Single molecule conductance through multiple π-π stacked benzene rings determined with direct electrode to benzene ring connections

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Supplementary Information

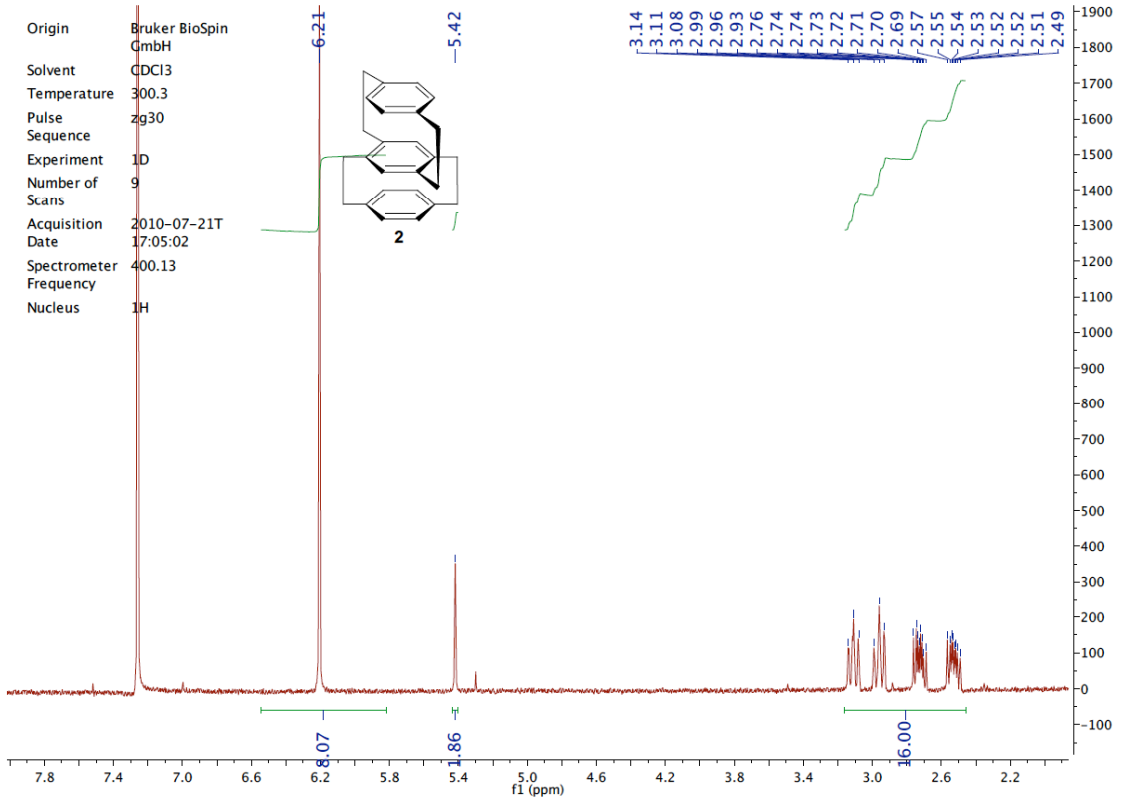
General Information:

Chemicals: Solvents, inorganic salts, and organic reagents were purchased from commercial sources and used without further purification unless otherwise mentioned.

Chromatography: Merck pre-coated 0.25 mm silica plates containing a 254 nm fluorescence indicator were used for analytical thin-layer chromatography. Flash chromatography was performed on 230-400 mesh silica (SiliaFlash® P60) from Silicycle.

Spectroscopy: NMR spectra were obtained on a Bruker DPX 300 or 400 MHz spectrometer. Spectra were analyzed with the MestreNova Software (Version 6.1). CI-MS spectra were taken on a Nermag R-10-10 instrument. FAB MS spectra were taken on a JEOL JMS-DX-303 HF instrument using either glycerol or p-nitrobenzyl alcohol as matrices. Matrix assisted laser desorption ionization (MALDI) mass spectra were acquired using an Applied Biosystems Voyager DE Pro time-of-flight mass spectrometer. Positive ion mass spectra were acquired in the linear mode using a nitrogen laser (337nm). Instrument settings were as follows: accelerating voltage, 21,000 volts; grid voltage, 95%; guide wire, 0.05%; extraction delay time, 200 nsec. All data processing was performed using Applied Biosystems Data Explorer v 4.0.0.0.

