Supplemental Material for

Crystal Structures and Electronic States of High-Pressure-Synthesized \((1-x)\text{PbVO}_3-x\text{BiCrO}_3\) Solid Solutions

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Figure S1 Evolution of the lattice parameters of the monoclinic phase of the (1−x)PbVO<sub>3</sub>−xBiCrO<sub>3</sub> solid solutions. (a) a- (red) and c- (blue) axis-lengths. (b) b- axis length (c) β-angle (d) unit cell volume. The lattice parameters of BiCrO<sub>3</sub> were obtained from Ref. 7. The parameters of shadowed region are questionable because their values were not precisely determined because of peak overlaps.
### Table S1  
Lattice parameters of the monoclinic phase (C2/c) of the (1−x)PbVO₃–xBiCrO₃ solid solutions (x = 7/8–3/8).

| Composition     | a (Å)  | b (Å)  | c (Å)  | β (deg.) | Unit cell volume (Å³) |
|-----------------|--------|--------|--------|----------|-----------------------|
| 1/8PbVO₃-7/8BiCrO₃ | 9.531(3) | 5.4950(6) | 9.530(3) | 108.848(9) | 472.4(2) |
| 2/8PbVO₃-6/8BiCrO₃ | 9.545(3) | 5.5093(8) | 9.536(4) | 109.04(1) | 474.0(3) |
| *3/8PbVO₃-5/8BiCrO₃ | 9.61(1)  | 5.5085(7) | 9.612(9) | 109.44(3) | 479.8(7) |
| *4/8PbVO₃-4/8BiCrO₃ | 9.59(3)  | 5.511(8)  | 9.59(3)  | 109.33(8) | 479(2)   |
| *5/8PbVO₃-3/8BiCrO₃ | 9.58(1)  | 5.533(4)  | 9.541(5) | 109.51(7) | 477.1(7) |

*The parameters are questionable because their values are not determined precisely owing to peak overlaps.

### Table S2  
Lattice parameters of the tetragonal (P4mm) phase of the (1−x)PbVO₃–xBiCrO₃ solid solutions (x = 4/8–1/8).

| Composition     | a (Å)  | c (Å)  | c/a    | Unit cell volume (Å³) |
|-----------------|--------|--------|--------|-----------------------|
| 4/8PbVO₃-4/8BiCrO₃ | 3.899(1) | 3.991(1) | 1.0235(6) | 60.69(3) |
| 5/8PbVO₃-3/8BiCrO₃ | 3.8918(6) | 4.0735(6) | 1.0467(4) | 61.70(2) |
| 6/8PbVO₃-2/8BiCrO₃ | 3.8723(7) | 4.257(1)  | 1.0992(6) | 63.83(2) |
| 7/8PbVO₃-1/8BiCrO₃ | 3.83568(5) | 4.4490(1) | 1.1599(4) | 65.455(2) |
Table S3 Refined structural parameters of \( \frac{1}{8}\text{PbVO}_3 - \frac{7}{8}\text{BiCrO}_3 \).

| Site     | Wyckoff position | \( x \)   | \( y \)   | \( z \)   | \( U_{\text{iso}} \) (Å\(^2\)) |
|----------|-----------------|-----------|-----------|-----------|-------------------------------|
| Pb, Bi   | 8f              | 0.1308(4) | 0.2604(10)| 0.1282(5) | 0.0178(5)                    |
| V1, Cr1  | 4e              | 0.5       | 0.274(5)  | 0.75      | 0.0093(15)                   |
| V2, Cr2  | 4d              | 0.25      | 0.25      | 0.5       | 0.0093(15)                   |
| O1       | 8f              | 0.101(3)  | 0.179(8)  | 0.565(3)  | 0.0063                       |
| O2       | 8f              | 0.127(8)  | 0.478(18) | 0.379(10) | 0.0063                       |
| O3       | 8f              | 0.353(4)  | 0.459(18) | 0.135(5)  | 0.0063                       |

\( R_{wp} = 14.835\% \), \( R_p = 10.344\% \), \( S = 6.5383 \). Space group: \( C2/c \) (No. 15), \( Z = 4 \), Occupation factors of all sites were fixed to the formula. Lattice parameters are provided in Table S1. The isotropic atomic displacement parameters (\( U_{\text{iso}} \)) of O sites were fixed to 0.0063 Å\(^2\).

