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Supporting information for article:

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Giorgia Confalonieri, Vincenzo Buscaglia, GianCarlo Capitani, Giovanna Canu, Nicola Rotiroti, Andrea Bernasconi, Alessandro Pavese and Monica Dapiaggi

Supporting Information

Local distortion and octahedral tilting in $BaCe_xTi_{1-x}O_3$ perovskite

Authors

Giorgia Confalonieri[a1]*, Vincenzo Buscaglia[b], GianCarlo Capitani[c], Giovanna Canu[b], Nicola Rotiroti[a], Andrea Bernasconi[d], Alessandro Pavese[e] and Monica Dapiaggi[a]

Correspondence email: giorgia.confalonieri@unito.it

Results and Discussion - Oxygen disorder and tilt model

The following tables report:

- Ti/Ce-oxygen bond lengths for each octahedron type obtained by tilt model.
- Average bond length, distortion index (Baur, 1974), quadratic elongation (Robinson *et al.*, 1971) and the bond angle variance (Robinson *et al.*, 1971) for each octahedron type obtained by tilt model
- Range of octahedra O-O distances obtained by tilt model
- Angle variations in the octahedra faces obtained by tilt model
- Example of comparison between isotropic thermal parameters obtained on the average and local structure (simple and tilt model).

Table S1 x=0.05 at 200K (tilt model): characterization of cerium octahedra and titanium octahedra groups (Ti octahedra near to those with cerium (TiC), those far from cerium (TiF) and those between these two last groups (TiB)). Ce/Ti bond lengths, average Ce/Ti bond lengths, polyhedra volume, distortion index, quadratic elongation and bond angle variance are reported. Parameters of TiC and TiB groups are affected by high correlation.

***x*=0.05 200K**							
Ce-O		*TiC: Ti-O*		*TiB: Ti-O*		*TiF: Ti-O*	
l(Ce3-O108)	2.143 Å	l(Ti3-O4)	1.915 Å	l(Ti5-O136)	2.330 Å	l(Ti4-O133)	2.049 Å
l(Ce3-O172)	2.143 Å	l(Ti3-O1)	1.772 Å	l(Ti5-O8)	2.330 Å	l(Ti4-O5)	2.049 Å
l(Ce3-O44)	2.143 Å	l(Ti3-O68)	1.813 Å	l(Ti5-O72)	2.043 Å	l(Ti4-O69)	2.049 Å
l(Ce3-O41)	2.143 Å	l(Ti3-O132)	1.813 Å	l(Ti5-O5)	1.991 Å	l(Ti4-O6)	1.989 Å
l(Ce3-O176)	2.143 Å	l(Ti3-O136)	1.772 Å	l(Ti5-O140)	1.991 Å	l(Ti4-O137)	1.989 Å
l(Ce3-O124)	2.143 Å	l(Ti3-O84)	1.77 Å	l(Ti5-O88)	1.991 Å	l(Ti4-O85)	1.989 Å
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Average bond length (Å)	2.14	Average bond length (Å)	1.81	Average bond length (Å)	2.11	Average bond length (Å)	2.02
Polyhedral volume ($Å^3$)	13.13	Polyhedral volume ($Å^3$)	7.26	Polyhedral volume ($Å^3$)	12.31	Polyhedral volume ($Å^3$)	10.88
Distortion index (bond length)	0	Distortion index (bond length)	0.02	Distortion index (bond length)	0.07	Distortion index (bond length)	0.02
Quadratic elongation	1	Quadratic elongation	1.06	Quadratic elongation	1.02	Quadratic elongation	1.00
Bond angle variance ($deg.^2$)	0.02	Bond angle variance ($deg.^2$)	167.50	Bond angle variance ($deg.^2$)	39.69	Bond angle variance ($deg.^2$)	23.03

Table S2 x=0.05 at 300K (tilt model): characterization of cerium octahedra and titanium octahedra groups (Ti octahedra near to those with cerium (TiC), those far from cerium (TiF) and those between these two last groups (TiB). Ce/Ti bond lengths, average Ce/Ti bond lengths, polyhedra volume, distortion index, quadratic elongation and bond angle variance are reported. Parameters of TiC and TiB groups are affected by high correlation.

