Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Reactivity of silica supported zirconium hydride with N_2O and CO_2 probe molecules: a computational point of view.

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Supplementary materials

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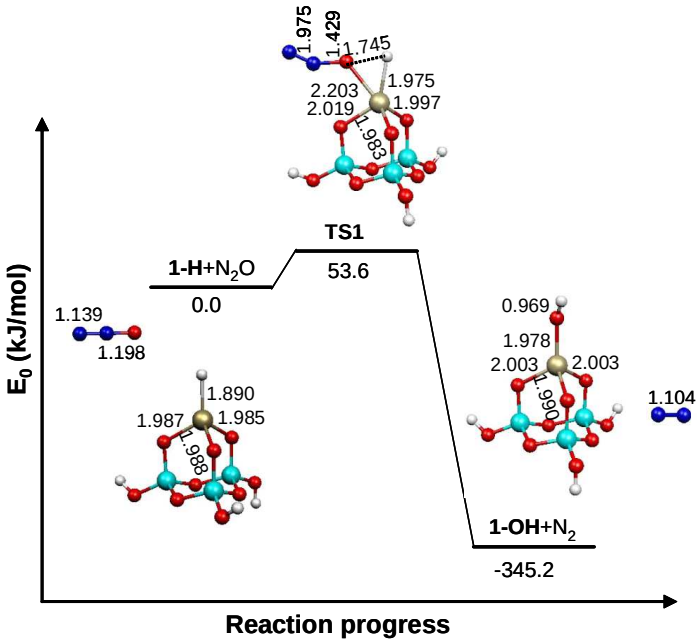

Figure S 1 : Energy profile of the reaction between **1-H** and N_2O, and relevant distances (Å).

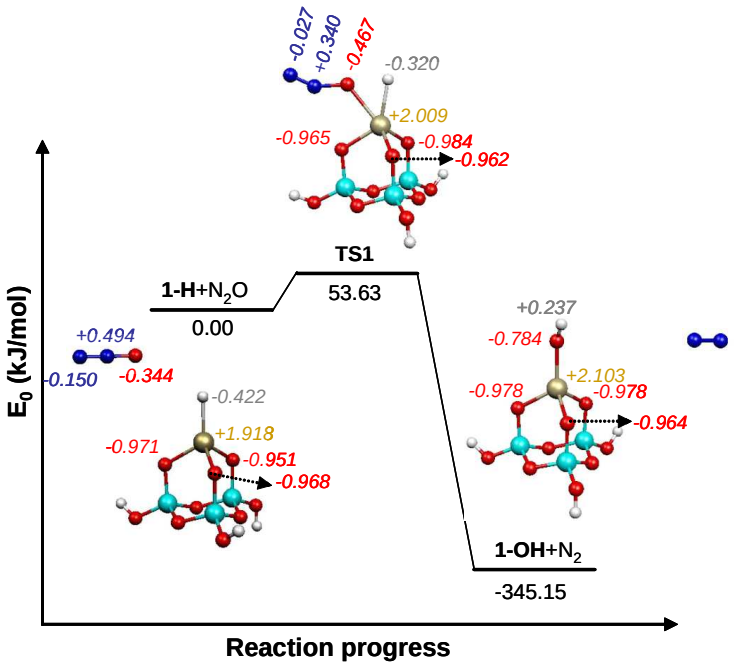

Figure S 2 : Energy profile of the reaction between **1-H** and N_2O, and relevant charges (italic).

