Alkylation of 1,3,5-Tribromobenzene by Cycloheptyl Bromide via Suzuki Coupling Reaction

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Carbon has several known allotropes, graphite, diamond, amorphous; there are also cylindrical nanotubes and spherical fullerenes. Scientists are trying to make another hypothetical allotrope that is called schwarzite, a 3d porous material made out of carbon heptagons, which does not exist in nature. Scientists failed to make it similar to the preparation of nanotubes, fullerene, but there is hope to make Schwarzites through bottom up synthesis. When graphene planes are attached to each other they form graphene. When seven membered rings are incorporated in graphene structure, it starts curving and may form a 3d structure. Thus, it will require some hexagons in the graphene to be replaced with heptagons. For that reason cycloheptane needs to be combined in trimers; one of the molecules is 1,3,5-tricycloheptyl benzene. This molecule was prepared by Suzuki coupling reaction between 1,3,5 tribromobenzene and cycloheptane-boronic acid. Commercially available bromocycloheptane was converted into boronic acid via a Grignard reaction synthesis. For the Suzuki coupling reaction catalyzed by palladium, the following were tried: two different palladium catalysts, Pd(PPh3)3 and Pd(dppf)2CL; two different solvents, THF and DMFA; and three different bases, triethylamine, potassium carbonate, and dimethylformamide. After many trials it was found that potassium ethoxide and solvent THF works best. The product was purified and isolated by column chromatography and characterized by 1H and 13C NMR This compound was successfully prepared and it will be used as the precursor for making the building blocks for the construction of schwarzites. Research will be continued in constructing schwarzites using 1, 3, 5-tricycloheptyl benzene.

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