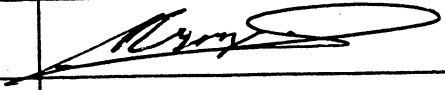


NMR SPECTROMETRY

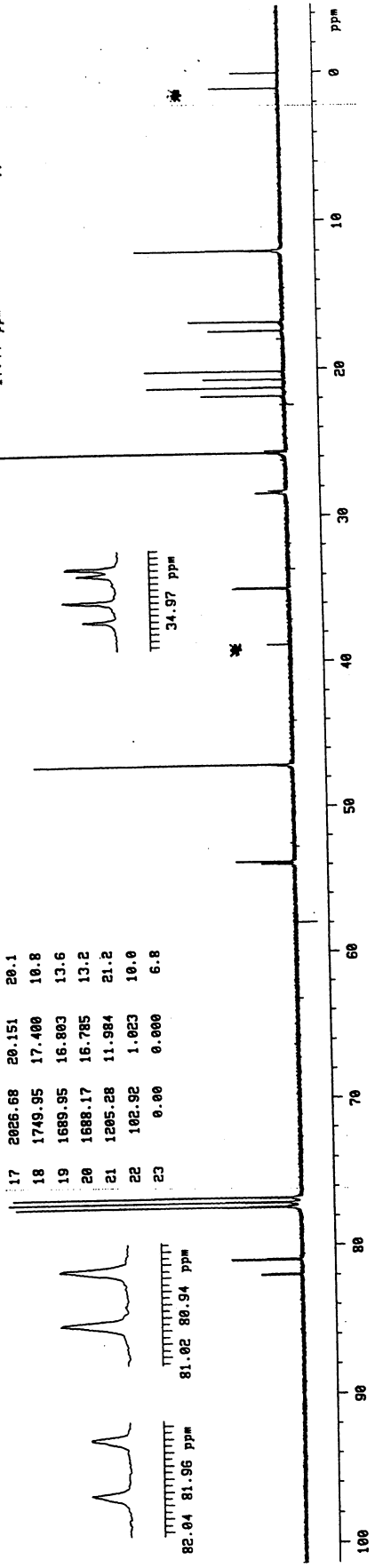
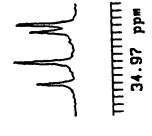
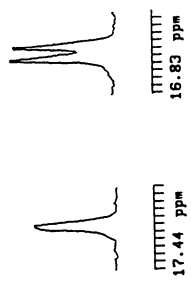
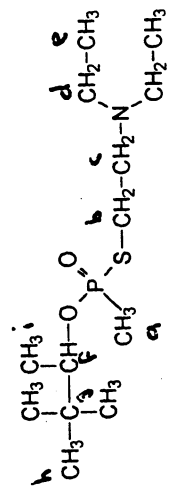
Contributor's name and address:	S.H. van Krimpen TNO Prins Maurits Laboratory P.O. Box 45 2280 AA Rijswijk The Netherlands
Secretariat identification code	6-3-275
Signature	
Chemical information:	
Chemical name	1,2,2-trimethylpropyl S-2-diethyl-aminoethyl methylphosphonothiolate
CAS register number (optional)	
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	¹³ C
Sample temperature	30 °C
Spectral width (Hz)	10655.3
Data points in Fourier transformed spectrum	128K
Repetition time (optional)	3.1 s
Pulse angle (μs and degrees) (optional)	13.2/60
Line width of a certain line (e.g. TMS) (optional)	0.5 Hz
Window function (e.g. line broadening) (optional)	0.2 Hz
Date of experiment (optional)	14 March 96
Data points in FID (optional)	64K

13C-NMR c1218c13) 20mg 1,2,2-trimethyl-
propyl phosphonothioate (2 enantiomers)
21419085.004 /rn.407/436/200

Solvent: CDCl3
Temp: 30.0 C / 303.1 K
User: pm1
File: c12182
VNR-400S "pm1vnr"
PULSE SEQUENCE
Pulse 80.0 sec
Pulse delay 1.00 sec
Width 10555.3 Hz
18000 repetitions
OBSERVE c13, 100.568008 MHz
DECOUPLE H1, 399.3571662 MHz
Power: auto on
SOLVENT DECOUPLING
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.2 Hz
SI size 131072
Total time 15.4 hours

SPECTRAL LINES for th=6.5
rfl= 460.0 rfp= 0.0
TMS internal

nr	Hz	ppm	intensity
1	8143.62	80.972	10.0
2	8135.33	80.889	10.1
3	7779.74	77.354	41.0
4	7747.88	77.037	42.1
5	7715.85	76.718	41.4
6	5410.33	53.795	8.3
7	5405.94	53.751	8.4
8	4737.69	47.107	37.5
9	4734.93	47.079	21.3
10	3516.00	34.959	8.1
11	3510.79	34.908	7.6
12	2585.66	25.769	103.1
13	2583.87	25.691	64.8
14	2194.96	21.824	12.0
15	2138.21	21.260	19.9
16	2082.45	20.706	11.6
17	2026.68	20.151	20.1
18	1749.95	17.400	10.8
19	1689.95	16.803	13.6
20	1688.17	16.785	13.2
21	1205.28	11.984	21.2
22	102.92	1.023	10.0
23	0.00	0.000	6.8



a: 20.8(21.4) ppm
b: 28.6(28.4) ppm
c: 53.9(54.1) ppm
d: 47.2(47.2) ppm
e: 12.1(12.1) ppm
f: 81.1(82.1) ppm
g: 35.1(35.1) ppm
h: 25.8(25.8) ppm
i: 16.9(17.5) ppm
J(aP) : 111.5(112.5) Hz
J(bP) : ca 2.5(ca 2.5)Hz
J(cP) : 4.4(4.1) Hz
J(fP) : 8.3(8.6) Hz
J(gP) : 5.2(7.3) Hz
J(iP) 1.8(0.0) Hz

1,2,2-trimethylpropyl S-2-diethylaminoethyl
methylphosphonothioate (2 enantiomers)
Concentration ca.26 mg/0.7 ml CDCl3
Reference TMS internal; resolution: 0.5 Hz