

Supporting Information

Size-dependent stability toward dissociation and ligand binding energies of phosphine-ligated gold cluster ions

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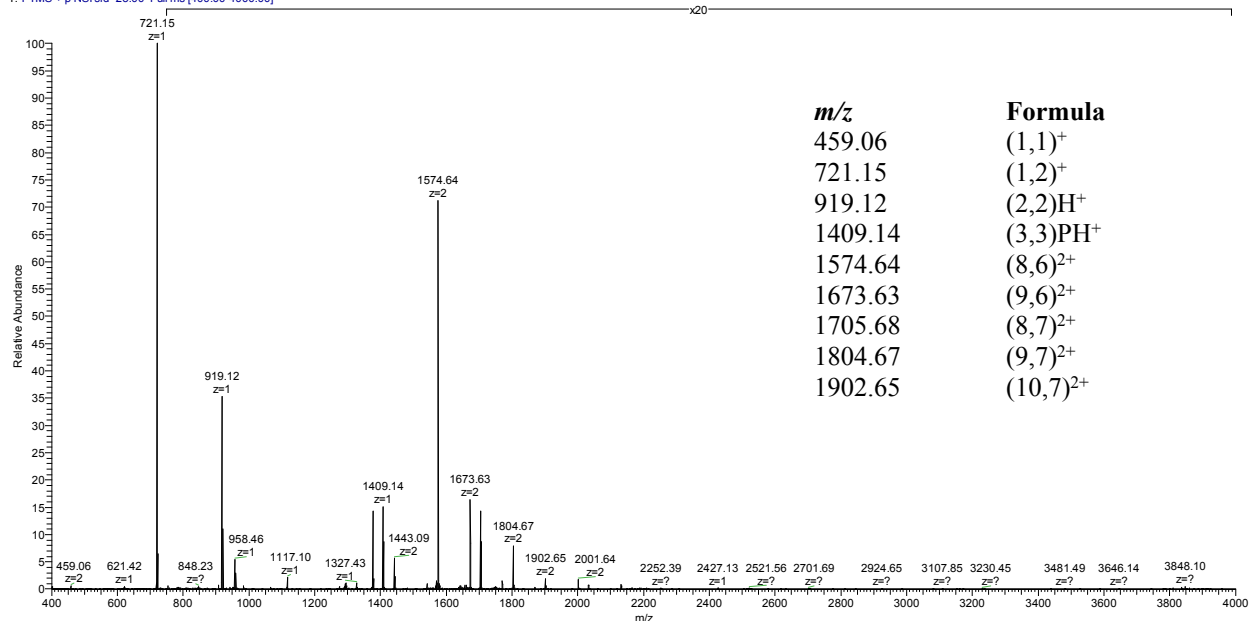


Figure S1. A typical positive mode ESI mass spectrum of subnanometer TPP-ligated gold clusters synthesized in methanol containing 0.2 μ M borane *tert*-butylamine reducing agent.

