

Electronic Supplementary Information (ESI)

Perspectives on the energy landscape of Au-Cl binary system from the structural phase diagram of Au_xCl_y ($x + y = 20$)

By

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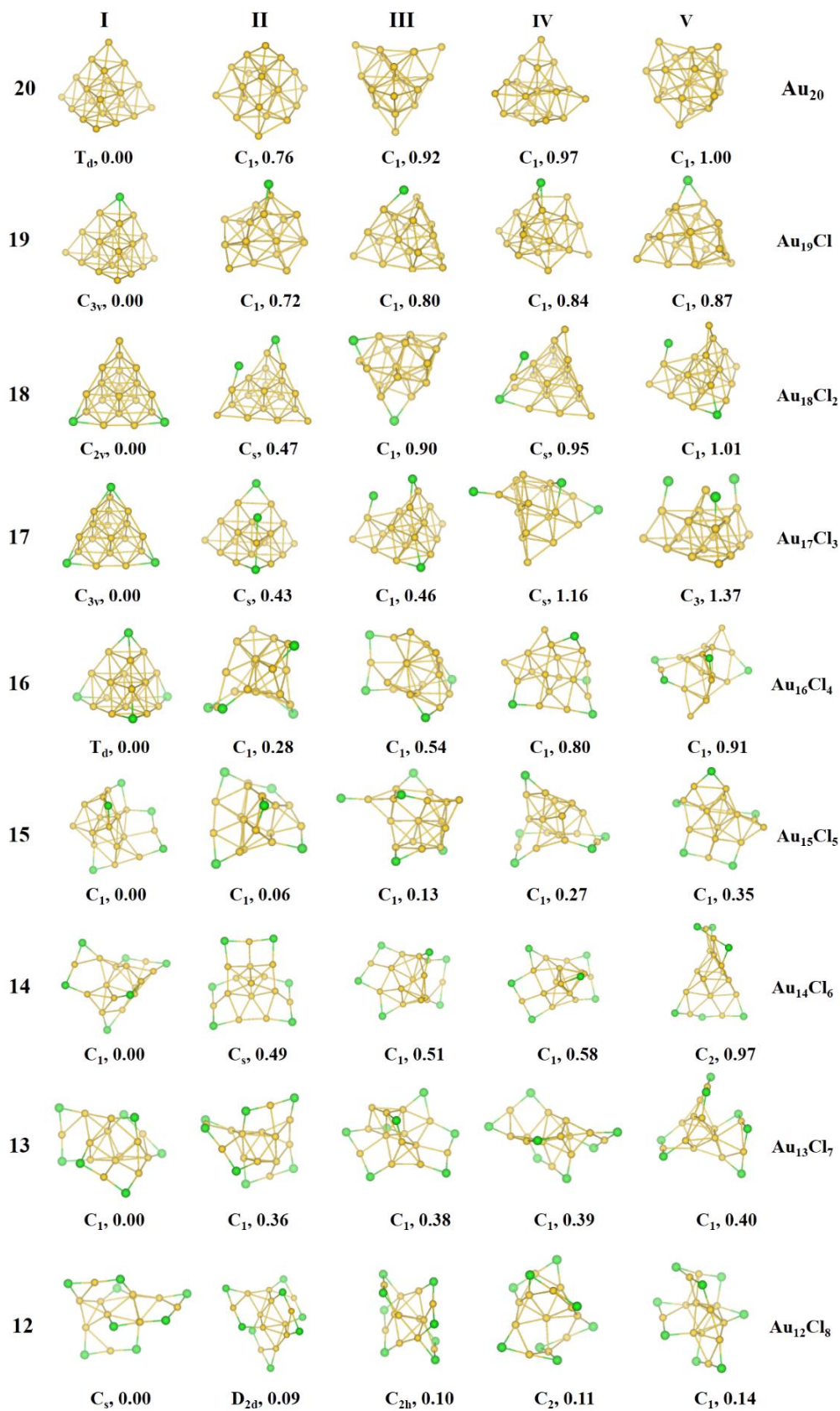


Fig. S1 Optimized structures and relative stability of Au₁₂Cl₈-Au₂₀ at TPSS/Def2-TZVP (Au) and 6-311G* (Cl) level of theory. Au, yellow, Cl, green.

