Supplementary Material

Gadolinium chloride hexahydrate and its intercalation into synthetic saponite: structure, characterization and slow magnetic relaxation of the intercalated sample

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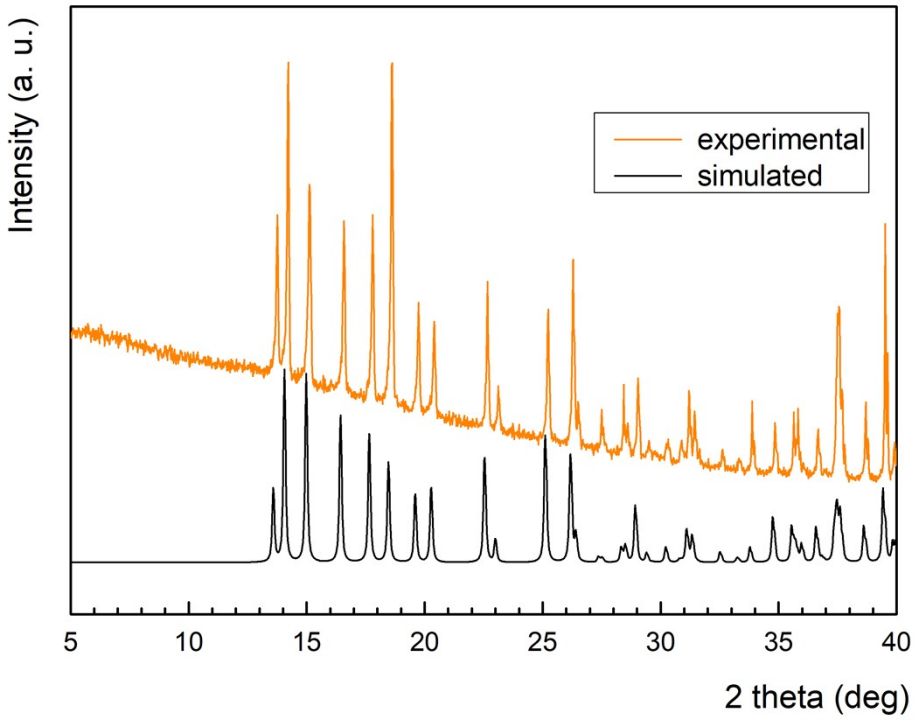
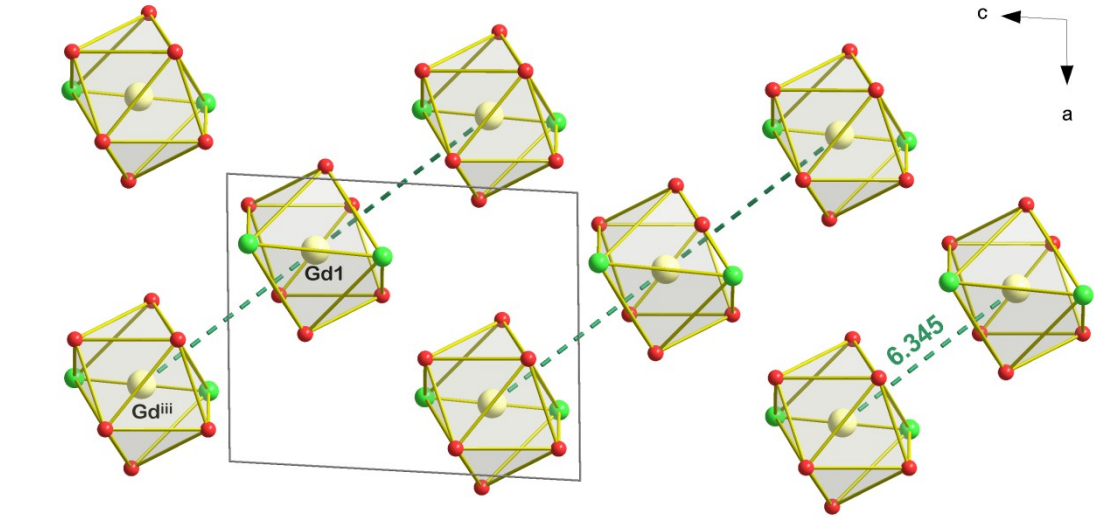
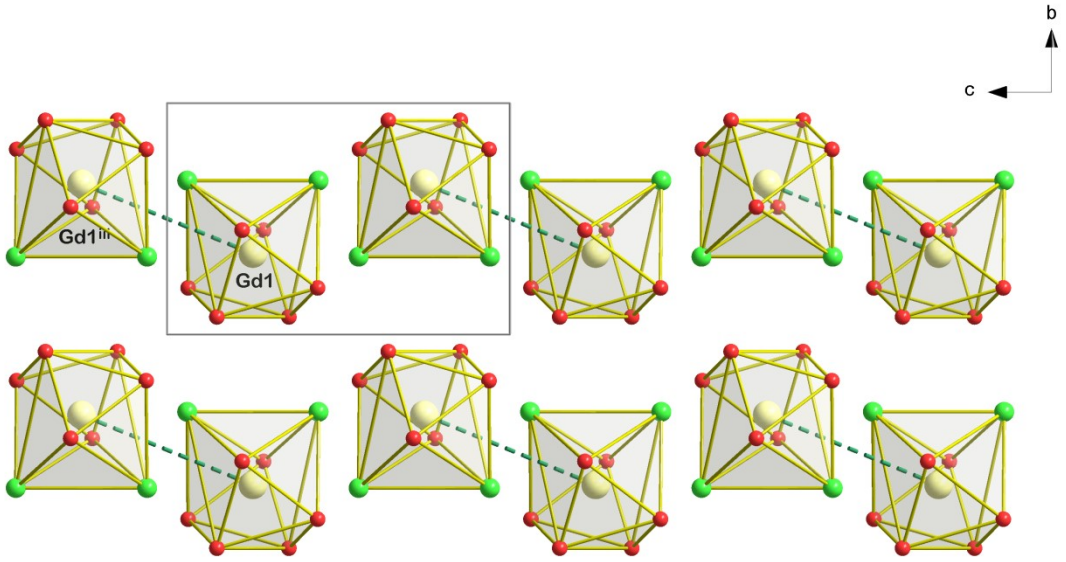


