[As@Ni12@As20]3- and [Sn@Cu12@Sn20]12- clusters. Related structures with different construction philosophy

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[Sn@Cu12@Sn20]12- and [As@Ni12@As20]3- structures display highly spherical shapes according to A@B12@A20. Their analysis denote similar features in the electronic structure construction, however the resulting charge distribution exhibits large differences accounting for the different electronic requirements of such concentric structures. This leads to different electronic distribution in the overall system, where the composition of relevant electronic shells and charge distribution in the whole cluster is an important point to take into account in addition to well developed electron count rules. © 2015 Elsevier B.V. All rights reserved.