NMR-Spectra: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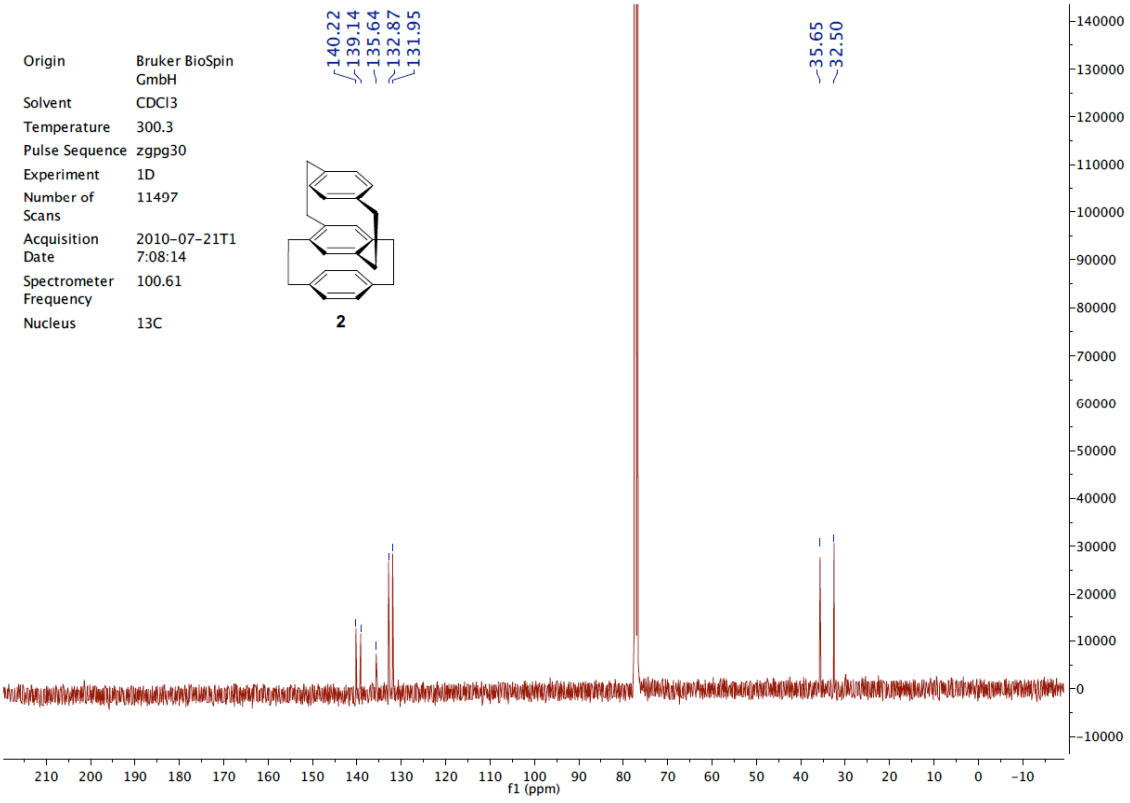
Pulse Sequence zg30
Experiment 1D
Number of Scans 9
Acquisition Date 2010-07-21T 17:05:02
Spectrometer Frequency 400.13
Nucleus 1H
6.21
5.42
3.14
3.11
3.08
2.99
2.96
2.93
2.76
2.74
2.74
2.73
2.72
2.71
2.70
2.69
2.57
2.55
2.54
2.53
2.52
2.52
2.51
2.49
2
8.07
1.86
16.00
f1 (ppm)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Spectrometer Frequency 100.61
Nucleus 13C
