



16:12:57 08-12-23

Simulated 2,3-Dibromopropanoic acid signal.

Experiment Information

Parameter	F1
Nucleus	^1H
Transmitter Frequency (MHz)	500
Sweep Width (Hz)	600
Sweep Width (ppm)	1.2
Transmitter Offset (Hz)	2050
Transmitter Offset (ppm)	4.1

4.600 - 4.400 ppm

Osc.	a	ϕ ($^\circ$)	f (Hz)	f (ppm)	η (s^{-1})	f
1	1.0004 $\pm 1.3876 \times 10^{-3}$	8.2802×10^{-2} $\pm 7.9531 \times 10^{-2}$	2.2344×10^3 $\pm 2.0361 \times 10^{-3}$	4.4688 $\pm 4.0723 \times 10^{-6}$	6.9995 $\pm 1.2772 \times 10^{-2}$	1.0023
2	0.99842 $\pm 1.4413 \times 10^{-3}$	2.5957×10^{-2} $\pm 8.2878 \times 10^{-2}$	2.243×10^3 $\pm 2.0799 \times 10^{-3}$	4.486 $\pm 4.1598 \times 10^{-6}$	6.9913 $\pm 1.3017 \times 10^{-2}$	1.0005
3	1.0002 $\pm 1.4456 \times 10^{-3}$	-6.5178×10^{-3} $\pm 8.2881 \times 10^{-2}$	2.257×10^3 $\pm 2.0863 \times 10^{-3}$	4.514 $\pm 4.1726 \times 10^{-6}$	7.0169 $\pm 1.3082 \times 10^{-2}$	1.0017
4	0.99804 $\pm 1.3876 \times 10^{-3}$	4.9217×10^{-2} $\pm 7.9756 \times 10^{-2}$	2.2656×10^3 $\pm 2.0404 \times 10^{-3}$	4.5312 $\pm 4.0808 \times 10^{-6}$	6.9955 $\pm 1.279 \times 10^{-2}$	1

4.020 - 3.820 ppm

Osc.	a	ϕ ($^{\circ}$)	f (Hz)	f (ppm)	η (s $^{-1}$)	f
1	1.0035 $\pm 1.2575 \times 10^{-3}$	-1.1133×10^{-3} $\pm 7.1748 \times 10^{-2}$	1.9386×10^3 $\pm 1.9405 \times 10^{-3}$	3.8772 $\pm 3.881 \times 10^{-6}$	7.0167 $\pm 1.2206 \times 10^{-2}$	1.0052
2	0.99852 $\pm 3.8331 \times 10^{-3}$	-2.1454×10^{-2} ± 0.22074	1.9588×10^3 $\pm 3.6287 \times 10^{-3}$	3.9176 $\pm 7.2574 \times 10^{-6}$	7.0111 $\pm 2.2801 \times 10^{-2}$	1.0003
3	1.0026 $\pm 3.8441 \times 10^{-3}$	-2.4786×10^{-2} ± 0.21966	1.9612×10^3 $\pm 3.6347 \times 10^{-3}$	3.9224 $\pm 7.2695 \times 10^{-6}$	7.0301 $\pm 2.2765 \times 10^{-2}$	1.004
4	1.0009 $\pm 1.2561 \times 10^{-3}$	-6.9312×10^{-2} $\pm 7.1886 \times 10^{-2}$	1.9814×10^3 $\pm 1.9407 \times 10^{-3}$	3.9628 $\pm 3.8815 \times 10^{-6}$	7.0042 $\pm 1.2203 \times 10^{-2}$	1.0028


3.800 - 3.600 ppm

Osc.	a	ϕ ($^{\circ}$)	f (Hz)	f (ppm)	η (s $^{-1}$)	f
1	1.0015 $\pm 1.3836 \times 10^{-3}$	6.6528×10^{-2} $\pm 7.9181 \times 10^{-2}$	1.8356×10^3 $\pm 2.0225 \times 10^{-3}$	3.6712 $\pm 4.045 \times 10^{-6}$	7.0086 $\pm 1.2697 \times 10^{-2}$	1.0032
2	0.99953 $\pm 1.4671 \times 10^{-3}$	-6.1993×10^{-3} $\pm 8.407 \times 10^{-2}$	1.8442×10^3 $\pm 2.081 \times 10^{-3}$	3.6884 $\pm 4.162 \times 10^{-6}$	6.9937 $\pm 1.3079 \times 10^{-2}$	1.0016
3	1.0023 $\pm 1.4693 \times 10^{-3}$	5.367×10^{-2} $\pm 8.412 \times 10^{-2}$	1.8558×10^3 $\pm 2.0914 \times 10^{-3}$	3.7116 $\pm 4.1828 \times 10^{-6}$	7.0212 $\pm 1.3102 \times 10^{-2}$	1.0038
4	0.99981 $\pm 1.3837 \times 10^{-3}$	4.9889×10^{-2} $\pm 7.9332 \times 10^{-2}$	1.8644×10^3 $\pm 2.0249 \times 10^{-3}$	3.7288 $\pm 4.0498 \times 10^{-6}$	7.0057 $\pm 1.2713 \times 10^{-2}$	1.0016


Estimation performed using NMR-EsPy.

Author: Simon Hulse

For more information:

 <https://foroozandehgroup.github.io/NMR-EsPy>

 <https://github.com/foroozandehgroup/NMR-EsPy>

 simon.hulse@chem.ox.ac.uk

If used in a publication, please cite:

Simon G. Hulse, Mohammadali Foroozandeh. *"Newton meets Ockham: Parameter estimation and model selection of NMR data with NMR-EsPy"*. J. Magn. Reson. 338 (2022) 107173.

<https://doi.org/10.1016/j.jmr.2022.107173>