Supporting Information for

Solid Solutions CaF_2-YF_3 with Fluorite Structure Prepared on the Sol-Gel Route: Investigation by Multinuclear MAS NMR Spectroscopy

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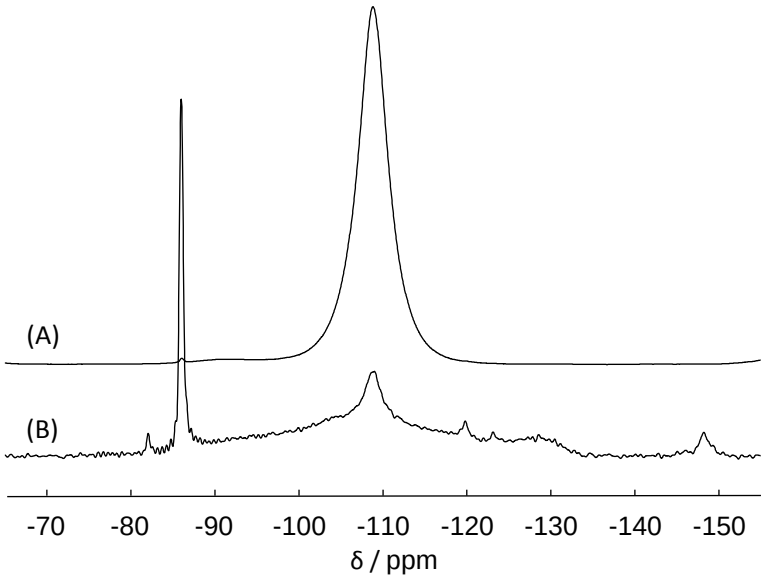

Figure S1. ^{19}F MAS NMR spectra of **2** CaF_2-s ($Ca_{0.999}Sm_{0.001}F_{2.001}$). (A) single pulse, (B) rs-echo L0=30.

Table S1. Cubic lattice parameters extracted from XRD in dependence of the Y-doping level.

Name	Lattice parameter
CaF_2	a = 5.463 Å
CaF_2:Y05-s	a = 5.469 Å
CaF_2:Y10-s	a = 5.481 Å
CaF_2:Y20-s	a = 5.499 Å
CaF_2:Y40-s	a = 5.533 Å

Table S2. Calculation of the metal-fluoride distances needed for Figure 5.

Cubic lattice constant of CaF_2	a_0 = 5.463 Å
Coordinates of the metal ions forming an octahedron	(0, 0.5, 0.5) (1, 0.5, 0.5) (0.5, 0, 0.5) (0.5, 1, 0.5) (0.5, 0.5, 0) (0.5, 0.5, 1)
Coordinates of the defect fluoride ion (for x = 0.5, all of these fluorides are located in the middle of the octahedron)	24*e* (*x*, 0.5, 0.5) 32*f* (*x*, *x*, *x*) 48*i* (*x*, *x*, 0.5)
Calculation of $d_{M\text{-}F}$ between F at (a_1, a_2, a_3) and M at (b_1, b_2, b_3)	$d_{M\text{-}F} = a_0 \left(\sum_{i=1}^{3} (a_i - b_i)^2 \right)^{\frac{1}{2}}$

Table S3. Site occupation frequencies (s.o.f.) needed for cubic $Ca_{1-x}Y_xF_{2+x}$ (x = 0...0.40) to fulfill the condition that all additional fluoride ions are located in well-defined clusters ($Fm\bar{3}m$, Z = 4). *wyck*: Wyckoff position (first number is the multiplicity), *s.o.f.*: site occupation frequency.

atom	*wyck*	***s.o.f.* 8:12:0**	***s.o.f.* 8:12:1**
Ca	4*a*	$1 - x$	$1 - x$
Y	4*a*	x	x
F*n*	8*c*	$1 - x$	$1 - \frac{4}{5}x$
F´	32*f*	0	$\frac{1}{40}x$
F´´	48*i*	$\frac{1}{4}x$	$\frac{1}{5}x$