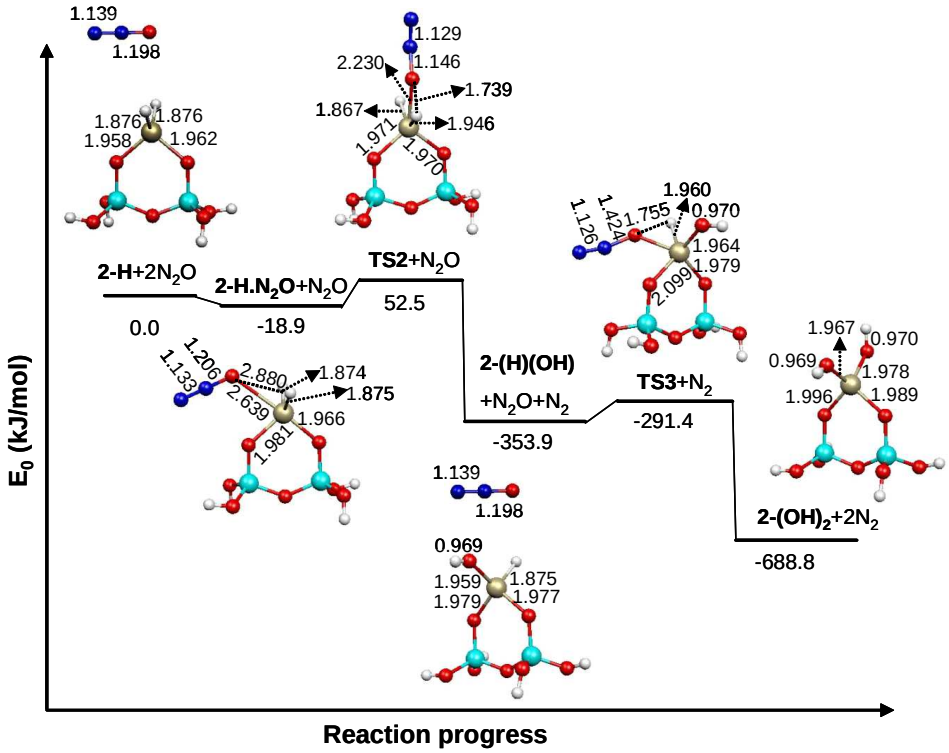

Figure S 3 : Energy profile of the reaction between **2-H** and two N_2O, and relevant distances (Å).

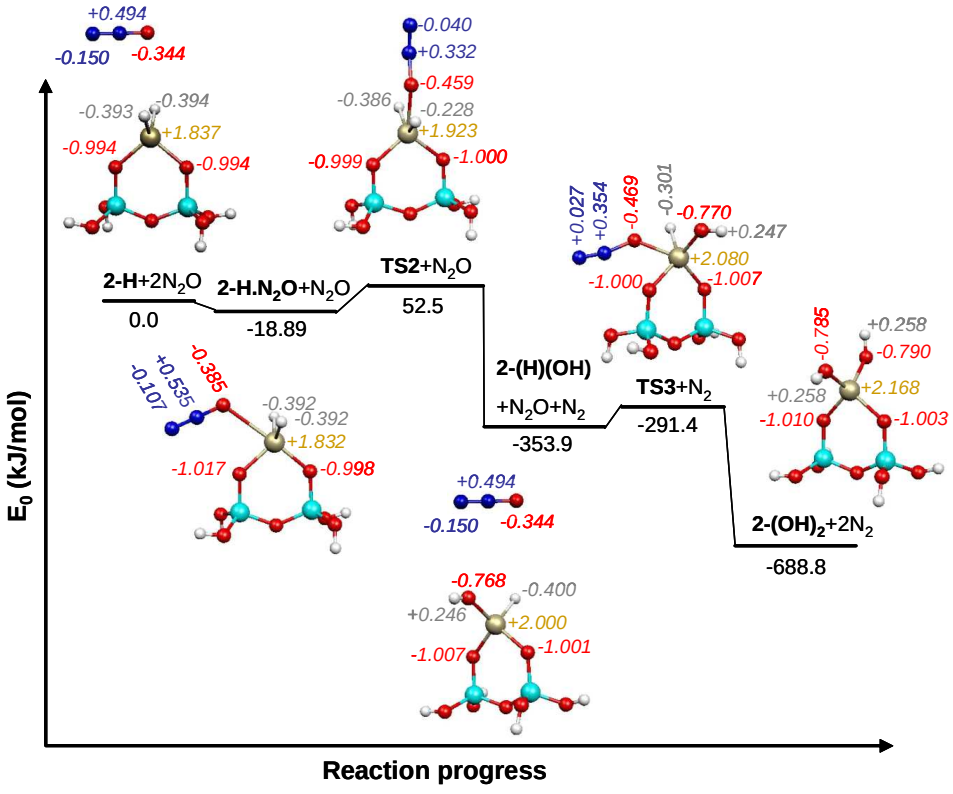

Figure S 4 : Energy profile of the reaction between **2-OH** and two N_2O, and relevant charges (italic).

