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Title: Pd(II)-Catalyzed Directing-Group-Aided C-H Arylation and Alkylation of Pyrene Core: Synthesis of C1,C2- and C1,C10-Disubstituted Pyrene Motifs Authors: Dalal, Arup (/jspui/browse?type=author&value=Dalal%2C+Arup) Babu, Srinivasarao Arulananda (/jspui/browse? type=author&value=Babu%2C+Srinivasarao+Arulananda) Keywords: palladium - pyrene C-H arylation/alkylation Issue Date: 2021 Publisher: Thieme Citation: Synthesis, 53(18), 3307-3324. Abstract: We report the application of the Pd(II)-catalyzed, directing-group-aided C-H arylation/alkylation tactics to functionalize the pyrene core, especially, the relatively inaccessible C2 and K-region C10 positions of the pyrene core and augmentation of the library of pyrene derivatives with C1,C2- and C1,C10-disubstituted pyrene motifs. The Pd(II)-catalyzed β-C-H arylation/alkylation of the C2-position of pyrene-1-carboxamide possessing an 8-aminoquinoline directing group yielded various C1,C2-disubstituted pyrenes. Similarly, the Pd(II)-catalyzed selective γ-C-H arylation/alkylation of the C10-position of N-(pyren-1-yl)picolinamide, possessing a picolinamide directing group, yielded various C1,C10-disubstituted pyrenes. Examples of C(9)-H arylation of pyrene-1-carboxamide and the removal of the directing group after the C–H arylation/alkylation reactions were also shown. The structures of representative pyrene derivatives were confirmed by the X-ray structure analysis. Given the importance of the pyrene derivatives in various fields of chemical sciences, this report is a contribution towards augmentation of the library of pyrene derivatives with C1,C2- and C1,C10-disubstituted pyrene amide motifs.

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