

Visible Light-Driven H₂ Evolution with Cobalt Complexes in Aqueous Solution: Theoretical and Experimental Study

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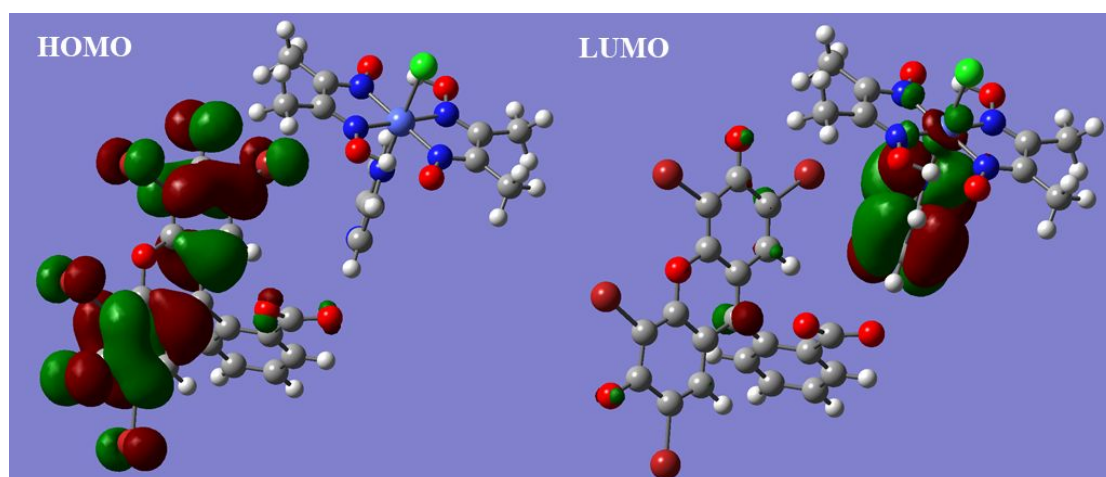


Figure S1. Computed the highest-occupied molecular orbital (HOMO) and the lowest-unoccupied molecular orbital (LUMO) of docking structure (**complex 13** and EY²⁻) in the ground state.

