Supplementary Material (ESI) for Chemical Communications

Accurate Heteronuclear *J*-Coupling Measurements in Dilute Spin Systems using the multiple-quantum filtered *J*-resolved experiment

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Electronic Supplementary Information

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Table 1. Atom Wickoff multiplicity for $Pb_5Cr_3F_{19}$[1] (Space Group n°108 I4cm, a = 14.384 Å, c = 7.408 Å).

Atom	Site
Pb1	16d
Pb2	4b
Cr1	8c
Cr2	4a
F1	16d
F2	16d
F3	16d
F4	8c
F5	8c
F6	8c
F7	4a

Table 2. Selected F-Pb bond distances (< 4 Å) in $Pb_5Cr_3F_{19}$.

F	Pb	d_{F-Pb}
F1 (unshared)	Pb1	2.4960
	Pb1	2.9311
	Pb1	3.3024
F2 (unshared)	Pb1	2.6189
	Pb1	2.6994
	Pb2	3.0239
F3 (unshared)	Pb1	2.1406
	Pb1	3.3879
	Pb1	3.4244
	Pb1	3.9140
F4 (unshared)	Pb1	2.5651
	Pb1	2.5651
F5 ("free")	Pb1	2.3558
	Pb1	2.3558
	Pb2	2.5222
	Pb2	3.5883
F6 (unshared)	Pb2	2.2671
	Pb2	2.4576
	Pb1	3.6189
	Pb1	3.6189
F7 (shared)	Pb1	3.4730
	Pb1	3.4730
	Pb1	3.4730
	Pb1	3.4730

Table 3. Line labels, relative intensity (%), isotropic chemical shift δ_{iso}/ppm as deduced from the ^{207}Pb decoupled ^{19}F MAS NMR spectrum reconstruction and line attributions (expected line intensity (%)) for $Pb_5Ga_3F_{19}$.

Line	Relative intensity	δ_{iso}	Site (expected line intensity)
1	4.6	-135	F7 (5.3)
2	9.1	-119	F4 or F6 (10.5)
3	21.5	-110	F1 or F2 or F3 (21.0)
4	22.1	-105	F1 or F2 or F3 (21.0)
5	24.1	-96	F1 or F2 or F3 (21.0)
6	8.5	-75	F4 or F6 (10.5)
7	10.1	-28	F5 (10.5)

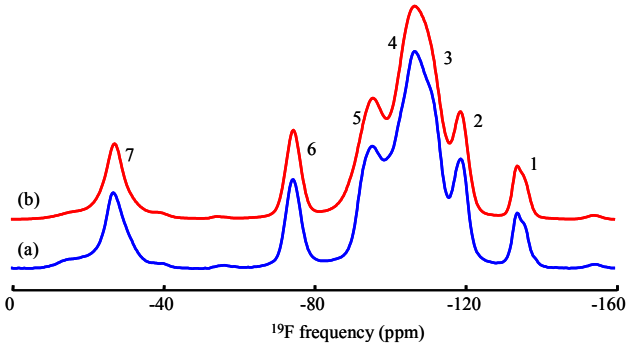

Figure 1. (a) experimental and (b) calculated ^{207}Pb decoupled ^{19}F MAS spectra of $Pb_5Ga_3F_{19}$ at spinning rate 30 kHz.

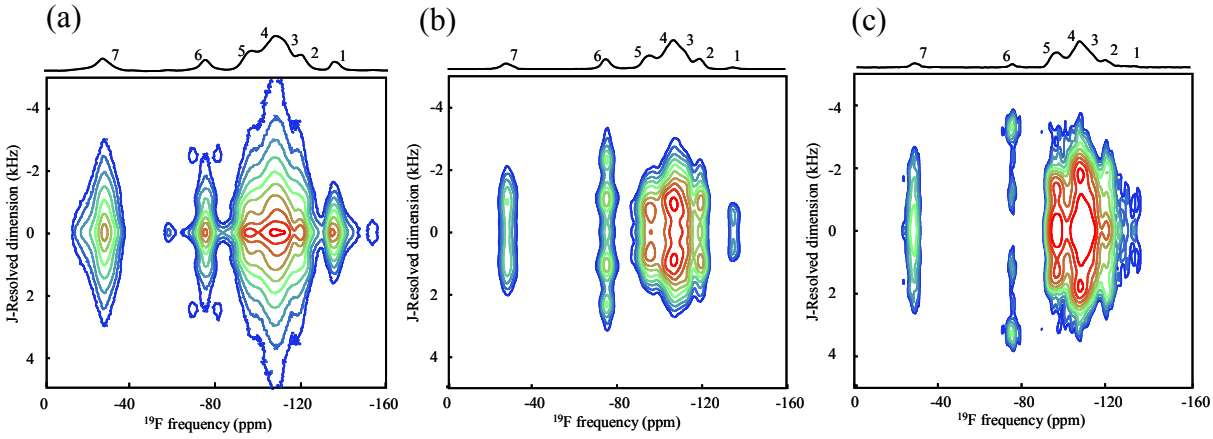

Figure 2. ^{19}F-^{207}Pb MAS (30 kHz) *J*-resolved spectra (a) without filtering, (b) with ^{207}Pb single-quantum filtering and (c) with ^{207}Pb double-quantum filtering.

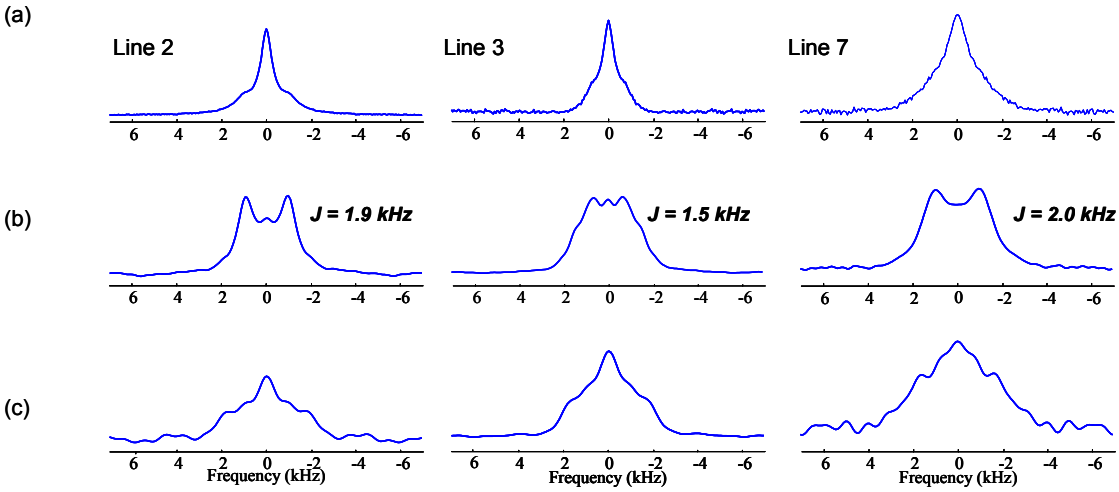

Figure 3. Cross-sections of the (a) 2D *J*-resolved, (b) ^{207}Pb single-quantum filtered 2D *J*-resolved and (c) ^{207}Pb double-quantum filtered 2D *J*-resolved MAS (30 kHz spinning frequency) spectra for some selected ^{19}F resonances of $Pb_5Ga_3F_{19}$.

Reference

1 J. Ravez, V. Andriamampianina, A. Simon, J. Grannec and S. C. Abrahams, *J. Appl. Phys.*, 1991, **70**, 1331.