***x*=0.05 300K**							
Ce-O		*TiC: Ti-O*		*TiB: Ti-O*		*TiF: Ti-O*	
l(Ce3-O108)	2.151 Å	l(Ti3-O4)	1.917 Å	l(Ti5-O136)	2.391 Å	l(Ti4-O133)	2.057 Å
l(Ce3-O172)	2.151 Å	l(Ti3-O1)	1.783 Å	l(Ti5-O8)	2.052 Å	l(Ti4-O5)	2.057 Å
l(Ce3-O44)	2.151 Å	l(Ti3-O68)	1.783 Å	l(Ti5-O72)	2.052 Å	l(Ti4-O69)	2.057 Å
l(Ce3-O41)	2.151 Å	l(Ti3-O132)	1.735 Å	l(Ti5-O5)	2.304 Å	l(Ti4-O6)	1.981 Å
l(Ce3-O176)	2.151 Å	l(Ti3-O136)	1.735 Å	l(Ti5-O140)	2.304 Å	l(Ti4-O137)	1.981 Å
l(Ce3-O124)	2.151 Å	l(Ti3-O84)	1.735 Å	l(Ti5-O88)	2.304 Å	l(Ti4-O85)	1.981 Å
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Average bond length (Å)	2.15	Average bond length (Å)	1.78	Average bond length (Å)	2.23	Average bond length (Å)	2.02
Polyhedral volume ($Å^3$)	13.27	Polyhedral volume ($Å^3$)	6.72	Polyhedral volume ($Å^3$)	14.26	Polyhedral volume ($Å^3$)	10.90
Distortion index (bond length)	0	Distortion index (bond length)	0.03	Distortion index (bond length)	0.05	Distortion index (bond length)	0.02
Quadratic elongation	1.00	Quadratic elongation	1.08	Quadratic elongation	1.03	Quadratic elongation	1.00
Bond angle variance ($deg.^2$)	0.29	Bond angle variance ($deg.^2$)	217.41	Bond angle variance ($deg.^2$)	97.98	Bond angle variance ($deg.^2$)	17.25

Table S3 x=0.05 at 350K (tilt model): characterization of cerium octahedra and titanium octahedra groups (Ti octahedra near to those with cerium (TiC), those far from cerium (TiF) and those between these two last groups (TiB). Ce/Ti bond lengths, average Ce/Ti bond lengths, polyhedra volume, distortion index, quadratic elongation and bond angle variance are reported. Parameters of TiC and TiB groups are affected by high correlation.

***x*=0.05 350K**							
Ce-O		*TiC: Ti-O*		*TiB: Ti-O*		*TiF: Ti-O*	
l(Ce3-O108)	2.143 Å	l(Ti3-O4)	1.921 Å	l(Ti5-O136)	2.325 Å	l(Ti4-O133)	2.046 Å
l(Ce3-O172)	2.143 Å	l(Ti3-O1)	1.786 Å	l(Ti5-O8)	2.049 Å	l(Ti4-O5)	2.046 Å
l(Ce3-O44)	2.143 Å	l(Ti3-O68)	1.828 Å	l(Ti5-O72)	2.049 Å	l(Ti4-O69)	2.046 Å
l(Ce3-O41)	2.143 Å	l(Ti3-O132)	1.828 Å	l(Ti5-O5)	2.254 Å	l(Ti4-O6)	1.988 Å
l(Ce3-O176)	2.143 Å	l(Ti3-O136)	1.786 Å	l(Ti5-O140)	2.254 Å	l(Ti4-O137)	1.988 Å
l(Ce3-O124)	2.143 Å	l(Ti3-O84)	1.786 Å	l(Ti5-O88)	2.254 Å	l(Ti4-O85)	1.988 Å
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Average bond length (Å)	2.14	Average bond length (Å)	1.82	Average bond length (Å)	2.20	Average bond length (Å)	2.02
Polyhedral volume ($Å^3$)	13.08	Polyhedral volume ($Å^3$)	7.35	Polyhedral volume ($Å^3$)	13.51	Polyhedral volume ($Å^3$)	10.93
Distortion index (bond length)	0	Distortion index (bond length)	0.02	Distortion index (bond length)	0.05	Distortion index (bond length)	0.01
Quadratic elongation	1.00	Quadratic elongation	1.07	Quadratic elongation	1.03	Quadratic elongation	1.00
Bond angle variance ($deg.^2$)	6.10	Bond angle variance ($deg.^2$)	182.40	Bond angle variance ($deg.^2$)	113.37	Bond angle variance ($deg.^2$)	4.23

Table S4 x=0.05 at 380K (tilt model): characterization of cerium octahedra and titanium octahedra groups (Ti octahedra near to those with cerium (TiC), those far from cerium (TiF) and those between these two last groups (TiB). Ce/Ti bond lengths, average Ce/Ti bond lengths, polyhedra volume, distortion index, quadratic elongation and bond angle variance are reported. Parameters of TiC and TiB groups are affected by high correlation.

