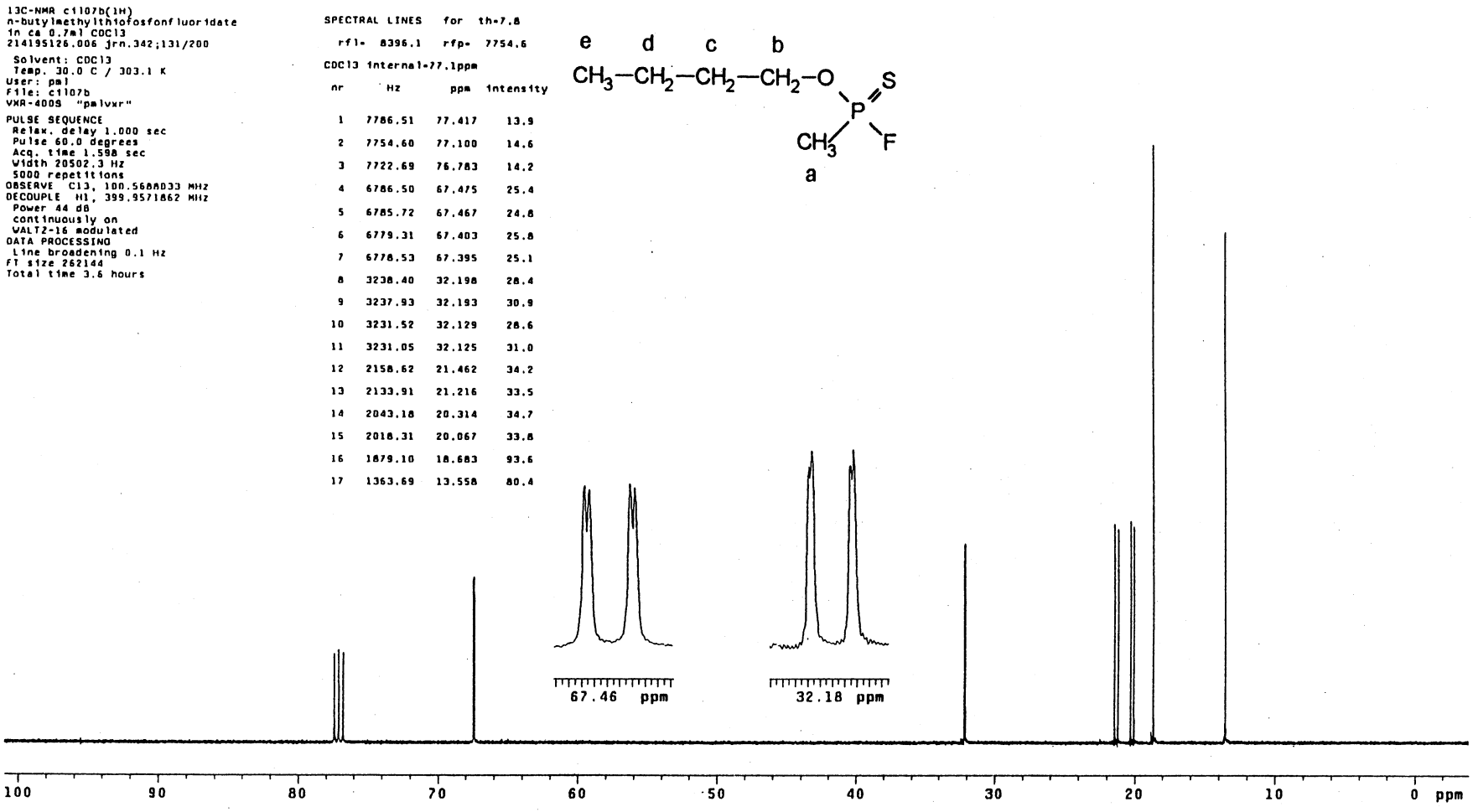

n-Butyl methylthiophosphonofluoridate
CAS 4241-36-5
Nucleus : $^{13}C\{1H\}$
Frequency : 100.6 MHz
Concentration : ca. 75 mg/0.7 ml $CDCl_3$
Ref. $CDCl_3$ internal 77.1 ppm. Res. : 0.8 Hz (13.6 ppm)
Instrument : Varian VXR 400S

Temperature : 30 °C
Spectral width : 20502.3 Hz
Data point (FID) : 64 K
Pulse angle : 13.0 µs (60°)
Number of pulses : 5000
Repetition time : 2.6 s
Line broadening : 0.1 Hz
Data points (spec) : 256 K

a: 20.8 ppm J(aP) : 115.5 Hz J(aF) : 24.8 Hz
b: 67.4 ppm J(bP) : 7.2 Hz J(bF) : 0.8 Hz
c: 32.1 ppm J(cP) : 6.9 Hz J(cF) : 0.5 Hz
d: 18.7 ppm
e: 13.6 ppm