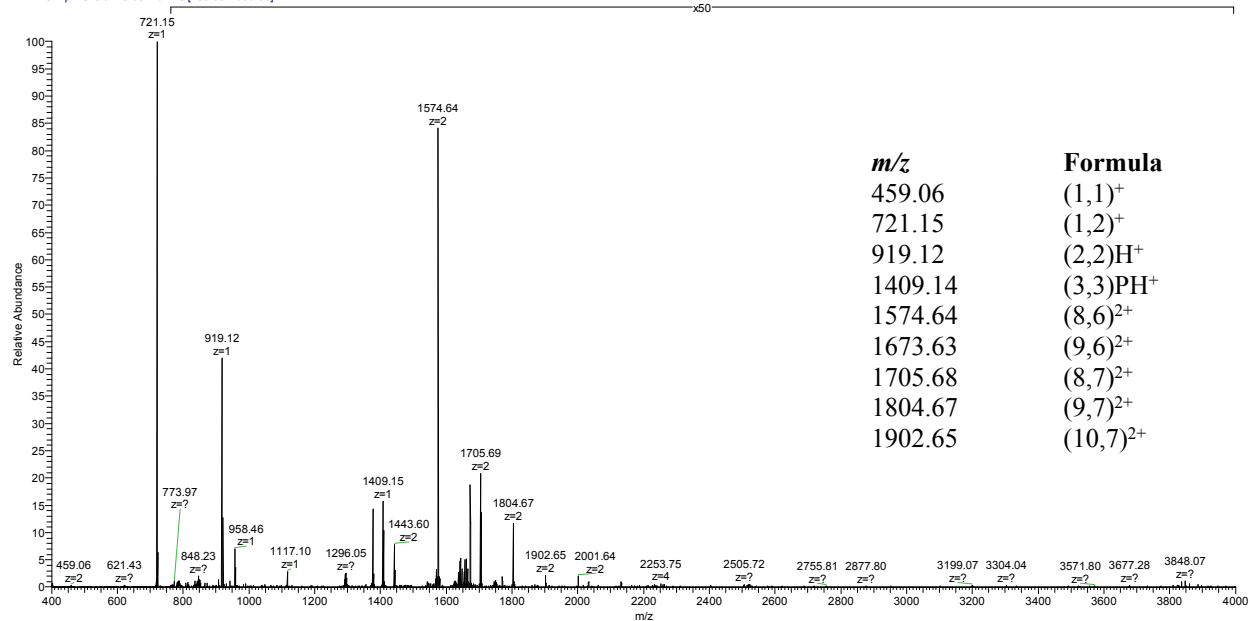


Figure S2. A typical positive mode ESI mass spectrum of subnanometer TPP-ligated gold clusters synthesized in methanol containing 0.5 μ M borane *tert*-butylamine reducing agent.

110813_AuPPh3_BTBA_8 #87-328 RT: 2.62-9.66 AV: 242 NL: 6.38E6
T: FTMS + p NSI Full ms [400.00-4000.00]

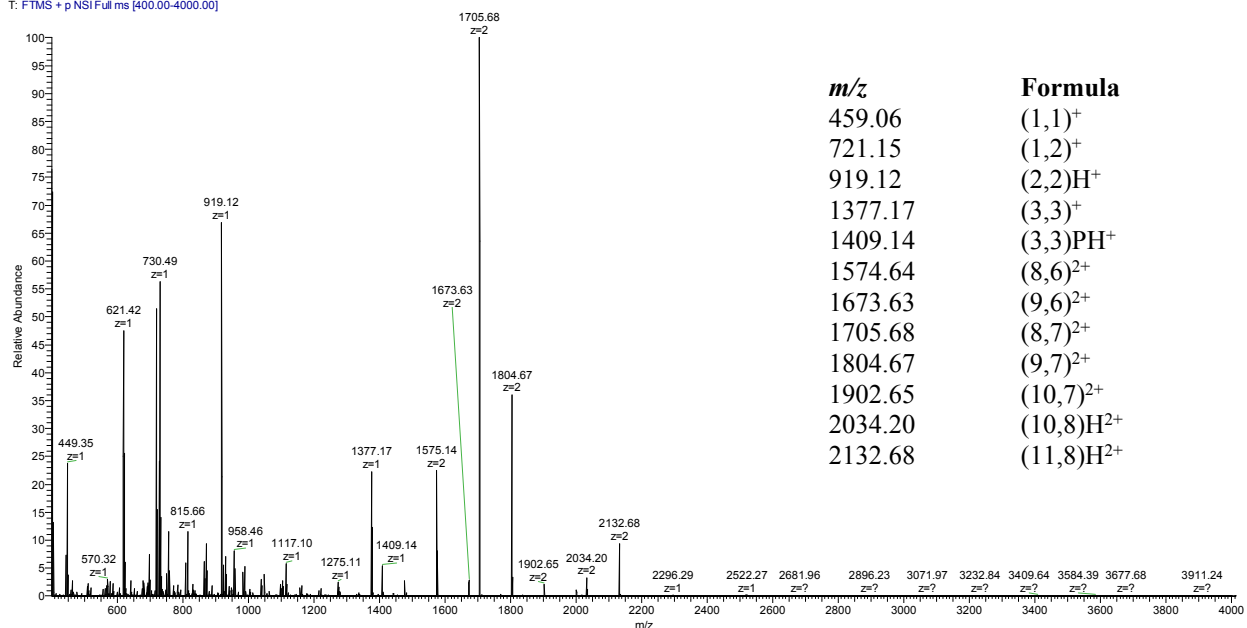


Figure S3. A typical positive mode ESI mass spectrum of subnanometer TPP-ligated gold clusters synthesized in methanol containing 1.0 μ M borane *tert*-butylamine reducing agent.

