Electronic supplementary information (ESI) in the manuscript

BiInO₃: a Polar Oxide with GdFeO₃-Type Perovskite Structure

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Table S1. O–In–O Bond Angles in BiInO₃ (Space Group *Pna2*₁)

Angle	
O1–In–O1	176.1
O2–In–O3	168.2
O2–In–O3	166.9
O1–In–O3	82.8
O1–In–O2	97.3
O1–In–O2	87.6
O1–In–O3	81.0
O1–In–O2	94.0
O1–In–O3	95.9
O1–In–O3	95.2
O1–In–O2	86.3
O2–In–O3	99.3
O2–In–O3	78.3
O2–In–O2	88.7
O3–In–O3	93.4

Table S2. Structure Parameters for BiInO₃ Refined in Space Group *Pnma*^a

Site	Wyckoff position	<i>x</i>	<i>y</i>	<i>z</i>	10 ² <i>U</i> (Å ²)
Bi	4 <i>c</i>	0.05998(18)	0.75	0.0086(4)	0.98(4)
In	4 <i>b</i>	0	0	0.5	1.66(6)
O1	4 <i>c</i>	−0.058(3)	0.75	0.379(2)	−1.2(3)
O2	8 <i>d</i>	0.174(3)	0.441(2)	0.186(3)	4.9(7)

^a Space group *Pnma* (No. 62); *Z* = 4; *a* = 5.95462(14) Å, *b* = 8.3864(2) Å, *c* = 5.60185(13) Å, and *V* = 279.745(11) Å³; *R*_{wp} = 12.78 %, *R*_p = 9.35 %, *R*_B = 7.72 %, *R*_F = 3.93 %, and *S* = *R*_{wp} / *R*_e = 3.45. Occupancy factors of all the sites are unity. The *y* coordinates were used to calculate the spontaneous polarization in BiInO₃.

Figure S1

DTA up to 800°C and DSC up to 550°C curves of BiInO₃. Note that the anomaly near 350°C was observed in many samples prepared at high pressure, for example, in BiAlO₃, BiGaO₃, and BiScO₃.