AROMATIC STABILITY ENERGY STUDIES ON FIVE-MEMBERED HETEROCYCLIC C_4H_4M (M = O, S, Se, Te, NH, PH, AsH AND SbH): DFT CALCULATIONS

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UDC 539.19;547.72;547.73;547.74;547.76

Energetic, geometric and magnetic criteria were applied to examine the stability and/or aromatic character for the cyclic molecules **C_4H_4M** (M = O, S, Se, Te, NH, PH, AsH and SbH) at B3LYP/6-311++G** and MP2/6-311++G** levels of theory. The isodesmic reactions and nuclear independent chemical shifts (NICS) calculations were utilized to examine the molecules for energetic and magnetic criteria, respectively. The isodesmic reaction energies reveal that thiophene (**C_4H_4S**, –23.269 kcal/mol) and pyrrole (**C_4H_4NH**, –20.804 kcal/mol) have the greatest aromatic stabilization energies and tellurophene (**C_4H_4Te**, –15.114 kcal/mol) and stibole (**C_4H_4SbH**, –1.169 kcal/mol) have the lowest aromatic stabilization energies in their corresponding groups at MP2/6-311++G**. The NICS calculations confirmed the results obtained through isodesmic reaction energies.

Keywords: aromatic character; isodesmic reaction; NICS; five-membered heterocycle; C_4H_4M.