Electronic Supporting Information

Thermal properties and phase transition behaviors of possible caloric materials $Bi_{0.95}Ln_{0.05}NiO_3$

Chen Chen,[a] Yoshihisa Kosugi,[a] Masato Goto,[a] and Yuichi Shimakawa*[a]

[a] *Institute for Chemical Research, Kyoto University, Gokasho, Uji, Kyoto 611-0011, Japan*

This supporting information consists of the refined structure parameters of $Bi_{0.95}Nd_{0.05}NiO_3$.at 450 K (Table S1) and 300 K (Table S2).

*∗Corresponding author E-mail : shimak@scl.kyoto-u.ac.jp

Table S1. Structural data obtained from the Rietveld refinement for $Bi_{0.95}Nd_{0.05}NiO_3$ at 450 K. Space group, *Pnma*, a = 5.54766(5) Å, b = 7.66767(7) Å, c = 5.35863(5) Å, α = β = γ = 90°, and R_{wp} = 11.7%.

Atom	x	y	z	g	B (Å^2)
Bi1	0.0528(2)	0.25	−0.0081(3)	0.95	0.72(2)
Nd1	0.0528(2)	0.25	−0.0081(3)	0.05	0.72(2)
Ni1	0	0	0.5	1	0.28(4)
O1	0.468(3)	0.25	0.088(3)	1	1.2(2)
O2	0.299(2)	0.043(1)	0.699(2)	1	1.2(2)

Table S2. Structural data obtained from the Rietveld refinement for $Bi_{0.95}Nd_{0.05}NiO_3$ at 300 K. Space group, $P\bar{1}$, a = 5.38711(5) Å, b = 5.64705(6) Å, c = 7.70295(8) Å, α = 91.9456(6)°, β = 89.8400(7)°, γ = 91.5717(6) °, and R_{wp}=8.9%.

Atom	x	y	z	g	B (Å^2)
Bi1	0.0089(3)	0.0500(2)	0.2345(2)	0.95	0.50(3)
Nd1	0.0089(3)	0.0500(2)	0.2345(2)	0.05	0.50(3)
Bi2	0.5114(3)	0.4420(2)	0.7264(2)	0.95	0.54(3)
Nd2	0.5114(3)	0.4420(2)	0.7264(2)	0.05	0.54(3)
Ni1	0.5	0	0	1	0.39(5)
Ni2	0	0.5	0	1	0.39(5)
Ni3	0.5	0	0.5	1	0.39(5)
Ni4	0	0.5	0.5	1	0.39(5)
O1	−0.144(4)	0.462(3)	0.252(2)	1	0.5(2)
O2	0.411(3)	0.078(3)	0.761(2)	1	0.5(2)
O3	0.833(3)	0.176(3)	−0.033(2)	1	0.5(2)
O4	0.314(4)	0.339(3)	0.078(2)	1	0.5(2)
O5	0.213(3)	0.783(3)	0.412(2)	1	0.5(2)
O6	0.678(4)	0.690(3)	0.543(2)	1	0.5(2)