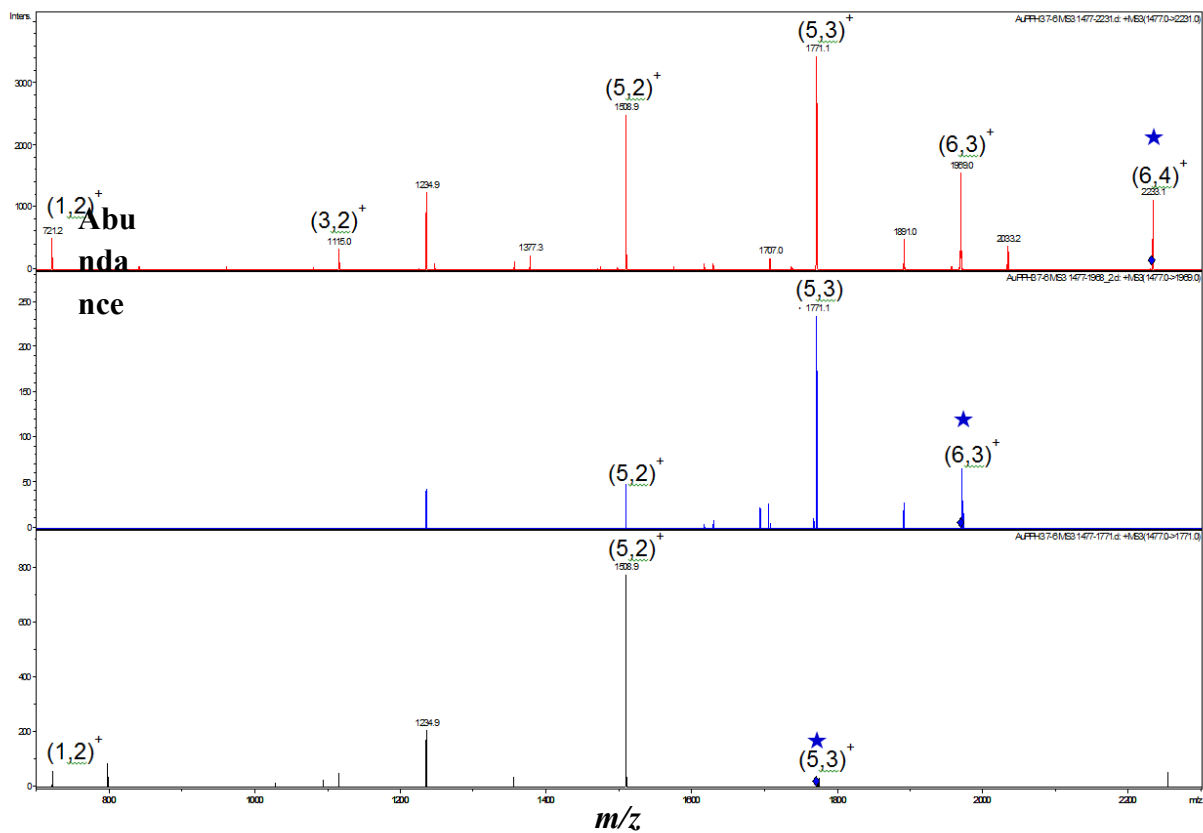


Figure S4. MS³ spectra of $(6,4)^+$, $(6,3)^+$ and $(5,3)^+$ product ions generated from the $(7,6)^{2+}$ precursor ion. The ions selected for dissociation are marked with a blue star.