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Table S4 Refined structural parameters of \( \frac{7}{8}\text{PbVO}_3 - \frac{1}{8}\text{BiCrO}_3 \) at a room temperature.

| Site     | Wyckoff position | \( x \)   | \( y \)   | \( z \)   | \( U_{\text{iso}} \) (Å\(^2\)) |
|----------|-----------------|-----------|-----------|-----------|-------------------------------|
| Pb, Bi   | 1a              | 0         | 0         | 0         | 0.0098(2)                    |
| V1, Cr1  | 1b              | 0.5       | 0.5       | 0.5651(8) | 0.0019(9)                   |
| O1       | 1b              | 0.5       | 0.5       | 0.184(2)  | 0.005(2)                    |
| O2       | 2c              | 0.5       | 0         | 0.669(1)  | 0.005(2)                    |

\( R_{wp} = 8.072\% \), \( R_p = 4.595\% \), \( S = 6.2865 \). Space group: \( P4mm \) (No. 99), \( Z = 1 \), \( P_S = 86 \mu \text{C/cm}^2 \) (point charge model), Occupation factors of all sites were fixed to the formula. Lattice parameters are provided in Table S2. The isotropic atomic displacement parameters (\( U_{\text{iso}} \)) of O sites were fixed as same.
Figure S2 Comparison of SXRD patterns of 6/8PbVO$_3$-2/8BiCrO$_3$ synthesized at 5 GPa (blue) and 7 GPa (red).
Figure S3 Comparison of the values of theoretical ($C_{\text{calc.}}$) and experimental ($C_{\text{exp.}}$) Curie constants of the $(1-x)\text{PbVO}_3-x\text{BiCrO}_3$ solid solutions ($x = 7/8-1/8$).
Table S5 Refined structural parameters of tetragonal phase of $7/8\text{PbVO}_3-1/8\text{BiCrO}_3$ at 700 K.

| Site  | Wyckoff position | x   | y   | z     | $U_{\text{iso}}$ (Å$^2$) |
|-------|------------------|-----|-----|-------|--------------------------|
| Pb, Bi| $1a$             | 0   | 0   | 0     | 0.0209(3)                |
| V1, Cr1| $1b$           | 0.5 | 0.5 | 0.5571(15) | 0.0099(15)          |
| O1    | $1b$             | 0.5 | 0.5 | 0.226(4) | 0.034(4)               |
| O2    | $2c$             | 0.5 | 0.5 | 0.682(2) | 0.034(4)               |

$R_p = 9.139\%$, $R_p = 5.967\%$, $S = 6.8911$. Space group: $P4mm$ (No. 99), $Z = 1$, $a = 3.84840(8)$ Å, $c = 4.48551(18)$ Å, unit cell volume = 66.431(3) Å$^3$. Occupation factors of all sites were fixed to the formula. The isotropic atomic displacement parameters ($U_{\text{iso}}$) of O sites were fixed as same.

Table S6 Refined structural parameters of cubic phase of $7/8\text{PbVO}_3-1/8\text{BiCrO}_3$ at 700 K.

| Site  | Wyckoff position | x   | y   | z     | $U_{\text{iso}}$ (Å$^2$) |
|-------|------------------|-----|-----|-------|--------------------------|
| Pb, Bi| $1a$             | 0   | 0   | 0     | 0.0098(2)                |
| V1, Cr1| $1b$           | 0.5 | 0.5 | 0.5   | 0.0019(9)               |
| O1    | $2c$             | 0.5 | 0.5 | 0.5   | 0.005(2)                |

Space group: $Pm-3m$ (No. 221), $Z = 1$, $a = 3.9387(1)$ Å, unit cell volume = 61.102(3) Å$^3$. Occupation factors of all sites were fixed to the formula.