Electronic Supplementary Material (ESI) for CrystEngComm.

Phase Transformation from α-Fe_2O_3 to Fe_3O_4 and $LiFeO_2$ by self-reduction of Fe (III) in Prussian Red in the presence of Alkali Hydroxides: Investigation on the Phase dependent Morphological and Magnetic properties

K Palani Thiruppathi[a] and Devaraj Nataraj[a,b*]

* Corresponding Author email: de.natraj2011@gmail.com

Table S1. The reaction parameters and precursor's mole concentrations for the various phases and morphologies of as prepared iron oxides.

Sample code	Iron Precursor $K_3[Fe(CN)_6]$ ($molL^{-1}$)*	Alkali Hydroxide name	Alkali Hydroxide ($molL^{-1}$)*	Hydrothermal reaction Temperature (˚C)	Hydrothermal reaction Time (h)	Crystalline Phase	Morphology
F1N1	0.01	NaOH	1	180	12	α-Fe_2O_3	Hexagonal disc
F1N5	0.01	NaOH	5	180	12	α-Fe_2O_3	Hexagonal disc
F1N7	0.01	NaOH	7	180	12	α-Fe_2O_3	Hexagonal disc
F1N13	0.01	NaOH	13	180	12	α-Fe_2O_3	Hierarchical sphere
F6N5	0.06	NaOH	5	180	12	α-Fe_2O_3 Fe_3O_4	Agglomerated ring with sphere
F9N5	0.09	NaOH	5	180	12	Fe_3O_4	Agglomerated Sphere
F1L1	0.01	$LiOH.H_2O$	1	180	12	$LiFe_5O_8$	Mixed flower
F1L2	0.01	$LiOH.H_2O$	2	180	12	$LiFeO_2$	Un matured sphere
F1L3	0.01	$LiOH.H_2O$	3	180	12	$LiFeO_2$	Un matured sphere
F1L7	0.01	$LiOH.H_2O$	7	180	12	$LiFeO_2$	Irregular sphere
F1N3	0.01	NaOH	3	180	6	α-Fe_2O_3	Hexagonal disc
F10N6	0.1	NaOH	6	180	6	Fe_3O_4	Sphere
F9N11	0.09	NaOH	11	180	6	Fe_3O_4	Irregular particle
F1L5	0.01	$LiOH.H_2O$	5	180	6	$LiFeO_2$	Irregular sphere

