Exploring the Low-lying Structures of $Au_n(CO)^+$ (n = 1-10): Adsorption and Stretching Frequencies of CO on Various Coordination Sites

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Figure S1

The low lying structures of $Au_6(CO)^+$. All structures were optimized at level I and the relative energies were recalculated at level II. Their electronic states and geometries are indicated. The numbers inside and outside of the parentheses indicate the relative energies from level I and level II, respectively. The structures with a terminal-bonded CO and a bridge-bonded CO are sequenced separately according to their relative energies from level II. Level I: B3LYP functional method with lanl2dz basis set for Au and 6-31G(d) basis sets for C and O. Level 2: B3LYP functional method with Aug-cc-PVTZ-PP basis set for Au and Aug-cc-PVTZ basis sets for C and O.

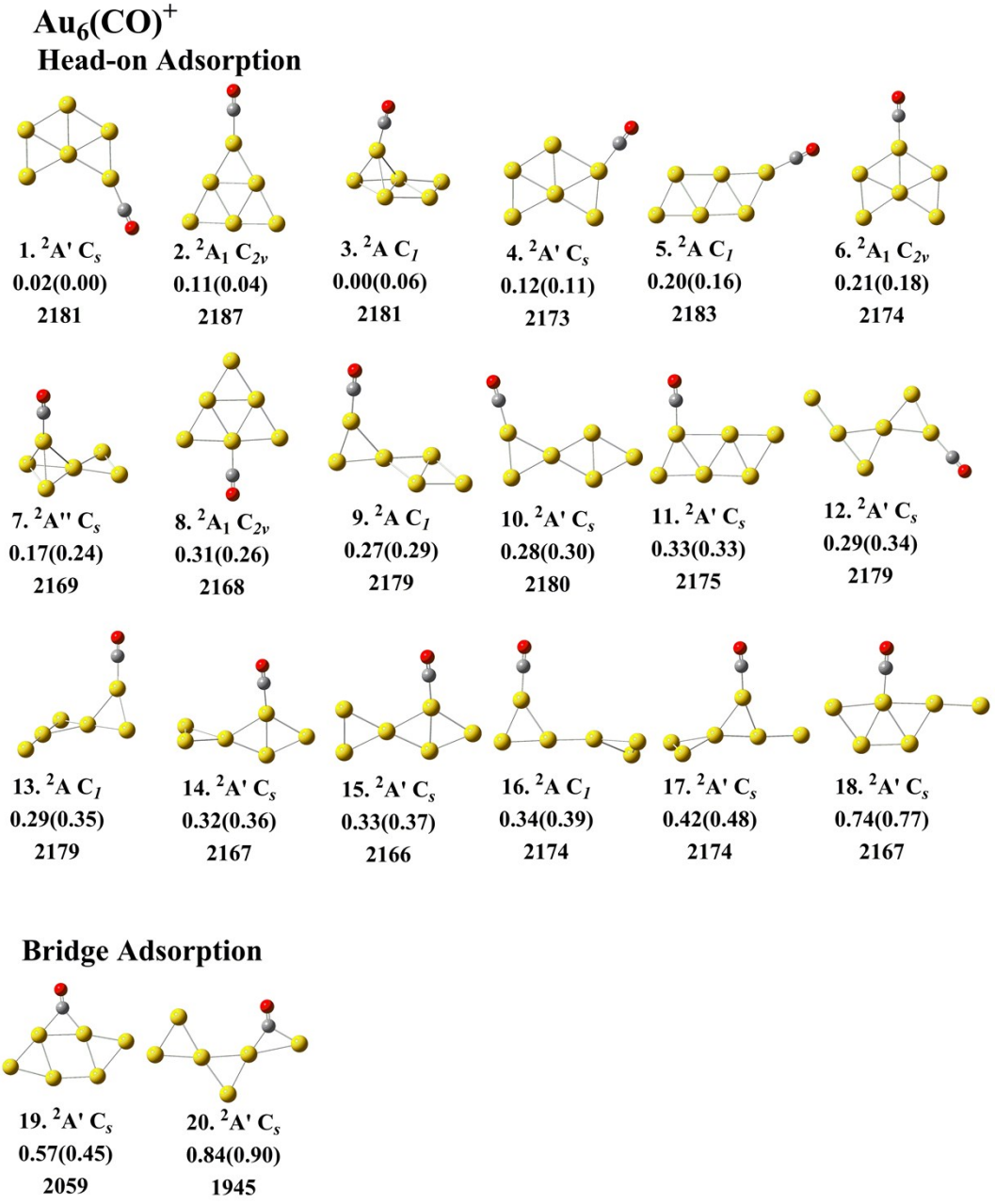

Figure S2

The low lying structures of $Au_7(CO)^+$ (similar to Figure S1).

