Electronic Supplementary Material (ESI) for CrystEngComm.

The Structural Effects of Alkaline- and Rare-Earth Elements Incorporation into the Thorium Molybdates

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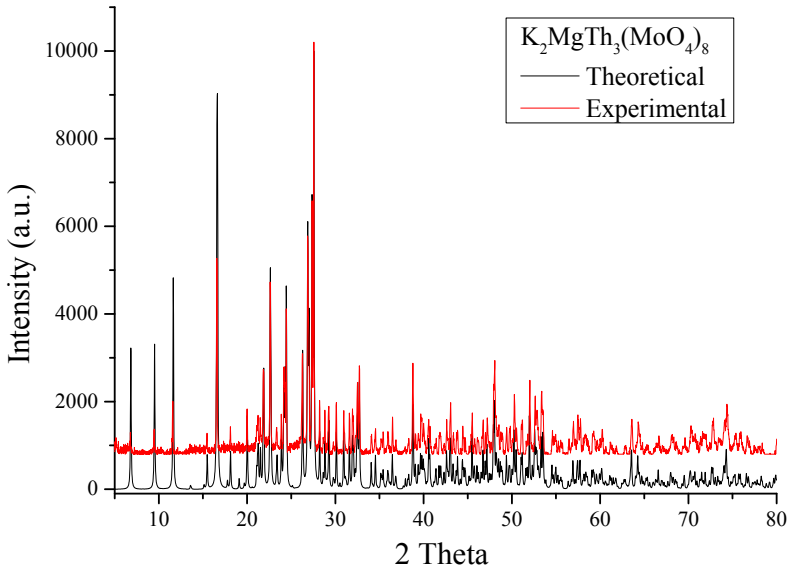
$K_2MgTh_3(MoO_4)_8$
Theoretical
Experimental
Intensity (a.u.)
2 Theta
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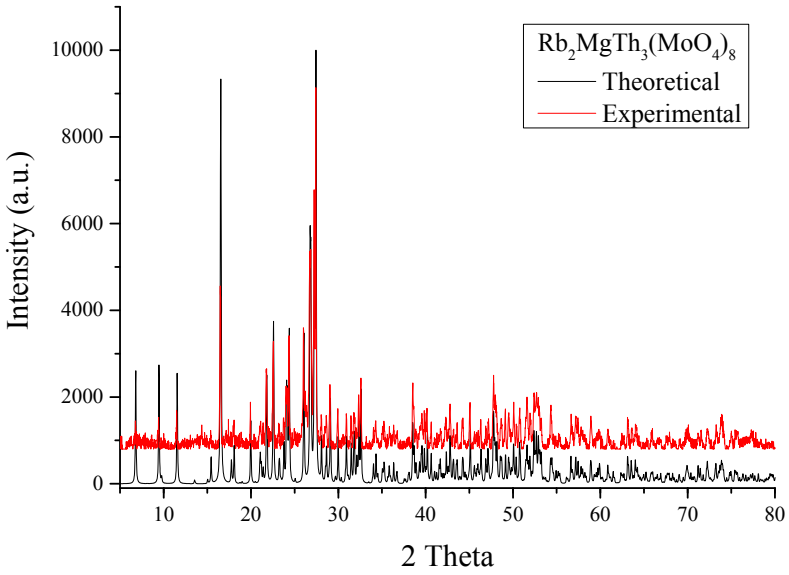
2000
4000
6000
8000
10000
10
20
30
40
50
60
70
80