* Both reactants were dissolved in 15 ml of double distilled water

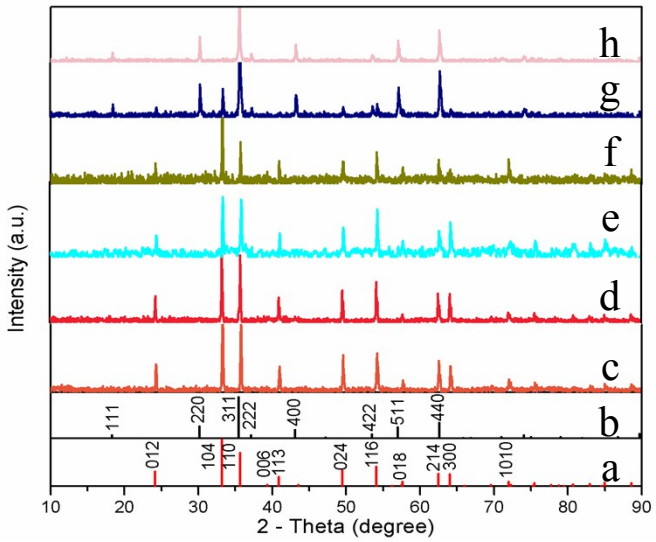
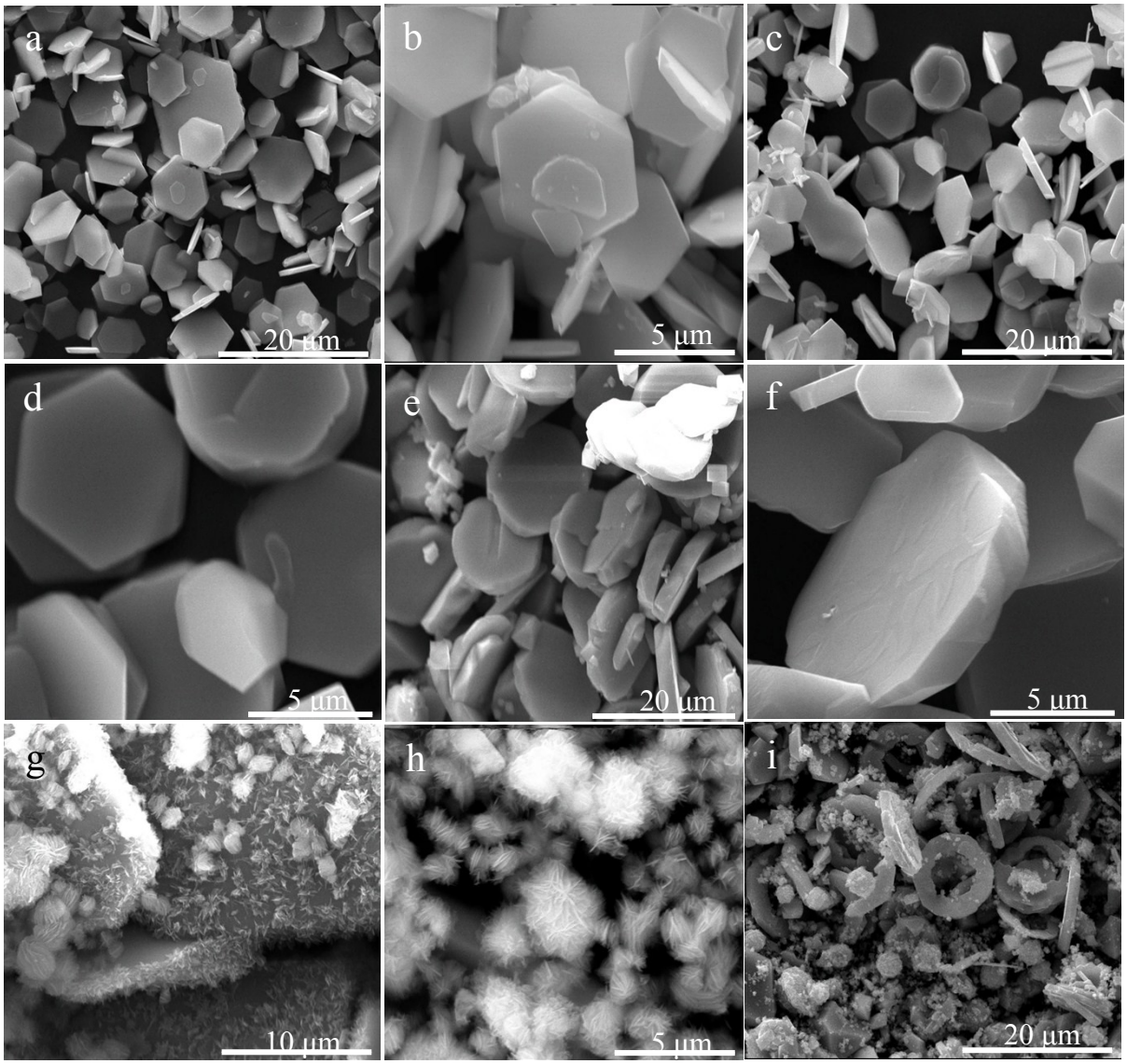


Figure S1. Powder X- Ray Diffraction pattern of phase evaluation from hematite (α-Fe_2O_3) to magnetite (Fe_3O_4) under different concentrations of $K_3[Fe(CN)_6]$ and NaOH. The JCPDS patterns (a) 87-1166 and (b) 65-3107 are represents the hematite and magnetite phases of iron oxides respectively. The various reactant concentrations are labeled as follows, (c) F1N1, (d) F1N5, (e) F1N7, (f) F1N13, (g) F6N5 and (h) F9N5.



