

¹³C-NMR cjh06b2(1H) + TSPA-d4 pH=ca 2
17.6mg v27 1n ca 0.7ml D2O + DCI
214196066.004 jrn.458;051/100

Solvent: D2O
Temp. 30.0 C / 303.1 K
User: pm1
File: cjh06b2
VXR-400S "pm1vvr"

PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 60.0 degrees
Acq. time 2.906 sec
Width 11277.1 Hz
6000 repetitions

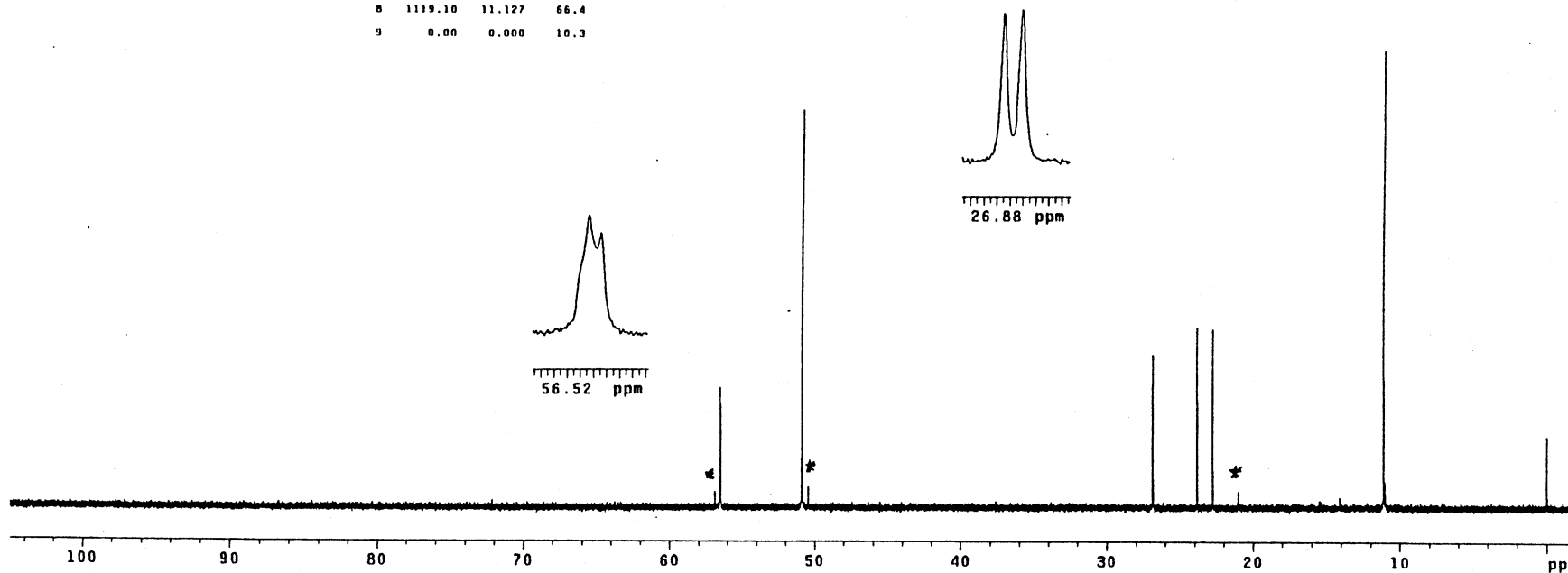
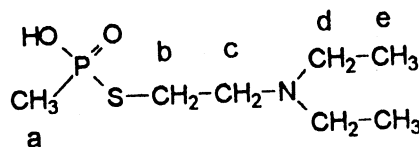
OBSERVE C13, 100.5671399 MHz
DECOUPLE H1, 399.9515670 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.1 Hz
FT size 262144
Total time 6.5 hours

SPECTRAL LINES for th=6.1

rfl= 719.2 rfp= 0.0

TSPA-d4=0.00ppm;dres=0.8Hz

nr	Hz	ppm	intensity
1	5680.94	56.486	17.3
2	5679.13	56.468	14.8
3	5117.13	50.880	57.6
4	2702.29	26.869	21.7
5	2699.54	26.842	22.1
6	2396.17	23.825	26.0
7	2288.96	22.759	25.6
8	1119.10	11.127	66.4
9	0.00	0.000	10.3



S-2-diethylaminoethyl methylphosphonothiolate
CAS
Nucleus : ¹³C{1H}
Frequency : 100.6 MHz
Concentration : 17.6 mg/0.7 ml D₂O + DCI (pH=2)
Reference TSPA-d4 internal. Res. : 0.8 Hz (TSPA-d4)
Instrument : Varian VXR 400S

Temperature : 30 °C
Spectral width : 11277.1 Hz
Data point (FID) : 64 K
Pulse angle : 12.3 μs (60°)
Number of pulses : 6000
Repetition time : 3.9 s
Line broadening : 0.1 Hz
Data points (spec) : 256 K

a: 23.3 ppm J(aP) : 107.2 Hz
b: 26.9 ppm J(bP) : 2.5 Hz
c: 56.5 ppm
d: 50.9 ppm
e: 11.1 ppm