



12:11:55 14-04-2021

Description

Example estimation result for NMR-EsPy docs.

Experiment Information

Sweep Width (Hz)	5494.51	
Sweep Width (ppm)	10.9861	
Transmitter Offset (Hz)	2249.21	
Transmitter Offset (ppm)	4.49722	
Transmitter Frequency (MHz)	500.132	
Basic Frequency (MHz)	500.13	
Nucleus	^{1}H	

Filter region (Hz): 2770.79 - 2710.76 Filter region (ppm): 5.54011 - 5.42008

Result

m	a _m	ϕ_m (rad)	f _m (Hz)	f _m (ppm)	$\eta_m~(\mathrm{s}^{-1})$	ſ	5/ 5
1	3.2947×10^4	0.03575	2.7198×10^{3}	5.4382	9.2827	2.9106×10^{9}	0.35233
	± 227.99	$\pm 3.6776 \times 10^{-3}$	$\pm\ 2.3079 \times 10^{-3}$	$\pm~4.6145 \times 10^{-6}$	$\pm \ 0.065552$	-	-
2	3.4676×10^4	0.018128	2.7253×10^{3}	5.4492	9.2969	3.0628×10^{9}	0.37075
	± 246.65	$\pm 4.9844 \times 10^{-3}$	$\pm 4.2789 \times 10^{-3}$	$\pm~8.5556 \times 10^{-6}$	± 0.066104	-	-
3	3.3345×10^4	0.013083	2.7284×10^{3}	5.4554	9.0494	2.9546×10^{9}	0.35765
	± 488.97	$\pm\ 5.8942 imes 10^{-3}$	$\pm~8.1909 \times 10^{-3}$	$\pm~1.6377 \times 10^{-5}$	$\pm \ 0.10245$	-	-

4	3.0111×10^{4}	-6.467×10^{-3}	2.7338×10^{3}	5.4662	8.8992	2.6733×10^{9}	0.32359
	± 375.37	$\pm~8.5845 \times 10^{-3}$	$\pm \ 0.011642$	$\pm\ 2.3278 \times 10^{-5}$	$\pm \ 0.091566$	-	_
5	3.1348×10^4	0.019111	2.7431×10^{3}	5.4848	7.609	2.834×10^{9}	0.34305
	\pm 201.12	$\pm \ 0.016456$	$\pm \ 0.018088$	$\pm \ 3.6167 \times 10^{-5}$	$\pm \ 0.051702$	-	-
6	3.3581×10^4	-7.7561×10^{-3}	2.7486×10^{3}	5.4957	7.6634	3.0335×10^{9}	0.36719
	\pm 389.2	$\pm\ 5.5778 \times 10^{-3}$	$\pm~6.9017 \times 10^{-3}$	$\pm 1.38 \times 10^{-5}$	$\pm~0.07508$	-	-
7	3.2942×10^4	-8.0157×10^{-3}	2.7535×10^{3}	5.5056	7.6245	2.9774×10^9	0.36041
	± 206.76	$\pm~6.3139 \times 10^{-3}$	$\pm 7.1993 \times 10^{-3}$	$\pm~1.4395 \times 10^{-5}$	$\pm \ 0.048888$	-	_
8	3.2182×10^4	-0.027252	2.7589×10^{3}	5.5164	7.932	2.8955×10^9	0.3505
	\pm 163.34	$\pm 4.0778 \times 10^{-3}$	$\pm 6.1219 \times 10^{-3}$	$\pm\ 1.2241 \times 10^{-5}$	± 0.046284	-	-
9	2.1404×10^3	1.6×10^{-3}	2.7664×10^{3}	5.5313	9.239	1.8919×10^{8}	0.022902
	\pm 123.46	$\pm 4.3689 \times 10^{-3}$	$\pm \ 0.095994$	$\pm 1.9194 \times 10^{-4}$	\pm 0.57799	-	-

Estimation performed using NMR-EsPy.

Author: Simon Hulse For more information:



https://nmr-espy.readthedocs.io/en/latest/



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



simon.hulse@chem.ox.ac.uk

If used in a publication, please cite:

No references yet...