

Spin-Flip Characterization of Furan Diradical Isomers
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Alternative sources of energy containing high percentages of heteroaromatic compounds can produce diradicals under combustion conditions, which is also true for the combustion of tobacco products. Regardless of their source, diradical combustion products are difficult to characterize experimentally due to their short lifetimes. Understanding the electronic structure of these species from a theoretical perspective would therefore provide a better understanding of their potential carcinogenic effects, which is critical to both moving safely from a fossil-fuel economy towards a renewable one and reducing preventable cancers caused by smoking. Towards this end, we characterize here the structures and energetics for the diradical isomers of furan using the spin-flip formulation of the equation-of-motion coupled cluster method with single and double substitutions (SF-EOM-CCSD) with Q-Chem. To better understand the stabilizing effects of through-bond and through-space coupling we also examined the natural orbitals for these systems, which demonstrate that through-bond and through-space coupling of radical centers is a source of stability for these species. Furthermore, we have also characterized the presence of aromaticity in these diradicals via nuclear-independent chemical shift (NICS) analysis, which we have performed using Gaussian16.