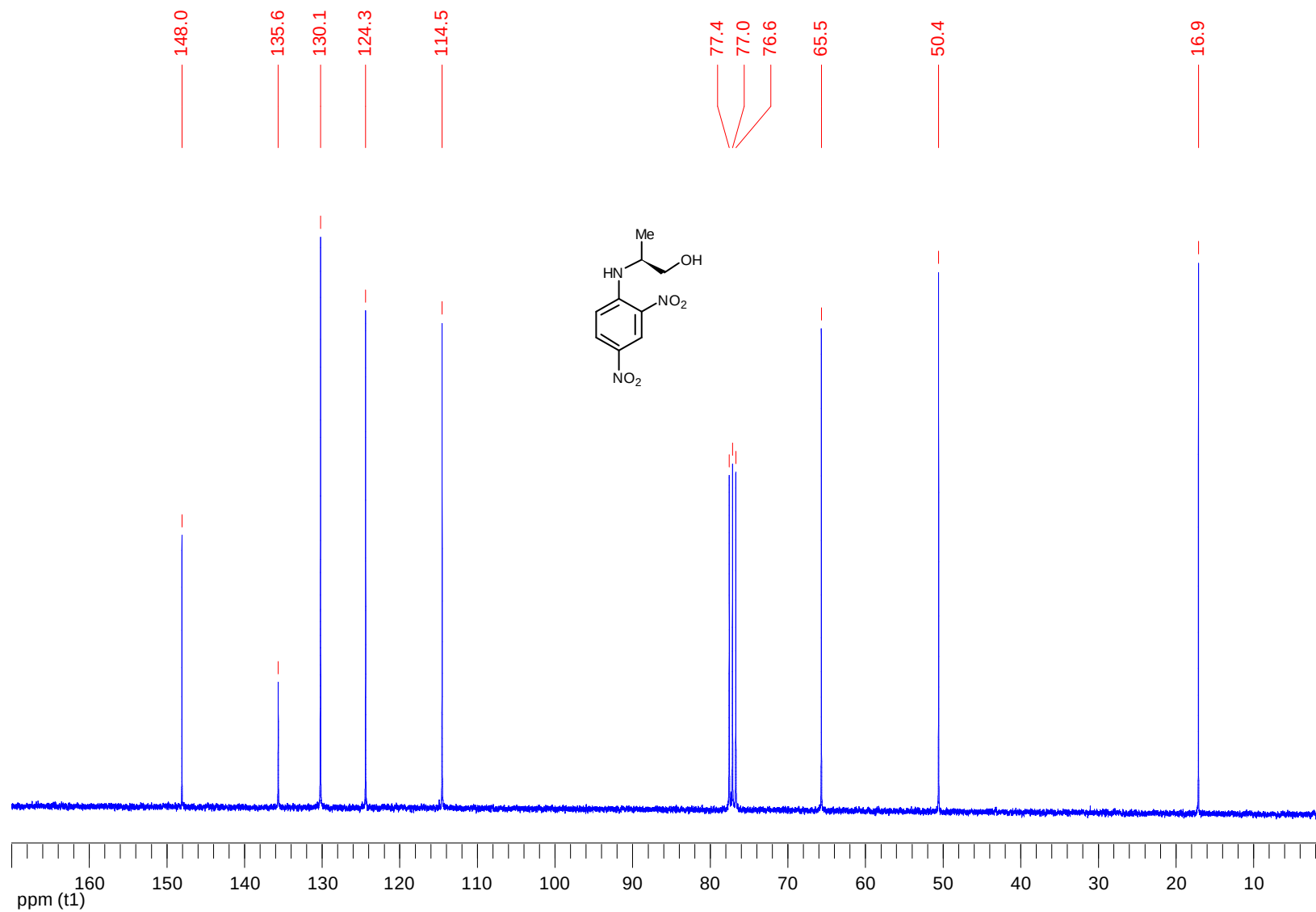
1-butoxy-2,4-dinitrobenzene (6) (^{13}C NMR, 75 MHz, CDCl_3).



