Supporting information

The effects of Sr content on the performance of $Nd_{1-x}Sr_xCoO_{3-\delta}$ air-electrode materials for intermediate temperature solid oxide fuel cells under operational conditions

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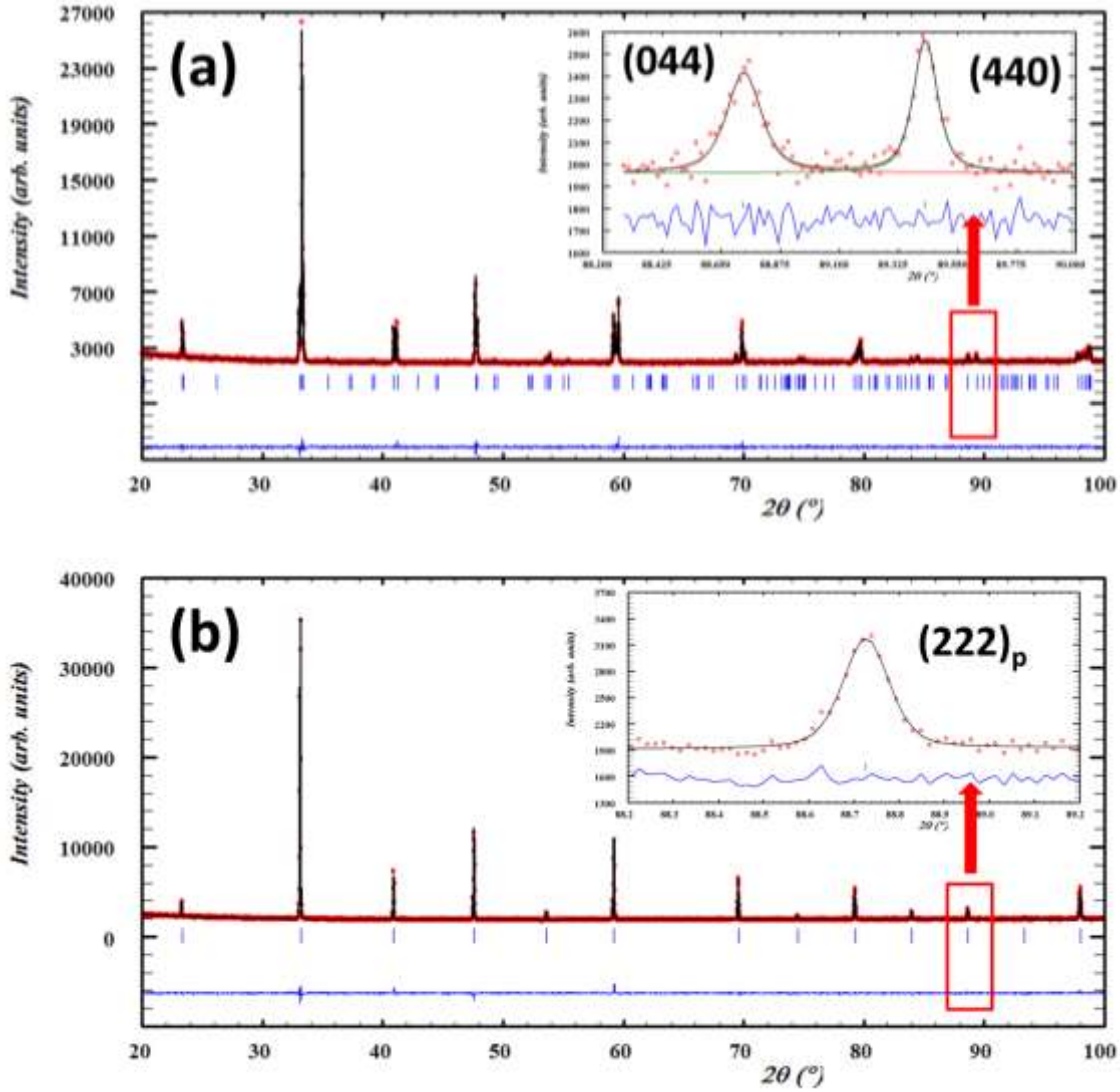

Figure S1. Experimental (red circles) and calculated (black continuous line) XRD patterns (and their difference, blue line at the bottom) for (a) $Nd_{2/3}Sr_{1/3}CoO_{3-\delta}$ (a) and (b) $Nd_{1/3}Sr_{2/3}CoO_{3-\delta}$ prepared in air. Vertical bars indicate the positions of Bragg peaks.

