Electronic Supporting Information (ESI): Electronic Transport in Antiaromatic Molecules

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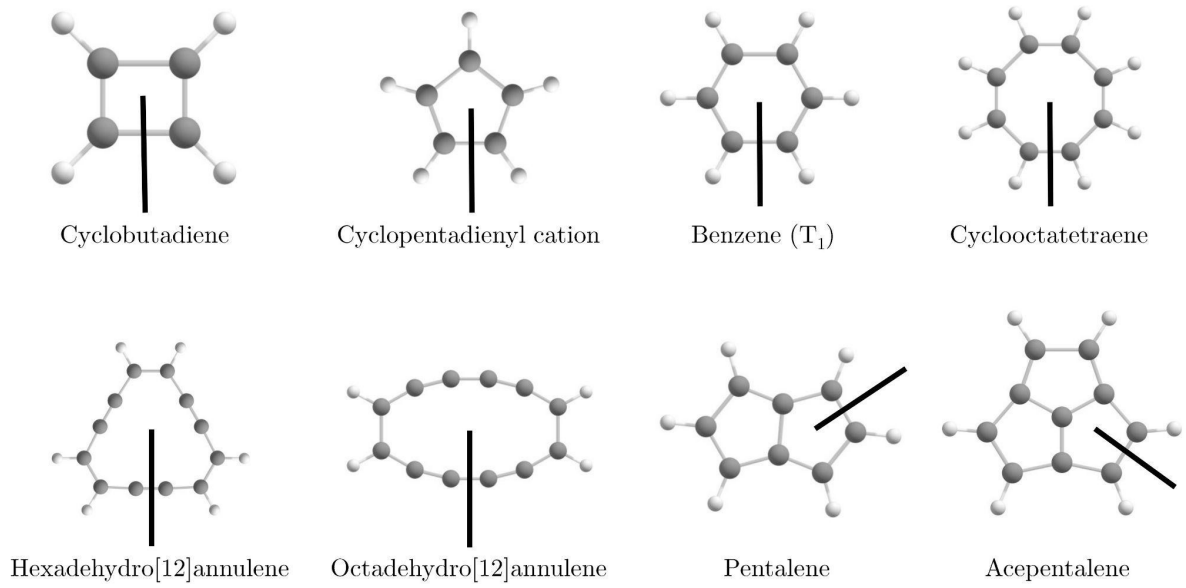

Figure S1. Integration planes used for GIMIC calculations across the studied molecular series. These planes were extended 8 Bohr above and below the molecular plane. Integration across these planes yields the net ring-current strength.