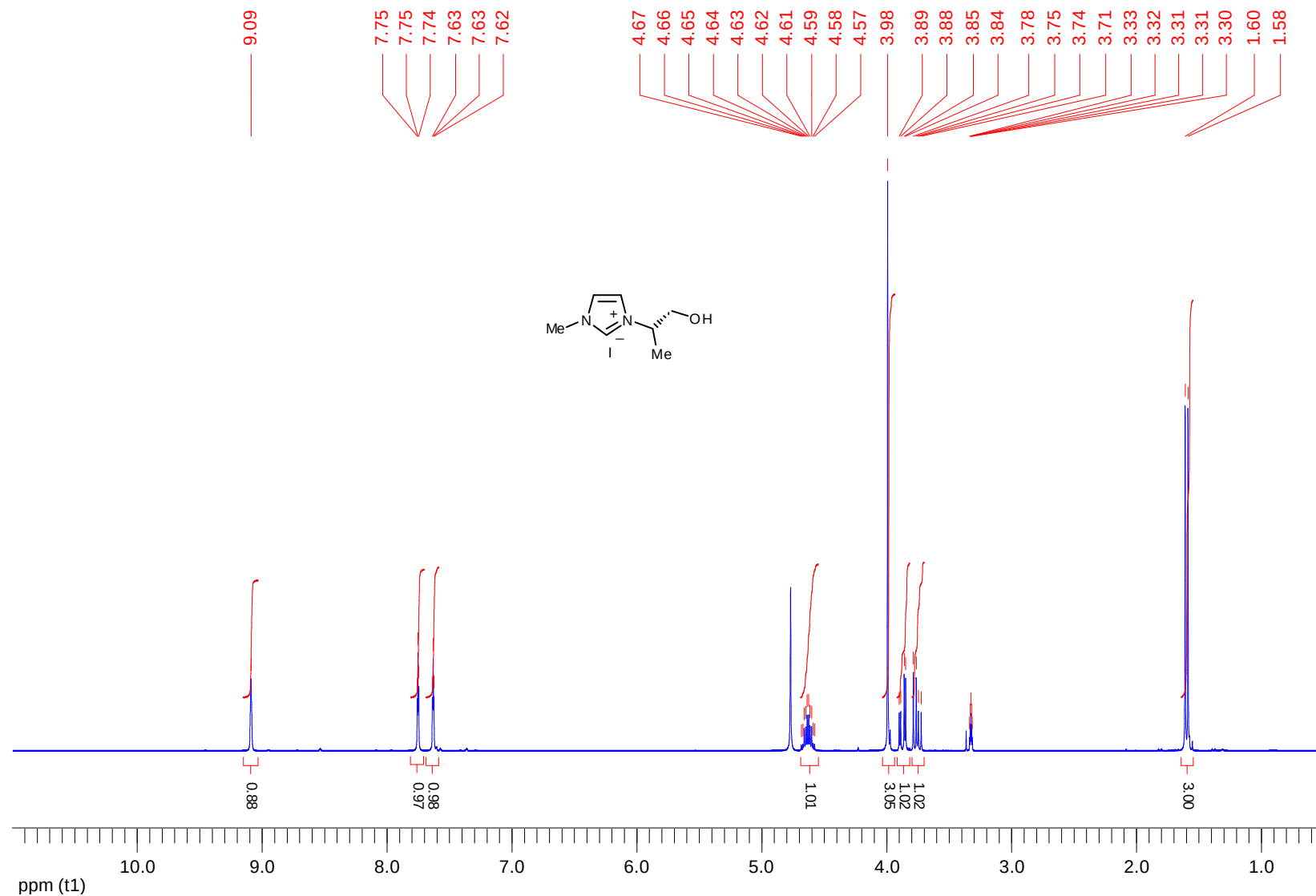
(S)-2-(2,4-dinitrophenylamino)propan-1-ol (7) (^1H NMR, 300 MHz, CDCl_3).



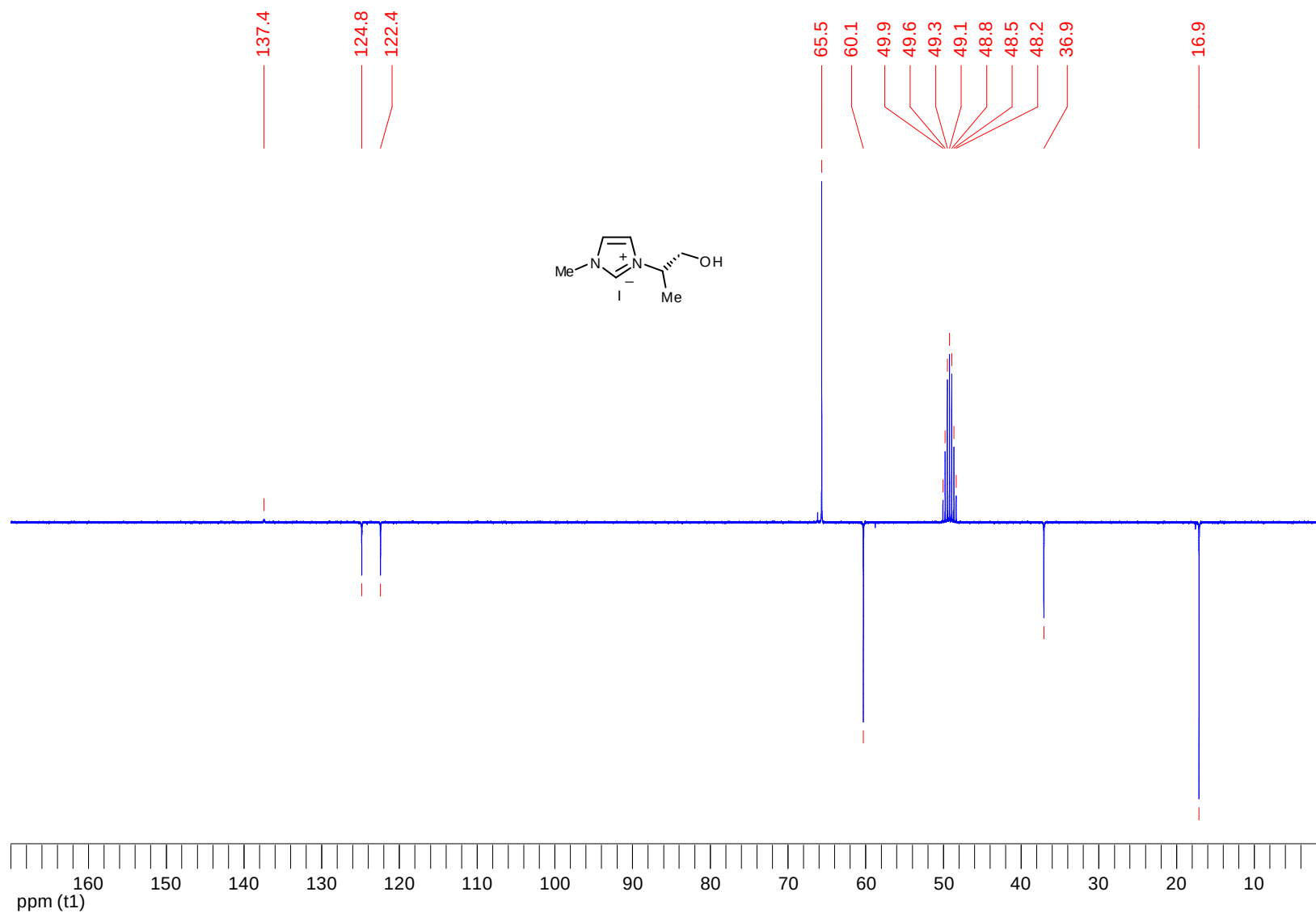
(S)-2-(2,4-dinitrophenylamino)propan-1-ol (7) (^{13}C NMR, 75 MHz, CDCl_3).



