

Supplementary Material for the paper:

Combustion synthesis of $\text{Ln}_{1-x}\text{M}_x\text{Cr}_{0.9}\text{Ni}_{0.1}\text{O}_3$ (Ln = La and/or Nd; M = Sr and/or Ca; $x \leq 0.25$) perovskites as anode materials for SOFCs.

**Luis Ortega-San-Martín^a, A. Morán-Ruiz^a, A. Wain^a, K. Vidal^a, A. Larrañaga^a,
M.A. Laguna-Bercero^c and M.I. Arriortua^a**

^aDepartamento de Ciencias, Sección Química, Pontificia Universidad Católica del Perú (PUCP), Av. Universitaria 1801, Lima 32, Perú.

^bFacultad de Ciencia y Tecnología, Universidad del País Vasco/Euskal Herriko Unibertsitatea (UPV/EHU), Sarriena s/n, 48940 Leioa, Spain.

^cCSIC-Universidad de Zaragoza, Instituto de Ciencia de Materiales de Aragón (ICMA), Pedro Cerbuna 12, 50009 Zaragoza, Spain.

Index of Figures and Tables

Tables S1 to S3. Lattice parameters, bond lengths, bond angles, density and atom occupancy, obtained from the Rietveld Refinement to the XRD Patterns for the compounds obtained using glycine, urea and sucrose as fuels, respectively.

Figures S1 and S3. Rietveld fits to the powder XRD data using orthorhombic *Pnma* space group for the compounds obtained using glycine (S1), urea (S2) and sucrose (S3) as combustion fuels.

Tables

Table S1. Lattice parameters, bond lengths, bond angles, density, atomic positions and R factor obtained by Rietveld Refinement to the XRD Patterns of the compounds obtained using glycine as fuel.

x	0.10	0.15	0.20	0.25
Symmetry	orthorhombic	orthorhombic	orthorhombic	orthorhombic
Space group	<i>Pnma</i>	<i>Pnma</i>	<i>Pnma</i>	<i>Pnma</i>
a(Å)	5.4721(4)	5.4693(4)	5.4545(1)	5.4542(1)
b(Å)	7.7513(5)	7.7501(7)	7.7196(2)	7.7184(2)
c(Å)	5.5101(3)	5.4997(5)	5.4902(1)	5.4897(1)
V (Å ³)	233.72(4)	233.12(5)	231.17(1)	231.10(1)
$\rho_{\text{the.}}(\text{g/cm}^3)^*$	6.674	6.547	6.452	6.312
A x	0.0169(2)	0.0183(2)	0.0144(2)	0.0139(2)
A z	-0.0029(5)	-0.0050(6)	-0.0025(5)	-0.0030(5)
Uiso(A)	1.99(4)	2.34(4)	2.81(4)	1.72(4)
Uiso(B)	1.68(5)	2.33(6)	2.30(5)	1.66(6)
O1 x	0.498(2)	0.497(2)	0.497(2)	0.500(2)
O1 z	0.057(2)	0.067(4)	0.060(2)	0.059(2)
O2 x	0.273(2)	0.278(3)	0.271(2)	0.273(2)
O2 y	0.034(1)	0.026(2)	0.029(1)	0.032(1)
O2 z	0.728(2)	0.722(2)	0.729(2)	0.727(2)
Uiso(O)	2.8(9)	3.6(2)	3.7(2)(5)	2.7(1)
<A-O> /Å	2.75(24)	2.75(25)	2.75(25)	2.75(25)
B-O1 /Å	1.963(2)	1.973(4)	1.958(2)	1.957(2)
<B-O2> /Å	1.97(2)	1.96(2)	1.95(2)	1.96(1)
<B-O ₁ -B> /°	162(1)	158(1)	161(1)	161(1)
<B-O ₂ -B> /°	161(1)	163(1)	163.7(5)	162.3(5)
R _{wp} (%)	8.7	9.4	8.4	9.5
R _p (%)	5.9	6.4	5.8	6.4
χ^2	2.1	2.8	2.3	2.5
R _F ² (%)	2.7	3.5	4.1	3.3

* Calculated assuming no oxygen deficiency

Table S2. Lattice parameters, bond lengths, bond angles, density, atomic positions and R factor obtained by Rietveld Refinement to the XRD Patterns of the compounds obtained using urea as fuel.

