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Copper-catalyzed cross-coupling of 1-haloalkyl-*o*-carboranes with grignard reagents: An efficient route to monosubstituted o-carborane derivatives

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Carboranes, a class of three-dimensional relatives of benzene, having many applications in medicine as boron neutron capture therapy agents, in supramolecular design/materials as building blocks, and in coordination/organometallic chemistry as unique ligands, which have received growing interest. However, their unique structures make derivatization difficult, which results in a limited application scope. Thus, it is important and necessary to develop new methodologies for the functionalization of carboranes. It is obvious that a cross-coupling of 1-haloalkyl-*o*-carboranes with alkyl and aryl Grignard reagents would be an ideal methodology for the synthesis of cage C-monosubstituted o-carborane compounds. We initially investigated the reaction conditions using 1-(2-bromoethyl)-o-carborane and n-BuMgBr as model substrates. The optimal conditions for the Cu-catalyzed synthesis of mono-substituted o-carboranes are as follows: 20 mol% $CuCl_2$ as the catalyst, 40 mol% PCy_3 as the ligand, 2.0 equiv. of Grignard reagents as the coupling partners of 1-haloalkyl-*o*-carboranes, and the reactions were performed at 25°C under N_2. After having optimized the model reaction, we were interested in extending the scope of the coupling reaction, and various *o*-carborane derivatives were prepared in good to excellent yields by using this copper-based procedure. The present copper-catalyzed protocol can be successfully used for the gram scale synthesis of 1-(*n*-hexyl)-*o*-carborane without an apparent decrease in the yield (4.0 g of product, 87.5% yield). The wide substrate scope makes this copper-based strategy remarkably practical for the synthesis of functional boron cluster compounds. We believe this general method will attract much attention and have broad applications in academic and industrial research.

Biography

Ju-You Lu has received his BS degree in Chemistry from Hunan University, China, in the year 2008 and PhD in Organic Chemistry from Tsinghua University, China, in the year 2013. He then worked as an Assistant Professor of Organic Chemistry at Xi'an Modern Chemistry Research Institute (MCRI), and joined the research group of Professor Jian Lu. He has been an Associate Professor at State Key Laboratory of Fluorine & Nitrogen Chemicals, MCRI, since 2016. His current research interests include the synthesis of functionalized carborane derivatives. He has contributed more than 20 peer-reviewed publications.

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