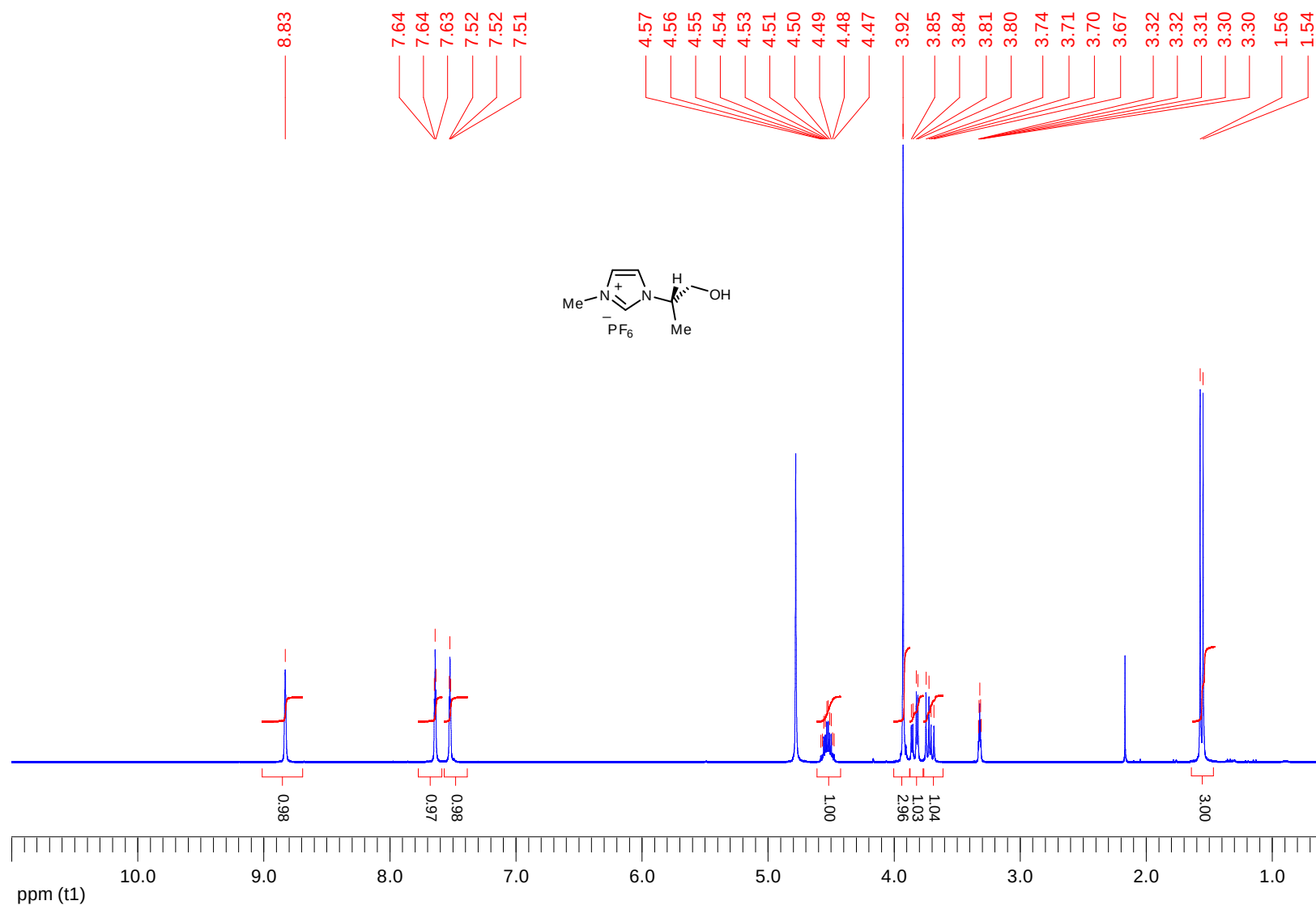
1-Methyl-3-[(2S)-1-hydroxy-2-propanyl]imidazolium iodide (9) (^1H NMR, 300 MHz, CD_3OD).



