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Supporting information for article:

Anomalous X-Ray Diffraction Study of Pr-substituted BaCeO3-δ

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In this document we included complementary information about the manuscript "**Anomalous X-Ray Diffraction Study of Pr-substituted $BaCeO_{3-\delta}$**". Some of this information has been also included as an example in the body of manuscript because it is relevant and improves the discussion.

The "Experimental" section of manuscript indicates that the XRD data at 10000 and 5962 eV were refined by Rietveld Method using multipattern fit mode of Fullprof Suite Tools. Three different models were tested (see details in the manuscript). Table S1 compares the goodness of fit obtained for $BaCe_{1-x}Pr_xO_{3-\delta}$ x = 0, 0.2, 0.4, 0.6 and 0.8 compounds from multipattern fit for Model I, II and III, at 10000 and 5962 eV. Three agreement factors are shown: the Profile Factor (R_p), the Weighted Profile Factor (R_{wp}) and the Reduced chi-square (χ^2). The discussion of the Models considerations and the justification of to select Model III is discussed in the manuscript. Table S2 indicates the structural parameters of Model III for all compositions. Structural data of x = 0.6 sample is described as an example in the manuscript.

References

J. Rodríguez-Carvajal (2000). Fullprof 2000: A program for Rietveld Refinement and Profile Matching Analysis of Complex Powder Diffraction Patterns; Laboratoire Léon Brillouin (CEA-CNRS).

Table S1 Goodness of fits from XRD multipattern fits at different energies. Each $BaCe_{1-x}Pr_xO_{3-\delta}$ x = 0, 0.2, 0.4, 0.6 and 0.8 composition was refined with the three Models

x = 0						
Model	**10000 eV**			**5962 eV**		
	R_p	R_{wp}	χ^2	R_p	R_{wp}	χ^2
I	-	-	-	-	-	-
II	**9.63**	**8.99**	**5.00**	**11.20**	**6.66**	**11.50**
III	-	-	-	-	-	-

x = 0.2						
Model	**10000 eV**			**5962 eV**		
	R_p	R_{wp}	χ^2	R_p	R_{wp}	χ^2
I	**9.84**	**8.87**	**4.35**	**13.90**	**9.44**	**19.30**
II	**9.44**	**8.40**	**3.92**	**13.70**	**9.18**	**18.30**
III	**9.99**	**8.74**	**4.24**	**12.80**	**8.52**	**15.17**

x = 0.4						
Model	**10000 eV**			**5962 eV**		
	R_p	R_{wp}	χ^2	R_p	R_{wp}	χ^2
I	**9.08**	**8.31**	**4.13**	**11.60**	**7.72**	**14.10**
II	**8.58**	**7.75**	**3.59**	**10.90**	**6.72**	**10.70**
III	**8.24**	**7.24**	**3.13**	**10.70**	**6.58**	**10.30**

x = 0.6						
Model	**10000 eV**			**5962 eV**		
	R_p	R_{wp}	χ^2	R_p	R_{wp}	χ^2
I	**8.38**	**8.01**	**3.78**	**13.00**	**9.59**	**21.50**
II	**7.68**	**6.88**	**2.79**	**10.50**	**6.32**	**9.37**
III	**7.75**	**6.92**	**2.83**	**10.40**	**6.16**	**8.90**

x = 0.8						
Model	**10000 eV**			**5962 eV**		
	R_p	R_{wp}	χ^2	R_p	R_{wp}	χ^2
I	**11.20**	**11.20**	**7.77**	**14.00**	**11.30**	**28.00**
II	**10.20**	**9.57**	**5.68**	**12.50**	**8.30**	**15.00**
III	**9.93**	**9.32**	**5.40**	**12.00**	**7.83**	**13.4**

Table S2 Structural parameters for $BaCe_{1-x}Pr_xO_{3-\delta}$ x = 0, 0.2, 0.4, 0.6 and 0.8 compositions obtained by using Model III. *Pnma* (N° 62) Space Group, $\alpha = \beta = \gamma = 90$.

