

# Spin-orbit effects on magnetically induced current densities in the M<sub>5</sub>

(M=N,P,As,Sb,Bi,Mc) clusters

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This study reports the spin-orbit effects on the aromaticity of the N-5, P-5, As-5, Sb-5, Bi-5, and Mc-5 anionic clusters via the magnetically induced current-density method. All-electron density functional theory (DFT) calculations were carried out using the four-component Dirac-Coulomb (DC) hamiltonian, including scalar and spin-orbit relativistic effects. The magnetic index of aromaticity was calculated by numerical integration over the current flow between two atoms in the pentagonal ring. These values were compared to the spin-free values (spin-orbit coupling switched off), in order to assess the spin-orbit effect on aromaticity. It was found that in the heavy anions, Bi-5, and Mc-5, there is a significant influence of the spin-orbit coupling. © 2018 Wiley Periodicals, Inc. © 2018

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