Electronic structure of five membered heterocyclic radicals – A computational study

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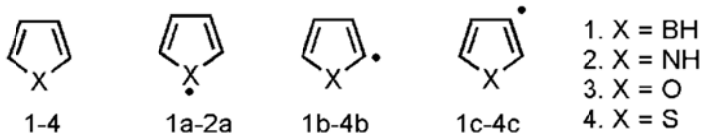
Abstract

Free radicals are one of the very important classes of reactive intermediates and are highly transient. They play an inevitable role in organic synthesis, polymer chemistry, atmospheric chemistry and biochemistry.[1] For instance, several radical based reactions such as photoredox catalysis, radical addition and radical cyclization are of great importance in field of organic synthesis.[2] Equally they play a vital role in biological processes like ageing. Not only the parent radical, but also many of their heteroatom rich ring opening products and fragments are equally interesting in the astrochemical point of view.

In our lab, we are currently focussing on heterocyclic radicals as they constitute the main building blocks of many biological systems (like nucleobases, aminoacids, etc) and biologically active drug molecules.[3] In a fundamental point of view, understanding the effect of heteroatoms in stability and reactivity of heterocyclic radicals is very interesting. Although experimental and theoretical studies have been reported on many heterocyclic radicals, the interaction between lone pair and the radical electron is not given proper attention.[4-5] Through this contribution, we present the computational studies on mono heteroatom containing five member heterocyclic radicals such as pyrrole, furan, thiophene, and borole radicals (**Scheme 1**). All the isomeric radicals of them have been considered. The primary focus has been given to the interaction between the lone pair(s) of the heteroatoms and the radical electron. A preliminary computational studies on these systems will be presented through this contribution.



Scheme 1. Parent heterocycles and the corresponding dehydro-borole, pyrrole, furan and thiophene radicals

References and Notes:

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