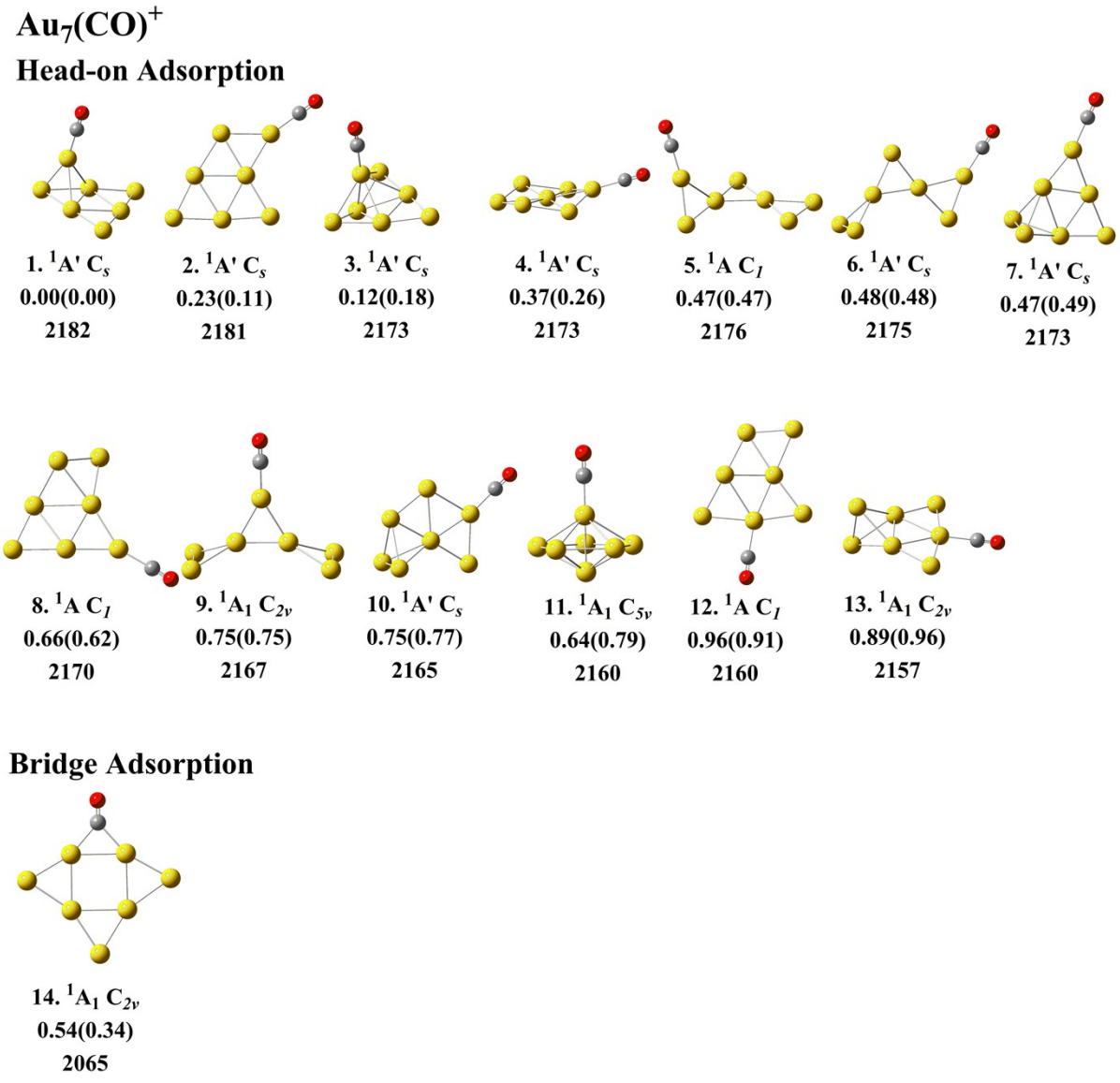

Figure S3

The low lying structures of $Au_8(CO)^+$ (similar to Figure S1).