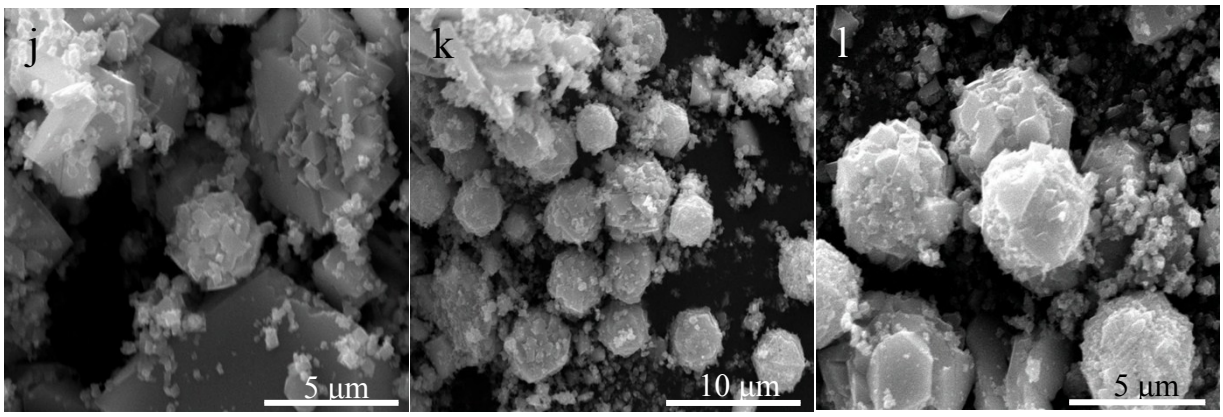


Figure S2. Scanning Electron Microscope images for various molar concentrations of $K_3[Fe(CN)_6]$ and NaOH based iron oxides. The images are labeled based on its sample code as follows, (a-b) F1N1, (c-d) F1N5, (e-f) F1N7, (g-h) F1N13, (i-j) F6N5 and (k-l) F9N5.

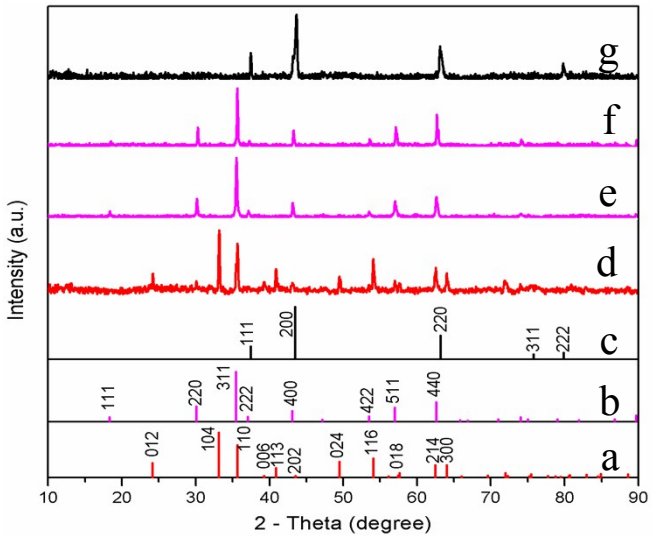
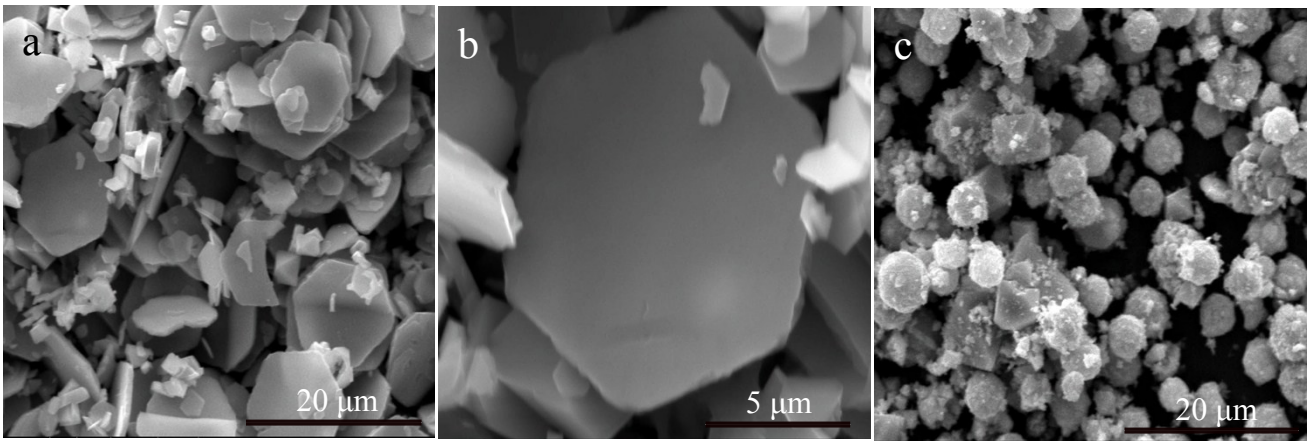