***x*=0.05 380K**							
Ce-O		*TiC: Ti-O*		*TiB: Ti-O*		*TiF: Ti-O*	
l(Ce3-O108)	2.150 Å	l(Ti3-O4)	1.914 Å	l(Ti5-O136)	2.335 Å	l(Ti4-O133)	2.047 Å
l(Ce3-O172)	2.150 Å	l(Ti3-O1)	1.776 Å	l(Ti5-O8)	2.047 Å	l(Ti4-O5)	2.047 Å
l(Ce3-O44)	2.15 Å	l(Ti3-O68)	1.818 Å	l(Ti5-O72)	2.047 Å	l(Ti4-O69)	2.047 Å
l(Ce3-O41)	2.150 Å	l(Ti3-O132)	1.8178 Å	l(Ti5-O5)	2.264 Å	l(Ti4-O6)	1.988 Å
l(Ce3-O176)	2.150 Å	l(Ti3-O136)	1.776 Å	l(Ti5-O140)	2.264 Å	l(Ti4-O137)	1.988 Å
l(Ce3-O124)	2.150 Å	l(Ti3-O84)	1.776 Å	l(Ti5-O88)	2.264 Å	l(Ti4-O85)	1.988 Å
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Average bond length (Å)	2.15	Average bond length (Å)	1.81	Average bond length (Å)	2.20	Average bond length (Å)	2.02
Polyhedral volume ($Å^3$)	13.19	Polyhedral volume ($Å^3$)	7.23	Polyhedral volume ($Å^3$)	13.68	Polyhedral volume ($Å^3$)	10.94
Distortion index (bond length)	0	Distortion index (bond length)	0.02	Distortion index (bond length)	0.05	Distortion index (bond length)	0.02
Quadratic elongation	1.00	Quadratic elongation	1.07	Quadratic elongation	1.03	Quadratic elongation	1.00
Bond angle variance ($deg.^2$)	11.85	Bond angle variance ($deg.^2$)	184.25	Bond angle variance ($deg.^2$)	100.69	Bond angle variance ($deg.^2$)	1.64

Table S5 x=0.05 at 420K (tilt model): characterization of cerium octahedra and titanium octahedra groups (Ti octahedra near to those with cerium (TiC), those far from cerium (TiF) and those between these two last groups (TiB). Ce/Ti bond lengths, average Ce/Ti bond lengths, polyhedra volume, distortion index, quadratic elongation and bond angle variance are reported. Parameters of Tic and TiB groups are affected by high correlation.

***x*=0.05 420K**							
Ce-O		*TiC: Ti-O*		*TiB: Ti-O*		*TiF: Ti-O*	
l(Ce3-O108)	2.145 Å	l(Ti3-O4)	1.923 Å	l(Ti5-O136)	2.302 Å	l(Ti4-O133)	2.047 Å
l(Ce3-O172)	2.145 Å	l(Ti3-O1)	1.810 Å	l(Ti5-O8)	2.047 Å	l(Ti4-O5)	2.047 Å
l(Ce3-O44)	2.145 Å	l(Ti3-O68)	1.852 Å	l(Ti5-O72)	2.047 Å	l(Ti4-O69)	2.047 Å
l(Ce3-O41)	2.145 Å	l(Ti3-O132)	1.852 Å	l(Ti5-O5)	2.232 Å	l(Ti4-O6)	1.989 Å
l(Ce3-O176)	2.145 Å	l(Ti3-O136)	1.810 Å	l(Ti5-O140)	2.232 Å	l(Ti4-O137)	1.989 Å
l(Ce3-O124)	2.145 Å	l(Ti3-O84)	1.810Å	l(Ti5-O88)	2.232 Å	l(Ti4-O85)	1.989 Å
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Average bond length (Å)	2.14	Average bond length (Å)	1.84	Average bond length (Å)	2.18	Average bond length (Å)	2.02
Polyhedral volume ($Å^3$)	13.03	Polyhedral volume ($Å^3$)	7.59	Polyhedral volume ($Å^3$)	13.27	Polyhedral volume ($Å^3$)	10.95
Distortion index (bond length)	0	Distortion index (bond length)	0.02	Distortion index (bond length)	0.04	Distortion index (bond length)	0.01
Quadratic elongation	1.01	Quadratic elongation	1.07	Quadratic elongation	1.03	Quadratic elongation	1.00
Bond angle variance ($deg.^2$)	22.74	Bond angle variance ($deg.^2$)	183.29	Bond angle variance ($deg.^2$)	105.37	Bond angle variance ($deg.^2$)	1.63