x	0.10	0.15	0.20	0.25
Symmetry	orthorhombic	orthorhombic	orthorhombic	orthorhombic
Space group	<i>Pnma</i>	<i>Pnma</i>	<i>Pnma</i>	<i>Pnma</i>
a(Å)	5.4706(2)	5.4645(4)	5.4585(3)	5.4519(2)
b(Å)	7.7500(3)	7.7434(7)	7.7305(5)	7.7140(4)
c(Å)	5.5078(2)	5.4941(4)	5.4939(3)	5.4861(2)
V (Å ³)	233.52(1)	232.48(2)	231.88(2)	230.72(2)
$\rho_{\text{the.}}(\text{g}/\text{cm}^3)^*$	6.676	6.565	6.432	6.316
A x	0.0175(2)	0.0172(2)	0.0140(2)	0.0145(2)
A z	-0.0032(5)	-0.0045(8)	-0.0031(7)	-0.0023(6)
Uiso(A)	1.92(3)	1.48(4)	1.22	0.79(4)
Uiso(B)	1.66(5)	1.17(5)	1.00(5)	0.51(5)
O1 x	0.495(2)	0.494(2)	0.497(2)	0.497(2)
O1 z	0.058(2)	0.065(4)	0.056(3)	0.062(3)
O2 x	0.279(2)	0.273(3)	0.272(2)	0.272(2)
O2 y	0.034(1)	0.028(2)	0.032(1)	0.030(1)
O2 z	0.727(2)	0.723(3)	0.727(2)	0.727(2)
Uiso(O)	2.4(2)	2.2(2)	1.8(2)	1.19(5)
<A-O> /Å	2.75(25)	2.75(25)	2.75(25)	2.75(25)
B-O1 /Å	1.967(1)	1.969(4)	1.957(2)	1.959(2)
<B-O2> /Å	1.97(1)	1.96(2)	1.96(2)	1.96(2)
<B-O ₁ -B> /°	160.2(7)	159(1)	162(1)	160(1)
<B-O ₂ -B> /°	160.6(5)	163(1)	162.1(6)	163.0(6)
R _{wp} (%)	8.1	8.8	8.4	5.8
R _p (%)	5.5	6.2	6.8	4.6
χ^2	2.2	2.4	2.2	2.4
R _F ² (%)	3.3	2.9	3.5	4.2

* Calculated assuming no oxygen deficiency

Table S3. Lattice parameters, bond lengths, bond angles, density, atomic positions and R factor obtained by Rietveld Refinement to the XRD Patterns of the compounds obtained using sucrose as fuel.

x	0.10	0.15	0.20	0.25
Symmetry	orthorhombic	orthorhombic	orthorhombic	orthorhombic
Space group	<i>Pnma</i>	<i>Pnma</i>	<i>Pnma</i>	<i>Pnma</i>
a(Å)	5.4696(5)	5.4652(4)	5.4597(6)	5.4553(7)
b(Å)	7.7483(7)	7.7392(6)	7.735(9)	7.7257(12)
c(Å)	5.5087(5)	5.5019(4)	5.4965(6)	5.4920(8)
V (Å ³)	233.46(6)	232.71(5)	232.15(3)	231.34(6)
$\rho_{\text{the.}}$ (g/cm ³)*	6.675	6.542	6.423	6.305
A x	0.0162(2)	0.0162(2)	0.0138(3)	0.0138(3)
A z	-0.0019(7)	-0.0024(6)	~0	~0
Uiso(A)	1.01(5)	1.42(4)	1.21(5)	1.19(5)
Uiso(B)	0.64(7)	1.10(6)	1.01(7)	0.98(7)
O1 x	0.502(2)	0.501(2)	0.497(3)	0.500(2)
O1 z	0.061(4)	0.056(3)	0.060(5)	0.073(4)
O2 x	0.271(3)	0.268(3)	0.273(4)	0.271(4)
O2 y	0.033(2)	0.036(2)	0.035(2)	0.023(2)
O2 z	0.729(3)	0.728(3)	0.732(4)	0.729(5)
Uiso(O)	1.6(2)	1.7(2)	1.2(2)	1.8(2)
<A-O> /Å	2.75(25)	2.75(24)	2.75(24)	2.74(22)
B-O1 /Å	1.966(3)	1.959(3)	1.963(4)	1.971(5)
<B-O2> /Å	1.96(3)	1.96(2)	1.96(3)	1.95(3)
<B-O ₁ -B> /°	160(1)	162(1)	161(1)	157(1)
<B-O ₂ -B> /°	162(1)	161.2(6)	162(1)	166(1)
R _{wp} (%)	11.2	10.8	11.2	11.1
R _p (%)	7.7	7.3	8.0	8.2
χ^2	2.2	2.4	2.2	2.3
R _F ² (%)	9.5	4.3	4.2	3.6

