Supporting Information:

High-Pressure Stabilized Post-Spinel Phase of $CdFe_2O_4$ with Distinct Magnetism from Its Ambient-Pressure Spinel Phase

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1. Supporting Figures

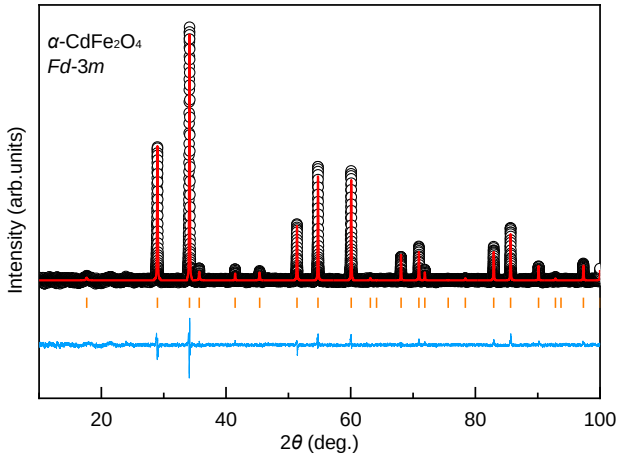

Figure S1. XRD patterns with Rietveld refinement results at room temperature for α-$CdFe_2O_4$. The observed (black circles), calculated (red line), and difference (blue line) patterns are shown. The allowed Bragg reflection with space group *Fd*-3*m*, are shown by the orange ticks.

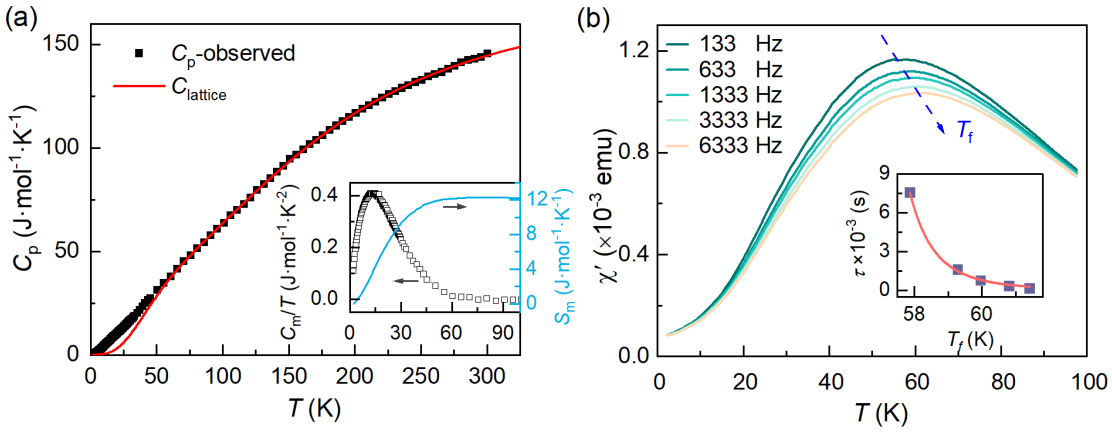

Figure S2. (a) Temperature dependence of specific heat $C_p(T)$ of α-$CdFe_2O_4$ in the wide temperature range from 2 to 300 K under zero field. The solid red line represents the lattice contribution $C_{lattice}$ from Debye-Einstein model. The inset shows the magnetic contribution to specific heat (left), plotted as $C_m/T \sim T$, obtained by subtracting $C_{lattice}$ from the observed total C_p. The magnetic entropy S (right) was evaluated by integrating C_m/T over the observed temperature range. (b) Temperature dependence of ac magnetization χ' at various frequencies for α-$CdFe_2O_4$. The fitting result yields $\tau_0 = 1.95\times10^{-8}$ s, $T_g = 54.5$ K, and $zv = 4.58$. The value of τ_0 in the range of 10^{-7}-10^{-10} s and the zv value confirm the spin cluster nature in α-$CdFe_2O_4$.

