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Title: Computational and Matrix Isolation Studies of Heterocyclic Radicals and Azoheteroarene Photoswitches

Authors: Sah, Chitranjan

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Abstract:

Free radicals are regarded as one of the important classes of highly reactive, short-lived intermediates containing an unpaired electron. The utility of these free radicals has been proposed by experimentalists and theoreticians in the field of organic synthesis, combustion chemistry, atmospheric chemistry, interstellar chemistry, and biological implications. Several approaches such as conjugation, spin delocalization, and introduction of heteroatoms have been adapted to enhance the stability as well as tuning the reactivity of radicals. In recent times, nitrogen-based heterocyclic radicals have gained immense importance for their various roles in reactive oxygen species (ROS), material chemistry, biofuels, and in constructing organic molecular-based magnets. Among the various heterocyclic radicals studied thus far, all of the radicals potentially resulted in two center-three electrons (2c-3e) interactions except for boryl and cyclopentadienyl radicals as shown in Scheme A.1.

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