Application of a planar superatom model on [Hg5(C(CF 3)2)]. Bonding and magnetic response considerations into a five-fold d10-d10 metal cycle

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Application of the planar superatom model to describe the electronic structure, and to gain insights into the stabilization of metal macrocycles supporting closed-shell d10-d10 interactions, is studied through analysis of the membered ring composed by Hg(ii) atoms, namely, [Hg(C(CF3)2)]5. Its electronic structure resembles the level sequence given for a planar jellium model, revealing an electronic configuration given by 1s2 1p4x,y 1d4xy,x2-y2. The analysis of the population of each level of the Hg5core, denotes a slight net bonding into the [Hg(C(CF3)2)]5 ring. However, stabilization is mainly supported by the balance given by a similar population of the jellium levels, which is suggested to be a different scheme for stabilizing d 10 macrocyclic clusters with metallophilic interactions, in the category of long d10-d10 contacts. The extension of the planar jellium model to the relativistic case, including spin-orbit coupling considering the D5h* point group, denotes the consequent splitting for levels with ? 0, namely, 1px,y and 1dxy,x 2-y2. In this framework, the electronic configuration is given by 1s1/22 1p3/22 1p 1/22 1d5/22 1d3/2 2, which contribute to the analysis of the electronic structure of planar clusters in terms of spin-orbit coupling, involving molecular spinors (j = ± s) instead of molecular orbitals (pure).