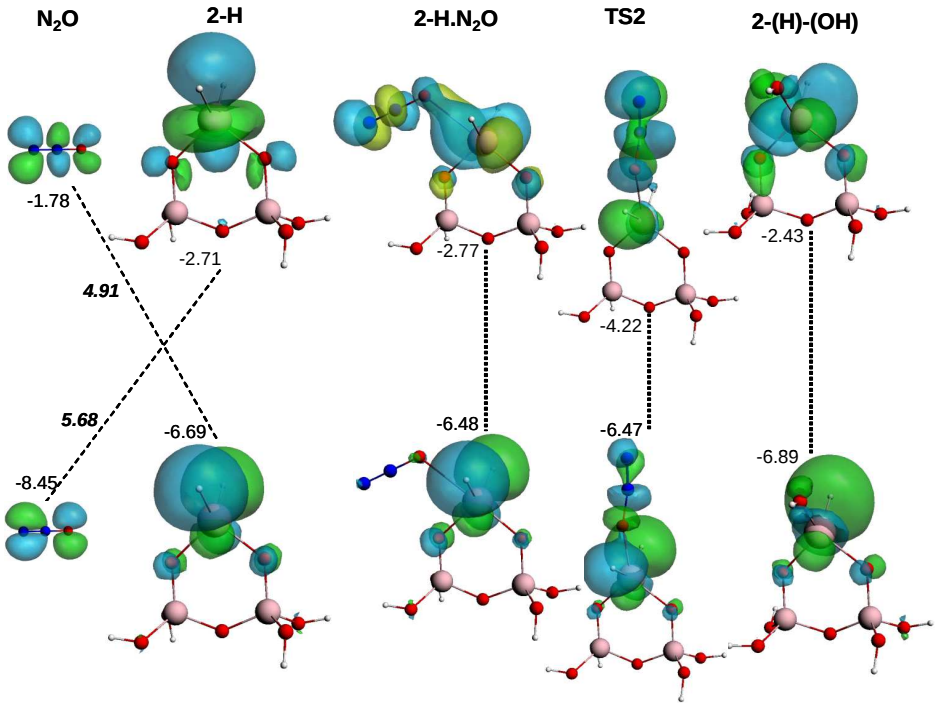

Figure S 5 : Changes in energy (eV) and shape of HOMOs and LUMOs of N_2O and **2-H** to **2-(H)-(OH)** via **TS2** (ΔE between HOMOs and LUMOs in italic).