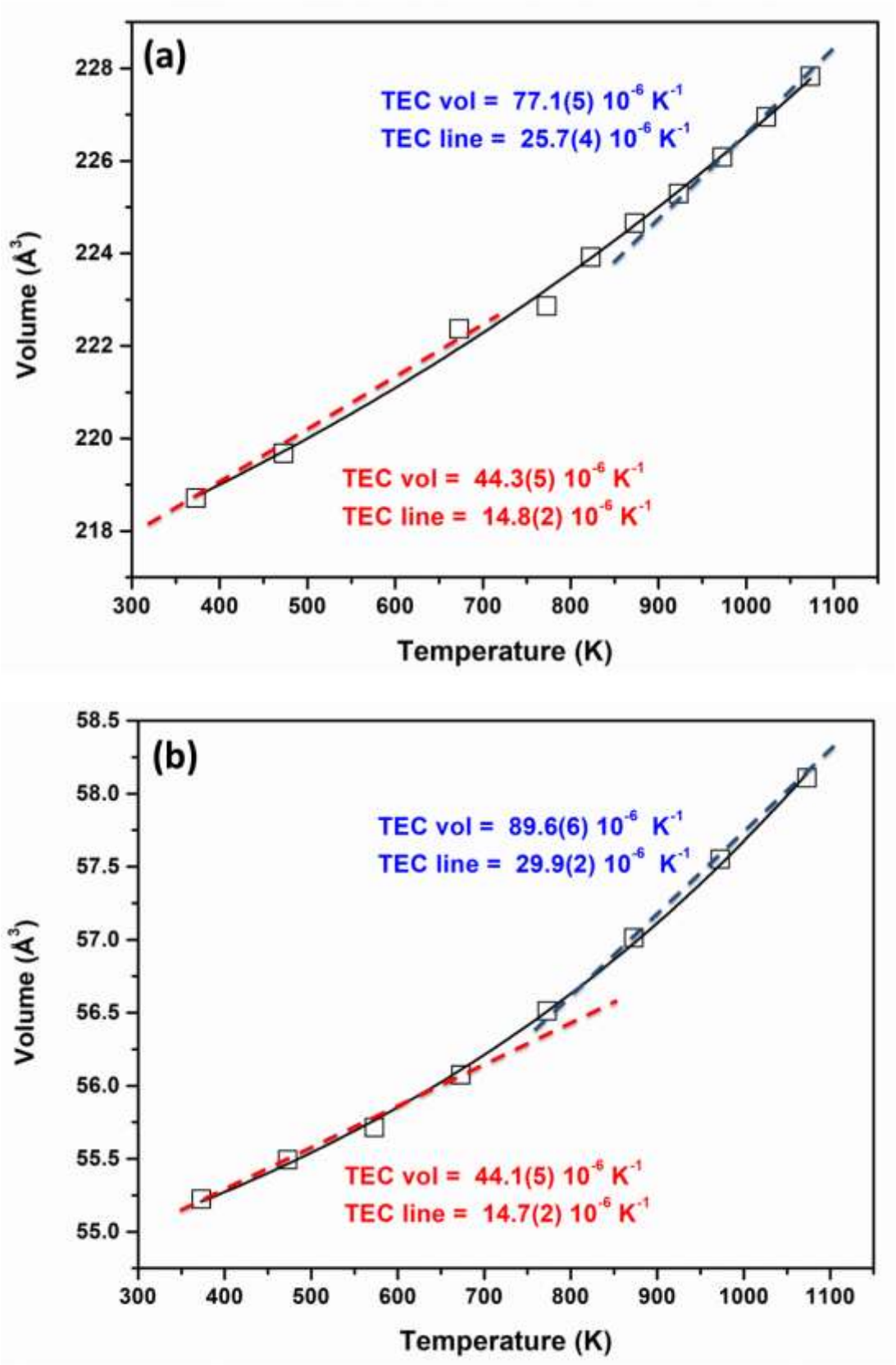

Figure S2. Thermal evolution of the unit cell volume of; (a) $Nd_{2/3}Sr_{1/3}CoO_{3-\delta}$ and (b) $Nd_{1/3}Sr_{2/3}CoO_{3-\delta}$ in air. Volume and linear TEC values at low and high temperature are calculated.