Table S6 x=0.10 at 100K (tilt model): characterization of cerium octahedra and titanium octahedra groups (Ti octahedra near (TiC) and those not near (TiB) to cerium polyhedra). Ce/Ti bond lengths, average Ce/Ti bond lengths, polyhedra volume, distortion index, quadratic elongation and bond angle variance are reported.

***x*=0.10 100K**					
Ce-O		*TiC: Ti-O*		*TiB: Ti-O*	
l(Ce5-O108)	2.139 Å	l(Ti25-O92)	2.051 Å	l(Ti22-O88)	2.062 Å
l(Ce5-O172)	2.13 Å	l(Ti25-O156)	2.051 Å	l(Ti22-O152)	2.062 Å
l(Ce5-O44)	2.139 Å	l(Ti25-O28)	2.051 Å	l(Ti22-O24)	2.062 Å
l(Ce5-O41)	2.139 Å	l(Ti25-O25)	2.018 Å	l(Ti22-O21)	2.016 Å
l(Ce5-O176)	2.139 Å	l(Ti25-O160)	2.018 Å	l(Ti22-O156)	2.016 Å
l(Ce5-O124)	2.139 Å	l(Ti25-O108)	1.890 Å	l(Ti22-O104)	2.016 Å
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Average bond length (Å)	2.14	Average bond length (Å)	2.01	Average bond length (Å)	2.04
Polyhedral volume (Å^3)	13.06	Polyhedral volume (Å^3)	10.62	Polyhedral volume (Å^3)	10.88
Distortion index (bond length)	0	Distortion index (bond length)	0.02	Distortion index (bond length)	0.01
Quadratic elongation	1	Quadratic elongation	1.02	Quadratic elongation	1.03
Bond angle variance (deg.^{2})	0.01	Bond angle variance (deg.^{2})	51.22	Bond angle variance (deg.^{2})	99.20

Table S7 x=0.10 at 200K (tilt model): characterization of cerium octahedra and titanium octahedra groups (Ti octahedra near (TiC) and those not near (TiB) to cerium polyhedra). Ce/Ti bond lengths, average Ce/Ti bond lengths, polyhedra volume, distortion index, quadratic elongation and bond angle variance are reported.

***x*=0.10 200K**					
Ce-O		*TiC: Ti-O*		*TiB: Ti-O*	
l(Ce5-O108)	2.169 Å	l(Ti25-O92)	2.061 Å	l(Ti22-O88)	2.076 Å
l(Ce5-O172)	2.169 Å	l(Ti25-O156)	2.061 Å	l(Ti22-O152)	2.076 Å
l(Ce5-O44)	2.169 Å	l(Ti25-O28)	2.061 Å	l(Ti22-O24)	2.076 Å
l(Ce5-O41)	2.169 Å	l(Ti25-O25)	2.010 Å	l(Ti22-O21)	2.006 Å
l(Ce5-O176)	2.169 Å	l(Ti25-O160)	2.010 Å	l(Ti22-O156)	2.006 Å
l(Ce5-O124)	2.169 Å	l(Ti25-O108)	1.853 Å	l(Ti22-O104)	2.006 Å
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Average bond length (Å)	2.169	Average bond length (Å)	2.01	Average bond length (Å)	2.04
Polyhedral volume (Å^3)	13.60	Polyhedral volume (Å^3)	10.58	Polyhedral volume (Å^3)	10.91
Distortion index (bond length)	0	Distortion index (bond length)	0.03	Distortion index (bond length)	0.02
Quadratic elongation	1	Quadratic elongation	1.02	Quadratic elongation	1.03
Bond angle variance (deg.^{2})	0.01	Bond angle variance (deg.^{2})	48.06	Bond angle variance (deg.^{2})	95.65

Table S8 x=0.10 at 300K (tilt model): characterization of cerium octahedra and titanium octahedra groups (Ti octahedra near (TiC) and those not near (TiB) to cerium polyhedra). Ce/Ti bond lengths, average Ce/Ti bond lengths, polyhedra volume, distortion index, quadratic elongation and bond angle variance are reported.

