

Supplementary information for

An unusual temperature induced isostructural phase
transition in Scheelite $\text{Li}_{0.5}\text{Ce}_{0.5}\text{MoO}_4$

Dipankar Saha,[†] Rajeev Ranjan,[‡] Diptikanta Swain,[§] Chandrabhas Narayana[§] and Tayur N.

Guru Row^{†,}*

[†]Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560 012, India.

[‡]Materials Engineering, Indian Institute of Science, Bangalore 560 012, India.

[§]Light Scattering Laboratory, Chemistry and Physics of Materials Unit, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Jakkur P.O., Bangalore 560064, India.

* Corresponding author: E-mail: ssctng@sscu.iisc.ernet.in Tel: +91-80-2292796 Fax: +91-80-3601310

Table S1. Intensity ratios between peaks of the main phase and surrogate phase.

Selected 2 θ Values	Peak intensity in %	
	Main Phase	Surrogate Phase
18.15	100	100
19.56	13.55	13.35
21.64	22.97	23.62
29.30	39.17	37.29
30.75	18.92	16.17
33.34	18.19	19.15
35.90	58.02	56.03
36.68	17.56	14.27

Table S2. List of oxygen coordinates after Rietveld refinements.

Temperature (°C)	Phase	<i>x</i>	<i>y</i>	<i>z</i>
550	1	0.246(1)	0.393(1)	0.043(1)
	2	0.243(2)	0.396(2)	0.044(2)
490	1	0.238(1)	0.392(1)	0.044(1)
	2	0.242(1)	0.376(2)	0.041(1)
450	1	0.242(2)	0.390(1)	0.042(1)
	2	0.240(1)	0.395(1)	0.042(2)
400		0.242(1)	0.389(2)	0.040(1)
300		0.240(1)	0.391(1)	0.043(1)
200		0.240(1)	0.393(1)	0.041(1)
100		0.244(1)	0.390(1)	0.042(1)
25		0.241(1)	0.394(1)	0.042(1)

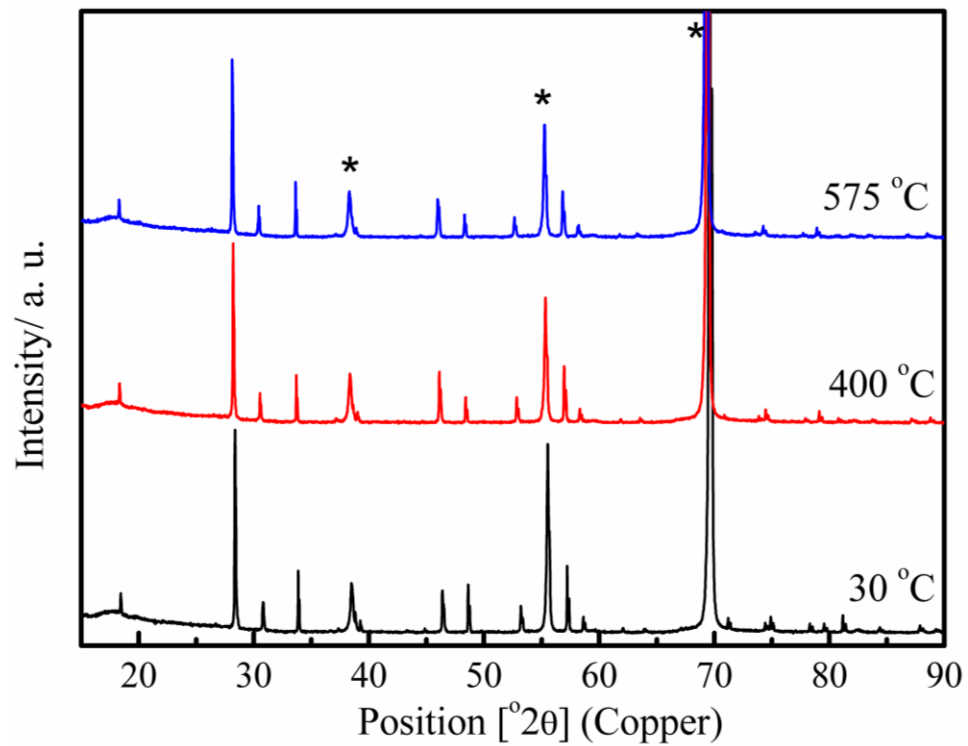


Figure S1 Laboratory powder X-ray diffractogram of LCM at different temperature

(* Bragg peaks from Ta strip).

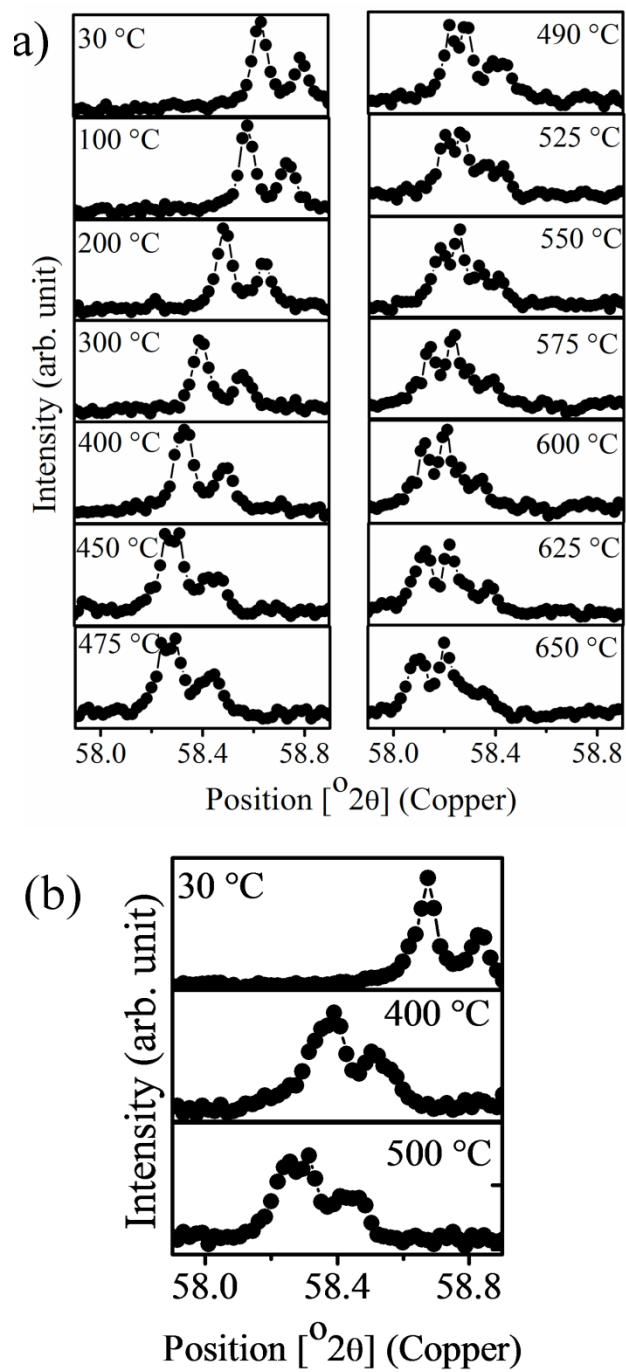


Figure S2 Laboratory powder X-ray diffractogram of LCM in a narrow 2θ interval at different temperature (a) Heating cycle (b) Cooling cycle.