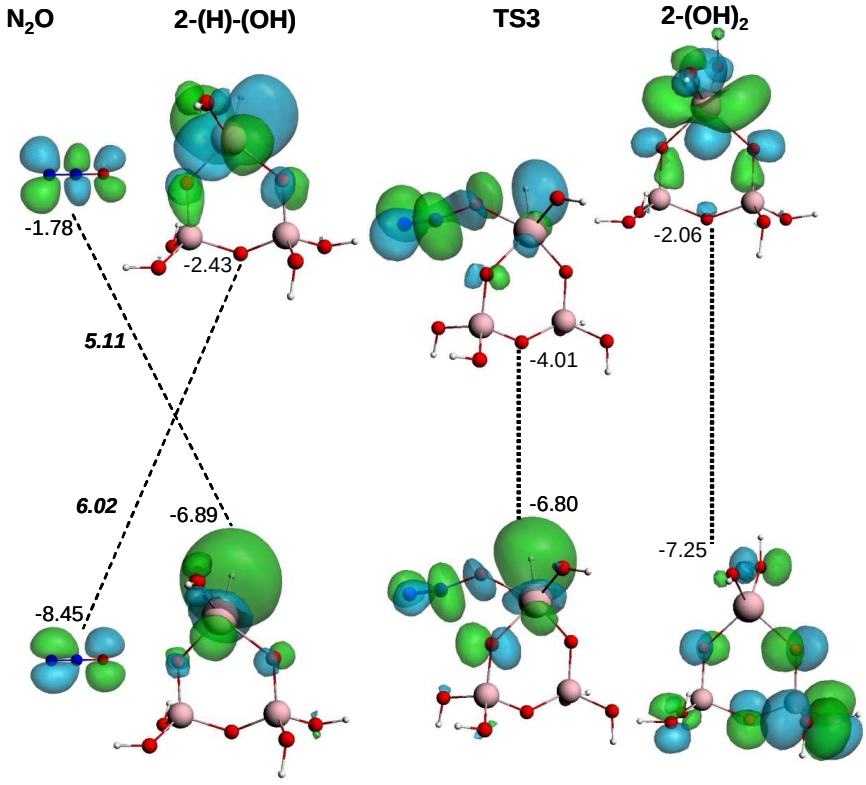

Figure S 6 : Changes in energy (eV) and shape of HOMOs and LUMOs of N_2O and **2-(H)-(OH)** to **2-$(OH)_2$** via **TS3** (ΔE between HOMOs and LUMOs in italic).

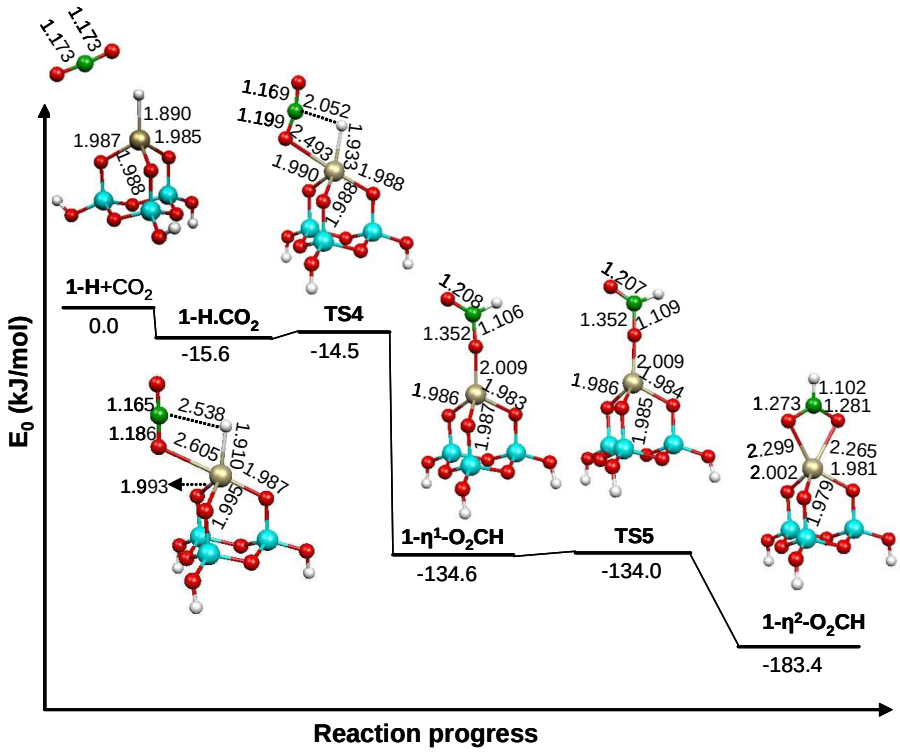

Figure S 7 : Energy profile of the reaction between **1-H** and first CO_2, and relevant distances (Å).

