Supplementary Material:

Pressure-induced structural changes and insulator-metal transition in layered bismuth triiodide, BiI₃: A combined experimental and theoretical study

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In figure S1, we have shown the variation of total energy of BiI₃ as a function of k-mesh. We have used Monkhorst-Pack k-mesh in our calculations. The plot in figure S1 shows that with 9×9×9 mesh of k-points, we indeed achieved convergence in total energy.

In figure S2, we have shown the evolution of the fractional coordinates (z component only) of two I atoms (each atom from two adjacent I planes as marked with red arrows in the unit cell) with pressure.
Figure S1. Variation of total energy of BiI$_3$ with Monkhorst-Pack k-mesh.

Figure S2. Evolution of fractional coordinates (z-component) of two of the six I atoms (indicated with red arrows in the unit cell of BiI$_3$) with pressure.