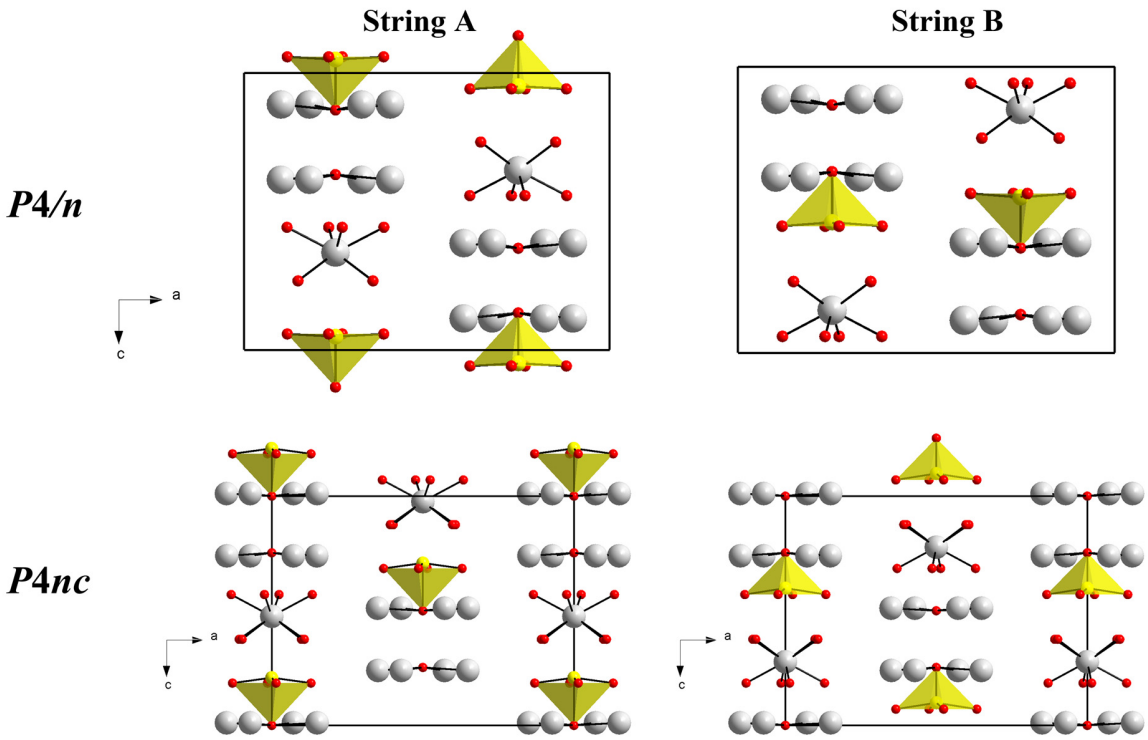

Figure S1. Depiction of the String A and String B arrangements in space groups *P*4/*n* and *P*4*nc*. The strings propagate along the fourfold axes at x = 1/4, y = 1/4, z and x = 3/4, y = 3/4, z in *P*4/*n*, and at the origin at x = 0, y = 0 , z and x = 1/2, y = 1/2, z in *P*4*nc*.

Additional details of test refinements of I and II for space group evaluation:

The first test refinements were performed in *P*4*nc*, where the atoms of String A and String B were identified and separated into two domains using the PART command in SHELX. For Compound **I**, free refinement of the string occupancies resulted in 61.8% and 38.2%, which is close to even distribution. The final R1 converged on 3.81% with a Flack parameter of 0.54(11), an indicator of either an inversion twin or a center of symmetry being present. The PLATON software suggested increasing to space group *P*4/*nnc*, and no twin law was identified. An inversion twin was applied with 53.7% as the majority domain contribution. This did not significantly improve the R1 value. With everything accounted for, the solution still had 7 nonpositive definite (NPD) atoms in *P*4*nc* (compared to zero NPD atoms in *P*4/*nnc*). The higher R values and poorer displacement parameters in *P*4*nc* suggest such an assignment incorrect for **I**. The same analysis was performed with **II**, which had 56% and 44% string occupancies and a resulting R1 of 5.12%. With the Flack parameter of 0.477(28), PLATON was used once more, which found no twin law and again suggested *P*4/*nnc* higher symmetry. The applied inversion twin had almost 50% distribution for each domain, but there remained 33 NPD atoms in this solution. For both compounds, *P*4*nc* was insufficient to model the diffraction data.

The second test refinements were performed in space group *P*4/*n*, with the same method used to identify the string atoms and determine the string occupancies. For Compound **I**, the string occupancies refined to 61.2% and 38.8% respectively, similar to refinement in *P*4*nc*; the final R1 converged on 4.44%. The F_o^2 values were significantly higher than the F_c^2 values, which are an indicator of incorrect space group or that a twin domain is not accounted for. PLATON did not find any applicable twin law that may bring the F^2 values into better agreement, and suggested increasing symmetry to *P*4/*nnc*. There were no remaining NPD atoms, but the discrepancy in the

F_o^2 and F_c^2 combined with the 1% better R1 value in *P*4*/nnc* suggest the higher symmetry space group is correct. For Compound **II**, the string distribution was approximately 50%, indicating no preference for long range ordering. The final R1 converged at 5.74%, with similar problems between the F^2 values. Since no twin law was found, no inversion twin could be applied, and 7 atoms remained NPD after refinement, *P*4*/n* was similarly ruled out for **II**. After comparison of the glide plane violating reflections and test refinements in lower symmetries, it was found that the *P*4*/nnc* model best described the diffraction data of both compounds.