On the assignment of ^{19}F MAS NMR spectra of fluoroaluminates using through-space spectral edition of ^{19}F-^{27}Al and ^{19}F-^{19}F connectivities

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Electronic Supplementary Information

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Table 1. F-F distances (d_{F-F}<3.6 Å) calculated from the optimized structure of β-$BaAlF_5$.[1]

Atom		Distance (Å)	Atom		Distance (Å)
F 1	F 6	2.4736	F 5	F 6	2.5016
	F 2	2.5774		F 3	2.5838
	F 7	2.5898		F 2	2.5897
	F 3	2.5925		F 8	2.5952
	F 4	2.5996		F 9	2.5990
	F 5	2.6108		F 10	2.6045
	F 10	2.6229		F 1	2.6108
	F 5	2.6382		F 1	2.6382
	F 9	3.0021		F 4	2.9972
	F 6	3.1199		F 6	3.3252
F 2	F 4	2.5008	F 6	F 1	2.4736
	F 8	2.5564		F 5	2.5016
	F 1	2.5774		F 9	2.5768
	F 5	2.5897		F 7	2.6043
	F 6	2.7512		F 2	2.7512
	F 8	3.0141		F 1	3.1199
	F 4	3.0884		F 6	3.1363
	F 2	3.1129		F 5	3.3252
	F 2	3.2350		F 6	3.3739
	F 3	3.5947		F 8	3.4909
F 3	F 8	2.5296	F 7	F 9	2.5787
	F 4	2.5800		F 1	2.5898
	F 5	2.5838		F 10	2.6029
	F 1	2.5925		F 6	2.6043
	F 7	2.8806		F 9	2.6591
	F 10	2.8947		F 3	2.8806
	F 10	2.8994		F 4	2.9115
	F 10	3.0361		F 8	3.3695
	F 9	3.3151		F 10	3.4472
	F 9	3.4378	F 8	F 4	2.5104
	F 2	3.5947		F 3	2.5296
F 4	F 2	2.5008		F 2	2.5564
	F 8	2.5105		F 5	2.5952
	F 3	2.5800		F 4	2.7234
	F 1	2.5996		F 9	2.8644
	F 8	2.7234		F 2	3.0141
	F 7	2.9115		F 7	3.3695
	F 5	2.9972		F 6	3.4909
	F 2	3.0884		F 10	3.5856
	F 10	3.3346			

Table 1. Continued.

Atom		Distance (Å)	Atom		Distance (Å)
F 9	F 6	2.5768	F 10	F 7	2.6029
	F 7	2.5787		F 5	2.6045
	F 5	2.5990		F 9	2.6081
	F 10	2.6081		F 1	2.6229
	F 7	2.6591		F 3	2.8947
	F 8	2.8644		F 3	2.8994
	F 1	3.0021		F 3	3.0361
	F 3	3.3151		F 4	3.3346
	F 10	3.4101		F 9	3.4101
	F 3	3.4378		F 7	3.4472
				F 8	3.5856

Table 2. F-F distances (d_{F-F}<3.6 Å) calculated from the optimized structure of $Ba_3Al_2F_{12}$.[1]

Atom		Distance (Å)	Atom		Distance (Å)
F 1	F 6	2.4945	F 5	F 2	2.5215
	F 6	2.4945		F 6	2.5420
	F 2	2.5564		F 7	2.6031
	F 2	2.5564		F 8	2.6201
	F 1	2.5591		F 6	2.7238
	F 8	2.6022		F 8	2.8516
	F 8	2.6022		F 3	3.1849
	F 7	2.6091		F 4	3.1895
	F 7	2.6091	F 6	F 1	2.4945
F 2	F 5	2.5215		F 5	2.5420
	F 5	2.5215		F 7	2.5496
	F 1	2.5564		F 2	2.5589
	F 1	2.5564		F 5	2.7238
	F 6	2.5589		F 3	3.0575
	F 6	2.5589		F 8	3.2090
	F 8	2.5954		F 4	3.2169
	F 8	2.5954		F 8	3.5262
	F 4	3.3262		F 7	3.5626
	F 4	3.5537	F 7	F 6	2.5496
F 3	F 3	2.8954		F 7	2.5551
	F 7	3.0129		F 8	2.5859
	F 7	3.0129		F 5	2.6031
	F 6	3.0575		F 1	2.6091
	F 6	3.0575		F 7	2.7931
	F 5	3.1849		F 4	2.9424
	F 5	3.1849		F 3	3.0129
	F 8	3.2642		F 6	3.5626
	F 8	3.2642	F 8	F 7	2.5859
	F 8	3.3241		F 2	2.5954
	F 8	3.3241		F 1	2.6022
F 4	F 7	2.9424		F 5	2.6201
	F 7	2.9424		F 8	2.8208
	F 4	2.9883		F 5	2.8516
	F 5	3.1895		F 6	3.2090
	F 5	3.1895		F 3	3.2642
	F 6	3.2169		F 3	3.3241
	F 6	3.2169		F 6	3.5262
	F 2	3.3262		F 4	3.5295
	F 8	3.5295			
	F 8	3.5295			
	F 2	3.5537			

Table 3. F-F distances (d_{F-F}<3.6 Å) calculated from the optimized structure of α-$CaAlF_5$.[1]

Atom		Distance (Å)
F1	F2	2.5206
	F2	2.5206
	F3	2.5699
	F3	2.5699
	F3	2.5785
	F3	2.5785
	F2	2.6970
	F2	2.6970
	F3	3.4556
	F3	3.4556
F2	F3	2.5142
	F1	2.5206
	F3	2.5521
	F1	2.6970
	F2	2.7646
	F3	3.0321
	F3	3.1362
	F3	3.1850
	F2	3.2076
	F3	3.3356
F3	F2	2.5142
	F2	2.5521
	F1	2.5699
	F1	2.5785
	F2	3.0321
	F2	3.1362
	F2	3.1850
	F2	3.3356
	F1	3.4556
	F3	3.5076
	F3	3.5300

Reference

1 M. Body, C. Legein, J.-Y. Buzaré, G. Silly, P. Blaha, C. Martineau, F. Calvayrac, *J. Phys. Chem. A*, 2007, **111**, 11873-11884.