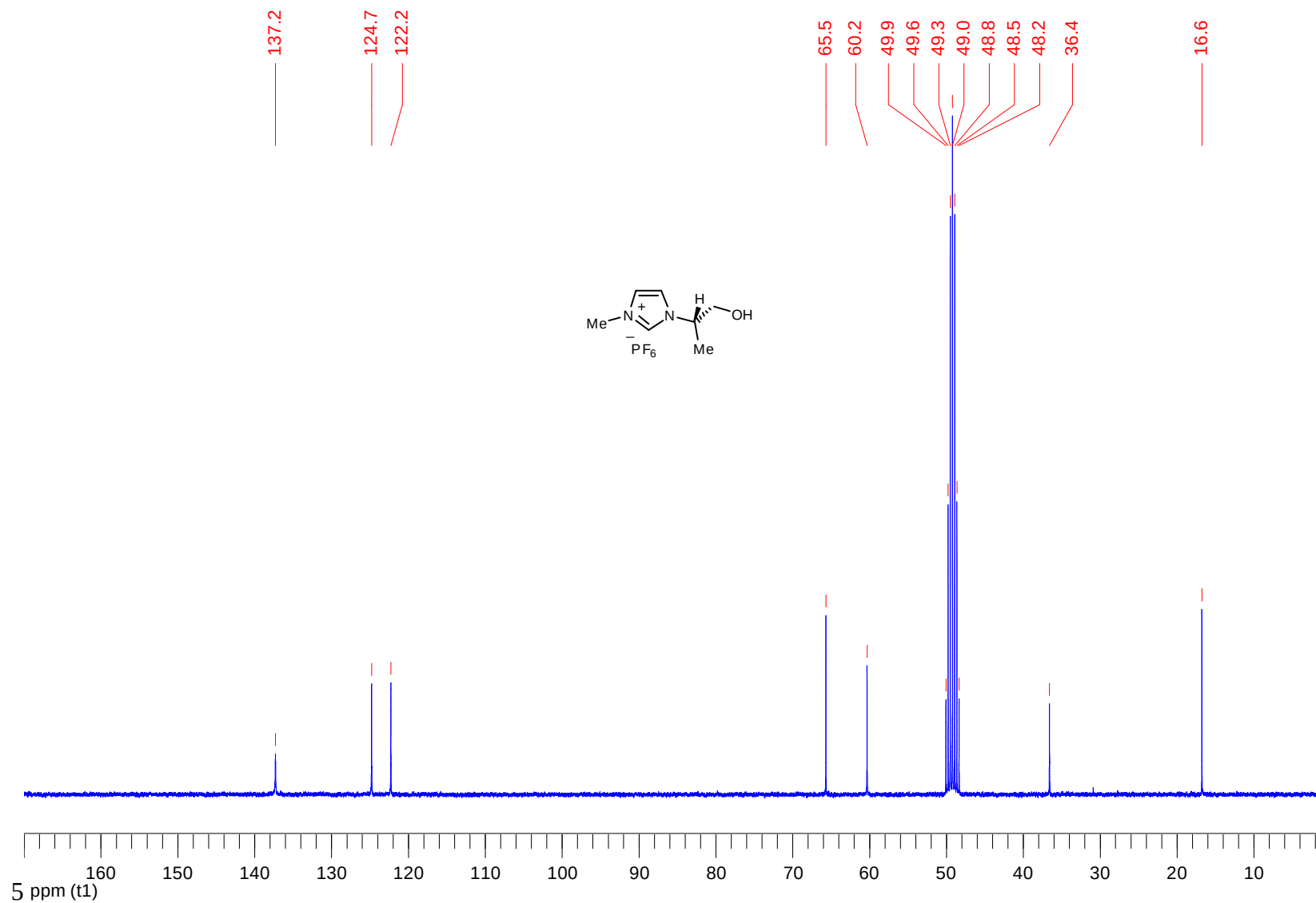
1-Methyl-3-[(2*S*)-1-hydroxy-2-propanyl]imidazolium iodide (9) (^{13}C NMR, 75 MHz, CD_3OD).



1-Methyl-3-[(2S)-1-hydroxy-2-propanyl]imidazolium hexafluorophosphate (10) (^1H NMR, 300 MHz, CD_3OD).

