Aromatic character of [Au13]5+ and [MAu12]4+/6+ (M = Pd, Pt) cores in ligand protected gold nanoclusters-interplay between spherical and planar ?-aromatics

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The most characteristic feature of planar ?-aromatics is the ability to sustain a long-range shielding cone under a magnetic field oriented in a specific direction. In this article, we showed that similar magnetic responses can be found in ?-aromatic and spherical aromatic systems. For [Au13]5+, long-range characteristics of the induced magnetic field in the bare icosahedral core are revealed, which are also found in the ligand protected [Au25(SH)18]- model, proving its spherical aromatic properties, also supported by the AdNDP analysis. Such properties are given by the 8-ve of the structural core satisfying the Hirsch 2(N + 1)2 rule, which is also found in the isoelectronic [M@Au12]4+ core, a part of the [MAu24(SR)18]2- (M = Pd, Pt) cluster. This contrasts with the [M@Au12]6+ core in [MAu24(SR)18]0 (M = Pd, Pt), representing 6-ve superatoms, which exhibit characteristics of planar ?-aromatics. Our results support the spherical aromatic character of stable superatoms, whereas the 6-ve intermediate electron counts satisfy the 4N + 2 rule (applicable for both ?- and ?-aromatics), showing the reversable and controlled interplay between 3D spherical and 2D ?-aromatic clusters. © 2019 the Owner Societies.