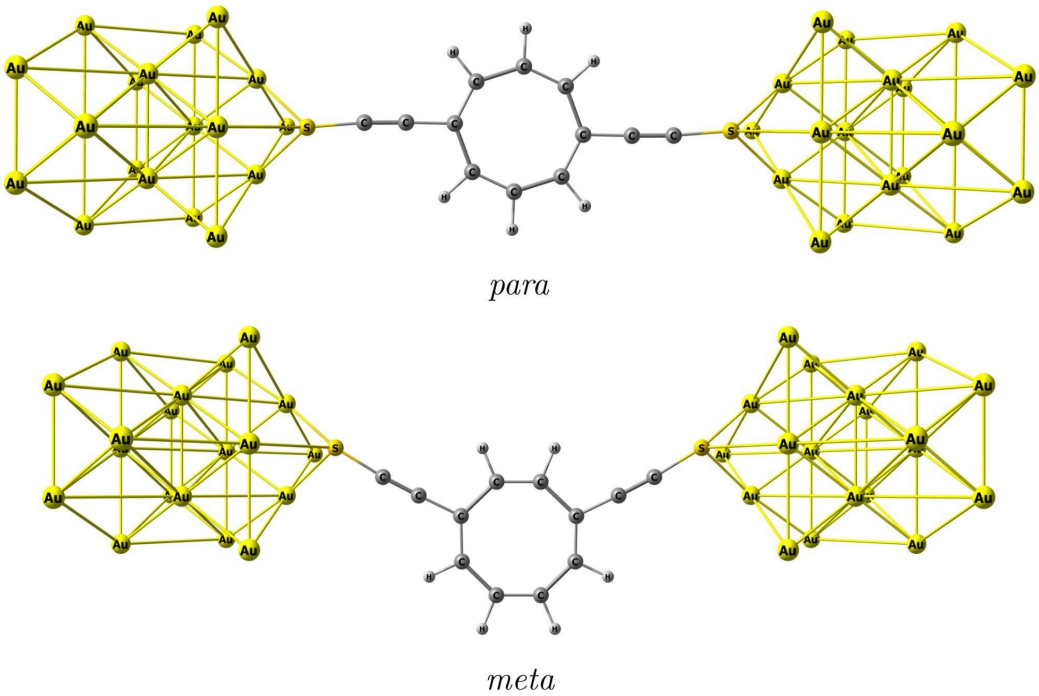

Figure S2. Schematic representation of the molecular junction construction (for COT) and the computational models used for transport analysis. Representative simplified model as shown in the transmission plots (Figure 4), where the electrodes are truncated at the sulfur atoms for visual clarity, while the electronic effect of the clusters is implicitly included in the NEGF-DFT formalism.

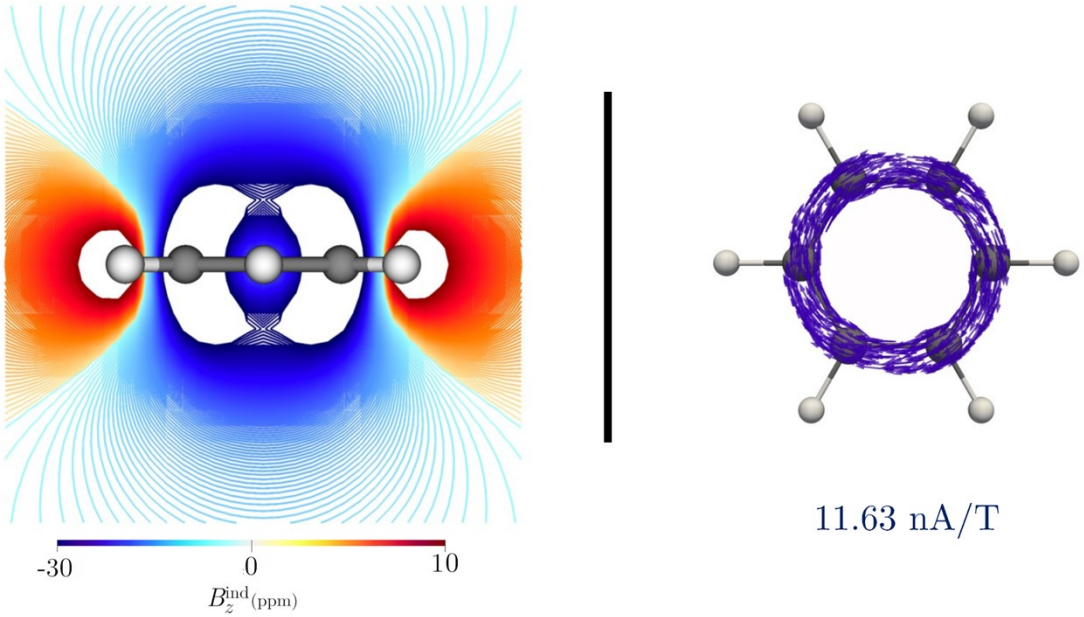

Figure S3. In the left panel: $B^{\mathrm{ind}}{}_z$ isolines for benzene in its ground state plotted in a transversal plane showing its shielding cone (negative values < -30 ppm). Surrounded white areas represent $B^{\mathrm{ind}}{}_z$ values that are out of scale. In the right panel: $\mathbf{J}^{\mathrm{ind}}$ map with its ring-current strength indicated.

