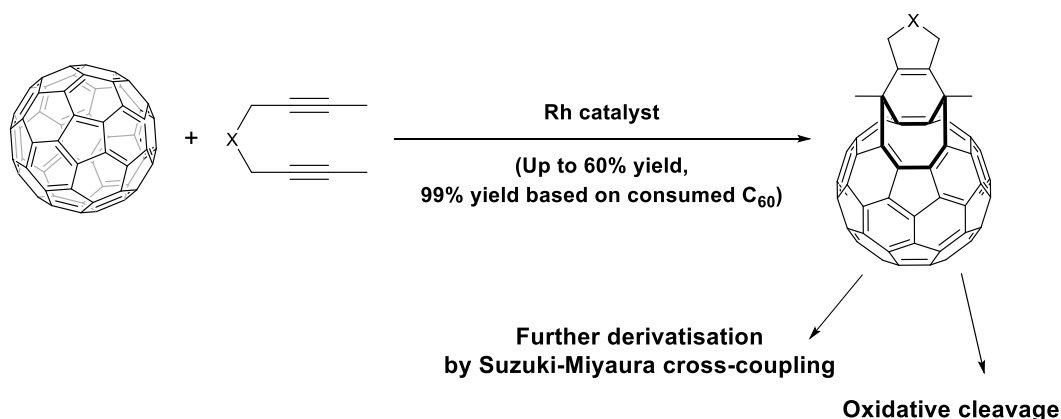


SYNTHESIS OF OPEN-CAGE FULLERENE DERIVATIVES BY RHODIUM(I)-CATALYZED [2+2+2] CYCLOADDITION OF C₆₀ AND DIYNES

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Since the discovery of C₆₀ in 1985 [1], fullerenes have attracted the attention of chemists due to their unique structure, properties and reactivity, along with their potential applications in a variety of fields ranging from materials science to biomedicine [2–5]. Many functionalized fullerene derivatives resulting from the structural modification of the fullerene cage have been reported over the last 30 years. Specifically, fullerene derivatives resulting from cycloaddition reactions involving [6,6] junctions of C₆₀ have been reported [6]. The preparation of cyclohexadiene-fused C₆₀ derivatives can be achieved by [2+2+2] cycloaddition reactions of C₆₀ with alkynes [7–9]. These compounds have been found to be important intermediates in the synthesis of so-called open-cage fullerenes [10]. Here, we report the first example of [2+2+2] cycloaddition involving C₆₀ and diynes under catalytic conditions promoted by a rhodium(I) catalyst, which leads to the formation of a series of open-cage bisfulleroids. The products obtained can be subjected to oxidative cleavage when exposed to light and O₂. Additionally, further derivatisation by Suzuki-Miyaura cross-coupling reaction has also been achieved. The mechanism of the process has been studied by means of DFT calculations [11].



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