# Many-body effects on the structures and stability of Ba2+Xen (n=1-39, 54) clusters

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## Abstract

The structures and relative stabilities of mixed Ba2+ Xe-n (n = 1-39, 54) clusters have been theoretically studied using basin-hopping global optimization. Analytical potential energy surfaces were constructed from ab initio or experimental data, assuming either purely additive interactions or including many-body polarization effects and the mutual contribution of self-consistent induced dipoles. For both models the stable structures are characterized by the barium cation being coated by a shell of xenon atoms, as expected from simple energetic arguments. Icosahedral packing is dominantly found, the exceptional stability of the icosahedral motif at n = 12 being further manifested at the size n = 32 where the basic icosahedron is surrounded by a dodecahedral cage, and at n = 54 where the transition to multilayer Mackay icosahedra has occurred. Interactions between induced dipoles generally tend to decrease the Xe-Xe binding, leading to different solvation patterns at small sizes but also favoring polyicosahedral growth. Besides attenuating relative energetic stability, many-body effects affect the structures by expanding the clusters by a few percents and allowing them to deform more. (C) 2014 AIP Publishing LLC.

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