* Calculated assuming no oxygen deficiency

Figure S1

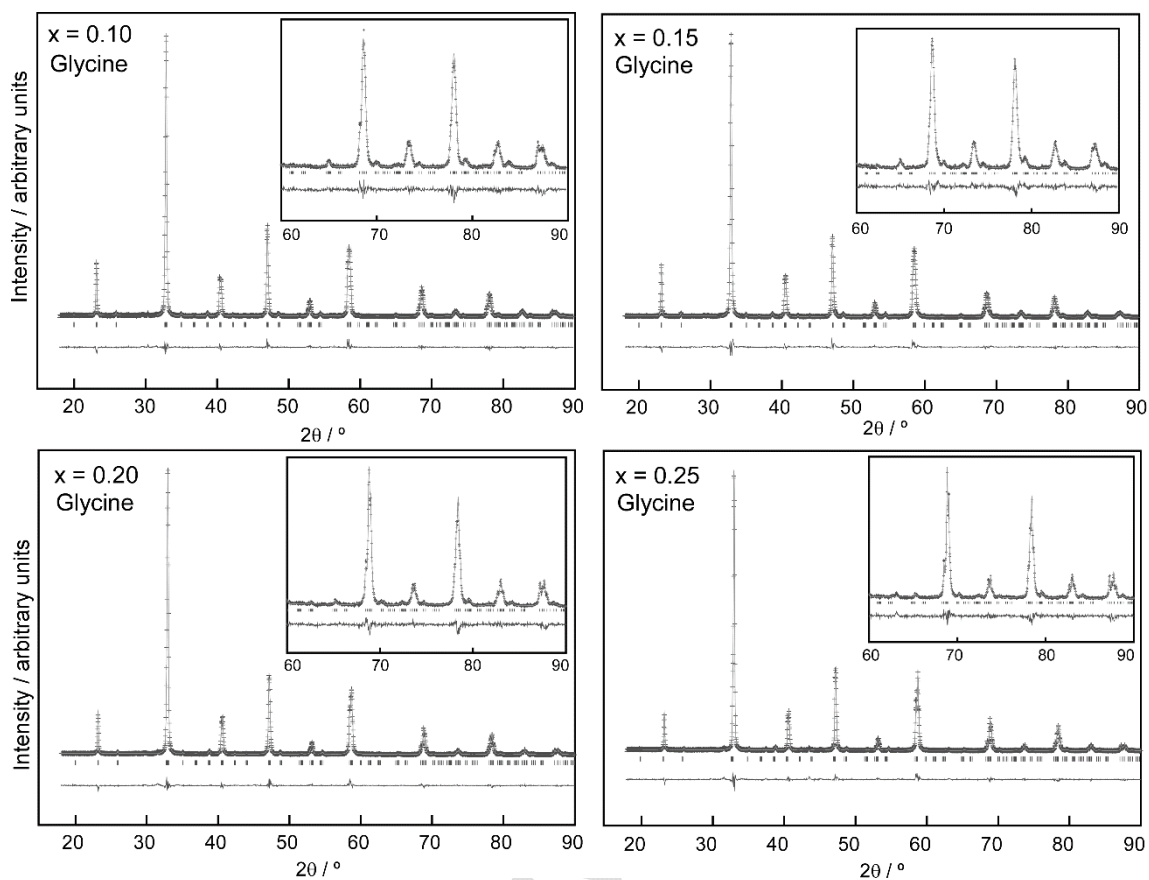


Figure S2