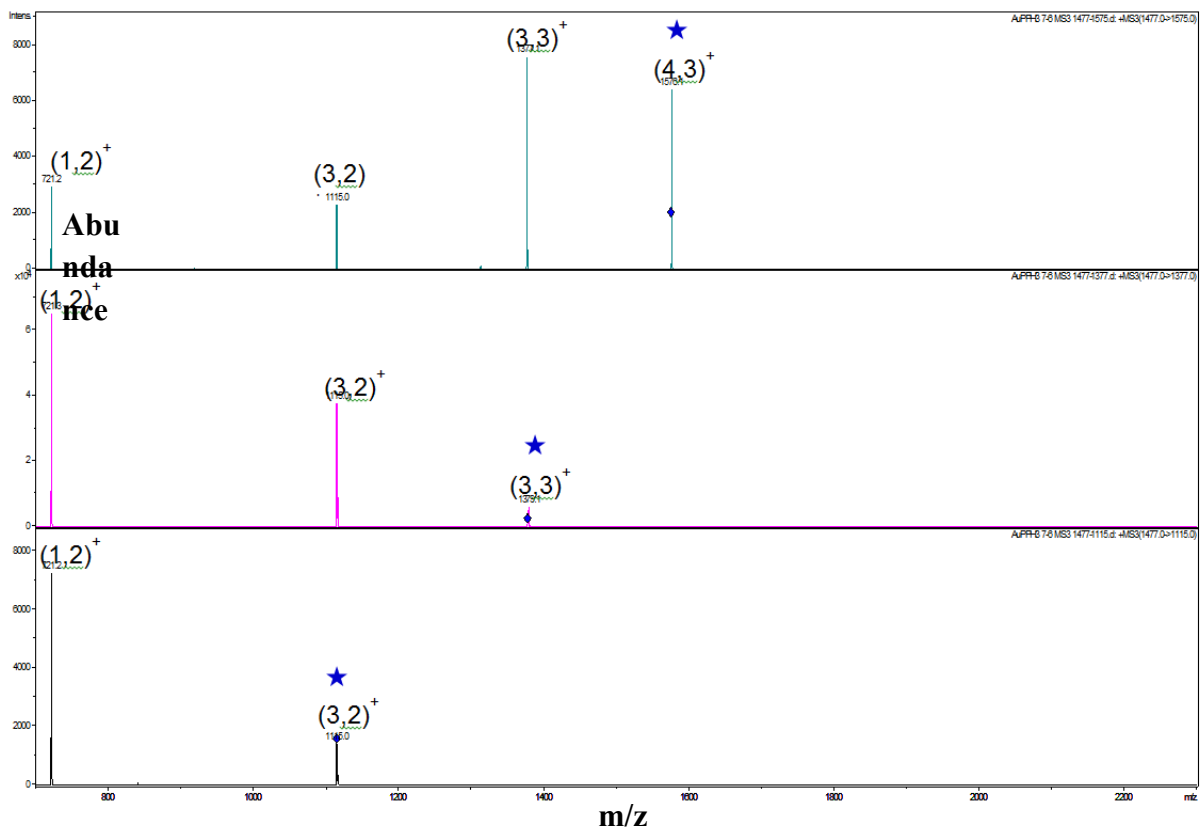
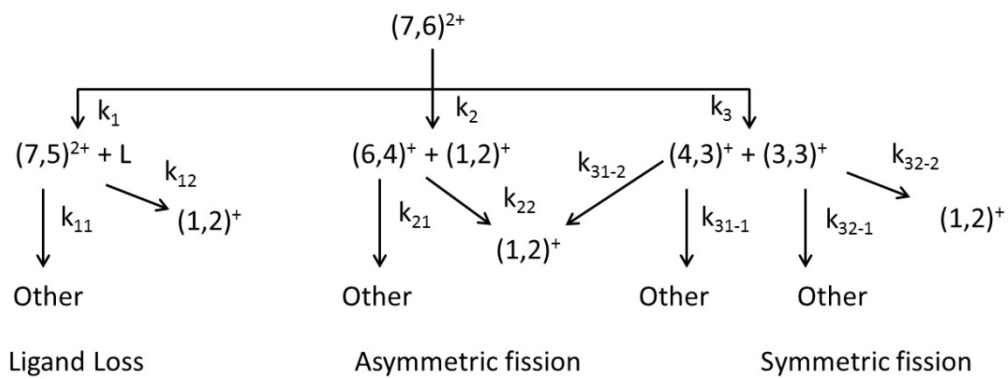
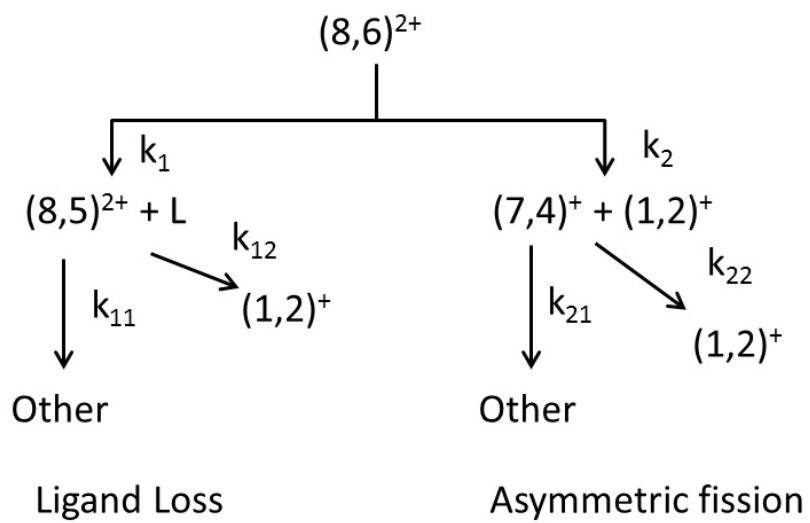