$Rb_2MgTh_3(MoO_4)_8$
Theoretical
Experimental
Intensity (a.u.)
2 Theta
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4000
6000
8000
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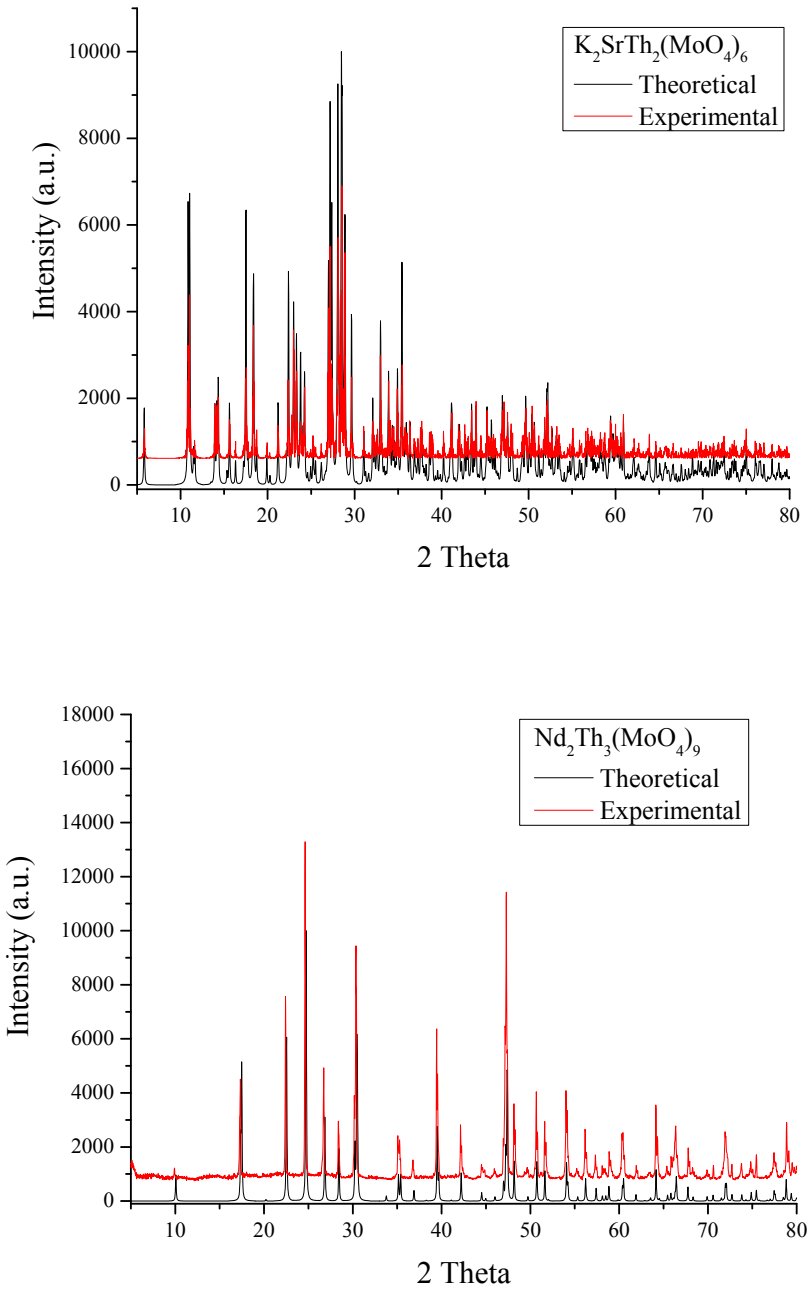


Figure 1. Comparison of PXRD patterns for $K_2MgTh_3(MoO_4)_8$, $Rb_2MgTh_3(MoO_4)_8$, $K_2SrTh_2(MoO_4)_6$ and $Nd_2Th_3(MoO_4)_9$, respectively.

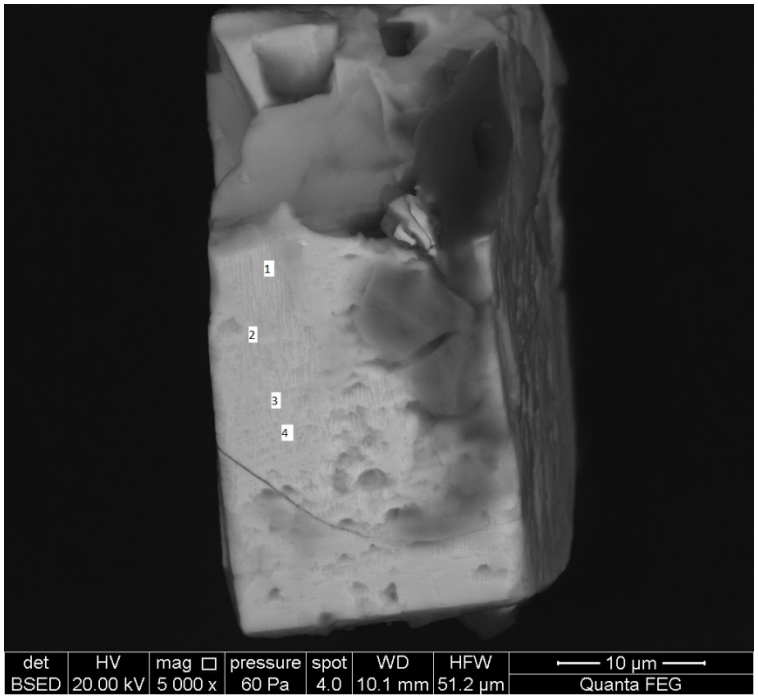


Figure S2(a) BSE image and EDS measuring points for $K_2MgTh_3(MoO_4)_8$

Table S1 (a). Atomic ratios of $K_2MgTh_3(MoO_4)_8$ (Th is kept constant as 3)

	K	Mg	Th	Mo
Point1	2.33	0.87	3	8.53
Point2	2.32	0.98	3	8.43
Point3	2.43	0.95	3	8.68
Point4	2.23	0.92	3	8.43
Average	2.33	0.93	3	8.52

