# On the role of heteroatoms in aromatic rings. Insights from 10? main group elements heterorings [(EH)2S2N4]Q (E = C, P, B, Si, Al and q = 0, -2)

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Inclusion of heteroatoms into a ring skeleton obtained unique electronic features, which differ from the respective isoelectronic organic counterparts, increasing the versatility of aromatic molecules. Herein, we evaluate the role of heteroatoms on the electronic and magnetic properties in a number of inorganic 10?-electron eight-member aromatic rings involving the isoelectronic [(EH)2S2N4]q (E = C, P, B, Si, Al) series using density functional methods. The inclusion of different heteroatoms with increasing electronegativity increased the aromatic behavior in relation to the representative 10?-electron [C8H8]2- organic ring. A deeper analysis on the magnetic response to an applied magnetic field, in terms of individual ?-orbitals contributions, revealed that the differentiation in aromaticity originates from orbitals with major contributions from pz of heteroatom E, whereas the diatropic contributions that arise from the S2N4 core remained similar throughout the series. Therefore, the effect of including a certain type of heteroatom can be addressed in terms of the variation and contribution of each individual ?-orbital, starting from the respective organic counterpart, which appears to be a convenient approach. The similar ?-aromatic character observed suggests the proposed hypothetical rings are feasible structures to explore synthetically. The less aromatic counterpart given by the Al counterpart should lead to a less stable ring in this series. 