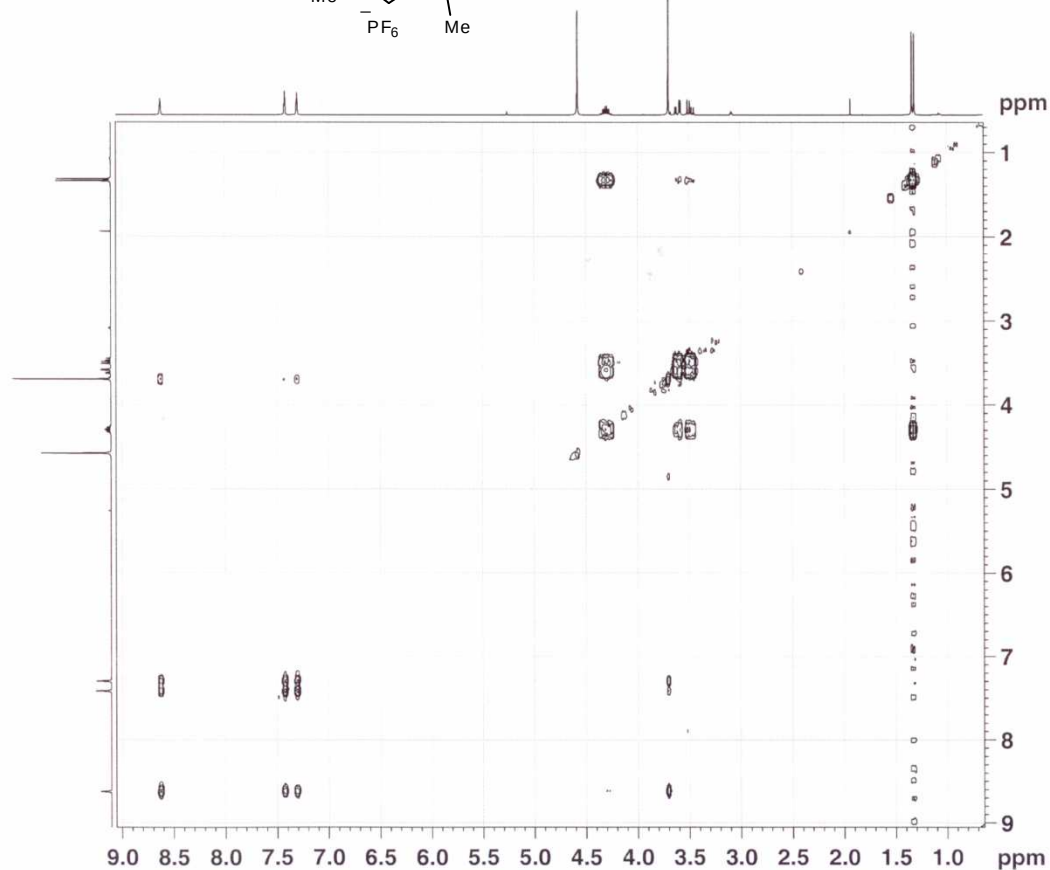
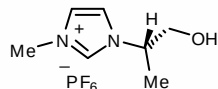


1-Methyl-3-[(2*S*)-1-hydroxy-2-propanyl]imidazolium hexafluorophosphate (10) (^{13}C NMR, 75 MHz, CD_3OD).



1-Methyl-3-[(2S)-1-hydroxy-2-propanyl]imidazolium hexafluorophosphate (10) (COSY, 300 MHz, CD₃OD).

COSY – J69Fc



Avance 300 a

Current Data Parameters
NAME: pastre_j_service300a
EXPNO: 35
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20080221
Time: 20.13
INSTRUM: spect
PROBHD: 5 mm BBO BB-1H
PULPROG: zgpg30
TD: 65536
SOLVENT: MeOD
NS: 4
DS: 4
SWH: 2525.252 Hz
FIDRES: 1.213013 Hz
AQ: 0.4055540 sec
RG: 101.6
DM: 198.000 usec
DE: 6.50 usec
TE: 300.2 K
DQ: 0.0000100 sec
D1: 1.87138498 sec
d13: 0.00000400 sec
D16: 0.00000000 sec
INQ: 0.00019600 sec

===== CHANNEL f1 =====
NUC1: 1H
P1: 11.20 usec
PL1: 0.00 dB
SFO1: 300.1325472 MHz

===== GRADIENT PULPROG =====
GPMAG: SINE.100
GPMAG2: SINE.100
GPMAG3: SINE.100
GPT1: 16.00 %
GPT2: 12.00 %
GPT3: 40.00 %
P16: 1000.00 usec

