

Metallophilicity Under Confinement: The Iminopyrrole Cage Promoting the $\text{Hg}^{\text{II}}\cdots\text{M}^{\text{II}}$ ($\text{M} = \text{Hg}, \text{Cd}$) Interactions

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Self-assembly of 2,5-diformylpyrrole, tris(2-aminoethyl)amine, and $\text{Cd}(\text{II})$ or $\text{Hg}(\text{II})$ affords homobimetallic cryptates. In contrast, the synthesis of heterobimetallic $\text{Zn}(\text{II})\text{--}\text{Cd}(\text{II})$ and $\text{Cd}(\text{II})\text{--}\text{Hg}(\text{II})$ cages requires a stepwise approach involving a monocadmium(II) precursor. The bis-mercury(II) cryptate exhibits a pronounced mercurophilic interaction, as evidenced by a short $\text{Hg}\cdots\text{Hg}$ separation of 3.0549(7) Å. Notably, a similarly close intracavity contact is observed for the $\text{Cd}(\text{II})\text{--}\text{Hg}(\text{II})$ system, with a $\text{M}\cdots\text{M}$ distance of ca. 3.1 Å. The participation of the metal centers in the attractive interaction—enforced by confinement within the iminopyrrole cage—was verified through the density functional theory (DFT) calculations of bond indices and was further corroborated by QTAIM analysis.

Słowa kluczowe

Ethers, Macrocyclic compounds, Metal clusters, Metals, Self organization

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