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Supporting information for article:

Incommensurate crystal structure of PbHfO3

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Table S1 Positional parameters in $PbHfO_3$ at 443 K

Atom	Wave	x	y	z	U_{eqv} (Å^2)
Hf1		0	0	0	0.012(4)
	s,1	-0.00464(13)	0	0	
	c,1	0	0	0	
	s,2	0	0.00005(2)	-0.00022(3)	
	c,2	0	0	0	
	s,3	-0.00097(3)	0	0	
	c,3	0	0	0	
Pb1†		0.0292(5)	0.75	0.50222(6)	0.0220(6)
	s,1	-0.00084(6)	0	-0.0004(4)	
	c,1	0.0042(4)	0	-0.00068(5)	
	s,2	0.00016(8)	0	0.0012(5)	
	c,2	0.0082(6)	0	-0.0004(6)	
O1		0	0.75	0.0467(11)	0.009(3)
	s,1	0.0200(9)	0	0	
	c,1	-0.0197(8)	0	0	
	s,2	0	0	-0.0019(5)	
	c,2	0	0	0.0005(5)	
	s,3	0.0043(6)	0	0	
	c,3	-0.0018(6)	0	0	
O2		0.25	0.0227(6)	0.25	0.0197(19)
	s,1	0.0137(9)	0	-0.0078(7)	
	c,1	0	-0.0097(4)	0	
	s,2	-0.0001(4)	0	-0.0004(4)	
	c,2	0	-0.0001(3)	0	
	s,3	0.0066(4)	0	-0.0062	
	c,3	0	0.0007(3)	0	

† The crenel function with parameters of occupancy, $x4_0 = 0.75$, $\Delta x4 = 0.5$ is used for Pb1 site.

Table S2 ADP harmonic parameters in $PbHfO_3$ at 443 K

Atom	Wave	U11	U22	U33	U12	U13	U23
Hf1		0.004(4)	0.031(11)	0.000811†	0	0	0.0035(9)
Pb1		0.0168(8)	0.0291(14)	0.0201(7)	0	-0.00184(10)	0
	s,1	0.00308(15)	-0.0008(4)	0.0002(3)	0	-0.0017(5)	0
	c,1	0.0000(9)	-0.0007(2)	-0.00087(15)	0	-0.00013(19)	0
	s,2	0.0012(2)	0.0000(5)	-0.0005(3)	0	-0.0003(7)	0
	c,2	-0.0111(18)	0.0002(12)	0.0014(7)	0	-0.0007(6)	0
O1		0.018(3)	0.009(9)	0.001445†	0	0	0
O2		0.018(3)	0.031(4)	0.010(3)	0	-0.000006†	0

† Parameter has been fixed.

Table S3 ADP nonzero and exceeding 1 s.u. anharmonic parameters of Hf1 in $PbHfO_3$ at 443 K

D1111	D1122	D1123	D2222	D2223	D2233	D3333
0.07(3)	0.015(8)	-0.0009(8)	0.07(4)	0.027(3)	0.008(6)	0.055(10)

F111111	F111123	F112222	F222222	F222223	F233333	F333333
0.13(5)	-0.0012(6)	0.018(8)	0.08(6)	0.045(5)	0.003(2)	0.09(2)