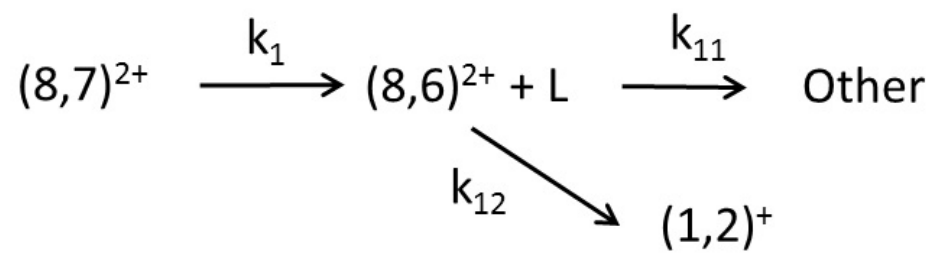
Figure S5. MS³ spectra of (4,3)⁺, (3,3)⁺ and (3,2)⁺ product ions generated from the (7,6)²⁺ precursor ion. The ions selected for dissociation are marked with a blue star.



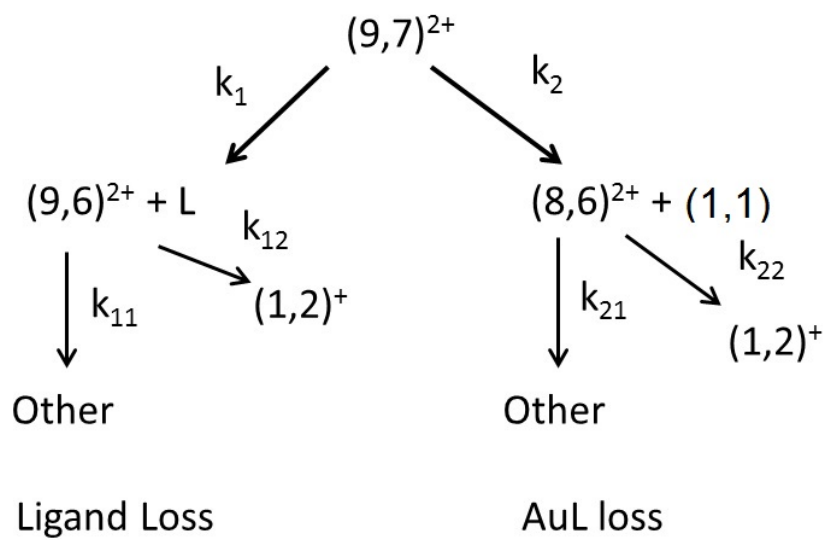
Scheme 1. Simplified kinetic scheme used for RRKM modeling of $(7,6)^{2+}$.



Scheme 2. Simplified kinetic scheme used for RRKM modeling of $(8,6)^{2+}$.



Scheme 3. Simplified kinetic scheme used for RRKM modeling of $(8,7)^{2+}$.



Scheme 4. Simplified kinetic scheme used for RRKM modeling of $(9,7)^{2+}$.