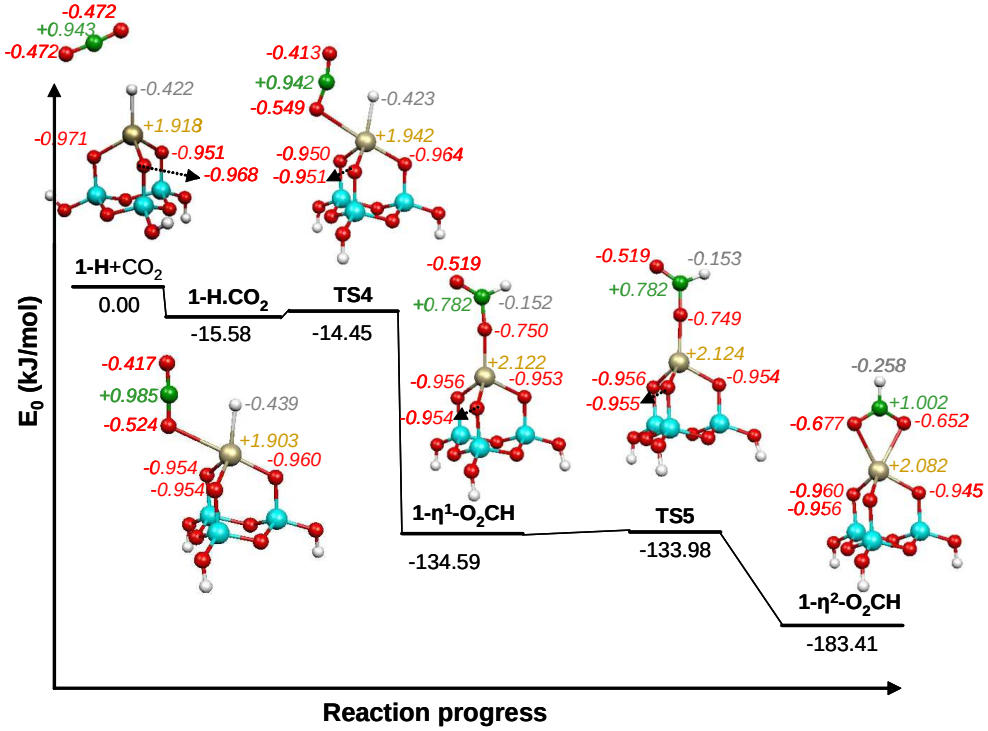

Figure S 8 : Energy profile of the reaction between **1-H** and first CO_2, and relevant charges (italic).

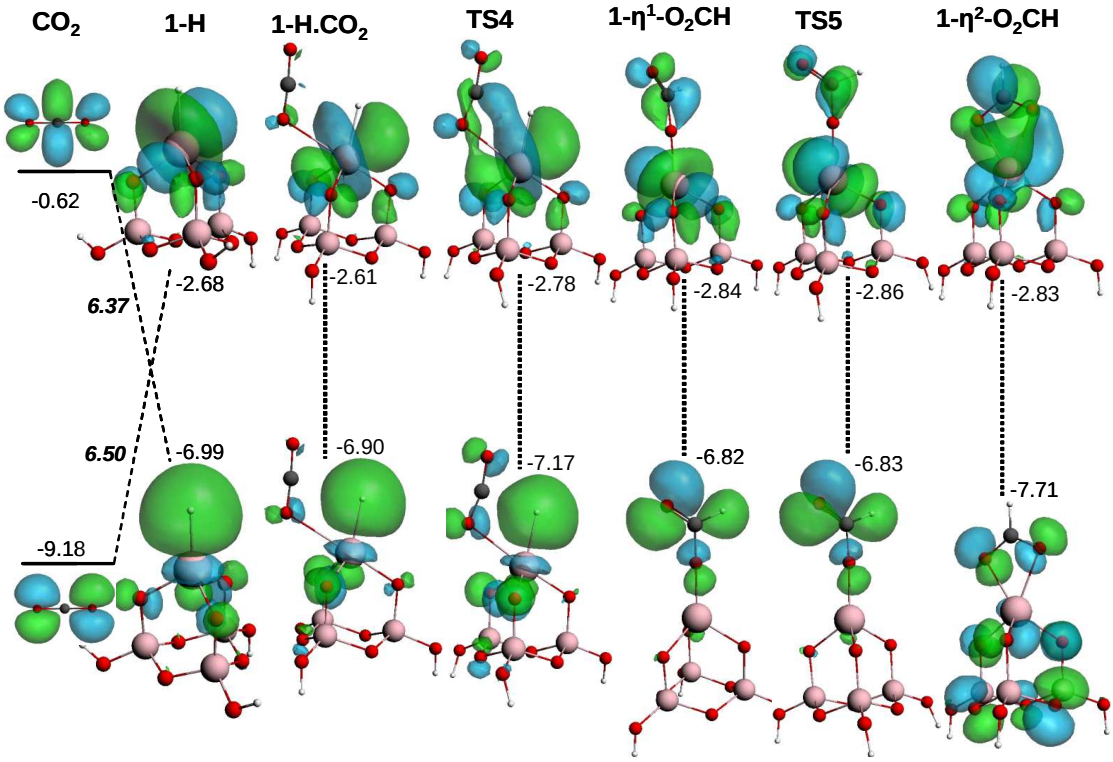

Figure S 9 : Changes in energy (eV) and shape of HOMOs and LUMOs of CO_2 and **1-H** to **1-η^1-O$_2$CH and 1-η^2-O$_2$CH** via **TS4** and **TS5** (ΔE between HOMOs and LUMOs in italic).

