

Electronic Supporting Information

for

Time and energy conserving solution combustion synthesis of nano $\text{Li}_{1.2}\text{Ni}_{0.13}\text{Co}_{0.13}\text{Mn}_{0.54}\text{O}_2$ cathode material and its performance in Li-ion batteries

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Electronic Supporting information Table - S1. Relevant thermodynamics data.

Compound	ΔH_f (KJ mol ⁻¹)
$\text{LiNO}_{3(c)}$	579.72
$\text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}_{(c)}$	539.63
$\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}_{(c)}$	54.66
$\text{Mn}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}_{(c)}$	311.2
$\text{CO}(\text{NH}_2)_2_{(c)}$	582.92
$\text{C}_2\text{H}_5\text{NO}_{2(c)}$	205.06
$\text{N}_{2(g)}$	0
$\text{CO}_{2(g)}$	393.5
$\text{H}_2\text{O}_{(g)}$	241.8
(C)=Crystalline	(g)= Gaseous

Electronic Supporting information Table - S2. pH observations of reaction mixtures before and after the pre heat treatment.

SI No	Combustion solution	Initial pH of the mixture	pH after heat treatment
1	Urea+ Nitrates solution	5.33	5.94
2	Glycine+ Nitrates solution	3.32	3.27
3	Mixed fuels+ Nitrates solution	3.22	6.74

Electronic Supporting information Table - S3. Structural parameters obtained from two phase rietveld refinement of XRD data for combustion synthesized $\text{Li}_{1.2}\text{Ni}_{0.13}\text{Mn}_{0.54}\text{Co}_{0.13}\text{O}_2$ heated at 850 °C and lattice parameter for solid state synthesized phase.

Phase 1: $\text{LiNi}_{1/3}\text{Co}_{1/3}\text{Mn}_{1/3}\text{O}_2$ ($R\bar{3}m$)					
Element	Site	Wyckoff positions			Occupancy
Li1	3b	0	0	0	0.9800
Ni1	3b	0	0	0	0.0200
Li2	3a	0	0	0.5	0.0200
Ni2	3a	0	0	0.5	0.3100
Mn1	3a	0	0	0.5	0.3350
Co1	3a	0	0	0.5	0.3366
O1	6c	0	0	0.2440	1.0000
a = 2.8487Å° c = 14.2216Å°					
Phase 2: Li_2MnO_3 (C2/m)					
Element	Site	Wyckoff positions			Occupancy
Li1	2b	0	0.5	0	0.8516
Mn1	2b	0	0.5	0	0.1261
Li2	2c	0	0	0.5	1.0080
Li3	4h	0	0.7149	0.5	1.1811
Mn2	4h	0	0.6740	0.5	0.0286
Li4	4g	0	0.0870	0	0.0840
Mn3	4g	0	0.1795	0	0.8507
O1	6c	0.2458	0	0.2130	1.0600
O2	8j	0.2491	0.3281	0.2429	2.0000
a = 4.9540Å° b = 8.5153Å° c = 5.0094Å° β = 108.88°					
Rwp = 10.2 Rp = 15.6 Chi 2 = 2.26 Phase ratio 5:5					
Solid –State synthesized phase					
$R\bar{3}m$:- a = b = 2.8453 Å°, c = 14.1906 Å°					
C2/m:- a = 4.9680 Å°, b = 8.4936 Å°, c = 5.0360 Å°, β = 110.2°					

Electronic Supporting information Fig– S1. FESEM image and Powder XRD pattern with Rietveld refinement of solid state synthesized $\text{Li}_{1.2}\text{Ni}_{0.13}\text{Mn}_{0.54}\text{Co}_{0.13}\text{O}_2$ sample. The XRD pattern shows experimental pattern (red dots), calculated patterns (black lines), the difference curve (pink line) and Bragg diffraction positions (yellow ticks for $R\bar{3}m$ space group and blue ticks for $C2/m$ space group). The inset of figure shows FESEM image.