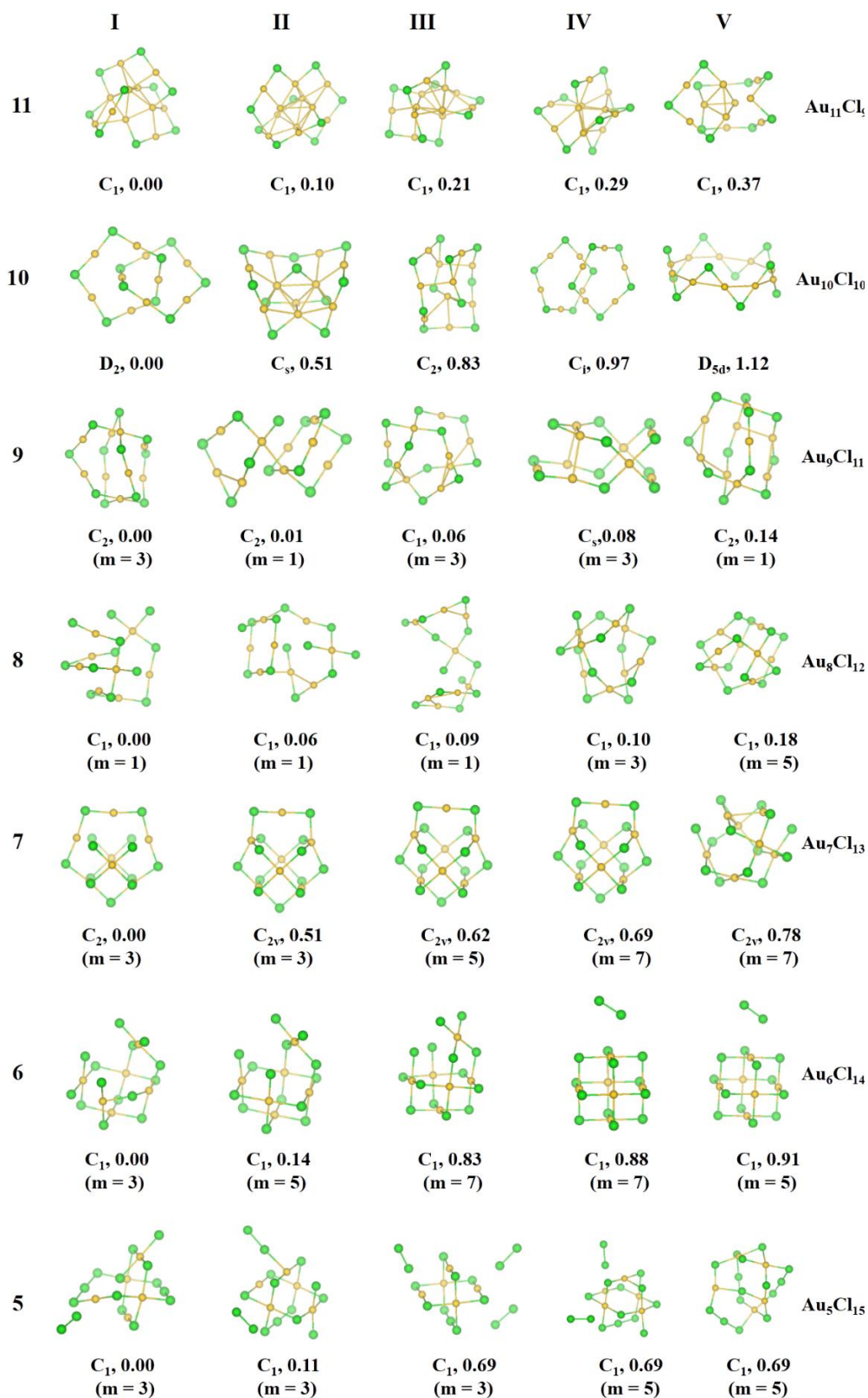


Fig. S2 Optimized structures and relative stability of $\text{Au}_5\text{Cl}_{15}$ - $\text{Au}_{11}\text{Cl}_9$ at TPSS/Def2-TZVP (Au) and 6-311G* (Cl) level of theory. Au, yellow, Cl, green. When $x \leq 9$, the multiplicity of the molecule is shown in the bracket.

