Supplemental Information

Atomic Gold Ions Clustered with Noble Gases: Helium, Neon, Argon, Krypton, and Xenon

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Fig. S1
Two-body potential energy curves derived from CCSD(T)/def2-TZVPP calculations for interactions between noble gas atoms (top panel) and between a gold cation and noble gas atom (low panel). The positions of the energy minima are highlighted by gray lines that help guide the eye.

Fig. S2
Time average of the radial density function (blue) and the cumulative number of solvent atoms versus distance from the ion (red) for He110Au+

Fig. S3
Time average of the radial density function (blue) and the cumulative number of solvent atoms versus distance from the ion (red) for Ar108Au+

Fig. S4
Dissociation energies of HeₙAu⁺ and ArₙAu⁺ clusters for the removal of the nᵗʰ rare gas atom. Selected magic numbers are highlighted and their structures are visualized in Fig. S5.

Fig. S5
Structures of select magic numbers observed in the calculated structures. The HeₙAu⁺ ions follow icosahedral symmetries and the ArₙAu⁺ systems have octahedral symmetries.
Fig. S2

Fig. S3

Fig. S4
Fig. S5