Supporting information

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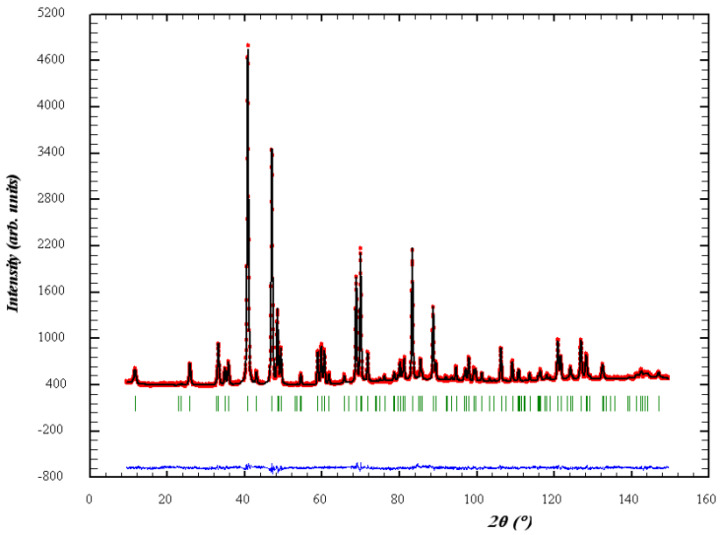
Title : "Oxygen diffusion mechanism in the mixed ion-electron conductor $NdBaCo_2O_{5+x}$"

Supporting information 1 : Rietveld plot of $NdBaCo_2O_{5+x}$ at 1173 K



Results of Rietveld analysis against neutron powder diffraction data collected at 1173 K in air on $NdBaCo_2O_{5+x}$ sample. The red circle symbols and the black line correspond to the observed and calculated intensities, respectively. Short vertical bars indicate the position of Bragg reflections within the *P*4/*mmm* space group (N°123). The difference between the observed and calculated profiles is plotted at the bottom. The wavelength of the incident neutrons beam is 1.594 Å.

Supporting information 2: Structural data

The $NdBaCo_2O_{5+x}$ structure has been refined within the *P*4/*mmm* space group (N°123).
At 1173 K, the refined structural parameters (all atoms refined anisotropically) are:

Atom	Wyckoff site	Occupancy factor	Fractional coordinates			U_{eq} (Å^2)
			x/*a*	*y*/*b*	*z*/*c*	
Nd	1*d*	1.0000	1/2	1/2	1/2	0.03452
Ba	1*c*	1.0000	1/2	1/2	0	0.03552
Co	2*g*	1.0000	0	0	0.2530(4)	0.03180
O1	1*a*	1.0000	0	0	0	0.03763
O2	1*b*	0.405(7)	0	0	1/2	0.05113
O3	4*i*	0.960(6)	0	1/2	0.29086(9)	0.04736

Refined formula: $NdBaCo_2O_{5.24(3)}$ ($x = 0.24(3)$) for $Z = 1$
Unit cell parameters: $a = 3.9741(14)$, $c = 7.729(3)$ Å, $V = 122.07(8)$ Å^3
Agreement factors: $R_{wp} = 2.04\%$, $R_p = 1.65$, $R_{exp} = 1.67$, $\chi^2 = 1.23$, $R_{Bragg} = 4.48\%$, $R_F = 2.39\%$, $R_{F2} = 2.62\%$ for 2734 observed points and 101 refined parameters

Supporting information 3: Molecular dynamics calculation details

Simulations were performed following the order: NST →NVT → NVE, where NST means constant Number of particles, Strain and Temperature, NVT means constant Number of particles, Volume and Temperature, NVE means constant Number of particles, Volume and Energy.

For each run, the simulation parameters were:

Simulation type	Total number of steps	Equilibration number of steps	Time step (ps)	Cut off Å	Extracted Information
NST	60 000	20 000	0.001	10	Supercell dimensions
NVT	60 000	20 000	0.001	10	Verification of supercell dimensions; Configuration for NVE simulation
NVE	2 000 000	20 000	0.001	10	Atoms trajectory

After NST simulations, the volume of the supercell was fixed according to simulations, forcing $a_{supercell}$ and $b_{supercell}$ dimensions to be equal. The consideration of supercell dimensions with $a_{supercell} \neq b_{supercell}$ led to very similar results in terms of oxygen diffusion coefficients and oxygen density maps.