Electronic Supplementary Material (ESI) for Dalton Transactions.

SUPPLEMENTARY INFORMATION

On the lack of Monoclinic Distortion in the Insulating Regime of $EuNiO_3$ and $GdNiO_3$ perovskites by high-angular resolution synchrotron x-ray diffraction: a comparison with $YNiO_3$

*Federico Serrano-Sánchez,[a] José Luis Martínez,[a] François Fauth,[b] José Antonio Alonso[a]**

[a] Instituto de Ciencia de Materiales de Madrid (ICMM). Consejo Superior de Investigaciones Científicas (CSIC). Sor Juana Inés de la Cruz 3, E-28049, Madrid, Spain.

[b] CELLS–ALBA Synchrotron, Cerdanyola del Valles, Barcelona, E-08290, Spain

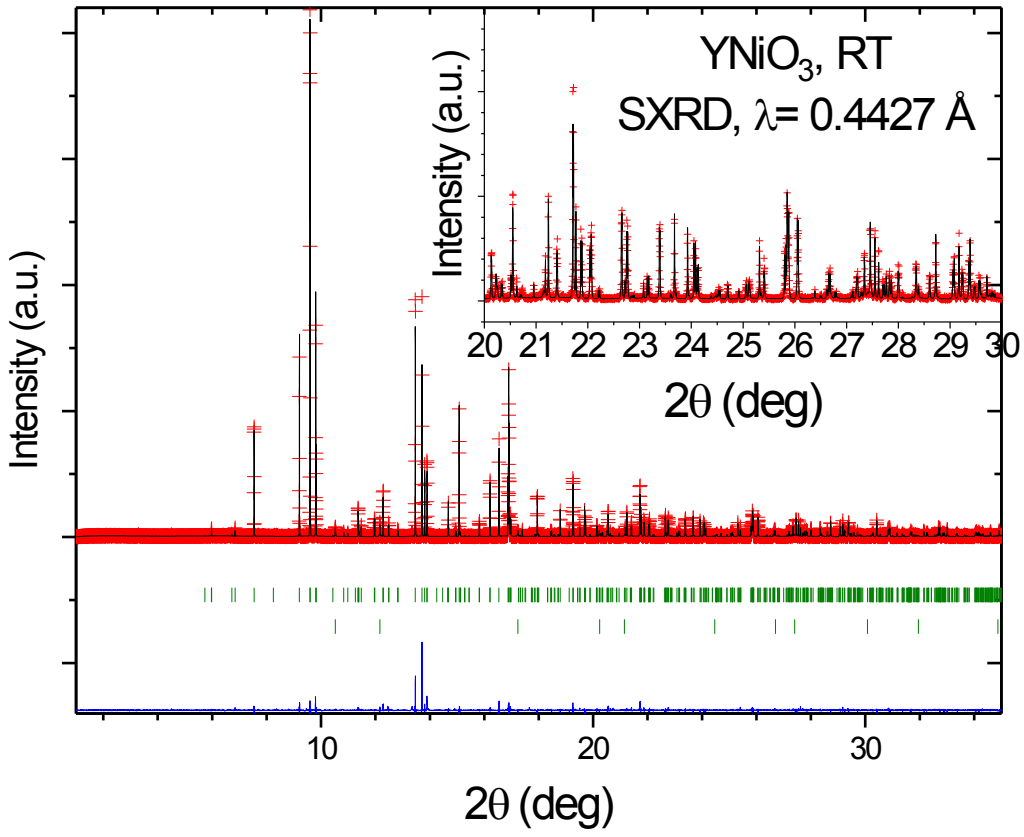

Figure S1. Rietveld plot from SXRD data for YNiO3 at RT, corresponding to the structural refinement in the monoclinic $P2_1/n$ space group. The insets show a close up of the high-angle region, highlighting the quality of the fit. The second series of Bragg reflections corresponds to a minor impurity of NiO.

Table S1. Structural parameters for $YNiO_3$, refined at RT from SXRD data.

Crystal data

Monoclinic, $P2_1/n$	$Z = 4$
$T = 295$ K	X-ray radiation
$a = 5.179998\ (13)$ Å	$b = 5.516174\ (14)$ Å
$c = 7.418316\ (19)$ Å	$\beta = 90.07594\ (15)°$
$V = 211.97\ (1)$ Å^3	

Refinement

$R_p = 13.36\%$	$R_{wp} = 18.141\%$
$R_{exp} = 12.43\%$	$R_{Bragg} = 7.20\%$
$\chi^2 = 2.13$	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}
Y	0.98165 (15)	0.07296 (12)	0.25011 (15)	0.00149 (18)
NI1	0.50000	0.00000	0.00000	0.0029 (5)
NI2	0.50000	0.00000	0.50000	0.0025 (5)
O1	0.1011 (9)	0.4661 (9)	0.2455 (9)	0.0001 (13)
O2	0.7003 (11)	0.3054 (13)	0.0471 (8)	−0.0009 (15)
O3	0.1884 (11)	0.1994 (13)	0.9499 (8)	0.0003 (16)