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Advances in the Parameter Space Concept for Crystal Structure Determination – a maximum resolution study

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We present a study of the maximum resolution of the PSC. As an example, a split position of La and Sr with $(0, 0, z = 0.3584)$ has been investigated in the potential high-T super-conductor $\text{La}_{0.5}\text{Sr}_{1.5}\text{MnO}_4$, I_4/mmm . Due to the difference in scattering power of La and Sr, a pseudosymmetric structure solution exists for approximately interchanged z -positions. Depending on the relative error of diffraction intensities, we present respective resolution limits for the split position.

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