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Metalation of Expanded Porphyrins: A Chemical Trigger Used To Produce Molecular Twisting and Möbius Aromaticity

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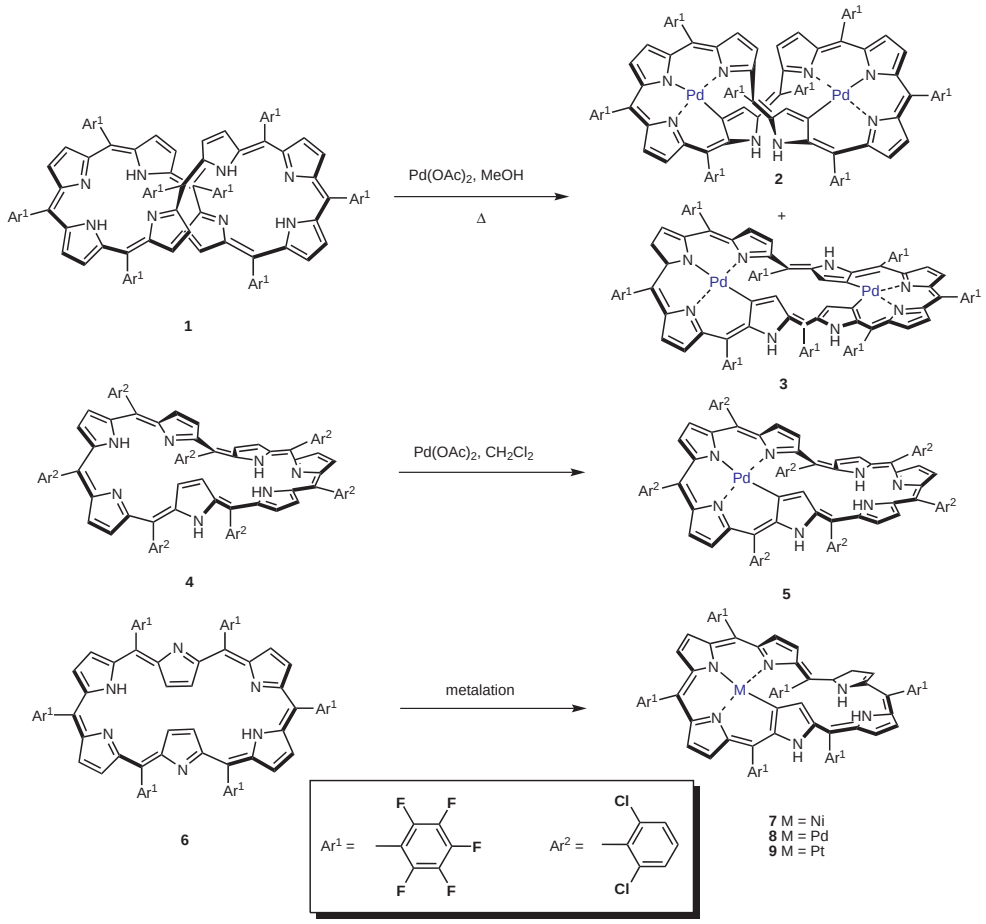
Metalation-Triggered Möbius Aromaticity



Significance: A new way to achieve complexes that exhibit Möbius aromaticity is described. Conjugated oligopyrrolic macrocycles (also known as expanded porphyrins) were locked into a twisted Möbius strip conformation using group 10 metals. Experimental and numerical studies reveal compounds **3**, **5**, and **7**–**9** as conformationally locked Möbius aromatic molecules.

Comment: Structures and aromaticity were confirmed via XRD (**2**, **3**, **5**), ^{1}H-NMR and UV/Vis. Significantly negative values of calculated NICS (Nucleus-Independent Chemical Shift) supported Möbius-type aromaticity for **3**, **5**, and **7**–**9**. A new method for the quantitative analysis of aromaticity based on the measurement of the TPA (two-photon absorption) cross-section ($\sigma^{(2)}$) by the open-aperture Z-scan method showed consistent results.

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