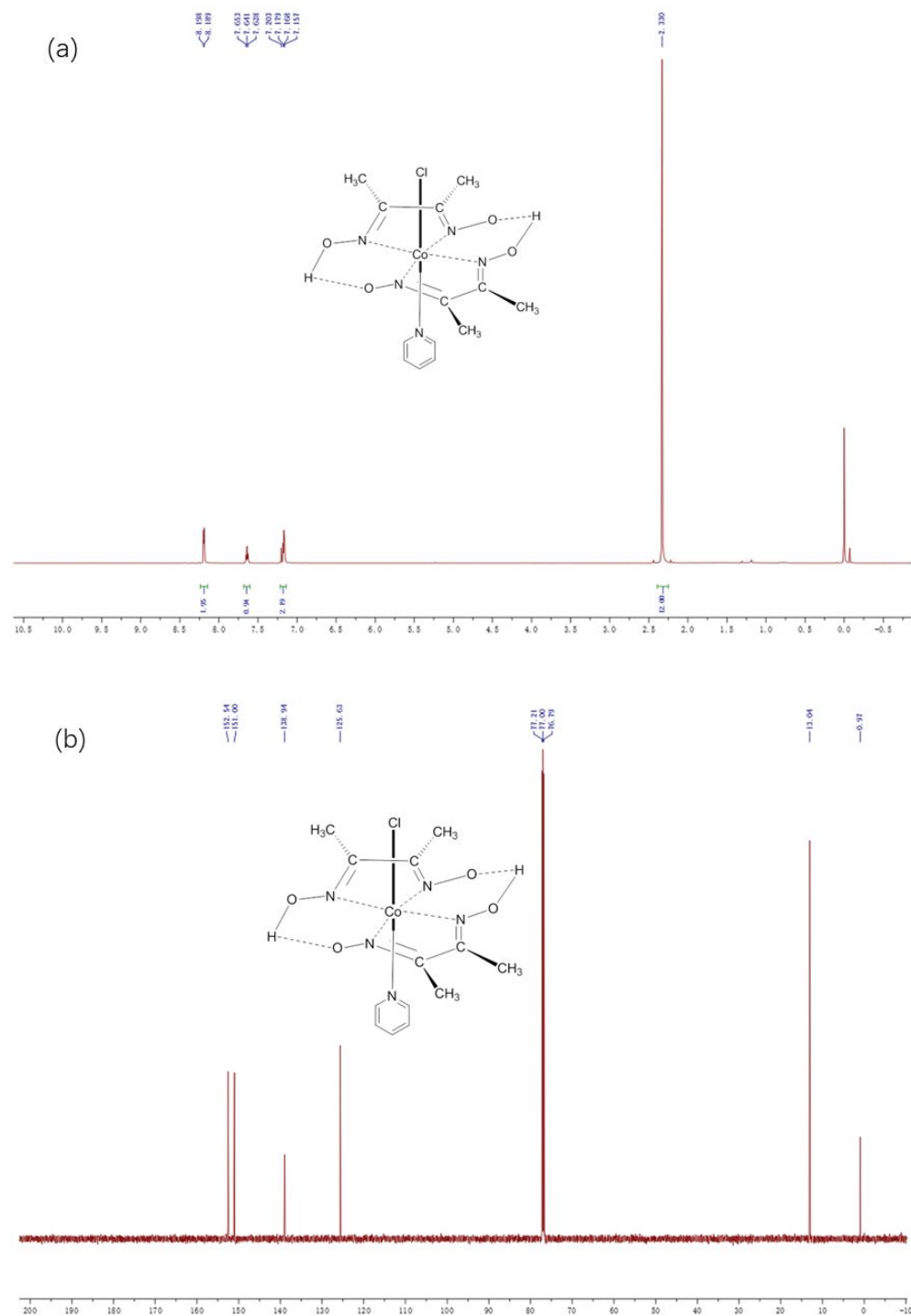
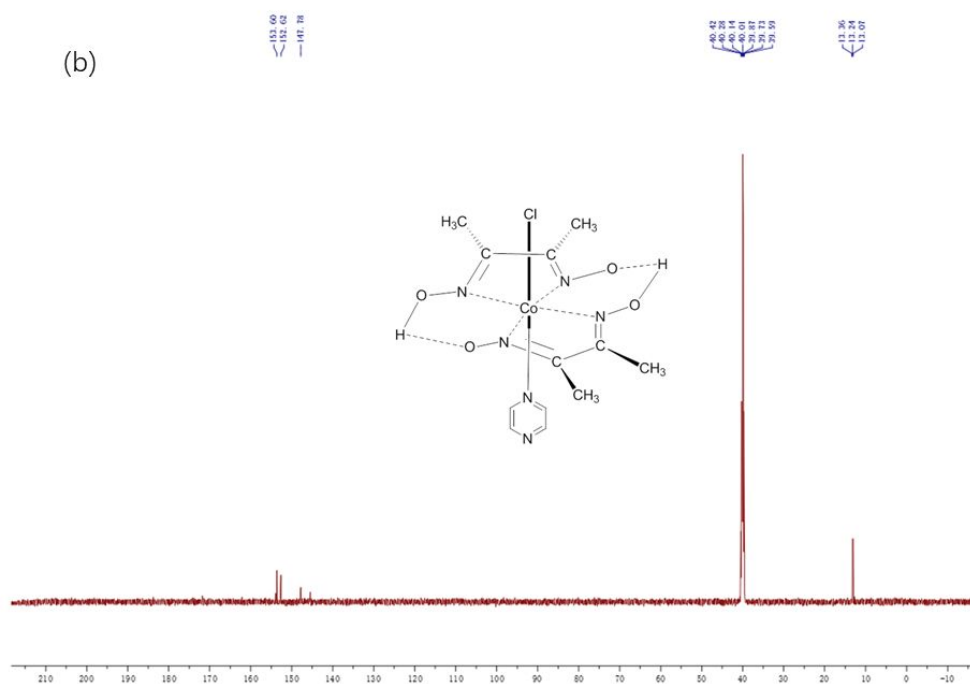


Figure S2. (a) ^1H NMR and (b) ^{13}C NMR of complex 1.