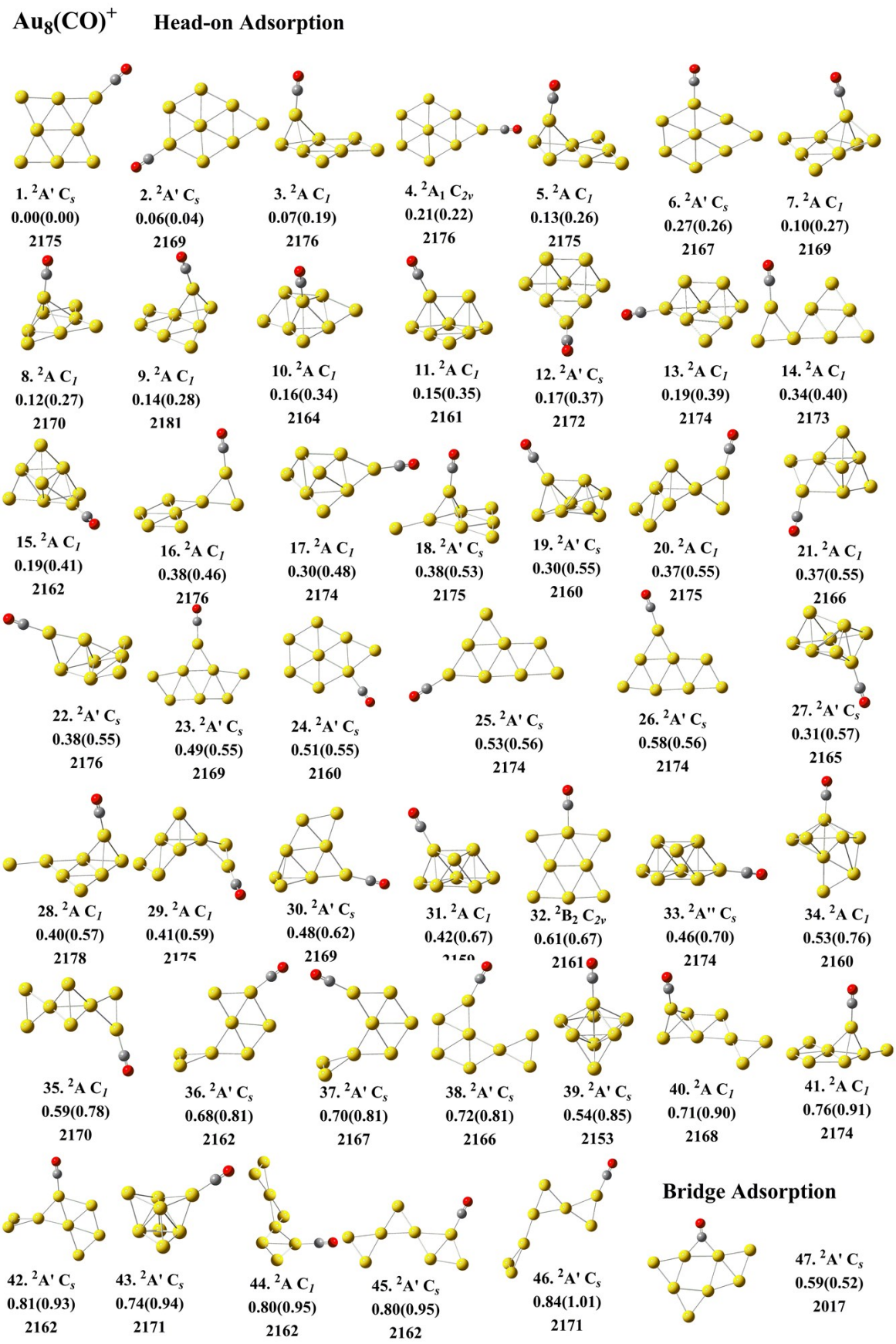

Figure S4

The low lying structures of $Au_9(CO)^+$ (similar to Figure S1).