Figure S3. XRD patterns of Reaction time (6hrs) dependent prepared iron oxides. Fig (a-c) shows the JCPDS patterns of α-Fe_2O_3 (87-1166), Fe_3O_4 (65-3107) and $LiFeO_2$ (74-2284) microcrystalites. The remaining patterns shows the (d) hematite hexagonal disc (F1N3-6), (e) magnetite truncated sphere (F10N6-6), (f) magnetite irregular particle (F9N11-6) and (g) irregular spherical $LiFeO_2$ (F1L5-6) crystalline structure.



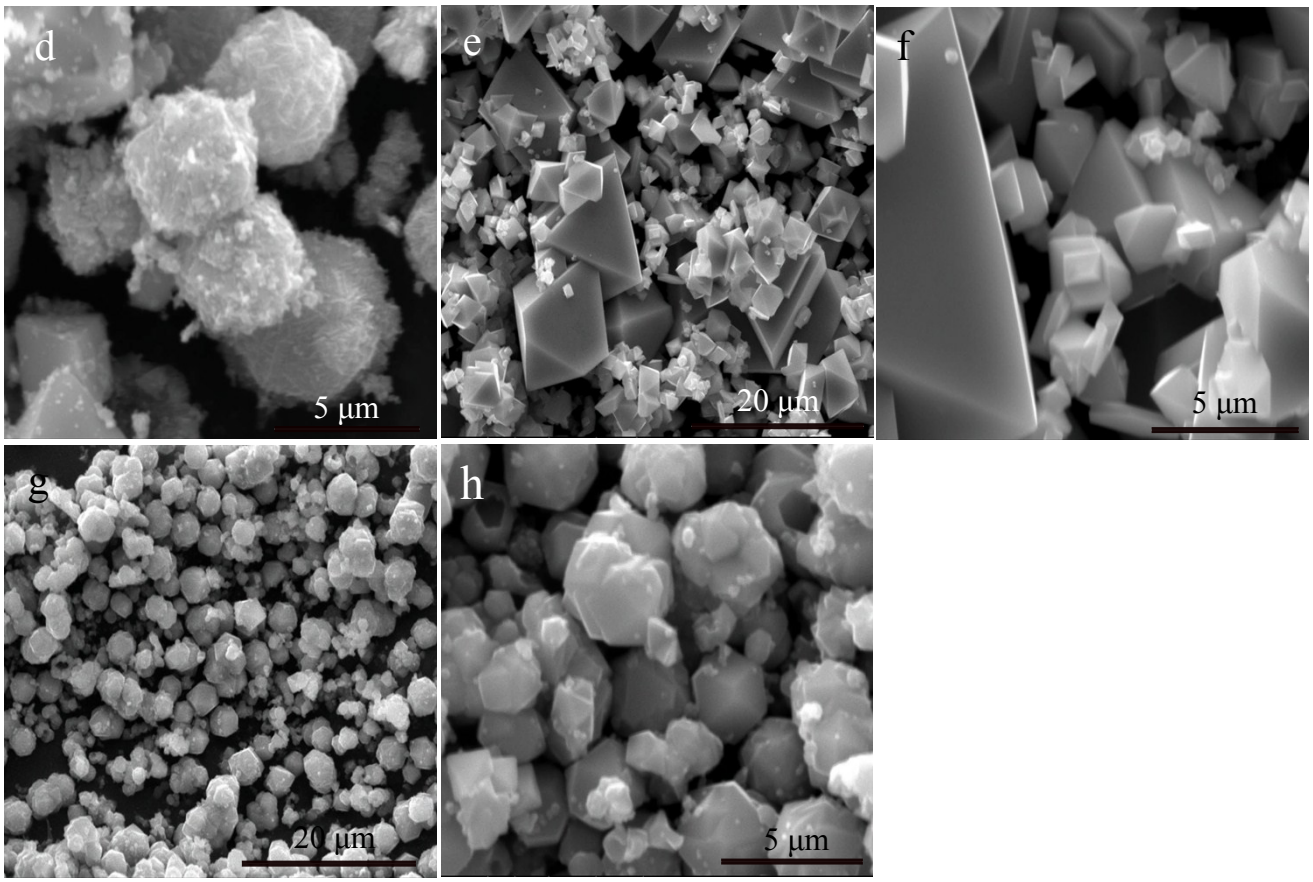


Figure S4. SEM images of iron oxides micro structures prepared from the 6hrs reaction time with 