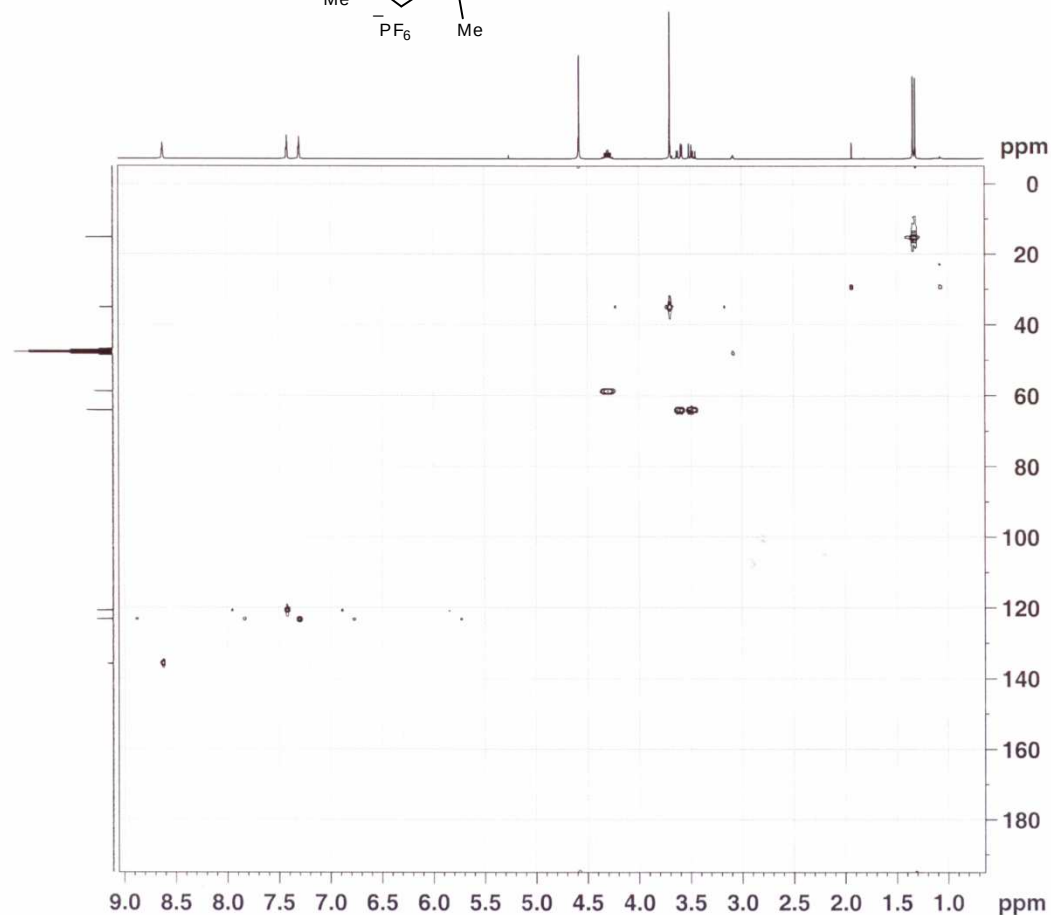
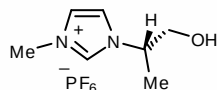
F1 - Acquisition parameters
RG: 1
TD: 65536
SFO1: 300.1315 MHz
FIDRES: 9.864257 Hz
SW: 8.414 ppm
F0MODE: QF

F2 - Processing parameters
SI: 32768
SF: 300.130723 MHz
WDW: EM
SSB: 0
LB: 0.00 Hz
GB: 0
PC: 1.40

F1 - Processing parameters
SI: 16384
SF: 300.130723 MHz
WDW: EM
SSB: 0
LB: 0.00 Hz
GB: 0

1-Methyl-3-[(2S)-1-hydroxy-2-propanyl]imidazolium hexafluorophosphate (10) (HSQC, 300 MHz, CD₃OD).

HSQC – J69Fc



Current Data Parameters
NAME pastre_1_service100a
EXPNO 16
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080225
Time 8.45
INSTRUM spect
PROBHD 5 mm BBO
PULPROG zgpg30
TD 1024
SOLVENT MeOD
NS 4
DS 16
SWH 2525.252 Hz
FIDRES 2.464047 Hz
AQ 0.125000 sec
RG 13004
DM 198.000 usec
DE 6.50 usec
TE 298.0 K
CLOCK 145.000000
d0 0.0000000 sec
d1 0.9480000 sec
d4 0.00172414 sec
d11 0.01000000 sec
d13 0.00004800 sec
d16 0.00020000 sec
DELTA 0.00122840 sec
DELTA1 0.00071614 sec
LNO 0.00003110 sec
PTCNT 128

***** CHANNEL f1 *****
NUC1 1H
P1 11.20 usec
P2 22.40 usec
P28 1000.00 usec
PL1 -1.00 dB
RF01 300.1315273 MHz

***** CHANNEL F2 *****
CPDPRG2 gprg4
NUC2 13C
P1 10.30 usec
P4 20.60 usec
PCPD2 100.00 usec
PL2 -1.00 dB
PL12 18.74 dB
RF02 75.4741984 MHz

