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Ring currents in *peri*odo-hydrocarbons

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A well-known example of doubly aromatic molecule is the hexaiodobenzene dication, $[C_6I_6]^{2+}$. Both, π-electrons in the benzene ring and σ-electrons in the outer ring formed by iodine atoms, induce diatropic currents (Fig. 1). In this work, the magnetically induced current densities were calculated for a series of *peri*odohydrocarbons. The current densities computed by means of the diamagnetic-zero variant of the continuous transformation of the origin of the current density (CTOCD-DZ) method were found to be a powerful tool for both qualitative and quantitative assessment of double aromaticity. The magnetic aspects of the double aromaticity were further compared with electronic aromaticity indices.

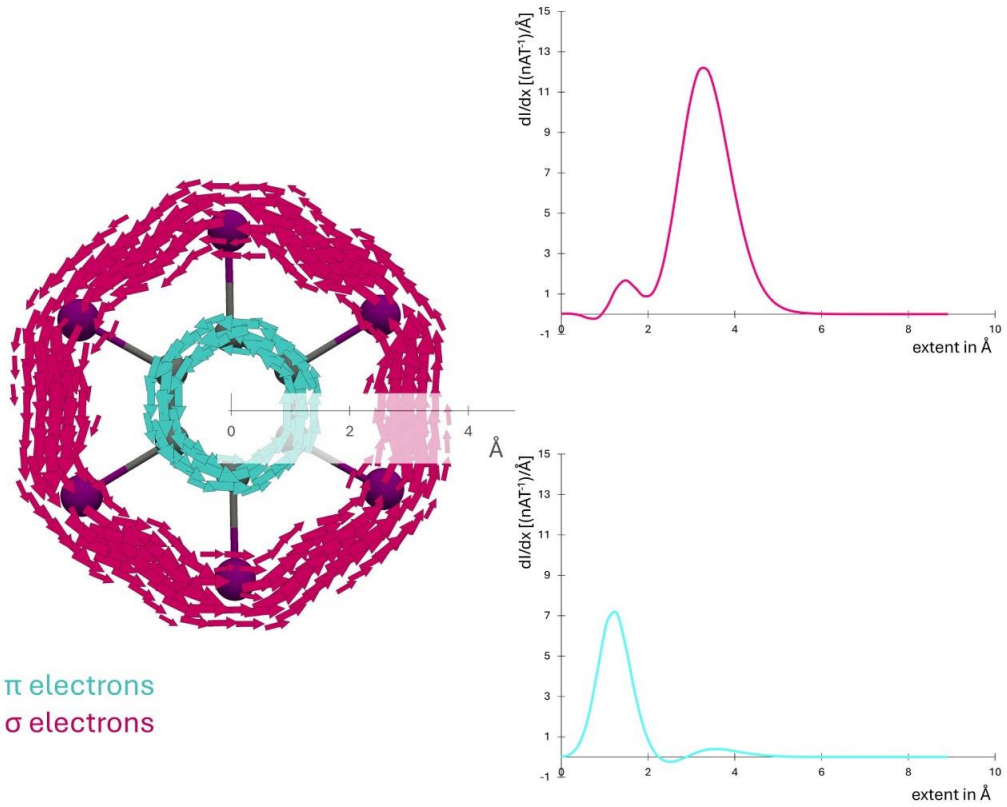

Figure 1. Map and bond current strength profiles of π (blue) and σ (red) current densities in $[C_6I_6]^{2+}$.