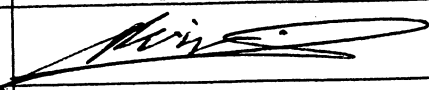


NMR SPECTROMETRY

Contributor's name and address:	S.H. van Krimpen TNO Prins Maurits Laboratory P.O. Box 45 2280 AA Rijswijk The Netherlands
Secretariat identification code	6-3-274
Signature	
Chemical information:	
Chemical name	1,2,2-trimethylpropyl S-2-diethyl-aminoethyl methylphosphonothiolate
CAS register number (optional)	
Chemical structure with numbering of atoms	see spectrum
Molecular formula (optional)	C ₁₃ H ₃₀ NO ₂ PS
Sample information:	
Sample purity (optional)	
Sample concentration (optional)	26mg/0.7ml
Solvent	CDCl ₃
pH (if relevant)	
Source (optional)	TNO-PML
Reference-chemical shift (internal/external)	TMS internal
Instrument information:	
Manufacturer	Varian
Model	VXR-400S
Spectrometer frequency ¹ H	400
Data system (optional)	Sun OS
Software version (optional)	VNMR 4.3B
Experimental information:	
Nucleus measured	¹ H
Sample temperature	30 °C
Spectral width (Hz)	6499.8
Data points in Fourier transformed spectrum	128K
Repetition time (optional)	8 s
Pulse angle (μs and degrees) (optional)	16.5/60
Line width of a certain line (e.g. TMS) (optional)	0.3 Hz
Window function (e.g. line broadening) (optional)	not used
Date of experiment (optional)	14 March 96
Data points in FID (optional)	64K

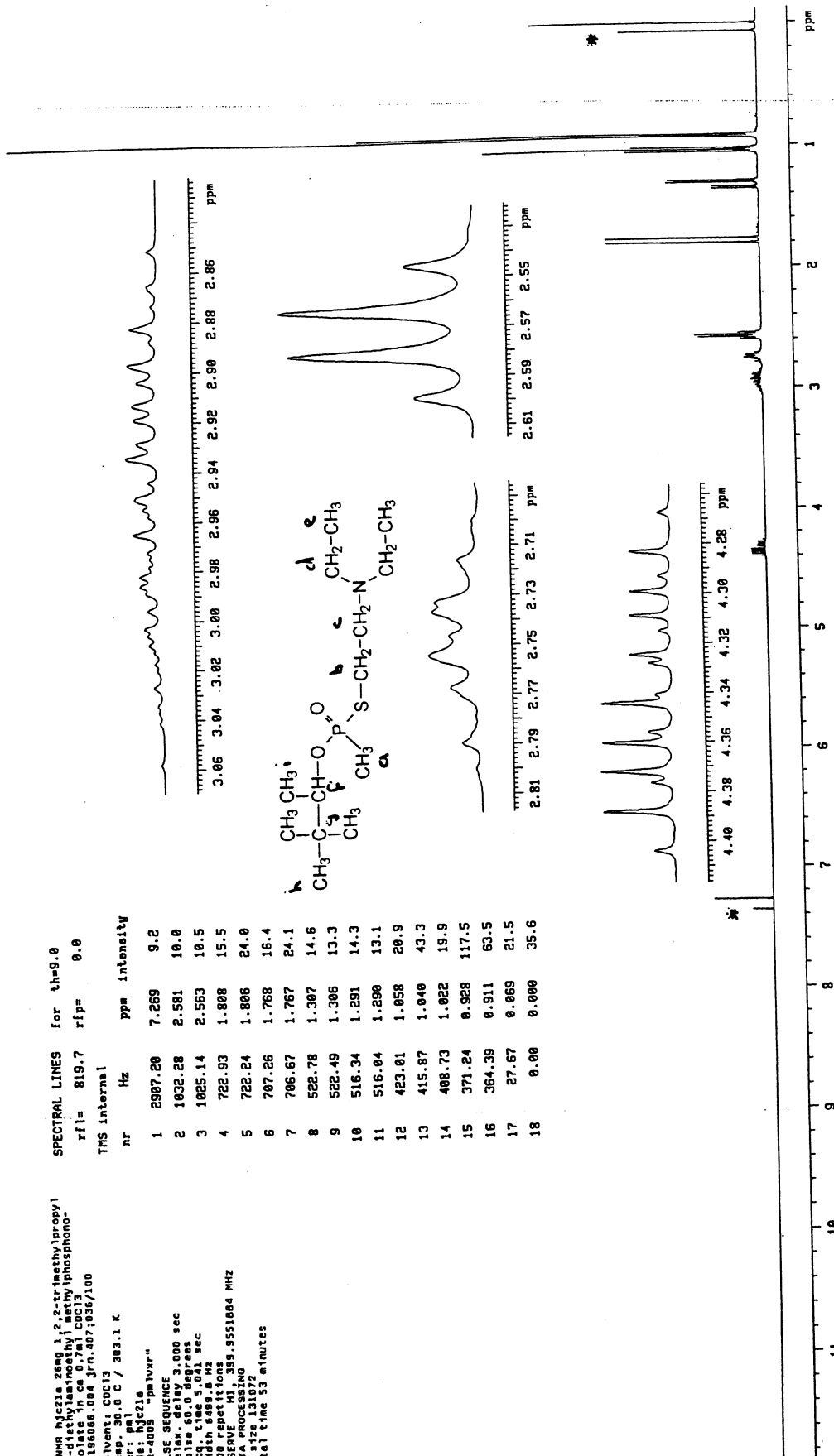
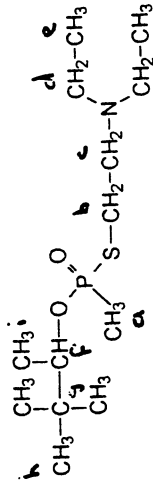
1H-NMR h1c1s1, 2500, 1, 2-trimethylpropyl
 S-2-diethylaminoethyl methylphosphono-
 thiolate in ca 0.7ml CDCl3
 21419686.004 Jrn.407;036/100

Solvent: CDCl3
 Temp: 30.0 C / 303.1 K
 User: mjczis
 File: h1c1s1
 VNR-400S 1pm1vvr"

PULSE SEQUENCE z, 900 sec
 Relax: 600 sec
 Acq. time 5.041 sec
 Width 6499.6 Hz
 400 repetitions
 OBSERVE: h1, 359.5551884 MHz
 PROCESSING
 FT size 131072
 Total time 53 minutes

SPECTRAL LINES for tk=9.0

nr	Hz	ppm	intensity
1	2907.20	7.269	9.2
2	1032.28	2.581	10.0
3	1025.14	2.563	10.5
4	722.93	1.808	15.5
5	722.24	1.806	24.0
6	707.26	1.768	16.4
7	706.67	1.767	24.1
8	522.78	1.307	14.6
9	522.49	1.306	13.3
10	516.34	1.291	14.3
11	516.04	1.290	13.1
12	423.01	1.058	20.9
13	415.87	1.040	43.3
14	408.73	1.022	19.9
15	371.24	0.928	117.5
16	364.39	0.911	63.5
17	27.67	0.069	21.5
18	0.00	0.000	35.6



1,2,2-trimethylpropyl S-2-diethylaminoethyl
 methylphosphonothiolate (2 enantiomers)
 Concentration ca. 26 mg/0.7 ml CDCl₃
 Reference TMS internal; resolution: 0.3 Hz