
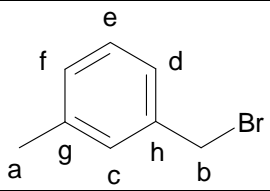


## NMR SPECTROMETRY

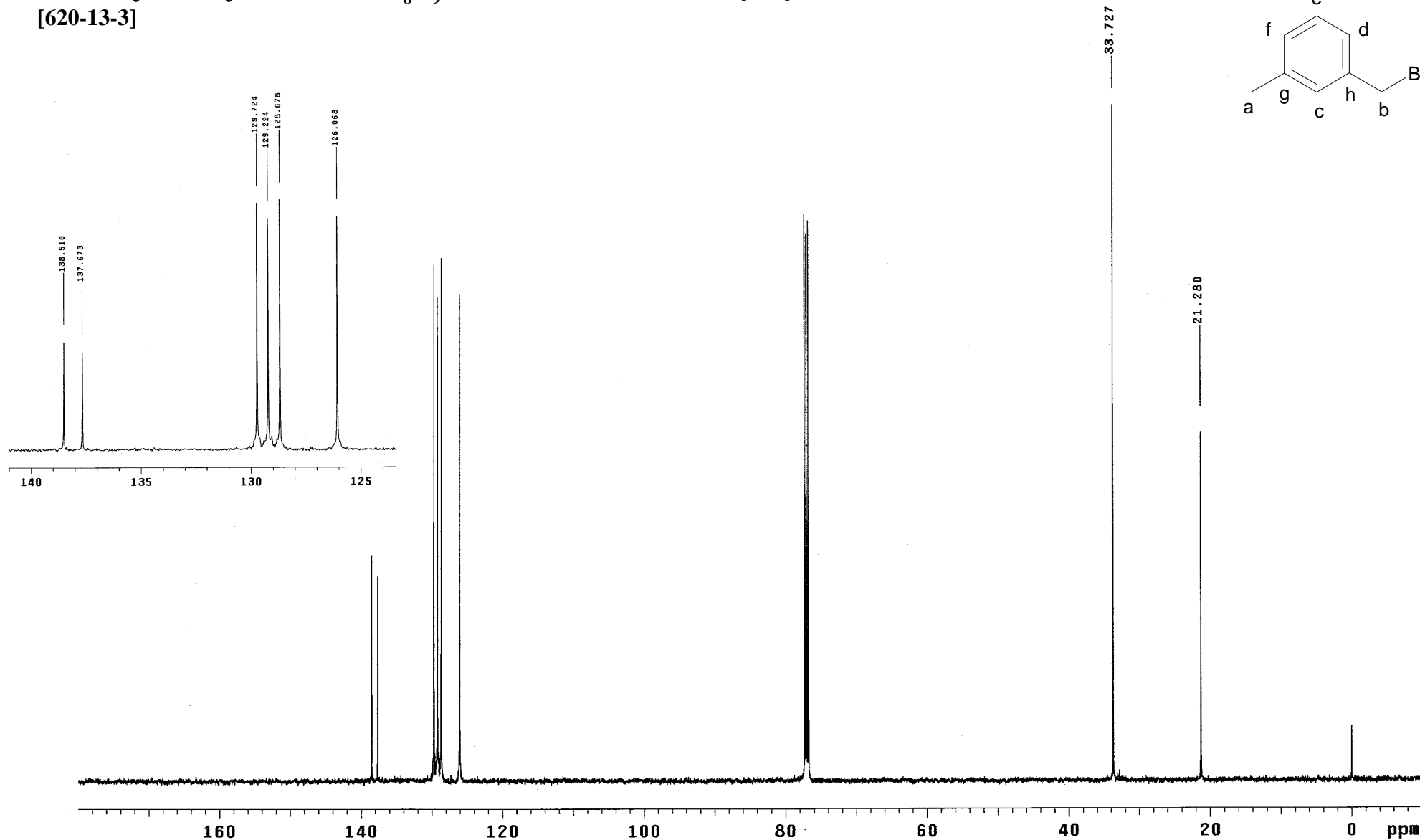
|  |  |                                       |
|--|--|---------------------------------------|
| <b>Contributor's name and address:</b>             |  | Verification Laboratory               |
| Secretariat identification code                    | 25-3-0018r (p1/3)  | DSO National Laboratories             |
| Signature  |                     | 11 Stockport Road<br>Singapore 117605 |
| <b>Chemical information:</b>                       |  |                                       |
| Chemical name                                      | 3-Methylbenzyl bromide   |                                       |
| Schedule number                                    |  |                                       |
| CAS registry number                                | 620-13-3   |                                       |
| Chemical structure with numbering of atoms         |                    |                                       |
| Molecular formula                                  | C <sub>8</sub> H <sub>9</sub> Br   |                                       |
| <b>Sample information:</b>                         |  |                                       |
| Sample purity                                      | 97 %   |                                       |
| Sample concentration                               | 69 mg/mL   |                                       |
| Solvent  | CDCl <sub>3</sub>  |                                       |
| pH   | -  |                                       |
| Source   | Merck  |                                       |
| Reference chemical shift (internal)                | TMS, 0 ppm   |                                       |
| <b>Instrument information:</b>                     |  |                                       |
| Manufacturer                                       | Varian, Inc.   |                                       |
| Model  | Inova 500 MHz  |                                       |
| Spectrometer frequency                             | 500 MHz  |                                       |
| Software version                                   | VNMR version 6.1C  |                                       |
| <b>Experimental information:</b>                   |  |                                       |
| Nucleus measured                                   | <sup>13</sup> C{ <sup>1</sup> H}   |                                       |
| Sample temperature                                 | 25 °C  |                                       |
| Spectral width (Hz)                                | 23923.4  |                                       |
| Data points in Fourier transformed spectrum        | 32768  |                                       |
| Repetition time                                    | 2.5 s  |                                       |
| Pulse angle (μs and degrees)                       | 4.125 μs, 45°  |                                       |
| Date of experiment                                 | 14 Apr 2005  |                                       |
| Data points in FID                                 | 23874  |                                       |
| Number of scans                                    | 720  |                                       |
| Baseline correction                                | Yes  |                                       |
| <b>Spectral information:</b>                       |  |                                       |
| Chemical shifts assigned except for acidic protons | Ca = 21.28, Cb = 33.73, Cc = 129.72, Cd = 126.06, Ce = 128.68, Cf = 129.22, Cg = 138.51, Ch = 137.67 |                                       |
| Coupling constants                                 |  |                                       |

25-3-0018r (p2/3)

# 3-Methyl benzyl bromide (C<sub>8</sub>H<sub>9</sub>Br)

[620-13-3]

## <sup>13</sup>C{<sup>1</sup>H} NMR



Res.Freq: 125.653 MHz  
Solvent: CDCl<sub>3</sub>  
Temperature: 25°C  
Concentration: 69 mg/mL  
Reference: TMS (internal)

Spectral Width: 35133.9 Hz  
Data points [FID]: 23874  
Data points [Spectrum]: 32768  
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: 21.28   | e: 128.68  |
| b: 33.73   | f: 129.22  |
| c: 129.72  | g: 138.51  |
| d: 126.06  | h: 137.67  |

**3-Methyl benzyl bromide (C<sub>8</sub>H<sub>9</sub>Br)**

[620-13-3]

