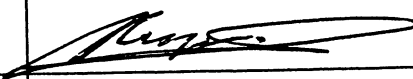
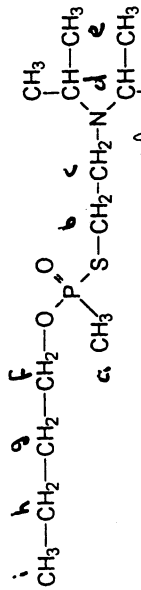


## NMR SPECTROMETRY

<b>Contributor's name and address:</b>	S.H. van Krimpen TNO Prins Maurits Laboratory P.O. Box 45 2280 AA Rijswijk The Netherlands
Secretariat identification code	6-3-278
Signature	
<b>Chemical information:</b>	
Chemical name	n-butyl S-2-diisopropylamino-ethyl methylphosphonothiolate
CAS register number (optional)	
Chemical structure with numbering of atoms	see spectrum
Molecular formula (optional)	C <sub>13</sub> H <sub>30</sub> NO <sub>2</sub> PS
<b>Sample information:</b>	
Sample purity (optional)	
Sample concentration (optional)	36.9mg/0.7ml
Solvent	CDCl <sub>3</sub>
pH (if relevant)	
Source (optional)	TNO-PML
Reference-chemical shift (internal/external)	TMS internal
<b>Instrument information:</b>	
Manufacturer	Varian
Model	VXR-400S
Spectrometer frequency <sup>1</sup> H	400
Data system (optional)	Sun OS
Software version (optional)	VNMR 4.3B
<b>Experimental information:</b>	
Nucleus measured	<sup>13</sup> C
Sample temperature	30 °C
Spectral width (Hz)	10655.3
Data points in Fourier transformed spectrum	128K
Repetition time (optional)	2.0 s
Pulse angle (μs and degrees) (optional)	13.2/60
Line width of a certain line (e.g. TMS) (optional)	0.7 Hz
Window function (e.g. line broadening) (optional)	0.2
Date of experiment (optional)	26 March 96
Data points in FID (optional)	32K



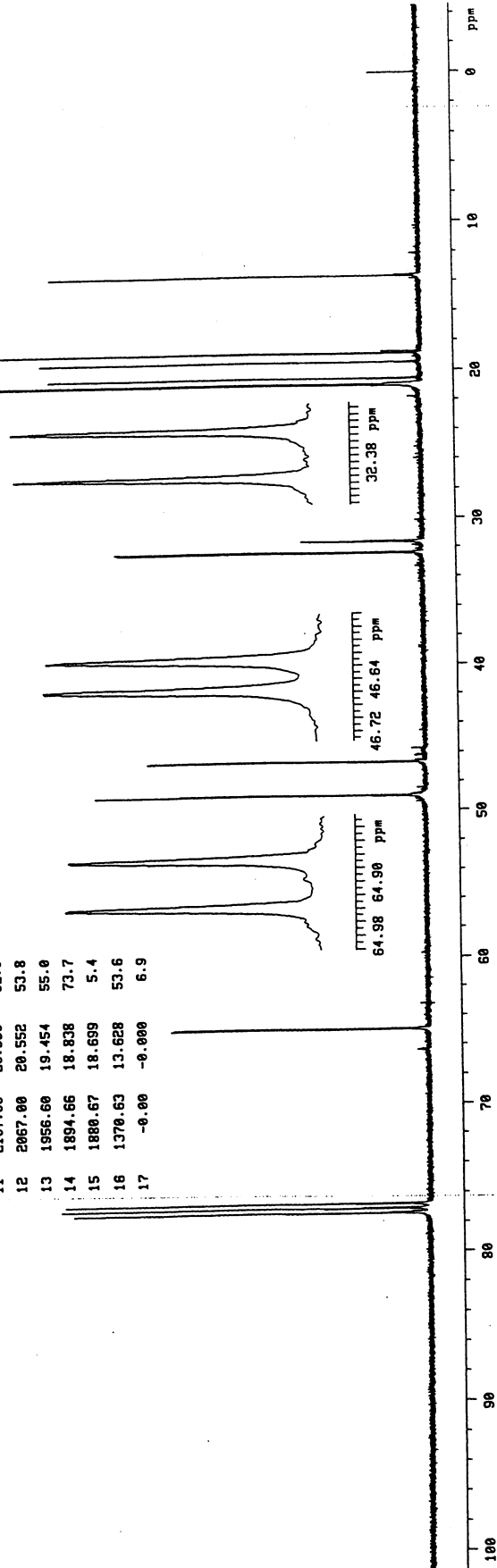
SPECTRAL LINES for t<sub>h</sub>=5.4

rfl= 459.6 rfp= 0.0

TMS=0.00ppm; dres=0.7Hz

nr	Hz	ppm	intensity
1	6531.22	64.940	37.0
2	6523.90	64.867	36.6
3	4921.75	48.937	47.6
4	4692.33	46.656	48.0
5	4687.78	46.610	39.6
6	3258.94	32.404	44.0
7	3251.95	32.334	44.4
8	3178.79	31.607	16.5
9	3176.51	31.584	17.5
10	2111.06	20.990	99.9
11	2107.00	20.950	92.0
12	2067.00	20.552	53.8
13	1956.60	19.454	55.0
14	1894.66	18.838	73.7
15	1880.67	18.699	5.4
16	1370.63	13.628	53.6
17	-0.00	-0.000	6.9

13C-NMR c.jc38b(1H)  
 36.9mg U6 in 0.7ml CDCl3  
 21419666.004 jrn.407;853/100  
 OBSERVE C13  
 FREQUENCY 100.574 MHz  
 SPECTRAL WIDTH 10655.3 Hz  
 ACQUISITION TIME 1.538 sec  
 RELAXATION DELAY 0.500 sec  
 PULSE WIDTH 13.2 usec  
 TEMPERATURE 30.0 deg. C.  
 NO. REPEATITIONS 25860  
 DECOUPLE H1  
 HIGH POWER 44  
 DECOUPLER CONTINUOUSLY ON  
 LALZ16 MODULATED  
 DOUBLE PRECISION ACQUISITION  
 DATA PROCESSING  
 LINE BROADENING 0.2 Hz  
 FT SIZE 131072  
 TOTAL ACQUISITION TIME 14.6 hours



**n-Butyl S-2-diisopropylaminoethyl methylphosphono-**  
**thiolate**  
 Concentration ca. 36.9 mg/0.7 ml CDCl<sub>3</sub>  
 Reference TMS internal; resolution: 0.7 Hz

a: 20.0 ppm  
 b: 31.6 ppm  
 c: 46.6 ppm  
 d: 48.9 ppm  
 e: 21.0/21.0 ppm

f: 64.9 ppm  
 g: 32.4 ppm  
 h: 18.8 ppm  
 i: 13.6 ppm

J(aP) : 110.4 Hz  
 J(bP) : 2.3 Hz  
 J(cP) : 4.6 Hz  
 J(fP) : 7.3 Hz  
 J(gP) : 7.0 Hz