

The nature of the Au-Rg bond in the $[\text{AuRg}_4]^{2+}$ (Rg=Ar, Kr and Xe) molecules.

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A topological analysis of the electron localisation function of the $[\text{AuRg}_4]^{2+}$ (Rg = Ar, Kr and Xe) molecules reveals the 'closed-shell' nature of the Au-Rg binding, which is dominated by electrostatic interactions. A similar finding is obtained by means of the AIM method where the Laplacian of the electron density computed for the bond critical point of the Au-Rg linkage is positive and decreases from 0.163 $[\text{AuAr}_4]^{2+}$ to 0.087 $[\text{AuXe}_4]^{2+}$. A charge separation according to the $\text{Au}^{+1.30}[\text{Ar}^{+0.18}]_4$, $\text{Au}^{+1.19}[\text{Kr}^{+0.20}]_4$ and $\text{Au}^{+0.29}[\text{Xe}^{+0.43}]_4$ formulas shows an increase of the positive charge on the rare-gas atom and accordingly decrease on the gold atom. The unpaired electron density is localised mainly on Au and the integrated spin density decreases from 0.28 e for $[\text{AuAr}_4]^{2+}$ to 0.16 e for $[\text{AuXe}_4]^{2+}$.

Adres publiczny

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