

Basicity of bisperhalophenyl aurates toward closed-shell metal ions:

Metallophilicity and additional interactions

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The interaction of bisperhalophenyl aurates $[\text{AuR}_2]^-$ ($\text{R} = \text{C}_6\text{F}_5$, $\text{C}_6\text{F}_3\text{Cl}_2$, and C_6Cl_5) with the closed-shell Ag^+ , Cu^+ , and Tl^+ ions has been studied theoretically and compared with the experimentally known X-ray diffraction crystal structures. Initially, the aurates have been fully optimized at MP2 level of theory in a D_{2h} symmetry. The analysis of the basicity of the three aurates $[\text{AuR}_2]^-$ ($\text{R} = \text{C}_6\text{F}_5$, $\text{C}_6\text{F}_3\text{Cl}_2$ and C_6Cl_5) against Ag^+ ions in a C_{2v} symmetry has been calculated in point-by-point bsse-corrected interaction energy analysis at HF and MP2 levels of theory. Taking into account the experimental observation of additional interactions between the heterometals and Cipro atoms at the perhalophenyl rings or halogen atoms at the ortho position of the perhalophenyl rings, dinuclear models of the type $[\text{AuR}_2]^- \cdots \text{Ag}^+$ ($\text{R} = \text{C}_6\text{Cl}_5$, and C_6F_5); $[\text{AuR}_2]^- \cdots \text{Cu}^+$ ($\text{R} = \text{C}_6\text{F}_5$, and C_6Cl_5) and $[\text{AuR}_2]^- \cdots \text{Tl}^+$ ($\text{R} = \text{C}_6\text{F}_5$, and C_6Cl_5) with a C_{2v} , C_2 , and C_s symmetries have been optimized at DFT-B3LYP level. The in