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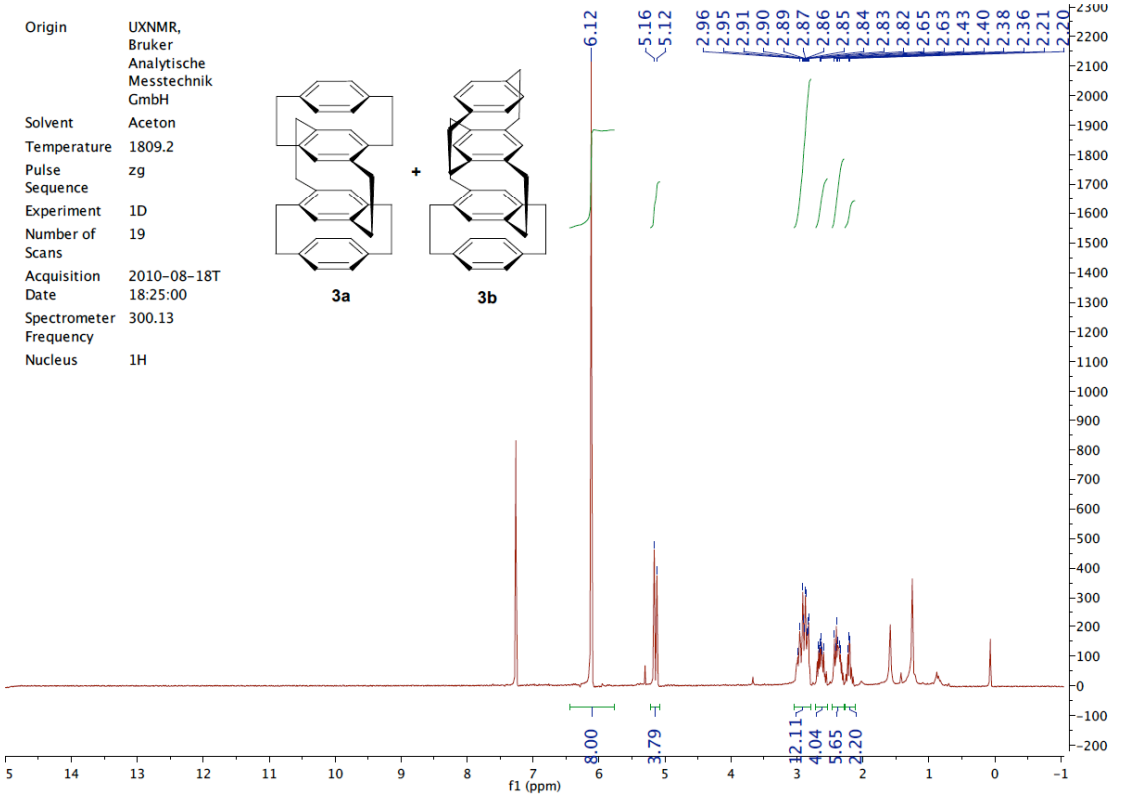
139.14
135.64
132.87
131.95
35.65
32.50
2
f1 (ppm)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Solvent Aceton
Temperature 1809.2
Pulse Sequence zg
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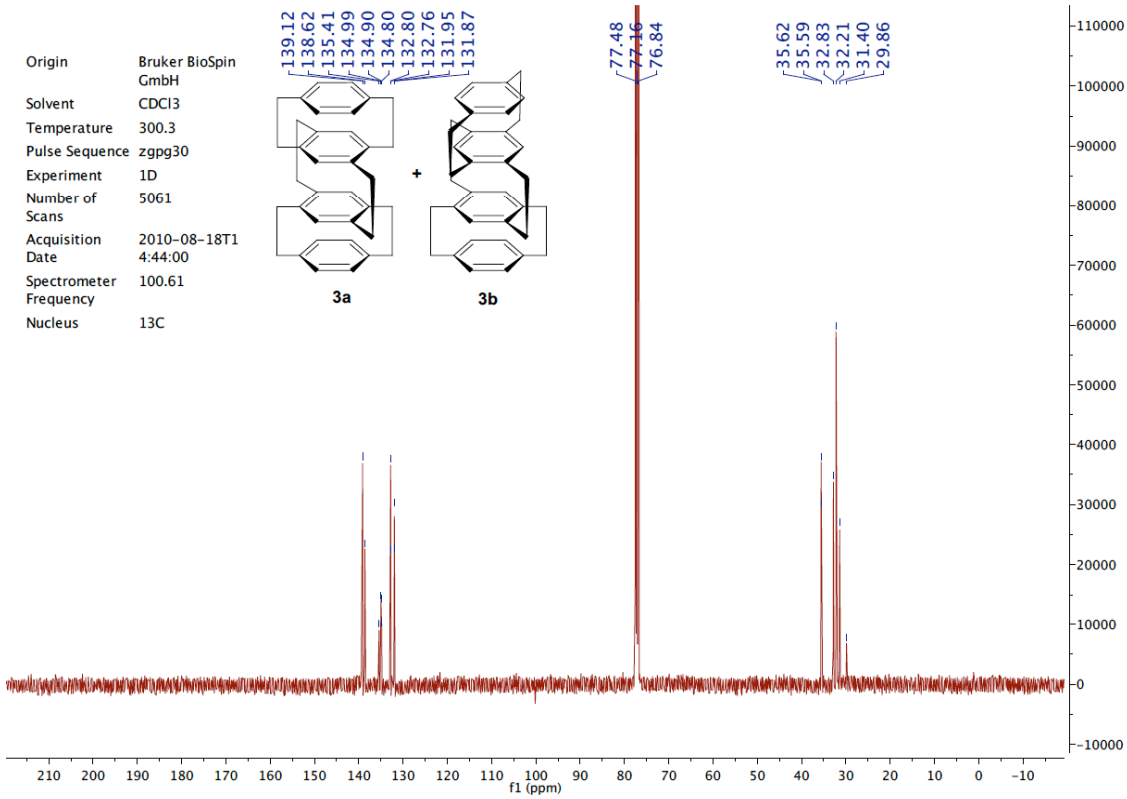
Acquisition Date 2010-08-18T 18:25:00
Spectrometer Frequency 300.13
Nucleus 1H
3a
3b
6.12
5.16
5.12
2.96
2.95
2.91
2.90
2.89
2.87
2.86
2.85
2.84
2.83
2.82