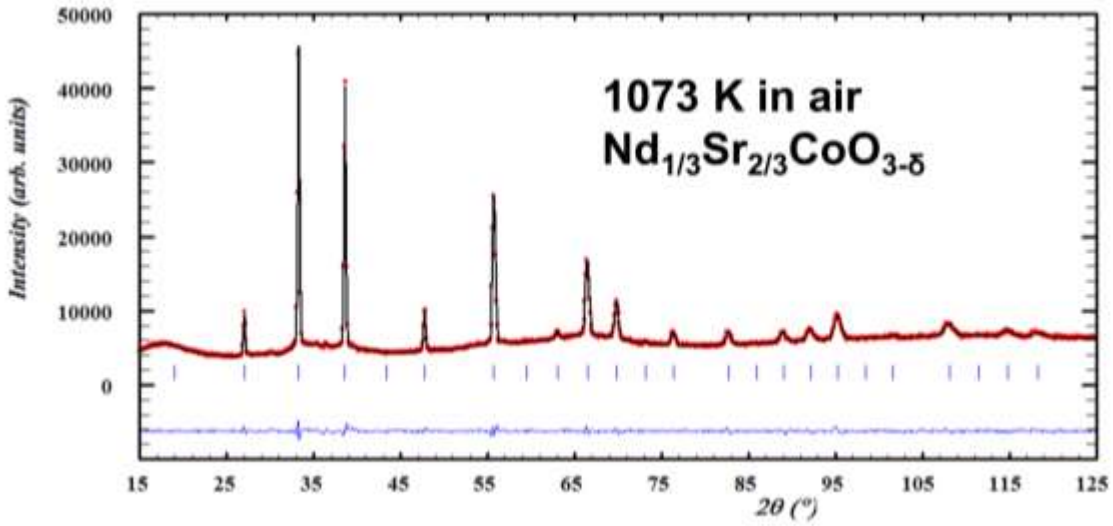

Figure S3. Experimental (red circles) and calculated (black continuous line) NPD patterns (and their difference, blue line at the bottom) for $Nd_{1/3}Sr_{2/3}CoO_{3-\delta}$ at 1073 K in air. Vertical bars indicate the positions of Bragg peaks.