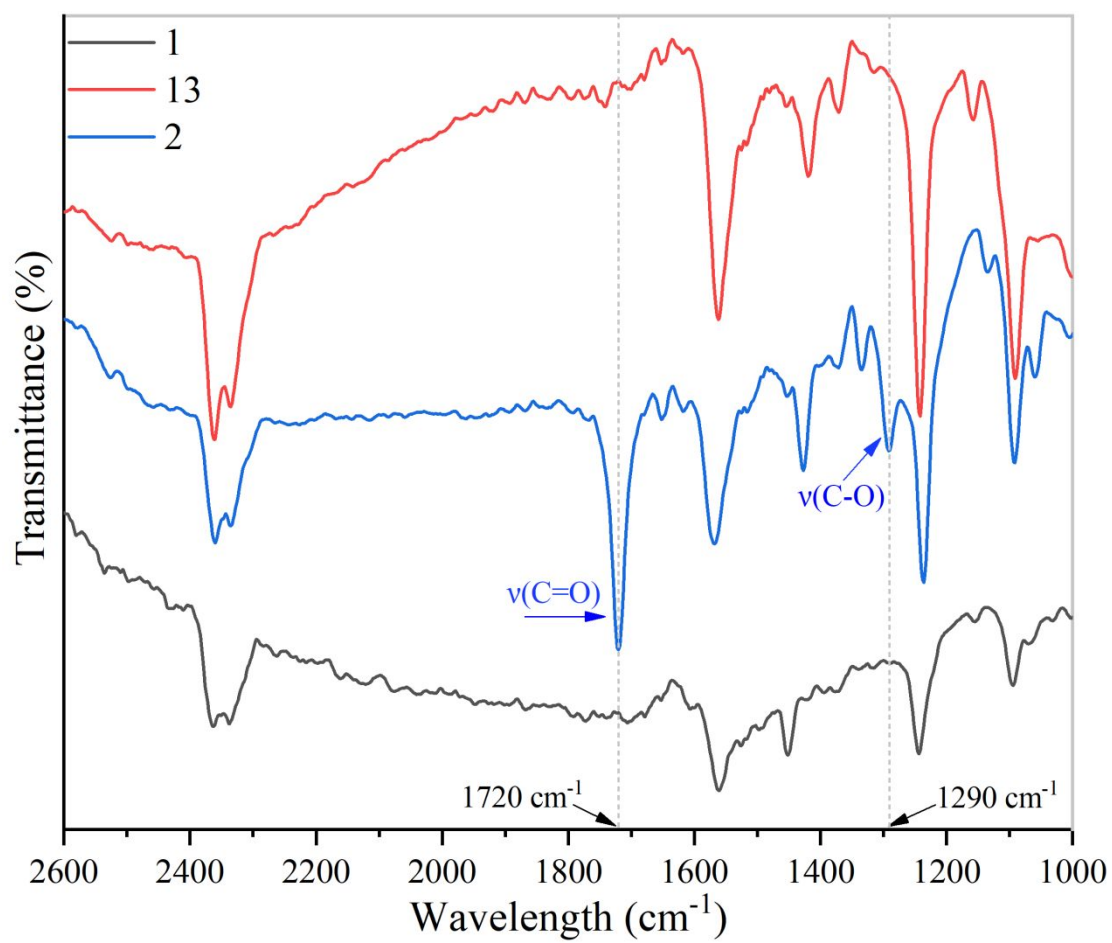


Figure S5. FT-IR of complexes 1, 2 and 13.