
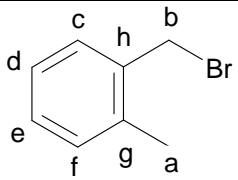


NMR SPECTROMETRY

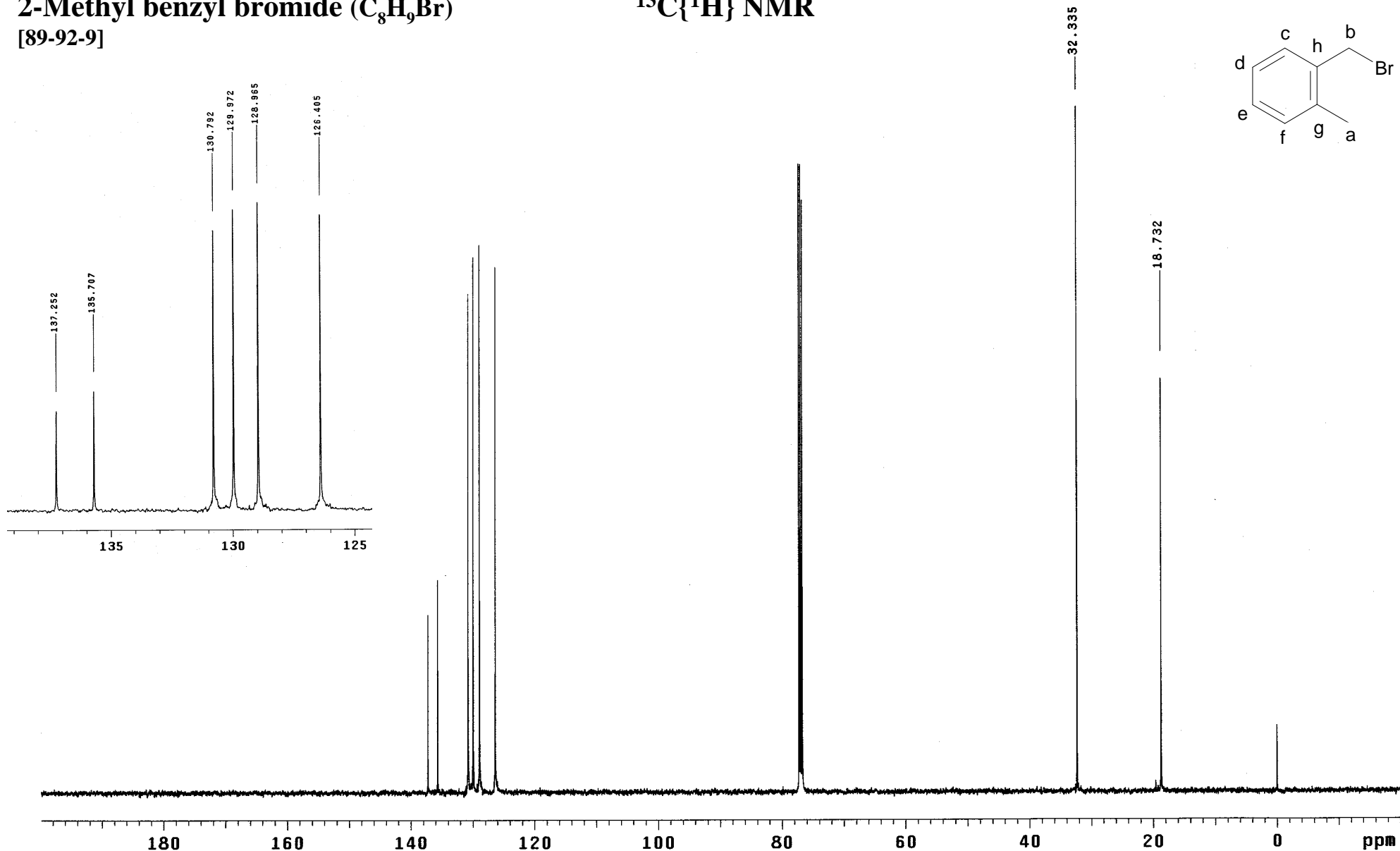
| | | |
|--|--|---------------------------------------|
| Contributor's name and address: | | Verification Laboratory |
| Secretariat identification code | 25-3-0016r (p1/3) | DSO National Laboratories |
| Signature |  | 11 Stockport Road Singapore 117605 |
| Chemical information: | | |
| Chemical name | 2-Methylbenzyl bromide | |
| Schedule number | | |
| CAS registry number | 89-92-9 | |
| Chemical structure with numbering of atoms |  | |
| Molecular formula | C ₈ H ₉ Br | |
| Sample information: | | |
| Sample purity | 98 % | |
| Sample concentration | 69 mg/mL | |
| Solvent | CDCl ₃ | |
| pH | - | |
| Source | Aldrich | |
| Reference chemical shift (Internal) | TMS, 0 ppm | |
| Instrument information: | | |
| Manufacturer | Varian, Inc. | |
| Model | Inova 500 MHz | |
| Spectrometer frequency | 500 MHz | |
| Software version | VNMR version 6.1C | |
| Experimental information: | | |
| Nucleus measured | ¹³ C{ ¹ H} | |
| Sample temperature | 25 °C | |
| Spectral width (Hz) | 35133.9 | |
| Data points in Fourier transformed spectrum | 65536 | |
| Repetition time | 2.5 s | |
| Pulse angle (μs and degrees) | 4.125 μs, 45° | |
| Date of experiment | 14 Apr 2005 | |
| Data points in FID | 35108 | |
| Number of scans | 720 | |
| Baseline correction | Yes | |
| Spectral information: | | |
| Chemical shifts (ppm) assigned except for acidic protons | Ca = 18.73, Cb = 32.34, Cc = 129.97, Cd = 126.41, Ce = 128.97, Cf = 130.79, Cg = 135.71, Ch = 137.25 | |
| Coupling constants (Hz) | - | |

25-3-0016r (p2/3)

2-Methyl benzyl bromide (C₈H₉Br)

[89-92-9]

¹³C{¹H} NMR



Res.Freq: 125.653 MHz
Solvent: CDCl₃
Temperature: 25°C
Concentration: 69 mg/mL
Reference: TMS (internal)

Spectral Width: 35133.9 Hz
Data points [FID]: 35108
Data points [Spectrum]: 65536
Pulse width: 4.125 μs, 45°
Number of Scans: 720

Line broadening: 2
Rep. time: 2.5 s
Resolution: 1.07 Hz (TMS)
Baseline correction: Yes
Instrument: Varian INOVA 500

| Nuc δ[ppm] | Nuc δ[ppm] |
|------------|------------|
| a: 18.73 | e: 128.97 |
| b: 32.34 | f: 130.79 |
| c: 129.97 | g: 135.71 |
| d: 126.41 | h: 137.25 |

25-3-0016r (p3/3)

2-Methyl benzyl bromide (C₈H₉Br)

[89-92-9]