2.65
2.63
2.43
2.40
2.38
2.36
2.21
2.20
8.00
3.79
12.11
4.04
5.65
2.20
f1 (ppm)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Solvent CDCl3
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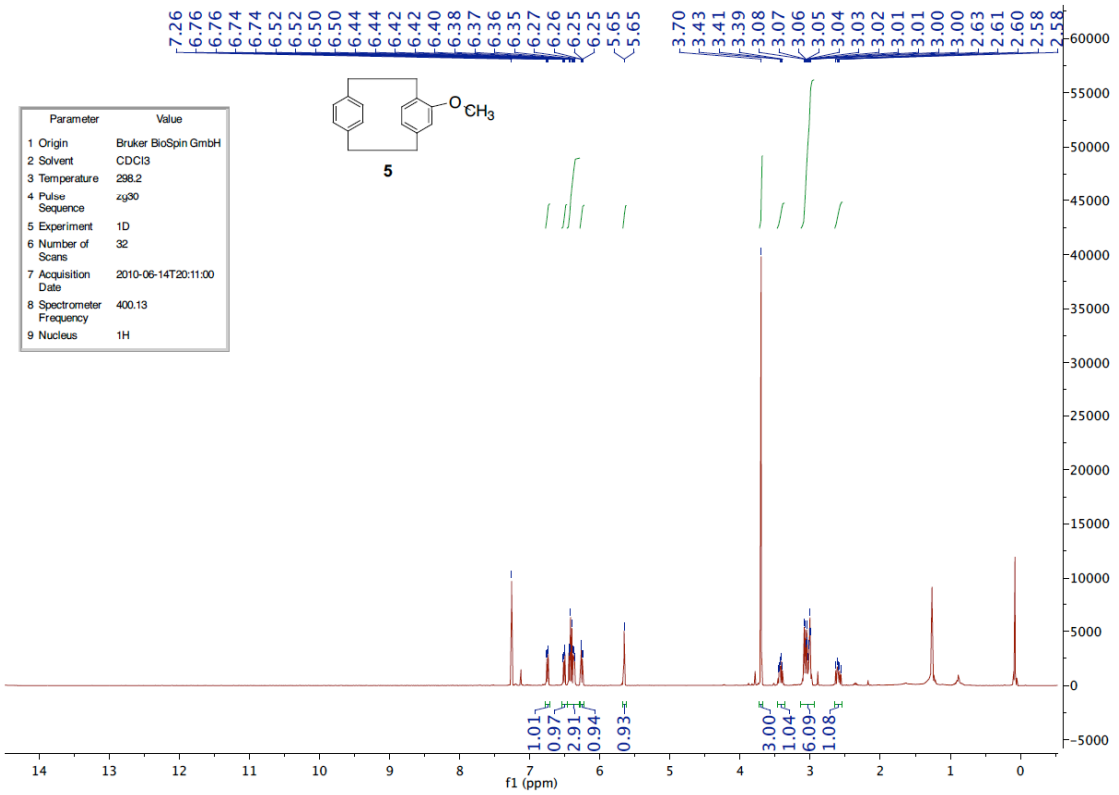
Acquisition Date 2010-08-18T14:44:00
Spectrometer Frequency 100.61
Nucleus 13C
3a
3b
139.12
138.62
135.41
134.99
134.90
134.80
132.80
132.76
131.95
131.87
77.48
77.16
76.84
35.62
35.59
32.83
32.21
31.40
29.86