***x*=0.10 300K**					
Ce-O		*TiC: Ti-O*		*TiB: Ti-O*	
l(Ce5-O108)	2.166 Å	l(Ti25-O92)	2.059 Å	l(Ti22-O88)	2.072 Å
l(Ce5-O172)	2.166 Å	l(Ti25-O156)	2.059 Å	l(Ti22-O152)	2.072 Å
l(Ce5-O44)	2.166 Å	l(Ti25-O28)	2.059 Å	l(Ti22-O24)	2.072 Å
l(Ce5-O41)	2.166 Å	l(Ti25-O25)	2.015 Å	l(Ti22-O21)	2.012 Å
l(Ce5-O176)	2.166 Å	l(Ti25-O160)	2.015 Å	l(Ti22-O156)	2.012 Å
l(Ce5-O124)	2.166 Å	l(Ti25-O108)	1.864 Å	l(Ti22-O104)	2.012 Å
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Average bond length (Å)	2.17	Average bond length (Å)	2.01	Average bond length (Å)	2.04
Polyhedral volume (Å^3)	13.54	Polyhedral volume (Å^3)	10.61	Polyhedral volume (Å^3)	10.93
Distortion index (bond length)	0	Distortion index (bond length)	0.03	Distortion index (bond length)	0.02
Quadratic elongation	1	Quadratic elongation	1.02	Quadratic elongation	1.03
Bond angle variance (deg.^{2})	0.00	Bond angle variance (deg.^{2})	48.60	Bond angle variance (deg.^{2})	98.51

Table S9 x=0.10 at 400K (tilt model): characterization of cerium octahedra and titanium octahedra groups (Ti octahedra near (TiC) and those not near (TiB) to cerium polyhedra). Ce/Ti bond lengths, average Ce/Ti bond lengths, polyhedra volume, distortion index, quadratic elongation and bond angle variance are reported.

***x*=0.10 400K**					
Ce-O		*TiC: Ti-O*		*TiB: Ti-O*	
l(Ce5-O108)	2.186 Å	l(Ti25-O92)	2.066 Å	l(Ti22-O88)	2.080 Å
l(Ce5-O172)	2.186 Å	l(Ti25-O156)	2.066 Å	l(Ti22-O152)	2.080 Å
l(Ce5-O44)	2.186 Å	l(Ti25-O28)	2.066 Å	l(Ti22-O24)	2.080 Å
l(Ce5-O41)	2.186 Å	l(Ti25-O25)	2.008 Å	l(Ti22-O21)	2.004 Å
l(Ce5-O176)	2.186 Å	l(Ti25-O160)	2.008 Å	l(Ti22-O156)	2.004 Å
l(Ce5-O124)	2.186 Å	l(Ti25-O108)	1.841 Å	l(Ti22-O104)	2.004 Å
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Average bond length (Å)	2.19	Average bond length (Å)	2.01	Average bond length (Å)	2.04
Polyhedral volume (Å^3)	13.88	Polyhedral volume (Å^3)	10.62	Polyhedral volume (Å^3)	10.98
Distortion index (bond length)	0	Distortion index (bond length)	0.03	Distortion index (bond length)	0.02
Quadratic elongation	1.00	Quadratic elongation	1.01	Quadratic elongation	1.02
Bond angle variance (deg.^{2})	7.87	Bond angle variance (deg.^{2})	37.48	Bond angle variance (deg.^{2})	86.61

Table S10 x=0.20 at 100K (tilt model): characterization of cerium octahedra and titanium octahedra (TiC). Ce/Ti bond lengths, average Ce/Ti bond lengths, polyhedra volume, distortion index, quadratic elongation and bond angle variance are reported.

***x*=0.20 100K**			
Ce-O		*TiC: Ti-O*	
l(Ce2-O16)	2.152 Å	l(Ti1-O2)	1.939 Å
l(Ce2-O24)	2.152 Å	l(Ti1-O10)	2.075 Å
l(Ce2-O8)	2.152 Å	l(Ti1-O18)	2.075 Å
l(Ce2-O7)	2.152 Å	l(Ti1-O1)	1.949 Å
l(Ce2-O22)	2.152 Å	l(Ti1-O20)	2.075 Å
l(Ce2-O12)	2.152 Å	l(Ti1-O14)	2.075 Å
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Average bond length (Å)	2.15	Average bond length (Å)	2.03
Polyhedral volume ($Å^3$)	13.27	Polyhedral volume ($Å^3$)	10.86
Distortion index (bond length)	0	Distortion index (bond length)	0.03
Quadratic elongation	1.00	Quadratic elongation	1.02
Bond angle variance ($deg.^2$)	4.28	Bond angle variance ($deg.^2$)	65.81

Table S11 x=0.20 at 200K (tilt model): characterization of cerium octahedra and titanium octahedra (TiC). Ce/Ti bond lengths, average Ce/Ti bond lengths, polyhedra volume, distortion index, quadratic elongation and bond angle variance are reported.