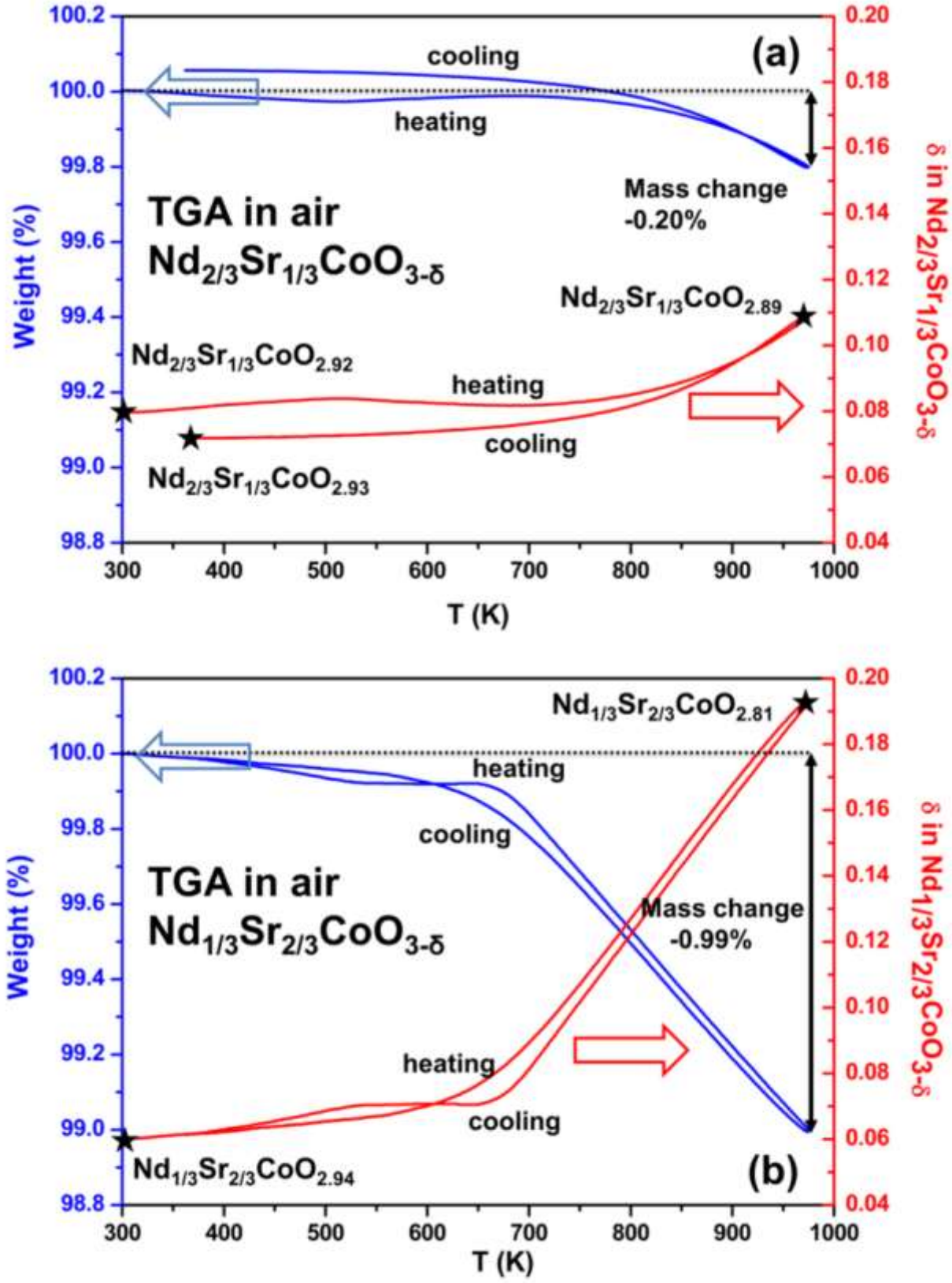

Figure S4: Percentage mass loss (blue, primary y-axis) and oxygen loss (red, secondary axis) in air as a function of temperature for (a) $Nd_{2/3}Sr_{1/3}CoO_{3-\delta}$ (a) and (b) $Nd_{1/3}Sr_{2/3}CoO_{3-\delta}$.

Table S1. Nominal and experimental (determined by EDS) compositions for the $Nd_{2/3}Sr_{1/3}CoO_{3-\delta}$, sample used for NPD and electrical characterization.

Element	Nominal composition (atom %)	Experimental composition (atom %)
Nd	13.3	13.5(2)
Sr	6.7	6.6(2)
Co	20.0	19.8(3)
O	60.0	59.6(3)

Table S2. Nominal and experimental (determined by EDS) compositions for the $Nd_{1/3}Sr_{2/3}CoO_{3-\delta}$, sample used for NPD and electrical characterization.

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Element	Nominal composition (atom %)	Experimental composition (atom %)
Nd	6.7	6.9(2)
Sr	13.3	13.1(3)
Co	20.0	20.0(1)
O	60.0	59.7(3)

Table S3. Structural parameters for Nd1-xSrxCoO3-δ obtained from joint fitting of NPD and XRD data. Agreement factors are given for the fitting of NPD data.

Sample	x= 1/3 [a]			x = 2/3 [b]			
Space Group	Pnma			**Space Group**	Pm-3m		
***a* (Å)**	5.3570(2)			***a* (Å)**	3.81479 (5)		
***b* (Å)**	7.5863(2)						
c (Å)	5.4061(2)						
Volume (Å^3)	219.70(1)			**Volume (Å^3)**	55.515(1)		
A position	4c	**O1 position**	4c	**A position**	1b	**O1 position**	3d
Occ Sr/Nd	0.33(1)/0.66(1)	**Occ**	0.994(4)	**Occ Sr/Nd**	0.66(1)/0.33(1)	**Occ**	0.983(3)
X	0.0134(4)	**X**	0.4954(6)	**U*100 (Å^2)**	0.76(2)	**U*100 (Å^2)**	0.29(4)
Z	-0.0024(4)	**Z**	0.0578(4)	**B position**	1a		
U*100 (Å^2)	0.46(1)	**U*100 (Å^2)**	0.62(2)	**Occ Co**	1		
B position	4a	**O2 position**	8d	**U*100 (Å^2)**	0.40(3)		
Occ Co	1	**Occ**	0.951(7)				
U*100 (Å^2)	0.15(2)	**X**	0.2721(3)				
		Y	0.0313(2)				
		Z	0.7294(3)				
		U*100 (Å^2)	0.62(2)				