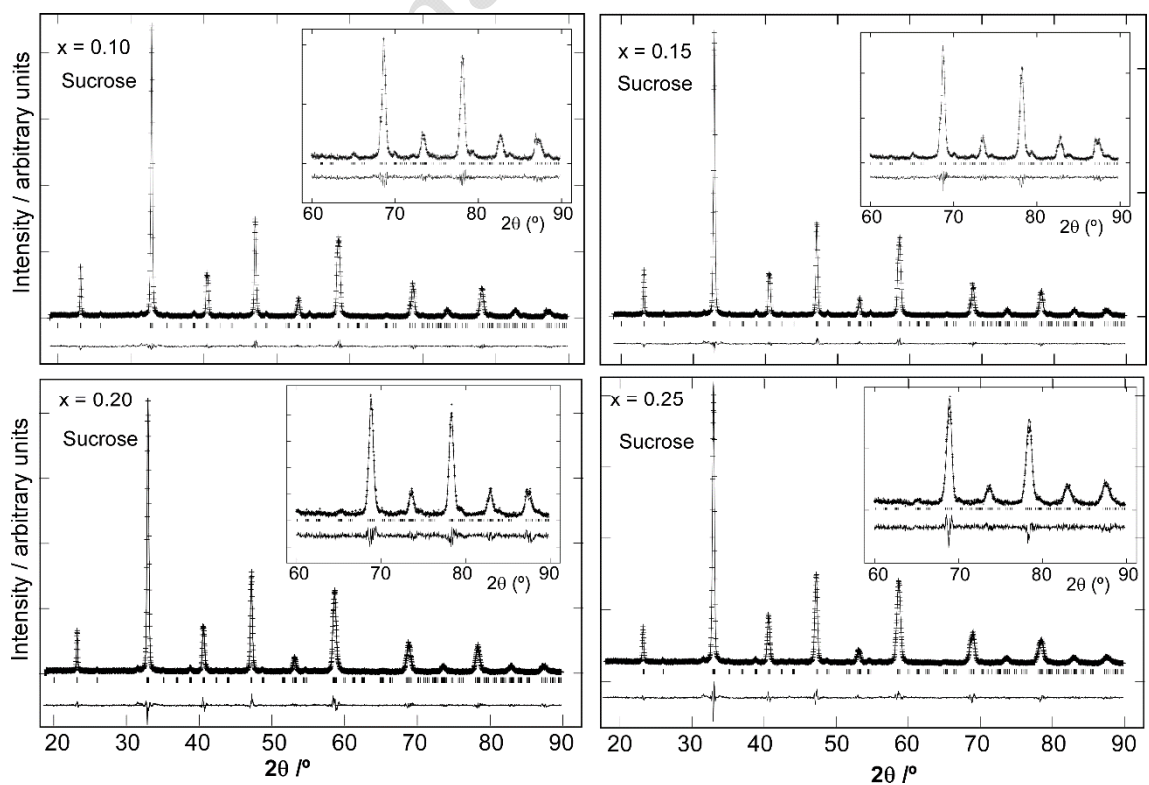
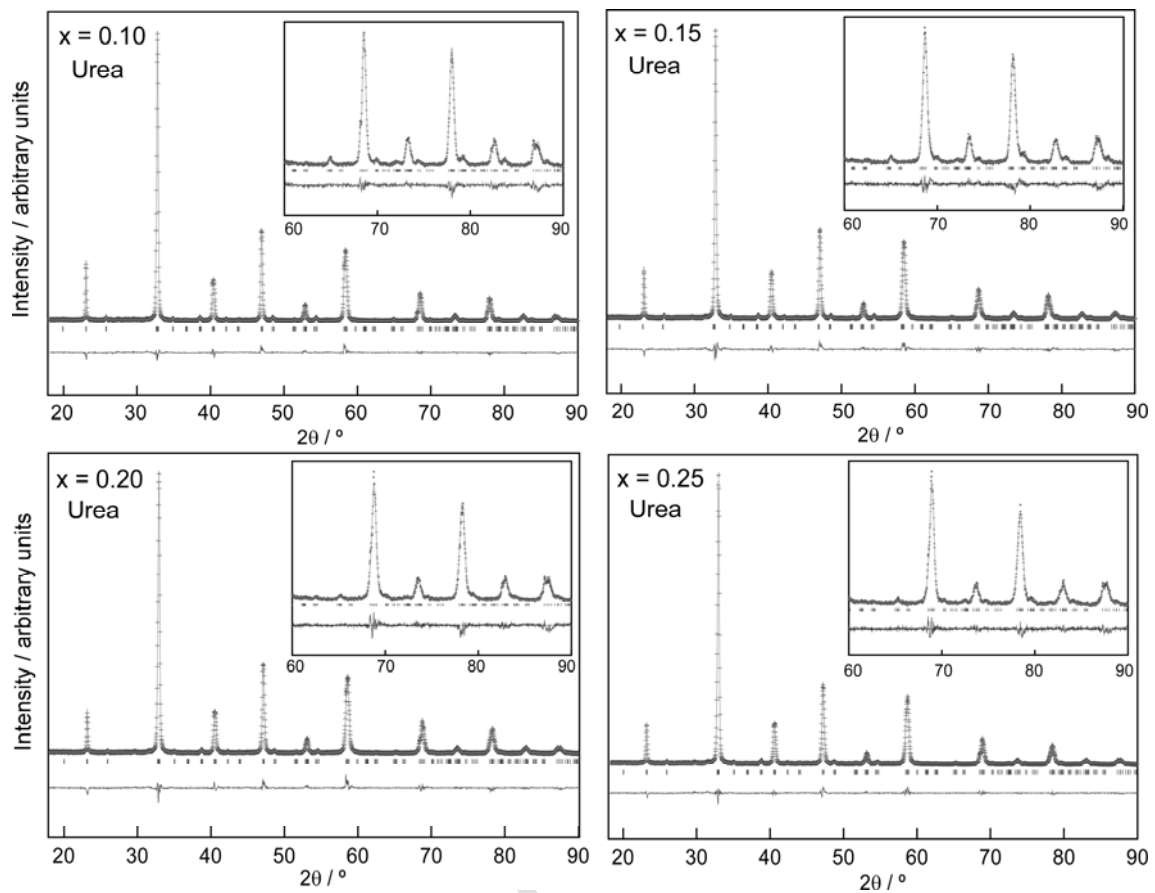


Figure S3



as Original