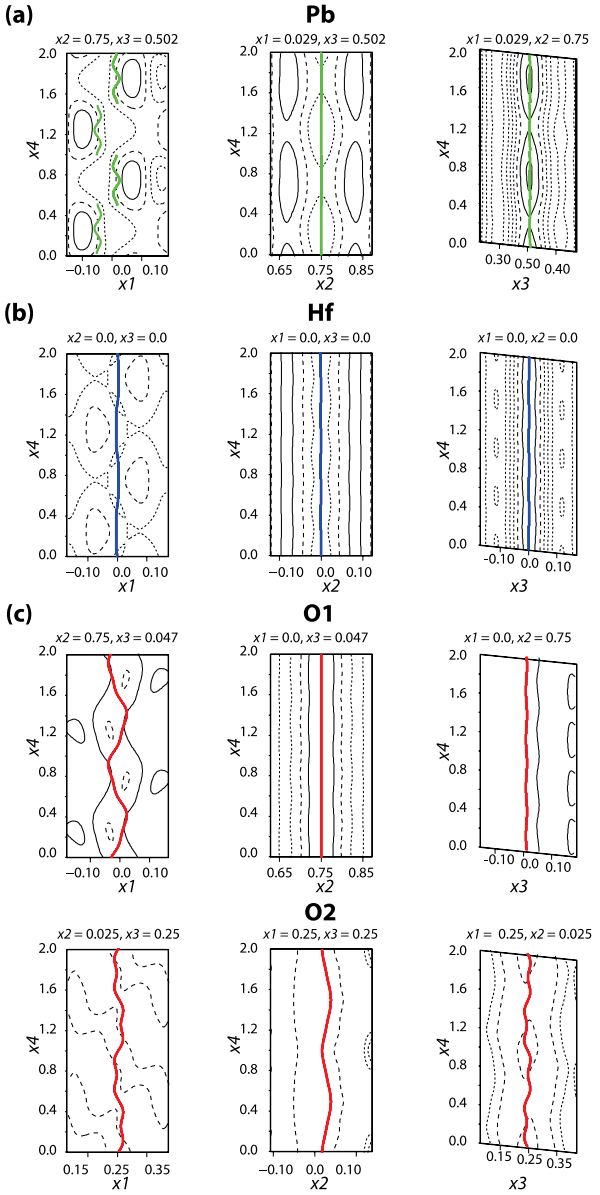

Figure S1 The residual electron density maps (black solid lines) for (a) Pb, (b) Hf and (c) O atoms in the *x*1-*x*4, *x*2-*x*4 and *x*3-*x*4 sections. The contour steps are 0.5 e Å^{-3}. Green, blue and red solid lines correspond to the Pb, Hf and O position modulation, respectively.

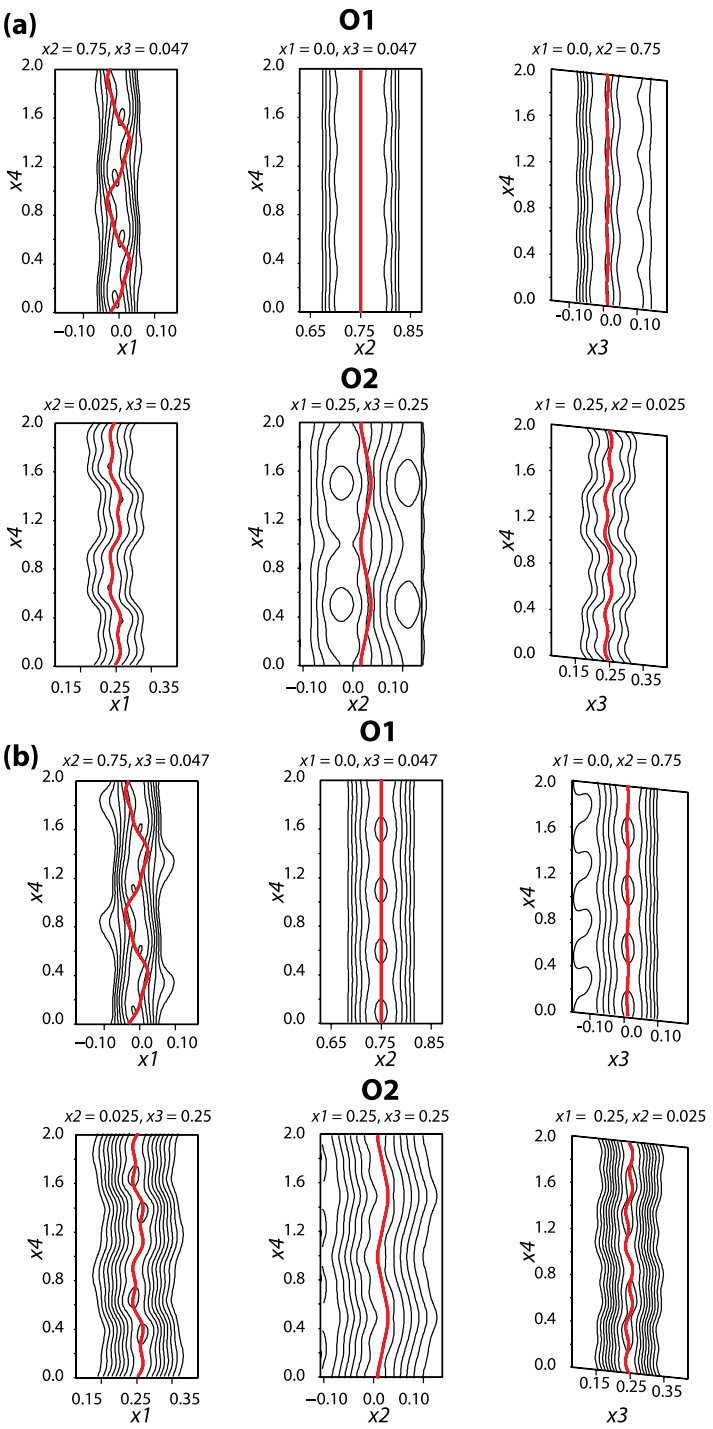

Figure S2 The experimental Fourier electron density maps (black solid lines) for O atoms calculated (a) using all reflections and (b) without seven strongest main reflections: (2400), (0420), (2040), (1610), (1230), (0040) and (0060). The contour step is 2 e Å^{-3}. Red solid lines correspond to the position modulation.