x = 0

a = 6.21664(7) Å, b = 8.77789(9) Å, c = 6.23629(9) Å

Atoms	Wyckoff position	Atomic positions			Occ.	Anisotropic Vibrations x 10^2 (Å^2)		
		x	y	z		U_{11}	U_{22}	U_{33}
Ba	4c	0.0166(1)	0.25	-0.0043(1)	1	1.02(1)	0.81(1)	0.19(1)
Ce	4b	0	0	0.5	1	0.25(1)	0.54(2)	0.16(1)
O1	4c	-0.021(1)	0.25	0.428(1)	1	Isotropic Vibration U_{iso} x 10^2 (Å^2) 0.70(5)		
O2	8d	0.278(1)	0.039(1)	0.723(1)	1			

x = 0.2

a = 6.21025(7) Å, b = 8.76826(9) Å, c = 6.22886(9) Å

Atoms	Wyckoff position	Atomic positions			Occ.	Anisotropic Vibrations x 10^2 (Å^2)		
		x	y	z		U_{11}	U_{22}	U_{33}
Ba	4c	0.0152(1)	0.25	-0.0047(2)	0.999(1)	0.94(2)	0.61(1)	0.45(1)
Pr1					0.001(1)			
Ce	4b	0	0	0.5	0.799(1)	0.39(1)	0.43(1)	0.28(2)
Pr2					0.199(1)			
O1	4c	-0.017(1)	0.25	0.424(1)	1	Isotropic Vibration U_{iso} x 10^2 (Å^2) 0.57(8)		
O2	8d	0.267(1)	0.046(1)	0.730(1)	1			

x = 0.4

a = 6.20345(7) Å, b = 8.75952(9) Å, c = 6.22537(9) Å

Atoms	Wyckoff position	Atomic positions			Occ.	Anisotropic Vibrations x 10^2 (Å^2)		
		x	y	z		U_{11}	U_{22}	U_{33}
Ba	4c	0.0145(1)	0.25	-0.0044(1)	0.995(1)	1.30(2)	0.90(1)	0.39(1)
Pr1					0.005(1)			
Ce	4b	0	0	0.5	0.597(1)	0.47(2)	0.85(1)	0.61(2)
Pr2					0.394(1)			

O1	**4c**	**-0.015(1)**	**0.25**	**0.427(1)**	**1**	**Isotropic Vibration** U_{iso} **x** 10^2 **(Å^2)** **0.51(7)**
O2	**8d**	**0.275(1)**	**0.042(1)**	**0.726(1)**	**1**	

x = 0.6

a = 6.19647(7) Å, b = 8.74999(9) Å, c = 6.22045(9) Å

Atoms	**Wyckoff position**	**Atomic positions**			**Occ.**	**Anisotropic Vibrations x 10^2 (Å^2)**		
		x	**y**	**z**		U_{11}	U_{22}	U_{33}
Ba	**4c**	**0.0145(1)**	**0.25**	**-0.0044(1)**	**0.991(1)**	**0.99(1)**	**0.99(1)**	**0.21(1)**
Pr1					**0.009(1)**			
Ce	**4b**	**0**	**0**	**0.5**	**0.396(1)**	**0.32(2)**	**0.48(1)**	**0.26(2)**
Pr2					**0.585(1)**			
O1	**4c**	**-0.011(1)**	**0.25**	**0.430(1)**	**1**	**Isotropic Vibration** U_{iso} **x** 10^2 **(Å^2)** **0.29(6)**		
O2	**8d**	**0.276(1)**	**0.042(1)**	**0.724(1)**	**1**			

x = 0.8

a = 6.18949(7) Å, b = 8.74009(9) Å, c = 6.21421(9) Å

Atoms	**Wyckoff position**	**Atomic positions**			**Occ.**	**Anisotropic Vibrations x 10^2 (Å^2)**		
		x	**y**	**z**		U_{11}	U_{22}	U_{33}
Ba	**4c**	**0.0134(1)**	**0.25**	**-0.0041(1)**	**0.985(1)**	**1.20(2)**	**0.84(2)**	**0.90(1)**
Pr1					**0.015(1)**			
Ce	**4b**	**0**	**0**	**0.5**	**0.197(1)**	**0.40(2)**	**0.26(1)**	**0.32(2)**
Pr2					**0.773(1)**			
O1	**4c**	**-0.013(1)**	**0.25**	**0.430(1)**	**1**	**Isotropic Vibration** U_{iso} **x** 10^2 **(Å^2)** **0.19(3)**		
O2	**8d**	**0.271(1)**	**0.035(1)**	**0.732(1)**	**1**			