f1 (ppm)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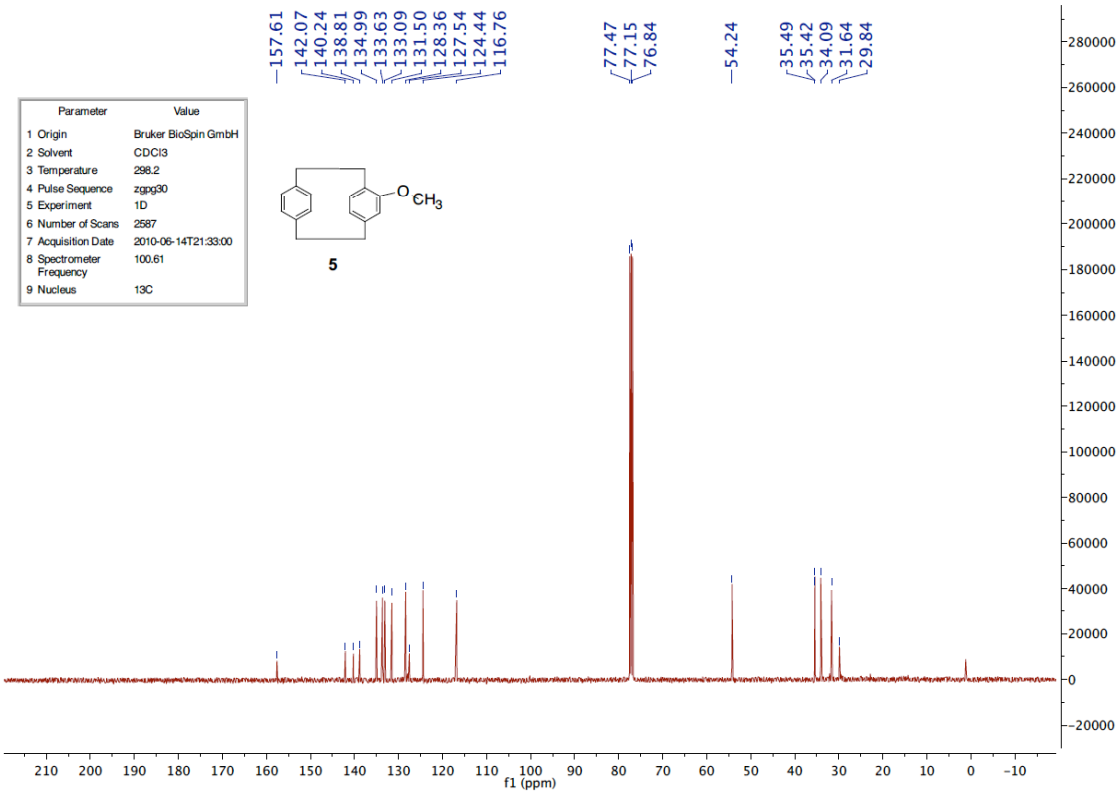
3.70 3.43 3.41 3.39 3.08 3.07 3.06 3.05 3.04 3.03 3.02 3.01 3.01 3.00 3.00 2.63 2.61 2.60 2.58 2.58
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Pulse Sequence zg30
5 Experiment 1D
6 Number of Scans 32
7 Acquisition Date 2010-06-14T20:11:00
8 Spectrometer Frequency 400.13
9 Nucleus 1H
O CH3
5
1.01 0.97 2.91 0.94 0.93 3.00 1.04 6.09 1.08
f1 (ppm)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77.47 77.15 76.84
54.24
