Magnetic Structures of $NaFePO_4$ Maricite and Triphylite Polymorphs for Sodium-ion Batteries

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Supplementary Information

Table S1. Basis vectors for the 4*c*(x,0.75,z) site of the *Pnma(62)* space group and the propagation vector k=(0,0,0). The atomic positions are Fe1 (x,y,z), Fe2 (-x+1/2,-y,z+1/2), Fe3(-x,y+1/2,-z), and Fe4(x+1/2,-y+1/2,-z+1/2). The ordering modes are A(+--+), C(++--), F(++++), and G(+-+-).

IR	Basis vectors	Shubnikov group
Γ1	Gy	Pnma
Γ2	AxCz	Pn'm'a'
Γ3	GxFz	Pn'm'a
Γ4	Ay	Pnma'
Γ5	Fy	Pn'ma'
Γ6	CxAz	Pnm'a
Γ7	FxGz	Pnm'a'
Γ8	Cy	Pn'ma

Table S2. Basis vectors for the 4*a*(0,0,0) site of the *Pnma(62)* space group and the propagation vector k=(1/2,0,1/2). The atomic positions are Fe1 (x,y,z), Fe2 (-x+1/2,-y,z+1/2), Fe3(-x,y+1/2,-z), and Fe4(x+1/2,-y+1/2,-z+1/2). Only non-zero values are given.

IR	Basis vector	Fe1			Fe2			Fe3			Fe4		
		m_x	m_y	m_z	m_x	m_y	m_z	m_x	m_y	m_z	m_x	m_y	m_z
Γ1	ψ_1	1			i			-1			-i		
	ψ_2		1			i			1			i	
	ψ_3			1			-i			-1			i
Γ3	ψ_1	1			i			1			i		
	ψ_2		1			i			-1			-i	
	ψ_3			1			-i			-1			-i
Γ5	ψ_1	1			-i			-1			i		
	ψ_2		1			-i			1			-i	
	ψ_3			1			i			-1			-i
Γ7	ψ_1	1			-i			1			-i		
	ψ_2		1			-i			-1			i	
	ψ_3			1			i			1			i

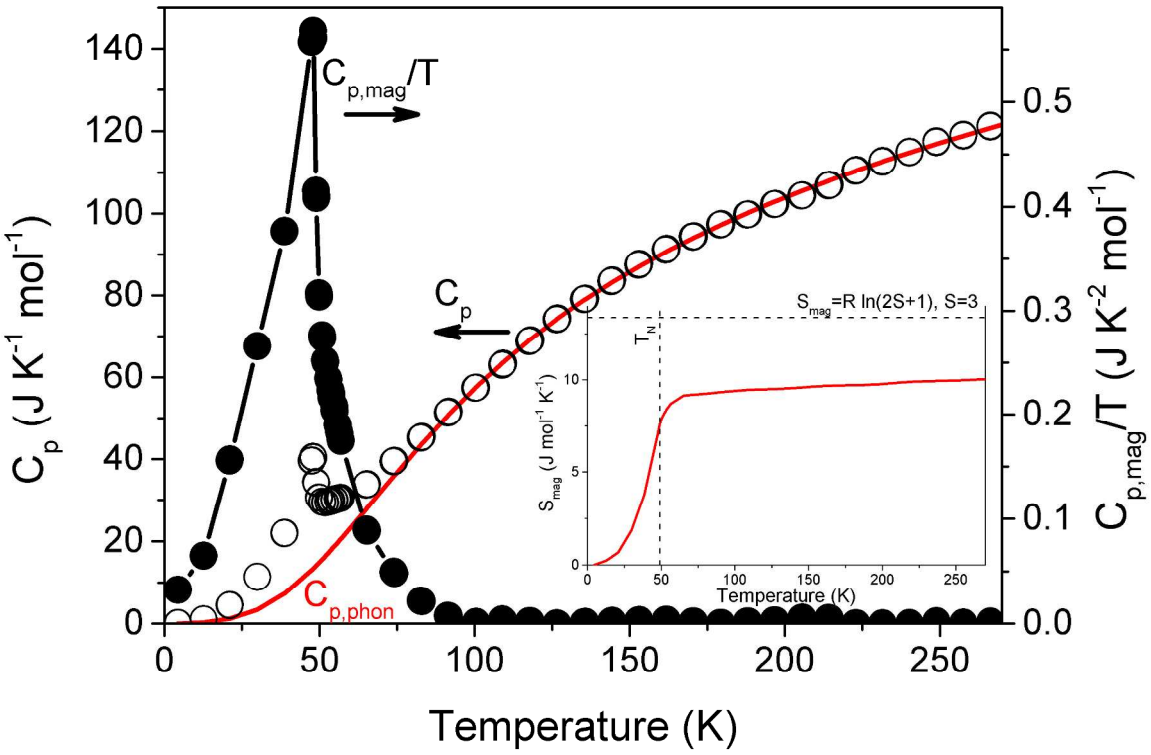

Figure S1. Total (open symbols) and magnetic specific heat (filled symbols) obtained by subtracting the lattice contribution (solid line) for t-$NaFePO_4$. Inset: magnetic entropy obtained by integrating Cp,mag/T vs T. The horizontal and vertical lines show the theoretical value for spin S=2 and ordering temperature, respectively.