Supplementary Information for "High pO_2 Floating Zone Single Crystal Growth of the Perovskite Nickelate $PrNiO_3$"

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In the main text, we considered the single crystal X-ray diffraction patterns (Figure 5) in pseudocubic symmetry. In doing so, we considered twinned orthorhombic (space group *Pbnm*) and monoclinic ($P2_1/n$) structures. When twinned, there are six matrix transformations that relate these two space groups to the pseudocubic axes:

$$M=\begin{bmatrix} -1/2 & 0 & 1/2 \\ 1/2 & 0 & 1/2 \\ 0 & 1/2 & 0 \end{bmatrix}, \begin{bmatrix} 1/2 & 0 & 1/2 \\ 1/2 & 0 & -1/2 \\ 0 & 1/2 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 1/2 & -1/2 \\ 0 & 1/2 & 1/2 \\ 1/2 & 0 & 0 \end{bmatrix},$$
$$\begin{bmatrix} 0 & 1/2 & 1/2 \\ 0 & -1/2 & 1/2 \\ 1/2 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 1/2 & -1/2 & 0 \\ 1/2 & 1/2 & 0 \\ 0 & 0 & 1/2 \end{bmatrix}, \begin{bmatrix} 1/2 & 1/2 & 0 \\ -1/2 & 1/2 & 0 \\ 0 & 0 & 1/2 \end{bmatrix},$$

such that $(\vec{a},\vec{b},\vec{c})_{pc} = (\vec{a},\vec{b},\vec{c})_{m,o}M$. The Miller indices transform by the same matrices such that $(h,k,l)_{pc} = (h,k,l)_{m,o}M$. The following reflection conditions exist for the Miller indices in the *Pbnm* space group: for 0*kl*, *k*=2*n* (where *n* is an integer); for *h*0*l*, *h*+*l*=2*n*; for *h*00, *h*=2*n*; for 0*k*0, *k*=2*n*; for 00*l*, *l*=2*n*. For the $P2_1/n$ space group, the 0*kl* condition is deleted, and all other conditions remain. When calculating the positions of systematic absences that are marked in Figure 5 of the main text, we transformed all allowed reflections for the *Pbnm* and $P2_1/n$ space groups to the pseudocubic coordinates using the above matrices.