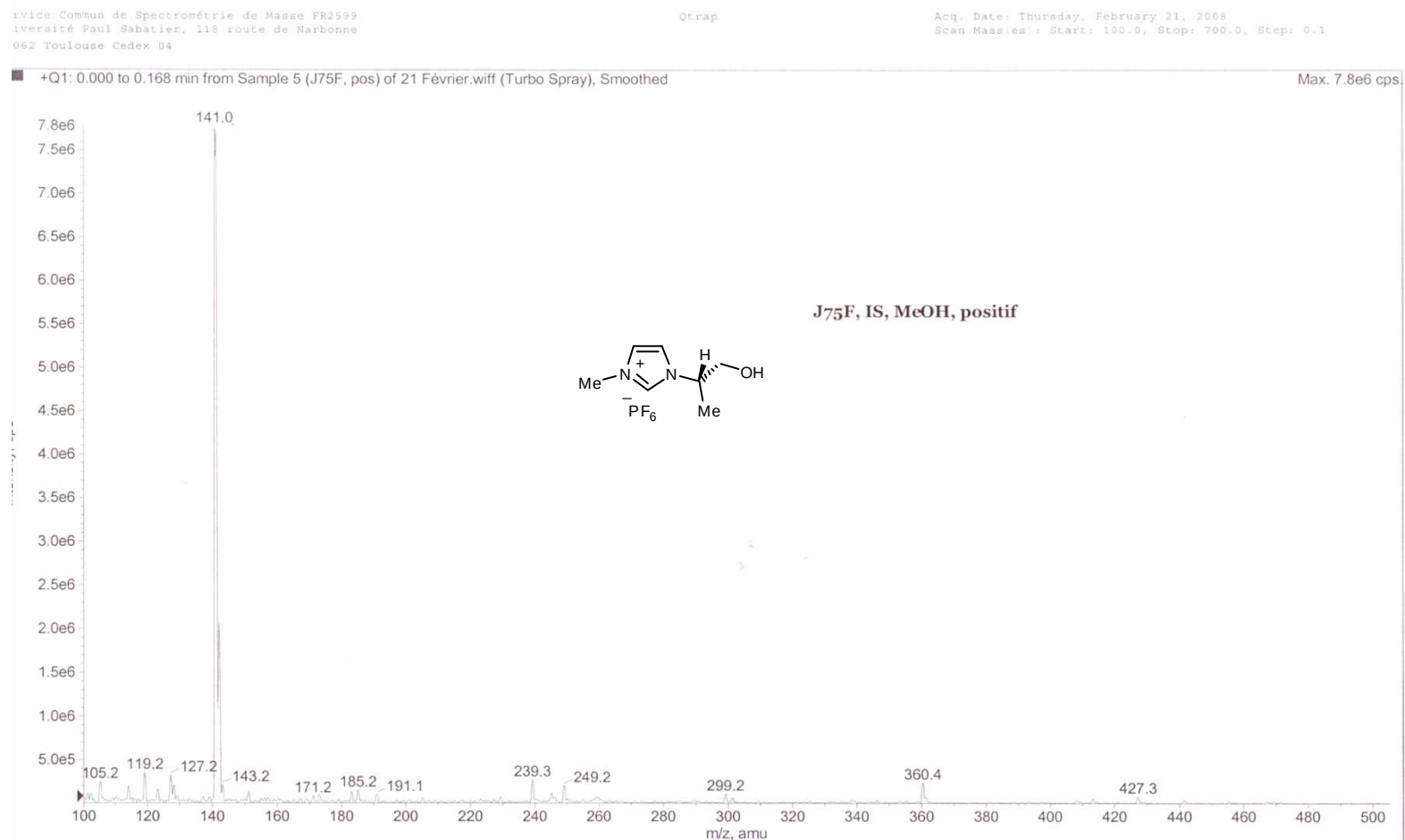
***** GRADIENT CHANNEL *****
GPRAMP1 SINE.100
GPRAMP2 SINE.100
GP21 80.00 s
GP22 20.10 s
P18 1000.00 usec

F1 - Acquisition parameters
ND0 2
TD 256
SF01 75.47492 MHz
FIDRES 59.00798 Hz
DM 0.125000
PRMODE Echo-Antiecho

F2 - Processing parameters
SI 2048
SF 300.1300723 MHz
WDW QDINE
SSB 0
GB 0
PC 1.40

F1 - Processing parameters
SI 2048
MC2 echo-antiecho
SF 75.4741984 MHz
WDW QDINE
SSB 0
LB 0.00 Hz
GB 0

1-Methyl-3-[(2S)-1-hydroxy-2-propanyl]imidazolium hexafluorophosphate (10) (ESI⁺).

