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Pentahexoctite: A New Two-dimensional Allotrope of Carbon AADITYA MANJANATH, Centre for Nano Science and Engineering/Materials Research Centre, Indian Institute of Science, BABU RAM SHARMA, ABHISHEK K. SINGH, Materials Research Centre, Indian Institute of Science — Structures with carbon atoms can be arranged in various shapes (polygons) that exhibit unique properties. This has spawned search in exploring such newer allotropes across dimensions. Although research has been extensive in bulk graphitic structures, there are several 2D allotropes that are yet to be unearthed. Here, we report a new allotrope consisting of 5-6-8 rings of carbon atoms, named as "pentahexoctite." This sp^2 hybridized 2D allotrope has mechanical strength comparable to graphene. Electronically, the sheet is metallic with direction-dependent flat and dispersive bands at the Fermi level. It serves as a precursor for a stable 1D nanotubes with chirality-dependent electronic and mechanical properties. With these unique properties, the pentahexoctite sheet is another exciting addition to the family of robust novel 2D allotropes of carbon.

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