180°C reaction temperature. The image details are represents with corresponding sample codes as follows, (a-b) F1N3-6, (c-d) F10N6-6, (e-f) F9N11-6 and (g-h) F1L5-6.

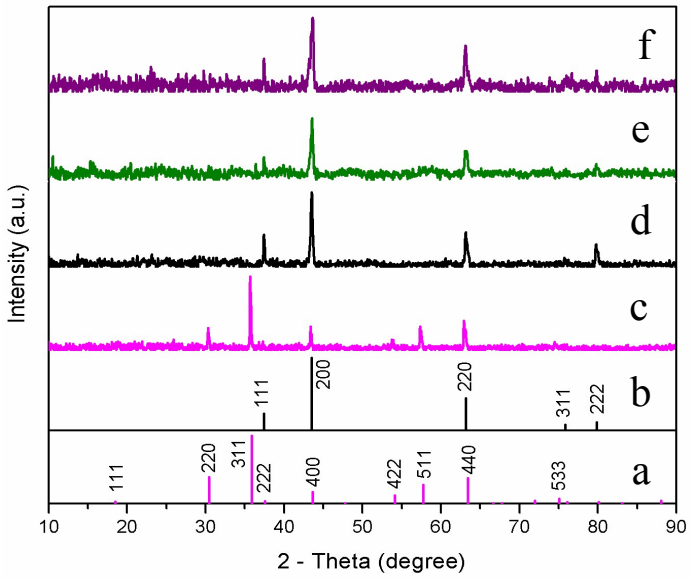


Figure S5. X-Ray diffraction patterns of different concentrations of $LiOH.H_2O$ based $LiFeO_2$ oxides. Fig.(a and b) shows the JCPDS card number for $LiFe_5O_8$ (76-1590) and $LiFeO_2$ (74-2284) phases. Various molar concentrations are shown as (c) 1 $molL^{-1}$ (F1L1), (d) 2 $molL^{-1}$ (F1L2), (e) 3 $molL^{-1}$ (F1L3) and (f) 7 $molL^{-1}$ (F1L7).