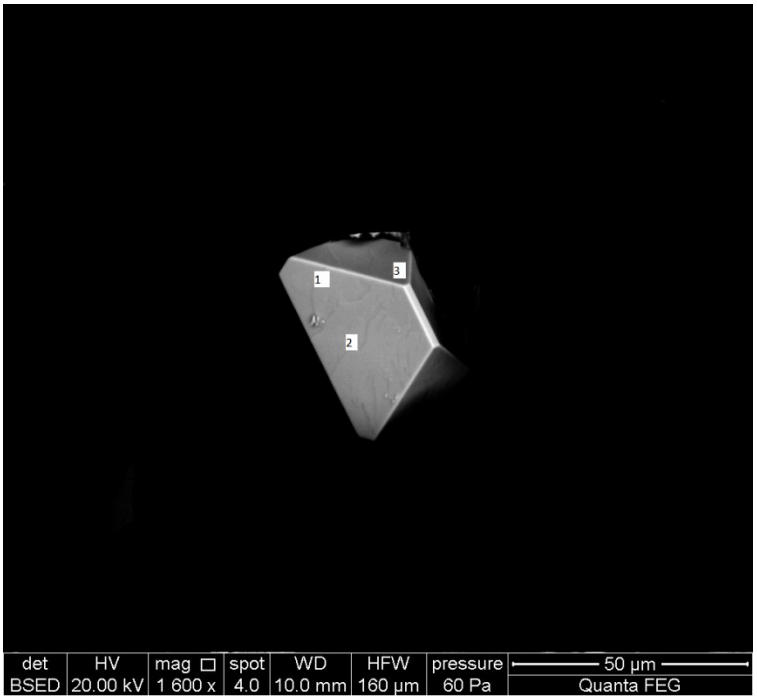


Figure S2(b). BSE image and EDS measuring points for $Rb_2MgTh_3(MoO_4)_8$

Table S1 (b). Atomic ratios of $Rb_2MgTh_3(MoO_4)_8$ (Th is kept constant as 3)

	Rb	Mg	Th	Mo
Point1	2.32	0.98	3	8.34
Point2	2.21	1.08	3	8.32
Point3	2.04	0.86	3	8.16
Average	2.19	0.97	3	8.27

Figure S2(c) BSE image and EDS measuring points for $K_2SrTh_2(MoO_4)_6$

Table S1 (c). Atomic ratios of $K_2SrTh_2(MoO_4)_6$ (Th is kept constant as 2)

	K	Sr	Th	Mo
Point1	2.11	0.98	2	6.06
Point2	2.04	0.78	2	6.13
Point3	2.22	0.79	2	6.16
Average	2.12	0.85	2	6.12