Figure S1 Comparison of the simulated XRPD analysis (black line) using single crystal data of **1-RT** calculated by program MERCURY [1] (calculated for $\lambda\alpha_1$=1.54060 Å and $\lambda\alpha_2$ =1.54443) and experimental XRPD analysis (orange line) of the bulk sample of **1**, measured at RT.

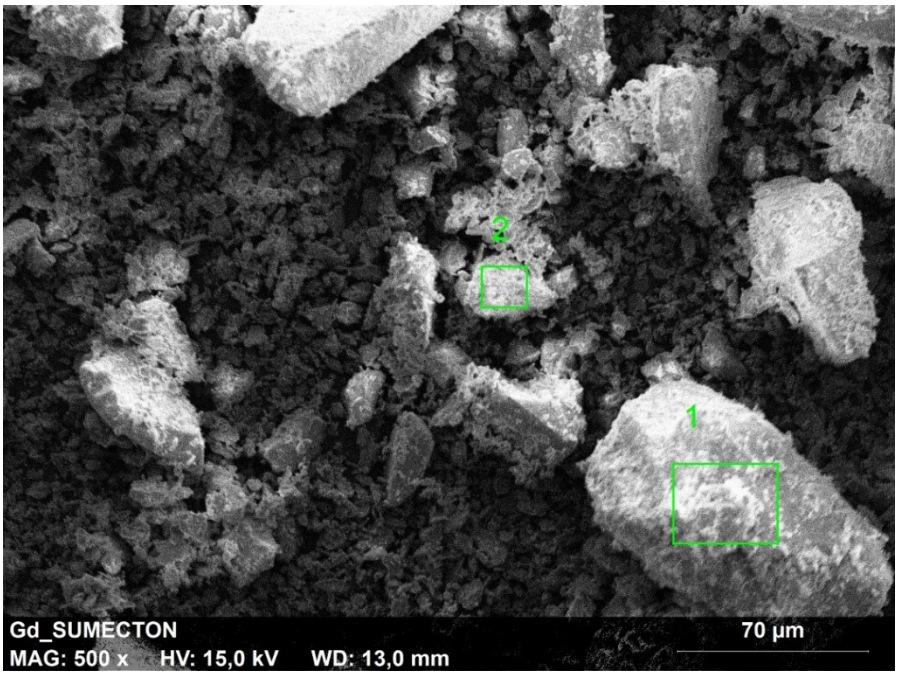


a)



b)

Figure S2 Gd(III) polyhedra arrangement in **1-LT**: **a)** in *ca* plane view, **b)** in *bc* plane view, the shortest distance of Gd···Gd is shown as green dashed line. Hydrogen bonds are omitted for clarity. Oxygen atoms are drawn as red balls and Chlorine atoms as green balls.



