

Electronic Supplementary Information

for

Raman spectroscopic study of anhydrous and hydrous REE phosphates, oxides, and hydroxides

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Supplementary Materials:

- Table S2 summary tables with reference data in xlsx format (ESI_TableS2)
- Folder containing reference raw spectra for all solids measured in this study (Suppl_rawfiles)
- Folder containing all Fityk files for peak deconvolution and fitting (Suppl_Fit)

Electronic Supplementary Information comprises an additional literature data compilation summarized in Table S1 with more reference data listed in a separate excel file (ESI_TableS2). We also provide a zip file (Suppl_rawfiles) with raw data (txt) for all solids measured in this study as xy tables, which can be used with a variety of software packages for direct comparison of spectra. We further provide Fityk files with the peak deconvolution used in this study (Suppl_Fit), which can be opened and viewed using the software package by Wojdyr (2010).

Table S1: Literature data compilation of previous Raman analyses for REE oxides, hydroxides and phosphates with more details given in the supplementary reference table (separate excel file).

Solid	Formula	Crystal system	Excitation laser (nm)	References
La-oxide	La ₂ O ₃	hexagonal	476.5, 488, 514.5, 524.5, 633, 647.1	1–5
Pr-oxide	Pr ₂ O ₃	hexagonal	457.9, 476.5, 496.5, 514.5, 520.8, 530.8	5
Nd-oxide	Nd ₂ O ₃	hexagonal	454.5, 457.9, 488, 514.5	3–5
Nd-oxide	Nd ₂ O ₃	monoclinic	na	6
Eu-oxide	Eu ₂ O ₃	monoclinic	532	7
Gd-oxide	Gd ₂ O ₃	monoclinic	514.5	8
Sc-oxide	Sc ₂ O ₃	monoclinic	na	9
Pr-oxide	Pr ₂ O ₃	isometric	457.9, 488, 514.5	10
Nd-oxide	Nd ₂ O ₃	isometric	457.9, 488, 514.5	10
Sm-oxide	Sm ₂ O ₃	isometric	488	10
Eu-oxide	Eu ₂ O ₃	isometric	457.9, 488, 514.5	10,11
Gd-oxide	Gd ₂ O ₃	isometric	457.9	10
Tb-oxide	Tb ₂ O ₃	isometric	457.9, 488, 514.5	10
Dy-oxide	Dy ₂ O ₃	isometric	457.9, 488, 501.7, 514.5, 632.8, 647.1	10–13
Ho-oxide	Ho ₂ O ₃	isometric	514.5, 568.2	10,12
Y-oxide	Y ₂ O ₃	isometric	457.9, 514.5, 568.2, 647.1	8,10,12,14–16
Er-oxide	Er ₂ O ₃	isometric	457.9	10
Tm-oxide	Tm ₂ O ₃	isometric	457.9, 488, 501.7, 514.5, 632.8	6,10,11,13
Yb-oxide	Yb ₂ O ₃	isometric	na	6
Lu-oxide	Lu ₂ O ₃	isometric	532	8,17

Sc-oxide	Sc ₂ O ₃	isometric	457.9	9,10,18,19
DyTm-oxide	Dy _{2-x} Tm _x O ₃	isometric	632.8	13
DyY-oxide	Dy _{2-x} Y _x O ₃	isometric	647.1	12
HoY-oxide	Ho _{2-x} Y _x O ₃	isometric	568.2	12
La-hydroxide	La(OH) ₃	hexagonal	na	20,21
Pr-hydroxide	Pr(OH) ₃	hexagonal	na	20
Nd-hydroxide	Nd(OH) ₃	hexagonal	514	20–22
Sm-hydroxide	Sm(OH) ₃	hexagonal	na	21
Eu-hydroxide	Eu(OH) ₃	hexagonal	na	21
Gd-hydroxide	Gd(OH) ₃	hexagonal	na	21
Tb-hydroxide	Tb(OH) ₃	hexagonal	na	21
Dy-hydroxide	Dy(OH) ₃	hexagonal	na	21
Xenotime-Gd	GdPO ₄	tetragonal	532	23
Xenotime-Tb	TbPO ₄	tetragonal	514.5, 532, 647	24–27
Xenotime-Dy	DyPO ₄	tetragonal	488, 532	24,27,28
Xenotime-Ho	HoPO ₄	tetragonal	514.5	24
Xenotime-Y	YPO ₄	tetragonal	514.5, 568, 633	24,29–32
Xenotime-Er	ErPO ₄	tetragonal	457.9, 532, 785	24,33,34
Xenotime-Tm	TmPO ₄	tetragonal	514.5	24,34
Xenotime-Yb	YbPO ₄	tetragonal	488, 532, 785	24,33
Xenotime-Lu	LuPO ₄	tetragonal	514.5	24
Xenotime-Sc	ScPO ₄	tetragonal	514.5, 568	29
Xenotime-GdDy	Gd _{1-x} Dy _x PO ₄	tetragonal	532	27
Xenotime-ErYb	Er _{1-x} Yb _x PO ₄	tetragonal	532, 785	33
Xenotime	REEPO ₄	tetragonal	473	35
Monazite-La	LaPO ₄	monoclinic	514, 532, 633	24,36–38
Monazite-Ce	CePO ₄	monoclinic	515, 632.8	36,37
Monazite-Pr	PrPO ₄	monoclinic	515, 632.8	36,37
Monazite-Nd	NdPO ₄	monoclinic	488	36
Monazite-Sm	SmPO ₄	monoclinic	514	36
Monazite-Eu	EuPO ₄	monoclinic	514	36
Monazite-Gd	GdPO ₄	monoclinic	514, 532	36
Monazite-LaEu	La _{1-x} Eu _x PO ₄	monoclinic	532, 633	38
Rhabdophane-La	LaPO ₄ *0.667H ₂ O	monoclinic	na	39
Rhabdophane-Nd	NdPO ₄ *0.667H ₂ O	monoclinic	na	39
Rhabdophane-Gd	GdPO ₄ *0.667H ₂ O	monoclinic	532	40

Abbreviations: na = information not available in the study.

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