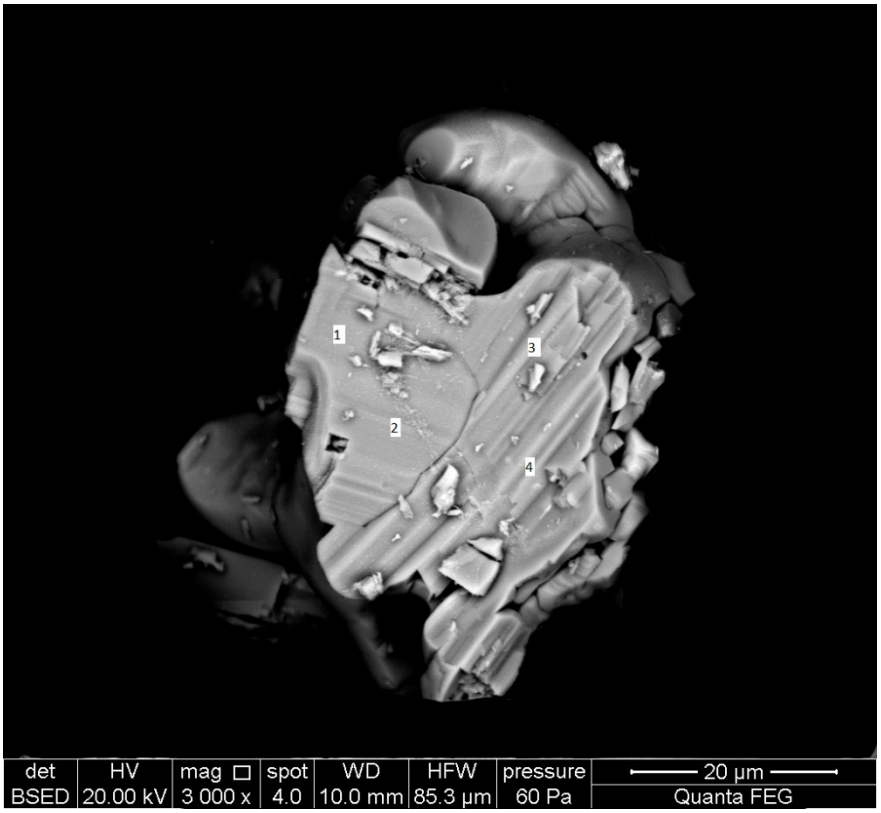


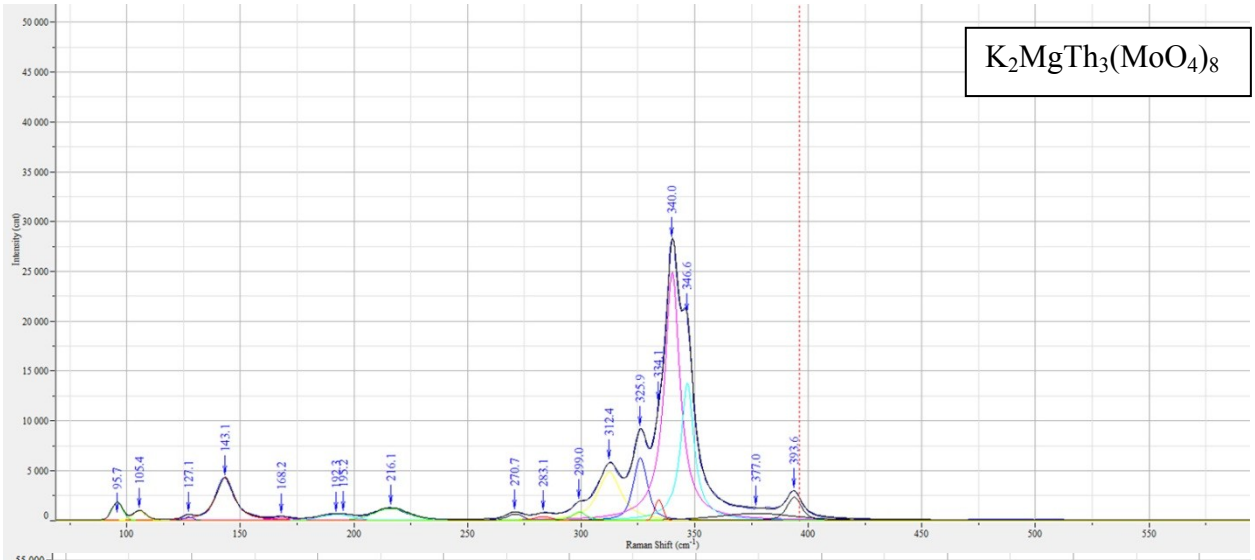
Figure S2(d) BSE image and EDS measuring points for $Nd_2Th_3(MoO_4)_9$

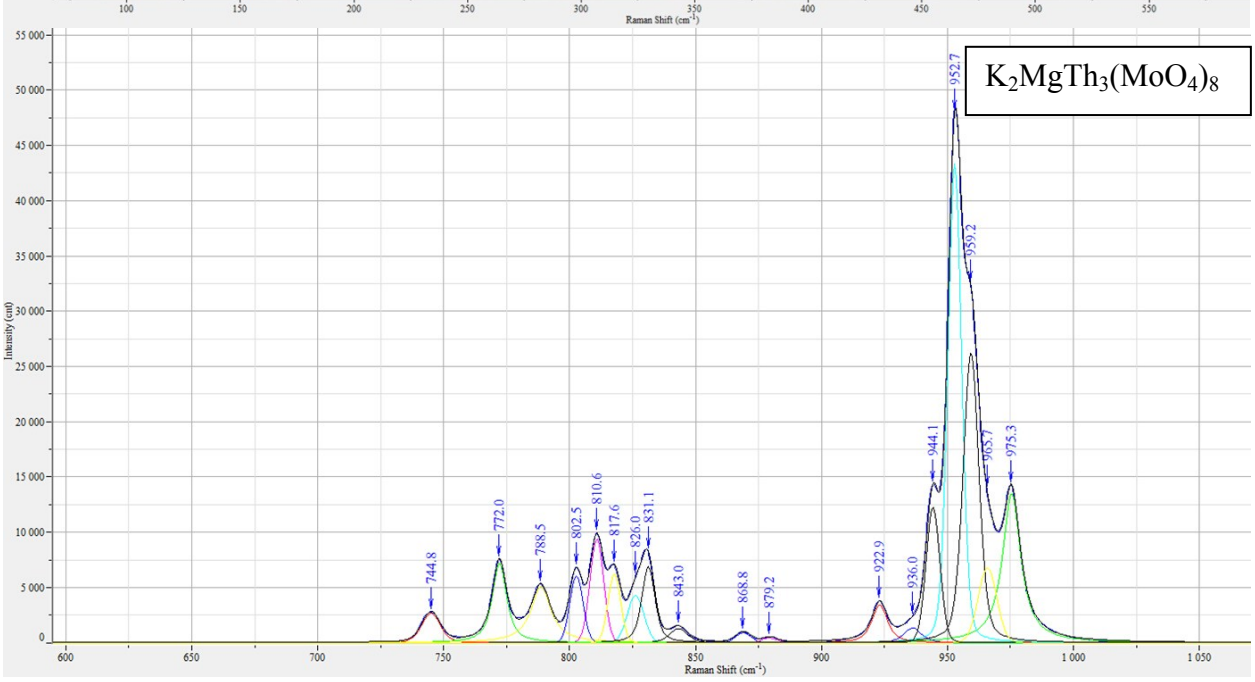
Table S1 (d). Atomic ratios of $Nd_2Th_3(MoO_4)_9$ (Th is kept constant as 3)