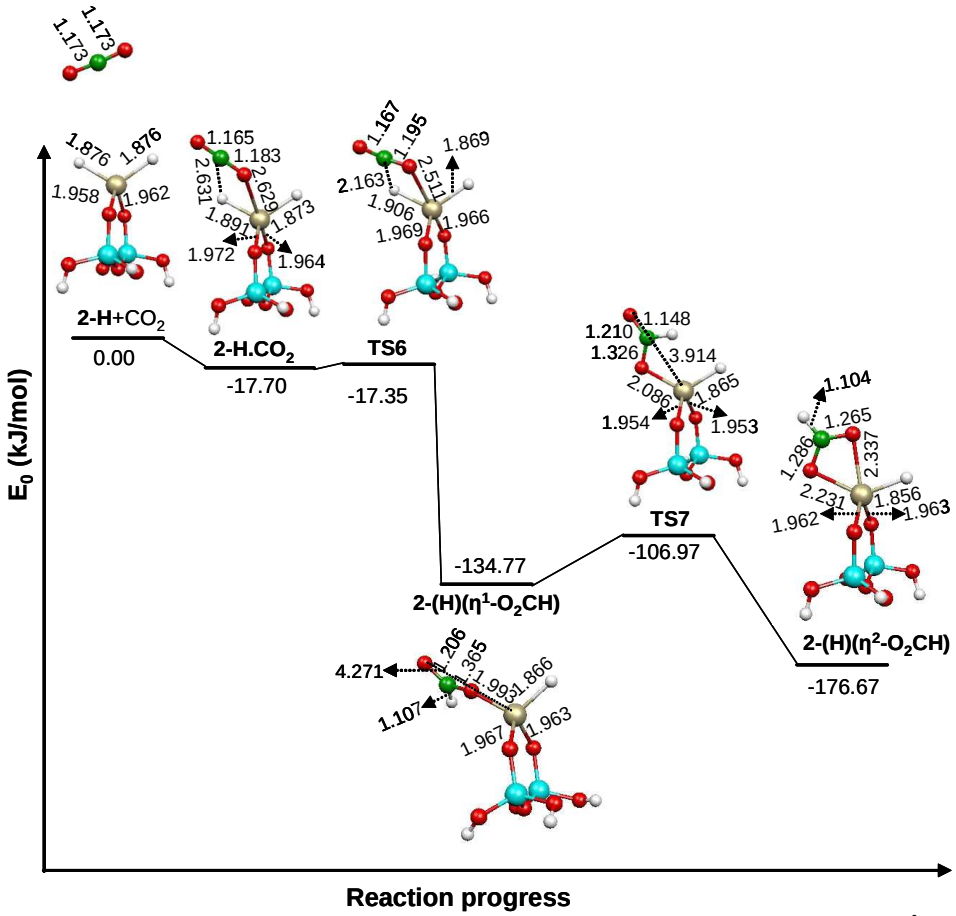

Figure S 10 : Energy profile of the reaction between **2-H** and first CO_2, and relevant distances (Å).

