

Supporting Information

for

Theoretical Investigation on CO Oxidation Catalyzed by a Copper Nanocluster

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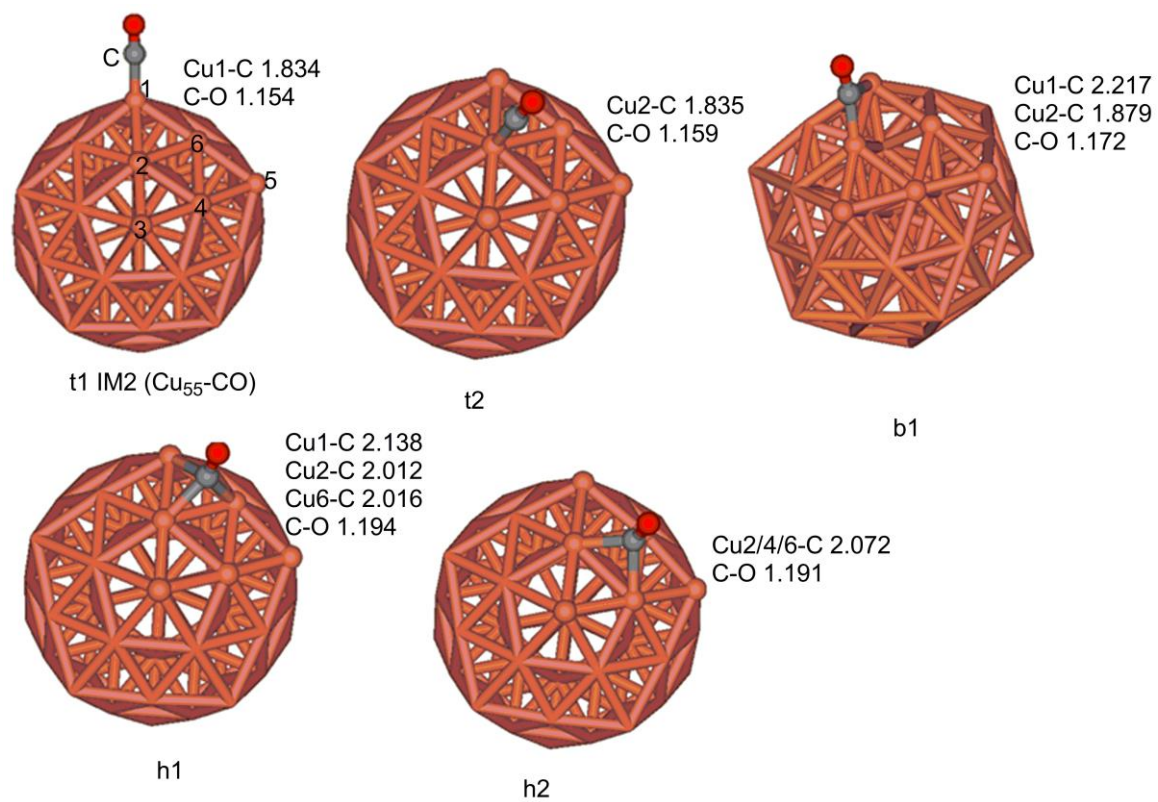


Fig. S1 The optimized structures and related parameters of CO adsorption on Cu_{55} cluster

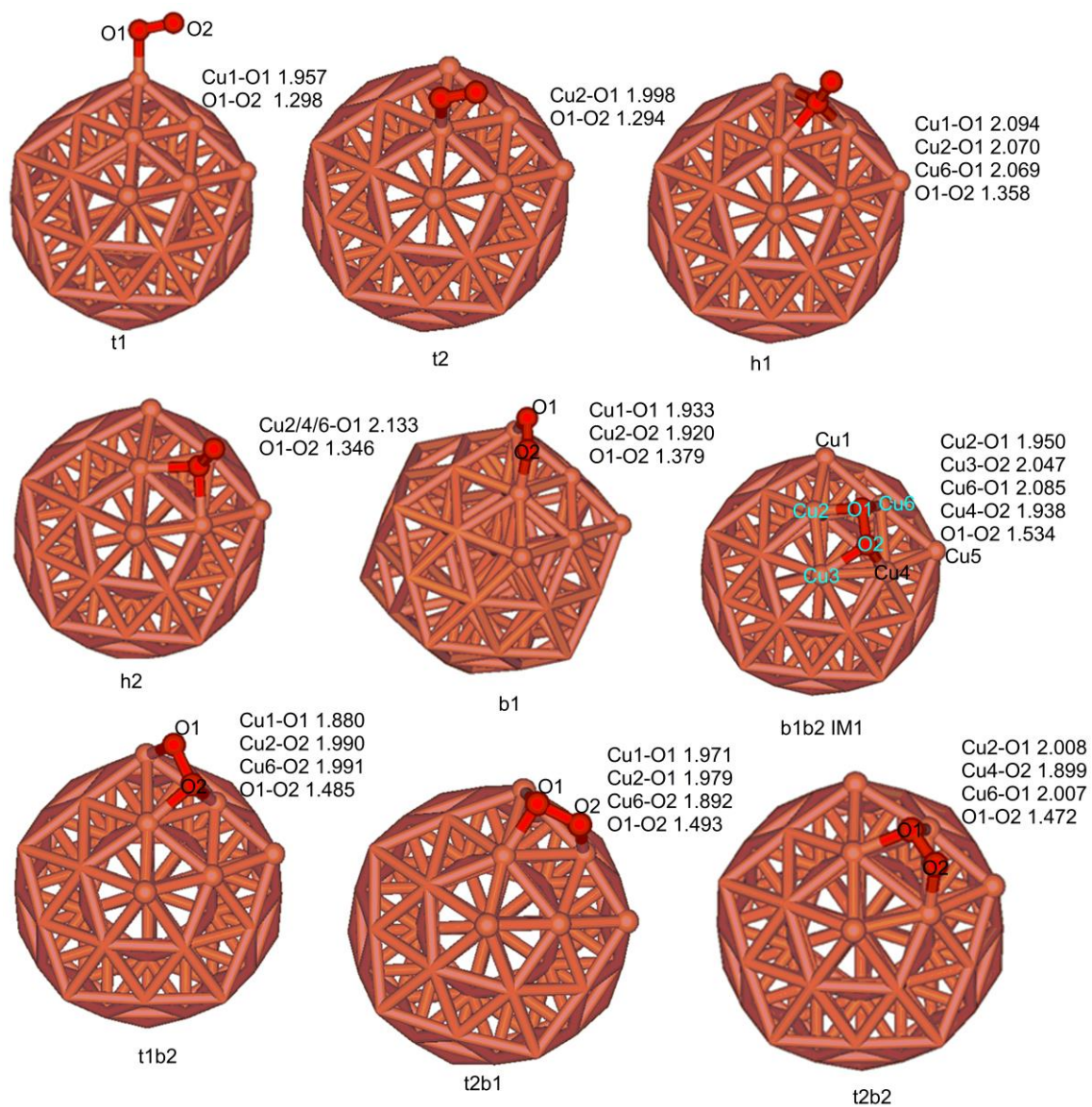


Fig. S2 The optimized structures and related parameters of O₂ adsorption on Cu₅₅ cluster