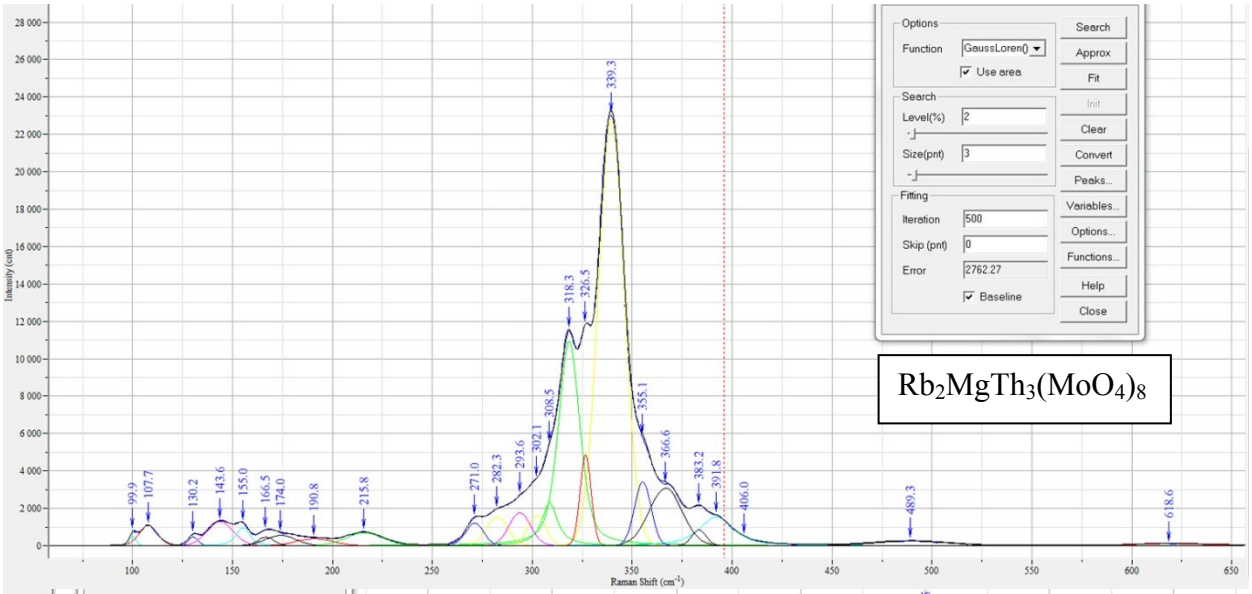
	Th	Mo	Nd
Point1	3	9.12	1.87
Point2	3	9.32	1.98
Point3	3	9.04	2.01
Point4	3	9.32	1.89
Average	3	9.20	1.94

Table S2. Raman shifts of $K_2MgTh_3(MoO_4)_8$, $Rb_2MgTh_3(MoO_4)_8$, $K_2SrTh_2(MoO_4)_6$ and $Nd_2Th_3(MoO_4)_9$, respectively. Abbreviations: s, strong; m, middle; w weak; sh, shoulder.

$K_2MgTh_3(MoO_4)_8$	$Rb_2MgTh_3(MoO_4)_8$	$Nd_2Th_3(MoO_4)_9$	$K_2SrTh_2(MoO_4)_6$
105w	100w	102w	110m
127w	108w	116w	115sh
143m	130w	123w	125m
168w	144w	133w	134m
192w	155w	142w	141m
195w	167w	151w	149sh
216w	174w	158w	155sh
271w	191w	178w	170w
283w	216w	201w	183m
299w	271w	211w	191sh
312m	282sh	224m	213w
326s	294sh	242m	219sh
334sh	302sh	252sh	243w
340s	309sh	270w	255w
347s	318s	285m	277sh
377w	327s	323m	285s
394w	339s	335w	298sh
745w	355sh	348m	310w
772m	367m	365w	319sh
789m	383w	374w	327sh
803m	392w	380w	333w
811m	406w	386w	341sh
818m	489w	414w	361sh
826sh	702w	449w	368sh
831m	744w	480w	377s
843w	751w	506w	390m
869w	757sh	524w	402sh
879w	764w	541w	409m
923w	772w	572w	420w
936sh	789m	607w	592w
944s	801m	631w	640w
953s	808sh	647w	659w
959s	818w	676w	717w
966sh	828w	715w	735w
975s	840w	727w	769s
	853w	758w	791m
	873w	789w	804m
	882w	797w	835m
	891w	805w	853sh
	908w	847w	903s
	922m	861m	956w
	930m	875w	
	937m	882w	
	951s	888m	
	957s	900w	
	963s	911m	
	970m	924w	
		932m	
		948m	
		954sh	
		965s	


$K_2MgTh_3(MoO_4)_8$
Intensity (cnt)
Raman Shift (cm⁻¹)
95.7
105.4
127.1
143.1
168.2
193.3
195.2
216.1
270.7
283.1
299.0
312.4
325.9
334.1
340.0
346.6
377.0
393.6


