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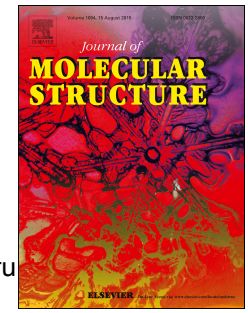

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ACCEPTED MANUSCRIPT

Computational study on fused five membered heterocyclic compounds containing tertiary oxygen

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ABSTRACT

The structure, stability and electronic properties of two fused five membered heterocyclic compounds containing tertiary oxygen have been investigated with quantum chemistry computation. The results show that 3*H*-4λ^3-furo[1,2-*a*]furan (M1) and 2a$^1\lambda^4$-oxacyclopenta[*cd*]pentalene (M2) both own three C-O bonds and especially in M2 the three C-O bonds and angles are approximately identical. The two compounds are comparatively stable and M2 with three pentacycles is more stable than compound M1 according to the C-O bond lengths, bond orders, Egap, electronegativity (χ), hardness (η), electrophilicity (ω), and aromaticity indexes. The aromaticity indexes such as NICS(0), NICS(1) and NICS(1)zz show that they both have strong aromaticity. The natural bonding orbital (NBO) analysis shows that oxygen atom takes hybrid orbitals composed of s and p orbital components to form σ(C-O) bonds in

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