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Title:	Bu4NI-Catalyzed, Radical-Induced Regioselective N-Alkylations and Arylations of Tetrazoles Using Organic Peroxides/Peresters
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Abstract:	Bu4NI-catalyzed regioselective N2-methylation, N2-alkylation, and N2-arylation of tetrazoles have been achieved using tert-butyl hydroperoxide (TBHP) as the methyl source, alkyl diacyl peroxides as the primary alkyl source, alkyl peresters as the secondary and tertiary alkyl sources, and aryl diacyl peroxides as the arylating source. These reactions proceed without pre-functionalization of tetrazole and in the absence of any metal catalysts. Here, peroxides serve the dual role of oxidants as well as alkylating or arylating agents. Based on DFT calculations, it was found that spin density, transition-state barriers (kinetic control), and thermodynamic stability of the products (thermodynamic control) play essential roles in the observed regioselectivity during N-alkylation. This radical-mediated process is amenable to a broad range of substrates and provides products in moderate to good yields.
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