***x*=0.20 200K**			
Ce-O		*TiC: Ti-O*	
l(Ce2-O16)	2.154 Å	l(Ti1-O2)	1.940 Å
l(Ce2-O24)	2.154 Å	l(Ti1-O10)	2.074 Å
l(Ce2-O8)	2.154 Å	l(Ti1-O18)	2.074 Å
l(Ce2-O7)	2.154 Å	l(Ti1-O1)	1.946 Å
l(Ce2-O22)	2.154 Å	l(Ti1-O20)	2.071 Å
l(Ce2-O12)	2.154 Å	l(Ti1-O14)	2.071 Å
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Average bond length (Å)	2.15	Average bond length (Å)	2.03
Polyhedral volume ($Å^3$)	13.32	Polyhedral volume ($Å^3$)	10.87
Distortion index (bond length)	0	Distortion index (bond length)	0.03
Quadratic elongation	1.00	Quadratic elongation	1.02
Bond angle variance ($deg.^2$)	0.82	Bond angle variance ($deg.^2$)	55.12

Table S12 x=0.20 at 300K (tilt model): characterization of cerium octahedra and titanium octahedra (TiC). Ce/Ti bond lengths, average Ce/Ti bond lengths, polyhedra volume, distortion index, quadratic elongation and bond angle variance are reported.

***x*=0.20 300K**			
Ce-O		*TiC: Ti-O*	
l(Ce2-O16)	2.165 Å	l(Ti1-O2)	2.081 Å
l(Ce2-O24)	2.165 Å	l(Ti1-O10)	2.081 Å
l(Ce2-O8)	2.165 Å	l(Ti1-O18)	1.931 Å
l(Ce2-O7)	2.165 Å	l(Ti1-O1)	1.940 Å
l(Ce2-O22)	2.165 Å	l(Ti1-O20)	2.063 Å
l(Ce2-O12)	2.165 Å	l(Ti1-O14)	2.063 Å
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Average bond length (Å)	2.17	Average bond length (Å)	2.03
Polyhedral volume ($Å^3$)	13.53	Polyhedral volume ($Å^3$)	10.84
Distortion index (bond length)	0	Distortion index (bond length)	0.03
Quadratic elongation	1	Quadratic elongation	1.02
Bond angle variance ($deg.^2$)	0.12	Bond angle variance ($deg.^2$)	50.72

Table S13 x=0.20 at 400K (tilt model): characterization of cerium octahedra and titanium octahedra (TiC). Ce/Ti bond lengths, average Ce/Ti bond lengths, polyhedra volume, distortion index, quadratic elongation and bond angle variance are reported.

***x*=0.20 400K**			
Ce-O		*TiC: Ti-O*	
l(Ce2-O16)	2.176 Å	l(Ti1-O2)	2.081 Å
l(Ce2-O24)	2.176 Å	l(Ti1-O10)	2.081 Å
l(Ce2-O8)	2.176 Å	l(Ti1-O18)	1.924 Å
l(Ce2-O7)	2.176 Å	l(Ti1-O1)	1.932 Å
l(Ce2-O22)	2.176 Å	l(Ti1-O20)	2.064 Å
l(Ce2-O12)	2.176 Å	l(Ti1-O14)	2.064 Å
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Average bond length (Å)	2.176	Average bond length (Å)	2.02
Polyhedral volume ($Å^3$)	13.73	Polyhedral volume ($Å^3$)	10.82
Distortion index (bond length)	0	Distortion index (bond length)	0.03
Quadratic elongation	1	Quadratic elongation	1.02
Bond angle variance ($deg.^2$)	0.17	Bond angle variance ($deg.^2$)	47.87

Table S14 x=0.30 at 100K (tilt model): characterization of cerium octahedra and titanium octahedra (TiC). Ce/Ti bond lengths, average Ce/Ti bond lengths, polyhedra volume, distortion index, quadratic elongation and bond angle variance are reported.