$K_2MgTh_3(MoO_4)_8$
Intensity (cnt)
Raman Shift (cm⁻¹)
744.8
772.0
788.5
802.5
810.6
817.6
826.0
831.1
843.0
868.8
879.2
922.9
936.0
944.1
952.7
959.2
965.7
975.3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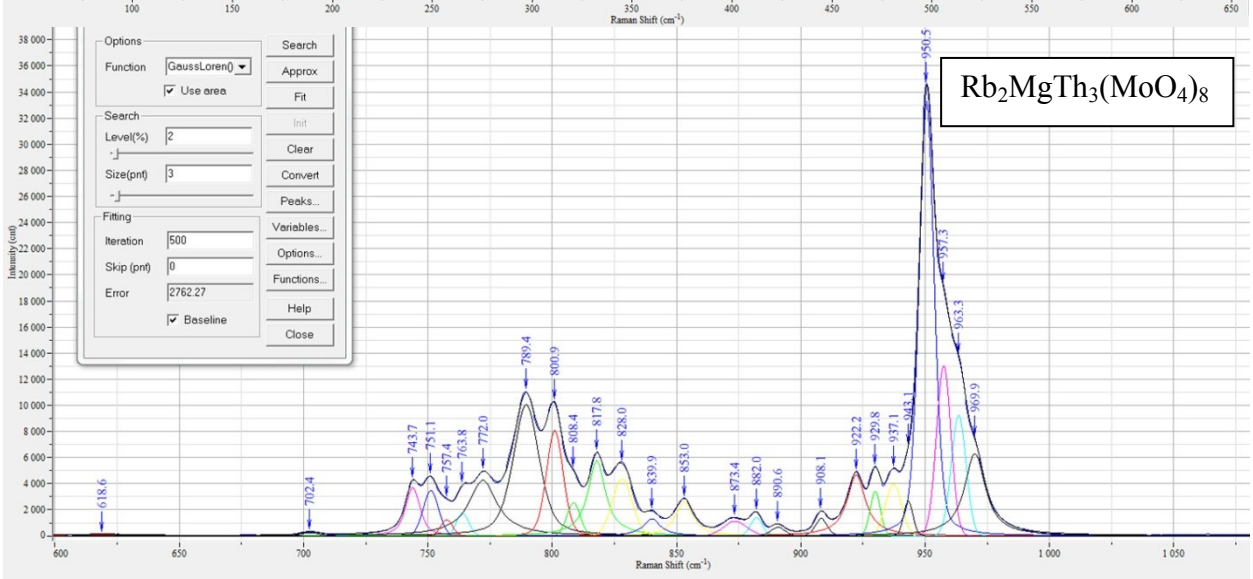
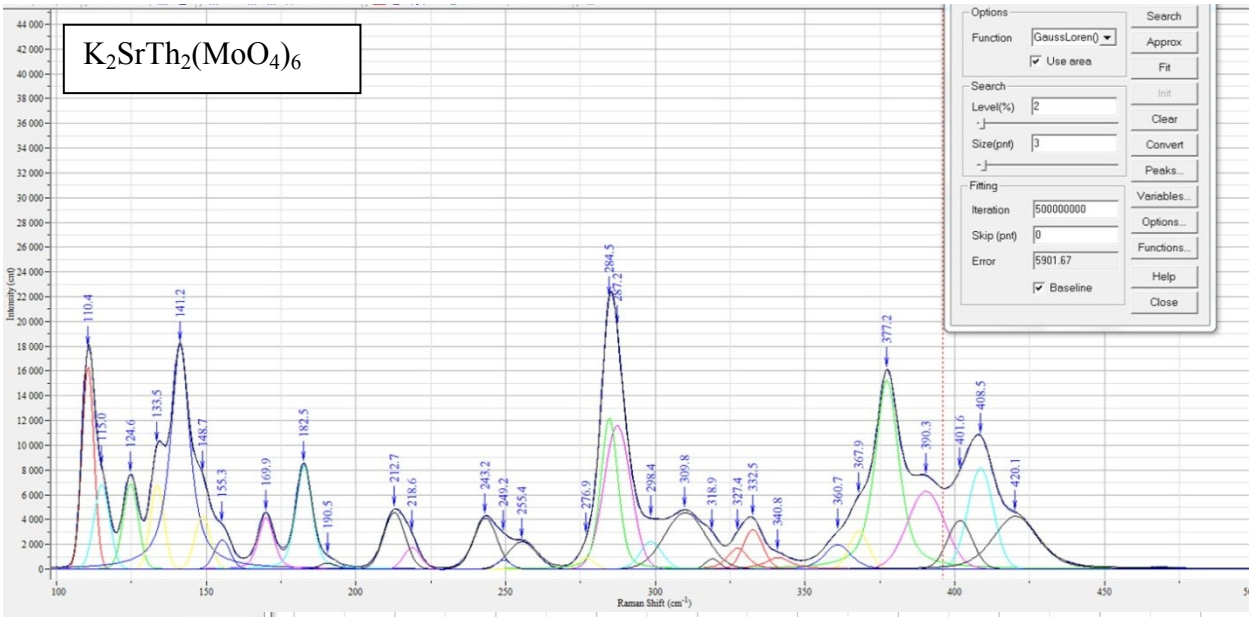