2. Supporting Tables

Table S1. Crystallographic parameters of α-$CdFe_2O_4$ and β-$CdFe_2O_4$ refined from XRD pattern at Room temperature.

atom	site	*x*	*y*	*z*	Occupancy	U_{iso} (100×Å^2)
α-$CdFe_2O_4$ phase [a]						
Cd	8*b*	0.5	0.5	0.5	1	0.68(2)
Fe	16*c*	0.125	0.125	0.125	1	0.27(4)
O	32*e*	0.2354(6)	0.2354(6)	0.2354(6)	1	0.40(2)
β-$CdFe_2O_4$ phase [b]						
Cd	4*c*	0.2412(1)	0.25	0.6526(2)	1	0.57(2)
Fe1	4*c*	0.0880(4)	0.25	0.3922(3)	1	0.30(3)
Fe2	4*c*	0.5677(3)	0.25	0.6140(3)	1	0.30(3)
O1	4*c*	0.0834(1)	0.25	0.0651(9)	1	0.6 [c]
O2	4*c*	0.2889(9)	0.25	0.3382(9)	1	0.6 [c]
O3	4*c*	0.3867(1)	0.25	0.0277(1)	1	0.6 [c]
O4	4*c*	0.4850(2)	0.25	0.7679(6)	1	0.6 [c]

[a] α-$CdFe_2O_4$'s lattice parameters: $a = b = c$ =8.7041(8). V =659.43(4) Å^3, R_p = 1.84, R_{wp} = 2.67, χ^2 = 2.704.

[b] β-$CdFe_2O_4$'s lattice parameters: a = 9.2331(1), b = 2.9935(2), c = 10.6753(2). V = 295.06(1), R_p = 1.70, R_{wp} = 2.63, χ^2 = 5.875.

[c] Fixed in the refinement.

Table S2. Selected bond lengths and angles bond-valence sum (BVS) calculations for α-$CdFe_2O_4$ and β-$CdFe_2O_4$. [a]

α-$CdFe_2O_4$ phase					
Fe-O (Å)	2.056(2)	BVS (Fe)	2.73	∠Fe-O-Fe (°)	96.82(9)
Cd-O (Å)	2.102(3)	BVS (Cd)	2.34	Fe-Fe (Å)	3.075(1)
β-$CdFe_2O_4$ phase					
Fe1-O (Å)	1.943(9) 2.046(8) 2.094(7) × 2 2.112(1) × 2	Fe2-O (Å)	1.811(1) 1.917(9) 2.062(6) × 2 2.113(6) × 2	Cd-O (Å)	2.395(8) × 2 2.498(8) × 2 2.326(6) × 2 2.567(2) 2.512(2)
BVS(Fe1)	3.14	BVS(Fe2)	3.2	BVS (Cd)	1.91
Fe1-Fe1 (Å)		2.993(2) 3.189 (6)	Fe2-Fe2 (Å)		2.993(2) 3.119(5)
Fe1-Fe2 (Å)		3.514(5) 3.624(4)	∠Fe1-O-Fe2 (°)		123.0(7) 134.4(6)
∠Fe1-O-Fe1 (°)		100.8(4) 90.3(5) 91.3(4)	∠Fe2-O-Fe2 (°)		101.3(4) 90.2(3) 93.0(1)

[a]The BVS values (V_i) were calculated using the formula $V_i = \sum_j S_{ij}$, and S_{ij} = exp[(r_0-r_{ij})/0.37], where the values of r_0 = 1.765 for Fe and 1.904 for Cd was used.

Table S3. The fitting results of the Debye-Einstein model[A] and the conventional dynamic slowing down model[B] for α-$CdFe_2O_4$.[a,b]

Model A		Model B	
Parameter	Value	Parameter	Value
a	3.0	τ_0	1.95×10^{-8} s
b	4.1	T_g	54.5K
T_D	274 K	zv	4.58
T_E	639 K		

[a]The formula for model A is $C_p = a\frac{9R}{x_D{}^3}\int_0^{x_D}\frac{x^4e^x}{(e^x\text{-}1)^2}dx + b\ 3R\frac{x_E{}^2e^{x_E}}{(e^{x_E}\text{-}1)^2}$, where R is the universal gas constant, a and b are the number of vibrating modes per f.u., $x_D = T_D/T$, $x_E = T_E/T$, and T_D and T_E are Debye and Einstein temperature, respectively.

[b]The formula for model B is $\tau_f/\tau_0 = (T_{ac}/T_g\text{-}1)^{-zv}$, where $\tau_f = 1/f$ is the maximum relaxation time related with the measured frequency f, τ_0 the spin flipping relaxation time, T_g the extrapolated freezing temperature at $f = 0$, and zv the dynamic exponent.