[a] Pnma (#62): 8d (x y z), 4c (x ¼ z), 4a (0 0 0),

χ^2= 1.55, R_{wp}= 4.12%, R_{exp}= 3.30%, R_B= 6.56%,

Composition: $Nd_{0.66(1)}Sr_{0.33(1)}CoO_{2.896(4)}$

[b] Pm-3m (#221): 1a (000), 1b (½ ½ ½), 3d (½ 0 0)

χ^2= 1.54, R_{wp}= 4.10%, R_{exp}= 3.34%, R_B= 2.41%,

Composition: $Nd_{0.33(1)}Sr_{0.66(1)}CoO_{2.949(2)}$

Table S4. Selected structural information for Nd1-xSrxCoO3-δ (x=1/3, 2/3) obtained from NPD data. Angles are given in degrees and distances in Å (up to 3.50 Å); distortion Δ of the BOn polyhedra and Bond Valence Sums [1], are reported as $\Delta=1/n\ \Sigma j=1,n\ \{(dn - <d>)/<d>\}2$ where <d> is the average B-O distance. The quadratic elongation λ is given by $\lambda= \Sigma j=1,n\ (li/l0)2/n$ and the bond-angle variance σ is given by $\sigma = \Sigma j=1,n\ (\theta i- \theta 0)2/(n-1)$ where l0 and θ0 are the cation-anion bond lengths and cation-anion-cation bond angles in regular coordination polyhedra, respectively, and li and θi are the cation-anion bond lengths and cation-anion-cation bond angles of bond i [2].

$Nd_{0.67(1)}Sr_{0.33(1)}CoO_{2.896(4)}$				$Nd_{0.33(1)}Sr_{0.67(1)}CoO_{2.949(2)}$			
[a] **Tilt angle θ**			13.23(4)	**Tilt angle θ**			-
[b] **Tilt angle φ**			13.23(4)	**Tilt angle φ**			-
[c] **Tilt angle μ**			8.6(1)	**Tilt angle μ**			-
CoO_6 octahedron		(Nd/sr)O_n polyhedron		**CoO_6 octahedron**		(Nd/Sr)O_n polyhedron	
B-O1 x 2	1.9221(4)	(Nd/Sr)-O1 x 1	2.602(3)	**B-O1 x 6**	1.9074(1)	(Nd/Sr)-O1 x 12	2.6975(5)
B-O2 x 4	1.927(2)	(Nd/Sr)-O1 x 1	2.794(3)				
		(Nd/Sr)-O1 x 1	3.004(4)				
Average B-O	1.9235(5)	(Nd/Sr)-O1 x 1	2.405(3)	**Average B-O**	1.9074(1)		
Octahedron volume ($Å^3$)	9.4878	(Nd/Sr)-O2 x 2	2.603(4)	**Octahedron volume ($Å^3$)**	9.2525		
Distortion B-O_6 x 10^4	0.036	(Nd/Sr)-O2 x 2	2.435(4)	**Distortion B-O_6 x 10^4**	-		
Quadratic elongation	1.0002	(Nd/Sr)-O2 x 2	3.012(2)	**Quadratic elongation**	1.0000		
Bond angle variance	0.8354 deg^2	(Nd/Sr)-O2 x 2	2.729(2)	**Bond angle variance**	-		
BVS	3.26(5)	Average (Nd/Sr)-O	2.697(5)	**BVS**	3.43(4)	Average (Nd/Sr)-O	2.6975(5)
		BVS	2.93(4)			BVS	2.51(2)

a with [110], b with [1-10],

References:

(1) Zachariasen, W. H. The Crystal Structure of Monoclinic Metaboric Acid. *Acta Cryst.* **1963**, *16*, 385-389.

(2) K. Robinson, Gibbs, G. V. & Ribbe, P. H., *Science*, **1971**, *172*, 567-570