35.49 35.42 34.09 31.64 29.84
Parameter Value
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2 Solvent CDCl3
3 Temperature 298.2
4 Pulse Sequence zgpg30
5 Experiment 1D
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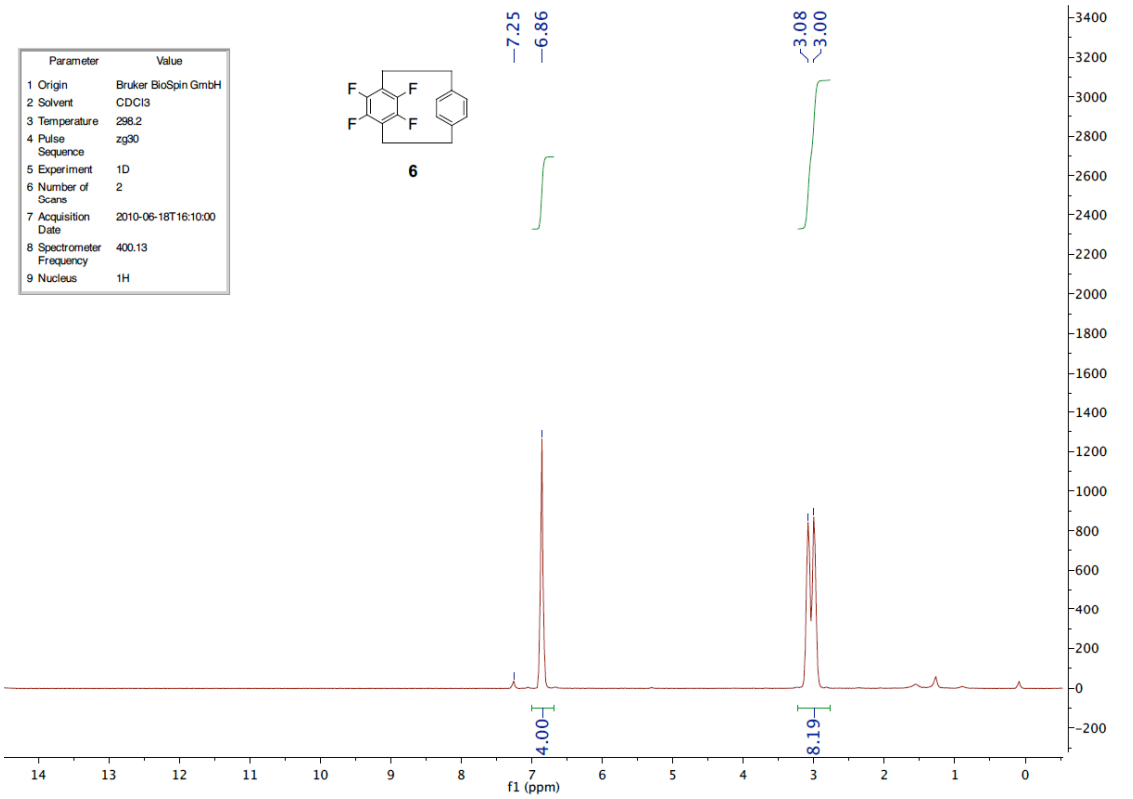
8 Spectrometer Frequency 100.61
9 Nucleus 13C
O CH3
5
f1 (ppm)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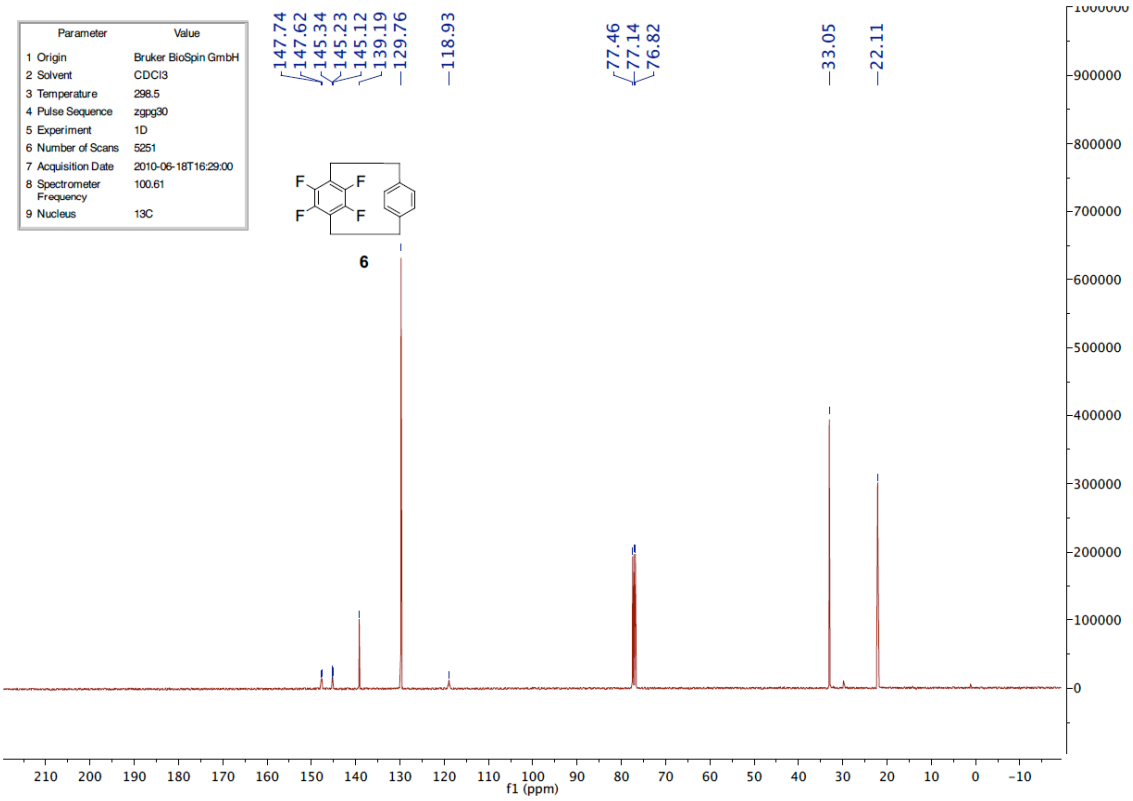
3 Temperature 298.2
4 Pulse Sequence zg30
5 Experiment 1D
6 Number of Scans 2
7 Acquisition Date 2010-06-18T16:10:00
8 Spectrometer Frequency 400.13
9 Nucleus 1H
F
F
F
F
6
7.25
6.86
3.08
3.00
4.00
8.19
f1 (ppm)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2 Solvent CDCl3
3 Temperature 298.5
4 Pulse Sequence zgpg30
5 Experiment 1D
6 Number of Scans 5251
7 Acquisition Date 2010-06-18T16:29:00
8 Spectrometer Frequency 100.61
9 Nucleus 13C
F
F
F
F
6
147.74
147.62
145.34
145.23
145.12
139.19
129.76
118.93
77.46
77.14
76.82
33.05
22.11
f1 (ppm)