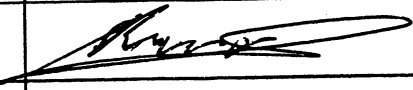


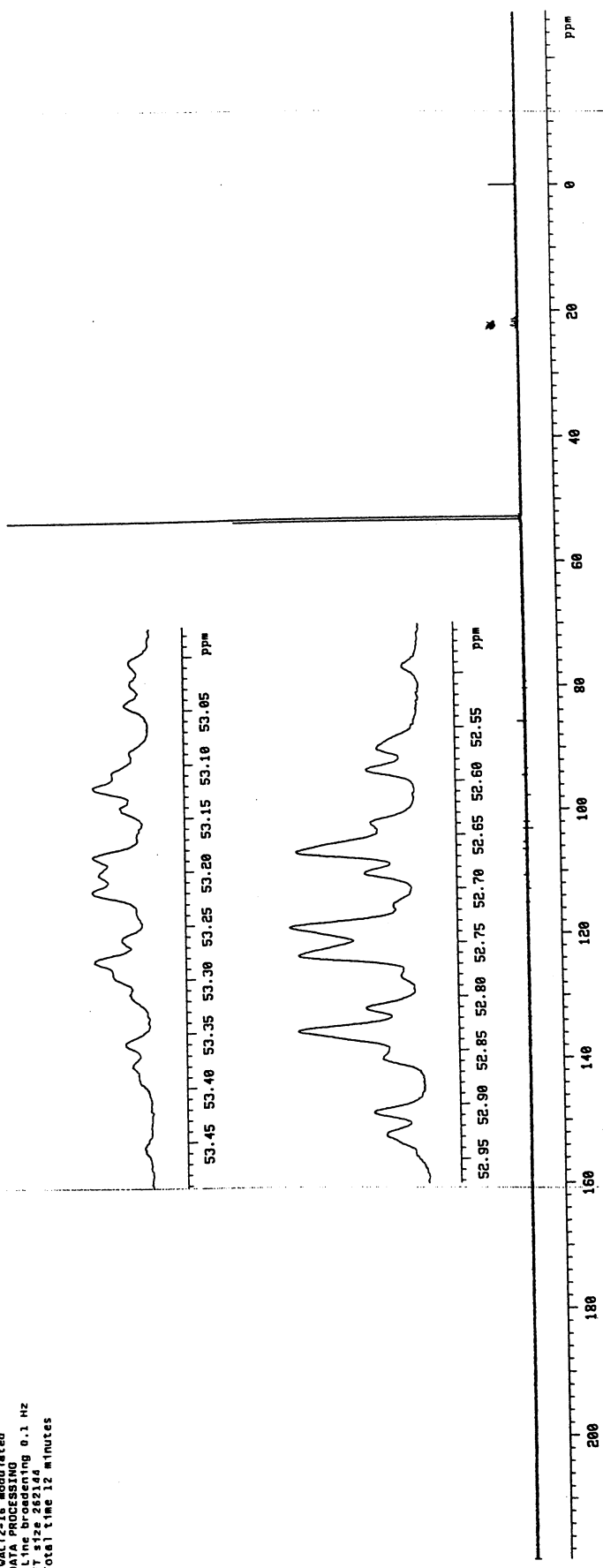
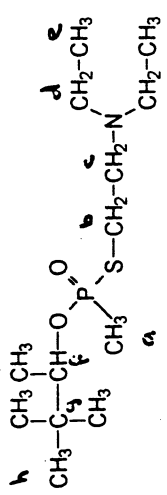
NMR SPECTROMETRY

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	6-3-276
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)	C13H30NO2PS
Sample information:	
Sample purity (optional)	
Sample concentration (optional)	26mg/0.7ml
Solvent	CDCl3
pH (if relevant)	
Source (optional)	TNO-PML
Reference-chemical shift (internal/external)	H3PO4 external
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	31P
Sample temperature	30 °C
Spectral width (Hz)	40000
Data points in Fourier transformed spectrum	256K
Repetition time (optional)	5 s
Pulse angle (µs and degrees) (optional)	10.3/60
Line width of a certain line (e.g. TMS) (optional)	1.2 Hz
Window function (e.g. line broadening) (optional)	0.1 Hz
Date of experiment (optional)	15 March 96
Data points in FID (optional)	128000

31P-NMR p1c21b2(1v) + H3PO4 26mg 1,2,2-trimethylpropyl S-2-diethylaminoethyl methylphosphonothiolate (2 enantiomers) Concentration ca. 26 mg/0.7 ml CDCl3
 214156066 004 3rn.407:036/100
 Solvent: CDCl3
 Temp: 30.0 C / 303.1 K
 User: pm1
 File: p1c21b2
 VNR-4005 "pm1var"
 PULSE SEQUENCE
 Relax. delay 3.400 sec
 Pulse 50.0 degrees
 Width 40000.0 Hz
 144 Repetitions
 OBSERVE P31, 161.9047166 MHz
 DECOUPLE H1, 399.9571985 MHz
 Acquisition
 off during delay
 VOLTAGE-15 modulated
 DATA PROCESSING
 Line broadening 0.1 Hz
 Gain 12.8212
 Total time 12 minutes

SPECTRAL LINES for t=2.6
 r1= 4442.2 rfp= 0.0
 H3PO4 external; dres 52.8ppm=1.2Hz
 nr Hz ppm intensity

1	8614.57	53.203	42.4
2	8541.32	52.750	75.8
3	0.00	0.000	3.8



P: 52.8(53.2) ppm J(aP) :15.6(15.6) Hz

1,2,2-trimethylpropyl S-2-diethylaminoethyl methylphosphonothiolate (2 enantiomers)
 Concentration ca. 26 mg/0.7 ml CDCl3
 Reference H3PO4 external. Resolution 52.8 ppm: 1.2 Hz