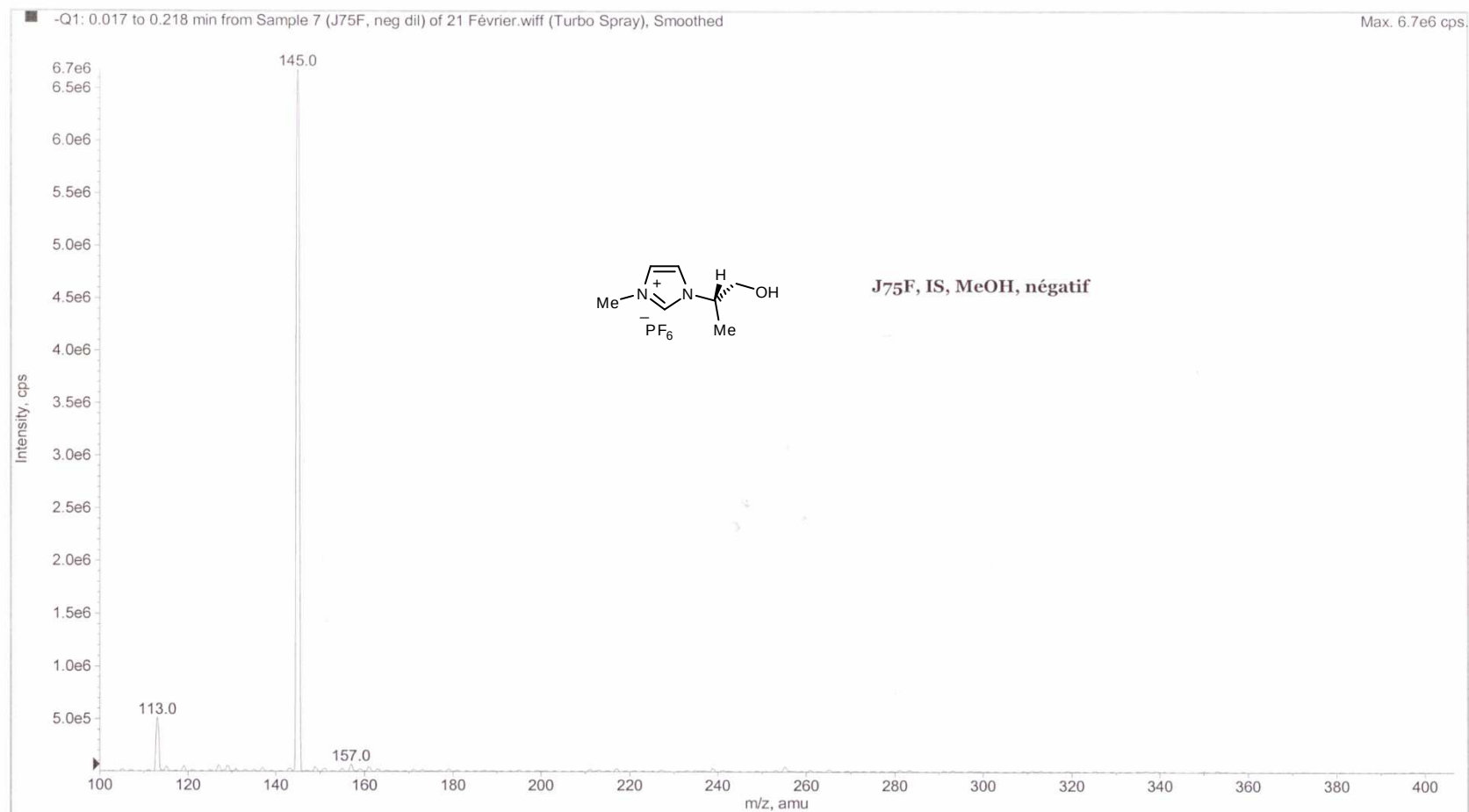


1-Methyl-3-[(2S)-1-hydroxy-2-propanyl]imidazolium hexafluorophosphate (10) (ESI⁻).

Service Commun de Spectrométrie de Masse FR2599
Université Paul Sabatier, 118 route de Narbonne
31062 Toulouse Cedex 04

Qtrap

Acq. Date: Thursday, February 21, 2008
Scan Mass(es): Start: 100.0, Stop: 700.0, Step: 0.1



1-Methyl-3-[(2S)-1-hydroxy-2-propanyl]imidazolium hexafluorophosphate (10) (HRMS, ESI⁺).

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

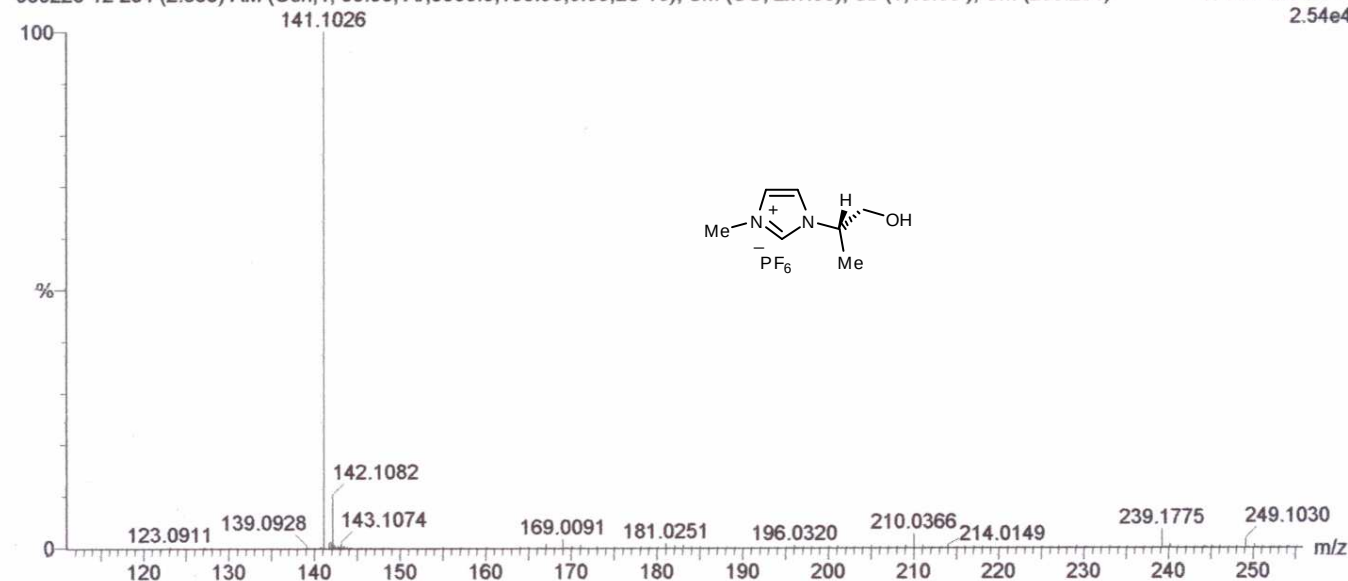
Monoisotopic Mass, Odd and Even Electron Ions

121 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)

J75F

080228-12 254 (2.865) AM (Cen,4, 80.00, Ar,5000.0,196.96,0.80,LS 10); Sm (SG, 2x1.00); Sb (1,40.00); Cm (238:254)

1: TOF MS ES+
2.54e4



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
141.1026	141.1028	-0.2	-1.3	2.5	1	C7 H13 N2 O
	141.1014	1.2	8.2	3.0	2	C5 H11 N5
	141.1004	2.2	15.7	-0.5	3	C5 H14 N2 O Na