NMR-ESPY

17:02:04 09-01-23
Simulated 2,3-Dibromopropanoic acid signal.

Experiment Information

Parameter	F1
Nucleus	^{1}H
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 (°)	f(Hz)	f(ppm)	η(s^{-1})	$\int$
1	1.0003 $\pm 1.2584 \times 10^{-3}$	6.4781×10^{-2} $\pm 7.2235 \times 10^{-2}$	2.2344×10^{3} $\pm 1.8524 \times 10^{-3}$	4.4688 $\pm 3.7047 \times 10^{-6}$	7.0095 $\pm 1.1596 \times 10^{-2}$	1.005
2	1.0011 $\pm 1.3095 \times 10^{-3}$	3.4463×10^{-2} $\pm 7.4913 \times 10^{-2}$	2.243×10^{3} $\pm 1.8811 \times 10^{-3}$	4.486 $\pm 3.7622 \times 10^{-6}$	7.0011 $\pm 1.1819 \times 10^{-2}$	1.006
3	0.999 02 $\pm 1.3071 \times 10^{-3}$	1.6175×10^{-2} $\pm 7.4975 \times 10^{-2}$	2.257×10^{3} $\pm 1.8788 \times 10^{-3}$	4.514 $\pm 3.7576 \times 10^{-6}$	6.9856 $\pm 1.1799 \times 10^{-2}$	1.0042
4	1.0004 $\pm 1.2592 \times 10^{-3}$	$-0.104\,44$ $\pm 7.2085 \times 10^{-2}$	2.2656×10^{3} $\pm 1.8456 \times 10^{-3}$	4.5312 $\pm 3.6913 \times 10^{-6}$	7.0057 $\pm 1.161 \times 10^{-2}$	1.0052

4.020 - 3.820 ppm

Osc.	a	ϕ (°)	f(Hz)	f(ppm)	η(s^{-1})	$\int$
1	1.0022 $\pm 1.174 \times 10^{-3}$	4.1216×10^{-2} $\pm 6.7046 \times 10^{-2}$	1.9386×10^{3} $\pm 1.8112 \times 10^{-3}$	3.8772 $\pm 3.6224 \times 10^{-6}$	7.0109 $\pm 1.1406 \times 10^{-2}$	1.007
2	0.9947 $\pm 3.5837 \times 10^{-3}$	-4.2748×10^{-2} $\pm 0.206\,12$	1.9588×10^{3} $\pm 3.3896 \times 10^{-3}$	3.9176 $\pm 6.7791 \times 10^{-6}$	6.9866 $\pm 2.1226 \times 10^{-2}$	1
3	1.008 $\pm 3.5889 \times 10^{-3}$	-5.7939×10^{-2} $\pm 0.204\,39$	1.9612×10^{3} $\pm 3.3774 \times 10^{-3}$	3.9224 $\pm 6.7549 \times 10^{-6}$	7.0448 $\pm 2.1273 \times 10^{-2}$	1.0121
4	1.0009 $\pm 1.1735 \times 10^{-3}$	-4.0908×10^{-2} $\pm 6.7195 \times 10^{-2}$	1.9814×10^{3} $\pm 1.8172 \times 10^{-3}$	3.9628 $\pm 3.6344 \times 10^{-6}$	7.0131 $\pm 1.141 \times 10^{-2}$	1.0056

3.800 - 3.600 ppm

Osc.	a	ϕ (°)	f(Hz)	f(ppm)	η(s^{-1})	$\int$
1	1.0018 $\pm 1.3135 \times 10^{-3}$	9.1221×10^{-2} $\pm 7.5016 \times 10^{-2}$	1.8356×10^{3} $\pm 1.9168 \times 10^{-3}$	3.6712 $\pm 3.8335 \times 10^{-6}$	7.0187 $\pm 1.2077 \times 10^{-2}$	1.0063
2	1.0003 $\pm 1.3915 \times 10^{-3}$	$0.142\,56$ $\pm 7.9603 \times 10^{-2}$	1.8442×10^{3} $\pm 1.9697 \times 10^{-3}$	3.6884 $\pm 3.9394 \times 10^{-6}$	6.9968 $\pm 1.2406 \times 10^{-2}$	1.0053
3	1.0024 $\pm 1.3942 \times 10^{-3}$	9.0623×10^{-2} $\pm 7.9693 \times 10^{-2}$	1.8558×10^{3} $\pm 1.9815 \times 10^{-3}$	3.7116 $\pm 3.9631 \times 10^{-6}$	7.0281 $\pm 1.2451 \times 10^{-2}$	1.0068
4	1.0008 $\pm 1.3112 \times 10^{-3}$	5.2478×10^{-2} $\pm 7.5047 \times 10^{-2}$	1.8644×10^{3} $\pm 1.9136 \times 10^{-3}$	3.7288 $\pm 3.8272 \times 10^{-6}$	7.0007 $\pm 1.203 \times 10^{-2}$	1.0058

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

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