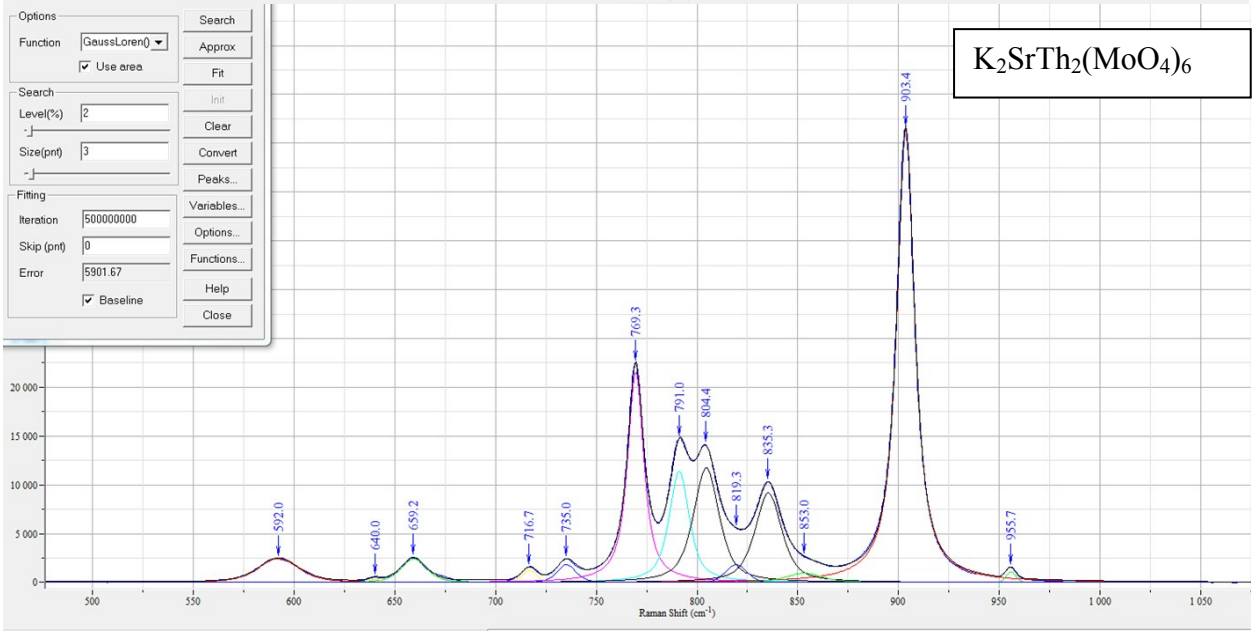
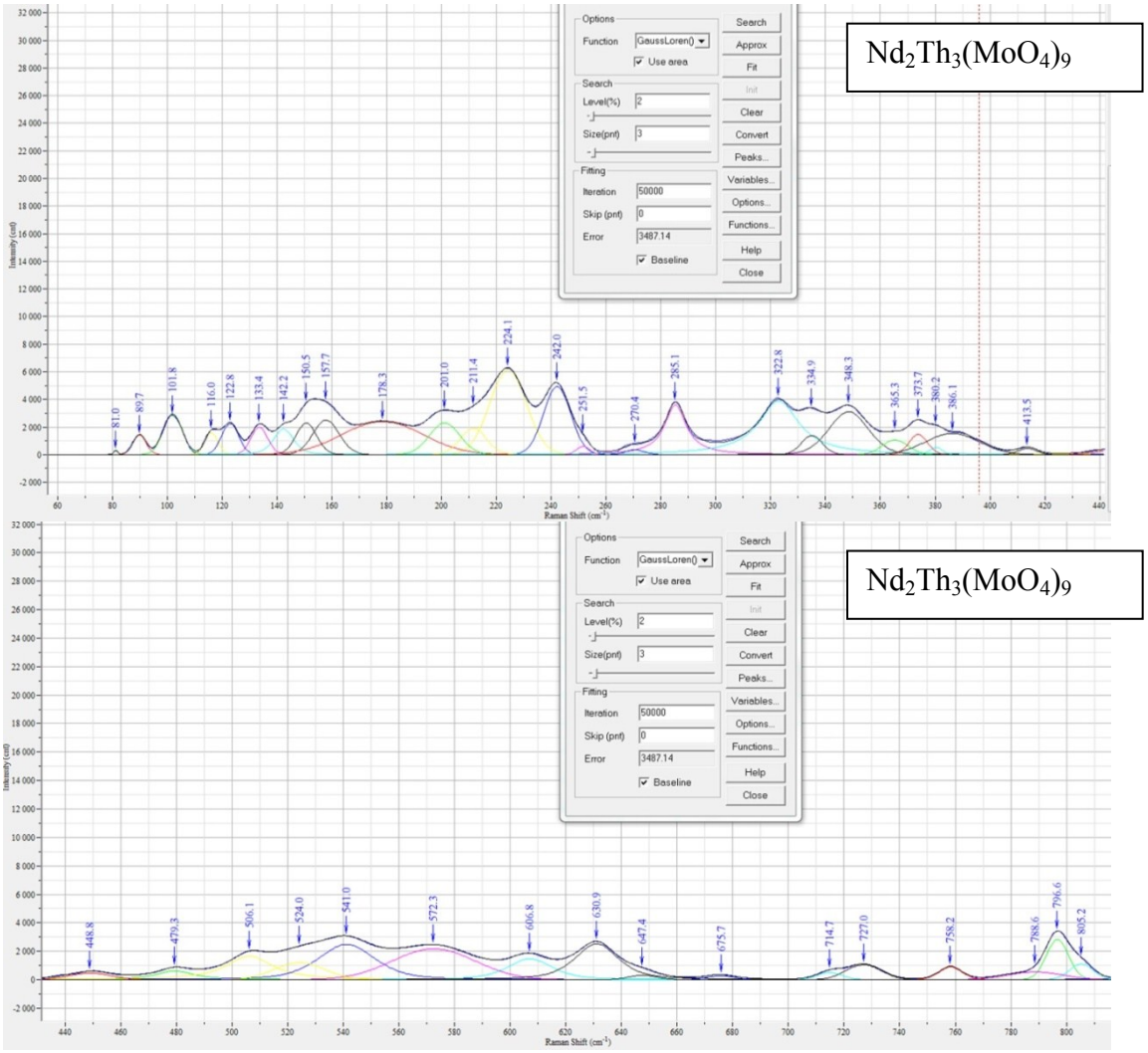
Use area
Search
Level(%) 2
Size(pnt) 3
Fitting
Iteration 500
Skip (pnt) 0
Error 2762.27
Baseline
Search
Approx
Fit
Init
Clear
Convert
Peaks...
Variables...
Options...
Functions...
Help
Close
Rb2MgTh3(MoO4)8
Intensity (cnt)
Raman Shift (cm-1)