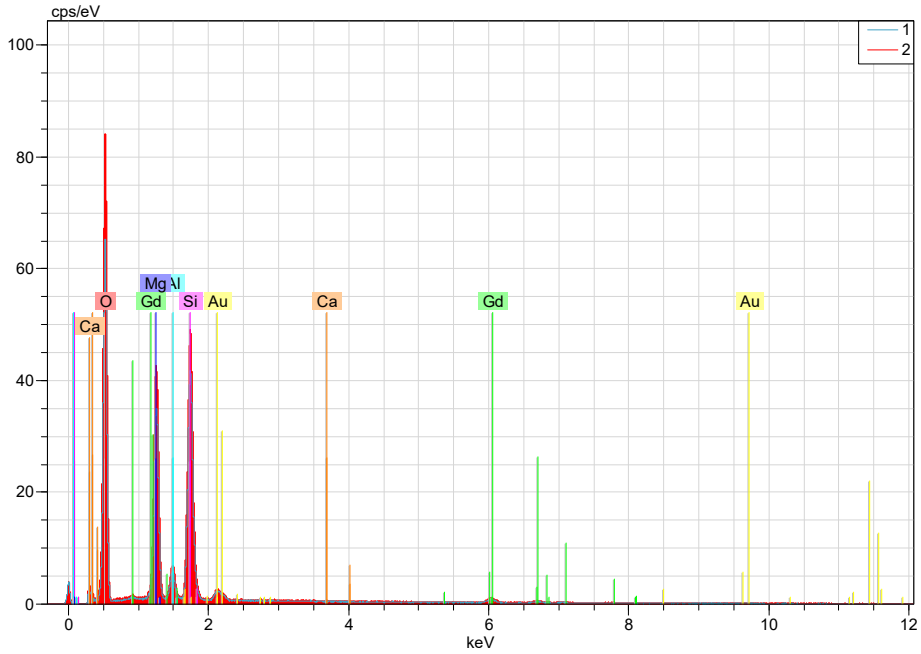


Figure S3 Results of EDX experiment of **Gd-Sap**.

Bruker AXS Microanalysis GmbH, Germany
Quantification results
Mass percent (%)

Spectrum	O	Mg	Al	Si	Ca	Gd	Au
1	53.39	18.78	2.89	25.09	0.08	5.85	4.36
2	55.88	16.77	2.56	22.41	0.09	5.77	3.35
Mean value:	54.63	17.77	2.73	23.75	0.09	5.81	3.86
Sigma:	1.76	1.42	0.23	1.89	0.01	0.06	0.72
Sigma mean:	1.24	1.01	0.16	1.34	0.01	0.04	0.51

Table S1 Results of the SHAPE [2] calculations defining the polyhedron shape of Gd(III) ion in complex **1**.

Polyhedron Shape	**TT-8**	**JSD-8**	**BTPR-8**	**JBTPR-8**	**JETBPY-8**	**JGBF-8**
(**1-LT**)	11.003	5.472	2.447	3.540	28.616	17.017
(**1-RT**)	10.967	5.450	2.440	3.520	28.653	17.022
	TDD-8	**SAPR-8**	**CU-8**	**HBPY-8**	**HPY-8**	**OP-8**
(**1-LT**)	1.902	**1.084**	10.847	17.059	23.723	29.918
(**1-RT**)	1.895	**1.067**	10.795	17.033	23.704	29.889

Additional text - abbreviations used for polyhedron shape definition in **Table S1**:

TT-8	12 Td	Triakis tetrahedron
JSD-8	11 D2d	Snub diphenoid J84
BTPR-8	10 C2v	Biaugmented trigonal prism
JBTPR-8	9 C2v	Biaugmented trigonal prism J50
JETBPY-8	8 D3h	Johnson elongated triangular bipyramid J14
JGBF-8	7 D2d	Johnson gyrobifastigium J26
TDD-8	6 D2d	Triangular dodecahedron
SAPR-8	5 D4d	Square antiprism
CU-8	4 Oh	Cube
HBP-8	3 D6h	Hexagonal bipyramid
HPY-8	2 C7v	Heptagonal pyramid
OP-8	1 D8h	Octagon

References

[1] C. F. Macrae, I. Sovago, S. J. Cottrell, P. T. A. Galek, P. McCabe, E. Pidcock, M. Platings, G. P. Shields, J. S. Stevens, M. Towler and P. A. Wood, *Mercury 4.0*: from visualization to analysis, design and prediction, *J. Appl. Cryst.,* 2020*,* **53**, 226-235.

[2] M. Llunell, D. Casanova, J. Cirera, P. Alemany, S. Alvarez (2013). SHAPE Program for the Stereochemical Analysis of Molecular Fragments by Means of Continuous Shape Measures and Associated Tools, Version 2.1 (2013). Universitat de Barcelona, Barcelona, Spain.