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Carbon Dioxide Reduction Mechanism on the Ru-based Electrocatalysts $[Ru(bpy)_2(CO)_2]^{2+}$: Insights from First-principles Theory

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Supporting Information

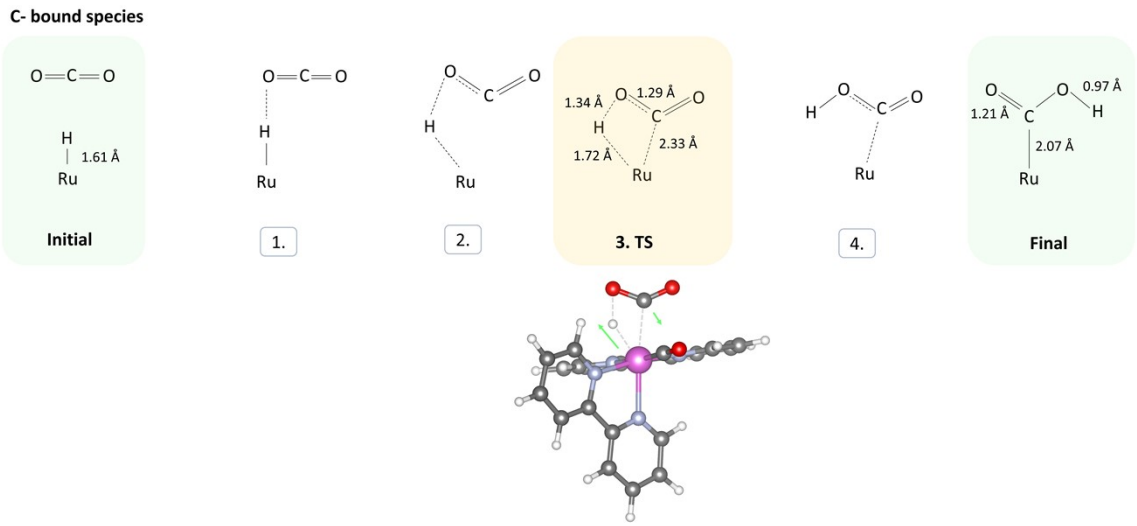

Figure S1- Schematic representation of the reaction mechanism leading to the formation of the C-bound species (**18**) from the hydride complex (**7**), being the activation barrier estimated as +52.03 kcal/mol. In detail, the transition state structure is depicted alongside the vectors that represent the negative frequency mode (- 1352 cm^{-1}). Color code: lilac (ruthenium), grey (carbon), blue (nitrogen), red (oxygen) and white (hydrogen).

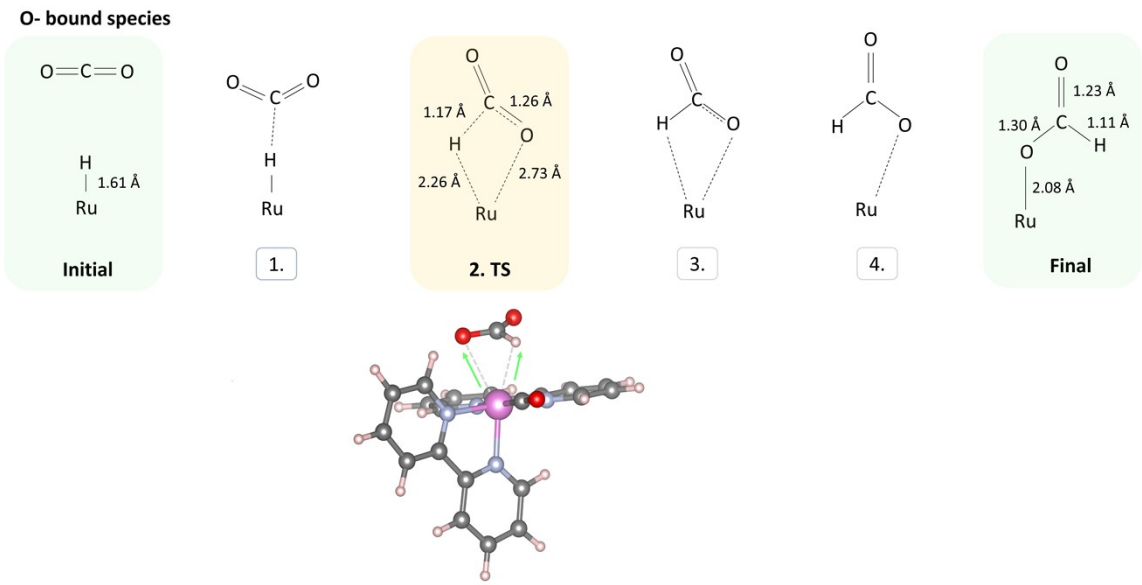

Figure S2- Schematic representation of the reaction mechanism leading to the formation of the O-bound species (**19**) from the hydride complex (**7**), being the activation barrier estimated as +32.91 kcal/mol. In detail, the transition state structure is depicted alongside the vectors that represent the negative frequency mode (- 492 cm^{-1}). Color code: lilac (ruthenium), grey (carbon), blue (nitrogen), red (oxygen) and white (hydrogen).