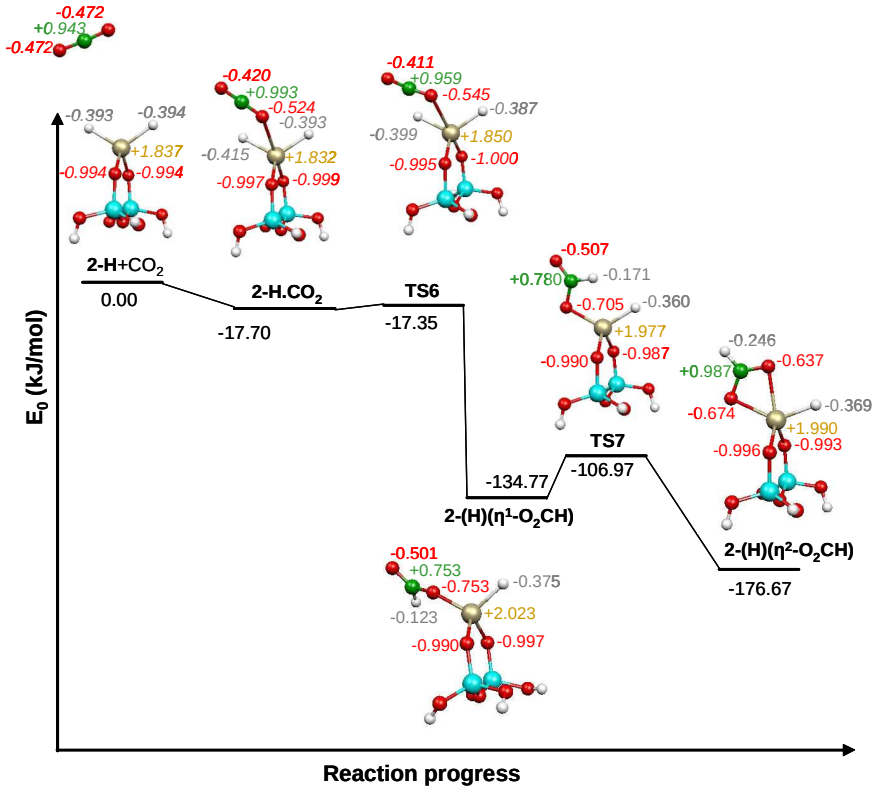

Figure S 11 : Energy profile of the reaction between **2-H** and first CO_2, and relevant charges (italic).

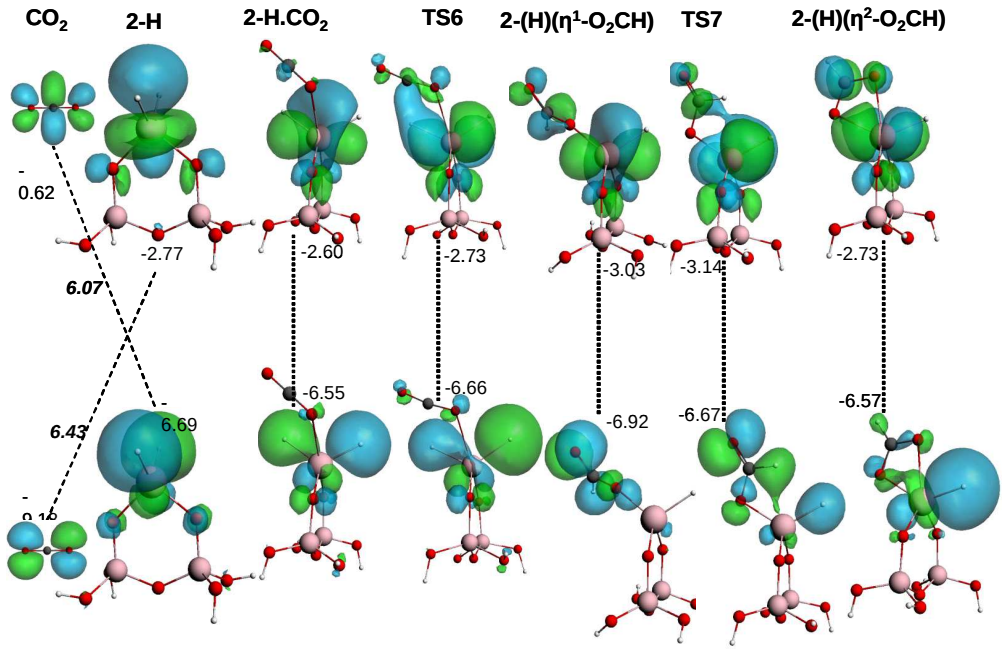

Figure S 12 : Changes in energy (eV) and shape of HOMOs and LUMOs of N_2O and **2-H** to **2-(H)(η^1-O$_2$CH)** and **2-(H)(η^2-O$_2$CH)** via **TS6**and **TS7** (ΔE between HOMOs and LUMOs in italic).