***x*=0.30 100K**			
Ce-O		*TiC: Ti-O*	
l(Ce2-O16)	2.240 Å	l(Ti1-O2)	1.890 Å
l(Ce2-O24)	2.240 Å	l(Ti1-O10)	1.901 Å
l(Ce2-O8)	2.240 Å	l(Ti1-O18)	1.901 Å
l(Ce2-O7)	2.240 Å	l(Ti1-O1)	1.890 Å
l(Ce2-O22)	2.240 Å	l(Ti1-O20)	1.901 Å
l(Ce2-O12)	2.240 Å	l(Ti1-O14)	1.890 Å
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Average bond length (Å)	2.24	Average bond length (Å)	1.90
Polyhedral volume ($Å^3$)	14.89	Polyhedral volume ($Å^3$)	9.04
Distortion index (bond length)	0	Distortion index (bond length)	0.00
Quadratic elongation	1.00	Quadratic elongation	1.00
Bond angle variance ($deg.^2$)	14.82	Bond angle variance ($deg.^2$)	9.58

Table S15 x=0.30 at 200K (tilt model): characterization of cerium octahedra and titanium octahedra (TiC). Ce/Ti bond lengths, average Ce/Ti bond lengths, polyhedra volume, distortion index, quadratic elongation and bond angle variance are reported.

***x*=0.30 200K**			
Ce-O		*TiC: Ti-O*	
l(Ce2-O16)	2.220 Å	l(Ti1-O2)	1.917 Å
l(Ce2-O24)	2.220 Å	l(Ti1-O10)	1.925 Å
l(Ce2-O8)	2.220 Å	l(Ti1-O18)	1.925 Å
l(Ce2-O7)	2.220 Å	l(Ti1-O1)	1.917 Å
l(Ce2-O22)	2.220 Å	l(Ti1-O20)	1.925 Å
l(Ce2-O12)	2.220 Å	l(Ti1-O14)	1.917 Å
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Average bond length (Å)	2.22	Average bond length (Å)	1.92
Polyhedral volume ($Å^3$)	14.41	Polyhedral volume ($Å^3$)	9.37
Distortion index (bond length)	0	Distortion index (bond length)	0.00
Quadratic elongation	1.00	Quadratic elongation	1.00
Bond angle variance ($deg.^2$)	29.01	Bond angle variance ($deg.^2$)	21.54

Table S16 x=0.30 at 300K (tilt model): characterization of cerium octahedra and titanium octahedra (TiC). Ce/Ti bond lengths, average Ce/Ti bond lengths, polyhedra volume, distortion index, quadratic elongation and bond angle variance are reported.

***x*=0.30 300K**			
Ce-O		*TiC: Ti-O*	
l(Ce2-O16)	2.191 Å	l(Ti1-O2)	1.958 Å
l(Ce2-O24)	2.191 Å	l(Ti1-O10)	1.954 Å
l(Ce2-O8)	2.191 Å	l(Ti1-O18)	1.954 Å
l(Ce2-O7)	2.191 Å	l(Ti1-O1)	1.958 Å
l(Ce2-O22)	2.191 Å	l(Ti1-O20)	1.954 Å
l(Ce2-O12)	2.191 Å	l(Ti1-O14)	1.958 Å
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Average bond length (Å)	2.19	Average bond length (Å)	1.96
Polyhedral volume ($Å^3$)	13.79	Polyhedral volume ($Å^3$)	9.84
Distortion index (bond length)	0	Distortion index (bond length)	0.00
Quadratic elongation	1.01	Quadratic elongation	1.00
Bond angle variance ($deg.^2$)	43.23	Bond angle variance ($deg.^2$)	31.99

Table S17 x=0.30 at 400K (tilt model): characterization of cerium octahedra and titanium octahedra (TiC). Ce/Ti bond lengths, average Ce/Ti bond lengths, polyhedra volume, distortion index, quadratic elongation and bond angle variance are reported.