Rb2MgTh3(MoO4)8
Intensity (cnt)
Raman Shift (cm-1)


$K_2SrTh_2(MoO_4)_6$
Options
Function
GaussLoren()
Use area
Search
Level(%)
Size(pnt)
Fitting
Iteration
Skip (pnt)
Error
Baseline
Search
Approx
Fit
Init
Clear
Convert
Peaks...
Variables...
Options...
Functions...
Help
Close
Intensity (cnt)
Raman Shift (cm-1)


$K_2SrTh_2(MoO_4)_6$
Raman Shift (cm-1)



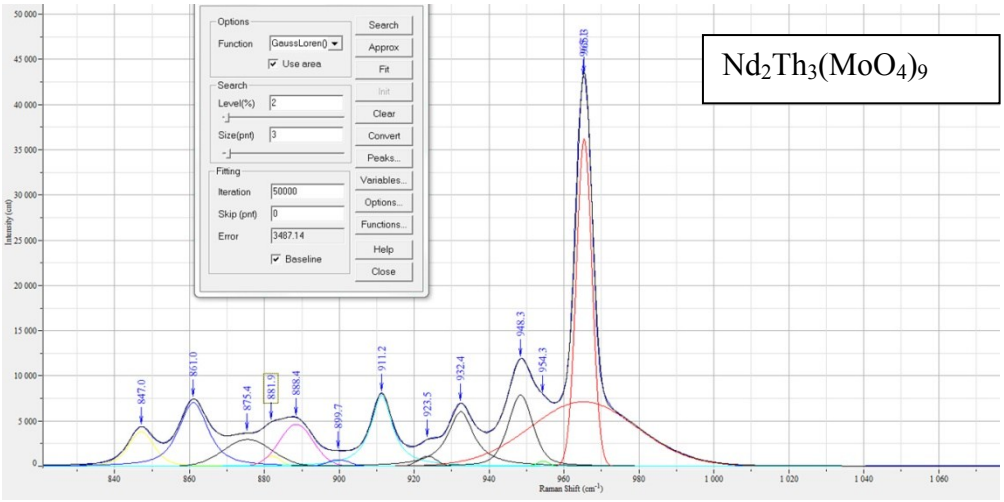


Figure S3. The complete Raman fitting results for $K_2MgTh_3(MoO_4)_8$, $Rb_2MgTh_3(MoO_4)_8$, $K_2SrTh_2(MoO_4)_6$ and $Nd_2Th_3(MoO_4)_9$, respectively.

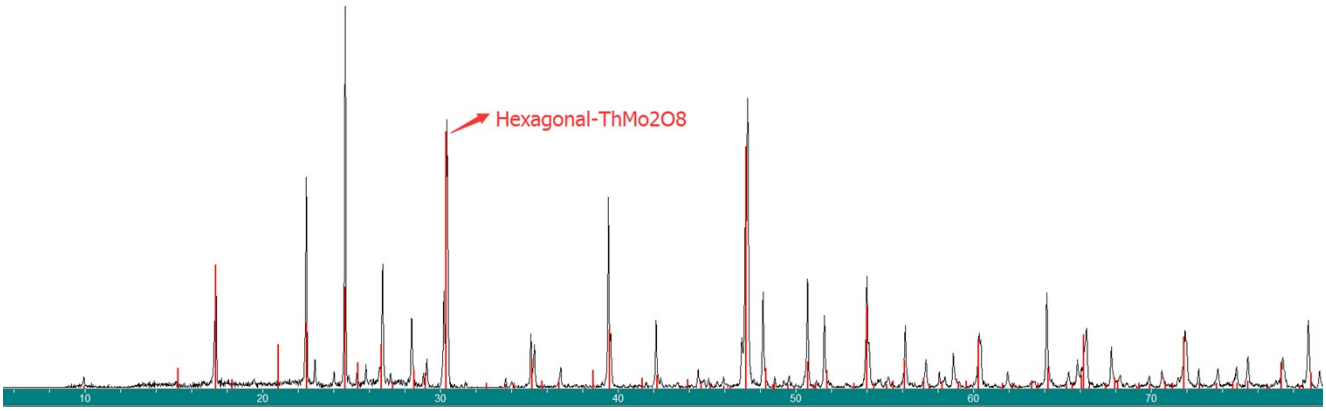


Figure S4. Powder X-ray diffraction pattern of reaction products after heating $Nd_2Th_3(MoO_4)_9$ across the first endothermic peak (667(5) °C), showing that the main phase that has been generated due to decomposition is hexagonal $ThMo_2O_8$.