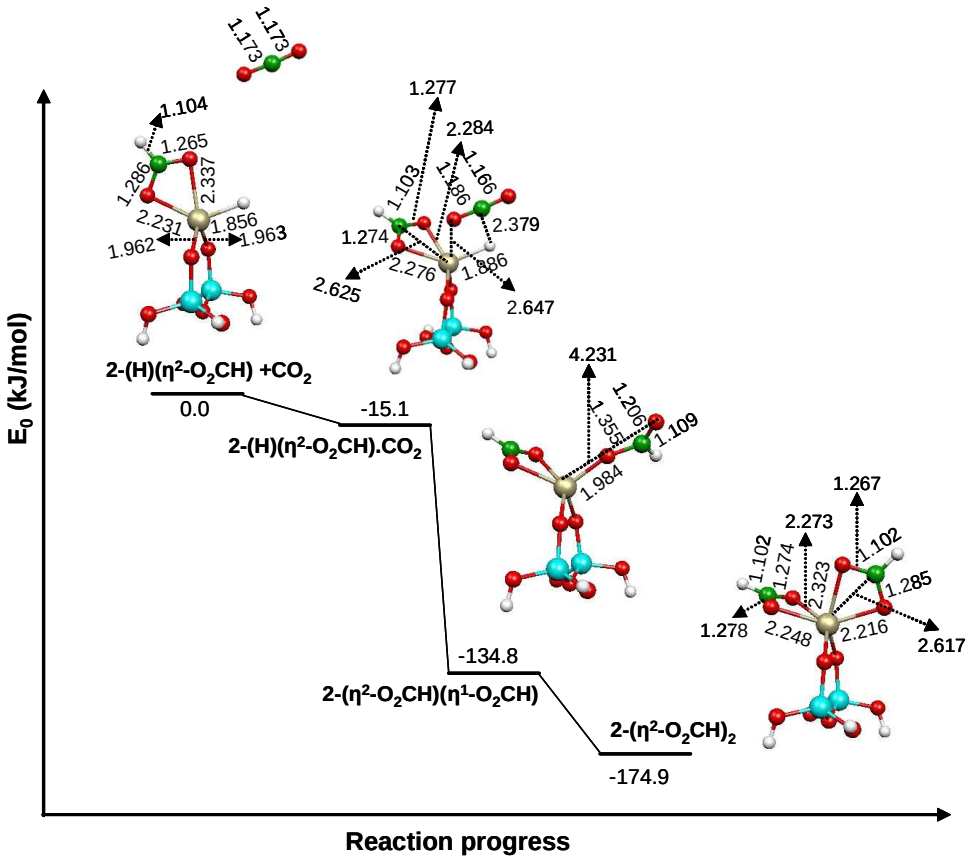

Figure S 13 : Energy profile of the reaction between **2-(H)(η^2-O$_2$CH)** and second CO_2, and relevant distances (Å).

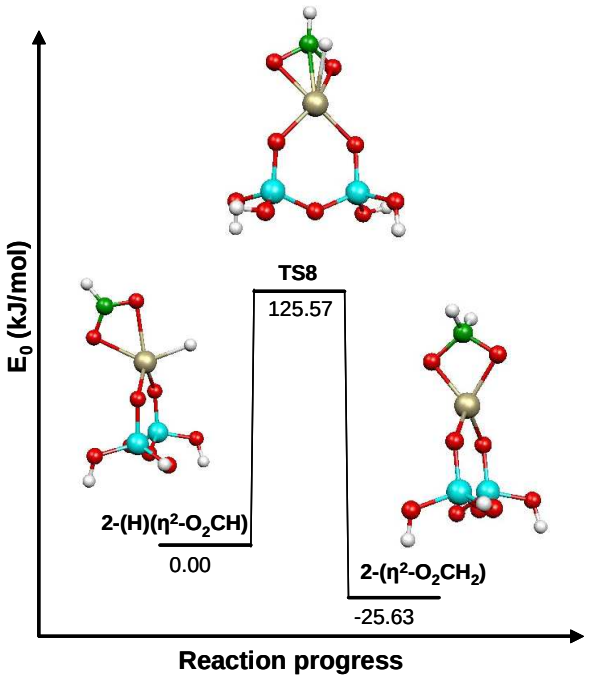

Figure S 14 : Energy profile for hydrogen transfer in **2-(H)(η^2-O$_2$CH).**