***x*=0.30 400K**			
Ce-O		*TiC: Ti-O*	
l(Ce2-O16)	2.119 Å	l(Ti1-O2)	2.035 Å
l(Ce2-O24)	2.119 Å	l(Ti1-O10)	2.044 Å
l(Ce2-O8)	2.119 Å	l(Ti1-O18)	2.044 Å
l(Ce2-O7)	2.119 Å	l(Ti1-O1)	2.035 Å
l(Ce2-O22)	2.119 Å	l(Ti1-O20)	2.044 Å
l(Ce2-O12)	2.119 Å	l(Ti1-O14)	2.035 Å
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Average bond length (Å)	2.12	Average bond length (Å)	2.034
Polyhedral volume ($Å^3$)	12.32	Polyhedral volume ($Å^3$)	11.06
Distortion index (bond length)	0	Distortion index (bond length)	0.00
Quadratic elongation	1.02	Quadratic elongation	1.02
Bond angle variance ($deg.^2$)	76.01	Bond angle variance ($deg.^2$)	50.61

Table S18 Range of octahedra oxygen-oxygen bond distances obtained refining different data set by tilt model. Values obtained by referenced $BaTiO_3$ rhombohedral structure at 100K (Kwei *et al.*, 1993) are also reported. Values in *x*=0.05, are affected by the high correlation of some oxygen parameters as explained in the text.

$BaTiO_3$		x=0.05		x=0.10		x=0.20		x=0.30	
Temp. (K)	Distance range (Å)	Temp. (K)	Distance range (Å)	Temp. (K)	Distance range (Å)	Temp. (K)	Distance range (Å)	Temp. (K)	Distance range (Å)
100	2.78-2.88	200	2.21-3.17	100	2.63-3.11	100	2.54-3.29	100	2.61-3.27
		300	2.12-3.23	200	2.64-3.11	200	2.57-3.26	200	2.61-3.28
		350	2.22-3.25	300	2.64-3.12	300	2.59-3.24	300	2.63-3.26
		380	2.21-3.23	400	2.57-3.20	400	2.603.23	400	2.71-3.21
		420	2.25-3.21						

Table S19 Angle variations in the octahedra faces obtained refining different data set by tilt model. Values obtained by referenced $BaTiO_3$ rhombohedral structure at 100K (Kwei *et al.*, 1993) are also reported. Values in *x*=0.05, are affected by the high correlation of some oxygen parameters as explained in the text.

$BaTiO_3$		x=0.05		x=0.10		x=0.20		x=0.30	
Temp. (K)	Angle range (°)	Temp. (K)	Angle range (°)	Temp. (K)	Angle range (°)	Temp. (K)	Angle range (°)	Temp. (K)	Angle range (°)
100	58.66-60.95	200	48.07-80.77	100	50.07-70.29	100	49.39-73.21	100	55.92-63.53
		300	46.31-82.62	200	50.26-69.93	200	50.34-72.58	200	54.38-65.41
		350	47.81-80.01	300	50.11-70.01	300	50.55-72.11	300	53.22-66.68
		380	47.78-79.93	400	50.70-69.13	400	50.68-71.90	400	51.19-68.56
		420	48.44-79.62						

Table S20 Comparison of isotropic thermal parameter values obtained on the average structure and on the local (simple and tilt model) for the sample x=0.10.

x=0.10	Temp. (K)	Uiso Ba ($Å^2$)	Uiso Ti ($Å^2$)	Uiso Ce ($Å^2$)	Uiso O ($Å^2$)
Average	100 K	0.003(4)	0.006(1)	0.006(1)	0.0101(5)
Local simple model		0.003(3)	0.005(1)	0.03(3)	0.02(1)
Local tilt model		0.003(3)	0.005(2)	0.009(1)	0.014(3)
Average	200 K	0.0055(5)	0.008(1)	0.008(1)	0.0124(1)
Local simple model		0.004(4)	0.004(1)	0.03(4)	0.02(1)
Local tilt model		0.004(3)	0.006(9)	0.008(4)	0.015(3)
Average	300 K	0.0073(8)	0.009(4)	0.009(4)	0.009(1)
Local simple model		0.005(8)	0.005(7)	0.009(3)	0.026(1)
Local tilt model		0.005(5)	0.008(1)	0.009(3)	0.015(4)
Average	400 K	0.0098(5)	0.0125(1)	0.0125(1)	0.0196(4)
Local simple model		0.007(1)	0.009(6)	0.006(2)	0.025(6)
Local tilt model		0.006(7)	0.008(2)	0.009(3)	0.015(4)

References of Supporting Information

Baur, W. (1974). *Acta Cryst. B* **30**, 1195-1215.
Kwei, G. H., Lawson, A. C., Billinge, S. J. L. & Cheong, S. W. (1993). *J. Phys. Chem.* **97**, 2368-2377.
Robinson, K., Gibbs, G. V. & Ribbe, P. H. (1971). *Science* **172**, 567-570.