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Crystal structure of \mathbf{Rb}_4\mathbf{C}_{60} under pressure¹ ASHFIA HUQ, Oak Ridge National Laboratory, PETER W. STEPHENS, Stony Brook University — We show that $\mathbf{Rb}_4\mathbf{C}_{60}$ transforms from its orientationally disordered tetragonal structure at ambient pressure to an orthorhombic phase in the neighborhood of 0.4 GPa. Lattice parameters, interfullerene distances, and closest Rb-C distances evolve continuously up to 2.2 GPa. Rietveld refinements establish that the high pressure phase is isostructural to $\mathbf{Cs}_4\mathbf{C}_{60}$. The previously observed conducting phase at 0.8 GPa is therefore structurally distinct from the ambient pressure insulator.

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> Ashfia Huq Oak Ridge National Laboratory

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