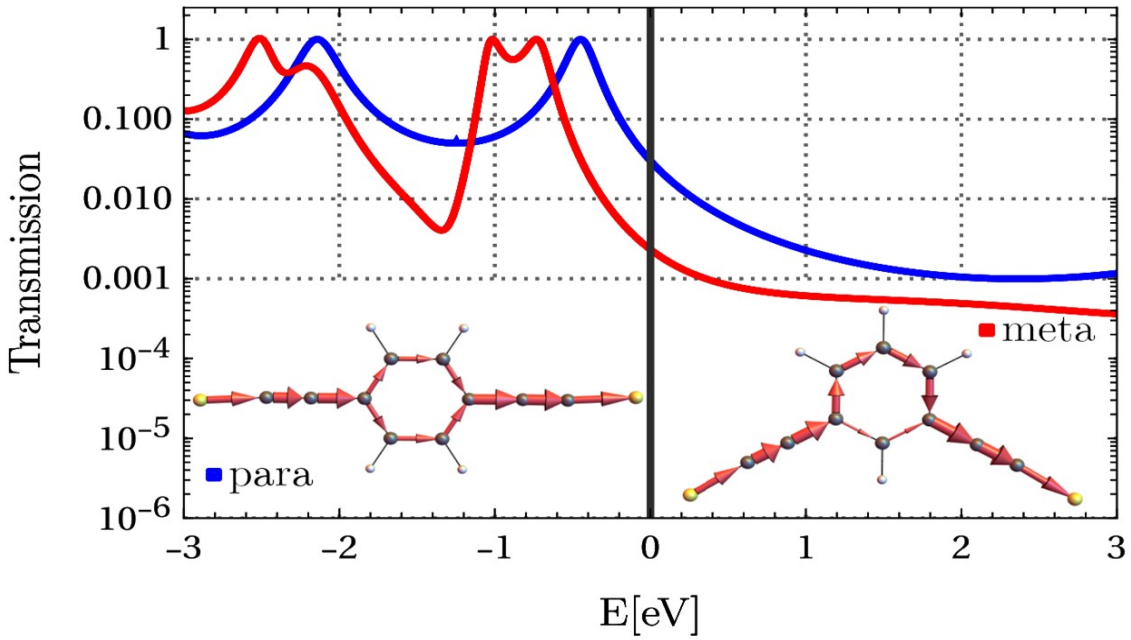

Figure S4. NEGF-DFT transmission spectra calculated for benzene in its ground state, using the different type connections to gold electrodes. Local current flow is also displayed with red arrows on molecules. The plots show electron transmission as a function of energy relative to the Fermi level (E = 0 eV) displayed with a vertical line.

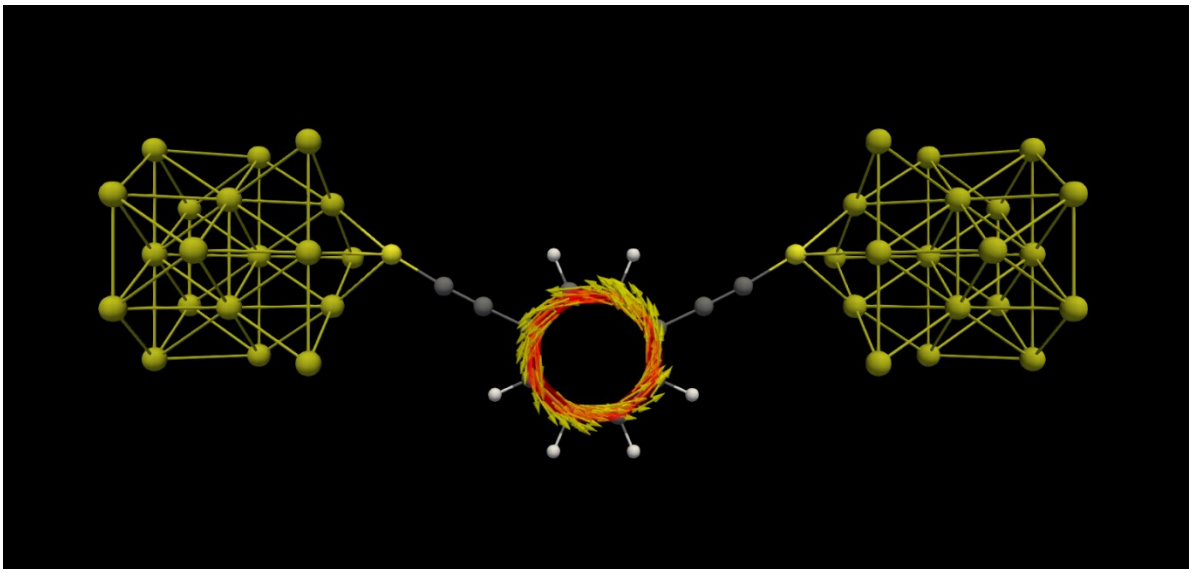

Figure S5. J^{ind} maps for *meta* configuration of COT including ethynyl-thiolate linkers and Au_{19} clusters. The persistent and strong paratropic ring current is maintained despite the connections.