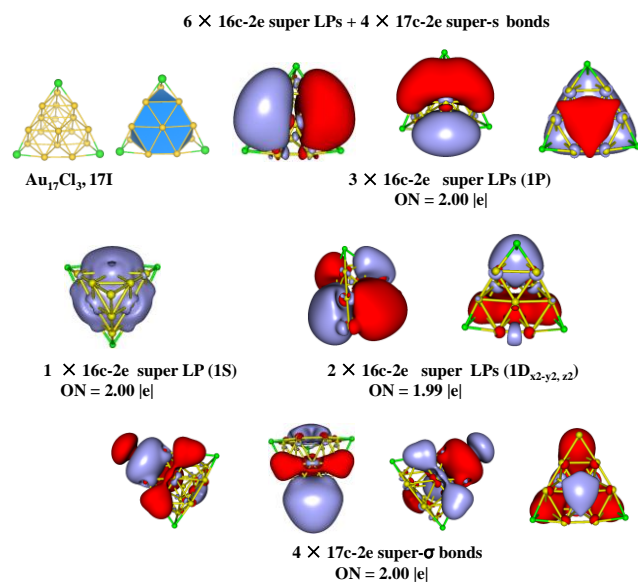


Fig. S3 Superatomic-molecule model and AdNDP localized natural bonding orbitals of 17I.

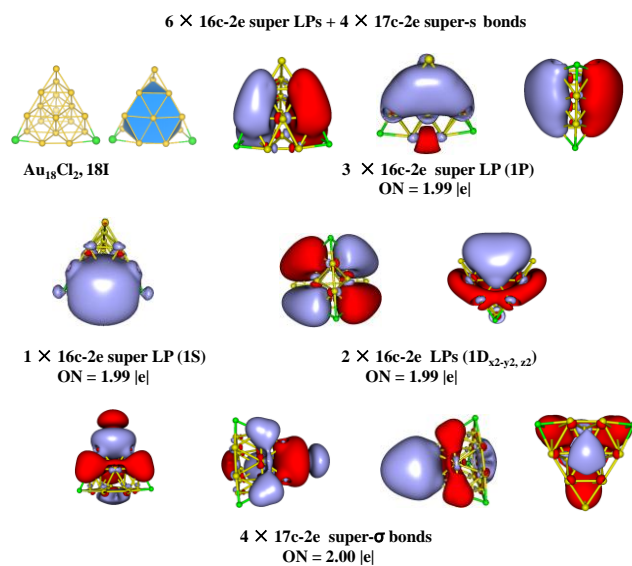


Fig. S4 Superatomic-molecule model and AdNDP localized natural bonding orbitals of 18I.

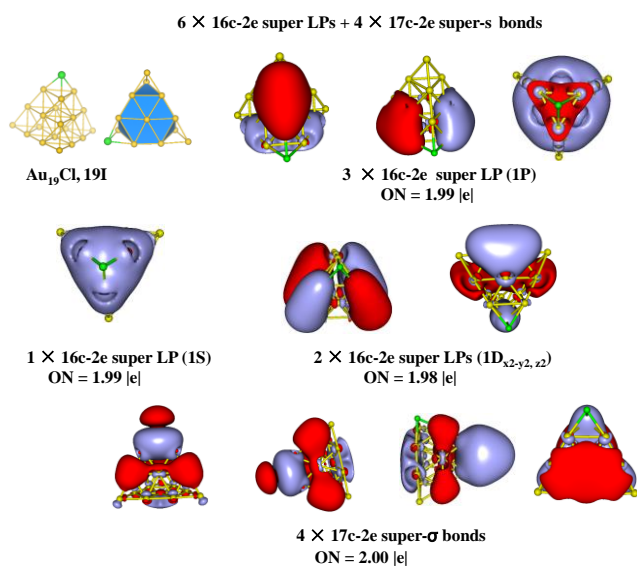


Fig. S5 Supratomic-molecule model and AdNDP localized natural bonding orbitals of 19I.