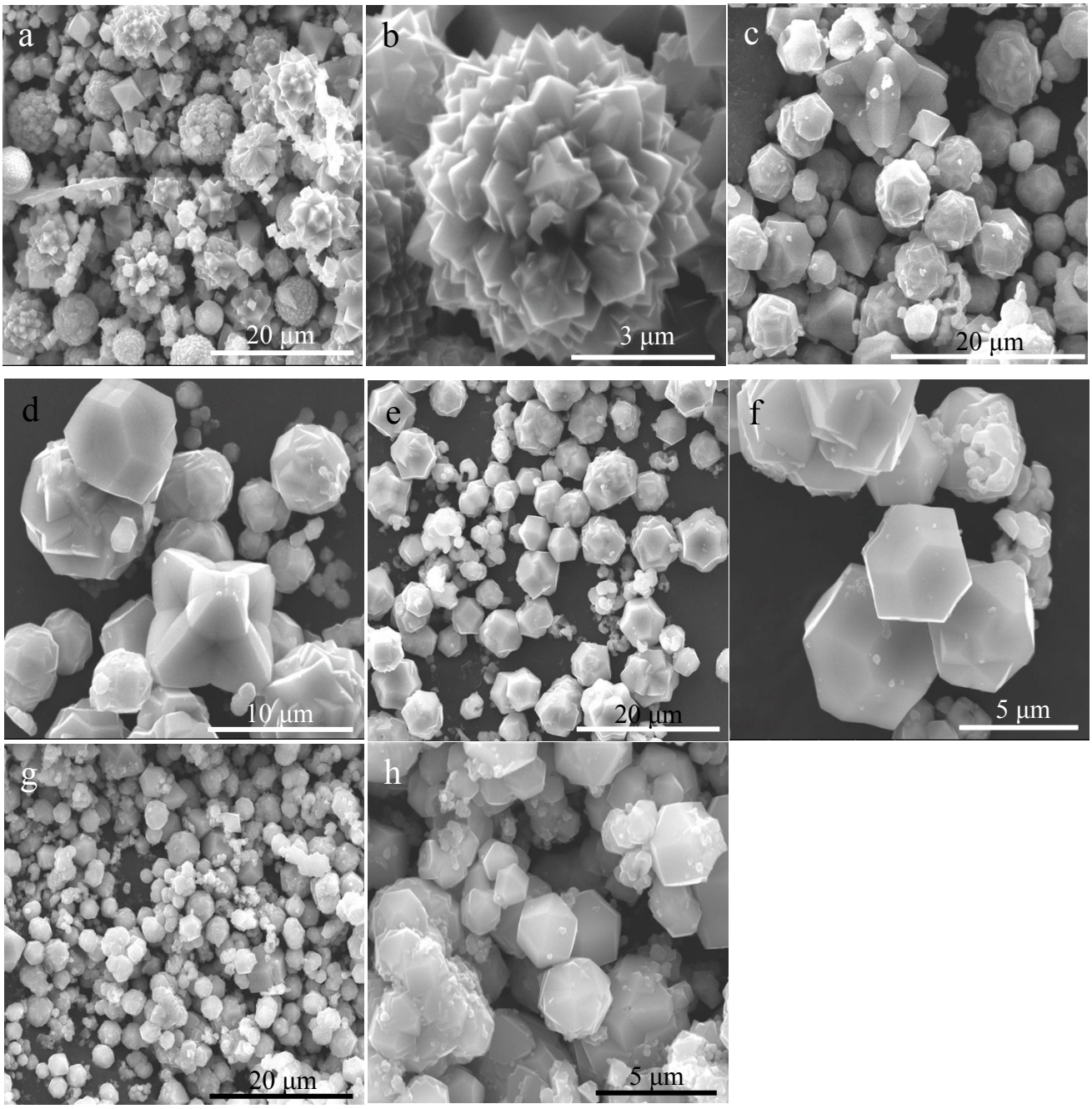


Figure S6. Scanning Electron Microscope images for various mole concentrations of $LiOH.H_2O$ with constant $K_3[Fe(CN)_6]$ iron (III) source. The images with two different magnifications are labeled as follows, (a-b) 1 $molL^{-1}$ (F1L1), (c-d) 2 $molL^{-1}$ (F1L2), (e-f) 3 $molL^{-1}$ (F1L3) and (g-h) 7 $molL^{-1}$ (F1L7).