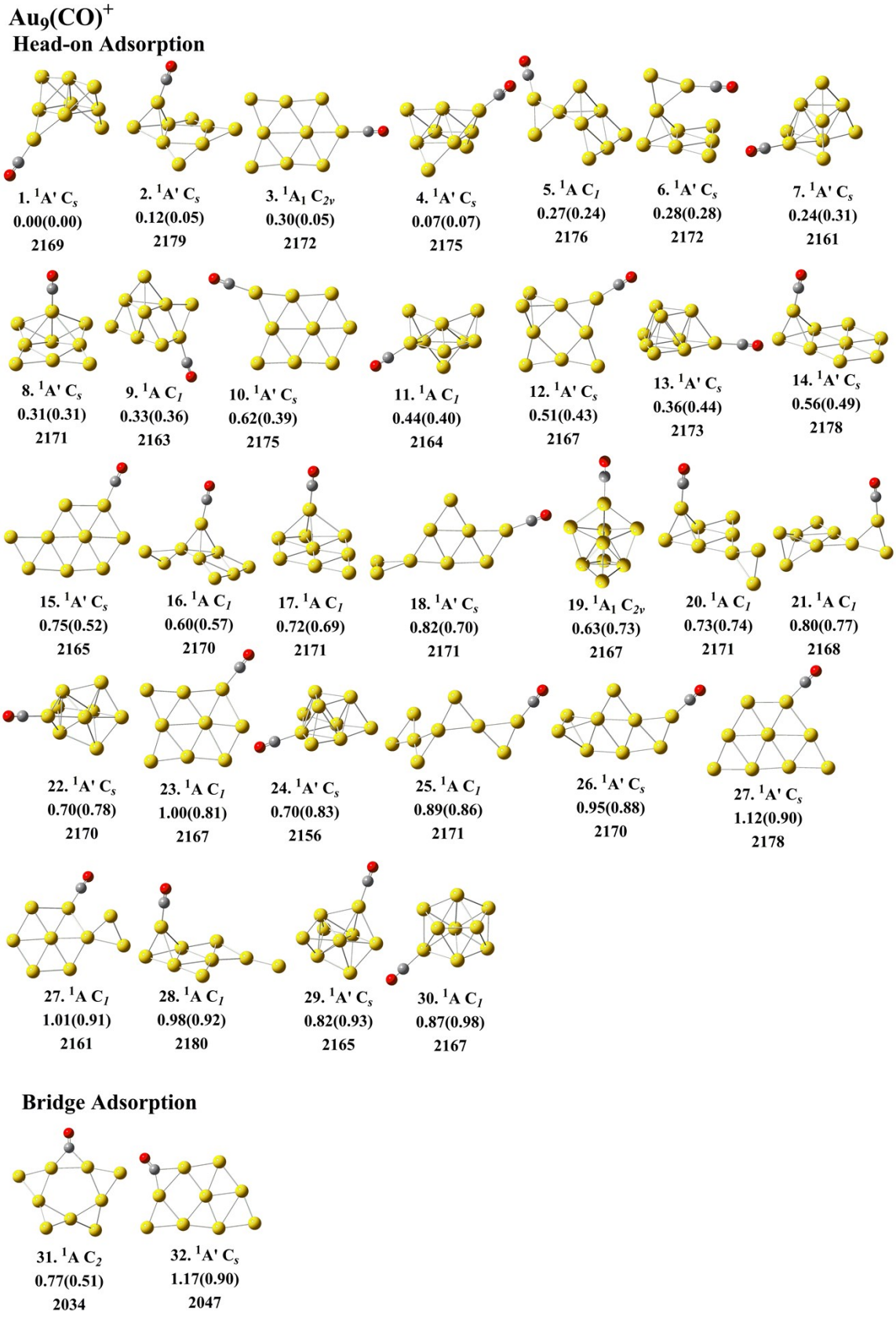

Figure S5

The low lying structures of $Au_{10}(CO)^+$ (similar to Figure S1).