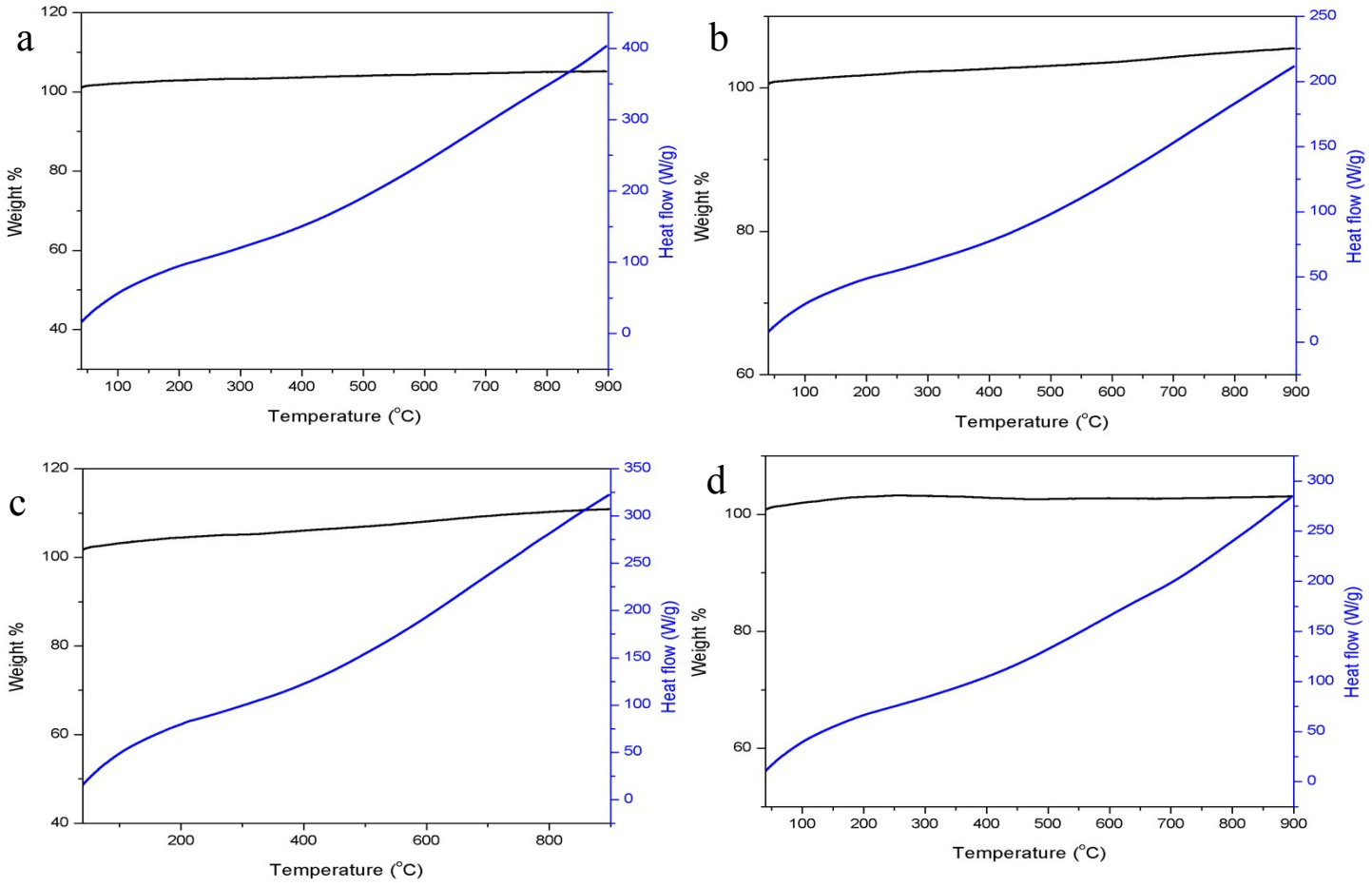


Figure S7. TG and DSC Spectra of samples code (a) F1N3, (b) F10N6, (c) F9N11 and (d) F1L5.